



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:27 AM GMT

PDB ID : 1F4H  
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (ORTHORHOMBIC)  
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.  
Deposited on : 2000-06-07  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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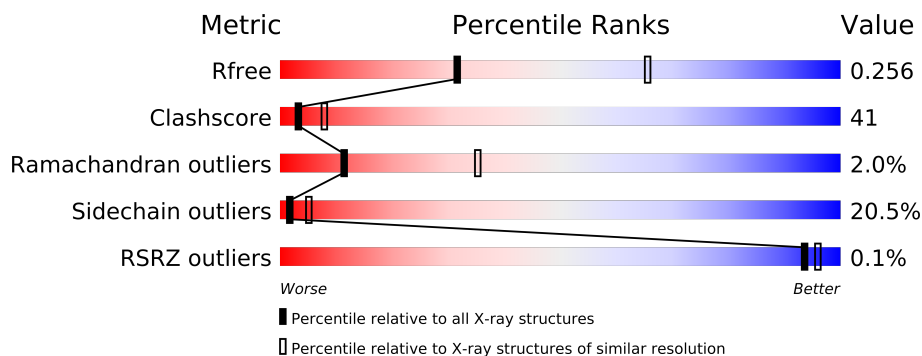
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1021	
1	B	1021	
1	C	1021	
1	D	1021	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	3002	-	X
2	MG	D	3002	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33805 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	B	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	C	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	D	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

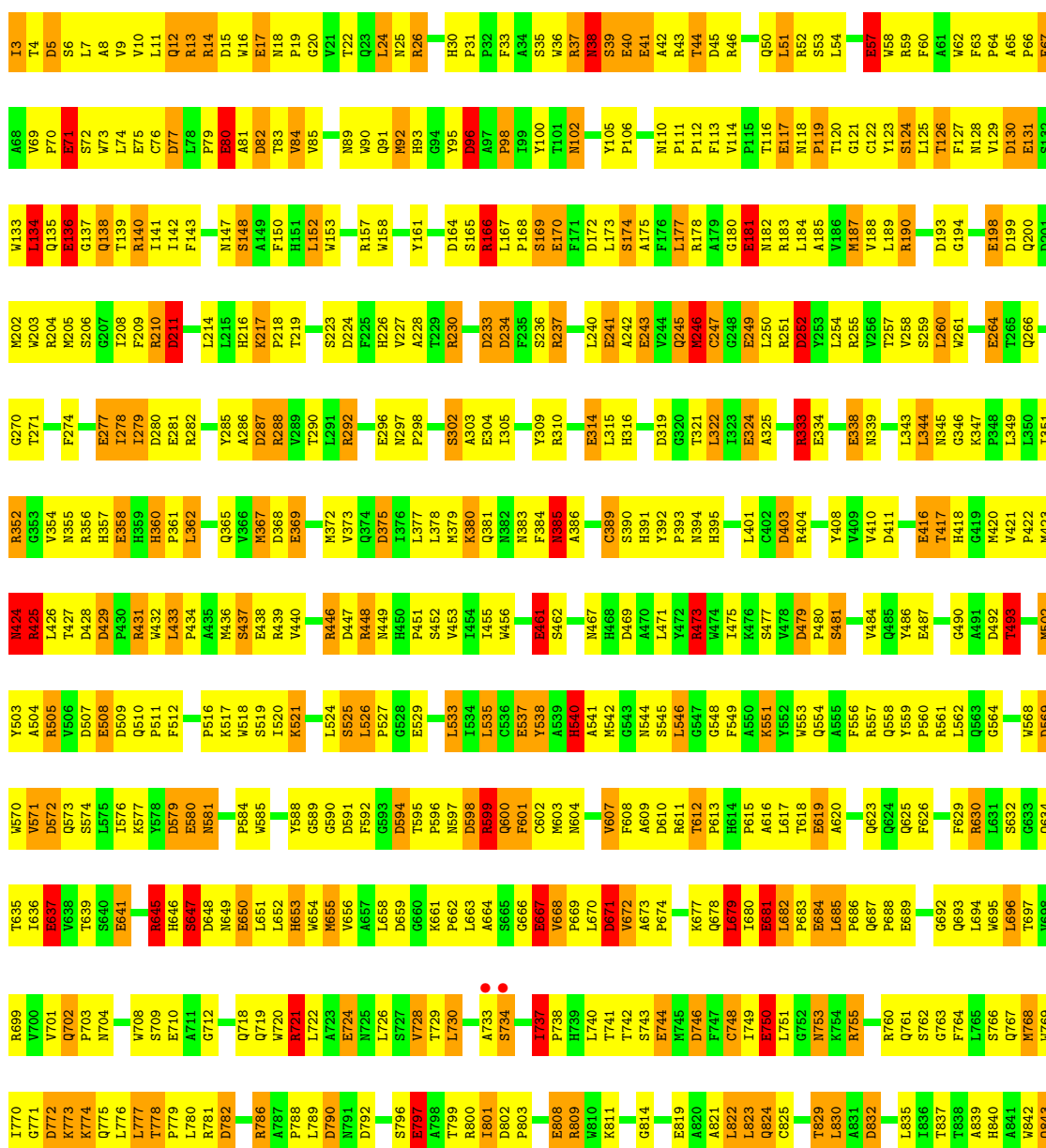
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		
3	B	202	Total	O	0	0
			202	202		
3	C	220	Total	O	0	0
			220	220		
3	D	212	Total	O	0	0
			212	212		

### 3 Residue-property plots

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

#### • Molecule 1: BETA-GALACTOSIDASE

Chain A:









S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000	S1001	S1002	S1003	S1004	A1005	E1006	S1007	S1008	S1009	S1010	A1011	G1012	G1013	S1014	Y1014	S1017	L1018	L1019	V1019	W1020	C1021	M1020	Q1022	K1023	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000	S1001	S1002	S1003	S1004	S1005	S1006	S1007	S1008	S1009	S1010	S1011	S1012	S1013	S1014	S1015	S1016	S1017	S1018	S1019	S1020	S1021	S1022	S1023	S1024	S1025	S1026	S1027	S1028	S1029	S1030	S1031	S1032	S1033	S1034	S1035	S1036	S1037	S1038	S1039	S1040	S1041	S1042	S1043	S1044	S1045	S1046	S1047	S1048	S1049	S1050	S1051	S1052	S1053	S1054	S1055	S1056	S1057	S1058	S1059	S1060	S1061	S1062	S1063	S1064	S1065	S1066	S1067	S1068	S1069	S1070	S1071	S1072	S1073	S1074	S1075	S1076	S1077	S1078	S1079	S1080	S1081	S1082	S1083	S1084	S1085	S1086	S1087	S1088	S1089	S1090	S1091	S1092	S1093	S1094	S1095	S1096	S1097	S1098	S1099	S1100	S1101	S1102	S1103	S1104	S1105	S1106	S1107	S1108	S1109	S1110	S1111	S1112	S1113	S1114	S1115	S1116	S1117	S1118	S1119	S1120	S1121	S1122	S1123	S1124	S1125	S1126	S1127	S1128	S1129	S1130	S1131	S1132	S1133	S1134	S1135	S1136	S1137	S1138	S1139	S1140	S1141	S1142	S1143	S1144	S1145	S1146	S1147	S1148	S1149	S1150	S1151	S1152	S1153	S1154	S1155	S1156	S1157	S1158	S1159	S1160	S1161	S1162	S1163	S1164	S1165	S1166	S1167	S1168	S1169	S1170	S1171	S1172	S1173	S1174	S1175	S1176	S1177	S1178	S1179	S1180	S1181	S1182	S1183	S1184	S1185	S1186	S1187	S1188	S1189	S1190	S1191	S1192	S1193	S1194	S1195	S1196	S1197	S1198	S1199	S1200	S1201	S1202	S1203	S1204	S1205	S1206	S1207	S1208	S1209	S1210	S1211	S1212	S1213	S1214	S1215	S1216	S1217	S1218	S1219	S1220	S1221	S1222	S1223	S1224	S1225	S1226	S1227	S1228	S1229	S1230	S1231	S1232	S1233	S1234	S1235	S1236	S1237	S1238	S1239	S1240	S1241	S1242	S1243	S1244	S1245	S1246	S1247	S1248	S1249	S1250	S1251	S1252	S1253	S1254	S1255	S1256	S1257	S1258	S1259	S1260	S1261	S1262	S1263	S1264	S1265	S1266	S1267	S1268	S1269	S1270	S1271	S1272	S1273	S1274	S1275	S1276	S1277	S1278	S1279	S1280	S1281	S1282	S1283	S1284	S1285	S1286	S1287	S1288	S1289	S1290	S1291	S1292	S1293	S1294	S1295	S1296	S1297	S1298	S1299	S1300	S1301	S1302	S1303	S1304	S1305	S1306	S1307	S1308	S1309	S1310	S1311	S1312	S1313	S1314	S1315	S1316	S1317	S1318	S1319	S1320	S1321	S1322	S1323	S1324	S1325	S1326	S1327	S1328	S1329	S1330	S1331	S1332	S1333	S1334	S1335	S1336	S1337	S1338	S1339	S1340	S1341	S1342	S1343	S1344	S1345	S1346	S1347	S1348	S1349	S1350	S1351	S1352	S1353	S1354	S1355	S1356	S1357	S1358	S1359	S1360	S1361	S1362	S1363	S1364	S1365	S1366	S1367	S1368	S1369	S1370	S1371	S1372	S1373	S1374	S1375	S1376	S1377	S1378	S1379	S1380	S1381	S1382	S1383	S1384	S1385	S1386	S1387	S1388	S1389	S1390	S1391	S1392	S1393	S1394	S1395	S1396	S1397	S1398	S1399	S1400	S1401	S1402	S1403	S1404	S1405	S1406	S1407	S1408	S1409	S1410	S1411	S1412	S1413	S1414	S1415	S1416	S1417	S1418	S1419	S1420	S1421	S1422	S1423	S1424	S1425	S1426	S1427	S1428	S1429	S1430	S1431	S1432	S1433	S1434	S1435	S1436	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447	S1448	S1449	S1450	S1451	S1452	S1453	S1454	S1455	S1456	S1457	S1458	S1459	S1460	S1461	S1462	S1463	S1464	S1465	S1466	S1467	S1468	S1469	S1470	S1471	S1472	S1473	S1474	S1475	S1476	S1477	S1478	S1479	S1480	S1481	S1482	S1483	S1484	S1485	S1486	S1487	S1488	S1489	S1490	S1491	S1492	S1493	S1494	S1495	S1496	S1497	S1498	S1499	S1500	S1501	S1502	S1503	S1504	S1505	S1506	S1507	S1508	S1509	S1510	S1511	S1512	S1513	S1514	S1515	S1516	S1517	S1518	S1519	S1520	S1521	S1522	S1523	S1524	S1525	S1526	S1527	S1528	S1529	S1530	S1531	S1532	S1533	S1534	S1535	S1536	S1537	S1538	S1539	S1540	S1541	S1542	S1543	S1544	S1545	S1546	S1547	S1548	S1549	S1550	S1551	S1552	S1553	S1554	S1555	S1556	S1557	S1558	S1559	S1560	S1561	S1562	S1563	S1564	S1565	S1566	S1567	S1568	S1569	S1570	S1571	S1572	S1573	S1574	S1575	S1576	S1577	S1578	S1579	S1580	S1581	S1582	S1583	S1584	S1585	S1586	S1587	S1588	S1589	S1590	S1591	S1592	S1593	S1594	S1595	S1596	S1597	S1598	S1599	S1600	S1601	S1602	S1603	S1604	S1605	S1606	S1607	S1608	S1609	S1610	S1611	S1612	S1613	S1614	S1615	S1616	S1617	S1618	S1619	S1620	S1621	S1622	S1623	S1624	S1625	S1626	S1627	S1628	S1629	S1630	S1631	S1632	S1633	S1634	S1635	S1636	S1637	S1638	S1639	S1640	S1641	S1642	S1643	S1644	S1645	S1646	S1647	S1648	S1649	S1650	S1651	S1652	S1653	S1654	S1655	S1656	S1657	S1658	S1659	S1660	S1661	S1662	S1663	S1664	S1665	S1666	S1667	S1668	S1669	S1670	S1671	S1672	S1673	S1674	S1675	S1676	S1677	S1678	S1679	S1680	S1681	S1682	S1683	S1684	S1685	S1686	S1687	S1688	S1689	S1690	S1691	S1692	S1693	S1694	S1695	S1696	S1697	S1698	S1699	S1700	S1701	S1702	S1703	S1704	S1705	S1706	S1707	S1708	S1709	S1710	S1711	S1712	S1713	S1714	S1715	S1716	S1717	S1718	S1719	S1720	S1721	S1722	S1723	S1724	S1725	S1726	S1727	S1728	S1729	S1730	S1731	S1732	S1733	S1734	S1735	S1736	S1737	S1738	S1739	S1740	S1741	S1742	S1743	S1744	S1745	S1746	S1747	S1748	S1749	S1750	S1751	S1752	S1753	S1754	S1755	S1756	S1757	S1758	S1759	S1760	S1761	S1762	S1763	S1764	S1765	S1766	S1767	S1768	S1769	S1770	S1771	S1772	S1773	S1774	S1775	S1776	S1777	S1778	S1779	S1780	S1781	S1782	S1783	S1784	S1785	S1786	S1787	S1788	S1789	S1790	S1791	S1792	S1793	S1794	S1795	S1796	S1797	S1798	S1799	S1800	S1801	S1802	S1803	S1804	S1805	S1806	S1807	S1808	S1809	S1810	S1811	S1812	S1813	S1814	S1815	S1816	S1817	S1818	S1819	S1820	S1821	S1822	S1823	S1824	S1825	S1826	S1827	S1828	S1829	S1830	S1831	S1832	S1833	S1834	S1835	S1836	S1837	S1838	S1839	S1840	S1841	S1842	S1843	S1844	S1845	S1846	S1847	S1848	S1849	S1850	S1851	S1852	S1853	S1854	S1855	S1856	S1857	S1858	S1859	S1860	S1861	S1862	S1863	S1864	S1865	S1866	S1867	S1868	S1869	S1870	S1871	S1872	S1873	S1874	S1875	S1876	S1877	S1878	S1879	S1880	S1881	S1882	S1883	S1884	S1885	S1886	S1887	S1888	S1889	S1890	S1891	S1892	S1893	S1894	S1895	S1896	S1897	S1898	S1899	S1900	S1901	S1902	S1903	S1904	S1905	S1906	S1907	S1908	S1909	S1910	S1911	S1912	S1913	S1914	S1915	S1916	S1917	S1918	S1919	S1920	S1921	S1922	S1923	S1924	S1925	S1926	S1927	S1928	S1929	S1930	S1931	S1932	S1933	S1934	S1935	S1936	S1937	S1938	S1939	S1940	S1941	S1942	S1943	S1944	S1945	S1946	S1947	S1948	S1949	S1950	S1951	S1952	S1953	S1954	S1955	S1956	S1957	S1958	S1959	S1960	S1961	S1962	S1963	S1964	S1965	S1966	S1967	S1968	S1969	S1970	S1971	S1972	S1973	S1974	S1975	S1976	S1977	S1978	S1979	S1980	S1981	S1982	S1983	S1984	S1985	S1986	S1987	S1988	S1989	S1990	S1991	S1992	S1993	S1994	S1995	S1996	S1997	S1998	S1999	S2000	S2001	S2002	S2003	S2004	S2005	S2006	S2007	S2008	S2009	S2010	S2011	S2012	S2013	S2014	S2015	S2016	S2017	S2018	S2019	S2020	S2021	S2022	S2023	S2024	S2025	S2026	S2027	S2028	S2029	S2030	S2031	S2032	S2033	S2034	S2035	S2036	S2037	S2038	S2039	S2040	S2041	S2042	S2043	S2044	S2045	S2046	S2047	S2048	S2049	S2050	S2051	S2052	S2053	S2054	S2055	S2056	S2057	S2058	S2059	S2060	S2061	S2062	S2063	S2064	S2065	S2066	S2067	S2068	S2069	S2070	S2071	S2072	S2073	S2074	S2075	S2076	S2077	S2078	S2079	S2080	S2081	S2082	S2083	S2084	S2085	S2086	S2087	S2088	S2089	S2090	S2091	S2092	S2093	S2094	S2095	S2096	S2097	S2098	S2099	S2100	S2101	S2102	S2103	S2104	S2105	S2106	S2107	S2108	S2109	S2110	S2111	S2112	S2113	S2114	S2115	S2116	S2117	S2118	S2119	S2120	S2121	S2122	S2123	S2124	S2125	S2126	S2127	S2128	S2129	S2130	S2131	S2132	S2133	S2134	S2135	S2136	S2137	S2138	S2139	S2140	S2141	S2142	S2143	S2144	S2145	S2146	S2147	S2148	S2149	S2150	S2151	S2152	S2153	S2154	S2155	S2156	S2157	S2158	S2159	S2160	S2161	S2162	S2163	S2164	S2165	S2166	S2167	S2168	S2169	S2170	S2171	S2172	S2173	S2174	S2175	S2176	S2177	S2178	S2179	S2180	S2181	S2182	S2183	S2184	S2185	S2186	S2187	S2188	S2189	S2190	S2191	S2192	S2193	S2194	S2195	S2196	S2197	S2198	S2199	S2200	S2201	S2202	S2203	S2204	S2205	S2206	S2207	S2208	S2209	S2210	S2211	S2212	S2213	S2214	S2215	S2216	S2217	S2218	S2219	S2220	S2221	S2222	S2223	S2224	S2225	S2226	S2227	S2228	S2229	S2230	S2231	S2232	S2233	S2234	S2235	S2236	S2237	S2238	S2239	S2240	S2241	S2242	S2243	S2244	S2245	S2246	S2247	S2248	S2249	S2250	S2251	S2252	S2253	S2254	S2255	S2256	S2257	S2258	S2259	S2260	S2261	S2262	S2263	S2264	S2265	S2266	S2267	S2268	S2269	S2270	S2271	S2272	S2273	S2274	S2275	S2276	S2277	S2278	S2279	S2280	S2281	S2282	S2283	S2284	S2285	S2286	S2287	S2288	S2289	S2290	S2291	S2292	S2293	S2294	S2295	S2296	S2297	S2298
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.40Å 173.40Å 204.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.97 – 2.82	Depositor EDS
% Data completeness (in resolution range)	88.0 (25.00-2.80) 80.5 (24.97-2.82)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.80Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.137 , 0.279 0.124 , 0.256	Depositor DCC
$R_{free}$ test set	1590 reflections (1.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 112.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 105768 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	33805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2179e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.11	56/8515 (0.7%)	1.72	186/11615 (1.6%)
1	B	1.09	53/8515 (0.6%)	1.69	174/11615 (1.5%)
1	C	1.08	49/8515 (0.6%)	1.69	187/11615 (1.6%)
1	D	1.10	54/8515 (0.6%)	1.70	183/11615 (1.6%)
All	All	1.09	212/34060 (0.6%)	1.70	730/46460 (1.6%)

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	2	0
1	B	1	0
1	C	4	1
1	D	1	0
All	All	8	1

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	249	GLU	CD-OE2	8.77	1.35	1.25
1	B	241	GLU	CD-OE2	8.07	1.34	1.25
1	C	508	GLU	CD-OE2	8.02	1.34	1.25
1	D	181	GLU	CD-OE2	7.94	1.34	1.25
1	A	198	GLU	CD-OE2	7.86	1.34	1.25
1	A	358	GLU	CD-OE2	7.77	1.34	1.25
1	A	487	GLU	CD-OE2	7.74	1.34	1.25
1	D	75	GLU	CD-OE2	7.71	1.34	1.25
1	B	75	GLU	CD-OE2	7.61	1.34	1.25
1	C	243	GLU	CD-OE2	7.61	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	GLU	CD-OE2	7.55	1.33	1.25
1	D	797	GLU	CD-OE2	7.54	1.33	1.25
1	D	314	GLU	CD-OE2	7.51	1.33	1.25
1	C	296	GLU	CD-OE2	7.48	1.33	1.25
1	D	619	GLU	CD-OE2	7.48	1.33	1.25
1	D	40	GLU	CD-OE2	7.45	1.33	1.25
1	C	75	GLU	CD-OE2	7.38	1.33	1.25
1	C	710	GLU	CD-OE2	7.30	1.33	1.25
1	C	744	GLU	CD-OE2	7.30	1.33	1.25
1	B	181	GLU	CD-OE2	7.30	1.33	1.25
1	D	537	GLU	CD-OE2	7.28	1.33	1.25
1	B	508	GLU	CD-OE2	7.27	1.33	1.25
1	D	724	GLU	CD-OE2	7.26	1.33	1.25
1	A	241	GLU	CD-OE2	7.26	1.33	1.25
1	A	281	GLU	CD-OE2	7.19	1.33	1.25
1	D	170	GLU	CD-OE2	7.16	1.33	1.25
1	B	650	GLU	CD-OE2	7.16	1.33	1.25
1	B	40	GLU	CD-OE2	7.08	1.33	1.25
1	C	314	GLU	CD-OE2	7.08	1.33	1.25
1	A	750	GLU	CD-OE2	7.06	1.33	1.25
1	C	338	GLU	CD-OE2	7.04	1.33	1.25
1	B	264	GLU	CD-OE2	6.99	1.33	1.25
1	C	667	GLU	CD-OE2	6.98	1.33	1.25
1	B	67	GLU	CD-OE2	6.96	1.33	1.25
1	B	797	GLU	CD-OE2	6.95	1.33	1.25
1	B	136	GLU	CD-OE2	6.95	1.33	1.25
1	D	338	GLU	CD-OE2	6.95	1.33	1.25
1	B	416	GLU	CD-OE2	6.92	1.33	1.25
1	C	904	GLU	CD-OE2	6.83	1.33	1.25
1	A	681	GLU	CD-OE2	6.77	1.33	1.25
1	A	943	GLU	CD-OE2	6.76	1.33	1.25
1	C	637	GLU	CD-OE2	6.73	1.33	1.25
1	D	969	GLU	CD-OE2	6.71	1.33	1.25
1	A	979	GLU	CD-OE2	6.69	1.33	1.25
1	D	667	GLU	CD-OE2	6.69	1.33	1.25
1	A	75	GLU	CD-OE2	6.69	1.33	1.25
1	D	71	GLU	CD-OE2	6.69	1.33	1.25
1	B	744	GLU	CD-OE2	6.67	1.32	1.25
1	D	681	GLU	CD-OE2	6.64	1.32	1.25
1	B	57	GLU	CD-OE2	6.63	1.32	1.25
1	C	681	GLU	CD-OE2	6.62	1.32	1.25
1	D	1006	GLU	CD-OE2	6.60	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1006	GLU	CD-OE2	6.58	1.32	1.25
1	A	529	GLU	CD-OE2	6.58	1.32	1.25
1	D	710	GLU	CD-OE2	6.57	1.32	1.25
1	D	264	GLU	CD-OE2	6.57	1.32	1.25
1	B	369	GLU	CD-OE2	6.54	1.32	1.25
1	C	358	GLU	CD-OE2	6.52	1.32	1.25
1	D	744	GLU	CD-OE2	6.52	1.32	1.25
1	D	243	GLU	CD-OE2	6.52	1.32	1.25
1	A	871	GLU	CD-OE2	6.50	1.32	1.25
1	B	619	GLU	CD-OE2	6.50	1.32	1.25
1	C	641	GLU	CD-OE2	6.45	1.32	1.25
1	C	934	GLU	CD-OE2	6.45	1.32	1.25
1	C	281	GLU	CD-OE2	6.44	1.32	1.25
1	B	667	GLU	CD-OE2	6.43	1.32	1.25
1	B	537	GLU	CD-OE2	6.43	1.32	1.25
1	D	41	GLU	CD-OE2	6.43	1.32	1.25
1	A	80	GLU	CD-OE2	6.41	1.32	1.25
1	B	641	GLU	CD-OE2	6.39	1.32	1.25
1	B	871	GLU	CD-OE2	6.34	1.32	1.25
1	C	438	GLU	CD-OE2	6.33	1.32	1.25
1	A	969	GLU	CD-OE2	6.31	1.32	1.25
1	B	979	GLU	CD-OE2	6.29	1.32	1.25
1	A	508	GLU	CD-OE2	6.27	1.32	1.25
1	D	438	GLU	CD-OE2	6.26	1.32	1.25
1	D	750	GLU	CD-OE2	6.25	1.32	1.25
1	B	681	GLU	CD-OE2	6.23	1.32	1.25
1	A	438	GLU	CD-OE2	6.19	1.32	1.25
1	A	249	GLU	CD-OE2	6.19	1.32	1.25
1	B	80	GLU	CD-OE2	6.18	1.32	1.25
1	C	808	GLU	CD-OE2	6.16	1.32	1.25
1	A	264	GLU	CD-OE2	6.14	1.32	1.25
1	D	979	GLU	CD-OE2	6.13	1.32	1.25
1	B	710	GLU	CD-OE2	6.13	1.32	1.25
1	A	57	GLU	CD-OE2	6.12	1.32	1.25
1	A	724	GLU	CD-OE2	6.11	1.32	1.25
1	C	724	GLU	CD-OE2	6.10	1.32	1.25
1	A	744	GLU	CD-OE2	6.09	1.32	1.25
1	C	57	GLU	CD-OE2	6.08	1.32	1.25
1	B	969	GLU	CD-OE2	6.06	1.32	1.25
1	C	170	GLU	CD-OE2	6.06	1.32	1.25
1	D	241	GLU	CD-OE2	6.05	1.32	1.25
1	C	71	GLU	CD-OE2	6.03	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	198	GLU	CD-OE2	6.01	1.32	1.25
1	C	67	GLU	CD-OE2	5.99	1.32	1.25
1	B	412	GLU	CD-OE2	5.98	1.32	1.25
1	A	667	GLU	CD-OE2	5.97	1.32	1.25
1	B	637	GLU	CD-OE2	5.96	1.32	1.25
1	D	808	GLU	CD-OE2	5.95	1.32	1.25
1	C	181	GLU	CD-OE2	5.94	1.32	1.25
1	B	934	GLU	CD-OE2	5.93	1.32	1.25
1	A	641	GLU	CD-OE2	5.92	1.32	1.25
1	A	797	GLU	CD-OE2	5.92	1.32	1.25
1	B	943	GLU	CD-OE2	5.92	1.32	1.25
1	C	334	GLU	CD-OE2	5.92	1.32	1.25
1	A	710	GLU	CD-OE2	5.91	1.32	1.25
1	D	80	GLU	CD-OE2	5.91	1.32	1.25
1	C	979	GLU	CD-OE2	5.91	1.32	1.25
1	B	334	GLU	CD-OE2	5.90	1.32	1.25
1	B	750	GLU	CD-OE2	5.90	1.32	1.25
1	D	369	GLU	CD-OE2	5.89	1.32	1.25
1	C	487	GLU	CD-OE2	5.87	1.32	1.25
1	D	508	GLU	CD-OE2	5.84	1.32	1.25
1	C	264	GLU	CD-OE2	5.84	1.32	1.25
1	D	17	GLU	CD-OE2	5.84	1.32	1.25
1	C	241	GLU	CD-OE2	5.83	1.32	1.25
1	A	334	GLU	CD-OE2	5.82	1.32	1.25
1	A	40	GLU	CD-OE2	5.82	1.32	1.25
1	D	650	GLU	CD-OE2	5.81	1.32	1.25
1	A	369	GLU	CD-OE2	5.79	1.32	1.25
1	A	904	GLU	CD-OE2	5.79	1.32	1.25
1	B	529	GLU	CD-OE2	5.79	1.32	1.25
1	C	943	GLU	CD-OE2	5.79	1.32	1.25
1	D	296	GLU	CD-OE2	5.78	1.32	1.25
1	B	904	GLU	CD-OE2	5.76	1.31	1.25
1	B	724	GLU	CD-OE2	5.75	1.31	1.25
1	A	170	GLU	CD-OE2	5.72	1.31	1.25
1	C	537	GLU	CD-OE2	5.71	1.31	1.25
1	A	537	GLU	CD-OE2	5.71	1.31	1.25
1	C	41	GLU	CD-OE2	5.71	1.31	1.25
1	C	750	GLU	CD-OE2	5.70	1.31	1.25
1	B	338	GLU	CD-OE2	5.69	1.31	1.25
1	B	358	GLU	CD-OE2	5.68	1.31	1.25
1	C	797	GLU	CD-OE2	5.67	1.31	1.25
1	C	969	GLU	CD-OE2	5.67	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	GLU	CD-OE2	5.67	1.31	1.25
1	A	416	GLU	CD-OE2	5.67	1.31	1.25
1	B	41	GLU	CD-OE2	5.66	1.31	1.25
1	B	808	GLU	CD-OE2	5.61	1.31	1.25
1	B	314	GLU	CD-OE2	5.60	1.31	1.25
1	C	304	GLU	CD-OE2	5.60	1.31	1.25
1	A	181	GLU	CD-OE2	5.60	1.31	1.25
1	D	461	GLU	CD-OE2	5.59	1.31	1.25
1	B	243	GLU	CD-OE2	5.57	1.31	1.25
1	A	338	GLU	CD-OE2	5.57	1.31	1.25
1	A	71	GLU	CD-OE2	5.57	1.31	1.25
1	A	314	GLU	CD-OE2	5.56	1.31	1.25
1	D	136	GLU	CD-OE2	5.56	1.31	1.25
1	A	41	GLU	CD-OE2	5.55	1.31	1.25
1	A	296	GLU	CD-OE2	5.55	1.31	1.25
1	B	461	GLU	CD-OE2	5.54	1.31	1.25
1	C	198	GLU	CD-OE2	5.53	1.31	1.25
1	C	136	GLU	CD-OE2	5.53	1.31	1.25
1	A	650	GLU	CD-OE2	5.46	1.31	1.25
1	D	461	GLU	CD-OE1	-5.39	1.19	1.25
1	D	304	GLU	CD-OE1	-5.39	1.19	1.25
1	D	943	GLU	CD-OE2	5.39	1.31	1.25
1	A	117	GLU	CD-OE2	5.39	1.31	1.25
1	A	17	GLU	CD-OE2	5.38	1.31	1.25
1	D	131	GLU	CD-OE2	5.37	1.31	1.25
1	D	529	GLU	CD-OE2	5.37	1.31	1.25
1	D	819	GLU	CD-OE2	5.35	1.31	1.25
1	C	277	GLU	CD-OE2	5.35	1.31	1.25
1	A	637	GLU	CD-OE2	5.34	1.31	1.25
1	D	980	GLU	CD-OE2	5.33	1.31	1.25
1	D	689	GLU	CD-OE2	5.31	1.31	1.25
1	A	131	GLU	CD-OE2	5.30	1.31	1.25
1	B	438	GLU	CD-OE2	5.30	1.31	1.25
1	C	580	GLU	CD-OE2	5.29	1.31	1.25
1	A	980	GLU	CD-OE2	5.29	1.31	1.25
1	B	689	GLU	CD-OE2	5.29	1.31	1.25
1	D	117	GLU	CD-OE2	5.28	1.31	1.25
1	C	131	GLU	CD-OE2	5.27	1.31	1.25
1	C	684	GLU	CD-OE2	5.27	1.31	1.25
1	C	980	GLU	CD-OE2	5.27	1.31	1.25
1	D	893	GLU	CD-OE2	5.26	1.31	1.25
1	C	893	GLU	CD-OE2	5.26	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	819	GLU	CD-OE2	5.26	1.31	1.25
1	B	980	GLU	CD-OE2	5.26	1.31	1.25
1	C	689	GLU	CD-OE2	5.26	1.31	1.25
1	B	277	GLU	CD-OE2	5.25	1.31	1.25
1	D	684	GLU	CD-OE2	5.25	1.31	1.25
1	A	684	GLU	CD-OE2	5.25	1.31	1.25
1	D	580	GLU	CD-OE2	5.24	1.31	1.25
1	C	619	GLU	CD-OE2	5.23	1.31	1.25
1	B	131	GLU	CD-OE2	5.22	1.31	1.25
1	B	819	GLU	CD-OE2	5.22	1.31	1.25
1	B	893	GLU	CD-OE2	5.22	1.31	1.25
1	A	136	GLU	CD-OE2	5.21	1.31	1.25
1	B	326	GLU	CD-OE2	5.21	1.31	1.25
1	A	689	GLU	CD-OE2	5.21	1.31	1.25
1	A	893	GLU	CD-OE2	5.20	1.31	1.25
1	B	684	GLU	CD-OE2	5.20	1.31	1.25
1	C	819	GLU	CD-OE2	5.20	1.31	1.25
1	A	580	GLU	CD-OE2	5.19	1.31	1.25
1	B	304	GLU	CD-OE2	5.18	1.31	1.25
1	D	67	GLU	CD-OE2	5.18	1.31	1.25
1	D	277	GLU	CD-OE2	5.18	1.31	1.25
1	A	324	GLU	CD-OE2	5.17	1.31	1.25
1	B	580	GLU	CD-OE2	5.17	1.31	1.25
1	A	277	GLU	CD-OE2	5.17	1.31	1.25
1	D	934	GLU	CD-OE2	5.16	1.31	1.25
1	B	296	GLU	CD-OE2	5.15	1.31	1.25
1	C	871	GLU	CD-OE2	5.15	1.31	1.25
1	A	808	GLU	CD-OE2	5.14	1.31	1.25
1	A	243	GLU	CD-OE2	5.14	1.31	1.25
1	D	871	GLU	CD-OE2	5.11	1.31	1.25
1	D	281	GLU	CD-OE2	5.05	1.31	1.25
1	D	412	GLU	CD-OE2	5.04	1.31	1.25
1	D	637	GLU	CD-OE2	5.03	1.31	1.25
1	A	619	GLU	CD-OE2	5.02	1.31	1.25

