Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 01:22 AM EDT

PDB ID	:	5GUG
Title	:	Crystal structure of inositol 1,4,5-trisphosphate receptor large cytosolic domain with inositol 1,4,5-trisphosphate
Authors	:	Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on	:	2016-08-29
Resolution	:	7.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

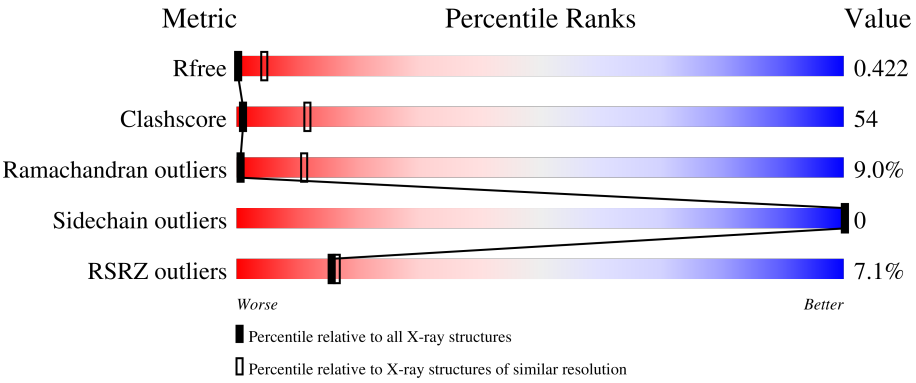
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2217	6% 43% 30% · 22%
1	B	2217	5% 43% 30% 5% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	I3P	B	3000	-	-	-	X

2 Entry composition

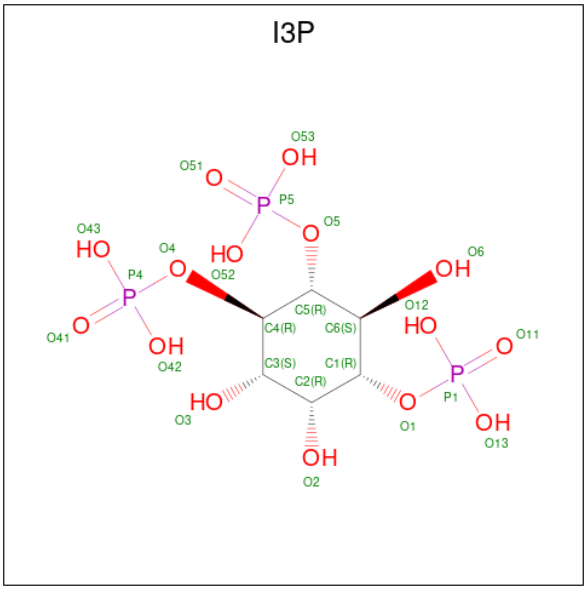
There are 2 unique types of molecules in this entry. The entry contains 25117 atoms, of which 7810 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1721	Total	C	H	N	O	S	0	0	0
			12529	5147	3897	1746	1738	1			
1	B	1720	Total	C	H	N	O	S	0	0	0
			12522	5144	3895	1745	1737	1			

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).



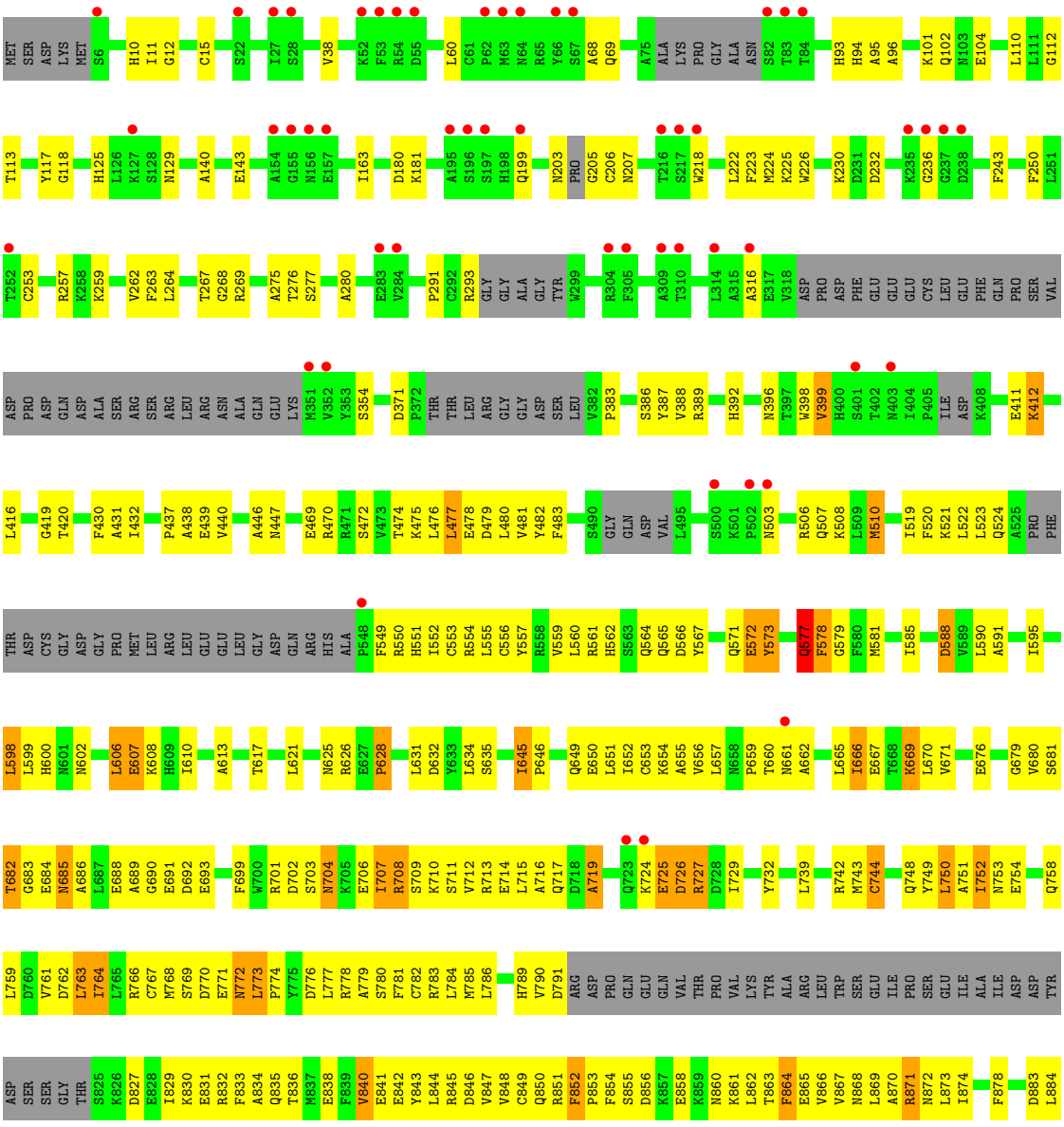
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			33	6	9	15	3		
2	B	1	Total	C	H	O	P	0	0
			33	6	9	15	3		

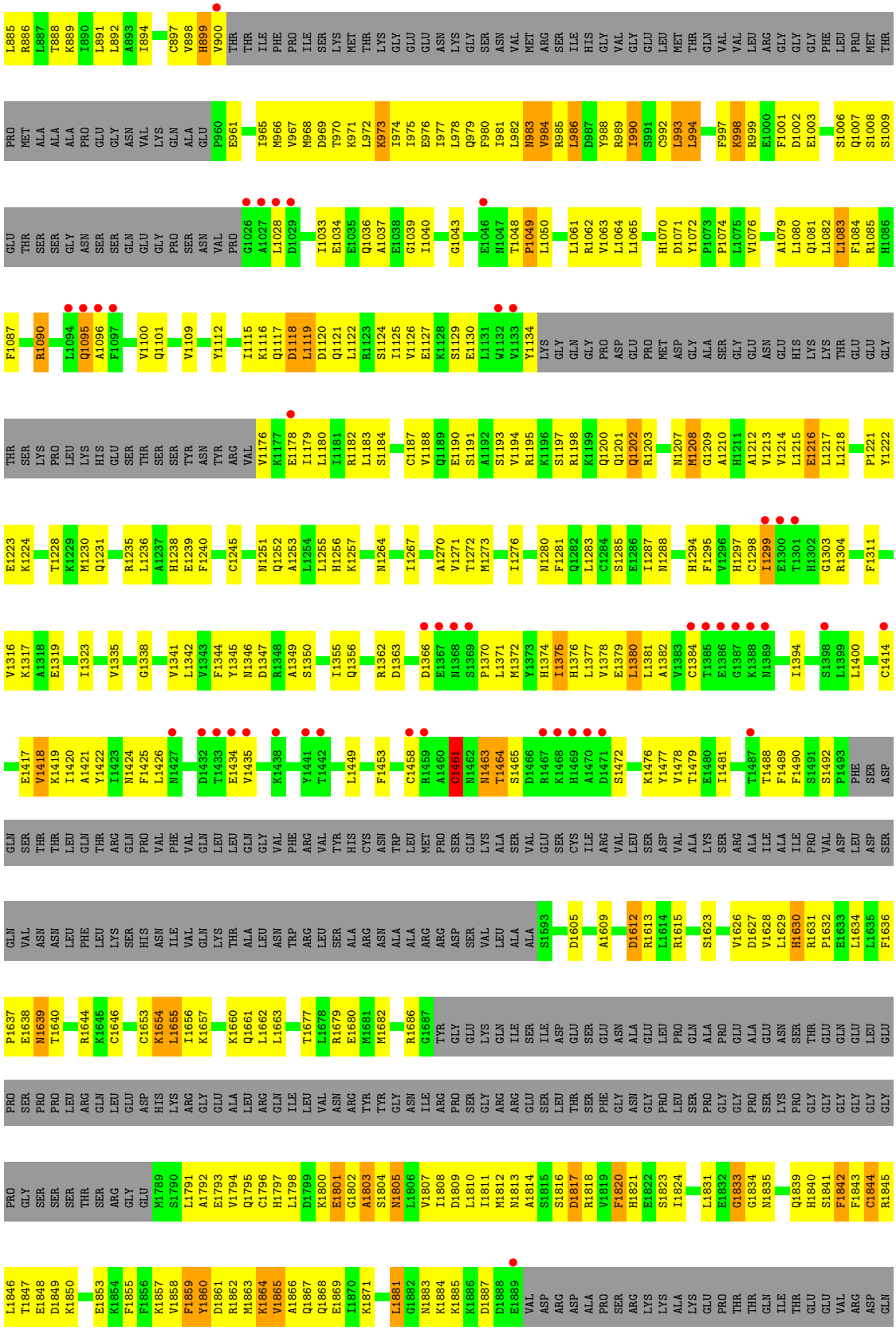
3 Residue-property plots (i)

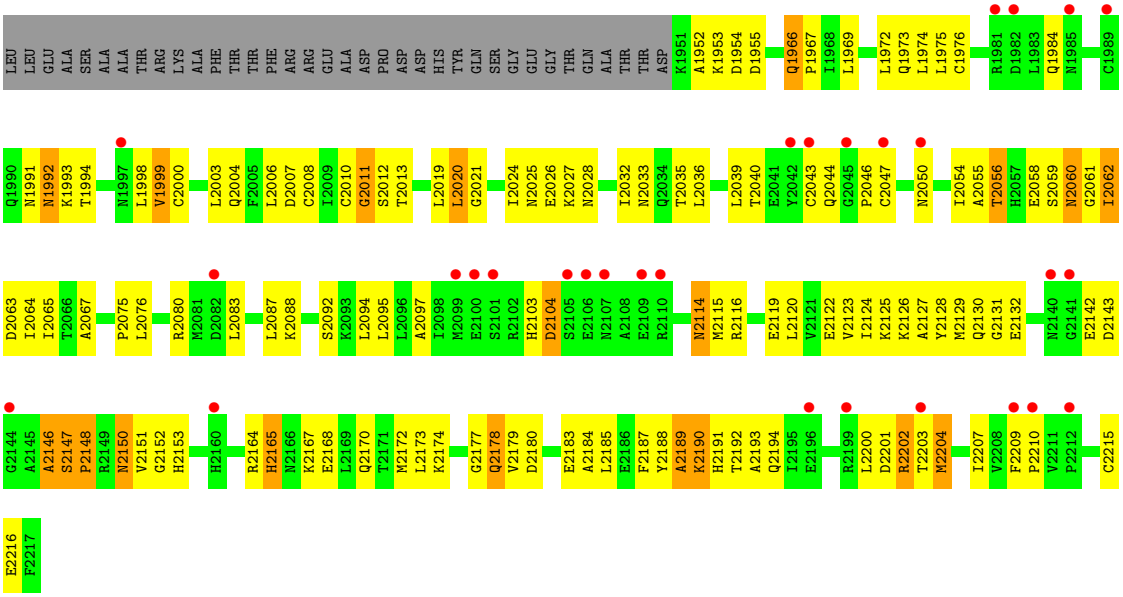
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain A:

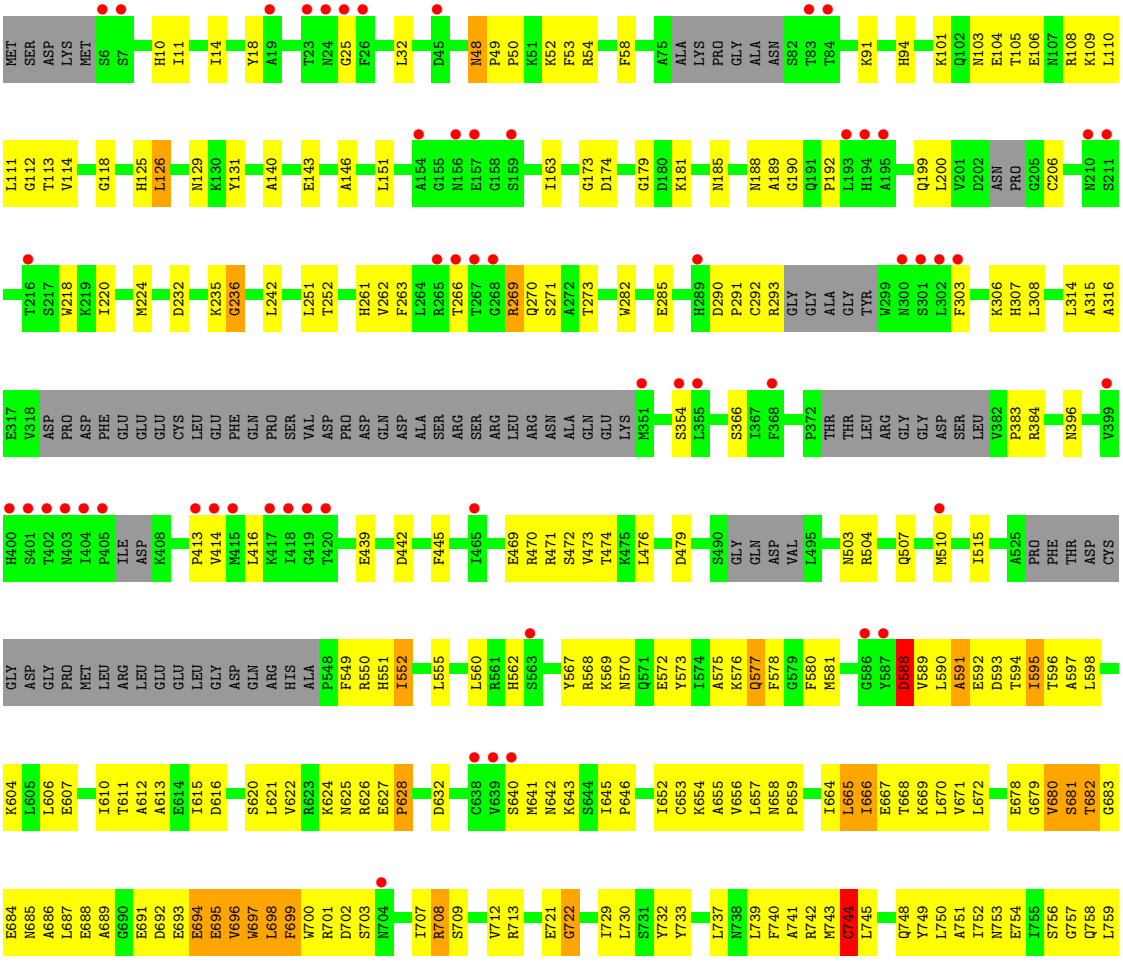


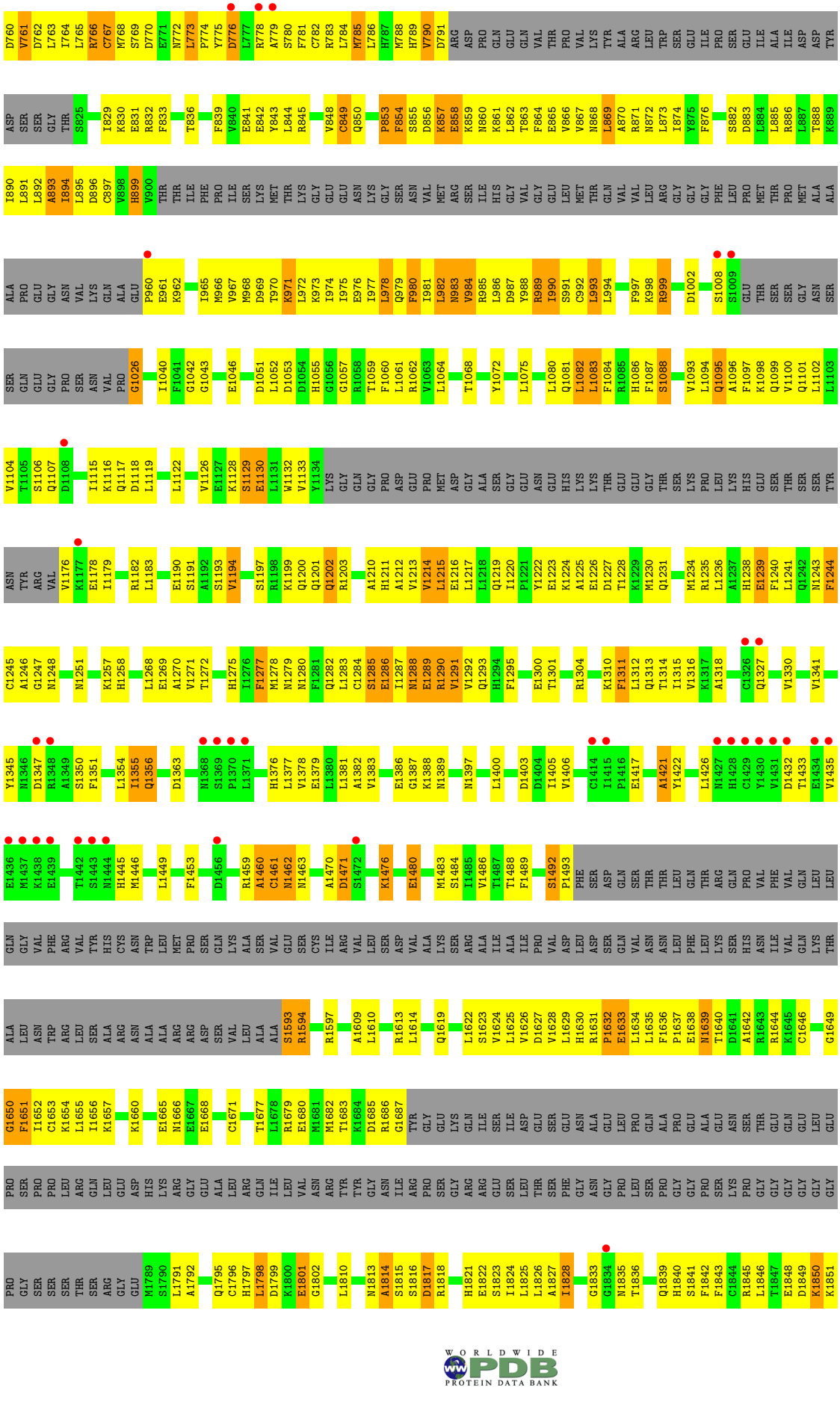

L885 R886 L887 T888 K889 T890 L891 L892 A893 I894 C897 V898 H899 V900 THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU LEU MET THR GLN VAL VAL LEU ARG GLY GLY GLY PHE LEU PRO MET THR
PRO MET ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E961 I965 M966 V967 M968 D969 T970 K971 L972 K973 I974 I975 E976 I977 L978 Q979 F980 I981 L982 N983 V984 R985 L986 D987 Y988 R989 I990 S991 C992 L993 L994 F997 K998 R999 E1000 F1001 D1002 E1003 S1006 Q1007 S1008 S1009
GLU THR SER SER GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL PRO G1026 A1027 L1028 D1029 I1033 E1034 E1035 Q1036 A1037 E1038 G1039 I1040 G1043 E1046 N1047 T1048 P1049 L1050 L1061 R1062 V1063 L1064 L1065 H1070 D1071 Y1072 P1073 P1074 L1075 V1076 A1079 L1080 Q1081 L1082 L1083 F1084 R1085 H1086
F1087 R1090 L1094 Q1095 A1096 F1097 V1100 Q1101 V1109 Y1112 I1115 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 R1123 S1124 I1125 V1126 E1127 K1128 S1129 E1130 L1131 W1132 V1133 Y1134 LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU GLU ASN GLU HIS LYS LYS THR GLU GLU GLY
THR SER LYS PRO LEU LYS HIS GLU SER THR SER TYR ASN TYR ARG VAL V1176 K1177 E1178 I1179 L1180 I1181 R1182 L1183 S1184 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 K1199 Q1200 Q1201 Q1202 R1203 N1207 M1208 G1209 A1210 H1211 A1212 V1213 V1214 L1215 E1216 L1217 L1218 P1221 Y1222
E1223 K1224 T1228 K1229 M1230 Q1231 R1235 L1236 A1237 H1238 E1239 F1240 C1245 N1251 Q1252 A1253 L1254 L1255 H1256 K1257 N1264 I1267 A1270 V1271 T1272 M1273 I1276 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 H1294 F1295 V1296 H1297 C1298 I1299 E1300 T1301 H1302 G1303 R1304 F1311
V1316 K1317 A1318 E1319 I1323 V1335 G1338 V1341 L1342 V1343 F1344 Y1345 N1346 D1347 R1348 A1349 S1350 I1355 Q1356 R1362 D1363 D1366 E1367 N1368 S1369 P1370 L1371 M1372 Y1373 H1374 I1375 H1376 L1377 V1378 E1379 L1380 L1381 A1382 V1383 C1384 T1385 E1386 G1387 K1388 N1389 I1394 S1398 L1399 L1400 C1414