All (730) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	D	210	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	D	425	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	D	668	VAL	C-N-CD	-13.14	91.69	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ARG	NE-CZ-NH1	13.13	126.87	120.30
1	A	557	ARG	NE-CZ-NH2	-12.49	114.05	120.30
1	B	507	ASP	CB-CG-OD2	-12.47	107.08	118.30
1	B	908	ASP	CB-CG-OD2	-12.45	107.09	118.30
1	B	809[A]	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	B	809[B]	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	C	809[A]	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	C	809[B]	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	D	251	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	A	424	ASN	CB-CA-C	-11.55	87.29	110.40
1	D	509	ASP	CB-CG-OD2	-11.52	107.93	118.30
1	B	356	ARG	NE-CZ-NH1	11.45	126.02	120.30
1	A	287	ASP	CB-CG-OD1	11.23	128.41	118.30
1	B	385	ASN	CB-CA-C	-10.82	88.75	110.40
1	D	938	ARG	N-CA-CB	10.69	129.84	110.60
1	D	792	ASP	CB-CG-OD2	-10.67	108.70	118.30
1	A	385	ASN	CB-CA-C	-10.62	89.17	110.40
1	B	356	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	A	199	ASP	CB-CG-OD2	-10.57	108.79	118.30
1	A	881	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	A	938	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	C	659	ASP	CB-CG-OD1	10.21	127.48	118.30
1	C	659	ASP	CB-CG-OD2	-10.17	109.14	118.30
1	B	479	ASP	CB-CG-OD2	-10.14	109.18	118.30
1	A	310	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	B	237	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	356	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	A	881	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	C	46	ARG	C-N-CD	-10.03	98.53	120.60
1	D	385	ASN	N-CA-CB	-10.01	92.58	110.60
1	D	507	ASP	CB-CG-OD2	-9.93	109.37	118.30
1	A	287	ASP	CB-CG-OD2	-9.84	109.45	118.30
1	C	210	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	D	909	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	B	507	ASP	CB-CG-OD1	9.73	127.06	118.30
1	B	46	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	C	144	ASP	CB-CG-OD2	-9.56	109.69	118.30
1	A	509	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	A	952	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	428	ASP	CB-CG-OD2	-9.49	109.76	118.30
1	B	473	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	D	287	ASP	CB-CG-OD2	-9.39	109.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	782	ASP	CB-CG-OD1	9.32	126.69	118.30
1	B	908	ASP	CB-CG-OD1	9.26	126.64	118.30
1	B	996	ASP	CB-CG-OD2	-9.25	109.98	118.30
1	A	645	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	C	429	ASP	CB-CG-OD1	9.06	126.45	118.30
1	A	809[A]	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	809[B]	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	D	792	ASP	CB-CG-OD1	9.00	126.40	118.30
1	A	446	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	C	26	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	A	429	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	A	659	ASP	CB-CG-OD2	-8.79	110.38	118.30
1	B	46	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	D	531	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	D	572	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	D	492	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	B	881	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	319	ASP	CB-CG-OD2	-8.66	110.50	118.30
1	D	881	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	A	310	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	C	973	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	782	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	D	875	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	A	448	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	C	431[A]	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	C	431[B]	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	D	648	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	C	997	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	C	447	ASP	CB-CG-OD2	-8.43	110.72	118.30
1	C	672	VAL	CB-CA-C	-8.38	95.47	111.40
1	C	599	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	792	ASP	CB-CG-OD2	-8.34	110.79	118.30
1	C	402	CYS	CA-CB-SG	-8.33	99.01	114.00
1	A	908	ASP	CB-CG-OD1	8.28	125.75	118.30
1	D	172	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	A	591	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	B	716	ALA	CB-CA-C	-8.27	97.70	110.10
1	D	579	ASP	CB-CG-OD1	8.24	125.72	118.30
1	A	671	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	13	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	D	26	ARG	NE-CZ-NH1	8.21	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	ASP	CB-CG-OD1	8.17	125.66	118.30
1	D	924	ASP	CB-CG-OD1	8.16	125.65	118.30
1	D	431[A]	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	D	431[B]	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	211	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	B	164	ASP	N-CA-CB	8.10	125.19	110.60
1	A	233	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	C	916	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	B	442	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	B	469	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	C	403	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	C	917	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	448	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	C	403	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	572	ASP	CB-CG-OD1	7.98	125.48	118.30
1	A	252	ASP	CB-CG-OD1	7.97	125.47	118.30
1	C	26	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	591	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	A	952	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	572	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	13	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	668	VAL	C-N-CD	-7.92	103.18	120.60
1	D	210	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	859	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	569	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	492	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	A	479	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	A	792	ASP	CB-CG-OD1	7.85	125.37	118.30
1	D	579	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	B	212	VAL	CA-CB-CG1	-7.78	99.23	110.90
1	B	1004	SER	N-CA-CB	7.77	122.15	110.50
1	A	193	ASP	CB-CG-OD1	7.74	125.27	118.30
1	D	924	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	C	429	ASP	CB-CG-OD2	-7.73	111.35	118.30
1	A	360	HIS	C-N-CD	-7.72	103.61	120.60
1	D	233	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	987	ASP	CB-CG-OD1	7.71	125.24	118.30
1	D	828	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	252	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	493	THR	CA-CB-CG2	-7.69	101.63	112.40
1	C	126	THR	CA-CB-CG2	-7.69	101.64	112.40
1	B	411	ASP	CB-CG-OD1	7.68	125.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	671	ASP	CB-CA-C	7.67	125.75	110.40
1	C	144	ASP	CB-CG-OD1	7.67	125.20	118.30
1	D	610	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	B	411	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	C	237	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	D	388	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	C	509	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	721	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	D	448	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	651	LEU	CB-CA-C	-7.59	95.78	110.20
1	A	659	ASP	CB-CG-OD1	7.58	125.13	118.30
1	A	790	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	403	ASP	CB-CG-OD1	7.57	125.12	118.30
1	D	917	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	C	750	GLU	N-CA-CB	7.56	124.20	110.60
1	D	659	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	D	509	ASP	CB-CG-OD1	7.55	125.10	118.30
1	A	857	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	385	ASN	N-CA-CB	-7.55	97.01	110.60
1	B	671	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	D	45	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	C	802	ASP	CB-CG-OD1	7.53	125.08	118.30
1	C	15	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	D	594	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	D	45	ASP	CB-CG-OD1	7.48	125.03	118.30
1	D	881	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	C	591	ASP	CB-CG-OD1	7.46	125.02	118.30
1	B	954	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	D	750	GLU	N-CA-CB	7.45	124.01	110.60
1	D	782	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	C	486	TYR	CB-CG-CD1	-7.43	116.54	121.00
1	A	938	ARG	N-CA-CB	7.42	123.96	110.60
1	A	908	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	375	ASP	CB-CG-OD2	-7.41	111.64	118.30
1	D	610	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	329	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	B	287	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	C	164	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	D	336	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	909	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	579	ASP	CB-CG-OD1	7.33	124.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	A	924	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	B	497	ASP	CB-CG-OD1	7.33	124.89	118.30
1	B	491	ALA	N-CA-CB	7.32	120.35	110.10
1	B	352	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	507	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	648	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	C	591	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	B	140	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	C	5	ASP	CB-CG-OD1	7.28	124.85	118.30
1	C	503	TYR	CB-CG-CD1	7.28	125.37	121.00
1	D	929	TYR	CB-CG-CD1	7.28	125.37	121.00
1	C	211	ASP	CB-CG-OD1	7.27	124.85	118.30
1	B	591	ASP	CB-CG-OD1	7.27	124.84	118.30
1	D	292	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	C	1006	GLU	CG-CD-OE2	-7.26	103.77	118.30
1	D	919	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	233	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	403	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	C	997	ASP	CB-CG-OD1	7.21	124.79	118.30
1	D	233	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	C	329	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	D	572	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	557	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	B	15	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	D	360	HIS	C-N-CD	-7.16	104.85	120.60
1	B	497	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	82	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	509	ASP	CB-CG-OD1	7.14	124.72	118.30
1	B	400	THR	CA-CB-CG2	-7.13	102.42	112.40
1	B	832	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	291	LEU	CB-CA-C	7.12	123.72	110.20
1	A	553	TRP	CA-CB-CG	-7.11	100.19	113.70
1	B	199	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	479	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	594	ASP	CB-CG-OD1	7.08	124.68	118.30
1	B	598	ASP	CB-CG-OD1	7.08	124.68	118.30
1	D	96	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	C	130	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	D	571	VAL	CB-CA-C	-7.05	98.00	111.40
1	C	792	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	292	ARG	NE-CZ-NH2	-7.05	116.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	721	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	679	LEU	CA-CB-CG	-7.03	99.12	115.30
1	B	919	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	A	166	ARG	N-CA-CB	7.02	123.24	110.60
1	D	403	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	987	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	746	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	15	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	630	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	233	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C	282	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	737	ILE	CB-CA-C	6.97	125.55	111.60
1	B	610	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	D	594	ASP	CB-CG-OD1	6.97	124.57	118.30
1	C	46	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	973	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	482	ARG	C-N-CD	-6.96	105.30	120.60
1	C	333	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	C	924	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	D	591	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	C	82	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	479	ASP	CB-CG-OD1	6.92	124.53	118.30
1	D	671	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	166	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	D	77	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	746	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	368	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	D	745	MET	CB-CA-C	-6.90	96.59	110.40
1	A	572	ASP	CB-CG-OD2	-6.89	112.09	118.30
1	D	287	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	790	ASP	CB-CG-OD1	6.89	124.50	118.30
1	D	13	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	15	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	172	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	D	424	ASN	CB-CA-C	-6.85	96.70	110.40
1	C	492	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	D	280	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	B	43	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	411	ASP	CB-CG-OD1	6.84	124.45	118.30
1	C	157	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	C	568	TRP	CA-CB-CG	-6.82	100.73	113.70
1	A	938	ARG	NE-CZ-NH1	6.82	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	211	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	C	579	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	D	853	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	190	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	911	THR	CA-CB-CG2	-6.75	102.95	112.40
1	D	875	ASP	CB-CG-OD1	6.71	124.34	118.30
1	D	607	VAL	CA-CB-CG1	-6.70	100.84	110.90
1	D	832	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	D	782	ASP	CB-CG-OD1	6.68	124.31	118.30
1	C	251	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	D	802	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	82	ASP	CB-CG-OD1	6.67	124.30	118.30
1	D	166	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	786	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	352	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	B	987	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	919	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	859	ASP	CB-CG-OD1	6.64	124.28	118.30
1	D	118	ASN	N-CA-CB	-6.63	98.67	110.60
1	B	375	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	D	671	ASP	CB-CG-OD1	6.63	124.27	118.30
1	D	403	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	859	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	D	292	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	509	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	187	MET	N-CA-CB	6.56	122.41	110.60
1	D	429	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	118	ASN	CB-CA-C	6.55	123.50	110.40
1	B	448	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	C	828	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	D	431[A]	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	D	431[B]	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	942	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	368	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	C	336	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	402	CYS	CA-CB-SG	-6.53	102.25	114.00
1	D	5	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	C	5	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	C	110	ASN	N-CA-CB	6.52	122.34	110.60
1	A	594	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	C	1006	GLU	CG-CD-OE1	6.52	131.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	857	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	249	GLU	CG-CD-OE2	-6.50	105.30	118.30
1	A	386	ALA	N-CA-CB	-6.50	101.00	110.10
1	C	760	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	386	ALA	CB-CA-C	-6.48	100.38	110.10
1	C	832	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	C	439	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	D	265	THR	N-CA-CB	-6.46	98.02	110.30
1	C	916	ASP	CB-CG-OD1	6.46	124.11	118.30
1	D	557	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	252	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	875	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	77	ASP	CB-CG-OD1	6.44	124.09	118.30
1	D	226	HIS	CB-CA-C	-6.43	97.54	110.40
1	C	226	HIS	CB-CA-C	-6.42	97.55	110.40
1	C	233	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	37	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	D	43	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	432	TRP	CA-CB-CG	-6.39	101.56	113.70
1	A	38	ASN	N-CA-CB	6.38	122.09	110.60
1	B	802	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	C	404	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	D	929	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	C	494	THR	CA-CB-CG2	-6.38	103.47	112.40
1	D	790	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	472	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	B	142	ILE	CB-CA-C	-6.38	98.85	111.60
1	D	908	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	C	908	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	C	310	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	D	230	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	D	859	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	B	183	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	869	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	D	809[A]	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	D	809[B]	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	598	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	B	287	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	252	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	247	CYS	CA-CB-SG	-6.32	102.62	114.00
1	A	175	ALA	CB-CA-C	-6.32	100.63	110.10
1	A	319	ASP	CB-CG-OD1	6.31	123.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	591	ASP	CB-CG-OD1	6.31	123.97	118.30
1	B	368	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	164	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	504	ALA	CB-CA-C	6.30	119.55	110.10
1	C	446	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	629	PHE	CB-CA-C	-6.28	97.83	110.40
1	D	760	ARG	N-CA-CB	6.28	121.90	110.60
1	C	737	ILE	N-CA-CB	6.28	125.23	110.80
1	D	5	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	287	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	A	44	THR	CA-CB-CG2	-6.27	103.62	112.40
1	C	517	LYS	CB-CA-C	6.27	122.94	110.40
1	A	533	LEU	CB-CG-CD1	6.26	121.65	111.00
1	B	531	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	598	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	B	234	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	D	954	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	C	980	GLU	N-CA-CB	6.25	121.84	110.60
1	C	600	GLN	N-CA-CB	6.24	121.82	110.60
1	A	130	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	869	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	750	GLU	N-CA-CB	6.21	121.78	110.60
1	C	857	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	368	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	234	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	446	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	13	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	77	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	164	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	954	ASP	CB-CG-OD1	6.15	123.84	118.30
1	D	130	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	D	863	GLN	N-CA-CB	-6.15	99.53	110.60
1	B	954	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	204	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	130	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	832	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	473	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	772	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	744	GLU	CB-CA-C	6.12	122.64	110.40
1	D	144	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	D	492	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	MET	N-CA-CB	6.11	121.59	110.60
1	B	786	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	D	997	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	553	TRP	CA-CB-CG	-6.09	102.13	113.70
1	B	746	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	310	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	755	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	193	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	C	431[A]	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	C	431[B]	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	C	673	ALA	CB-CA-C	6.07	119.21	110.10
1	B	249	GLU	CA-C-N	-6.07	103.84	117.20
1	D	288	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	C	512	PHE	C-N-CD	-6.07	107.25	120.60
1	B	561	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	571	VAL	CB-CA-C	-6.06	99.88	111.40
1	C	486	TYR	CB-CG-CD2	6.06	124.64	121.00
1	C	147	ASN	N-CA-CB	-6.05	99.70	110.60
1	A	389	CYS	CA-CB-SG	-6.05	103.11	114.00
1	D	550	ALA	N-CA-CB	6.05	118.57	110.10
1	A	954	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	832	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	B	140	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	579	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	C	518	TRP	CB-CA-C	-6.03	98.34	110.40
1	D	838	THR	CA-CB-CG2	-6.03	103.96	112.40
1	D	917	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	5	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	C	204	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	237	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	469	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	599	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	859	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	249	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	C	671	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	473	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	832	ASP	CB-CG-OD1	6.00	123.69	118.30
1	A	687	GLN	CB-CA-C	5.99	122.39	110.40
1	C	572	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	772	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	5	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	591	ASP	CB-CG-OD1	5.99	123.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	996	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	D	439	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	859	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	D	772	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	505	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	C	428	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	226	HIS	CB-CA-C	-5.96	98.48	110.40
1	A	786	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	C	404	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	C	199	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	639	THR	CA-CB-CG2	-5.95	104.07	112.40
1	D	252	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	D	598	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	772	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	B	538	TYR	CB-CG-CD1	-5.94	117.43	121.00
1	B	672	VAL	CB-CA-C	-5.94	100.11	111.40
1	D	249	GLU	CA-C-N	-5.93	104.14	117.20
1	B	859	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	237	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	996	ASP	CB-CG-OD1	5.93	123.63	118.30
1	C	802	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	881	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	429	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	509	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	96	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	96	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	24	LEU	CB-CG-CD1	5.90	121.03	111.00
1	B	782	ASP	CB-CG-OD1	5.90	123.61	118.30
1	D	569	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	166	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	96	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	746	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	392	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	325	ALA	N-CA-CB	5.88	118.33	110.10
1	D	679	LEU	CA-CB-CG	-5.87	101.81	115.30
1	C	291	LEU	N-CA-CB	5.87	122.13	110.40
1	A	246	MET	CG-SD-CE	-5.86	90.82	100.20
1	B	455	ILE	CB-CA-C	-5.85	99.89	111.60
1	D	553	TRP	CA-CB-CG	-5.85	102.58	113.70
1	B	230	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	166	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	164	ASP	CB-CG-OD1	5.85	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	D	404	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	368	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	996	ASP	CB-CG-OD1	5.84	123.56	118.30
1	C	497	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	190	ARG	N-CA-CB	5.83	121.09	110.60
1	A	996	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	319	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	952	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	389	CYS	CA-CB-SG	-5.81	103.54	114.00
1	D	648	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	638	VAL	CB-CA-C	-5.81	100.37	111.40
1	C	285	TYR	CB-CG-CD2	5.80	124.48	121.00
1	B	509	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	817	GLN	N-CA-CB	5.79	121.01	110.60
1	B	598	ASP	N-CA-CB	5.78	121.01	110.60
1	D	164	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	13	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	924	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	448	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	164	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	429	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	210	ARG	N-CA-CB	5.75	120.96	110.60
1	C	469	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	924	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	610	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	857	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	506	VAL	CA-CB-CG1	-5.74	102.29	110.90
1	B	428	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	D	427	THR	CA-CB-CG2	-5.73	104.38	112.40
1	D	598	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	659	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	D	363	HIS	CA-CB-CG	-5.72	103.87	113.60
1	D	954	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	1006	GLU	CB-CA-C	-5.71	98.99	110.40
1	B	792	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	326	GLU	N-CA-CB	5.70	120.86	110.60
1	C	594	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	230	ARG	CB-CA-C	-5.69	99.02	110.40
1	A	916	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	403	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	C	451	PRO	N-CA-CB	5.68	110.12	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	SER	N-CA-CB	5.68	119.02	110.50
1	C	388	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	876	THR	CA-CB-CG2	5.66	120.33	112.40
1	D	255	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	45	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	997	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	26	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	B	234	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	292	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	828	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	734	SER	C-N-CA	-5.60	107.70	121.70
1	B	648	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	538	TYR	CB-CG-CD2	5.59	124.36	121.00
1	A	772	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	45	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	790	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	439	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	344	LEU	N-CA-CB	5.58	121.55	110.40
1	A	782	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	424	ASN	N-CA-CB	-5.57	100.58	110.60
1	A	579	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	781	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	233	ASP	N-CA-CB	5.56	120.61	110.60
1	C	96	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	193	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	5	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	C	485	GLN	N-CA-CB	5.56	120.60	110.60
1	B	249	GLU	O-C-N	5.55	131.59	122.70
1	D	661	LYS	N-CA-CB	5.55	120.60	110.60
1	A	916	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	598	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	875	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	D	421	VAL	CB-CA-C	-5.55	100.86	111.40
1	B	144	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	772	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	249	GLU	N-CA-CB	5.54	120.58	110.60
1	D	952	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	1018	LEU	CB-CA-C	-5.53	99.69	110.20
1	B	130	ASP	CB-CG-OD1	5.53	123.27	118.30
1	B	204	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	329	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	479	ASP	C-N-CD	-5.53	108.44	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1006	GLU	N-CA-CB	5.52	120.54	110.60
1	B	442	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	828	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	D	772	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	431[A]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	431[B]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	769	TRP	CB-CA-C	-5.51	99.39	110.40
1	D	77	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	979	GLU	CB-CA-C	5.50	121.41	110.40
1	C	411	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	832	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	423	MET	C-N-CA	5.50	135.44	121.70
1	B	245	GLN	N-CA-CB	5.49	120.48	110.60
1	A	961	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	82	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C	100	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	C	954	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	560	PRO	CA-N-CD	-5.47	103.85	111.50
1	B	997	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	439	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	980	GLU	N-CA-CB	5.46	120.43	110.60
1	A	919	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	409	VAL	CA-CB-CG1	5.46	119.08	110.90
1	C	772	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	251	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	126	THR	CA-CB-CG2	-5.44	104.78	112.40
1	B	645	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	319	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	533	LEU	CB-CA-C	5.44	120.53	110.20
1	B	280	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	802	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	D	748	CYS	N-CA-CB	5.42	120.35	110.60
1	A	612	THR	CA-CB-CG2	-5.42	104.82	112.40
1	C	581	ASN	N-CA-CB	5.41	120.34	110.60
1	B	653[A]	HIS	CA-CB-CG	-5.41	104.41	113.60
1	B	653[B]	HIS	CA-CB-CG	-5.41	104.41	113.60
1	B	252	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	375	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	115	PRO	CA-N-CD	-5.40	103.94	111.50
1	B	478	VAL	CA-CB-CG1	-5.38	102.83	110.90
1	A	417	THR	CA-CB-CG2	-5.38	104.87	112.40
1	A	702	GLN	CA-CB-CG	-5.37	101.58	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	211	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	954	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	746	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	569	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	37	ARG	CB-CA-C	5.35	121.09	110.40
1	D	204	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	946	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	A	686	PRO	C-N-CA	-5.33	108.36	121.70
1	B	594	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	671	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	850	PHE	CB-CA-C	-5.33	99.75	110.40
1	D	37	ARG	CB-CA-C	5.33	121.05	110.40
1	D	411	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	B	864	MET	N-CA-CB	5.33	120.19	110.60
1	D	949	HIS	CA-CB-CG	-5.33	104.55	113.60
1	C	553	TRP	CA-CB-CG	-5.32	103.58	113.70
1	D	375	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	C	987	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	829	THR	N-CA-CB	5.32	120.41	110.30
1	C	537	GLU	N-CA-CB	5.32	120.18	110.60
1	C	409	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	C	287	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	853	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	233	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	671	ASP	N-CA-CB	5.31	120.15	110.60
1	B	787	ALA	C-N-CD	-5.31	108.92	120.60
1	C	356	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	333	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	352	ARG	N-CA-C	-5.30	96.69	111.00
1	B	916	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	D	659	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	894	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	172	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	407	LEU	CB-CG-CD2	-5.29	102.02	111.00
1	D	965	GLN	N-CA-CB	5.28	120.11	110.60
1	A	746	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	44	THR	CA-CB-CG2	-5.28	105.01	112.40
1	A	505	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	509	ASP	N-CA-CB	5.27	120.09	110.60
1	B	561	ARG	CD-NE-CZ	5.27	130.98	123.60
1	A	1004	SER	N-CA-CB	5.27	118.41	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	924	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	199	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	C	210	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	134	LEU	N-CA-CB	5.26	120.92	110.40
1	C	392	TYR	CB-CG-CD1	5.26	124.16	121.00
1	D	190	ARG	N-CA-CB	5.25	120.04	110.60
1	D	832	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	687	GLN	N-CA-CB	5.24	120.03	110.60
1	D	100	TYR	CA-CB-CG	-5.23	103.46	113.40
1	B	37	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	531	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	15	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	404	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	903[A]	GLN	N-CA-CB	5.22	120.00	110.60
1	C	903[B]	GLN	N-CA-CB	5.22	120.00	110.60
1	B	190	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	170	GLU	N-CA-CB	5.22	120.00	110.60
1	D	227	VAL	CA-CB-CG1	-5.22	103.07	110.90
1	C	610	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	687	GLN	N-CA-CB	5.21	119.99	110.60
1	D	193	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	258	VAL	O-C-N	5.21	131.04	122.70
1	B	336	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	D	853	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	881	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	126	THR	CA-CB-CG2	-5.20	105.12	112.40
1	A	96	ASP	CB-CG-OD1	5.20	122.97	118.30
1	C	492	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	396	PRO	N-CA-CB	5.19	109.53	103.30
1	B	747	PHE	N-CA-C	-5.18	97.01	111.00
1	B	972	HIS	N-CA-CB	5.18	119.93	110.60
1	B	1019	VAL	CA-CB-CG1	-5.18	103.13	110.90
1	B	980	GLU	N-CA-CB	5.18	119.92	110.60
1	C	193	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	C	255	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	280	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	300	LEU	CA-C-N	-5.17	105.83	117.20
1	B	659	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	425	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	610	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	96	ASP	CB-CG-OD1	5.16	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	C	735	HIS	CB-CA-C	5.15	120.70	110.40
1	D	201	ASP	CB-CG-OD1	5.15	122.93	118.30
1	D	721	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	610	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	D	210	ARG	CD-NE-CZ	5.14	130.80	123.60
1	C	130	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	639	THR	CA-CB-CG2	-5.14	105.21	112.40
1	D	234	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	128	ASN	CA-CB-CG	-5.12	102.14	113.40
1	B	494	THR	CA-CB-CG2	-5.12	105.24	112.40
1	C	59	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	507	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	486	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	C	909	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	356	ARG	CD-NE-CZ	5.11	130.75	123.60
1	D	756	TRP	CB-CA-C	-5.11	100.18	110.40
1	D	1018	LEU	CB-CA-C	-5.11	100.49	110.20
1	B	172	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	368	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	908	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	500	CYS	CA-CB-SG	-5.10	104.82	114.00
1	C	924	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	916	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	234	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	748	CYS	N-CA-CB	5.09	119.76	110.60
1	A	98	PRO	N-CA-C	-5.08	98.88	112.10
1	C	435	ALA	CB-CA-C	-5.08	102.48	110.10
1	D	223	SER	CB-CA-C	5.07	119.73	110.10
1	B	829	THR	CA-CB-CG2	-5.07	105.31	112.40
1	B	857	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	569	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	321	THR	CA-CB-CG2	-5.06	105.32	112.40
1	B	164	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	997	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	D	672	VAL	CB-CA-C	-5.05	101.81	111.40
1	A	598	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	132	SER	N-CA-CB	5.04	118.06	110.50
1	C	400	THR	CA-CB-CG2	-5.04	105.35	112.40
1	A	428	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	425	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	385	ASN	CB-CA-C	-5.01	100.37	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	826	THR	CA-CB-CG2	-5.01	105.39	112.40
1	C	648	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	D	554	GLN	CB-CA-C	5.01	120.42	110.40
1	A	755	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	230	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	B	237	ARG	CD-NE-CZ	5.00	130.60	123.60
1	B	314	GLU	N-CA-CB	5.00	119.61	110.60
1	C	901	GLY	N-CA-C	-5.00	100.59	113.10
1	C	908	ASP	CB-CG-OD1	5.00	122.80	118.30
1	D	894	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	A	5	ASP	CB-CG-OD1	5.00	122.80	118.30
1	C	842	TRP	N-CA-CB	5.00	119.60	110.60

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	166	ARG	CA
1	A	187	MET	CA
1	B	118	ASN	CA
1	C	291	LEU	CA
1	C	503	TYR	CA
1	C	735	HIS	CA
1	C	980	GLU	CA
1	D	938	ARG	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	352	ARG	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8238	0	7824	643	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8238	0	7824	695	0
1	C	8238	0	7824	667	0
1	D	8238	0	7823	632	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	211	0	0	13	0
3	B	202	0	0	12	0
3	C	220	0	0	24	0
3	D	212	0	0	13	0
All	All	33805	0	31295	2582	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