E1417 V1418 K1419 I1420 A1421 Y1422 I1423 N1424 F1425 L1426 N1427 D1432 T1433 E1434 V1435 K1438 Y1441 T1442 L1449 F1453 C1458 R1459 A1460 C1461 N1462 N1463 T1464 S1465 D1466 R1467 K1468 H1469 A1470 D1471 S1472 K1476 Y1477 V1478 T1479 E1480 I1481 T1487 T1488 F1489 F1490 S1491 S1492 P1493 PHE SER ASP
GLN SER THR THR LEU GLN THR ARG GLN PRO VAL PHE VAL GLN LEU LEU GLN GLY VAL PHE ARG VAL TYR HIS CYS ASN TRP LEU MET PRO SER GLN LYS ALA SER VAL GLU SER CYS ILE ARG VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP LEU ASP SER
GLN VAL ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA LEU ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ASP SER VAL LEU ALA ALA S1593 D1605 A1609 D1612 R1613 L1614 R1615 S1623 V1626 D1627 V1628 L1629 H1630 R1631 P1632 E1633 L1634 L1635 F1636
P1637 E1638 N1639 T1640 R1644 K1645 C1646 C1653 K1654 L1655 T1656 K1657 K1660 Q1661 L1662 L1663 T1677 L1678 R1679 E1680 M1681 M1682 R1686 G1687 TYR GLY GLU LYS GLN ILE SER ILE ASP GLU SER GLU ASN ALA GLU LEU PRO GLN ALA PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU
PRO SER PRO PRO LEU ARG GLN LEU GLU ASP HIS LYS ARG GLY GLU ALA LEU ARG GLN ILE LEU VAL ASN ARG TYR GLY ASN ILE ARG PRO GLU SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER GLY LYS PRO GLY GLY GLY GLY GLY
PRO GLY SER SER THR SER ARG GLY GLU M1789 S1790 L1791 A1792 E1793 V1794 Q1795 C1796 H1797 L1798 D1799 K1800 E1801 G1802 A1803 S1804 N1805 L1806 V1807 I1808 D1809 L1810 I1811 M1812 N1813 A1814 S1815 S1816 D1817 R1818 V1819 F1820 H1821 E1822 S1823 I1824 L1831 E1832 G1833 G1834 N1835 Q1839 H1840 S1841 F1842 F1843 C1844 R1845
L1846 T1847 E1848 D1849 K1850 E1853 K1854 F1855 F1856 K1857 V1858 F1859 Y1860 D1861 R1862 M1863 K1864 V1865 A1866 Q1867 Q1868 E1869 I1870 K1871 L1881 G1882 N1883 K1884 K1885 K1886 D1887 D1888 E1889 VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU VAL ARG ASP GLN