All (2582) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:LEU:HB3	1:A:177:LEU:HD21	1.21	1.17
1:B:427:THR:HA	1:B:436:MET:HE1	1.26	1.14
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.24	1.12
1:D:427:THR:HA	1:D:436:MET:HE1	1.32	1.11
1:A:777:LEU:HD21	1:A:889:ALA:HB2	1.28	1.10
1:A:7:LEU:HD21	1:A:74:LEU:HD21	1.32	1.09
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.21	1.07
1:A:944:LEU:HD12	1:A:945:ASN:H	1.20	1.04
1:C:362:LEU:HD21	1:C:576:ILE:HD12	1.39	1.03
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.21	1.03
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.39	1.03
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.39	1.03
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.34	1.02
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.39	1.02
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.44	0.99
1:B:858:ILE:HD13	1:B:864:MET:HB3	1.42	0.99
1:C:693:GLN:HG2	1:C:721:ARG:HD3	1.44	0.99
1:D:830:LEU:HD21	1:D:835:LEU:HB2	1.43	0.98
1:B:650:GLU:HB3	1:B:670:LEU:HD12	1.43	0.98
1:B:7:LEU:HD23	1:B:74:LEU:HD11	1.44	0.98
1:C:777:LEU:HD21	1:C:889:ALA:HB2	1.42	0.97
1:A:928:PRO:HB2	1:A:973:ARG:HH12	1.26	0.97
1:D:597:ASN:HD22	1:D:599:ARG:H	1.13	0.96
1:D:597:ASN:ND2	1:D:599:ARG:H	1.64	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:830:LEU:HD21	1:B:835:LEU:HB2	1.47	0.96
1:D:984:LEU:HD21	1:D:986:ILE:HD11	1.44	0.95
1:B:367:MET:HB3	1:B:372:MET:HE3	1.48	0.95
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.44	0.95
1:B:595:THR:HG23	1:B:596:PRO:HA	1.50	0.93
1:C:568:TRP:HE1	1:C:604:ASN:ND2	1.66	0.93
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.51	0.93
1:D:251:ARG:HH11	1:D:251:ARG:HG3	1.31	0.93
1:A:360:HIS:ND1	1:A:361:PRO:HD2	1.84	0.92
1:B:730:LEU:HD12	1:B:730:LEU:H	1.32	0.92
1:D:230:ARG:HG3	1:D:230:ARG:HH11	1.34	0.92
1:C:581:ASN:HD22	1:C:583:ASN:ND2	1.66	0.92
1:B:427:THR:HA	1:B:436:MET:CE	2.00	0.92
1:C:26:ARG:HD2	1:C:169:SER:HA	1.51	0.91
1:B:559:TYR:HB2	1:B:562:LEU:HD12	1.50	0.91
1:A:851:ILE:HD12	1:B:726:LEU:HD13	1.50	0.91
1:B:118:ASN:HB2	1:B:191:TRP:HD1	1.32	0.91
1:C:237:ARG:HB3	1:C:237:ARG:NH1	1.84	0.91
1:A:26:ARG:HH11	1:A:169:SER:HB3	1.37	0.90
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.35	0.90
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.33	0.90
1:D:352:ARG:HB2	1:D:385:ASN:HB2	1.53	0.90
1:B:830:LEU:CD2	1:B:835:LEU:HB2	2.02	0.90
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.36	0.90
1:C:427:THR:HA	1:C:436:MET:CE	2.02	0.90
1:C:1004:SER:HB3	1:C:1006:GLU:OE2	1.71	0.89
1:B:778:THR:HG22	1:B:779:PRO:HD2	1.54	0.89
1:A:227:VAL:HG13	1:A:240:LEU:HD11	1.54	0.89
1:A:427:THR:HA	1:A:436:MET:CE	2.03	0.89
1:B:89:ASN:ND2	1:B:205:MET:HB3	1.87	0.89
1:D:427:THR:HA	1:D:436:MET:CE	2.01	0.88
1:A:944:LEU:HD12	1:A:945:ASN:N	1.86	0.88
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.55	0.88
1:B:786:ARG:HD3	1:B:880:ALA:HB1	1.55	0.88
1:D:114:VAL:HG13	1:D:115:PRO:HD2	1.56	0.88
1:C:734:SER:HB3	1:C:860:GLY:CA	2.03	0.88
1:C:928:PRO:HB2	1:C:973:ARG:NH1	1.87	0.88
1:B:282:ARG:HH12	1:C:419:GLY:HA2	1.38	0.88
1:C:653[A]:HIS:CE1	1:C:667:GLU:HG2	2.09	0.87
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.57	0.87
1:D:830:LEU:CD2	1:D:835:LEU:HB2	2.05	0.86
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.10	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.55	0.86
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.57	0.86
1:A:38:ASN:HD22	1:A:41:GLU:H	1.22	0.86
1:C:730:LEU:HD12	1:C:730:LEU:H	1.40	0.86
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.90	0.86
1:B:444:VAL:O	1:B:448:ARG:HB3	1.77	0.85
1:B:734:SER:CB	1:B:860:GLY:HA3	2.06	0.85
1:A:740:LEU:HD12	1:A:741:THR:H	1.41	0.85
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.12	0.85
1:B:842:TRP:CZ3	1:B:852:SER:HB2	2.11	0.85
1:B:589:GLY:HA3	1:B:599:ARG:HA	1.58	0.84
1:C:362:LEU:CD2	1:C:576:ILE:HD12	2.07	0.84
1:D:102:ASN:ND2	1:D:201:ASP:HB2	1.90	0.84
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.59	0.84
1:A:7:LEU:CD2	1:A:74:LEU:HD21	2.06	0.84
1:D:650:GLU:HB3	1:D:670:LEU:CD1	2.08	0.84
1:A:930:VAL:HA	1:A:973:ARG:CD	2.08	0.84
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.58	0.84
1:A:134:LEU:HD22	1:A:134:LEU:H	1.43	0.84
1:D:240:LEU:HD23	1:D:293:LEU:HD12	1.59	0.84
1:C:360:HIS:ND1	1:C:361:PRO:HD2	1.93	0.84
1:D:360:HIS:ND1	1:D:361:PRO:HD2	1.93	0.83
1:B:693:GLN:HG2	1:B:721:ARG:HD3	1.60	0.83
1:A:777:LEU:HD21	1:A:889:ALA:CB	2.08	0.83
1:C:597:ASN:HD22	1:C:599:ARG:H	1.25	0.83
1:D:559:TYR:HB2	1:D:562:LEU:CD1	2.08	0.83
1:A:38:ASN:ND2	1:A:41:GLU:H	1.76	0.83
1:C:776:LEU:C	1:C:777:LEU:HD23	1.99	0.82
1:A:746:ASP:CA	1:A:760:ARG:HG3	2.08	0.82
1:B:693:GLN:HG2	1:B:721:ARG:CD	2.08	0.82
1:C:902:PRO:HD2	1:C:903[B]:GLN:HG3	1.60	0.82
1:D:533:LEU:HD12	1:D:534:ILE:N	1.94	0.82
1:C:102:ASN:ND2	1:C:201:ASP:HB2	1.94	0.82
1:C:255:ARG:HG2	1:C:255:ARG:HH11	1.45	0.82
1:D:255:ARG:HH11	1:D:255:ARG:HG2	1.43	0.82
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.45	0.82
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.09	0.82
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.62	0.82
1:B:118:ASN:HB2	1:B:191:TRP:CD1	2.15	0.82
1:A:658:LEU:HD22	1:A:688:PRO:HG2	1.59	0.82
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.62	0.81
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.26	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:141:ILE:HD13	1:B:143:PHE:CZ	2.16	0.81
1:C:9:VAL:O	1:C:12:GLN:HB3	1.81	0.81
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.61	0.81
1:A:878:HIS:CD2	1:A:1010:SER:HB3	2.16	0.81
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.45	0.81
1:B:655:MET:HG3	1:B:656:VAL:N	1.95	0.81
1:A:436:MET:CE	1:A:467:ASN:HD22	1.93	0.80
1:C:125:LEU:HG	1:C:126:THR:N	1.95	0.80
1:C:777:LEU:HD21	1:C:889:ALA:CB	2.10	0.80
1:A:9:VAL:O	1:A:12:GLN:HB3	1.80	0.80
1:D:525:SER:HB2	3:D:4202:HOH:O	1.81	0.80
1:B:658:LEU:HG	1:B:661:LYS:NZ	1.96	0.80
1:A:635:THR:HG21	1:A:679:LEU:HD13	1.64	0.80
1:A:7:LEU:CD1	1:A:69:VAL:HG12	2.11	0.80
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.62	0.80
1:C:135:GLN:HE21	1:C:135:GLN:HA	1.44	0.80
1:C:942:ARG:HA	1:C:953:GLY:O	1.82	0.80
1:C:347:LYS:NZ	1:C:675:GLN:HG3	1.97	0.80
1:D:984:LEU:CD2	1:D:986:ILE:HD11	2.12	0.80
1:B:662:PRO:O	1:B:663:LEU:HD23	1.81	0.80
1:B:840:HIS:HB2	1:B:842:TRP:CZ3	2.16	0.80
1:A:24:LEU:HB2	1:A:161:TYR:HB3	1.62	0.80
1:B:856:TYR:HB3	1:B:864:MET:CE	2.13	0.80
1:C:685:LEU:HD23	1:C:686:PRO:HD3	1.62	0.80
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.46	0.80
1:A:856:TYR:HB3	1:A:864:MET:CE	2.12	0.79
1:B:299:LYS:HB3	1:B:307:ASN:ND2	1.96	0.79
1:D:322:LEU:HD22	1:D:323:ILE:H	1.46	0.79
1:C:427:THR:HA	1:C:436:MET:HE1	1.64	0.79
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.97	0.79
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.64	0.79
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.17	0.79
1:D:282:ARG:HG3	1:D:282:ARG:HH11	1.47	0.79
1:A:367:MET:HB3	1:A:372:MET:CE	2.12	0.79
1:D:237:ARG:HH11	1:D:237:ARG:CB	1.95	0.79
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.17	0.78
1:A:696:LEU:HD12	1:A:697:THR:N	1.97	0.78
1:A:599:ARG:NH1	1:A:600:GLN:HE22	1.81	0.78
1:C:105:TYR:HB3	1:C:106:PRO:HD2	1.65	0.78
1:A:202:MET:HA	1:A:573:GLN:HE22	1.47	0.78
1:D:237:ARG:HH11	1:D:237:ARG:HB2	1.47	0.78
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.17	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:225:PHE:HB3	1:B:244:VAL:HG13	1.65	0.78
1:D:890:GLN:NE2	1:D:890:GLN:H	1.81	0.78
1:B:102:ASN:ND2	1:B:201:ASP:HB2	1.99	0.78
1:B:786:ARG:HA	1:B:964:GLN:OE1	1.84	0.78
1:C:53:SER:O	1:C:54:LEU:HD23	1.84	0.78
1:C:945:ASN:OD1	1:C:950:GLN:HB2	1.83	0.78
1:D:102:ASN:HD22	1:D:201:ASP:HB2	1.49	0.78
1:D:52[B]:ARG:HG3	1:D:133:TRP:CH2	2.19	0.78
1:A:52[B]:ARG:HH22	1:A:130:ASP:HB2	1.47	0.78
1:A:928:PRO:HB2	1:A:973:ARG:NH1	1.99	0.77
1:C:167:LEU:HD21	1:C:393:PRO:HG2	1.66	0.77
1:C:258:VAL:HG23	1:C:291:LEU:HD11	1.66	0.77
1:A:777:LEU:CD2	1:A:889:ALA:HB2	2.11	0.77
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.31	0.77
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.66	0.77
1:C:577:LYS:HD3	1:C:585:TRP:CZ2	2.19	0.77
1:C:581:ASN:HD22	1:C:583:ASN:HD22	1.31	0.77
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.67	0.77
1:C:764:PHE:CD2	1:C:781:ARG:HB3	2.19	0.77
1:B:433:LEU:HB2	1:B:467:ASN:OD1	1.84	0.77
1:B:89:ASN:HD22	1:B:205:MET:HB3	1.50	0.77
1:B:422:PRO:CG	1:C:279:ILE:HD11	2.13	0.77
1:D:5:ASP:OD2	1:D:157:ARG:HA	1.84	0.77
1:A:427:THR:HA	1:A:436:MET:HE2	1.65	0.77
1:D:114:VAL:CG1	1:D:115:PRO:HD2	2.15	0.77
1:B:597:ASN:HD22	1:B:599:ARG:H	1.33	0.77
1:A:950:GLN:OE1	1:A:952:ARG:HD3	1.85	0.77
1:C:581:ASN:ND2	1:C:583:ASN:ND2	2.32	0.77
1:B:656:VAL:HG12	1:B:694:LEU:HD11	1.67	0.77
1:A:878:HIS:HB3	1:A:1009:LEU:O	1.85	0.77
1:C:210:ARG:HD3	3:C:4036:HOH:O	1.84	0.76
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.64	0.76
1:C:446:ARG:HG2	1:C:447:ASP:OD1	1.85	0.76
1:D:777:LEU:HD21	1:D:889:ALA:HB2	1.67	0.76
1:C:167:LEU:HB3	1:C:168:PRO:HD2	1.67	0.76
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.68	0.76
1:C:258:VAL:CG2	1:C:291:LEU:HD11	2.16	0.76
1:A:598:ASP:O	1:A:601:PHE:HB2	1.85	0.76
1:B:423:MET:HB2	1:C:282:ARG:HG3	1.66	0.76
1:B:457:SER:HA	1:B:485:GLN:O	1.84	0.76
1:B:458:LEU:HB2	1:B:486:TYR:HB2	1.67	0.76
1:C:749:ILE:O	1:C:755:ARG:HG3	1.86	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:797:GLU:O	1:B:801:ILE:HD12	1.86	0.75
1:C:778:THR:HB	1:C:887:GLN:HB3	1.68	0.75
1:C:930:VAL:HA	1:C:973:ARG:HG2	1.68	0.75
1:A:740:LEU:HD12	1:A:741:THR:N	2.01	0.75
1:B:43:ARG:HG2	1:B:43:ARG:NH1	1.99	0.75
1:A:634:GLN:HB3	1:A:685:LEU:HD11	1.66	0.75
1:D:835:LEU:CD1	1:D:857:ARG:HB2	2.16	0.75
1:C:135:GLN:NE2	1:C:135:GLN:HA	1.96	0.75
1:C:797:GLU:O	1:C:801:ILE:HD12	1.85	0.75
1:B:433:LEU:HD12	1:B:433:LEU:O	1.86	0.75
1:B:758:PHE:CE2	1:B:765:LEU:HB2	2.21	0.75
1:B:251:ARG:H	1:B:254:LEU:HD12	1.51	0.75
1:C:128:ASN:HA	1:C:180:GLY:O	1.87	0.75
1:D:1004:SER:HB3	1:D:1006:GLU:OE2	1.86	0.75
1:C:427:THR:HA	1:C:436:MET:HE2	1.69	0.74
1:A:511:PRO:HA	1:A:516:PRO:HB3	1.69	0.74
1:D:77:ASP:C	1:D:78:LEU:HD23	2.08	0.74
1:A:778:THR:HG23	1:A:779:PRO:HD2	1.69	0.74
1:A:769:TRP:HE1	1:A:774:LYS:HD2	1.52	0.74
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.01	0.74
1:A:769:TRP:NE1	1:A:774:LYS:HD2	2.02	0.74
1:B:577:LYS:HD3	1:B:585:TRP:CZ2	2.22	0.74
1:C:499:ILE:HB	1:C:533:LEU:HB2	1.69	0.74
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.69	0.74
1:B:835:LEU:C	1:B:836:ILE:HD13	2.07	0.74
1:C:77:ASP:O	1:C:78:LEU:HD23	1.87	0.74
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.67	0.74
1:B:3:ILE:HG23	1:B:4:THR:H	1.51	0.74
1:D:166:ARG:HD3	3:D:4035:HOH:O	1.86	0.74
1:A:100:TYR:CE2	1:A:602:CYS:HB3	2.22	0.74
1:C:375:ASP:O	1:C:379:MET:HG3	1.86	0.74
1:D:655:MET:HG3	1:D:656:VAL:N	1.99	0.74
1:D:890:GLN:NE2	1:D:890:GLN:N	2.36	0.74
1:B:740:LEU:HD12	1:B:748:CYS:O	1.88	0.74
1:A:420:MET:HE2	1:A:426:LEU:HG	1.70	0.74
1:C:655:MET:HE1	1:C:662:PRO:HB3	1.68	0.74
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.02	0.74
1:A:637:GLU:HB2	1:A:679:LEU:HD21	1.69	0.73
1:D:403:ASP:OD1	1:D:451:PRO:HD2	1.88	0.73
1:C:581:ASN:ND2	1:C:583:ASN:HD22	1.83	0.73
1:C:416:GLU:HG3	1:C:460:ASN:O	1.88	0.73
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.17	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:217:LYS:HG2	1:C:218:PRO:HD2	1.68	0.73
1:A:41:GLU:HG2	1:A:46:ARG:NH1	2.03	0.73
1:A:546:LEU:HD22	1:A:616:ALA:HB1	1.68	0.73
1:C:777:LEU:CD2	1:C:889:ALA:HB2	2.17	0.73
1:D:658:LEU:CG	1:D:661:LYS:HZ2	2.02	0.73
1:B:796:SER:HB2	1:B:802:ASP:HB3	1.69	0.73
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.89	0.73
1:A:224:ASP:HB3	1:A:245:GLN:HG3	1.69	0.73
1:B:367:MET:HB3	1:B:372:MET:CE	2.19	0.73
1:A:770:ILE:HD12	1:A:775:GLN:NE2	2.02	0.72
1:D:26:ARG:HD3	1:D:169:SER:HB3	1.69	0.72
1:C:342:LEU:O	1:C:343:LEU:HD23	1.89	0.72
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	1.89	0.72
1:A:367:MET:HB3	1:A:372:MET:HE3	1.69	0.72
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.19	0.72
1:B:777:LEU:HD11	1:B:889:ALA:HA	1.69	0.72
1:D:655:MET:HE1	1:D:662:PRO:HB3	1.71	0.72
1:C:114:VAL:HG13	1:C:115:PRO:HD2	1.69	0.72
1:B:942:ARG:HA	1:B:953:GLY:O	1.89	0.72
1:A:683:PRO:O	1:A:684:GLU:C	2.24	0.72
1:C:148:SER:HB3	1:C:190:ARG:O	1.89	0.72
1:B:427:THR:CA	1:B:436:MET:HE1	2.15	0.72
1:A:646:HIS:O	1:A:648:ASP:N	2.22	0.72
1:B:696:LEU:HB2	1:B:722:LEU:HD11	1.71	0.72
1:D:658:LEU:HG	1:D:661:LYS:HZ2	1.55	0.72
1:B:6:SER:OG	1:B:9:VAL:HB	1.88	0.72
1:B:748:CYS:C	1:B:749:ILE:HD12	2.10	0.72
1:C:873:ALA:O	1:C:876:THR:HG22	1.90	0.72
1:A:5:ASP:OD2	1:A:157:ARG:HA	1.90	0.72
1:B:114:VAL:CG1	1:B:191:TRP:HB2	2.20	0.72
1:D:52[B]:ARG:HG3	1:D:133:TRP:HH2	1.53	0.72
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.71	0.72
1:C:836:ILE:HD13	1:C:836:ILE:N	2.05	0.72
1:D:531:ARG:O	1:D:561:ARG:NH1	2.22	0.72
1:C:134:LEU:N	1:C:134:LEU:HD23	2.04	0.72
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.55	0.72
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.53	0.72
1:D:38:ASN:ND2	1:D:41:GLU:H	1.88	0.72
1:B:230:ARG:HG3	1:B:230:ARG:NH1	2.03	0.71
1:B:422:PRO:HG3	1:C:279:ILE:HD11	1.71	0.71
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.54	0.71
1:C:894:ARG:NH2	1:C:921:PRO:HD3	2.05	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.71	0.71
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.01	0.71
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.23	0.71
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.71	0.71
1:C:737:ILE:HD12	1:C:738:PRO:O	1.89	0.71
1:B:849:LEU:N	1:B:849:LEU:HD23	2.06	0.71
1:B:836:ILE:HD13	1:B:836:ILE:N	2.03	0.71
1:A:708:TRP:CZ3	1:A:709:SER:HB3	2.25	0.71
1:B:464:HIS:HB2	1:B:489:GLY:HA3	1.71	0.71
1:B:858:ILE:CD1	1:B:864:MET:HB3	2.18	0.71
1:C:100:TYR:HB2	1:C:203:TRP:CD2	2.25	0.71
1:C:767:GLN:HG3	1:C:768:MET:N	2.04	0.71
1:A:650:GLU:HA	1:A:701:VAL:O	1.90	0.71
1:A:383:ASN:ND2	1:A:625:GLN:HA	2.06	0.71
1:A:570:TRP:CD1	1:A:571:VAL:HG22	2.25	0.71
1:D:251:ARG:NH1	1:D:251:ARG:HG3	2.03	0.71
1:C:53:SER:C	1:C:54:LEU:HD23	2.09	0.71
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.26	0.71
1:A:230:ARG:HB3	1:A:230:ARG:HH11	1.55	0.71
1:A:427:THR:HA	1:A:436:MET:HE1	1.70	0.71
1:C:888:LEU:O	1:C:981:GLY:HA3	1.91	0.71
1:A:647:SER:OG	1:A:672:VAL:HG23	1.91	0.71
1:B:651:LEU:CD1	1:B:703:PRO:HG3	2.21	0.71
1:A:742:THR:HG22	1:A:743:SER:H	1.55	0.71
1:A:93:HIS:HB3	1:A:95:TYR:HE1	1.56	0.70
1:A:878:HIS:NE2	1:A:1010:SER:HB3	2.06	0.70
1:D:568:TRP:HE1	1:D:604:ASN:ND2	1.87	0.70
1:B:282:ARG:HH12	1:C:419:GLY:CA	2.05	0.70
1:B:152:LEU:O	1:B:159:VAL:HG23	1.90	0.70
1:C:856:TYR:HB3	1:C:864:MET:CE	2.21	0.70
1:A:734:SER:HB2	1:A:860:GLY:HA3	1.73	0.70
1:C:620:ALA:O	1:C:624:GLN:HG3	1.91	0.70
1:D:836:ILE:N	1:D:836:ILE:HD13	2.07	0.70
1:A:152:LEU:HG	1:A:153:TRP:N	2.05	0.70
1:D:835:LEU:C	1:D:836:ILE:HD13	2.12	0.70
1:C:989:PHE:CE1	1:C:1014:TYR:HB3	2.26	0.70
1:A:242:ALA:O	1:A:290:THR:HA	1.92	0.70
1:D:734:SER:HB2	1:D:860:GLY:HA3	1.73	0.70
1:D:499:ILE:HG22	1:D:501:PRO:CD	2.19	0.69
1:D:859:ASP:OD1	1:D:861:SER:HB2	1.92	0.69
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.89	0.69
1:A:11:LEU:HD23	1:A:11:LEU:N	2.07	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.75	0.69
1:D:827:ALA:CB	1:D:836:ILE:HD12	2.22	0.69
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.26	0.69
1:A:763:GLY:HA3	1:A:822:LEU:HD21	1.75	0.69
1:B:553:TRP:O	1:B:557:ARG:HG3	1.92	0.69
1:A:473:ARG:O	1:A:473:ARG:HD3	1.92	0.69
1:D:835:LEU:HD12	1:D:857:ARG:HB2	1.74	0.69
1:A:134:LEU:N	1:A:134:LEU:HD22	2.07	0.69
1:B:383:ASN:ND2	1:B:621:LYS:HG3	2.08	0.69
1:D:62:TRP:CD1	1:D:95:TYR:HB3	2.28	0.69
1:A:678:GLN:C	1:A:679:LEU:HD23	2.13	0.69
1:B:576:ILE:HD13	1:B:584:PRO:HB3	1.75	0.69
1:C:662:PRO:C	1:C:663:LEU:HD23	2.13	0.69
1:A:991:MET:HG2	1:A:992:GLY:N	2.07	0.69
1:C:850:PHE:HD2	1:C:872:VAL:HG13	1.57	0.69
1:C:12:GLN:HG3	1:C:13:ARG:N	2.08	0.69
1:B:355:ASN:OD1	1:B:388:ARG:HD3	1.92	0.69
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.75	0.69
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.16	0.69
1:B:824:GLN:O	1:B:838:THR:HA	1.92	0.69
1:C:457:SER:HA	1:C:485:GLN:O	1.93	0.69
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.75	0.69
1:C:1018:LEU:HD23	1:C:1018:LEU:N	2.08	0.69
1:C:110:ASN:O	1:C:113:PHE:N	2.26	0.69
1:A:737:ILE:HG13	1:A:738:PRO:HD2	1.73	0.69
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.27	0.69
1:C:738:PRO:HA	1:C:751:LEU:HB2	1.74	0.68
1:C:830:LEU:HB2	1:C:833:ALA:O	1.93	0.68
1:C:245:GLN:HB3	1:C:288:ARG:HG2	1.75	0.68
1:C:38:ASN:ND2	1:C:41:GLU:H	1.90	0.68
1:A:210:ARG:HD3	3:A:4019:HOH:O	1.93	0.68
1:B:63:PHE:CD1	1:B:69:VAL:HG22	2.28	0.68
1:B:17:GLU:HG2	1:B:114:VAL:HG23	1.74	0.68
1:D:657:ALA:O	1:D:694:LEU:HD12	1.94	0.68
1:A:202:MET:CA	1:A:573:GLN:HE22	2.05	0.68
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.75	0.68
1:B:255:ARG:NH1	1:B:255:ARG:HG2	2.08	0.68
1:D:210:ARG:HD3	3:D:4036:HOH:O	1.91	0.68
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.26	0.68
1:A:287:ASP:CG	1:D:425:ARG:HH22	1.96	0.68
1:A:510:GLN:HB2	1:A:517:LYS:HB2	1.76	0.68
1:D:129:VAL:HG23	1:D:182:ASN:HD22	1.56	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:531:ARG:O	1:C:561:ARG:NH1	2.27	0.68
1:D:166:ARG:HG3	1:D:392:TYR:CG	2.29	0.68
1:A:635:THR:CG2	1:A:679:LEU:HD13	2.24	0.68
1:D:786:ARG:HA	1:D:964:GLN:OE1	1.94	0.68
1:C:649:ASN:OD1	1:C:703:PRO:HD2	1.94	0.68
1:A:314:GLU:HB3	1:A:322:LEU:HD21	1.75	0.67
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.75	0.67
1:D:187:MET:HG3	1:D:187:MET:O	1.93	0.67
1:C:356:ARG:HD2	1:C:379:MET:CE	2.24	0.67
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.29	0.67
1:D:654:TRP:HZ3	1:D:656:VAL:HG23	1.59	0.67
1:D:24:LEU:HB2	1:D:161:TYR:HB3	1.77	0.67
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.23	0.67
1:D:856:TYR:HB3	1:D:864:MET:HE2	1.76	0.67
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.29	0.67
1:A:595:THR:HG23	1:A:596:PRO:HA	1.76	0.67
1:D:71:GLU:O	1:D:72:SER:C	2.32	0.67
1:B:651:LEU:HD13	1:B:703:PRO:HG3	1.75	0.67
1:A:742:THR:HG22	1:A:743:SER:N	2.08	0.67
1:C:166:ARG:O	1:C:210:ARG:NH2	2.28	0.67
1:D:43:ARG:O	1:D:310:ARG:HD3	1.94	0.67
1:C:187:MET:O	1:C:187:MET:HG3	1.95	0.67
1:C:140:ARG:NH1	1:C:170:GLU:OE1	2.27	0.67
1:A:59:ARG:NH2	1:A:81:ALA:O	2.27	0.67
1:C:35:SER:OG	1:C:37:ARG:NH1	2.27	0.67
1:B:928:PRO:HB2	1:B:973:ARG:NH1	2.10	0.67
1:D:658:LEU:HD22	1:D:688:PRO:HG2	1.77	0.67
1:C:80:GLU:OE2	1:C:80:GLU:N	2.28	0.67
1:B:822:LEU:HD12	1:B:824:GLN:H	1.60	0.67
1:D:87:PRO:HB3	1:D:210:ARG:O	1.95	0.67
1:D:949:HIS:HB2	1:D:951:TRP:CH2	2.30	0.67
1:B:128:ASN:HA	1:B:180:GLY:O	1.94	0.67
1:A:436:MET:HE3	1:A:467:ASN:HD22	1.60	0.67
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.28	0.67
1:B:3:ILE:HG23	1:B:4:THR:N	2.10	0.67
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.30	0.67
1:A:962:TYR:HD2	1:A:966:GLN:HE22	1.42	0.67
1:D:933:SER:O	1:D:934:GLU:C	2.31	0.67
1:B:738:PRO:HB2	1:B:834:VAL:HG23	1.76	0.67
1:A:128:ASN:HA	1:A:180:GLY:O	1.95	0.67
1:B:824:GLN:OE1	1:B:837:THR:HG21	1.94	0.67
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.29	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:654:TRP:CZ3	1:A:656:VAL:HG23	2.31	0.66
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.77	0.66
1:C:542:MET:HE3	1:C:601:PHE:HA	1.77	0.66
1:C:542:MET:HA	1:C:604:ASN:HA	1.77	0.66
1:A:410:VAL:HG22	1:A:455:ILE:HB	1.75	0.66
1:A:436:MET:HE1	1:A:467:ASN:HD22	1.58	0.66
1:B:576:ILE:HG23	1:B:577:LYS:N	2.11	0.66
1:D:894:ARG:NH2	1:D:921:PRO:HD3	2.10	0.66
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.29	0.66
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.31	0.66
1:B:587:ALA:HB1	1:B:592:PHE:CE1	2.30	0.66
1:A:786:ARG:HG2	1:A:880:ALA:HB1	1.77	0.66
1:A:928:PRO:O	1:A:973:ARG:NH1	2.29	0.66
1:B:114:VAL:HG13	1:B:191:TRP:HB2	1.76	0.66
1:B:777:LEU:CG	1:B:889:ALA:HA	2.26	0.66
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.78	0.66
1:D:603:MET:HE1	1:D:930:VAL:CG1	2.26	0.66
1:B:576:ILE:CD1	1:B:584:PRO:HB3	2.25	0.66
1:B:807:VAL:O	1:B:811:LYS:HB2	1.95	0.66
1:C:879:PRO:HD2	1:C:1009:LEU:HB2	1.78	0.66
1:A:775:GLN:OE1	1:A:890:GLN:NE2	2.29	0.66
1:D:657:ALA:HB2	1:D:662:PRO:HA	1.77	0.66
1:B:577:LYS:HD3	1:B:585:TRP:HZ2	1.61	0.66
1:A:824:GLN:HG3	1:A:825:CYS:N	2.08	0.66
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.92	0.66
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.78	0.66
1:D:499:ILE:CG2	1:D:501:PRO:HD3	2.21	0.66
1:C:360:HIS:CE1	1:C:361:PRO:HD2	2.30	0.66
1:A:693:GLN:HG2	1:A:721:ARG:CD	2.26	0.66
1:C:347:LYS:HZ1	1:C:675:GLN:HG3	1.59	0.66
1:C:43:ARG:HG2	1:C:43:ARG:NH1	2.11	0.66
1:B:883:GLY:HA2	1:B:1016:TYR:OH	1.95	0.66
1:D:202:MET:HA	1:D:573:GLN:HE22	1.60	0.66
1:C:166:ARG:CG	1:C:392:TYR:HB2	2.26	0.66
1:C:856:TYR:HD2	1:C:864:MET:HE1	1.61	0.66
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.26	0.66
1:B:15:ASP:HB3	1:B:21:VAL:HG11	1.78	0.66
1:D:780:LEU:HA	1:D:886:CYS:HB3	1.76	0.66
1:B:211:ASP:OD1	1:B:211:ASP:N	2.28	0.66
1:D:875:ASP:OD2	1:D:875:ASP:N	2.27	0.66
1:A:432:TRP:O	1:A:436:MET:HG3	1.94	0.66
1:A:693:GLN:HG2	1:A:721:ARG:HD3	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:30:HIS:ND1	1:C:31:PRO:O	2.25	0.66
1:A:776:LEU:C	1:A:777:LEU:HD23	2.17	0.65
1:D:36:TRP:NE1	1:D:46:ARG:O	2.28	0.65
1:A:654:TRP:HZ3	1:A:656:VAL:HG23	1.60	0.65
1:B:237:ARG:NH1	1:B:296:GLU:OE2	2.29	0.65
1:D:547:GLY:HA2	1:D:908:ASP:O	1.96	0.65
1:D:429:ASP:OD1	1:D:431[A]:ARG:HG3	1.96	0.65
1:A:949:HIS:CD2	1:A:1020:TRP:HE1	2.15	0.65
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.32	0.65
1:B:537:GLU:HG2	1:B:568:TRP:HE3	1.59	0.65
1:B:866:ILE:HB	1:B:1018:LEU:HB2	1.77	0.65
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.78	0.65
1:B:856:TYR:HB3	1:B:864:MET:HE1	1.78	0.65
1:A:637:GLU:HA	1:A:679:LEU:CD2	2.26	0.65
1:B:355:ASN:O	1:B:569:ASP:HB2	1.97	0.65
1:C:161:TYR:OH	1:C:163:GLN:NE2	2.29	0.65
1:D:257:THR:HA	1:D:270:GLY:O	1.96	0.65
1:C:902:PRO:O	1:C:938:ARG:NH1	2.30	0.65
1:B:254:LEU:O	1:B:255:ARG:NH1	2.30	0.65
1:B:750:GLU:OE1	1:B:750:GLU:N	2.28	0.65
1:D:668:VAL:HG11	1:D:680:ILE:HD13	1.78	0.65
1:C:7:LEU:N	1:C:71:GLU:OE2	2.30	0.65
1:B:38:ASN:O	1:B:38:ASN:ND2	2.29	0.65
1:C:380:LYS:HE2	3:C:4077:HOH:O	1.97	0.65
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.05	0.65
1:A:440:VAL:HG21	1:A:471:LEU:HD13	1.79	0.65
1:A:851:ILE:HD12	1:B:726:LEU:CD1	2.24	0.65
1:C:900:LEU:HA	1:C:914:CYS:O	1.97	0.65
1:C:420:MET:CE	1:C:425:ARG:HB3	2.27	0.65
1:B:833:ALA:HB1	1:B:858:ILE:O	1.97	0.65
1:B:140:ARG:NH1	1:B:170:GLU:OE1	2.28	0.65
1:C:770:ILE:O	1:C:773:LYS:HD2	1.97	0.65
1:A:535:LEU:HD22	1:A:538:TYR:HB3	1.77	0.65
1:D:245:GLN:HB3	3:D:6016:HOH:O	1.96	0.65
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.27	0.65
1:B:595:THR:HG23	1:B:596:PRO:CA	2.26	0.65
1:C:668:VAL:HG12	1:C:669:PRO:HD2	1.79	0.65
1:D:403:ASP:CG	1:D:451:PRO:HD2	2.17	0.65
1:C:856:TYR:CD2	1:C:864:MET:HE1	2.32	0.65
1:A:770:ILE:HD12	1:A:775:GLN:CD	2.17	0.65
1:B:141:ILE:HG12	1:B:142:ILE:H	1.62	0.65
1:D:11:LEU:HD21	1:D:187:MET:CE	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:908:ASP:HB3	1:A:1007:PHE:CD1	2.32	0.65
1:C:932:PRO:HG2	1:C:970:THR:O	1.97	0.64
1:C:436:MET:HE1	1:C:467:ASN:HB2	1.79	0.64
1:A:287:ASP:OD2	1:D:425:ARG:NH2	2.31	0.64
1:A:748:CYS:C	1:A:749:ILE:HD12	2.17	0.64
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.78	0.64
1:C:246:MET:HE2	1:C:287:ASP:CB	2.26	0.64
1:D:46:ARG:CB	1:D:47:PRO:HD2	2.25	0.64
1:C:251:ARG:O	1:C:253:TYR:N	2.30	0.64
1:B:693:GLN:HG2	1:B:721:ARG:HD2	1.79	0.64
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.32	0.64
1:A:894:ARG:HD3	1:A:919:ASP:OD1	1.97	0.64
1:A:282:ARG:HG3	1:A:282:ARG:HH11	1.62	0.64
1:D:460:ASN:ND2	1:D:461:GLU:HG2	2.12	0.64
1:C:436:MET:CE	1:C:467:ASN:HD22	2.09	0.64
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.78	0.64
1:D:93:HIS:HB3	1:D:95:TYR:HE1	1.62	0.64
1:B:789:LEU:N	1:B:792:ASP:OD2	2.29	0.64
1:A:937:LEU:HD21	1:A:956:GLN:HB3	1.80	0.64
1:C:418:HIS:ND1	1:C:461:GLU:HG3	2.12	0.64
1:C:10:VAL:HG12	1:C:11:LEU:N	2.12	0.64
1:D:763:GLY:HA3	1:D:822:LEU:HD21	1.80	0.64
1:B:844:HIS:C	1:B:845:GLN:HG2	2.18	0.64
1:C:437:SER:O	1:C:441:THR:HG23	1.97	0.64
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.78	0.64
1:C:833:ALA:HB1	1:C:858:ILE:O	1.97	0.64
1:B:950:GLN:OE1	1:B:952:ARG:NH1	2.31	0.64
1:A:35:SER:OG	1:A:37:ARG:NH1	2.31	0.64
1:B:805:ALA:HB3	1:B:808:GLU:HB2	1.80	0.64
1:A:635:THR:HA	1:A:680:ILE:O	1.98	0.64
1:C:148:SER:OG	1:C:192:SER:HB3	1.97	0.64
1:C:850:PHE:CD2	1:C:872:VAL:HG13	2.33	0.64
1:D:350:LEU:N	3:D:4120:HOH:O	2.29	0.64
1:B:200:GLN:N	1:B:200:GLN:OE1	2.30	0.64
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.95	0.64
1:A:202:MET:CB	1:A:573:GLN:HE22	2.11	0.64
1:C:764:PHE:CE2	1:C:781:ARG:HB3	2.32	0.64
1:D:776:LEU:C	1:D:777:LEU:HD23	2.19	0.64
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.31	0.64
1:A:62:TRP:CZ2	1:A:119:PRO:HB3	2.33	0.64
1:D:11:LEU:HD21	1:D:187:MET:HE1	1.79	0.64
1:A:7:LEU:N	1:A:71:GLU:OE2	2.32	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:380:LYS:HE2	3:A:4042:HOH:O	1.98	0.63
1:A:6:SER:HB2	1:A:71:GLU:OE2	1.98	0.63
1:D:655:MET:CE	1:D:662:PRO:HB3	2.27	0.63
1:C:167:LEU:HD21	1:C:393:PRO:CG	2.27	0.63
1:A:618:THR:HG22	1:A:912:ALA:HB1	1.79	0.63
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.26	0.63
1:A:240:LEU:CD2	1:A:260:LEU:HD22	2.28	0.63
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.80	0.63
1:B:385:ASN:HB3	1:B:408:TYR:CD1	2.33	0.63
1:C:588:TYR:O	1:C:591:ASP:HB2	1.98	0.63
1:C:777:LEU:N	1:C:777:LEU:HD23	2.11	0.63
1:D:377:LEU:CD2	1:D:708:TRP:HA	2.29	0.63
1:A:678:GLN:O	1:A:679:LEU:HD23	1.98	0.63
1:A:856:TYR:HD2	1:A:864:MET:HE1	1.62	0.63
1:C:499:ILE:HD11	1:C:529:GLU:OE1	1.99	0.63
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.01	0.63
1:C:870:VAL:HG12	1:C:871:GLU:N	2.14	0.63
1:B:100:TYR:HB2	1:B:203:TRP:CE3	2.33	0.63
1:C:167:LEU:CD2	1:C:393:PRO:HB2	2.29	0.63
1:B:701:VAL:O	1:B:703:PRO:HD3	1.97	0.63
1:D:336:ARG:HH21	1:D:338:GLU:CD	2.01	0.63
1:B:842:TRP:HZ3	1:B:852:SER:HB2	1.61	0.63
1:A:789:LEU:CD1	1:A:993:ILE:HG22	2.29	0.63
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.32	0.63
1:A:823:LEU:HD22	1:B:728:VAL:HG12	1.80	0.63
1:A:38:ASN:ND2	1:A:41:GLU:HG3	2.14	0.63
1:A:749:ILE:HD12	1:A:749:ILE:N	2.14	0.63
1:B:673:ALA:HB1	1:B:674:PRO:CD	2.26	0.63
1:B:473:ARG:HD3	1:B:473:ARG:O	1.98	0.63
1:A:166:ARG:HD3	3:A:4018:HOH:O	1.98	0.63
1:C:43:ARG:NH2	1:C:264:GLU:OE2	2.32	0.63
1:B:374:GLN:O	1:B:378:LEU:HD12	1.99	0.63
1:B:282:ARG:NH1	1:C:418:HIS:O	2.28	0.63
1:A:304:GLU:C	1:A:305:ILE:HG13	2.18	0.63
1:B:658:LEU:HG	1:B:661:LYS:HZ1	1.62	0.63
1:C:433:LEU:HB3	1:C:434:PRO:CD	2.29	0.62
1:B:499:ILE:HB	1:B:533:LEU:HB2	1.80	0.62
1:A:502:MET:HB2	1:A:503:TYR:CD1	2.34	0.62
1:A:902:PRO:O	1:A:938:ARG:NH1	2.32	0.62
1:A:945:ASN:OD1	1:A:950:GLN:HB2	1.99	0.62
1:A:377:LEU:CD2	1:A:708:TRP:HA	2.29	0.62
1:D:52[A]:ARG:NH2	1:D:128:ASN:O	2.30	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:166:ARG:HG3	1:C:392:TYR:CG	2.33	0.62
1:B:383:ASN:HD22	1:B:621:LYS:HG3	1.63	0.62
1:C:502:MET:HA	1:C:537:GLU:O	2.00	0.62
1:C:431[B]:ARG:NH2	3:C:7516:HOH:O	2.32	0.62
1:D:827:ALA:HB2	1:D:836:ILE:HD12	1.81	0.62
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.81	0.62
1:B:204:ARG:N	1:B:204:ARG:HD3	2.13	0.62
1:A:7:LEU:HD11	1:A:69:VAL:HG12	1.80	0.62
1:D:100:TYR:HB3	1:D:589:GLY:HA2	1.80	0.62
1:D:603:MET:HE1	1:D:930:VAL:HG11	1.80	0.62
1:B:559:TYR:HB2	1:B:562:LEU:CD1	2.28	0.62
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.81	0.62
1:D:38:ASN:HD22	1:D:41:GLU:H	1.45	0.62
1:C:920:LEU:CB	1:C:921:PRO:HD2	2.28	0.62
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.02	0.62
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.82	0.62
1:A:38:ASN:HD21	1:A:40:GLU:HB2	1.65	0.62
1:D:42:ALA:O	1:D:310:ARG:NH1	2.33	0.62
1:D:904:GLU:HG2	1:D:909:ARG:HH22	1.64	0.62
1:B:424:ASN:OD1	1:C:279:ILE:HD12	2.00	0.62
1:D:38:ASN:HD21	1:D:40:GLU:HB2	1.63	0.62
1:D:103:VAL:HG22	1:D:418:HIS:CE1	2.34	0.62
1:B:35:SER:OG	1:B:37:ARG:NH1	2.32	0.62
1:D:467:ASN:O	1:D:471:LEU:HG	1.99	0.62
1:B:782:ASP:HB2	1:B:842:TRP:CZ2	2.34	0.62
1:C:167:LEU:HD21	1:C:393:PRO:CB	2.30	0.62
1:A:91:GLN:OE1	1:A:205:MET:HB3	2.00	0.62
1:A:403:ASP:OD1	1:A:451:PRO:HD2	2.00	0.62
1:A:663:LEU:HD23	1:A:663:LEU:N	2.13	0.62
1:D:274:PHE:HB3	1:D:286:ALA:O	2.00	0.62
1:D:693:GLN:HB3	1:D:721:ARG:HD3	1.82	0.62
1:C:833:ALA:CB	1:C:859:ASP:HA	2.30	0.62
1:C:776:LEU:O	1:C:777:LEU:HD23	1.99	0.62
1:A:928:PRO:CB	1:A:973:ARG:HH12	2.06	0.62
1:B:778:THR:HG22	1:B:779:PRO:CD	2.28	0.62
1:C:662:PRO:O	1:C:663:LEU:HD23	1.99	0.62
1:A:655:MET:CE	1:A:662:PRO:HB3	2.30	0.62
1:C:342:LEU:C	1:C:343:LEU:HD23	2.20	0.61
1:D:375:ASP:O	1:D:379:MET:HG3	1.99	0.61
1:D:437:SER:O	1:D:441:THR:HG23	1.99	0.61
1:A:856:TYR:CD2	1:A:864:MET:HE1	2.34	0.61
1:D:654:TRP:CZ3	1:D:656:VAL:HG23	2.35	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:989:PHE:HE1	1:C:1014:TYR:HB3	1.62	0.61
1:D:919:ASP:O	1:D:920:LEU:HD23	2.00	0.61
1:C:894:ARG:HD3	1:C:919:ASP:OD1	2.01	0.61
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.98	0.61
1:A:14:ARG:HA	1:A:16:TRP:CZ3	2.35	0.61
1:A:233:ASP:CG	1:C:233:ASP:HB3	2.21	0.61
1:C:22:THR:O	1:C:163:GLN:HG3	1.99	0.61
1:C:769:TRP:HA	1:C:773:LYS:O	1.99	0.61
1:A:613:PRO:HB3	1:A:617:LEU:HD23	1.83	0.61
1:A:143:PHE:O	1:A:168:PRO:HA	2.01	0.61
1:A:668:VAL:HG12	1:A:669:PRO:HD2	1.83	0.61
1:D:745:MET:HB2	1:D:746:ASP:OD2	2.01	0.61
1:C:141:ILE:HB	1:C:173:LEU:HD11	1.83	0.61
1:B:537:GLU:HG2	1:B:568:TRP:CE3	2.36	0.61
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.03	0.61
1:D:777:LEU:CD2	1:D:889:ALA:HB2	2.30	0.61
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.83	0.61
1:B:506:VAL:HA	1:B:520:ILE:HG12	1.81	0.61
1:D:196:TYR:O	1:D:417:THR:HG22	2.01	0.61
1:D:794:GLY:HA2	1:D:998:SER:O	2.00	0.61
1:A:874:SER:HB3	1:B:724:GLU:OE1	2.00	0.61
1:B:373:VAL:O	1:B:377:LEU:HG	2.00	0.61
1:B:141:ILE:HD13	1:B:143:PHE:CE1	2.35	0.61
1:A:662:PRO:C	1:A:663:LEU:HD23	2.19	0.61
1:B:129:VAL:HG12	1:B:134:LEU:HD11	1.81	0.61
1:B:542:MET:HB2	1:B:604:ASN:OD1	2.01	0.61
1:A:801:ILE:O	1:A:803:PRO:HD3	2.00	0.61
1:D:88:SER:HA	1:D:366:VAL:HG21	1.83	0.61
1:B:776:LEU:HB3	1:B:778:THR:O	2.00	0.61
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.36	0.61
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.11	0.61
1:C:357:HIS:HD2	1:C:392:TYR:OH	1.83	0.61
1:A:894:ARG:NH2	1:A:921:PRO:HD3	2.15	0.61
1:A:965:GLN:O	1:A:969:GLU:HG3	2.01	0.61
1:D:479:ASP:N	1:D:480:PRO:HD3	2.12	0.61
1:D:606:LEU:O	1:D:614:HIS:HB2	2.00	0.61
1:A:50:GLN:N	1:A:50:GLN:NE2	2.48	0.61
1:B:422:PRO:HD3	1:C:284:GLY:O	2.01	0.61
1:B:649:ASN:O	1:B:702:GLN:HG2	2.01	0.61
1:C:73:TRP:CZ2	1:C:185:ALA:HB1	2.35	0.61
1:A:52[B]:ARG:HG3	1:A:133:TRP:CH2	2.36	0.60
1:A:762:SER:OG	1:A:763:GLY:N	2.33	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:777:LEU:CD1	1:B:889:ALA:HA	2.29	0.60
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.01	0.60
1:C:557:ARG:HD2	3:C:4018:HOH:O	2.01	0.60
1:A:595:THR:CG2	1:A:596:PRO:HA	2.31	0.60
1:C:509:ASP:C	1:C:511:PRO:HD3	2.22	0.60
1:A:369:GLU:O	1:A:373:VAL:HG23	2.01	0.60
1:C:776:LEU:HD23	1:C:776:LEU:N	2.16	0.60
1:D:238:ALA:HB1	1:D:332:PHE:CE2	2.37	0.60
1:B:964:GLN:O	1:B:967:LEU:HB2	2.00	0.60
1:D:55:ASN:HD22	1:D:87:PRO:HD3	1.65	0.60
1:B:658:LEU:O	1:B:661:LYS:HE3	2.02	0.60
1:B:429:ASP:OD2	1:B:431[A]:ARG:HD3	2.02	0.60
1:D:533:LEU:HD12	1:D:533:LEU:C	2.21	0.60
1:C:928:PRO:O	1:C:973:ARG:NH1	2.34	0.60
1:B:589:GLY:HA3	1:B:599:ARG:CA	2.31	0.60
1:A:696:LEU:HB2	1:A:722:LEU:HD11	1.82	0.60
1:A:257:THR:OG1	1:A:271:THR:HG23	2.02	0.60
1:D:322:LEU:HD22	1:D:323:ILE:N	2.15	0.60
1:B:36:TRP:NE1	1:B:46:ARG:O	2.28	0.60
1:A:502:MET:HB2	1:A:503:TYR:CE1	2.36	0.60
1:D:424:ASN:ND2	1:D:464:HIS:O	2.33	0.60
1:A:930:VAL:HG22	1:A:973:ARG:CD	2.30	0.60
1:B:246:MET:HE2	1:B:287:ASP:HB2	1.82	0.60
1:D:62:TRP:HB2	1:D:95:TYR:CD2	2.37	0.60
1:B:217:LYS:HG2	1:B:218:PRO:HD2	1.83	0.60
1:D:89:ASN:O	1:D:92:MET:HB2	2.01	0.60
1:B:650:GLU:HG3	1:B:700:VAL:CG1	2.32	0.60
1:A:544:ASN:HB3	1:A:789:LEU:HD22	1.83	0.60
1:D:38:ASN:ND2	1:D:41:GLU:HG2	2.17	0.60
1:C:559:TYR:CB	1:C:562:LEU:HD12	2.31	0.60
1:C:129:VAL:HG12	1:C:134:LEU:HD21	1.84	0.60
1:A:737:ILE:CG1	1:A:738:PRO:HD2	2.30	0.60
1:B:949:HIS:HB2	1:B:951:TRP:CH2	2.37	0.60
1:B:78:LEU:O	1:B:81:ALA:N	2.30	0.60
1:C:775:GLN:C	1:C:776:LEU:HD23	2.22	0.60
1:B:127:PHE:O	1:B:182:ASN:N	2.34	0.60
1:C:949:HIS:HB2	1:C:951:TRP:CH2	2.36	0.60
1:C:3:ILE:O	1:C:6:SER:HB3	2.02	0.60
1:A:542:MET:HA	1:A:604:ASN:HA	1.83	0.60
1:C:881:ARG:HG3	1:C:882:ILE:N	2.15	0.60
1:C:153:TRP:HA	1:C:157:ARG:O	2.02	0.60
1:A:753:ASN:OD1	1:A:753:ASN:N	2.28	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:856:TYR:HB3	1:D:864:MET:CE	2.30	0.59
1:A:637:GLU:CB	1:A:679:LEU:HD21	2.32	0.59
1:D:129:VAL:HG23	1:D:182:ASN:ND2	2.16	0.59
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.99	0.59
1:D:540:HIS:CE1	1:D:542:MET:HB2	2.37	0.59
1:C:78:LEU:HB3	1:C:80:GLU:OE2	2.02	0.59
1:A:473:ARG:C	1:A:473:ARG:HD3	2.19	0.59
1:C:133:TRP:CE3	1:C:216:HIS:HB2	2.36	0.59
1:B:138:GLN:HG2	1:B:139:THR:N	2.16	0.59
1:B:897:TRP:HB3	1:B:944:LEU:HB2	1.84	0.59
1:D:100:TYR:HB2	1:D:203:TRP:CD2	2.37	0.59
1:A:701:VAL:O	1:A:703:PRO:HD3	2.02	0.59
1:D:504:ALA:HB3	1:D:535:LEU:HD21	1.83	0.59
1:D:138:GLN:HG2	1:D:138:GLN:O	1.99	0.59
1:B:658:LEU:O	1:B:659:ASP:C	2.40	0.59
1:D:658:LEU:CD2	1:D:661:LYS:HZ2	2.15	0.59
1:C:200:GLN:OE1	1:C:200:GLN:N	2.35	0.59
1:C:767:GLN:NE2	1:C:774:LYS:HG2	2.17	0.59
1:B:808:GLU:OE1	1:B:808:GLU:HA	2.03	0.59
1:D:881:ARG:HD3	1:D:987:ASP:OD1	2.02	0.59
1:A:777:LEU:N	1:A:777:LEU:HD23	2.17	0.59
1:C:835:LEU:C	1:C:836:ILE:HD13	2.22	0.59
1:B:377:LEU:N	1:B:377:LEU:HD23	2.16	0.59
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.35	0.59
1:A:217:LYS:HB3	1:A:218:PRO:HD2	1.83	0.59
1:D:588:TYR:HD2	1:D:603:MET:HE1	1.67	0.59
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.84	0.59
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.37	0.59
1:D:588:TYR:CD2	1:D:603:MET:HE1	2.37	0.59
1:B:372:MET:O	1:B:375:ASP:HB2	2.03	0.59
1:B:100:TYR:HB2	1:B:203:TRP:CD2	2.37	0.59
1:C:161:TYR:HE2	1:C:163:GLN:HE21	1.45	0.59
1:C:124:SER:HA	1:C:184:LEU:O	2.03	0.59
1:A:254:LEU:O	1:A:255:ARG:HG3	2.03	0.59
1:A:429:ASP:OD1	1:A:431[B]:ARG:HG3	2.03	0.59
1:B:746:ASP:OD2	1:B:757:GLN:NE2	2.30	0.59
1:C:763:GLY:HA3	1:C:822:LEU:HD13	1.85	0.59
1:A:619:GLU:HG2	1:A:909:ARG:HG2	1.83	0.59
1:D:651:LEU:HD12	1:D:668:VAL:O	2.02	0.59
1:B:217:LYS:NZ	1:B:324:GLU:OE1	2.35	0.59
1:A:138:GLN:O	1:A:216:HIS:HA	2.02	0.59
1:A:505:ARG:HB2	1:A:508:GLU:O	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:256:VAL:O	1:B:271:THR:HA	2.03	0.59
1:C:347:LYS:HZ2	1:C:675:GLN:HG3	1.67	0.59
1:B:300:LEU:N	1:B:307:ASN:HD22	2.00	0.59
1:C:167:LEU:HB3	1:C:168:PRO:CD	2.33	0.59
1:C:881:ARG:HD3	1:C:987:ASP:OD1	2.02	0.59
1:B:634:GLN:O	1:B:682:LEU:HB2	2.02	0.59
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.37	0.58
1:B:573:GLN:HB2	1:B:602:CYS:O	2.03	0.58
1:D:658:LEU:HG	1:D:661:LYS:NZ	2.18	0.58
1:A:626:PHE:O	1:A:641:GLU:HB2	2.02	0.58
1:B:786:ARG:CD	1:B:880:ALA:HB1	2.31	0.58
1:B:141:ILE:HG23	1:B:143:PHE:HE1	1.67	0.58
1:D:52[A]:ARG:HG2	1:D:52[A]:ARG:HH11	1.68	0.58
1:D:7:LEU:HG	1:D:74:LEU:HD11	1.84	0.58
1:B:314:GLU:HB3	1:B:322:LEU:HD21	1.86	0.58
1:D:352:ARG:CB	1:D:385:ASN:HB2	2.29	0.58
1:D:38:ASN:HB3	1:D:41:GLU:HG3	1.85	0.58
1:B:51:LEU:HD12	1:B:214:LEU:O	2.02	0.58
1:D:672:VAL:HG13	1:D:678:GLN:HB2	1.85	0.58
1:A:261:TRP:HZ3	1:A:264:GLU:O	1.86	0.58
1:B:739[A]:HIS:CD2	1:B:740:LEU:H	2.21	0.58
1:B:37:ARG:HG2	1:B:50:GLN:NE2	2.17	0.58
1:B:145:GLY:HA3	1:B:210:ARG:HG3	1.85	0.58
1:C:400:THR:O	1:C:403:ASP:HB2	2.03	0.58
1:A:930:VAL:HG22	1:A:973:ARG:HD3	1.84	0.58
1:B:698:VAL:O	1:B:717:TRP:HB2	2.04	0.58
1:C:38:ASN:HD21	1:C:41:GLU:H	1.50	0.58
1:B:570:TRP:CD1	1:B:571:VAL:HG13	2.38	0.58
1:D:868:VAL:HG12	1:D:869:ASP:N	2.18	0.58
1:C:579:ASP:OD1	1:C:583:ASN:N	2.33	0.58
1:D:78:LEU:N	1:D:78:LEU:HD23	2.15	0.58
1:D:635:THR:HA	1:D:680:ILE:O	2.04	0.58
1:A:906:TYR:CZ	1:A:937:LEU:HB2	2.38	0.58
1:B:217:LYS:HE2	1:B:326:GLU:OE2	2.04	0.58
1:D:749:ILE:O	1:D:755:ARG:HG3	2.04	0.58
1:A:246:MET:HB3	1:A:274:PHE:CZ	2.38	0.58
1:D:965:GLN:HE21	1:D:969:GLU:CD	2.07	0.58
1:D:304:GLU:C	1:D:305:ILE:HG13	2.23	0.58
1:C:721:ARG:HG3	1:C:721:ARG:HH11	1.69	0.58
1:D:100:TYR:HD2	1:D:589:GLY:HA3	1.68	0.58
1:A:433:LEU:HD12	1:A:433:LEU:O	2.03	0.58
1:C:420:MET:HE2	1:C:425:ARG:HB3	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:ARG:CB	1:A:230:ARG:HH11	2.17	0.58
1:B:385:ASN:HB3	1:B:408:TYR:HD1	1.67	0.58
1:D:867:THR:HB	3:D:4146:HOH:O	2.02	0.58
1:D:654:TRP:HE3	1:D:655:MET:N	2.02	0.58
1:D:777:LEU:HD21	1:D:889:ALA:CB	2.33	0.58
1:D:331:GLY:HA3	1:D:451:PRO:HB3	1.85	0.58
1:C:537:GLU:HA	1:C:566:PHE:O	2.03	0.58
1:C:896:ASN:HA	1:C:918:TRP:O	2.03	0.58
1:B:416:GLU:HA	1:B:460:ASN:O	2.04	0.58
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.02	0.58
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.85	0.58
1:D:649:ASN:O	1:D:702:GLN:HG3	2.03	0.58
1:A:433:LEU:HB3	1:A:434:PRO:CD	2.33	0.58
1:A:599:ARG:HH12	1:A:600:GLN:HE22	1.50	0.58
1:A:599:ARG:NH1	1:A:600:GLN:NE2	2.52	0.58
1:B:536:CYS:O	1:B:566:PHE:HB2	2.04	0.58
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.03	0.58
1:C:421:VAL:O	1:C:425:ARG:HD2	2.04	0.58
1:D:656:VAL:HG12	1:D:694:LEU:HD11	1.85	0.58
1:C:27:LEU:HD12	1:C:170:GLU:HB3	1.85	0.58
1:B:286:ALA:HB1	3:B:4439:HOH:O	2.03	0.58
1:C:746:ASP:HA	1:C:760:ARG:HG2	1.86	0.58
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.51	0.57
1:B:398:TRP:HA	1:B:401:LEU:HD12	1.86	0.57
1:D:673:ALA:O	1:D:674:PRO:C	2.41	0.57
1:B:91:GLN:HB3	1:B:98:PRO:HG3	1.86	0.57
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.04	0.57
1:C:486:TYR:CZ	1:C:488:GLY:HA3	2.38	0.57
1:A:502:MET:HA	1:A:537:GLU:O	2.04	0.57
1:C:804:ASN:O	1:C:809[A]:ARG:NH1	2.30	0.57
1:A:882:ILE:O	1:A:882:ILE:HG22	2.04	0.57
1:A:69:VAL:HG13	1:A:70:PRO:HD2	1.86	0.57
1:B:856:TYR:HB3	1:B:864:MET:HE2	1.86	0.57
1:B:840:HIS:ND1	1:B:840:HIS:N	2.50	0.57
1:A:202:MET:HE2	1:A:365:GLN:NE2	2.19	0.57
1:B:225:PHE:HA	1:B:243:GLU:O	2.04	0.57
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.39	0.57
1:A:3:ILE:HD12	1:A:3:ILE:O	2.04	0.57
1:C:726:LEU:HD12	1:D:848:THR:HG22	1.86	0.57
1:A:490:GLY:N	3:A:4007:HOH:O	2.31	0.57
1:A:637:GLU:HA	1:A:679:LEU:HD21	1.84	0.57
1:C:347:LYS:HE3	1:C:643:LEU:O	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:510:GLN:O	1:C:517:LYS:N	2.31	0.57
1:D:446:ARG:HG2	1:D:447:ASP:OD1	2.04	0.57
1:A:767:GLN:HG3	1:A:768:MET:N	2.19	0.57
1:A:7:LEU:HD13	1:A:69:VAL:HG12	1.86	0.57
1:B:579:ASP:CG	1:B:583:ASN:HB2	2.24	0.57
1:D:903[B]:GLN:HE22	1:D:913:ALA:HA	1.68	0.57
1:B:929:TYR:O	1:B:931:PHE:N	2.37	0.57
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.34	0.57
1:A:202:MET:O	1:A:204:ARG:HD3	2.05	0.57
1:B:237:ARG:HB2	1:B:237:ARG:HH11	1.69	0.57
1:A:136:GLU:O	1:A:216:HIS:HE1	1.88	0.57
1:C:897:TRP:HB2	1:C:943:GLU:O	2.04	0.57
1:A:375:ASP:O	1:A:379:MET:HG3	2.04	0.57
1:D:141:ILE:HG13	1:D:213:SER:O	2.04	0.57
1:B:114:VAL:HG13	1:B:191:TRP:CB	2.34	0.57
1:A:672:VAL:HG13	1:A:678:GLN:HB2	1.86	0.57
1:A:737:ILE:HD12	1:A:832:ASP:C	2.25	0.57
1:B:138:GLN:N	1:B:217:LYS:O	2.38	0.57
1:C:746:ASP:CA	1:C:760:ARG:HG2	2.35	0.57
1:C:198:GLU:OE2	1:C:439:ARG:NH1	2.35	0.57
1:D:444:VAL:O	1:D:448:ARG:HB3	2.04	0.57
1:C:775:GLN:OE1	1:C:890:GLN:NE2	2.38	0.57
1:D:673:ALA:HB1	1:D:674:PRO:CD	2.32	0.57
1:B:777:LEU:HD21	1:B:889:ALA:CB	2.35	0.57
1:C:948:PRO:O	1:C:1022:GLN:HA	2.04	0.57
1:D:511:PRO:HA	1:D:516:PRO:HB3	1.86	0.57
1:C:258:VAL:N	1:C:270:GLY:O	2.29	0.57
1:C:246:MET:HE2	1:C:287:ASP:HB3	1.87	0.57
1:C:36:TRP:CD1	1:C:41:GLU:HB3	2.39	0.57
1:D:894:ARG:HD3	1:D:919:ASP:OD1	2.04	0.57
1:B:391:HIS:HA	1:B:412:GLU:OE1	2.05	0.57
1:C:608:PHE:O	1:C:611:ARG:N	2.32	0.57
1:A:599:ARG:HD2	1:A:600:GLN:OE1	2.05	0.57
1:C:167:LEU:HD21	1:C:393:PRO:HB2	1.86	0.57
1:A:392:TYR:HB2	1:A:393:PRO:HD2	1.86	0.57
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.25	0.57
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.25	0.57
1:C:234:ASP:O	1:C:235:PHE:HB2	2.04	0.57
1:C:622:HIS:HD2	1:C:625:GLN:OE1	1.87	0.57
1:A:750:GLU:HB3	1:A:755:ARG:HG3	1.86	0.56
1:D:653[B]:HIS:HD2	1:D:667:GLU:HG3	1.69	0.56
1:A:599:ARG:HB2	1:A:600:GLN:OE1	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:102:ASN:C	1:A:102:ASN:HD22	2.07	0.56
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.40	0.56
1:B:945:ASN:OD1	1:B:950:GLN:HB2	2.04	0.56
1:D:749:ILE:N	1:D:749:ILE:HD12	2.20	0.56
1:B:399:TYR:HB3	1:B:450:HIS:CD2	2.39	0.56
1:D:230:ARG:CG	1:D:230:ARG:HH11	2.12	0.56
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.17	0.56
1:D:7:LEU:O	1:D:11:LEU:HB2	2.06	0.56
1:B:422:PRO:HG3	1:C:279:ILE:CD1	2.35	0.56
1:A:737:ILE:HG13	1:A:738:PRO:CD	2.36	0.56
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.89	0.56
1:A:894:ARG:CZ	1:A:921:PRO:HD3	2.36	0.56
1:B:80:GLU:OE2	1:B:80:GLU:N	2.39	0.56
1:D:767:GLN:HG3	1:D:768:MET:N	2.19	0.56
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.05	0.56
1:D:393:PRO:HD2	1:D:414:ASN:HB2	1.86	0.56
1:B:505:ARG:HG2	1:B:996:ASP:OD2	2.04	0.56
1:A:844:HIS:C	1:A:845:GLN:HG2	2.24	0.56
1:A:237:ARG:HH11	1:A:237:ARG:HB2	1.70	0.56
1:B:141:ILE:HB	1:B:173:LEU:HD12	1.87	0.56
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.05	0.56
1:A:60:PHE:HA	1:A:122:CYS:O	2.06	0.56
1:B:1019:VAL:HG12	1:B:1019:VAL:O	2.03	0.56
1:C:573:GLN:HB2	1:C:602:CYS:O	2.05	0.56
1:A:693:GLN:NE2	1:A:721:ARG:HH11	2.03	0.56
1:B:251:ARG:H	1:B:254:LEU:CD1	2.18	0.56
1:C:833:ALA:HB2	1:C:859:ASP:HA	1.87	0.56
1:A:282:ARG:HB2	1:D:422:PRO:HA	1.87	0.56
1:D:110:ASN:O	1:D:113:PHE:HB2	2.06	0.56
1:B:888:LEU:N	1:B:982:THR:O	2.27	0.56
1:D:306:PRO:O	1:D:307:ASN:C	2.36	0.56
1:D:522:LYS:O	1:D:522:LYS:HG2	2.05	0.56
1:C:721:ARG:HH11	1:C:721:ARG:CG	2.19	0.56
1:D:836:ILE:HG22	1:D:837:THR:N	2.20	0.56
1:C:432:TRP:O	1:C:433:LEU:C	2.42	0.56
1:D:316:HIS:HD2	1:D:317:THR:O	1.88	0.56
1:B:38:ASN:ND2	1:B:41:GLU:H	2.03	0.56
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.73	0.56
1:A:930:VAL:HA	1:A:973:ARG:HD2	1.86	0.56
1:C:577:LYS:HD3	1:C:585:TRP:CH2	2.41	0.56
1:A:200:GLN:N	1:A:200:GLN:OE1	2.34	0.56
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.32	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:358:GLU:HB3	1:A:367:MET:HG2	1.88	0.56
1:D:777:LEU:HD23	1:D:777:LEU:N	2.21	0.56
1:A:987:ASP:OD2	1:A:990:HIS:HD2	1.88	0.56
1:A:422:PRO:HG2	1:D:285:TYR:CZ	2.40	0.56
1:A:84:VAL:HG13	1:A:85:VAL:N	2.20	0.56
1:A:426:LEU:HD22	1:A:432:TRP:CE2	2.41	0.56
1:A:437:SER:HA	1:A:471:LEU:HD21	1.88	0.56
1:C:256:VAL:O	1:C:271:THR:HA	2.06	0.56
1:A:90:TRP:CD1	1:A:95:TYR:HB2	2.41	0.56
1:D:895:VAL:O	1:D:919:ASP:HA	2.06	0.56
1:C:807:VAL:HG13	1:C:808:GLU:N	2.21	0.56
1:A:693:GLN:CG	1:A:721:ARG:HD3	2.35	0.56
1:C:356:ARG:HD3	3:C:4139:HOH:O	2.04	0.56
1:B:630:ARG:HB3	1:B:630:ARG:CZ	2.35	0.56
1:C:721:ARG:HE	1:D:874:SER:CB	2.18	0.55
1:A:693:GLN:HG3	1:A:724:GLU:HG3	1.87	0.55
1:A:421:VAL:HG13	1:D:282:ARG:O	2.06	0.55
1:C:836:ILE:HG22	1:C:837:THR:N	2.20	0.55
1:B:822:LEU:HD12	1:B:823:LEU:H	1.71	0.55
1:D:416:GLU:OE1	1:D:418:HIS:HB2	2.06	0.55
1:C:354:VAL:HG22	1:C:355:ASN:N	2.21	0.55
1:B:929:TYR:O	1:B:930:VAL:C	2.43	0.55
1:B:767:GLN:HG3	1:B:768:MET:N	2.18	0.55
1:B:309:TYR:HB2	1:B:330:VAL:HG12	1.88	0.55
1:B:367:MET:CE	1:B:372:MET:HG2	2.36	0.55
1:B:658:LEU:HG	1:B:661:LYS:HZ2	1.69	0.55
1:B:299:LYS:C	1:B:307:ASN:HD22	2.10	0.55
1:D:693:GLN:HB2	1:D:695:TRP:HE1	1.71	0.55
1:D:133:TRP:C	1:D:134:LEU:HD23	2.26	0.55
1:B:357:HIS:HD2	1:B:392:TYR:OH	1.89	0.55
1:B:213:SER:O	1:B:214:LEU:HD23	2.06	0.55
1:D:344:LEU:HG	1:D:345:ASN:N	2.19	0.55
1:B:397:LEU:O	1:B:398:TRP:C	2.45	0.55
1:D:75:GLU:OE1	1:D:75:GLU:HA	2.06	0.55
1:B:38:ASN:HD21	1:B:41:GLU:H	1.54	0.55
1:C:881:ARG:C	1:C:882:ILE:HG13	2.26	0.55
1:A:946:TYR:HH	1:A:982:THR:HG1	1.53	0.55
1:D:769:TRP:HE1	1:D:774:LYS:HE2	1.71	0.55
1:B:710:GLU:OE2	1:B:710:GLU:HA	2.05	0.55
1:C:597:ASN:ND2	1:C:599:ARG:H	2.00	0.55
1:A:377:LEU:HD22	1:A:708:TRP:CA	2.36	0.55
1:A:202:MET:HA	1:A:573:GLN:NE2	2.18	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:907:PRO:HD3	1:A:939:CYS:SG	2.45	0.55
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.37	0.55
1:B:200:GLN:CB	1:B:202:MET:HG2	2.36	0.55
1:B:385:ASN:O	1:B:408:TYR:N	2.28	0.55
1:A:540:HIS:C	1:A:542:MET:H	2.09	0.55
1:D:578:TYR:HA	1:D:583:ASN:O	2.07	0.55
1:D:344:LEU:HD23	1:D:644:PHE:CZ	2.41	0.55
1:D:737:ILE:HG13	1:D:738:PRO:N	2.20	0.55
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.88	0.55
1:A:427:THR:O	1:A:467:ASN:HB2	2.07	0.55
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.36	0.55
1:C:397:LEU:O	1:C:398:TRP:C	2.45	0.55
1:B:510:GLN:HB2	1:B:517:LYS:HB2	1.87	0.55
1:C:382:ASN:O	1:C:621:LYS:HA	2.06	0.55
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.88	0.55
1:D:984:LEU:HD21	1:D:986:ILE:CD1	2.27	0.55
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.74	0.55
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.53	0.55
1:A:379:MET:HB3	1:A:384:PHE:HB2	1.88	0.55
1:D:142:ILE:O	1:D:212:VAL:HA	2.06	0.55
1:D:512:PHE:HE1	1:D:517:LYS:HG3	1.71	0.55
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.42	0.55
1:A:52[B]:ARG:NH2	1:A:130:ASP:HB2	2.21	0.55
1:C:27:LEU:HD12	1:C:170:GLU:CB	2.37	0.55
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.89	0.55
1:D:878:HIS:CD2	1:D:1010:SER:HB3	2.41	0.55
1:B:258:VAL:HA	1:B:312:VAL:O	2.07	0.55
1:B:227:VAL:HG11	1:B:330:VAL:CG2	2.36	0.55
1:D:344:LEU:HD23	1:D:644:PHE:CE1	2.42	0.55
1:B:974:HIS:O	1:B:975:LEU:HD23	2.07	0.55
1:C:523:TRP:O	1:C:526:LEU:HB2	2.07	0.55
1:A:352:ARG:O	1:A:385:ASN:HB2	2.07	0.55
1:C:629:PHE:CD1	1:C:629:PHE:N	2.75	0.55
1:D:432:TRP:O	1:D:436:MET:HG3	2.06	0.55
1:A:381:GLN:NE2	1:A:708:TRP:O	2.40	0.55
1:D:656:VAL:CG1	1:D:694:LEU:HD11	2.37	0.55
1:C:393:PRO:HD3	1:C:412:GLU:O	2.07	0.55
1:C:376:ILE:HG22	1:C:377:LEU:N	2.21	0.55
1:D:95:TYR:N	1:D:95:TYR:CD1	2.75	0.55
1:D:457:SER:HA	1:D:485:GLN:O	2.07	0.55
1:B:246:MET:HE2	1:B:246:MET:O	2.06	0.55
1:D:333:ARG:HA	1:D:345:ASN:OD1	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:69:VAL:CG1	1:D:70:PRO:HD2	2.37	0.55
1:A:282:ARG:NH1	1:D:420:MET:O	2.39	0.55
1:A:925:MET:HE3	1:A:925:MET:HA	1.88	0.55
1:C:23:GLN:O	1:C:24:LEU:HD13	2.07	0.55
1:C:29:ALA:HB3	1:C:445:GLN:OE1	2.06	0.55
1:C:742:THR:HG22	1:C:743:SER:H	1.71	0.55
1:A:511:PRO:HA	1:A:516:PRO:CB	2.37	0.54
1:B:212:VAL:HG12	1:B:213:SER:N	2.19	0.54
1:C:432:TRP:N	1:C:432:TRP:CD1	2.71	0.54
1:B:141:ILE:HG23	1:B:143:PHE:CE1	2.42	0.54
1:C:438:GLU:O	1:C:442:ARG:HG3	2.08	0.54
1:A:762:SER:O	1:A:822:LEU:HD23	2.08	0.54
1:D:416:GLU:OE1	1:D:461:GLU:HG3	2.06	0.54
1:B:51:LEU:HD13	1:B:215:LEU:HB2	1.89	0.54
1:D:782:ASP:HA	1:D:884:LEU:HD23	1.88	0.54
1:A:890:GLN:O	1:A:891:VAL:HG23	2.07	0.54
1:C:568:TRP:NE1	1:C:604:ASN:ND2	2.46	0.54
1:B:152:LEU:C	1:B:159:VAL:HG23	2.28	0.54
1:D:155:ASN:ND2	1:D:182:ASN:OD1	2.29	0.54
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	2.24	0.54
1:A:274:PHE:HB3	1:A:286:ALA:O	2.08	0.54
1:D:852:SER:HB2	1:D:870:VAL:HG22	1.89	0.54
1:D:528:GLY:O	1:D:530:THR:HG23	2.06	0.54
1:A:80:GLU:H	1:A:80:GLU:CD	2.11	0.54
1:B:662:PRO:C	1:B:663:LEU:HD23	2.27	0.54
1:B:424:ASN:HB3	1:C:285:TYR:OH	2.07	0.54
1:C:240:LEU:HG	1:C:241:GLU:N	2.21	0.54
1:A:7:LEU:HD21	1:A:74:LEU:CD2	2.23	0.54
1:B:840:HIS:HB2	1:B:842:TRP:CH2	2.43	0.54
1:C:256:VAL:HG12	1:C:257:THR:N	2.21	0.54
1:C:876:THR:HA	3:C:4521:HOH:O	2.07	0.54
1:D:801:ILE:HG23	1:D:808:GLU:CD	2.27	0.54
1:A:63:PHE:CB	1:A:64:PRO:HD2	2.26	0.54
1:B:143:PHE:HB3	3:B:4101:HOH:O	2.07	0.54
1:B:777:LEU:HD21	1:B:889:ALA:HA	1.88	0.54
1:B:751:LEU:HD23	1:B:751:LEU:O	2.07	0.54
1:D:893:GLU:O	1:D:921:PRO:HA	2.07	0.54
1:D:904:GLU:HG2	1:D:909:ARG:NH2	2.22	0.54
1:D:246:MET:HG2	1:D:274:PHE:CZ	2.43	0.54
1:C:995:GLY:O	1:C:997:ASP:N	2.41	0.54
1:C:685:LEU:O	1:C:687:GLN:HG3	2.08	0.54
1:A:570:TRP:HD1	1:A:571:VAL:HG22	1.69	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:134:LEU:O	1:B:135:GLN:C	2.43	0.54
1:B:897:TRP:CB	1:B:944:LEU:HB2	2.38	0.54
1:C:802:ASP:O	1:C:808:GLU:HG3	2.07	0.54
1:B:493:THR:HG23	3:B:4020:HOH:O	2.08	0.54
1:B:670:LEU:HD11	1:B:700:VAL:HG22	1.90	0.54
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.41	0.54
1:B:655:MET:O	1:B:696:LEU:HD12	2.08	0.54
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.43	0.54
1:B:200:GLN:HB3	1:B:202:MET:HG2	1.90	0.54
1:A:652:LEU:HD12	1:A:699:ARG:O	2.07	0.54
1:B:429:ASP:OD1	1:B:431[B]:ARG:HG3	2.08	0.54
1:B:774:LYS:HB2	1:B:774:LYS:NZ	2.23	0.54
1:D:742:THR:HG22	1:D:743:SER:N	2.22	0.54
1:C:478:VAL:HG12	1:C:479:ASP:N	2.21	0.54
1:B:114:VAL:HG12	1:B:115:PRO:N	2.23	0.54
1:A:228:ALA:O	1:A:240:LEU:HD12	2.08	0.54
1:A:93:HIS:HB3	1:A:95:TYR:CE1	2.39	0.54
1:B:822:LEU:HD12	1:B:823:LEU:N	2.23	0.54
1:D:763:GLY:CA	1:D:822:LEU:HD21	2.37	0.54
1:C:748:CYS:SG	1:C:757:GLN:HG3	2.48	0.54
1:D:696:LEU:HD12	1:D:697:THR:N	2.23	0.54
1:A:198:GLU:HB3	3:A:4060:HOH:O	2.07	0.54
1:B:916:ASP:HB3	1:B:918:TRP:CZ2	2.42	0.54
1:B:894:ARG:CZ	1:B:921:PRO:HD3	2.38	0.54
1:C:168:PRO:O	1:C:442:ARG:NH2	2.38	0.54
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	2.26	0.54
1:A:138:GLN:OE1	1:A:140:ARG:NH2	2.39	0.54
1:B:955:PHE:HB2	1:B:987:ASP:O	2.06	0.54
1:C:789:LEU:HG	1:C:792:ASP:OD2	2.08	0.54
1:B:246:MET:HE2	1:B:287:ASP:CB	2.38	0.53
1:C:801:ILE:O	1:C:803:PRO:HD3	2.08	0.53
1:D:23:GLN:HB3	1:D:26:ARG:HH21	1.73	0.53
1:B:58:TRP:CE3	1:B:123:TYR:HB3	2.43	0.53
1:B:420:MET:HE2	1:B:426:LEU:HG	1.91	0.53
1:D:745:MET:O	1:D:760:ARG:N	2.38	0.53
1:A:930:VAL:HG22	1:A:973:ARG:NE	2.23	0.53
1:D:573:GLN:HB2	1:D:602:CYS:O	2.08	0.53
1:C:420:MET:HE2	1:C:426:LEU:HG	1.90	0.53
1:D:890:GLN:H	1:D:890:GLN:CD	2.11	0.53
1:D:890:GLN:HE21	1:D:890:GLN:N	2.06	0.53
1:B:769:TRP:NE1	1:B:774:LYS:HG3	2.23	0.53
1:C:658:LEU:HD12	1:C:659:ASP:N	2.23	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:639:THR:OG1	1:D:677:LYS:HE2	2.09	0.53
1:D:757:GLN:HG2	1:D:758:PHE:N	2.22	0.53
1:D:597:ASN:HD22	1:D:599:ARG:N	1.95	0.53
1:D:238:ALA:HB2	1:D:298:PRO:HG3	1.90	0.53
1:A:224:ASP:HB3	1:A:245:GLN:CG	2.37	0.53
1:C:463:GLY:HA2	3:C:7509:HOH:O	2.08	0.53
1:D:737:ILE:HG13	1:D:738:PRO:CD	2.38	0.53
1:B:868:VAL:HG12	1:B:869:ASP:N	2.23	0.53
1:B:59:ARG:O	1:B:124:SER:N	2.39	0.53
1:B:440:VAL:CG1	1:B:475:ILE:HD11	2.38	0.53
1:C:734:SER:HB3	1:C:860:GLY:N	2.23	0.53
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	2.26	0.53
1:B:592:PHE:CD1	1:B:592:PHE:N	2.76	0.53
1:D:937:LEU:HA	1:D:958:ASN:HB3	1.89	0.53
1:C:58:TRP:CE3	1:C:123:TYR:HB3	2.43	0.53
1:A:53:SER:C	1:A:54:LEU:HD23	2.29	0.53
1:B:658:LEU:C	1:B:661:LYS:HE3	2.29	0.53
1:A:856:TYR:HB3	1:A:864:MET:HE3	1.89	0.53
1:A:52[B]:ARG:HG3	1:A:133:TRP:HH2	1.73	0.53
1:D:683:PRO:O	1:D:685:LEU:HG	2.08	0.53
1:D:524:LEU:O	1:D:561:ARG:NH2	2.41	0.53
1:C:856:TYR:HD2	1:C:864:MET:CE	2.21	0.53
1:A:257:THR:HA	1:A:270:GLY:O	2.08	0.53
1:C:590:GLY:HA2	1:C:594:ASP:O	2.09	0.53
1:C:930:VAL:O	1:C:932:PRO:HD3	2.08	0.53
1:A:240:LEU:HD23	1:A:260:LEU:HD22	1.89	0.53
1:A:38:ASN:HD22	1:A:41:GLU:HG3	1.73	0.53
1:C:254:LEU:O	1:C:255:ARG:NH1	2.42	0.53
1:D:71:GLU:O	1:D:73:TRP:N	2.41	0.53
1:C:10:VAL:O	1:C:11:LEU:C	2.43	0.53
1:A:962:TYR:HD2	1:A:966:GLN:NE2	2.06	0.53
1:C:770:ILE:HD11	1:C:1022:GLN:HG2	1.90	0.53
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.90	0.53
1:C:694:LEU:HD12	1:C:695:TRP:H	1.74	0.53
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.33	0.53
1:B:143:PHE:CD1	1:B:143:PHE:N	2.76	0.53
1:B:660:GLY:O	1:B:662:PRO:HD3	2.09	0.53
1:C:11:LEU:HD21	1:C:187:MET:CE	2.39	0.53
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.90	0.53
1:D:946:TYR:CE2	1:D:982:THR:HG21	2.43	0.53
1:A:891:VAL:HG12	1:A:891:VAL:O	2.09	0.53
1:A:856:TYR:HD2	1:A:864:MET:CE	2.21	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:429:ASP:OD1	1:C:431[A]:ARG:HG3	2.09	0.53
1:C:658:LEU:O	1:C:661:LYS:HE3	2.09	0.53
1:A:607:VAL:HG23	1:A:608:PHE:O	2.08	0.53
1:D:654:TRP:CE3	1:D:655:MET:N	2.77	0.53
1:B:739[A]:HIS:CD2	1:B:740:LEU:N	2.77	0.53
1:D:429:ASP:OD1	1:D:431[B]:ARG:HG3	2.09	0.53
1:A:507:ASP:OD1	1:A:521:LYS:HE2	2.08	0.53
1:D:501:PRO:HD2	1:D:533:LEU:HD13	1.90	0.53
1:C:261:TRP:HA	1:C:267:VAL:HG23	1.91	0.53
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.38	0.53
1:A:734:SER:HB2	1:A:860:GLY:CA	2.38	0.53
1:D:356:ARG:HD2	1:D:379:MET:CE	2.39	0.53
1:A:579:ASP:C	1:A:581:ASN:H	2.13	0.53
1:B:221:GLN:O	1:B:221:GLN:HG2	1.95	0.53
1:D:99:ILE:O	1:D:204:ARG:N	2.41	0.52
1:B:30:HIS:CE1	1:B:33:PHE:CD1	2.97	0.52
1:C:673:ALA:HB1	1:C:674:PRO:CD	2.36	0.52
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.44	0.52
1:D:161:TYR:OH	1:D:163:GLN:NE2	2.33	0.52
1:C:835:LEU:HD12	1:C:836:ILE:N	2.24	0.52
1:B:275:GLY:HA2	1:B:286:ALA:HA	1.92	0.52
1:A:416:GLU:OE1	1:A:418:HIS:HB2	2.09	0.52
1:C:241:GLU:HG3	1:C:292:ARG:HG2	1.91	0.52
1:C:59:ARG:NH2	1:C:81:ALA:O	2.42	0.52
1:D:127:PHE:HE1	1:D:129:VAL:HG22	1.73	0.52
1:B:866:ILE:O	1:B:1018:LEU:N	2.32	0.52
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.77	0.52
1:D:878:HIS:NE2	1:D:1010:SER:HB3	2.24	0.52
1:A:140:ARG:HG2	1:A:141:ILE:N	2.23	0.52
1:A:126:THR:HA	1:A:182:ASN:O	2.10	0.52
1:D:77:ASP:O	1:D:78:LEU:HD23	2.10	0.52
1:D:948:PRO:HG2	1:D:949:HIS:CE1	2.44	0.52
1:A:53:SER:O	1:A:54:LEU:HD23	2.10	0.52
1:C:176:PHE:N	1:C:176:PHE:CD1	2.76	0.52
1:D:473:ARG:O	1:D:473:ARG:HD3	2.10	0.52
1:C:734:SER:CB	1:C:860:GLY:HA3	2.27	0.52
1:C:652:LEU:HB2	1:C:670:LEU:HD21	1.91	0.52
1:A:38:ASN:ND2	1:A:41:GLU:N	2.54	0.52
1:B:839:ALA:HA	1:B:852:SER:O	2.09	0.52
1:A:502:MET:HB3	1:A:537:GLU:HB2	1.91	0.52
1:A:548:GLY:O	1:A:551:LYS:HB2	2.09	0.52
1:D:746:ASP:HA	1:D:760:ARG:CG	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:497:ASP:O	1:B:531:ARG:HG2	2.09	0.52
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.74	0.52
1:D:62:TRP:CG	1:D:95:TYR:HB3	2.44	0.52
1:B:784:PHE:HA	1:B:881:ARG:O	2.09	0.52
1:D:486:TYR:CZ	1:D:488:GLY:HA3	2.44	0.52
1:C:878:HIS:ND1	3:C:4074:HOH:O	2.30	0.52
1:A:389:CYS:HB3	1:A:394:ASN:ND2	2.24	0.52
1:A:6:SER:OG	1:A:8:ALA:HB3	2.10	0.52
1:D:959:ILE:O	1:D:959:ILE:HG23	2.09	0.52
1:A:420:MET:HE2	1:A:426:LEU:CG	2.37	0.52
1:D:114:VAL:CG1	1:D:191:TRP:HB2	2.39	0.52
1:B:422:PRO:HG2	1:B:424:ASN:HB3	1.89	0.52
1:C:373:VAL:HG12	1:C:377:LEU:HD11	1.90	0.52
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.28	0.52
1:D:464:HIS:HB2	1:D:489:GLY:HA3	1.91	0.52
1:B:78:LEU:O	1:B:80:GLU:N	2.42	0.52
1:C:353:GLY:HA2	1:C:386:ALA:O	2.09	0.52
1:D:415:ILE:HG12	1:D:439:ARG:HD2	1.91	0.52
3:C:4115:HOH:O	1:D:525:SER:HA	2.10	0.52
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.22	0.52
1:B:578:TYR:HA	1:B:583:ASN:O	2.09	0.52
1:C:751:LEU:HD23	1:C:751:LEU:C	2.30	0.52
1:A:58:TRP:N	1:A:84:VAL:O	2.42	0.52
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.44	0.52
1:D:650:GLU:HA	1:D:701:VAL:O	2.10	0.52
1:A:433:LEU:HD12	1:A:433:LEU:C	2.30	0.52
1:B:685:LEU:HB3	1:B:686:PRO:CD	2.36	0.52
1:C:373:VAL:O	1:C:377:LEU:HG	2.09	0.52
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.44	0.52
1:D:23:GLN:O	1:D:24:LEU:HD13	2.10	0.52
1:C:858:ILE:HA	1:C:863:GLN:O	2.09	0.52
1:A:128:ASN:HD22	1:A:181:GLU:N	2.06	0.52
1:A:652:LEU:O	1:A:667:GLU:HA	2.10	0.52
1:A:138:GLN:HG2	1:A:139:THR:N	2.20	0.52
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.23	0.52
1:A:18:ASN:OD1	1:A:20:GLY:N	2.40	0.52
1:D:826:THR:OG1	1:D:826:THR:O	2.27	0.52
1:B:11:LEU:HD21	1:B:187:MET:CE	2.40	0.52
1:C:133:TRP:HA	1:C:216:HIS:CE1	2.45	0.52
1:C:319:ASP:OD1	1:C:321:THR:OG1	2.27	0.52
1:B:759:ASN:OD1	1:B:761:GLN:N	2.29	0.52
1:D:499:ILE:O	1:D:533:LEU:HD13	2.11	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:399:TYR:HB2	1:B:450:HIS:NE2	2.25	0.52
1:C:255:ARG:HH11	1:C:255:ARG:CG	2.20	0.52
1:C:166:ARG:O	1:C:167:LEU:HD23	2.10	0.52
1:D:41:GLU:OE2	1:D:46:ARG:NH1	2.43	0.52
1:C:856:TYR:HB3	1:C:864:MET:HE1	1.90	0.52
1:D:512:PHE:CE1	1:D:517:LYS:HG3	2.44	0.52
1:C:960:SER:HA	3:C:4030:HOH:O	2.10	0.52
1:B:29:ALA:HB3	1:B:445:GLN:HG3	1.92	0.52
1:B:856:TYR:CD1	1:B:856:TYR:N	2.78	0.51
1:D:230:ARG:O	1:D:238:ALA:HA	2.09	0.51
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.72	0.51
1:D:655:MET:HA	1:D:665:SER:HA	1.92	0.51
1:C:258:VAL:CB	1:C:291:LEU:HD11	2.40	0.51
1:A:383:ASN:HD22	1:A:625:GLN:HA	1.74	0.51
1:C:497:ASP:O	1:C:531:ARG:HG2	2.10	0.51
1:B:41:GLU:HA	1:B:46:ARG:HB2	1.92	0.51
1:C:84:VAL:HG22	1:C:93:HIS:ND1	2.25	0.51
1:A:948:PRO:O	1:A:1022:GLN:HA	2.10	0.51
1:D:666:GLY:O	1:D:667:GLU:HG3	2.10	0.51
1:D:685:LEU:CB	1:D:686:PRO:HD2	2.37	0.51
1:B:916:ASP:HB3	1:B:918:TRP:CE2	2.44	0.51
1:C:99:ILE:CG2	1:C:101:THR:HG22	2.40	0.51
1:B:234:ASP:O	1:B:235:PHE:HB2	2.10	0.51
1:A:989:PHE:N	1:A:989:PHE:CD1	2.79	0.51
1:B:733:ALA:O	1:B:734:SER:C	2.48	0.51
1:A:12:GLN:HG3	1:A:13:ARG:N	2.26	0.51
1:A:991:MET:HG2	1:A:992:GLY:H	1.73	0.51
1:B:823:LEU:HD11	1:B:841:ALA:HB2	1.91	0.51
1:D:55:ASN:OD1	1:D:211:ASP:HB3	2.11	0.51
1:D:966:GLN:NE2	1:D:979:GLU:OE2	2.44	0.51
1:D:399:TYR:CE1	1:D:446:ARG:NH2	2.79	0.51
1:D:906:TYR:O	1:D:907:PRO:C	2.49	0.51
1:C:44:THR:O	1:C:45:ASP:C	2.46	0.51
1:B:141:ILE:HG12	1:B:142:ILE:N	2.25	0.51
1:D:72:SER:O	1:D:75:GLU:N	2.42	0.51
1:B:458:LEU:HD11	1:B:472:TYR:HB2	1.93	0.51
1:B:35:SER:O	1:B:50:GLN:NE2	2.42	0.51
1:A:124:SER:HA	1:A:184:LEU:O	2.11	0.51
1:A:1020:TRP:HD1	1:A:1021:CYS:H	1.56	0.51
1:B:521:LYS:HD3	1:B:559:TYR:CZ	2.45	0.51
1:A:636:ILE:N	1:A:680:ILE:O	2.35	0.51
1:A:24:LEU:O	1:A:25:ASN:HB2	2.08	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:567:VAL:HG12	1:B:568:TRP:N	2.25	0.51
1:C:883:GLY:HA2	1:C:1016:TYR:OH	2.10	0.51
1:A:11:LEU:HD23	1:A:11:LEU:H	1.76	0.51
1:B:650:GLU:CB	1:B:670:LEU:HD12	2.28	0.51
1:A:106:PRO:HG3	1:A:204:ARG:HG3	1.93	0.51
1:C:649:ASN:O	1:C:702:GLN:HG3	2.10	0.51
1:D:878:HIS:HB3	1:D:879:PRO:HD2	1.92	0.51
1:A:416:GLU:OE1	1:A:461:GLU:OE2	2.29	0.51
1:C:515:VAL:O	1:C:515:VAL:HG23	2.10	0.51
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.14	0.51
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.93	0.51
1:C:1009:LEU:HD23	1:C:1009:LEU:N	2.25	0.51
1:D:472:TYR:O	1:D:476:LYS:HG2	2.10	0.51
1:D:577:LYS:O	1:D:584:PRO:HA	2.10	0.51
1:C:513:PRO:O	1:C:514:ALA:HB3	2.11	0.51
1:B:433:LEU:HD12	1:B:433:LEU:C	2.29	0.51
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.43	0.51
1:A:41:GLU:HG2	1:A:46:ARG:HH11	1.76	0.51
1:D:254:LEU:C	1:D:255:ARG:HG2	2.31	0.51
1:A:858:ILE:HG12	1:A:864:MET:HB3	1.92	0.51
1:C:261:TRP:CD1	1:C:261:TRP:N	2.79	0.51
1:D:42:ALA:O	1:D:43:ARG:C	2.47	0.51
1:D:636:ILE:N	1:D:680:ILE:O	2.37	0.51
1:B:533:LEU:HD12	1:B:533:LEU:C	2.30	0.51
1:C:505:ARG:HB3	3:C:4226:HOH:O	2.11	0.51
1:C:741:THR:HG22	1:C:741:THR:O	2.09	0.51
1:B:956:GLN:O	1:B:987:ASP:N	2.29	0.51
1:A:585:TRP:CE3	1:A:974:HIS:CE1	2.99	0.51
1:B:979:GLU:O	1:B:980:GLU:C	2.49	0.51
1:D:655:MET:HE3	1:D:664:ALA:O	2.10	0.51
1:B:11:LEU:N	1:B:11:LEU:HD23	2.25	0.51
1:C:585:TRP:CE3	1:C:974:HIS:CE1	2.98	0.51
1:C:499:ILE:HB	1:C:533:LEU:CB	2.40	0.51
1:C:701:VAL:HG12	1:C:702:GLN:N	2.26	0.51
1:A:128:ASN:HD22	1:A:180:GLY:C	2.14	0.51
1:B:36:TRP:CD1	1:B:41:GLU:HB3	2.46	0.51
1:D:697:THR:HG22	1:D:698:VAL:N	2.26	0.51
1:D:37:ARG:HD3	1:D:50:GLN:NE2	2.26	0.51
1:B:851:ILE:O	1:B:870:VAL:HA	2.11	0.51
1:B:427:THR:O	1:B:467:ASN:HB2	2.11	0.51
1:A:233:ASP:OD2	1:C:233:ASP:HB3	2.11	0.51
1:C:600:GLN:HB3	1:C:603:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:143:PHE:O	1:B:168:PRO:HA	2.11	0.51
1:D:13:ARG:O	1:D:14:ARG:C	2.47	0.51
1:C:43:ARG:HD2	1:C:261:TRP:CE2	2.46	0.51
1:A:613:PRO:HB3	1:A:617:LEU:CD2	2.40	0.51
1:A:50:GLN:H	1:A:50:GLN:NE2	2.08	0.51
1:B:894:ARG:NH1	1:B:921:PRO:HD3	2.26	0.51
1:A:234:ASP:OD1	1:A:236:SER:OG	2.28	0.51
1:B:217:LYS:HG2	1:B:218:PRO:CD	2.42	0.50
1:C:610:ASP:OD2	1:C:610:ASP:N	2.41	0.50
1:D:200:GLN:N	1:D:200:GLN:OE1	2.43	0.50
1:B:959:ILE:HG23	1:B:959:ILE:O	2.12	0.50
1:C:963:SER:OG	1:C:979:GLU:OE2	2.28	0.50
1:B:910:LEU:C	1:B:910:LEU:HD12	2.32	0.50
1:A:426:LEU:HD22	1:A:432:TRP:NE1	2.26	0.50
1:A:613:PRO:CB	1:A:617:LEU:HD23	2.40	0.50
1:B:429:ASP:CG	1:B:431[A]:ARG:HD3	2.32	0.50
1:A:80:GLU:N	1:A:80:GLU:OE2	2.30	0.50
1:C:229:THR:HA	1:C:239:VAL:O	2.10	0.50
1:B:58:TRP:HE3	1:B:123:TYR:HB3	1.76	0.50
1:D:475:ILE:O	1:D:476:LYS:C	2.49	0.50
1:B:788:PRO:HD3	1:B:968:MET:HG3	1.91	0.50
1:D:130:ASP:OD2	1:D:132:SER:OG	2.29	0.50
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.29	0.50
1:B:733:ALA:O	1:B:734:SER:O	2.30	0.50
1:A:746:ASP:HA	1:A:760:ARG:CG	2.29	0.50
1:B:600:GLN:C	1:B:602:CYS:H	2.15	0.50
1:C:143:PHE:O	1:C:168:PRO:HA	2.11	0.50
1:C:258:VAL:HB	1:C:291:LEU:CD1	2.41	0.50
1:C:111:PRO:HG3	1:C:196:TYR:CE2	2.46	0.50
1:D:446:ARG:HG2	1:D:446:ARG:O	2.11	0.50
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.29	0.50
1:D:234:ASP:O	1:D:235:PHE:HB2	2.11	0.50
1:B:577:LYS:HB3	1:B:585:TRP:CE2	2.46	0.50
1:C:506:VAL:HA	1:C:520:ILE:HG12	1.93	0.50
1:A:959:ILE:HA	3:A:4028:HOH:O	2.11	0.50
1:A:590:GLY:HA2	1:A:594:ASP:CG	2.32	0.50
1:B:399:TYR:CB	1:B:450:HIS:CD2	2.95	0.50
1:B:102:ASN:HD22	1:B:102:ASN:C	2.15	0.50
1:B:638:VAL:O	1:B:677:LYS:HA	2.11	0.50
1:A:887:GLN:HB2	1:A:983:TRP:CD2	2.47	0.50
1:A:719:GLN:HE22	1:A:915:PHE:H	1.59	0.50
1:D:225:PHE:HA	1:D:243:GLU:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:821:ALA:O	1:A:840:HIS:HA	2.10	0.50
1:A:847:LYS:HD2	1:A:848:THR:N	2.27	0.50
1:D:3:ILE:O	1:D:3:ILE:HD12	2.12	0.50
1:B:118:ASN:CB	1:B:191:TRP:HD1	2.14	0.50
1:B:701:VAL:CG1	1:B:702:GLN:N	2.73	0.50
1:C:649:ASN:ND2	1:C:702:GLN:HG2	2.26	0.50
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.12	0.50
1:A:797:GLU:O	1:A:800:ARG:O	2.29	0.50
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.94	0.50
1:C:925:MET:HE3	1:C:925:MET:HA	1.94	0.50
1:B:674:PRO:C	1:B:675:GLN:HG2	2.32	0.50
1:A:658:LEU:N	1:A:661:LYS:O	2.38	0.50
1:A:202:MET:HB3	1:A:573:GLN:HE22	1.76	0.50
1:A:652:LEU:N	1:A:668:VAL:O	2.36	0.50
1:B:571:VAL:HG11	1:B:611:ARG:CZ	2.41	0.50
1:C:21:VAL:HG13	1:C:24:LEU:HD13	1.94	0.50
1:C:103:VAL:HG12	1:C:104:THR:N	2.27	0.50
1:D:16:TRP:O	1:D:193:ASP:N	2.44	0.50
1:A:36:TRP:CE2	1:A:42:ALA:HA	2.46	0.50
1:B:163:GLN:OE1	1:B:193:ASP:OD1	2.30	0.50
1:A:211:ASP:N	1:A:211:ASP:OD1	2.25	0.50
1:A:629:PHE:CD1	1:A:629:PHE:N	2.79	0.50
1:B:645:ARG:NH2	1:B:650:GLU:OE2	2.42	0.50
1:D:588:TYR:HB2	1:D:602:CYS:SG	2.52	0.50
1:B:696:LEU:HD12	1:B:697:THR:N	2.27	0.50
1:A:647:SER:OG	1:A:672:VAL:O	2.30	0.50
1:A:856:TYR:N	1:A:856:TYR:CD1	2.79	0.50
1:C:726:LEU:HD11	1:D:873:ALA:HB2	1.93	0.50
1:C:386:ALA:HB2	1:C:408:TYR:HB2	1.94	0.50
1:C:966:GLN:NE2	1:C:979:GLU:OE2	2.31	0.50
1:D:33:PHE:HA	1:D:326:GLU:OE1	2.11	0.50
1:D:598:ASP:C	1:D:599:ARG:HG3	2.33	0.50
1:A:682:LEU:HB3	1:A:683:PRO:HD2	1.93	0.50
1:D:822:LEU:HD12	1:D:824:GLN:N	2.27	0.50
1:A:217:LYS:NZ	1:A:324:GLU:OE2	2.44	0.50
1:A:808:GLU:HA	1:A:808:GLU:OE1	2.11	0.50
1:D:670:LEU:HA	1:D:678:GLN:OE1	2.11	0.49
1:C:416:GLU:OE1	1:C:418:HIS:HB2	2.12	0.49
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.11	0.49
1:C:134:LEU:CD2	1:C:134:LEU:N	2.75	0.49
1:B:653[B]:HIS:HD2	1:B:666:GLY:O	1.96	0.49
1:A:90:TRP:NE1	1:A:96:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:382:ASN:O	1:B:383:ASN:HB2	2.12	0.49
1:D:581:ASN:HD22	1:D:583:ASN:HD21	1.59	0.49
1:D:808:GLU:HA	1:D:808:GLU:OE1	2.10	0.49
1:B:769:TRP:CE3	1:B:769:TRP:N	2.80	0.49
1:C:842:TRP:N	1:C:842:TRP:CE3	2.80	0.49
1:A:726:LEU:CD1	1:B:873:ALA:HB2	2.42	0.49
1:A:995:GLY:O	1:A:997:ASP:N	2.45	0.49
1:A:524:LEU:HD22	1:A:561:ARG:HB3	1.94	0.49
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.47	0.49
1:B:696:LEU:HD12	1:B:697:THR:H	1.77	0.49
1:B:577:LYS:HB3	1:B:585:TRP:CZ2	2.47	0.49
1:B:649:ASN:O	1:B:702:GLN:HA	2.12	0.49
1:D:334:GLU:CD	1:D:336:ARG:HD3	2.33	0.49
1:C:502:MET:CB	1:C:537:GLU:HG3	2.42	0.49
1:D:540:HIS:HE1	1:D:542:MET:HB2	1.76	0.49
1:C:746:ASP:N	1:C:760:ARG:HG2	2.27	0.49
1:D:784:PHE:CD1	1:D:850:PHE:CE1	3.00	0.49
1:D:716:ALA:O	1:D:717:TRP:HB3	2.12	0.49
1:C:867:THR:O	1:C:867:THR:HG22	2.12	0.49
1:A:89:ASN:O	1:A:92:MET:HB2	2.12	0.49
1:A:360:HIS:CE1	1:A:361:PRO:HD2	2.46	0.49
1:C:579:ASP:OD1	1:C:583:ASN:HB2	2.12	0.49
1:B:166:ARG:CG	1:B:392:TYR:HB2	2.40	0.49
1:A:141:ILE:O	1:A:141:ILE:HG23	2.11	0.49
1:D:870:VAL:HG12	1:D:871:GLU:N	2.27	0.49
1:B:906:TYR:CD2	1:B:937:LEU:HD22	2.47	0.49
1:A:718:GLN:HG3	1:A:719:GLN:N	2.27	0.49
1:B:351:ILE:O	1:B:351:ILE:HG22	2.11	0.49
1:A:890:GLN:OE1	1:A:949:HIS:HE1	1.94	0.49
1:B:141:ILE:HB	1:B:173:LEU:CD1	2.43	0.49
1:A:634:GLN:OE1	1:A:685:LEU:HD12	2.13	0.49
1:C:78:LEU:O	1:C:81:ALA:HB3	2.12	0.49
1:B:15:ASP:HB3	1:B:21:VAL:CG1	2.43	0.49
1:B:14:ARG:HG2	1:B:16:TRP:CZ2	2.47	0.49
1:B:622:HIS:HD2	1:B:625:GLN:OE1	1.95	0.49
1:B:474:TRP:CZ2	1:B:478:VAL:HG21	2.47	0.49
1:B:176:PHE:N	1:B:176:PHE:CD1	2.79	0.49
1:B:7:LEU:N	1:B:71:GLU:OE2	2.46	0.49
1:A:878:HIS:HD2	1:A:1008:GLN:HB3	1.77	0.49
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.47	0.49
1:C:399:TYR:N	1:C:399:TYR:CD1	2.80	0.49
1:C:858:ILE:HG12	1:C:864:MET:HB3	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:63:PHE:HB3	1:D:64:PRO:CD	2.42	0.49
1:A:556:PHE:CD1	1:A:564:GLY:HA2	2.47	0.49
1:A:878:HIS:HB2	3:A:4054:HOH:O	2.12	0.49
1:B:73:TRP:CH2	1:B:187:MET:HB3	2.47	0.49
1:C:589:GLY:C	1:C:591:ASP:H	2.16	0.49
1:C:856:TYR:CD1	1:C:856:TYR:N	2.79	0.49
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.93	0.49
1:D:786:ARG:O	1:D:788:PRO:HD3	2.13	0.49
1:D:373:VAL:O	1:D:374:GLN:C	2.49	0.49
1:B:133:TRP:CD1	1:B:133:TRP:N	2.78	0.49
1:C:859:ASP:OD1	1:C:861:SER:OG	2.27	0.49
1:D:762:SER:C	1:D:822:LEU:HD23	2.33	0.49
1:B:730:LEU:H	1:B:730:LEU:CD1	2.00	0.49
1:A:26:ARG:NH1	1:A:169:SER:HB3	2.18	0.49
1:C:652:LEU:O	1:C:667:GLU:HA	2.13	0.49
1:B:423:MET:CB	1:C:282:ARG:HG3	2.41	0.49
1:C:961:ARG:HG3	1:C:961:ARG:NH1	2.27	0.49
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.76	0.49
1:B:894:ARG:HD2	1:B:919:ASP:OD1	2.13	0.49
1:C:84:VAL:HG13	1:C:85:VAL:N	2.27	0.49
1:A:446:ARG:HG2	1:A:447:ASP:OD1	2.13	0.49
1:B:305:ILE:O	1:B:305:ILE:HG22	2.13	0.49
1:A:479:ASP:OD1	1:A:481:SER:HB3	2.13	0.49
1:C:339:ASN:HB3	3:C:4161:HOH:O	2.13	0.49
1:D:261:TRP:CD1	1:D:261:TRP:N	2.80	0.49
1:C:728:VAL:HG23	1:C:728:VAL:O	2.12	0.49
1:A:208:ILE:HG22	1:A:208:ILE:O	2.12	0.49
1:D:100:TYR:O	1:D:597:ASN:HB2	2.13	0.49
1:D:357:HIS:HD2	1:D:392:TYR:OH	1.96	0.49
1:D:238:ALA:HB1	1:D:332:PHE:HE2	1.77	0.49
1:C:261:TRP:CH2	1:C:266:GLN:HG3	2.47	0.49
1:B:153:TRP:HA	1:B:157:ARG:O	2.13	0.49
1:C:455:ILE:HG22	1:C:456:TRP:N	2.27	0.49
1:D:211:ASP:OD1	1:D:211:ASP:N	2.45	0.49
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.48	0.49
1:C:127:PHE:CD2	1:C:127:PHE:N	2.80	0.49
1:B:510:GLN:HB3	1:B:512:PHE:CZ	2.46	0.49
1:B:788:PRO:CD	1:B:968:MET:HG3	2.43	0.49
1:D:513:PRO:O	1:D:514:ALA:HB3	2.12	0.49
1:B:434:PRO:O	1:B:435:ALA:C	2.50	0.48
1:A:134:LEU:CD2	1:A:134:LEU:H	2.21	0.48
1:B:777:LEU:CD2	1:B:889:ALA:HA	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:512:PHE:HE1	1:A:517:LYS:HE2	1.78	0.48
1:A:881:ARG:NH1	1:A:987:ASP:OD2	2.40	0.48
1:C:65:ALA:HB1	1:C:66:PRO:CD	2.43	0.48
1:A:282:ARG:HG3	1:D:420:MET:O	2.13	0.48
1:B:932:PRO:HG2	1:B:970:THR:O	2.13	0.48
1:B:959:ILE:HD12	1:B:984:LEU:HD13	1.95	0.48
1:B:397:LEU:O	1:B:400:THR:N	2.46	0.48
1:B:282:ARG:NH1	1:C:419:GLY:HA2	2.19	0.48
1:C:242:ALA:O	1:C:291:LEU:N	2.46	0.48
1:D:62:TRP:HB2	1:D:95:TYR:HD2	1.78	0.48
1:A:62:TRP:HZ2	1:A:119:PRO:HB3	1.78	0.48
1:B:80:GLU:CD	1:B:80:GLU:H	2.16	0.48
1:C:387:VAL:HG11	1:C:398:TRP:HZ2	1.79	0.48
1:A:995:GLY:H	1:A:1002:SER:HB2	1.78	0.48
1:C:689:GLU:O	1:C:690:SER:O	2.31	0.48
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.57	0.48
1:C:685:LEU:CD2	1:C:686:PRO:HD3	2.38	0.48
1:A:683:PRO:O	1:A:685:LEU:N	2.46	0.48
1:C:367:MET:HE2	1:C:372:MET:HG2	1.96	0.48
1:A:822:LEU:HD11	1:A:824:GLN:O	2.14	0.48
1:B:126:THR:HA	1:B:182:ASN:O	2.13	0.48
1:A:897:TRP:CE2	1:A:918:TRP:HD1	2.30	0.48
1:C:995:GLY:O	1:C:996:ASP:C	2.50	0.48
1:D:309:TYR:CD1	1:D:309:TYR:N	2.81	0.48
1:A:769:TRP:HA	1:A:773:LYS:O	2.12	0.48
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.48	0.48
1:B:598:ASP:C	1:B:599:ARG:HG3	2.34	0.48
1:C:141:ILE:HD13	1:C:143:PHE:CZ	2.48	0.48
1:B:581:ASN:ND2	1:B:583:ASN:ND2	2.61	0.48
1:D:949:HIS:HB2	1:D:951:TRP:CZ3	2.48	0.48
1:C:429:ASP:OD1	1:C:431[B]:ARG:HG3	2.13	0.48
1:D:937:LEU:HG	1:D:938:ARG:N	2.28	0.48
1:D:853:ARG:NH1	1:D:871:GLU:OE2	2.47	0.48
1:C:58:TRP:HE3	1:C:123:TYR:HB3	1.78	0.48
1:D:638:VAL:HG23	1:D:678:GLN:O	2.13	0.48
1:C:730:LEU:CD1	1:C:730:LEU:H	2.15	0.48
1:B:838:THR:HG21	3:B:4178:HOH:O	2.14	0.48
1:A:786:ARG:HG2	1:A:880:ALA:CB	2.41	0.48
1:B:807:VAL:HA	1:B:810:TRP:CE3	2.49	0.48
1:B:454:ILE:HG13	1:B:455:ILE:HG13	1.95	0.48
1:B:609:ALA:O	1:B:611:ARG:NH1	2.44	0.48
1:D:769:TRP:NE1	1:D:774:LYS:HE2	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:229:THR:HG22	1:C:240:LEU:HA	1.95	0.48
1:D:8:ALA:O	1:D:12:GLN:HB3	2.14	0.48
1:D:368:ASP:O	1:D:372:MET:HG3	2.12	0.48
1:C:929:TYR:HB3	3:C:4108:HOH:O	2.12	0.48
1:A:434:PRO:O	1:A:437:SER:HB3	2.14	0.48
1:B:92:MET:O	1:B:93:HIS:HD2	1.97	0.48
1:D:105:TYR:CZ	1:D:199:ASP:HB2	2.48	0.48
1:B:721:ARG:HH11	1:B:721:ARG:HB2	1.79	0.48
1:A:696:LEU:C	1:A:696:LEU:HD12	2.34	0.48
1:C:944:LEU:O	1:C:950:GLN:HA	2.13	0.48
1:A:823:LEU:CD2	1:B:728:VAL:HG12	2.44	0.48
1:D:937:LEU:HG	1:D:938:ARG:H	1.76	0.48
1:B:441:THR:HG22	1:B:474:TRP:CH2	2.48	0.48
1:B:683:PRO:O	1:B:684:GLU:C	2.51	0.48
1:D:143:PHE:O	1:D:168:PRO:HA	2.14	0.48
1:C:652:LEU:CB	1:C:670:LEU:HD21	2.43	0.48
1:C:287:ASP:N	1:C:287:ASP:OD1	2.33	0.48
1:B:255:ARG:HB2	1:B:316:HIS:NE2	2.29	0.48
1:C:133:TRP:N	1:C:133:TRP:CD1	2.80	0.48
1:B:737:ILE:HG13	1:B:738:PRO:N	2.19	0.48
1:B:908:ASP:OD1	1:B:993:ILE:HG12	2.13	0.48
1:D:867:THR:HG22	1:D:867:THR:O	2.13	0.48
1:C:292:ARG:HG3	1:C:292:ARG:NH1	2.27	0.48
1:A:592:PHE:HB2	1:A:594:ASP:OD1	2.14	0.48
1:C:869:ASP:OD1	1:C:1015:HIS:ND1	2.42	0.48
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.49	0.48
1:D:757:GLN:O	1:D:765:LEU:HD12	2.14	0.48
1:B:91:GLN:HE21	1:B:190:ARG:NH1	2.10	0.48
1:B:62:TRP:CD1	1:B:95:TYR:HB3	2.48	0.48
1:B:721:ARG:HH11	1:B:721:ARG:CB	2.27	0.48
1:C:598:ASP:C	1:C:599:ARG:HG2	2.34	0.48
1:B:254:LEU:C	1:B:255:ARG:HH11	2.16	0.48
1:C:190:ARG:HG3	1:C:206:SER:OG	2.13	0.48
1:C:767:GLN:CG	1:C:768:MET:N	2.75	0.48
1:A:823:LEU:HD12	1:A:839:ALA:HB1	1.95	0.48
1:C:510:GLN:N	1:C:511:PRO:HD3	2.28	0.48
1:D:141:ILE:O	1:D:170:GLU:HA	2.13	0.48
1:B:409:VAL:HG23	1:B:452:SER:HB2	1.95	0.48
1:B:872:VAL:HG23	1:B:1012:GLY:O	2.13	0.48
1:C:144:ASP:HB3	3:C:4082:HOH:O	2.13	0.48
1:D:972:HIS:HB2	1:D:974:HIS:CE1	2.49	0.48
1:A:241:GLU:HG3	1:A:292:ARG:HG3	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:LEU:O	1:A:174:SER:C	2.51	0.48
1:A:100:TYR:HB2	1:A:203:TRP:CD2	2.49	0.48
1:C:88:SER:HA	1:C:366:VAL:HG21	1.95	0.48
1:C:864:MET:HG3	1:C:1020:TRP:HB3	1.96	0.48
1:B:26:ARG:HD2	1:B:169:SER:HA	1.96	0.48
1:D:637:GLU:HB2	1:D:679:LEU:HD21	1.95	0.48
1:D:352:ARG:HB2	1:D:385:ASN:CB	2.35	0.48
1:B:9:VAL:CG1	1:B:10:VAL:N	2.77	0.48
1:D:144:ASP:HB2	1:D:211:ASP:H	1.79	0.48
1:A:897:TRP:CE2	1:A:918:TRP:CD1	3.02	0.48
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.47	0.48
1:A:577:LYS:O	1:A:584:PRO:HA	2.13	0.48
1:B:349:LEU:O	1:B:563:GLN:HB3	2.14	0.48
1:D:638:VAL:CG2	1:D:678:GLN:HB3	2.44	0.47
1:D:588:TYR:O	1:D:589:GLY:C	2.52	0.47
1:B:30:HIS:ND1	1:B:33:PHE:CD1	2.82	0.47
1:D:889:ALA:HB3	1:D:890:GLN:HE22	1.79	0.47
1:B:651:LEU:O	1:B:701:VAL:N	2.32	0.47
1:A:897:TRP:HA	1:A:943:GLU:O	2.14	0.47
1:B:906:TYR:CZ	1:B:937:LEU:HB3	2.49	0.47
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.96	0.47
1:A:456:TRP:O	1:A:484:VAL:HA	2.14	0.47
1:B:105:TYR:CE2	1:B:196:TYR:HA	2.49	0.47
1:A:889:ALA:O	1:A:890:GLN:C	2.51	0.47
1:A:695:TRP:CE2	1:A:721:ARG:HG3	2.49	0.47
1:A:742:THR:CG2	1:A:743:SER:H	2.26	0.47
1:D:906:TYR:OH	1:D:935:ASN:HA	2.13	0.47
1:C:657:ALA:O	1:C:694:LEU:HD12	2.13	0.47
1:D:740:LEU:HA	1:D:748:CYS:O	2.14	0.47
1:D:610:ASP:OD2	1:D:612:THR:HG23	2.14	0.47
1:A:440:VAL:CG1	1:A:475:ILE:HD11	2.44	0.47
1:A:573:GLN:HB2	1:A:602:CYS:O	2.14	0.47
1:D:153:TRP:HA	1:D:157:ARG:O	2.13	0.47
1:A:763:GLY:HA3	1:A:822:LEU:HD23	1.93	0.47
1:C:894:ARG:CZ	1:C:921:PRO:HD3	2.44	0.47
1:D:55:ASN:ND2	1:D:87:PRO:HD3	2.28	0.47
1:D:1020:TRP:CD1	1:D:1021:CYS:N	2.79	0.47
1:C:7:LEU:HB2	1:C:71:GLU:CD	2.34	0.47
1:A:906:TYR:CE2	1:A:937:LEU:HB2	2.48	0.47
1:D:749:ILE:O	1:D:755:ARG:HA	2.14	0.47
1:D:515:VAL:N	1:D:516:PRO:HD3	2.29	0.47
1:A:285:TYR:HB2	1:A:288:ARG:HB2	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.97	0.47
1:C:100:TYR:CB	1:C:203:TRP:CE3	2.96	0.47
1:C:653[A]:HIS:ND1	1:C:667:GLU:HG2	2.28	0.47
1:D:282:ARG:CG	1:D:282:ARG:HH11	2.19	0.47
1:B:576:ILE:HD11	1:B:584:PRO:CB	2.44	0.47
1:C:533:LEU:HD12	1:C:533:LEU:C	2.34	0.47
1:B:153:TRP:HA	1:B:159:VAL:HG23	1.96	0.47
1:D:127:PHE:HE1	1:D:129:VAL:CG2	2.28	0.47
1:B:429:ASP:OD1	1:B:431[A]:ARG:HD3	2.15	0.47
1:B:51:LEU:CD1	1:B:215:LEU:HB2	2.44	0.47
1:C:610:ASP:O	1:C:611:ARG:HB2	2.15	0.47
1:D:742:THR:CG2	1:D:743:SER:N	2.78	0.47
1:C:84:VAL:HG13	1:C:85:VAL:O	2.14	0.47
1:C:506:VAL:HG22	1:C:520:ILE:HD11	1.97	0.47
1:B:902:PRO:O	1:B:938:ARG:NH1	2.44	0.47
1:D:943:GLU:HG2	1:D:944:LEU:N	2.27	0.47
1:A:928:PRO:CB	1:A:973:ARG:NH1	2.72	0.47
1:B:559:TYR:CD1	1:B:559:TYR:N	2.80	0.47
1:A:316:HIS:HB2	1:A:321:THR:O	2.14	0.47
1:B:425:ARG:HH22	1:C:287:ASP:CG	2.17	0.47
1:B:4:THR:O	1:B:9:VAL:HG11	2.13	0.47
1:D:331:GLY:HA3	1:D:451:PRO:CB	2.44	0.47
1:D:403:ASP:OD1	1:D:452:SER:OG	2.26	0.47
1:B:567:VAL:CG1	1:B:568:TRP:N	2.78	0.47
1:D:749:ILE:HG22	1:D:750:GLU:N	2.29	0.47
1:A:417:THR:O	1:A:418:HIS:C	2.49	0.47
1:C:99:ILE:HG22	1:C:101:THR:HG22	1.97	0.47
1:C:791:ASN:N	3:C:4072:HOH:O	2.40	0.47
1:B:904:GLU:HB2	1:B:936:GLY:HA2	1.97	0.47
1:C:146:VAL:O	1:C:165:SER:HA	2.14	0.47
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.15	0.47
1:B:278:ILE:N	1:B:278:ILE:HD12	2.29	0.47
1:B:98:PRO:HB3	1:B:205:MET:HG2	1.97	0.47
1:A:100:TYR:CD2	1:A:602:CYS:HB3	2.50	0.47
1:B:153:TRP:NE1	1:B:158:TRP:HB2	2.30	0.47
1:C:36:TRP:CD1	1:C:41:GLU:CB	2.98	0.47
1:B:737:ILE:C	1:B:751:LEU:HD12	2.34	0.47
1:D:881:ARG:HD2	3:D:4054:HOH:O	2.14	0.47
1:A:897:TRP:NE1	1:A:918:TRP:HD1	2.12	0.47
1:D:697:THR:CG2	1:D:698:VAL:N	2.78	0.47
1:B:941:THR:HG22	1:B:955:PHE:CZ	2.49	0.47
1:C:659:ASP:HB2	1:C:661:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:850:PHE:HD2	1:B:872:VAL:HG13	1.80	0.47
1:C:309:TYR:CD1	1:C:309:TYR:N	2.83	0.47
1:A:354:VAL:HG22	1:A:355:ASN:N	2.28	0.47
1:D:758:PHE:HZ	1:D:864:MET:HE1	1.80	0.47
1:D:166:ARG:CG	1:D:392:TYR:HB2	2.43	0.47
1:D:955:PHE:CD2	1:D:955:PHE:N	2.83	0.47
1:D:230:ARG:NH1	1:D:230:ARG:HG3	2.12	0.47
1:D:230:ARG:NH1	1:D:230:ARG:CG	2.76	0.47
1:B:559:TYR:HA	1:B:560:PRO:HD2	1.69	0.47
1:D:352:ARG:HG2	1:D:624:GLN:HB3	1.96	0.47
1:D:433:LEU:N	1:D:434:PRO:HD2	2.29	0.47
1:A:66:PRO:HD3	1:A:118:ASN:HB3	1.97	0.47
1:B:842:TRP:CH2	1:B:852:SER:HB2	2.47	0.47
1:B:201:ASP:HB3	3:B:4001:HOH:O	2.15	0.47
1:B:486:TYR:O	1:B:496:THR:HB	2.15	0.47
1:C:778:THR:CG2	1:C:779:PRO:N	2.78	0.47
1:A:822:LEU:HD11	1:A:824:GLN:C	2.34	0.47
1:C:133:TRP:CZ3	1:C:216:HIS:HB2	2.50	0.47
1:A:666:GLY:C	1:A:667:GLU:HG2	2.33	0.47
1:D:767:GLN:CG	1:D:768:MET:N	2.77	0.47
1:C:234:ASP:OD1	1:C:236:SER:OG	2.29	0.47
1:D:737:ILE:HG13	1:D:738:PRO:HD2	1.97	0.47
1:B:961:ARG:O	1:B:979:GLU:HG3	2.15	0.47
1:D:76:CYS:HA	3:D:4520:HOH:O	2.13	0.47
1:B:983:TRP:HA	1:B:983:TRP:CE3	2.49	0.47
1:C:143:PHE:CD1	1:C:143:PHE:N	2.83	0.47
1:C:391:HIS:HA	1:C:412:GLU:OE1	2.14	0.47
1:C:764:PHE:CE2	1:C:781:ARG:CB	2.98	0.47
1:C:250:LEU:HD11	1:C:287:ASP:HA	1.95	0.47
1:D:685:LEU:O	1:D:686:PRO:O	2.32	0.47
1:C:375:ASP:O	1:C:376:ILE:C	2.52	0.47
1:B:848:THR:C	1:B:849:LEU:HD23	2.35	0.47
1:A:937:LEU:HA	1:A:958:ASN:HB3	1.97	0.47
1:B:281:GLU:HG3	1:C:515:VAL:HG21	1.96	0.47
1:A:147:ASN:HB2	1:A:209:PHE:CE2	2.50	0.47
1:A:885:ASN:O	1:A:886:CYS:HB3	2.15	0.47
1:B:253:TYR:O	1:B:318:ALA:N	2.41	0.47
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.96	0.47
1:C:105:TYR:CE1	1:C:419:GLY:HA3	2.50	0.47
1:A:597:ASN:ND2	1:A:599:ARG:H	2.13	0.47
1:C:778:THR:HG23	1:C:779:PRO:HD2	1.97	0.47
1:A:778:THR:HA	1:A:779:PRO:HD3	1.77	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:111:PRO:HA	1:C:112:PRO:HA	1.58	0.47
1:C:147:ASN:HB2	1:C:209:PHE:CE2	2.50	0.47
1:C:1020:TRP:HD1	1:C:1021:CYS:H	1.62	0.47
1:D:636:ILE:O	1:D:680:ILE:N	2.39	0.47
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.18	0.47
1:A:77:ASP:HA	3:A:4068:HOH:O	2.15	0.47
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.49	0.47
1:C:651:LEU:CD2	1:C:653[A]:HIS:HE1	2.28	0.47
1:B:656:VAL:CG1	1:B:694:LEU:HD11	2.42	0.47
1:D:74:LEU:HD21	1:D:153:TRP:CE2	2.49	0.47
1:C:77:ASP:C	1:C:78:LEU:HD23	2.36	0.47
1:C:217:LYS:HG2	1:C:218:PRO:CD	2.43	0.47
1:B:701:VAL:HG12	1:B:702:GLN:N	2.29	0.47
1:B:550:ALA:O	1:B:553:TRP:N	2.48	0.47
1:C:647:SER:OG	1:C:672:VAL:HG23	2.15	0.47
1:D:617:LEU:HA	1:D:617:LEU:HD12	1.72	0.47
1:B:13:ARG:NH1	1:C:13:ARG:NH1	2.63	0.46
1:B:153:TRP:CD1	1:B:158:TRP:HA	2.50	0.46
1:C:649:ASN:O	1:C:702:GLN:HA	2.15	0.46
1:C:403:ASP:OD2	1:C:450:HIS:ND1	2.47	0.46
1:C:897:TRP:CH2	1:C:918:TRP:HB2	2.50	0.46
1:C:91:GLN:HG2	1:C:98:PRO:HA	1.96	0.46
1:A:278:ILE:CG2	1:A:279:ILE:N	2.78	0.46
1:D:229:THR:HA	1:D:239:VAL:O	2.15	0.46
1:C:721:ARG:NH1	1:C:721:ARG:HB2	2.31	0.46
1:C:970:THR:CG2	1:C:975:LEU:HB2	2.46	0.46
1:B:282:ARG:HG2	1:C:423:MET:HB2	1.97	0.46
1:A:693:GLN:HG2	1:A:721:ARG:HD2	1.95	0.46
1:A:702:GLN:O	1:A:712:GLY:N	2.34	0.46
1:A:571:VAL:HG12	1:A:609:ALA:HA	1.96	0.46
1:B:652:LEU:HA	1:B:699:ARG:O	2.15	0.46
1:A:223:SER:HB3	1:A:247:CYS:HB2	1.97	0.46