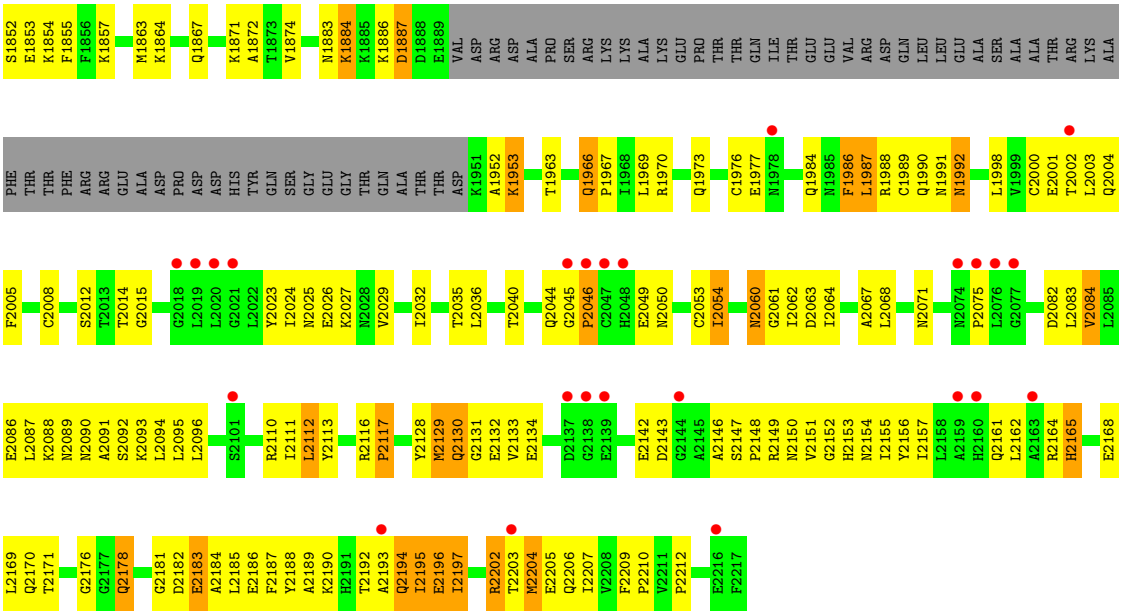


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain B:




D760 V761 D762 L763 I764 L765 R766 C767 M768 S769 D770 E771 N772 L773 P774 Y775 D776 L777 R778 A779 S780 F781 C782 R783 L784 M785 L786 H787 M788 H789 V790 D791 ARG ASP PRO GLN GLU ILE ALA ILE ASP ASP TYR
ASP SER SER GLY THR S825 I829 K830 E831 R832 F833 T836 F839 V840 E841 E842 Y843 L844 R845 V848 C849 Q850 P853 F854 S855 D856 K857 E858 K859 N860 K861 L862 T863 F864 E865 V866 V867 N868 L869 A870 R871 N872 L873 I874 Y875 F876 S882 D883 L884 L885 R886 L887 T888 K889
I890 L891 L892 A893 I894 L895 D896 C897 V898 H899 V900 THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY SER ASN VAL MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR PRO MET ALA ALA
ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E961 K962 I965 M966 V967 M968 D969 T970 K971 L972 K973 I974 I975 E976 I977 L978 Q979 F980 I981 L982 N983 V984 R985 L986 D987 Y988 R989 I990 S991 C992 L993 L994 F997 K998 R999 D1002 S1008 S1009 GLU THR SER SER GLY ASN SER
SER GLN GLU GLY PRO SER ASN VAL PRO G1026 I1040 F1041 G1042 G1043 E1046 D1051 L1052 D1053 D1054 H1055 G1056 G1057 R1058 T1059 F1060 L1061 R1062 V1063 L1064 T1068 Y1072 L1075 L1080 Q1081 L1082 L1083 F1084 R1085 H1086 F1087 S1088 V1093 L1094 Q1095 A1096 F1097 K1098 Q1099 V1100 Q1101 L1102 L1103
V1104 T1105 S1106 Q1107 D1108 I1115 K1116 Q1117 D1118 L1119 L1122 V1126 E1127 K1128 S1129 E1130 L1131 W1132 V1133 Y1134 LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER GLY TYR
ASN TYR ARG VAL V1176 K1177 E1178 I1179 R1182 L1183 E1190 S1191 A1192 S1193 V1194 S1197 R1198 K1199 Q1200 Q1201 Q1202 R1203 A1210 H1211 A1212 V1213 V1214 L1215 E1216 L1217 L1218 Q1219 I1220 P1221 Y1222 E1223 K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 M1234 R1235 L1236 A1237 H1238 E1239 F1240 L1241 Q1242 N1243 F1244
C1245 A1246 G1247 N1248 N1251 K1257 H1258 L1268 E1269 A1270 V1271 T1272 H1275 I1276 F1277 M1278 N1279 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 E1289 R1290 V1291 V1292 Q1293 H1294 F1295 E1300 T1301 R1304 K1310 F1311 L1312 Q1313 T1314 I1315 V1316 K1317 A1318 C1326 Q1327 V1330 V1341
Y1345 N1346 D1347 R1348 A1349 S1350 F1351 L1354 I1355 Q1356 D1363 N1368 S1369 P1370 L1371 H1376 L1377 V1378 E1379 L1380 L1381 A1382 V1383 E1386 G1387 K1388 N1389 N1397 L1400 D1403 D1404 I1405 V1406 C1414 I1415 P1416 E1417 A1421 Y1422 L1426 N1427 H1428 C1429 Y1430 V1431 D1432 T1433 E1434 V1435
E1436 M1437 K1438 E1439 T1442 S1443 N1444 H1445 M1446 L1449 F1453 D1456 R1459 A1460 C1461 N1462 N1463 A1470 D1471 S1472 K1476 E1480 M1483 S1484 I1485 V1486 T1487 T1488 F1489 S1492 P1493 PHE SER ASP GLN SER THR THR LEU GLN THR ARG GLN PRO VAL PHE VAL GLN LEU LEU
GLN GLY VAL PHE ARG VAL TYR HIS CYS ASN TRP LEU MET PRO SER GLN LYS ALA SER VAL GLU SER CYS ILE ARG VAL LEU SER ASP VAL ASP LEU ASP SER GLN GLN VAL ASN ASN LEU PHE LEU LYS SER ARG ALA ILE ALA ILE PRO VAL ASP LEU ASP SER GLN GLN LEU LYS THR
ALA LEU ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA S1593 R1594 R1597 A1609 L1610 R1613 L1614 Q1619 L1622 S1623 V1624 L1625 V1626 D1627 V1628 L1629 H1630 R1631 P1632 E1633 L1634 L1635 F1636 P1637 E1638 N1639 T1640 D1641 A1642 R1643 R1644 K1645 C1646 G1649
G1650 F1651 I1652 C1653 K1654 L1655 I1656 K1657 K1660 E1665 N1666 E1667 E1668 C1671 T1677 L1678 R1679 E1680 M1681 M1682 T1683 K1684 D1685 R1686 G1687 TYR GLY GLU LYS GLN ILE SER ILE ASP GLU SER GLU ASN ALA GLU LEU PRO GLN ALA PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU
PRO SER PRO PRO LEU ARG GLN LEU GLU ASP HIS LYS ARG GLY GLU ALA LEU ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG ARG GLU SER LEU THR SER GLU ASP GLY ASN GLY PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY
PRO GLY SER SER THR SER ARG GLY GLU M1789 S1790 L1791 A1792 Q1795 C1796 H1797 L1798 D1799 K1800 E1801 G1802 L1810 N1813 A1814 S1815 S1816 D1817 R1818 H1821 E1822 S1823 I1824 L1825 L1826 A1827 I1828 G1833 G1834 N1835 T1836 Q1839 H1840 S1841 F1842 F1843 C1844 R1845 L1846 T1847 E1848 D1849 K1850 K1851


S1852 E1853 K1854 F1855 F1856 K1857 M1863 K1864 Q1867 K1871 A1872 T1873 V1874 N1883 K1884 K1885 K1886 D1887 D1888 E1889
PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP
VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR ARG LYS ALA
K1951 A1952 K1953 T1963 Q1966 P1967 I1968 L1969 R1970 Q1973 C1976 E1977 N1978 Q1984 N1985 F1986 L1987 R1988 C1989 Q1990 N1991 N1992 L1998 V1999 C2000 E2001 T2002 L2003 Q2004
F2005 C2008 S2012 T2013 T2014 G2015 G2018 L2019 L2020 G2021 L2022 Y2023 I2024 N2025 E2026 K2027 N2028 V2029 I2032 T2035 L2036 T2040 Q2044 G2045 P2046 C2047 H2048 E2049 N2050 C2053 I2054 N2060 G2061 I2062 D2063 I2064 A2067 L2068 N2071 N2074 P2075 L2076 G2077 D2082 L2083 V2084 L2085
E2086 L2087 K2088 N2089 N2090 A2091 S2092 K2093 L2094 L2095 L2096 S2101 R2110 I2111 L2112 Y2113 R2116 P2117 Y2128 M2129 Q2130 G2131 E2132 V2133 E2134 D2137 G2138 E2139 E2142 D2143 G2144 A2145 A2146 S2147 P2148 R2149 N2150 V2151 G2152 H2153 N2154 I2155 Y2156 I2157 L2158 A2159 H2160 Q2161 L2162 A2163 R2164 H2165 E2168
L2169 Q2170 T2171 G2176 G2177 Q2178 G2181 D2182 E2183 A2184 L2185 E2186 F2187 Y2188 A2189 K2190 H2191 T2192 A2193 Q2194 I2195 E2196 I2197 R2202 T2203 M2204 E2205 Q2206 I2207 Y2208 F2209 P2210 Y2211 P2212 E2216 F2217

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.99Å 223.49Å 319.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 7.40 49.49 – 7.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.49-7.40) 85.7 (49.49-7.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 7.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.356 , 0.416 0.359 , 0.422	Depositor DCC
R_{free} test set	526 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	159.4	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 212.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.23$, $< L^2 > = 0.08$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.62	EDS
Total number of atoms	25117	wwPDB-VP
Average B, all atoms (Å^2)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: I3P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	9/8617 (0.1%)	0.84	6/11978 (0.1%)
1	B	0.71	6/8612 (0.1%)	0.83	5/11971 (0.0%)
All	All	0.71	15/17229 (0.1%)	0.83	11/23949 (0.0%)