1:B:1014:TYR:HE1	3:B:4057:HOH:O	1.96	0.46
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.50	0.46
1:C:899:GLY:O	1:C:915:PHE:HA	2.16	0.46
1:D:99:ILE:O	1:D:203:TRP:HA	2.16	0.46
1:C:102:ASN:C	1:C:102:ASN:HD22	2.19	0.46
1:D:661:LYS:HA	1:D:662:PRO:HD3	1.70	0.46
1:D:52[A]:ARG:HG2	1:D:52[A]:ARG:NH1	2.30	0.46
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.50	0.46
1:D:86:VAL:HA	1:D:87:PRO:C	2.34	0.46
1:B:883:GLY:HA2	1:B:1016:TYR:CZ	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:455:ILE:HG21	1:D:485:GLN:HG2	1.97	0.46
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.48	0.46
1:A:354:VAL:CG2	1:A:355:ASN:N	2.79	0.46
1:D:474:TRP:CZ2	1:D:478:VAL:HG21	2.50	0.46
1:A:927:THR:HA	1:A:928:PRO:HD3	1.47	0.46
1:B:782:ASP:HB2	1:B:842:TRP:HZ2	1.79	0.46
1:A:377:LEU:O	1:A:381:GLN:HB2	2.16	0.46
1:A:671:ASP:N	1:A:678:GLN:OE1	2.44	0.46
1:D:658:LEU:HD23	1:D:661:LYS:HZ2	1.80	0.46
1:D:78:LEU:HB2	1:D:81:ALA:HB2	1.98	0.46
1:B:4:THR:C	1:B:9:VAL:HG11	2.35	0.46
1:C:66:PRO:HD2	1:C:67:GLU:HG2	1.97	0.46
1:C:743:SER:OG	1:C:744:GLU:N	2.48	0.46
1:A:333:ARG:NH1	1:A:453:VAL:O	2.49	0.46
1:A:867:THR:HG22	1:A:867:THR:O	2.16	0.46
1:C:733:ALA:O	1:C:734:SER:C	2.54	0.46
1:B:730:LEU:HD12	1:B:730:LEU:N	2.16	0.46
1:A:38:ASN:HD21	1:A:40:GLU:CB	2.29	0.46
1:B:721:ARG:CB	1:B:721:ARG:NH1	2.78	0.46
1:B:740:LEU:HD13	1:B:749:ILE:HD11	1.96	0.46
1:B:274:PHE:HB3	1:B:286:ALA:O	2.16	0.46
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.16	0.46
1:C:721:ARG:CG	1:C:721:ARG:NH1	2.78	0.46
1:D:836:ILE:CG2	1:D:837:THR:N	2.78	0.46
1:D:588:TYR:CD2	1:D:603:MET:CE	2.99	0.46
1:A:701:VAL:HG12	1:A:702:GLN:N	2.31	0.46
1:B:738:PRO:HA	1:B:751:LEU:HB2	1.97	0.46
1:D:925:MET:HE3	1:D:938:ARG:CZ	2.45	0.46
1:C:959:ILE:O	1:C:959:ILE:HG23	2.14	0.46
1:C:362:LEU:CG	1:C:576:ILE:HD12	2.45	0.46
1:C:721:ARG:CB	1:C:721:ARG:NH1	2.79	0.46
1:B:375:ASP:HB3	1:B:379:MET:HE3	1.96	0.46
1:B:399:TYR:O	1:B:400:THR:C	2.53	0.46
1:B:246:MET:CE	1:B:287:ASP:HB3	2.45	0.46
1:D:73:TRP:CH2	1:D:187:MET:HB3	2.51	0.46
1:B:38:ASN:ND2	1:B:41:GLU:HB2	2.30	0.46
1:C:486:TYR:O	1:C:496:THR:HB	2.16	0.46
1:B:770:ILE:HG22	1:B:770:ILE:O	2.16	0.46
1:C:788:PRO:O	1:C:933:SER:HB2	2.16	0.46
1:D:463:GLY:HA2	3:D:7505:HOH:O	2.16	0.46
1:C:333:ARG:NH1	1:C:451:PRO:O	2.43	0.46
1:D:999:TRP:N	1:D:999:TRP:CD2	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:646:HIS:NE2	1:B:671:ASP:OD1	2.41	0.46
1:A:755:ARG:O	1:A:768:MET:HA	2.16	0.46
1:A:26:ARG:HD2	1:A:169:SER:HB3	1.97	0.46
1:C:600:GLN:NE2	1:C:790:ASP:OD1	2.49	0.46
1:A:427:THR:HG21	1:A:462:SER:HB3	1.97	0.46
1:A:693:GLN:NE2	1:A:721:ARG:NH1	2.64	0.46
1:D:421:VAL:O	1:D:425:ARG:HD2	2.16	0.46
1:A:906:TYR:CZ	1:A:937:LEU:CB	2.99	0.46
1:B:390:SER:HA	1:B:391:HIS:HA	1.79	0.46
1:A:394:ASN:O	1:A:395:HIS:C	2.52	0.46
1:B:538:TYR:O	1:B:539:ALA:HB3	2.15	0.46
1:D:536:CYS:C	1:D:537:GLU:HG3	2.36	0.46
1:B:367:MET:HE2	1:B:372:MET:HG2	1.97	0.46
1:A:255:ARG:N	1:A:316:HIS:O	2.45	0.46
1:D:352:ARG:HD2	1:D:352:ARG:HH11	1.58	0.46
1:A:118:ASN:O	1:A:120:THR:N	2.49	0.46
1:C:663:LEU:O	1:C:664:ALA:HB2	2.16	0.46
1:B:777:LEU:HD21	1:B:889:ALA:CA	2.46	0.46
1:C:920:LEU:CB	1:C:921:PRO:CD	2.94	0.46
1:C:37:ARG:HH22	1:C:216:HIS:CD2	2.34	0.46
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.45	0.46
1:C:380:LYS:HE3	1:C:406:GLY:O	2.15	0.46
1:A:209:PHE:H	1:A:209:PHE:HD2	1.61	0.46
1:A:125:LEU:O	1:A:183:ARG:HA	2.15	0.46
1:A:7:LEU:O	1:A:11:LEU:HG	2.15	0.46
1:C:232:ASN:O	1:C:233:ASP:C	2.53	0.46
1:C:568:TRP:C	1:C:568:TRP:CD1	2.89	0.46
1:A:436:MET:O	1:A:437:SER:C	2.52	0.46
1:C:420:MET:CE	1:C:426:LEU:HG	2.46	0.46
1:C:418:HIS:CG	1:C:461:GLU:HG3	2.51	0.46
1:A:696:LEU:HD12	1:A:697:THR:H	1.77	0.46
1:A:14:ARG:HG2	1:A:16:TRP:CZ2	2.50	0.46
1:B:881:ARG:O	1:B:882:ILE:HG13	2.16	0.46
1:A:764:PHE:CE2	1:A:840:HIS:CE1	3.04	0.46
1:C:842:TRP:N	1:C:842:TRP:HE3	2.14	0.46
1:C:689:GLU:O	1:C:690:SER:C	2.54	0.46
1:D:897:TRP:HA	1:D:943:GLU:O	2.16	0.46
1:C:331:GLY:N	1:C:451:PRO:HG3	2.31	0.46
1:A:842:TRP:HZ3	1:A:852:SER:HB3	1.81	0.46
1:A:111:PRO:HA	1:A:112:PRO:HA	1.55	0.46
1:A:679:LEU:HD23	1:A:679:LEU:N	2.04	0.45
1:D:654:TRP:CE2	1:D:666:GLY:N	2.85	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:422:PRO:HG2	1:B:424:ASN:CB	2.46	0.45
1:A:742:THR:CG2	1:A:743:SER:N	2.78	0.45
1:B:548:GLY:O	1:B:549:PHE:C	2.54	0.45
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.16	0.45
1:A:424:ASN:HB3	1:D:285:TYR:OH	2.16	0.45
1:C:299:LYS:HB2	1:C:309:TYR:OH	2.16	0.45
1:A:150:PHE:HB3	1:A:188:VAL:HA	1.97	0.45
1:C:225:PHE:HA	1:C:243:GLU:O	2.16	0.45
1:C:433:LEU:HA	1:C:433:LEU:HD12	1.64	0.45
1:B:89:ASN:O	1:B:92:MET:N	2.45	0.45
1:C:420:MET:HE3	1:C:425:ARG:HB3	1.96	0.45
1:B:656:VAL:O	1:B:657:ALA:HB2	2.15	0.45
1:D:133:TRP:O	1:D:134:LEU:HD23	2.17	0.45
1:C:499:ILE:HD11	1:C:529:GLU:CD	2.35	0.45
1:D:38:ASN:ND2	1:D:41:GLU:CG	2.79	0.45
1:A:737:ILE:CD1	1:A:832:ASP:HA	2.46	0.45
1:B:256:VAL:HG12	1:B:257:THR:N	2.32	0.45
1:B:970:THR:HG22	1:B:972:HIS:O	2.16	0.45
1:A:997:ASP:O	1:A:1002:SER:OG	2.34	0.45
1:D:999:TRP:N	1:D:999:TRP:CE3	2.84	0.45
1:B:292:ARG:HH11	1:B:292:ARG:CG	2.29	0.45
1:B:777:LEU:HG	1:B:889:ALA:HA	1.98	0.45
1:D:95:TYR:HD1	1:D:95:TYR:H	1.63	0.45
1:B:416:GLU:OE1	1:B:418:HIS:HB2	2.16	0.45
1:D:768:MET:HG2	1:D:775:GLN:HB2	1.97	0.45
1:D:455:ILE:CG2	1:D:456:TRP:N	2.78	0.45
1:A:479:ASP:N	1:A:480:PRO:HD3	2.31	0.45
1:B:791:ASN:HB2	3:B:4029:HOH:O	2.16	0.45
1:C:316:HIS:HB3	1:C:322:LEU:HD23	1.97	0.45
1:C:603:MET:HE3	1:C:930:VAL:HB	1.98	0.45
1:A:38:ASN:O	1:A:39:SER:C	2.54	0.45
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.52	0.45
1:A:202:MET:CE	1:A:365:GLN:NE2	2.79	0.45
1:B:421:VAL:O	1:B:425:ARG:NH1	2.39	0.45
1:B:3:ILE:C	1:B:5:ASP:H	2.20	0.45
1:D:129:VAL:CG2	1:D:182:ASN:ND2	2.79	0.45
1:D:824:GLN:O	1:D:838:THR:HA	2.17	0.45
1:C:303:ALA:CB	1:C:408:TYR:CZ	3.00	0.45
1:B:352:ARG:CZ	1:B:626:PHE:CE2	2.99	0.45
1:A:767:GLN:CG	1:A:768:MET:H	2.30	0.45
1:A:767:GLN:CG	1:A:768:MET:N	2.79	0.45
1:B:424:ASN:HB2	1:C:279:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:486:TYR:CE2	1:B:488:GLY:CA	2.99	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.73	0.45
1:C:37:ARG:HG2	1:C:50:GLN:NE2	2.30	0.45
1:D:649:ASN:OD1	1:D:703:PRO:HD2	2.17	0.45
1:B:84:VAL:CG1	1:B:85:VAL:N	2.79	0.45
1:D:147:ASN:HB2	1:D:209:PHE:CE2	2.51	0.45
1:B:7:LEU:CD2	1:B:74:LEU:HD11	2.31	0.45
1:D:599:ARG:HB2	1:D:600:GLN:H	1.43	0.45
1:B:91:GLN:NE2	1:B:190:ARG:CZ	2.79	0.45
1:B:661:LYS:HA	1:B:662:PRO:HD2	1.62	0.45
1:C:258:VAL:HB	1:C:291:LEU:HD11	1.99	0.45
1:C:455:ILE:CG2	1:C:456:TRP:N	2.80	0.45
1:D:127:PHE:CE1	1:D:129:VAL:HG22	2.51	0.45
1:B:587:ALA:HB1	1:B:592:PHE:HE1	1.80	0.45
1:B:807:VAL:HA	1:B:810:TRP:HE3	1.81	0.45
1:A:137:GLY:HA3	1:A:216:HIS:CE1	2.51	0.45
1:B:240:LEU:HD23	1:B:240:LEU:C	2.36	0.45
1:B:814:GLY:O	1:B:818:ALA:N	2.49	0.45
1:A:297:ASN:N	1:A:298:PRO:CD	2.77	0.45
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.81	0.45
1:D:407:LEU:HD23	1:D:407:LEU:HA	1.58	0.45
1:A:67:GLU:H	1:A:67:GLU:HG2	1.20	0.45
1:B:734:SER:HB3	1:B:860:GLY:CA	2.18	0.45
1:A:260:LEU:HD12	1:A:261:TRP:N	2.32	0.45
1:B:246:MET:HE1	1:B:287:ASP:HB3	1.99	0.45
1:A:377:LEU:HB3	1:A:381:GLN:HE22	1.82	0.45
1:D:658:LEU:O	1:D:661:LYS:HD2	2.17	0.45
1:A:789:LEU:HD11	1:A:993:ILE:CG2	2.41	0.45
1:D:786:ARG:NH2	1:D:792:ASP:OD1	2.44	0.45
1:C:570:TRP:CD1	1:C:571:VAL:CG2	2.99	0.45
1:D:824:GLN:CG	1:D:825:CYS:N	2.78	0.45
1:D:868:VAL:CG1	1:D:869:ASP:N	2.79	0.45
1:B:930:VAL:O	1:B:932:PRO:HD3	2.16	0.45
1:C:694:LEU:HD12	1:C:695:TRP:N	2.32	0.45
1:D:130:ASP:O	1:D:131:GLU:C	2.53	0.45
1:D:217:LYS:NZ	1:D:324:GLU:OE1	2.49	0.45
1:A:110:ASN:O	1:A:113:PHE:N	2.32	0.45
1:D:279:ILE:HD13	1:D:279:ILE:HG21	1.74	0.45
1:B:588:TYR:O	1:B:589:GLY:C	2.53	0.45
1:C:256:VAL:O	1:C:272:ALA:N	2.41	0.45
1:C:835:LEU:C	1:C:835:LEU:HD12	2.37	0.45
1:D:85:VAL:C	1:D:86:VAL:HG23	2.37	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:789:LEU:H	1:B:789:LEU:HG	1.66	0.45
1:B:408:TYR:HB3	1:B:454:ILE:CD1	2.47	0.45
1:D:769:TRP:HA	1:D:773:LYS:O	2.17	0.45
1:B:850:PHE:HA	1:B:871:GLU:O	2.16	0.45
1:A:449:ASN:HB2	3:A:4055:HOH:O	2.17	0.45
1:A:814:GLY:HA2	3:A:4138:HOH:O	2.16	0.45
1:D:507:ASP:OD1	1:D:521:LYS:HE2	2.17	0.45
1:C:545:SER:HB3	1:C:546:LEU:H	1.50	0.45
1:A:1023:LYS:HB2	1:A:1023:LYS:HE2	1.58	0.45
1:D:100:TYR:HB2	1:D:203:TRP:CE2	2.52	0.45
1:B:967:LEU:HA	1:B:967:LEU:HD23	1.56	0.45
1:C:256:VAL:CG1	1:C:257:THR:N	2.80	0.45
1:D:5:ASP:OD2	1:D:157:ARG:HG3	2.16	0.45
1:C:192:SER:O	1:C:195:SER:HB2	2.17	0.45
1:D:287:ASP:N	1:D:287:ASP:OD1	2.50	0.45
1:D:455:ILE:HG22	1:D:456:TRP:N	2.31	0.45
1:D:69:VAL:HG13	1:D:70:PRO:HD2	1.99	0.45
1:D:387:VAL:O	1:D:409:VAL:HA	2.17	0.45
1:D:571:VAL:HG11	1:D:611:ARG:NH1	2.32	0.45
1:A:360:HIS:CG	1:A:361:PRO:CD	3.00	0.45
1:B:694:LEU:O	1:B:721:ARG:HG3	2.17	0.45
1:A:608:PHE:HD1	1:A:612:THR:O	2.00	0.45
1:A:129:VAL:HG23	1:A:182:ASN:HD22	1.82	0.45
1:B:234:ASP:OD1	1:B:236:SER:OG	2.34	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.73	0.45
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.31	0.45
1:C:344:LEU:O	1:C:345:ASN:C	2.54	0.45
1:D:101:THR:HG23	1:D:204:ARG:NH2	2.32	0.44
1:C:427:THR:HG23	1:C:427:THR:H	1.36	0.44
1:B:782:ASP:OD1	1:B:854:LYS:HE3	2.16	0.44
1:D:658:LEU:HA	1:D:693:GLN:O	2.17	0.44
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.44
1:C:54:LEU:N	1:C:54:LEU:HD23	2.31	0.44
1:C:78:LEU:O	1:C:79:PRO:C	2.55	0.44
1:B:581:ASN:HD22	1:B:583:ASN:ND2	2.14	0.44
1:B:651:LEU:HD12	1:B:703:PRO:HG3	1.94	0.44
1:B:152:LEU:HG	1:B:159:VAL:HG21	1.98	0.44
1:D:84:VAL:HG22	1:D:93:HIS:CE1	2.51	0.44
1:C:120:THR:HG21	1:C:187:MET:SD	2.57	0.44
1:B:227:VAL:HG12	1:B:228:ALA:N	2.32	0.44
1:C:965:GLN:O	1:C:966:GLN:C	2.55	0.44
1:A:876:THR:O	1:A:877:PRO:C	2.55	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:VAL:HG13	1:C:70:PRO:HD2	1.99	0.44
1:D:902:PRO:HD3	1:D:918:TRP:CH2	2.52	0.44
1:A:116:THR:HA	3:A:4017:HOH:O	2.17	0.44
1:D:272:ALA:HA	1:D:273:PRO:HD3	1.56	0.44
1:D:757:GLN:CG	1:D:758:PHE:N	2.80	0.44
1:B:397:LEU:HA	1:B:397:LEU:HD12	1.55	0.44
1:D:282:ARG:CG	1:D:282:ARG:NH1	2.79	0.44
1:C:209:PHE:O	1:C:366:VAL:HG13	2.17	0.44
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.46	0.44
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.99	0.44
1:C:448:ARG:HH21	1:C:478:VAL:HG13	1.82	0.44
1:D:928:PRO:HB2	1:D:973:ARG:NH1	2.32	0.44
1:B:529:GLU:HG2	3:B:4084:HOH:O	2.17	0.44
1:B:935:ASN:N	1:B:935:ASN:HD22	2.16	0.44
1:A:949:HIS:HD2	1:A:1022:GLN:HE21	1.64	0.44
1:A:436:MET:HE1	1:A:467:ASN:ND2	2.31	0.44
1:B:395:HIS:HA	1:B:396:PRO:HD3	1.75	0.44
1:C:43:ARG:NH1	1:C:263:GLY:O	2.51	0.44
1:B:654:TRP:N	1:B:666:GLY:O	2.50	0.44
1:D:416:GLU:CD	1:D:461:GLU:HG3	2.37	0.44
1:B:929:TYR:HB3	3:B:4090:HOH:O	2.16	0.44
1:D:696:LEU:C	1:D:696:LEU:HD12	2.37	0.44
1:A:44:THR:O	1:A:45:ASP:C	2.54	0.44
1:D:856:TYR:CD1	1:D:856:TYR:N	2.84	0.44
1:D:559:TYR:HB2	1:D:562:LEU:CG	2.46	0.44
1:D:100:TYR:CD1	1:D:602:CYS:HB3	2.53	0.44
1:B:287:ASP:OD1	1:C:425:ARG:NH2	2.47	0.44
1:B:588:TYR:HD1	1:B:589:GLY:N	2.14	0.44
1:B:658:LEU:O	1:B:660:GLY:N	2.50	0.44
1:B:225:PHE:CB	1:B:244:VAL:HG13	2.40	0.44
1:B:822:LEU:HD12	1:B:824:GLN:N	2.30	0.44
1:C:354:VAL:O	1:C:387:VAL:HA	2.18	0.44
1:A:303:ALA:HB2	1:A:408:TYR:CZ	2.52	0.44
1:A:904:GLU:O	1:A:904:GLU:HG2	2.17	0.44
1:D:202:MET:O	1:D:204:ARG:HD3	2.18	0.44
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.53	0.44
1:A:309:TYR:N	1:A:309:TYR:CD1	2.86	0.44
1:B:282:ARG:O	1:C:421:VAL:HG13	2.17	0.44
1:A:658:LEU:HD12	1:A:693:GLN:O	2.17	0.44
1:B:140:ARG:HB2	1:B:171:PHE:O	2.17	0.44
1:A:60:PHE:HE1	1:A:121:GLY:HA3	1.83	0.44
1:C:190:ARG:HD3	1:C:191:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:429:ASP:HA	1:C:430:PRO:HD3	1.79	0.44
1:A:843:GLN:HB3	1:A:847:LYS:O	2.17	0.44
1:C:618:THR:HG22	1:C:912:ALA:CB	2.48	0.44
1:D:482:ARG:HA	1:D:483:PRO:HD2	1.62	0.44
1:A:344:LEU:HG	1:A:345:ASN:N	2.32	0.44
1:A:868:VAL:HG12	1:A:869:ASP:N	2.32	0.44
1:C:814:GLY:O	1:C:818:ALA:N	2.39	0.44
1:D:961:ARG:HB3	1:D:961:ARG:HE	1.73	0.44
1:B:836:ILE:O	1:B:855:THR:HA	2.18	0.44
1:A:658:LEU:HD11	1:A:692:GLY:O	2.18	0.44
1:C:455:ILE:HG21	1:C:485:GLN:HG2	2.00	0.44
1:D:471:LEU:HA	1:D:471:LEU:HD23	1.57	0.44
1:C:869:ASP:CG	1:C:1015:HIS:HD1	2.20	0.44
1:C:500:CYS:HA	1:C:534:ILE:O	2.17	0.44
1:C:758:PHE:CD1	1:C:758:PHE:N	2.85	0.44
1:B:948:PRO:O	1:B:1022:GLN:HA	2.17	0.44
1:D:678:GLN:O	1:D:679:LEU:HD23	2.17	0.44
1:D:238:ALA:CB	1:D:332:PHE:CE2	3.00	0.44
1:A:134:LEU:N	1:A:134:LEU:CD2	2.77	0.44
1:A:635:THR:OG1	1:A:681:GLU:HG2	2.18	0.44
1:D:658:LEU:CD2	1:D:661:LYS:NZ	2.80	0.44
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.87	0.44
1:B:422:PRO:HD2	1:C:285:TYR:CE2	2.53	0.44
1:D:64:PRO:O	1:D:65:ALA:HB2	2.17	0.44
1:D:936:GLY:O	1:D:937:LEU:C	2.55	0.44
1:B:505:ARG:CD	1:B:508:GLU:HG2	2.48	0.44
1:C:230:ARG:O	1:C:238:ALA:HA	2.18	0.44
1:D:242:ALA:O	1:D:290:THR:HA	2.17	0.44
1:B:229:THR:HA	1:B:239:VAL:O	2.17	0.44
1:C:967:LEU:HD11	3:C:4016:HOH:O	2.17	0.44
1:A:767:GLN:HG3	1:A:768:MET:H	1.83	0.44
1:D:202:MET:HE3	1:D:357:HIS:HD2	1.83	0.44
1:D:673:ALA:O	1:D:676:GLY:N	2.45	0.44
1:A:260:LEU:CD1	1:A:309:TYR:HB3	2.48	0.44
1:B:93:HIS:HB3	1:B:95:TYR:HE1	1.83	0.44
1:B:600:GLN:O	1:B:602:CYS:N	2.51	0.44
1:B:658:LEU:HD12	1:B:659:ASP:H	1.83	0.44
1:C:395:HIS:CE1	1:C:396:PRO:HD2	2.53	0.44
1:B:652:LEU:HD12	1:B:652:LEU:C	2.37	0.44
1:D:118:ASN:O	1:D:119:PRO:C	2.55	0.44
1:D:949:HIS:CB	1:D:951:TRP:CH2	3.01	0.44
1:A:663:LEU:O	1:A:664:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:258:VAL:HG22	1:B:313:VAL:HG22	2.00	0.44
1:B:213:SER:C	1:B:214:LEU:HD23	2.37	0.44
1:B:570:TRP:CE3	1:B:570:TRP:HA	2.53	0.44
1:C:746:ASP:OD2	1:C:757:GLN:NE2	2.45	0.44
1:D:435:ALA:O	1:D:439:ARG:HG3	2.16	0.44
1:A:588:TYR:CD2	1:A:603:MET:CE	3.01	0.44
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.76	0.44
1:B:925:MET:HB3	3:B:4027:HOH:O	2.18	0.44
1:A:260:LEU:HD11	1:A:309:TYR:CB	2.48	0.44
1:B:749:ILE:O	1:B:755:ARG:HG3	2.17	0.44
1:C:754:LYS:HA	1:C:769:TRP:O	2.18	0.44
1:B:212:VAL:CG1	1:B:213:SER:N	2.78	0.44
1:C:866:ILE:O	1:C:1017:GLN:HA	2.18	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.44
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.21	0.43
1:A:261:TRP:CH2	1:A:266:GLN:HB2	2.53	0.43
1:C:418:HIS:ND1	3:C:4156:HOH:O	2.35	0.43
1:C:420:MET:HE1	1:C:426:LEU:CD2	2.48	0.43
1:C:242:ALA:O	1:C:290:THR:HA	2.18	0.43
1:D:11:LEU:HD21	1:D:187:MET:HE2	1.97	0.43
1:B:3:ILE:CG2	1:B:4:THR:N	2.80	0.43
1:C:377:LEU:H	1:C:377:LEU:HG	1.53	0.43
1:B:749:ILE:O	1:B:755:ARG:HA	2.18	0.43
1:B:154:CYS:N	1:B:157:ARG:O	2.42	0.43
1:A:730:LEU:HD22	1:B:823:LEU:HB3	2.00	0.43
1:D:127:PHE:CE1	1:D:129:VAL:CG2	3.01	0.43
1:A:128:ASN:ND2	1:A:181:GLU:HA	2.33	0.43
1:C:463:GLY:O	1:C:488:GLY:HA3	2.18	0.43
1:A:899:GLY:O	1:A:918:TRP:NE1	2.49	0.43
1:D:770:ILE:O	1:D:770:ILE:HG22	2.17	0.43
1:B:278:ILE:H	1:B:278:ILE:HD12	1.81	0.43
1:B:963:SER:HB3	1:B:983:TRP:CZ2	2.53	0.43
1:A:518:TRP:CD1	1:A:526:LEU:HD21	2.53	0.43
1:C:311:ALA:O	1:C:327:ALA:HB1	2.18	0.43
1:B:650:GLU:HG3	1:B:700:VAL:HG13	1.99	0.43
1:B:118:ASN:HD21	1:B:189:LEU:HD22	1.82	0.43
1:C:432:TRP:O	1:C:436:MET:HG3	2.17	0.43
1:A:100:TYR:HB3	1:A:589:GLY:HA2	2.00	0.43
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.73	0.43
1:C:246:MET:HE2	1:C:287:ASP:HB2	1.97	0.43
1:C:129:VAL:CG1	1:C:134:LEU:HD21	2.47	0.43
1:B:125:LEU:HD23	1:B:127:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:888:LEU:HA	1:C:888:LEU:HD23	1.75	0.43
1:B:152:LEU:HG	1:B:159:VAL:CG2	2.47	0.43
1:C:830:LEU:HA	1:C:830:LEU:HD12	1.86	0.43
1:D:460:ASN:ND2	1:D:461:GLU:CG	2.78	0.43
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.83	0.43
1:A:525:SER:O	1:A:526:LEU:C	2.54	0.43
1:A:22:THR:HG22	3:A:4063:HOH:O	2.18	0.43
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.81	0.43
1:B:606:LEU:HB3	1:B:617:LEU:HD13	2.00	0.43
1:D:746:ASP:HB3	1:D:757:GLN:HE21	1.84	0.43
1:C:600:GLN:O	1:C:602:CYS:N	2.51	0.43
1:B:282:ARG:HB2	1:C:423:MET:N	2.33	0.43
1:B:577:LYS:NZ	1:B:591:ASP:O	2.31	0.43
1:C:876:THR:O	1:C:877:PRO:C	2.54	0.43
1:C:701:VAL:CG1	1:C:702:GLN:N	2.81	0.43
1:B:35:SER:HB2	1:B:217:LYS:HG3	2.00	0.43
1:D:815:HIS:HE1	1:D:877:PRO:O	2.01	0.43
1:C:303:ALA:HB2	1:C:408:TYR:CE2	2.52	0.43
1:A:995:GLY:O	1:A:996:ASP:C	2.56	0.43
1:C:941:THR:HG22	1:C:955:PHE:CZ	2.53	0.43
1:D:1023:LYS:HE3	1:D:1023:LYS:C	2.39	0.43
1:A:766:SER:O	1:A:767:GLN:HB2	2.19	0.43
1:C:232:ASN:OD1	1:C:237:ARG:N	2.45	0.43
1:D:959:ILE:HB	1:D:984:LEU:HD12	1.99	0.43
1:B:398:TRP:HA	1:B:398:TRP:CE3	2.52	0.43
1:C:105:TYR:HB3	1:C:106:PRO:CD	2.42	0.43
1:B:282:ARG:NH1	1:C:419:GLY:CA	2.77	0.43
1:A:599:ARG:NH1	1:A:600:GLN:OE1	2.51	0.43
1:B:472:TYR:CD2	1:B:473:ARG:N	2.86	0.43
1:C:396:PRO:O	1:C:399:TYR:HD1	2.01	0.43
1:C:807:VAL:CG1	1:C:808:GLU:N	2.81	0.43
1:B:629:PHE:HA	1:B:637:GLU:O	2.17	0.43
1:B:941:THR:HG22	1:B:955:PHE:CE1	2.53	0.43
1:D:37:ARG:CD	1:D:50:GLN:NE2	2.82	0.43
1:C:899:GLY:HA2	1:C:915:PHE:CD1	2.53	0.43
1:A:615:PRO:HG2	1:A:929:TYR:OH	2.19	0.43
1:D:576:ILE:HA	1:D:576:ILE:HD13	1.79	0.43
1:C:272:ALA:HB1	1:C:273:PRO:CD	2.47	0.43
1:D:653[B]:HIS:NE2	1:D:665:SER:HB2	2.33	0.43
1:D:237:ARG:CG	1:D:237:ARG:NH1	2.82	0.43
1:C:151:HIS:HB3	1:C:153:TRP:CZ3	2.54	0.43
1:A:200:GLN:HA	1:A:416:GLU:OE2	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:21:VAL:HG12	1:C:21:VAL:O	2.17	0.43
1:A:995:GLY:H	1:A:1002:SER:CB	2.32	0.43
1:D:289:VAL:HG22	1:D:290:THR:N	2.32	0.43
1:D:192:SER:OG	1:D:194:GLY:N	2.51	0.43
1:A:65:ALA:CB	1:A:66:PRO:CD	2.95	0.43
1:C:668:VAL:O	1:C:669:PRO:C	2.52	0.43
1:B:658:LEU:HD22	1:B:688:PRO:HG2	2.01	0.43
1:D:654:TRP:NE1	1:D:666:GLY:CA	2.76	0.43
1:C:870:VAL:CG1	1:C:871:GLU:N	2.80	0.43
1:D:334:GLU:OE1	1:D:336:ARG:HD3	2.19	0.43
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.41	0.43
1:A:540:HIS:O	1:A:542:MET:N	2.52	0.43
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.65	0.43
1:D:802:ASP:O	1:D:808:GLU:HG3	2.19	0.43
1:A:297:ASN:N	1:A:298:PRO:HD3	2.34	0.43
1:B:186:VAL:HG12	1:B:188:VAL:HG23	2.00	0.43
1:B:679:LEU:HD23	1:B:679:LEU:HA	1.60	0.43
1:A:976:LEU:HA	1:A:976:LEU:HD23	1.75	0.43
1:A:69:VAL:HA	1:A:70:PRO:HD3	1.74	0.43
1:B:858:ILE:HD11	1:B:864:MET:HE3	2.00	0.43
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.63	0.43
1:B:261:TRP:CZ2	1:B:266:GLN:HG3	2.53	0.43
1:B:40:GLU:OE2	1:B:43:ARG:NE	2.52	0.43
1:A:240:LEU:HD22	1:A:260:LEU:HD22	1.99	0.43
1:B:141:ILE:O	1:B:170:GLU:HA	2.19	0.43
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.87	0.43
1:C:167:LEU:HD23	1:C:393:PRO:HB2	1.99	0.43
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.21	0.43
1:C:702:GLN:O	1:C:712:GLY:N	2.51	0.43
1:C:11:LEU:HD23	1:C:11:LEU:HA	1.63	0.43
1:C:16:TRP:HA	1:C:161:TYR:OH	2.19	0.43
1:C:253:TYR:O	1:C:318:ALA:N	2.52	0.43
1:A:282:ARG:HG3	1:A:282:ARG:NH1	2.32	0.43
1:D:460:ASN:O	1:D:461:GLU:C	2.57	0.43
1:D:350:LEU:HA	1:D:350:LEU:HD12	1.85	0.43
1:D:883:GLY:HA3	1:D:987:ASP:HA	2.01	0.43
1:A:556:PHE:CE1	1:A:564:GLY:HA2	2.53	0.43
1:C:90:TRP:CZ3	1:C:121:GLY:HA3	2.54	0.43
1:B:109:VAL:HG23	3:B:4275:HOH:O	2.18	0.43
1:A:17:GLU:OE2	1:A:114:VAL:N	2.30	0.43
1:B:631:LEU:HG	1:B:632:SER:N	2.27	0.43
1:C:821:ALA:O	1:C:823:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:MET:HE2	1:A:426:LEU:CD1	2.49	0.43
1:D:654:TRP:CD1	1:D:666:GLY:HA3	2.53	0.43
1:A:210:ARG:NH1	1:A:358:GLU:OE1	2.52	0.43
1:C:131:GLU:O	1:C:134:LEU:N	2.44	0.43
1:C:40:GLU:O	1:C:43:ARG:N	2.51	0.43
1:C:502:MET:HB2	1:C:537:GLU:HG3	2.00	0.43
1:D:965:GLN:O	1:D:966:GLN:C	2.54	0.43
1:B:416:GLU:HA	1:B:462:SER:OG	2.19	0.43
1:A:58:TRP:CE3	1:A:123:TYR:HB3	2.54	0.43
1:C:227:VAL:HG12	1:C:228:ALA:N	2.33	0.43
1:C:230:ARG:HH21	1:C:241:GLU:CD	2.21	0.43
1:A:98:PRO:HD2	1:A:592:PHE:HB3	2.01	0.43
1:A:719:GLN:HE22	1:A:915:PHE:N	2.16	0.43
1:C:91:GLN:HG2	1:C:98:PRO:CA	2.49	0.43
1:C:600:GLN:HG2	1:C:931:PHE:HB2	2.01	0.43
1:D:240:LEU:O	1:D:292:ARG:HA	2.19	0.43
1:C:685:LEU:HA	1:C:685:LEU:HD23	1.64	0.43
1:D:657:ALA:HB1	1:D:661:LYS:C	2.39	0.43
1:A:546:LEU:HD23	1:A:619:GLU:HB3	2.00	0.43
1:B:152:LEU:O	1:B:159:VAL:N	2.33	0.43
1:C:859:ASP:CG	1:C:861:SER:HG	2.20	0.43
1:A:966:GLN:HB2	1:A:979:GLU:OE2	2.18	0.43
1:A:749:ILE:CD1	1:A:749:ILE:N	2.81	0.43
1:D:424:ASN:ND2	3:D:7510:HOH:O	2.52	0.43
1:A:141:ILE:HG12	1:A:142:ILE:N	2.33	0.43
1:B:630:ARG:HB2	1:B:637:GLU:HB3	1.99	0.43
1:B:906:TYR:HB3	1:B:907:PRO:CD	2.49	0.43
1:C:303:ALA:HB2	1:C:408:TYR:CZ	2.54	0.43
1:D:234:ASP:OD1	1:D:236:SER:OG	2.36	0.43
1:D:10:VAL:O	1:D:12:GLN:N	2.51	0.43
1:D:125:LEU:HG	1:D:126:THR:N	2.34	0.43
1:D:778:THR:HB	1:D:887:GLN:HB3	2.00	0.43
1:C:617:LEU:HA	1:C:617:LEU:HD12	1.71	0.43
1:C:434:PRO:HA	1:C:437:SER:HB3	2.01	0.43
1:C:730:LEU:HD12	1:C:730:LEU:N	2.14	0.43
1:B:30:HIS:CB	1:B:31:PRO:CD	2.97	0.43
1:B:423:MET:HB2	1:C:282:ARG:CG	2.44	0.43
1:D:77:ASP:OD1	1:D:183:ARG:NH2	2.50	0.43
1:D:904:GLU:HB2	1:D:936:GLY:HA2	2.00	0.43
1:B:80:GLU:N	1:B:80:GLU:CD	2.72	0.43
1:C:897:TRP:CZ3	1:C:918:TRP:HB2	2.54	0.43
1:D:502:MET:HA	1:D:537:GLU:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:380:LYS:HE2	3:D:4077:HOH:O	2.18	0.43
1:B:635:THR:CG2	1:B:636:ILE:N	2.81	0.43
1:D:967:LEU:HA	1:D:967:LEU:HD23	1.70	0.43
1:C:433:LEU:CB	1:C:434:PRO:HD3	2.40	0.42
1:C:434:PRO:O	1:C:437:SER:HB3	2.19	0.42
1:A:367:MET:HB3	1:A:372:MET:HE2	1.96	0.42
1:B:576:ILE:HD11	1:B:584:PRO:HB3	2.00	0.42
1:B:652:LEU:CD1	1:B:698:VAL:HB	2.49	0.42
1:D:952:ARG:NH1	1:D:1021:CYS:SG	2.91	0.42
1:A:3:ILE:HG13	1:A:4:THR:N	2.32	0.42
1:D:518:TRP:HB3	1:D:522:LYS:HD3	2.00	0.42
1:C:292:ARG:CG	1:C:292:ARG:HH11	2.31	0.42
1:B:881:ARG:C	1:B:882:ILE:HG13	2.40	0.42
1:C:789:LEU:HA	1:C:933:SER:CB	2.49	0.42
1:C:339:ASN:O	1:D:527:PRO:HB3	2.19	0.42
1:D:612:THR:HB	1:D:613:PRO:HD2	2.01	0.42
1:B:335:VAL:HG22	1:B:344:LEU:HD12	2.01	0.42
1:C:548:GLY:O	1:C:551:LYS:HB2	2.19	0.42
1:A:51:LEU:HG	1:A:51:LEU:O	2.19	0.42
1:B:100:TYR:CB	1:B:203:TRP:CE3	3.02	0.42
1:B:255:ARG:HB2	1:B:316:HIS:CD2	2.54	0.42
1:B:654:TRP:CZ2	1:B:666:GLY:HA3	2.54	0.42
1:A:737:ILE:HG13	1:A:738:PRO:N	2.34	0.42
1:D:786:ARG:HH21	1:D:792:ASP:CG	2.22	0.42
1:A:422:PRO:HG2	1:D:285:TYR:CE1	2.54	0.42
1:C:782:ASP:HB2	1:C:842:TRP:CZ2	2.53	0.42
1:C:815:HIS:HD2	1:C:849:LEU:HD13	1.84	0.42
1:D:382:ASN:HA	1:D:621:LYS:HD2	2.01	0.42
1:D:442:ARG:HH11	1:D:442:ARG:HD3	1.72	0.42
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.73	0.42
1:A:252:ASP:OD1	1:A:252:ASP:N	2.52	0.42
1:B:521:LYS:HD3	1:B:559:TYR:OH	2.20	0.42
1:C:255:ARG:HA	1:C:273:PRO:HA	2.00	0.42
1:A:357:HIS:HD2	1:A:392:TYR:OH	2.02	0.42
1:D:38:ASN:ND2	1:D:40:GLU:N	2.67	0.42
1:B:354:VAL:HG22	1:B:355:ASN:N	2.34	0.42
1:B:79:PRO:N	1:B:80:GLU:OE2	2.53	0.42
1:A:914:CYS:O	1:A:918:TRP:HZ2	2.01	0.42
1:A:194:GLY:O	1:A:198:GLU:HG3	2.19	0.42
1:A:726:LEU:HD12	1:B:873:ALA:HB2	1.99	0.42
1:B:304:GLU:O	1:B:305:ILE:HG13	2.19	0.42
1:A:278:ILE:HA	1:A:278:ILE:HD13	1.60	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:147:ASN:HA	1:D:148:SER:HA	1.71	0.42
1:A:588:TYR:CD2	1:A:603:MET:HE1	2.54	0.42
1:C:958:ASN:ND2	3:C:4153:HOH:O	2.51	0.42
1:D:303:ALA:HB1	1:D:406:GLY:O	2.20	0.42
1:C:422:PRO:HG2	1:C:424:ASN:HB2	2.00	0.42
1:C:722:LEU:HD23	1:C:722:LEU:HA	1.66	0.42
1:D:315:LEU:O	1:D:323:ILE:HB	2.19	0.42
1:B:496:THR:O	1:B:531:ARG:NH1	2.49	0.42
1:C:655:MET:HG3	1:C:655:MET:O	2.06	0.42
1:A:140:ARG:CG	1:A:141:ILE:N	2.79	0.42
1:D:852:SER:CB	1:D:870:VAL:HG22	2.49	0.42
1:B:24:LEU:HB2	1:B:161:TYR:HB3	1.99	0.42
1:D:308:LEU:HD23	1:D:330:VAL:O	2.19	0.42
1:D:377:LEU:HD22	1:D:708:TRP:CA	2.40	0.42
1:B:721:ARG:HB3	1:B:721:ARG:NH1	2.34	0.42
1:D:52[B]:ARG:CG	1:D:133:TRP:CH2	2.98	0.42
1:A:907:PRO:HA	1:A:910:LEU:HD23	2.02	0.42
1:C:881:ARG:HD3	1:C:987:ASP:CG	2.39	0.42
1:C:228:ALA:C	1:C:229:THR:HG23	2.40	0.42
1:D:906:TYR:CB	1:D:907:PRO:HD2	2.50	0.42
1:D:778:THR:HA	1:D:779:PRO:HD2	1.86	0.42
1:B:347:LYS:HE3	1:B:643:LEU:O	2.20	0.42
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.79	0.42
1:A:746:ASP:N	1:A:760:ARG:HG3	2.33	0.42
1:A:302:SER:HB2	1:A:304:GLU:H	1.83	0.42
1:A:680:ILE:O	1:A:680:ILE:HG22	2.15	0.42
1:C:663:LEU:HD23	1:C:663:LEU:N	2.31	0.42
1:C:114:VAL:HA	1:C:115:PRO:HD3	1.66	0.42
1:B:652:LEU:HG	1:B:652:LEU:O	2.19	0.42
1:C:961:ARG:HD2	1:C:981:GLY:O	2.20	0.42
1:B:822:LEU:HD21	1:B:825:CYS:HB2	2.01	0.42
1:C:870:VAL:HG12	1:C:871:GLU:H	1.84	0.42
1:A:652:LEU:HD12	1:A:652:LEU:HA	1.49	0.42
1:A:217:LYS:HB3	1:A:218:PRO:CD	2.47	0.42
1:D:814:GLY:O	1:D:815:HIS:C	2.58	0.42
1:B:941:THR:CG2	1:B:955:PHE:CE1	3.02	0.42
1:C:786:ARG:O	1:C:788:PRO:N	2.53	0.42
1:C:782:ASP:OD1	1:C:854:LYS:NZ	2.50	0.42
1:A:110:ASN:N	1:A:111:PRO:HD3	2.34	0.42
1:C:424:ASN:HD22	1:C:424:ASN:HA	1.29	0.42
1:B:317:THR:HG23	1:B:321:THR:O	2.19	0.42
1:A:338:GLU:O	1:A:339:ASN:HB3	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:652:LEU:HD12	1:D:700:VAL:CG2	2.50	0.42
1:A:942:ARG:HA	1:A:953:GLY:O	2.19	0.42
1:C:986:ILE:HD13	1:C:986:ILE:HG21	1.59	0.42
1:D:745:MET:HG2	1:D:745:MET:H	1.28	0.42
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.55	0.42
1:D:377:LEU:HD23	1:D:708:TRP:CB	2.50	0.42
1:A:658:LEU:CD2	1:A:688:PRO:HG2	2.39	0.42
1:B:3:ILE:O	1:B:6:SER:OG	2.29	0.42
1:A:825:CYS:HA	1:A:837:THR:O	2.20	0.42
1:B:736:ALA:O	1:B:737:ILE:HG22	2.20	0.42
1:B:737:ILE:CG1	1:B:738:PRO:N	2.80	0.42
1:D:979:GLU:O	1:D:980:GLU:C	2.57	0.42
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.34	0.42
1:D:197:LEU:HD12	1:D:439:ARG:NE	2.35	0.42
1:A:718:GLN:HG2	1:A:720:TRP:CZ2	2.55	0.42
1:C:63:PHE:CG	1:C:69:VAL:HG22	2.55	0.42
1:B:1022:GLN:OE1	1:B:1022:GLN:N	2.51	0.42
1:D:927:THR:HG21	1:D:929:TYR:CZ	2.55	0.42
1:A:343:LEU:HD22	1:A:346:GLY:O	2.19	0.42
1:B:994:GLY:HA3	1:B:1003:VAL:HG23	2.01	0.42
1:C:334:GLU:HG3	3:C:4209:HOH:O	2.19	0.42
1:D:208:ILE:HG22	1:D:208:ILE:O	2.20	0.42
1:C:415:ILE:HG21	1:C:415:ILE:HD13	1.74	0.42
1:D:864:MET:O	1:D:864:MET:HG3	2.19	0.42
1:D:955:PHE:CD1	1:D:986:ILE:CG2	3.02	0.42
1:D:77:ASP:OD1	1:D:183:ARG:NE	2.50	0.42
1:B:395:HIS:ND1	1:B:396:PRO:CD	2.79	0.42
1:A:166:ARG:HG3	1:A:392:TYR:CG	2.54	0.42
1:C:342:LEU:O	1:C:348:PRO:HA	2.19	0.42
1:D:356:ARG:HD2	1:D:379:MET:HE3	2.01	0.42
1:C:881:ARG:O	1:C:882:ILE:HG13	2.18	0.42
1:B:955:PHE:CD1	1:B:955:PHE:C	2.93	0.42
1:D:643:LEU:CD2	1:D:675:GLN:NE2	2.82	0.42
1:D:27:LEU:HD12	1:D:140:ARG:HD3	2.00	0.42
1:D:942:ARG:HA	1:D:953:GLY:O	2.20	0.42
1:C:149:ALA:HA	1:C:162:GLY:O	2.19	0.42
1:A:349:LEU:HA	1:A:349:LEU:HD23	1.91	0.42
1:A:637:GLU:CA	1:A:679:LEU:HD21	2.48	0.42
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.82	0.42
1:D:282:ARG:HG3	1:D:282:ARG:NH1	2.24	0.42
1:C:279:ILE:HD13	1:C:279:ILE:HG21	1.61	0.42
1:B:316:HIS:HB3	1:B:322:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:749:ILE:CG2	1:B:750:GLU:N	2.82	0.42
1:B:382:ASN:O	1:B:621:LYS:HA	2.19	0.42
1:B:166:ARG:HA	1:B:166:ARG:HD2	1.73	0.42
1:B:866:ILE:O	1:B:1017:GLN:HB2	2.19	0.42
1:C:382:ASN:HA	1:C:621:LYS:HD2	2.01	0.42
1:B:906:TYR:CE2	1:B:937:LEU:HD22	2.54	0.42
1:C:925:MET:HE2	1:C:925:MET:HB3	1.77	0.42
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.55	0.42
1:C:63:PHE:HA	1:C:64:PRO:HD3	1.38	0.42
1:A:869:ASP:CG	1:A:1015:HIS:HD1	2.23	0.42
1:C:118:ASN:HA	1:C:119:PRO:HD2	1.41	0.42
1:C:138:GLN:HA	1:C:174:SER:OG	2.19	0.42
1:C:721:ARG:CB	1:C:721:ARG:CZ	2.97	0.42
1:D:955:PHE:CD1	1:D:986:ILE:HG23	2.54	0.42
1:B:400:THR:O	1:B:403:ASP:HB2	2.20	0.42
1:D:300:LEU:HD22	1:D:332:PHE:O	2.20	0.42
1:A:240:LEU:HD22	1:A:260:LEU:CD2	2.49	0.42
1:B:658:LEU:HB3	1:B:661:LYS:HD2	2.02	0.42
1:D:734:SER:CB	1:D:860:GLY:HA3	2.46	0.42
1:B:393:PRO:HD2	1:B:414:ASN:HB2	2.02	0.42
1:C:11:LEU:HD21	1:C:187:MET:HE3	2.02	0.42
1:A:906:TYR:HB3	1:A:907:PRO:HD2	2.02	0.42
1:D:309:TYR:HD1	1:D:309:TYR:N	2.17	0.42
1:D:9:VAL:O	1:D:10:VAL:C	2.57	0.42
1:C:315:LEU:O	1:C:323:ILE:HB	2.20	0.42
1:B:524:LEU:HD22	1:B:561:ARG:CZ	2.50	0.42
1:B:900:LEU:HA	1:B:914:CYS:O	2.19	0.42
1:B:380:LYS:HE2	3:B:4077:HOH:O	2.19	0.42
1:A:856:TYR:CD2	1:A:864:MET:CE	3.01	0.41
1:B:550:ALA:O	1:B:551:LYS:C	2.59	0.41
1:D:822:LEU:HD11	1:D:824:GLN:O	2.20	0.41
1:B:768:MET:CE	1:B:770:ILE:CD1	2.97	0.41
1:C:526:LEU:HA	1:C:526:LEU:HD12	1.84	0.41
1:C:741:THR:HG22	1:C:742:THR:O	2.20	0.41
1:B:885:ASN:HB2	1:B:984:LEU:O	2.21	0.41
1:D:33:PHE:CD1	1:D:217:LYS:HE3	2.55	0.41
1:A:780:LEU:HD12	1:A:886:CYS:HB3	2.02	0.41
1:D:260:LEU:O	1:D:267:VAL:N	2.44	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.41	0.41
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.79	0.41
1:A:43:ARG:NH1	1:A:43:ARG:HG2	2.35	0.41
1:D:427:THR:HG22	1:D:436:MET:SD	2.61	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:851:ILE:O	1:A:870:VAL:HA	2.20	0.41
1:B:111:PRO:HA	1:B:112:PRO:HA	1.76	0.41
1:A:427:THR:CA	1:A:436:MET:HE1	2.47	0.41
1:B:173:LEU:O	1:B:175:ALA:N	2.53	0.41
1:B:419:GLY:C	1:C:282:ARG:NH1	2.74	0.41
1:A:167:LEU:HG	1:A:393:PRO:HG2	2.01	0.41
1:A:734:SER:CB	1:A:860:GLY:CA	2.97	0.41
1:B:455:ILE:HG22	1:B:456:TRP:N	2.35	0.41
1:C:536:CYS:O	1:C:566:PHE:HB2	2.19	0.41
1:A:651:LEU:HA	1:A:651:LEU:HD12	1.92	0.41
1:D:608:PHE:CD1	1:D:614:HIS:CD2	3.08	0.41
1:B:787:ALA:HA	1:B:788:PRO:HD3	1.72	0.41
1:C:322:LEU:HD23	1:C:322:LEU:HA	1.84	0.41
1:D:652:LEU:HD12	1:D:700:VAL:HG22	2.01	0.41
1:D:759:ASN:HB2	1:D:766:SER:OG	2.19	0.41
1:A:829:THR:C	1:A:830:LEU:HD13	2.40	0.41
1:B:42:ALA:O	1:B:310:ARG:NH1	2.53	0.41
1:D:177:LEU:HA	1:D:177:LEU:HD23	1.82	0.41
1:D:834:VAL:HG12	1:D:835:LEU:N	2.34	0.41
1:C:569:ASP:HB2	3:C:5099:HOH:O	2.21	0.41
1:B:63:PHE:HE1	1:B:122:CYS:HG	1.68	0.41
1:B:458:LEU:HD23	1:B:458:LEU:HA	1.65	0.41
1:C:207:GLY:O	1:C:209:PHE:N	2.54	0.41
1:C:766:SER:O	1:C:767:GLN:HB2	2.20	0.41
1:D:62:TRP:CZ2	1:D:119:PRO:HB3	2.56	0.41
1:B:392:TYR:HD1	1:B:393:PRO:O	2.03	0.41
1:C:292:ARG:CG	1:C:292:ARG:NH1	2.82	0.41
1:B:935:ASN:N	1:B:935:ASN:ND2	2.68	0.41
1:B:344:LEU:HG	1:B:345:ASN:N	2.34	0.41
1:B:513:PRO:O	1:B:514:ALA:HB3	2.20	0.41
1:D:252:ASP:OD1	1:D:252:ASP:N	2.51	0.41
1:B:670:LEU:HD11	1:B:700:VAL:CG2	2.51	0.41
1:B:368:ASP:O	1:B:372:MET:HG3	2.19	0.41
1:A:361:PRO:CD	1:A:362:LEU:H	2.33	0.41
1:A:316:HIS:HB3	1:A:322:LEU:HD23	2.01	0.41
1:D:654:TRP:HE1	1:D:666:GLY:HA3	1.84	0.41
1:A:358:GLU:HB3	1:A:367:MET:SD	2.61	0.41
1:D:7:LEU:HA	1:D:7:LEU:HD23	1.85	0.41
1:C:217:LYS:CG	1:C:218:PRO:CD	2.99	0.41
1:C:592:PHE:C	1:C:594:ASP:H	2.22	0.41
1:C:791:ASN:HB3	3:C:4270:HOH:O	2.20	0.41
1:D:232:ASN:O	1:D:233:ASP:C	2.57	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:640:SER:OG	1:B:642:TYR:HB2	2.20	0.41
1:D:262:GLN:O	1:D:262:GLN:HG2	2.19	0.41
1:B:875:ASP:N	1:B:875:ASP:OD2	2.53	0.41
1:D:751:LEU:C	1:D:751:LEU:HD23	2.40	0.41
1:A:351:ILE:N	1:A:351:ILE:HD13	2.35	0.41
1:B:356:ARG:HH22	1:B:367:MET:CE	2.33	0.41
1:C:928:PRO:O	1:C:929:TYR:C	2.58	0.41
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.77	0.41
1:B:579:ASP:OD2	1:B:583:ASN:HB2	2.21	0.41
1:B:568:TRP:C	1:B:568:TRP:CD1	2.93	0.41
1:D:62:TRP:CD1	1:D:95:TYR:CB	3.02	0.41
1:B:837:THR:CG2	1:B:838:THR:N	2.78	0.41
1:A:138:GLN:CG	1:A:139:THR:N	2.78	0.41
1:B:257:THR:O	1:B:313:VAL:HA	2.20	0.41
1:D:896:ASN:HA	1:D:918:TRP:O	2.21	0.41
1:A:526:LEU:O	1:A:527:PRO:C	2.56	0.41
1:C:46:ARG:HA	1:C:47:PRO:HD3	1.80	0.41
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.80	0.41
1:B:436:MET:HE1	1:B:467:ASN:HD22	1.86	0.41
1:D:858:ILE:HD11	1:D:864:MET:HE3	2.02	0.41
1:D:603:MET:HE1	1:D:930:VAL:HG12	2.03	0.41
1:A:38:ASN:ND2	1:A:40:GLU:N	2.68	0.41
1:B:598:ASP:O	1:B:599:ARG:C	2.57	0.41
1:B:658:LEU:CG	1:B:661:LYS:NZ	2.78	0.41
1:A:599:ARG:HB2	1:A:600:GLN:H	1.30	0.41
1:B:740:LEU:HA	1:B:748:CYS:O	2.20	0.41
1:A:734:SER:CB	1:A:860:GLY:HA3	2.45	0.41
1:B:549:PHE:O	1:B:553:TRP:HD1	2.04	0.41
1:D:763:GLY:CA	1:D:822:LEU:CD2	2.98	0.41
1:D:925:MET:CE	1:D:938:ARG:CZ	2.99	0.41
1:A:653[B]:HIS:CD2	1:A:666:GLY:O	2.74	0.41
1:B:897:TRP:HB2	1:B:943:GLU:O	2.21	0.41
1:D:956:GLN:HB2	1:D:987:ASP:HB2	2.02	0.41
1:A:896:ASN:HA	1:A:918:TRP:O	2.21	0.41
1:B:608:PHE:O	1:B:611:ARG:N	2.45	0.41
1:C:963:SER:HG	1:C:979:GLU:CD	2.24	0.41
1:C:46:ARG:CB	1:C:47:PRO:CD	2.98	0.41
1:C:152:LEU:N	1:C:160:GLY:O	2.54	0.41
1:D:706:THR:HG23	1:D:709:SER:OG	2.20	0.41
1:A:768:MET:HG2	1:A:775:GLN:HG3	2.03	0.41
1:D:765:LEU:O	1:D:765:LEU:HG	2.19	0.41
1:B:486:TYR:CZ	1:B:488:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:737:ILE:HD12	1:A:832:ASP:HA	2.03	0.41
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.85	0.41
1:B:682:LEU:HD23	1:B:682:LEU:HA	1.60	0.41
1:A:524:LEU:HD22	1:A:561:ARG:CB	2.50	0.41
1:D:27:LEU:HD12	1:D:140:ARG:NH1	2.35	0.41
1:D:730:LEU:HA	1:D:731:PRO:HD3	1.95	0.41
1:B:590:GLY:HA2	1:B:594:ASP:OD1	2.20	0.41
1:C:638:VAL:O	1:C:677:LYS:HA	2.21	0.41
1:B:1009:LEU:HD23	1:B:1009:LEU:N	2.34	0.41
1:A:775:GLN:O	1:A:889:ALA:N	2.53	0.41
1:A:930:VAL:CA	1:A:973:ARG:HD3	2.37	0.41
1:D:202:MET:HE3	1:D:357:HIS:CD2	2.56	0.41
1:B:375:ASP:O	1:B:376:ILE:C	2.57	0.41
1:D:300:LEU:HD23	1:D:332:PHE:HB3	2.02	0.41
1:B:17:GLU:O	1:B:112:PRO:HG2	2.21	0.41
1:D:105:TYR:HA	1:D:106:PRO:HD2	1.76	0.41
1:B:589:GLY:CA	1:B:599:ARG:HA	2.39	0.41
1:C:376:ILE:HD13	1:C:401:LEU:HB3	2.03	0.41
1:C:342:LEU:HA	1:C:342:LEU:HD12	1.67	0.41
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.49	0.41
1:B:103:VAL:HG22	1:B:418:HIS:CE1	2.56	0.41
1:C:726:LEU:CD1	1:D:848:THR:HG22	2.50	0.41
1:B:615:PRO:HG2	1:B:904:GLU:OE1	2.20	0.41
1:C:63:PHE:HB3	1:C:64:PRO:HD2	2.02	0.41
1:C:824:GLN:HG3	1:C:825:CYS:N	2.34	0.41
1:B:44:THR:O	1:B:45:ASP:HB3	2.21	0.41
1:A:434:PRO:HB3	1:D:434:PRO:HB3	2.03	0.41
1:B:142:ILE:HG21	1:B:142:ILE:HD13	1.87	0.41
1:A:13:ARG:NH1	1:D:13:ARG:NH1	2.69	0.41
1:C:342:LEU:HB3	1:C:563:GLN:HE22	1.86	0.41
1:C:190:ARG:HD3	1:C:191:TRP:CZ2	2.55	0.41
1:C:737:ILE:HB	1:C:738:PRO:HD2	2.02	0.41
1:A:153:TRP:CD1	1:A:158:TRP:HA	2.56	0.41
1:B:549:PHE:HE1	1:B:567:VAL:CG2	2.34	0.41
1:B:620:ALA:O	1:B:621:LYS:C	2.58	0.41
1:A:737:ILE:HD12	1:A:832:ASP:CA	2.51	0.41
1:D:56:GLY:O	1:D:85:VAL:HA	2.20	0.41
1:C:120:THR:CG2	1:C:187:MET:SD	3.09	0.41
1:C:35:SER:CB	1:C:37:ARG:NH1	2.84	0.41
1:D:904:GLU:CG	1:D:909:ARG:HH22	2.31	0.41
1:A:651:LEU:HD12	1:A:669:PRO:HA	2.03	0.41
1:C:3:ILE:C	1:C:5:ASP:H	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:768:MET:HG3	1:B:768:MET:O	2.18	0.41
1:A:946:TYR:OH	1:A:982:THR:OG1	2.30	0.41
1:D:870:VAL:CG1	1:D:871:GLU:N	2.84	0.41
1:C:226:HIS:CD2	1:C:448:ARG:HD2	2.56	0.41
1:C:176:PHE:HE1	3:C:4172:HOH:O	2.04	0.41
1:A:728:VAL:HG13	1:B:851:ILE:HD11	2.02	0.41
1:D:200:GLN:HG2	1:D:391:HIS:HB2	2.03	0.41
1:A:243:GLU:OE1	1:A:288:ARG:HD3	2.20	0.41
1:B:292:ARG:NH1	1:B:292:ARG:CG	2.84	0.41
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.51	0.41
1:C:194:GLY:O	1:C:197:LEU:HB2	2.21	0.41
1:C:567:VAL:H	1:C:567:VAL:HG23	1.67	0.41
1:C:482:ARG:HH11	1:C:482:ARG:HD2	1.60	0.41
1:C:952:ARG:CZ	1:C:952:ARG:CB	2.99	0.41
1:D:505:ARG:HH11	1:D:505:ARG:HD3	1.56	0.41
1:A:260:LEU:HD11	1:A:309:TYR:HB3	2.01	0.41
1:D:360:HIS:ND1	1:D:362:LEU:N	2.62	0.41
1:D:668:VAL:CG1	1:D:669:PRO:N	2.84	0.41
1:B:455:ILE:HD13	1:B:455:ILE:HG21	1.90	0.41
1:A:141:ILE:O	1:A:170:GLU:HA	2.21	0.41
1:B:417:THR:O	1:B:418:HIS:C	2.59	0.41
1:C:796:SER:HB2	1:C:802:ASP:HB3	2.03	0.41
1:A:782:ASP:OD2	1:A:852:SER:OG	2.29	0.41
1:D:209:PHE:N	1:D:209:PHE:CD2	2.80	0.41
1:A:769:TRP:HB3	1:A:771:GLY:O	2.21	0.40
1:A:7:LEU:HD13	1:A:69:VAL:CG1	2.51	0.40
1:D:679:LEU:HA	1:D:679:LEU:HD23	1.07	0.40
1:D:298:PRO:N	3:D:4211:HOH:O	2.54	0.40
1:B:421:VAL:HA	1:B:422:PRO:HA	1.85	0.40
1:C:195:SER:O	1:C:196:TYR:C	2.58	0.40
1:B:90:TRP:CD1	1:B:90:TRP:C	2.94	0.40
1:B:888:LEU:O	1:B:981:GLY:HA3	2.20	0.40
1:B:221:GLN:HB3	1:B:221:GLN:HE21	1.26	0.40
1:B:406:GLY:O	1:B:407:LEU:HD23	2.21	0.40
1:D:932:PRO:HG2	1:D:970:THR:O	2.21	0.40
1:A:390:SER:HA	1:A:391:HIS:HA	1.79	0.40
1:D:184:LEU:HA	1:D:184:LEU:HD23	1.74	0.40
1:B:476:LYS:HE3	1:B:476:LYS:HB3	1.82	0.40
1:A:775:GLN:CD	1:A:890:GLN:HE22	2.24	0.40
1:A:131:GLU:O	1:A:134:LEU:HD23	2.21	0.40
1:A:658:LEU:HD11	1:A:692:GLY:C	2.42	0.40
1:A:210:ARG:HD3	1:A:210:ARG:HH11	1.71	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:422:PRO:HB2	1:C:280:ASP:OD1	2.21	0.40
1:D:6:SER:HB2	1:D:71:GLU:OE2	2.21	0.40
1:C:373:VAL:HG12	1:C:373:VAL:O	2.20	0.40
1:A:763:GLY:CA	1:A:822:LEU:HD21	2.49	0.40
1:A:925:MET:HE1	1:A:938:ARG:CZ	2.52	0.40
1:C:510:GLN:HB3	1:C:512:PHE:CZ	2.57	0.40
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.57	0.40
1:C:815:HIS:CD2	1:C:849:LEU:HD13	2.56	0.40
1:B:607:VAL:HG12	1:B:613:PRO:HA	2.02	0.40
1:A:378:LEU:HA	1:A:378:LEU:HD23	1.61	0.40
1:A:1019:VAL:O	1:A:1019:VAL:HG12	2.20	0.40
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.65	0.40
1:B:433:LEU:O	1:B:437:SER:HB3	2.22	0.40
1:A:767:GLN:CD	1:A:774:LYS:HG2	2.42	0.40
1:D:559:TYR:HA	1:D:560:PRO:HD2	1.89	0.40
1:D:202:MET:CE	1:D:357:HIS:CD2	3.04	0.40
1:B:595:THR:CG2	1:B:596:PRO:CA	2.98	0.40
1:B:118:ASN:O	1:B:120:THR:OG1	2.39	0.40
1:C:100:TYR:HB2	1:C:203:TRP:CZ3	2.56	0.40
1:A:152:LEU:CG	1:A:153:TRP:N	2.81	0.40
1:A:30:HIS:CE1	1:A:33:PHE:CD1	3.10	0.40
1:C:502:MET:HB3	1:C:537:GLU:HG3	2.02	0.40
1:C:987:ASP:OD2	1:C:990:HIS:HD2	2.05	0.40
1:D:956:GLN:N	1:D:956:GLN:CD	2.74	0.40
1:A:898:LEU:HB2	1:A:917:ARG:NH2	2.36	0.40
1:B:881:ARG:HD3	1:B:987:ASP:OD2	2.22	0.40
1:D:476:LYS:H	1:D:476:LYS:HG2	1.60	0.40
1:C:490:GLY:N	3:C:4010:HOH:O	2.32	0.40
1:B:559:TYR:CB	1:B:562:LEU:HD12	2.35	0.40
1:D:352:ARG:O	1:D:385:ASN:HB2	2.22	0.40
1:D:106:PRO:HB2	1:D:191:TRP:CH2	2.56	0.40
1:B:599:ARG:HB2	1:B:600:GLN:H	1.20	0.40
1:C:835:LEU:HG	1:C:835:LEU:O	2.21	0.40
1:C:30:HIS:HE1	3:C:4191:HOH:O	2.04	0.40
1:A:559:TYR:HB2	1:A:562:LEU:CD1	2.52	0.40
1:C:118:ASN:HD21	1:C:189:LEU:CD2	2.34	0.40
1:B:900:LEU:HD13	1:B:913:ALA:HB3	2.02	0.40
1:B:369:GLU:O	1:B:370:GLN:C	2.60	0.40
1:A:57:GLU:HG2	1:A:83:THR:CG2	2.52	0.40
1:D:632:SER:O	1:D:634:GLN:N	2.55	0.40
1:A:788:PRO:O	1:A:933:SER:HB2	2.21	0.40
1:A:127:PHE:N	1:A:127:PHE:CD2	2.90	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:500:CYS:N	1:D:501:PRO:CD	2.85	0.40
1:D:559:TYR:CD1	1:D:559:TYR:N	2.90	0.40
1:B:376:ILE:CD1	1:B:401:LEU:HB3	2.51	0.40
1:B:251:ARG:O	1:B:254:LEU:HD12	2.22	0.40
1:C:834:VAL:HG12	1:C:835:LEU:N	2.37	0.40
1:C:961:ARG:HG3	1:C:961:ARG:HH11	1.85	0.40
1:D:651:LEU:HD13	1:D:651:LEU:HA	1.60	0.40
1:B:41:GLU:HG3	1:B:46:ARG:NH1	2.37	0.40
1:B:90:TRP:NE1	1:B:96:ASP:OD1	2.55	0.40
1:C:784:PHE:HA	1:C:881:ARG:O	2.22	0.40
1:A:995:GLY:HA3	3:A:4067:HOH:O	2.22	0.40
1:A:576:ILE:CG2	1:A:577:LYS:N	2.84	0.40
1:A:852:SER:OG	1:A:854:LYS:HE3	2.21	0.40
1:B:240:LEU:HG	1:B:241:GLU:N	2.36	0.40
1:A:623:GLN:NE2	1:A:911:THR:OG1	2.54	0.40
1:D:882:ILE:HB	1:D:989:PHE:HB2	2.04	0.40
1:A:572:ASP:C	1:A:574:SER:H	2.25	0.40
1:C:458:LEU:HD11	1:C:472:TYR:HB2	2.04	0.40
1:B:67:GLU:HG2	1:B:67:GLU:H	1.28	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1026/1021 (100%)	923 (90%)	86 (8%)	17 (2%)	14	42
1	B	1026/1021 (100%)	917 (89%)	89 (9%)	20 (2%)	12	37
1	C	1026/1021 (100%)	918 (90%)	82 (8%)	26 (2%)	9	28
1	D	1026/1021 (100%)	921 (90%)	85 (8%)	20 (2%)	12	37
All	All	4104/4084 (100%)	3679 (90%)	342 (8%)	83 (2%)	11	35

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	SER
1	A	733	ALA
1	A	734	SER
1	A	1005	ALA
1	B	79	PRO
1	B	164	ASP
1	B	174	SER
1	B	734	SER
1	B	930	VAL
1	C	252	ASP
1	C	425	ARG
1	C	493	THR
1	D	10	VAL
1	D	667	GLU
1	D	686	PRO
1	D	687	GLN
1	D	732	ALA
1	A	119	PRO
1	A	461	GLU
1	A	493	THR
1	B	601	PHE
1	B	659	ASP
1	B	733	ALA
1	B	831	ALA
1	C	46	ARG
1	C	79	PRO
1	C	690	SER
1	C	731	PRO
1	C	733	ALA
1	C	743	SER
1	C	746	ASP
1	D	11	LEU
1	D	461	GLU
1	D	815	HIS
1	A	252	ASP
1	A	541	ALA
1	A	601	PHE
1	B	77	ASP
1	B	95	TYR
1	B	425	ARG
1	C	47	PRO
1	C	119	PRO
1	C	601	PHE

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Mol	Chain	Res	Type
1	C	734	SER
1	C	742	THR
1	C	996	ASP
1	D	174	SER
1	D	273	PRO
1	D	546	LEU
1	A	10	VAL
1	A	79	PRO
1	A	540	HIS
1	A	890	GLN
1	B	398	TRP
1	B	546	LEU
1	B	690	SER
1	C	12	GLN
1	C	81	ALA
1	C	461	GLU
1	D	493	THR
1	D	909	ARG
1	A	599	ARG
1	B	383	ASN
1	B	891	VAL
1	C	208	ILE
1	C	211	ASP
1	C	233	ASP
1	D	14	ARG
1	D	72	SER
1	D	109	VAL
1	D	647	SER
1	A	174	SER
1	A	580	GLU
1	C	77	ASP
1	C	788	PRO
1	C	916	ASP
1	D	669	PRO
1	D	948	PRO
1	B	688	PRO
1	C	376	ILE
1	D	488	GLY
1	B	434	PRO
1	B	119	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	880/873 (101%)	700 (80%)	180 (20%)	2	5
1	B	880/873 (101%)	690 (78%)	190 (22%)	1	4
1	C	880/873 (101%)	703 (80%)	177 (20%)	2	5
1	D	880/873 (101%)	709 (81%)	171 (19%)	2	6
All	All	3520/3492 (101%)	2802 (80%)	718 (20%)	2	5