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	0	8
1	B	0	9
All	All	0	17

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	GLN	CD-NE2	-9.15	1.09	1.32
1	B	270	GLN	CD-OE1	-7.90	1.06	1.24
1	A	577	GLN	C-O	7.33	1.37	1.23
1	B	1026	GLY	C-O	-6.82	1.12	1.23
1	A	579	GLY	N-CA	-6.53	1.36	1.46
1	A	572	GLU	CB-CG	6.10	1.63	1.52
1	A	577	GLN	CA-C	6.05	1.68	1.52
1	A	717	GLN	CA-CB	-5.86	1.41	1.53
1	A	1118	ASP	CA-CB	5.44	1.66	1.53
1	B	1026	GLY	CA-C	-5.38	1.43	1.51
1	A	772	ASN	C-N	5.32	1.46	1.34
1	A	60	LEU	C-N	-5.21	1.22	1.34
1	B	261	HIS	C-N	-5.19	1.22	1.34
1	A	577	GLN	CA-CB	-5.09	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	588	ASP	C-O	5.04	1.32	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	577	GLN	C-N-CA	9.25	144.83	121.70
1	A	578	PHE	N-CA-CB	8.28	125.51	110.60
1	B	588	ASP	N-CA-C	6.75	129.24	111.00
1	B	588	ASP	N-CA-CB	-6.54	98.82	110.60
1	A	510	MET	CB-CG-SD	-5.91	94.68	112.40
1	A	772	ASN	CB-CA-C	5.88	122.16	110.40
1	B	1026	GLY	CA-C-O	-5.68	110.38	120.60
1	A	772	ASN	N-CA-C	-5.64	95.76	111.00
1	B	1476	LYS	N-CA-CB	-5.52	100.67	110.60
1	A	961	GLU	CB-CA-C	5.52	121.43	110.40
1	B	1884	LYS	N-CA-C	5.43	125.67	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	GLU	Peptide
1	A	1375	ILE	Peptide
1	A	1380	LEU	Peptide
1	A	1461	CYS	Peptide
1	A	2114	ASN	Peptide
1	A	2142	GLU	Peptide
1	A	577	GLN	Peptide
1	A	588	ASP	Peptide
1	B	1269	GLU	Peptide
1	B	1421	ALA	Peptide
1	B	1593	SER	Mainchain
1	B	1594	ARG	Peptide
1	B	1798	LEU	Peptide
1	B	577	GLN	Peptide
1	B	588	ASP	Peptide
1	B	744	CYS	Peptide
1	B	759	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8632	3897	3899	667	0
1	B	8627	3895	3898	687	0
2	A	24	9	9	6	0
2	B	24	9	9	1	0
All	All	17307	7810	7815	1353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