All (718) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	12	GLN
1	A	14	ARG
1	A	24	LEU
1	A	37	ARG
1	A	38	ASN
1	A	39	SER
1	A	51	LEU
1	A	57	GLU
1	A	67	GLU
1	A	71	GLU
1	A	72	SER
1	A	76	CYS
1	A	80	GLU
1	A	82	ASP
1	A	84	VAL
1	A	92	MET
1	A	96	ASP
1	A	102	ASN
1	A	117	GLU
1	A	124	SER
1	A	134	LEU
1	A	135	GLN
1	A	136	GLU
1	A	138	GLN
1	A	140	ARG

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Mol	Chain	Res	Type
1	A	148	SER
1	A	152	LEU
1	A	165	SER
1	A	166	ARG
1	A	169	SER
1	A	177	LEU
1	A	178	ARG
1	A	181	GLU
1	A	187	MET
1	A	189	LEU
1	A	190	ARG
1	A	206	SER
1	A	210	ARG
1	A	211	ASP
1	A	217	LYS
1	A	219	THR
1	A	230	ARG
1	A	237	ARG
1	A	245	GLN
1	A	246	MET
1	A	247	CYS
1	A	249	GLU
1	A	250	LEU
1	A	251	ARG
1	A	259	SER
1	A	260	LEU
1	A	277	GLU
1	A	278	ILE
1	A	279	ILE
1	A	280	ASP
1	A	288	ARG
1	A	302	SER
1	A	322	LEU
1	A	333	ARG
1	A	344	LEU
1	A	347	LYS
1	A	362	LEU
1	A	367	MET
1	A	380	LYS
1	A	385	ASN
1	A	424	ASN
1	A	425	ARG

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Mol	Chain	Res	Type
1	A	433	LEU
1	A	437	SER
1	A	448	ARG
1	A	452	SER
1	A	461	GLU
1	A	473	ARG
1	A	477	SER
1	A	481	SER
1	A	493	THR
1	A	502	MET
1	A	519	SER
1	A	520	ILE
1	A	521	LYS
1	A	525	SER
1	A	526	LEU
1	A	533	LEU
1	A	535	LEU
1	A	538	TYR
1	A	540	HIS
1	A	545	SER
1	A	546	LEU
1	A	551	LYS
1	A	554	GLN
1	A	558	GLN
1	A	571	VAL
1	A	581	ASN
1	A	599	ARG
1	A	600	GLN
1	A	607	VAL
1	A	611	ARG
1	A	630	ARG
1	A	632	SER
1	A	637	GLU
1	A	645	ARG
1	A	647	SER
1	A	653[A]	HIS
1	A	653[B]	HIS
1	A	655	MET
1	A	667	GLU
1	A	668	VAL
1	A	671	ASP
1	A	672	VAL

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Mol	Chain	Res	Type
1	A	677	LYS
1	A	679	LEU
1	A	681	GLU
1	A	682	LEU
1	A	685	LEU
1	A	694	LEU
1	A	696	LEU
1	A	704	ASN
1	A	721	ARG
1	A	728	VAL
1	A	729	THR
1	A	730	LEU
1	A	737	ILE
1	A	744	GLU
1	A	750	GLU
1	A	751	LEU
1	A	753	ASN
1	A	761	GLN
1	A	768	MET
1	A	772	ASP
1	A	773	LYS
1	A	774	LYS
1	A	777	LEU
1	A	778	THR
1	A	781	ARG
1	A	790	ASP
1	A	796	SER
1	A	797	GLU
1	A	799	THR
1	A	801	ILE
1	A	811	LYS
1	A	822	LEU
1	A	823	LEU
1	A	824	GLN
1	A	830	LEU
1	A	835	LEU
1	A	843	GLN
1	A	845	GLN
1	A	847	LYS
1	A	853	ARG
1	A	856	TYR
1	A	857	ARG

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Mol	Chain	Res	Type
1	A	858	ILE
1	A	859	ASP
1	A	861	SER
1	A	863	GLN
1	A	864	MET
1	A	867	THR
1	A	874	SER
1	A	876	THR
1	A	881	ARG
1	A	885	ASN
1	A	888	LEU
1	A	894	ARG
1	A	900	LEU
1	A	916	ASP
1	A	923	SER
1	A	925	MET
1	A	931	PHE
1	A	938	ARG
1	A	950	GLN
1	A	956	GLN
1	A	965	GLN
1	A	966	GLN
1	A	969	GLU
1	A	1004	SER
1	A	1006	GLU
1	A	1017	GLN
1	A	1018	LEU
1	A	1023	LYS
1	B	4	THR
1	B	7	LEU
1	B	9	VAL
1	B	11	LEU
1	B	14	ARG
1	B	24	LEU
1	B	25	ASN
1	B	37	ARG
1	B	38	ASN
1	B	39	SER
1	B	43	ARG
1	B	48	SER
1	B	49	GLN
1	B	53	SER

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Mol	Chain	Res	Type
1	B	67	GLU
1	B	71	GLU
1	B	75	GLU
1	B	76	CYS
1	B	80	GLU
1	B	82	ASP
1	B	83	THR
1	B	90	TRP
1	B	101	THR
1	B	102	ASN
1	B	108	THR
1	B	115	PRO
1	B	116	THR
1	B	117	GLU
1	B	118	ASN
1	B	123	TYR
1	B	124	SER
1	B	125	LEU
1	B	128	ASN
1	B	132	SER
1	B	134	LEU
1	B	135	GLN
1	B	138	GLN
1	B	141	ILE
1	B	143	PHE
1	B	159	VAL
1	B	181	GLU
1	B	187	MET
1	B	189	LEU
1	B	190	ARG
1	B	198	GLU
1	B	202	MET
1	B	210	ARG
1	B	211	ASP
1	B	213	SER
1	B	214	LEU
1	B	217	LYS
1	B	219	THR
1	B	220	THR
1	B	221	GLN
1	B	223	SER
1	B	226	HIS

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Mol	Chain	Res	Type
1	B	230	ARG
1	B	233	ASP
1	B	237	ARG
1	B	240	LEU
1	B	244	VAL
1	B	246	MET
1	B	247	CYS
1	B	249	GLU
1	B	250	LEU
1	B	252	ASP
1	B	255	ARG
1	B	266	GLN
1	B	280	ASP
1	B	292	ARG
1	B	310	ARG
1	B	314	GLU
1	B	322	LEU
1	B	324	GLU
1	B	330	VAL
1	B	333	ARG
1	B	338	GLU
1	B	357	HIS
1	B	362	LEU
1	B	394	ASN
1	B	424	ASN
1	B	425	ARG
1	B	445	GLN
1	B	448	ARG
1	B	460	ASN
1	B	472	TYR
1	B	473	ARG
1	B	476	LYS
1	B	507	ASP
1	B	508	GLU
1	B	509	ASP
1	B	519	SER
1	B	525	SER
1	B	526	LEU
1	B	529	GLU
1	B	531	ARG
1	B	532	PRO
1	B	533	LEU

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Mol	Chain	Res	Type
1	B	542	MET
1	B	545	SER
1	B	546	LEU
1	B	554	GLN
1	B	563	GLN
1	B	576	ILE
1	B	580	GLU
1	B	581	ASN
1	B	588	TYR
1	B	598	ASP
1	B	599	ARG
1	B	600	GLN
1	B	630	ARG
1	B	631	LEU
1	B	645	ARG
1	B	651	LEU
1	B	652	LEU
1	B	655	MET
1	B	658	LEU
1	B	661	LYS
1	B	663	LEU
1	B	672	VAL
1	B	681	GLU
1	B	687	GLN
1	B	690	SER
1	B	719	GLN
1	B	728	VAL
1	B	729	THR
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	745	MET
1	B	750	GLU
1	B	751	LEU
1	B	755	ARG
1	B	761	GLN
1	B	765	LEU
1	B	766	SER
1	B	768	MET
1	B	769	TRP
1	B	770	ILE
1	B	772	ASP

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Mol	Chain	Res	Type
1	B	773	LYS
1	B	774	LYS
1	B	778	THR
1	B	781	ARG
1	B	789	LEU
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	808	GLU
1	B	817	GLN
1	B	822	LEU
1	B	824	GLN
1	B	829	THR
1	B	837	THR
1	B	843	GLN
1	B	845	GLN
1	B	848	THR
1	B	852	SER
1	B	854	LYS
1	B	858	ILE
1	B	864	MET
1	B	866	ILE
1	B	867	THR
1	B	872	VAL
1	B	874	SER
1	B	876	THR
1	B	884	LEU
1	B	900	LEU
1	B	910	LEU
1	B	917	ARG
1	B	923	SER
1	B	926	TYR
1	B	934	GLU
1	B	938	ARG
1	B	942	ARG
1	B	944	LEU
1	B	950	GLN
1	B	958	ASN
1	B	965	GLN
1	B	971	SER
1	B	972	HIS
1	B	986	ILE

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Mol	Chain	Res	Type
1	B	991	MET
1	B	998	SER
1	B	1004	SER
1	B	1006	GLU
1	B	1009	LEU
1	B	1013	ARG
1	B	1018	LEU
1	B	1023	LYS
1	C	3	ILE
1	C	6	SER
1	C	24	LEU
1	C	27	LEU
1	C	35	SER
1	C	38	ASN
1	C	39	SER
1	C	49	GLN
1	C	55	ASN
1	C	67	GLU
1	C	71	GLU
1	C	72	SER
1	C	80	GLU
1	C	82	ASP
1	C	84	VAL
1	C	85	VAL
1	C	102	ASN
1	C	108	THR
1	C	109	VAL
1	C	114	VAL
1	C	116	THR
1	C	125	LEU
1	C	130	ASP
1	C	131	GLU
1	C	134	LEU
1	C	135	GLN
1	C	138	GLN
1	C	141	ILE
1	C	143	PHE
1	C	148	SER
1	C	163	GLN
1	C	165	SER
1	C	166	ARG
1	C	178	ARG

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Mol	Chain	Res	Type
1	C	187	MET
1	C	189	LEU
1	C	192	SER
1	C	195	SER
1	C	197	LEU
1	C	223	SER
1	C	230	ARG
1	C	236	SER
1	C	237	ARG
1	C	246	MET
1	C	249	GLU
1	C	251	ARG
1	C	252	ASP
1	C	253	TYR
1	C	255	ARG
1	C	259	SER
1	C	264	GLU
1	C	266	GLN
1	C	282	ARG
1	C	291	LEU
1	C	292	ARG
1	C	296	GLU
1	C	299	LYS
1	C	322	LEU
1	C	324	GLU
1	C	333	ARG
1	C	338	GLU
1	C	350	LEU
1	C	352	ARG
1	C	357	HIS
1	C	377	LEU
1	C	380	LYS
1	C	394	ASN
1	C	424	ASN
1	C	425	ARG
1	C	427	THR
1	C	431[A]	ARG
1	C	431[B]	ARG
1	C	437	SER
1	C	448	ARG
1	C	473	ARG
1	C	476	LYS

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Mol	Chain	Res	Type
1	C	503	TYR
1	C	508	GLU
1	C	517	LYS
1	C	519	SER
1	C	521	LYS
1	C	526	LEU
1	C	529	GLU
1	C	531	ARG
1	C	533	LEU
1	C	535	LEU
1	C	537	GLU
1	C	542	MET
1	C	545	SER
1	C	554	GLN
1	C	571	VAL
1	C	575	LEU
1	C	580	GLU
1	C	581	ASN
1	C	595	THR
1	C	600	GLN
1	C	604	ASN
1	C	618	THR
1	C	631	LEU
1	C	645	ARG
1	C	655	MET
1	C	670	LEU
1	C	671	ASP
1	C	672	VAL
1	C	675	GLN
1	C	677	LYS
1	C	687	GLN
1	C	690	SER
1	C	714	ILE
1	C	719	GLN
1	C	721	ARG
1	C	727	SER
1	C	730	LEU
1	C	735	HIS
1	C	737	ILE
1	C	742	THR
1	C	743	SER
1	C	744	GLU

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Mol	Chain	Res	Type
1	C	745	MET
1	C	750	GLU
1	C	751	LEU
1	C	760	ARG
1	C	761	GLN
1	C	765	LEU
1	C	768	MET
1	C	772	ASP
1	C	774	LYS
1	C	778	THR
1	C	779	PRO
1	C	781	ARG
1	C	789	LEU
1	C	797	GLU
1	C	800	ARG
1	C	801	ILE
1	C	811	LYS
1	C	817	GLN
1	C	823	LEU
1	C	824	GLN
1	C	828	ASP
1	C	829	THR
1	C	830	LEU
1	C	843	GLN
1	C	845	GLN
1	C	854	LYS
1	C	856	TYR
1	C	857	ARG
1	C	861	SER
1	C	863	GLN
1	C	864	MET
1	C	867	THR
1	C	869	ASP
1	C	871	GLU
1	C	874	SER
1	C	881	ARG
1	C	885	ASN
1	C	886	CYS
1	C	894	ARG
1	C	896	ASN
1	C	910	LEU
1	C	917	ARG

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Mol	Chain	Res	Type
1	C	920	LEU
1	C	921	PRO
1	C	923	SER
1	C	934	GLU
1	C	938	ARG
1	C	939	CYS
1	C	948	PRO
1	C	950	GLN
1	C	956	GLN
1	C	965	GLN
1	C	973	ARG
1	C	984	LEU
1	C	991	MET
1	C	998	SER
1	C	1006	GLU
1	C	1013	ARG
1	C	1018	LEU
1	D	3	ILE
1	D	11	LEU
1	D	12	GLN
1	D	13	ARG
1	D	24	LEU
1	D	37	ARG
1	D	38	ASN
1	D	39	SER
1	D	41	GLU
1	D	52[A]	ARG
1	D	52[B]	ARG
1	D	67	GLU
1	D	71	GLU
1	D	75	GLU
1	D	76	CYS
1	D	80	GLU
1	D	82	ASP
1	D	84	VAL
1	D	85	VAL
1	D	90	TRP
1	D	102	ASN
1	D	116	THR
1	D	117	GLU
1	D	125	LEU
1	D	128	ASN

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Mol	Chain	Res	Type
1	D	134	LEU
1	D	138	GLN
1	D	169	SER
1	D	187	MET
1	D	190	ARG
1	D	202	MET
1	D	211	ASP
1	D	213	SER
1	D	219	THR
1	D	230	ARG
1	D	236	SER
1	D	237	ARG
1	D	240	LEU
1	D	241	GLU
1	D	243	GLU
1	D	246	MET
1	D	247	CYS
1	D	249	GLU
1	D	252	ASP
1	D	255	ARG
1	D	277	GLU
1	D	278	ILE
1	D	279	ILE
1	D	288	ARG
1	D	289	VAL
1	D	292	ARG
1	D	309	TYR
1	D	310	ARG
1	D	314	GLU
1	D	319	ASP
1	D	322	LEU
1	D	333	ARG
1	D	342	LEU
1	D	344	LEU
1	D	352	ARG
1	D	378	LEU
1	D	380	LYS
1	D	385	ASN
1	D	424	ASN
1	D	425	ARG
1	D	437	SER
1	D	445	GLN

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Mol	Chain	Res	Type
1	D	448	ARG
1	D	473	ARG
1	D	476	LYS
1	D	477	SER
1	D	481	SER
1	D	505	ARG
1	D	516	PRO
1	D	519	SER
1	D	521	LYS
1	D	526	LEU
1	D	529	GLU
1	D	545	SER
1	D	546	LEU
1	D	554	GLN
1	D	559	TYR
1	D	571	VAL
1	D	580	GLU
1	D	581	ASN
1	D	594	ASP
1	D	595	THR
1	D	599	ARG
1	D	600	GLN
1	D	630	ARG
1	D	632	SER
1	D	638	VAL
1	D	639	THR
1	D	645	ARG
1	D	647	SER
1	D	651	LEU
1	D	652	LEU
1	D	655	MET
1	D	661	LYS
1	D	672	VAL
1	D	675	GLN
1	D	680	ILE
1	D	681	GLU
1	D	683	PRO
1	D	685	LEU
1	D	687	GLN
1	D	690	SER
1	D	696	LEU
1	D	701	VAL

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Mol	Chain	Res	Type
1	D	702	GLN
1	D	720	TRP
1	D	721	ARG
1	D	730	LEU
1	D	737	ILE
1	D	743	SER
1	D	745	MET
1	D	746	ASP
1	D	750	GLU
1	D	755	ARG
1	D	760	ARG
1	D	765	LEU
1	D	766	SER
1	D	768	MET
1	D	772	ASP
1	D	773	LYS
1	D	774	LYS
1	D	777	LEU
1	D	778	THR
1	D	797	GLU
1	D	799	THR
1	D	804	ASN
1	D	819	GLU
1	D	822	LEU
1	D	824	GLN
1	D	826	THR
1	D	829	THR
1	D	830	LEU
1	D	836	ILE
1	D	845	GLN
1	D	850	PHE
1	D	852	SER
1	D	853	ARG
1	D	854	LYS
1	D	867	THR
1	D	874	SER
1	D	875	ASP
1	D	876	THR
1	D	881	ARG
1	D	885	ASN
1	D	888	LEU
1	D	890	GLN

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Mol	Chain	Res	Type
1	D	894	ARG
1	D	904	GLU
1	D	910	LEU
1	D	923	SER
1	D	925	MET
1	D	934	GLU
1	D	938	ARG
1	D	956	GLN
1	D	959	ILE
1	D	961	ARG
1	D	968	MET
1	D	971	SER
1	D	986	ILE
1	D	991	MET
1	D	998	SER
1	D	1002	SER
1	D	1006	GLU
1	D	1013	ARG
1	D	1017	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	50	GLN
1	A	102	ASN
1	A	128	ASN
1	A	216	HIS
1	A	226	HIS
1	A	316	HIS
1	A	357	HIS
1	A	365	GLN
1	A	381	GLN
1	A	385	ASN
1	A	394	ASN
1	A	424	ASN
1	A	467	ASN
1	A	510	GLN
1	A	554	GLN
1	A	558	GLN
1	A	573	GLN

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Mol	Chain	Res	Type
1	A	581	ASN
1	A	597	ASN
1	A	614	HIS
1	A	622	HIS
1	A	623	GLN
1	A	693	GLN
1	A	704	ASN
1	A	718	GLN
1	A	863	GLN
1	A	878	HIS
1	A	887	GLN
1	A	949	HIS
1	A	965	GLN
1	A	990	HIS
1	A	1017	GLN
1	B	38	ASN
1	B	89	ASN
1	B	102	ASN
1	B	163	GLN
1	B	216	HIS
1	B	221	GLN
1	B	226	HIS
1	B	245	GLN
1	B	307	ASN
1	B	316	HIS
1	B	357	HIS
1	B	445	GLN
1	B	583	ASN
1	B	597	ASN
1	B	622	HIS
1	B	624	GLN
1	B	675	GLN
1	B	949	HIS
1	B	965	GLN
1	C	38	ASN
1	C	102	ASN
1	C	135	GLN
1	C	163	GLN
1	C	216	HIS
1	C	221	GLN
1	C	226	HIS
1	C	266	GLN

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Mol	Chain	Res	Type
1	C	316	HIS
1	C	357	HIS
1	C	424	ASN
1	C	467	ASN
1	C	554	GLN
1	C	563	GLN
1	C	583	ASN
1	C	597	ASN
1	C	604	ASN
1	C	622	HIS
1	C	624	GLN
1	C	817	GLN
1	C	863	GLN
1	C	949	HIS
1	C	965	GLN
1	C	990	HIS
1	C	1017	GLN
1	D	38	ASN
1	D	102	ASN
1	D	216	HIS
1	D	316	HIS
1	D	357	HIS
1	D	394	ASN
1	D	424	ASN
1	D	510	GLN
1	D	554	GLN
1	D	573	GLN
1	D	583	ASN
1	D	597	ASN
1	D	604	ASN
1	D	614	HIS
1	D	622	HIS
1	D	623	GLN
1	D	675	GLN
1	D	693	GLN
1	D	702	GLN
1	D	718	GLN
1	D	757	GLN
1	D	845	GLN
1	D	890	GLN
1	D	949	HIS
1	D	965	GLN



### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1021/1021 (100%)	-1.31	2 (0%) 93 95	2, 26, 68, 100	19 (1%)
1	B	1021/1021 (100%)	-1.21	0 100 100	4, 31, 72, 100	19 (1%)
1	C	1021/1021 (100%)	-1.25	1 (0%) 93 96	6, 28, 65, 100	19 (1%)
1	D	1021/1021 (100%)	-1.29	0 100 100	3, 26, 65, 100	19 (1%)
All	All	4084/4084 (100%)	-1.27	3 (0%) 93 96	2, 28, 68, 100	76 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	ALA	2.6
1	C	732	ALA	2.2
1	A	734	SER	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	3002	1/1	0.12	4.87	31,31,31,31	0
2	MG	D	3002	1/1	0.10	2.13	25,25,25,25	0
2	MG	A	3001	1/1	0.10	0.33	28,28,28,28	0
2	MG	B	3002	1/1	0.07	-0.18	36,36,36,36	0
2	MG	C	3002	1/1	0.07	-0.43	31,31,31,31	0
2	MG	D	3001	1/1	0.07	-0.67	40,40,40,40	0
2	MG	B	3001	1/1	0.04	-1.66	20,20,20,20	0
2	MG	C	3001	1/1	0.03	-2.11	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.