All (1353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2020:LEU:O	1:A:2024:ILE:N	1.57	1.38
1:B:863:THR:O	1:B:867:VAL:N	1.72	1.21
1:A:1210:ALA:O	1:A:1214:VAL:CB	1.89	1.20
1:A:1125:ILE:O	1:A:1129:SER:CB	1.91	1.19
1:B:1682:MET:O	1:B:1686:ARG:N	1.78	1.16
1:A:869:LEU:O	1:A:873:LEU:N	1.81	1.14
1:A:1864:LYS:O	1:A:1867:GLN:N	1.82	1.13
1:A:2124:ILE:O	1:A:2128:TYR:CB	2.00	1.09
1:A:866:VAL:O	1:A:870:ALA:N	1.87	1.08
1:A:2150:ASN:O	1:A:2153:HIS:N	1.87	1.08
1:B:1966:GLN:O	1:B:1970:ARG:CB	2.05	1.04
1:A:1421:ALA:O	1:A:1425:PHE:CB	2.04	1.04
1:A:1377:LEU:O	1:A:1381:LEU:CB	2.06	1.03
1:A:1231:GLN:O	1:A:1235:ARG:CB	2.05	1.03
1:A:1420:ILE:O	1:A:1424:ASN:CB	2.07	1.03
1:A:2125:LYS:O	1:A:2129:MET:CB	2.06	1.02
1:B:1635:LEU:O	1:B:1639:ASN:N	1.93	1.02
1:B:2061:GLY:O	1:B:2064:ILE:N	1.92	1.01
1:A:2147:SER:O	1:A:2151:VAL:CB	2.08	1.01
1:A:1371:LEU:O	1:A:1375:ILE:N	1.92	1.01
1:B:1231:GLN:O	1:B:1235:ARG:CB	2.09	1.00
1:A:1126:VAL:O	1:A:1130:GLU:CB	2.10	1.00
1:A:628:PRO:O	1:A:632:ASP:N	1.95	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:764:ILE:O	1:B:768:MET:N	1.96	0.98
1:A:1843:PHE:O	1:A:1846:LEU:N	1.93	0.98
1:A:1849:ASP:O	1:A:1853:GLU:N	1.96	0.98
1:B:2147:SER:O	1:B:2151:VAL:N	1.96	0.98
1:A:1252:GLN:O	1:A:1256:HIS:N	1.97	0.98
1:B:2091:ALA:O	1:B:2095:LEU:CB	2.12	0.97
1:B:2182:ASP:O	1:B:2185:LEU:N	1.97	0.97
1:B:763:LEU:O	1:B:767:CYS:N	1.97	0.97
1:A:844:LEU:O	1:A:847:VAL:N	1.98	0.96
1:A:476:LEU:O	1:A:479:ASP:N	1.98	0.96
1:A:978:LEU:O	1:A:982:LEU:N	1.98	0.95
1:B:785:MET:O	1:B:788:MET:N	1.99	0.95
1:A:976:GLU:O	1:A:980:PHE:N	2.00	0.94
1:A:868:ASN:O	1:A:872:ASN:N	1.99	0.94
1:B:782:CYS:O	1:B:785:MET:N	2.01	0.93
1:A:1867:GLN:O	1:A:1871:LYS:CB	2.16	0.93
1:B:620:SER:O	1:B:624:LYS:N	2.02	0.93
1:A:708:ARG:O	1:A:712:VAL:N	2.02	0.92
1:A:1179:ILE:O	1:A:1183:LEU:CB	2.17	0.92
1:B:780:SER:O	1:B:783:ARG:N	2.02	0.92
1:A:552:ILE:O	1:A:556:CYS:N	2.02	0.92
1:B:1417:GLU:O	1:B:1421:ALA:N	2.03	0.91
1:A:1472:SER:O	1:A:1476:LYS:CB	2.19	0.91
1:A:1820:PHE:O	1:A:1824:ILE:N	2.03	0.91
1:A:2188:TYR:O	1:A:2192:THR:CB	2.19	0.91
1:A:651:LEU:O	1:A:655:ALA:N	2.04	0.91
1:B:1096:ALA:O	1:B:1100:VAL:N	2.03	0.91
1:A:867:VAL:O	1:A:871:ARG:N	2.03	0.90
1:A:354:SER:HA	1:A:419:GLY:HA2	1.54	0.90
1:B:891:LEU:O	1:B:895:LEU:CB	2.19	0.90
1:B:1422:TYR:O	1:B:1426:LEU:CB	2.19	0.90
1:B:2050:ASN:O	1:B:2054:ILE:CB	2.19	0.90
1:B:476:LEU:O	1:B:479:ASP:N	2.05	0.90
1:A:1118:ASP:O	1:A:1121:GLN:N	2.05	0.89
1:A:650:GLU:O	1:A:654:LYS:N	2.06	0.89
1:B:621:LEU:O	1:B:625:ASN:N	2.07	0.88
1:A:2055:ALA:O	1:A:2059:SER:N	2.06	0.88
1:A:2021:GLY:O	1:A:2025:ASN:N	2.07	0.88
1:A:2128:TYR:O	1:A:2132:GLU:CB	2.22	0.88
1:A:125:HIS:O	1:A:129:ASN:N	2.07	0.88
1:B:665:LEU:O	1:B:671:VAL:N	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1986:PHE:O	1:B:1988:ARG:N	2.07	0.87
1:B:789:HIS:O	1:B:791:ASP:N	2.06	0.87
1:A:833:PHE:O	1:A:836:THR:N	2.07	0.87
1:A:1294:HIS:O	1:A:1298:CYS:N	2.06	0.87
1:B:866:VAL:O	1:B:870:ALA:N	2.07	0.87
1:B:1119:LEU:O	1:B:1122:LEU:N	2.07	0.87
1:A:1817:ASP:O	1:A:1821:HIS:N	2.05	0.87
1:B:1821:HIS:O	1:B:1825:LEU:N	2.08	0.87
1:B:1849:ASP:O	1:B:1852:SER:N	2.08	0.87
1:A:1862:ARG:O	1:A:1866:ALA:CB	2.23	0.86
1:A:585:ILE:HA	1:A:591:ALA:HB1	1.57	0.86
1:A:1417:GLU:O	1:A:1419:LYS:N	2.08	0.86
1:A:2126:LYS:O	1:A:2130:GLN:CB	2.24	0.86
1:B:2183:GLU:O	1:B:2187:PHE:CB	2.23	0.86
1:A:268:GLY:N	2:A:3000:I3P:O42	2.08	0.85
1:B:1797:HIS:O	1:B:1802:GLY:N	2.09	0.85
1:A:1116:LYS:O	1:A:1119:LEU:N	2.08	0.85
1:A:2076:LEU:HA	1:A:2080:ARG:CB	2.07	0.85
1:B:872:ASN:O	1:B:876:PHE:N	2.08	0.85
1:A:267:THR:OG1	2:A:3000:I3P:O41	1.94	0.85
1:A:710:LYS:O	1:A:714:GLU:N	2.10	0.84
1:B:1223:GLU:O	1:B:1271:VAL:CB	2.25	0.84
1:A:269:ARG:NH2	2:A:3000:I3P:O52	2.09	0.84
1:A:2004:GLN:O	1:A:2008:CYS:N	2.11	0.84
1:B:967:VAL:O	1:B:969:ASP:N	2.10	0.84
1:B:2148:PRO:O	1:B:2152:GLY:N	2.11	0.84
1:A:975:ILE:O	1:A:979:GLN:N	2.09	0.84
1:B:1211:HIS:O	1:B:1214:VAL:N	2.10	0.83
1:B:885:LEU:O	1:B:888:THR:N	2.09	0.83
1:B:1986:PHE:O	1:B:1989:CYS:N	2.12	0.83
1:A:1379:GLU:HA	1:A:1382:ALA:HB3	1.59	0.83
1:B:2128:TYR:O	1:B:2132:GLU:CB	2.26	0.83
1:B:552:ILE:O	1:B:555:LEU:N	2.11	0.83
1:A:1208:MET:O	1:A:1212:ALA:CB	2.26	0.83
1:A:773:LEU:CB	1:A:779:ALA:H	1.92	0.83
1:A:1792:ALA:O	1:A:1796:CYS:CB	2.27	0.82
1:A:773:LEU:CB	1:A:779:ALA:N	2.43	0.82
1:B:11:ILE:O	1:B:112:GLY:N	2.11	0.82
1:B:680:VAL:O	1:B:682:THR:N	2.12	0.82
1:B:773:LEU:O	1:B:775:TYR:N	2.12	0.82
1:B:988:TYR:O	1:B:990:ILE:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:GLN:O	1:A:573:TYR:N	2.13	0.81
1:A:1317:LYS:HA	1:A:1323:ILE:CB	2.09	0.81
1:A:665:LEU:O	1:A:671:VAL:N	2.14	0.81
1:A:1862:ARG:O	1:A:1866:ALA:HB3	1.78	0.81
1:B:864:PHE:O	1:B:868:ASN:N	2.13	0.81
1:B:2152:GLY:O	1:B:2156:TYR:CB	2.30	0.80
1:A:1118:ASP:O	1:A:1120:ASP:N	2.13	0.80
1:A:708:ARG:O	1:A:712:VAL:CB	2.29	0.80
1:A:982:LEU:O	1:A:986:LEU:N	2.14	0.79
1:B:1095:GLN:O	1:B:1099:GLN:N	2.13	0.79
1:B:1609:ALA:O	1:B:1613:ARG:CB	2.31	0.79
1:B:1638:GLU:O	1:B:1640:THR:N	2.15	0.79
1:A:1992:ASN:O	1:A:1994:THR:N	2.15	0.78
1:A:2007:ASP:O	1:A:2011:GLY:N	2.16	0.78
1:A:2036:LEU:O	1:A:2040:THR:CB	2.30	0.78
1:A:970:THR:O	1:A:973:LYS:CB	2.31	0.78
1:B:653:CYS:O	1:B:657:LEU:N	2.16	0.78
1:B:1101:GLN:O	1:B:1104:VAL:N	2.17	0.77
1:B:2060:ASN:O	1:B:2064:ILE:N	2.17	0.77
1:A:399:VAL:HA	1:A:420:THR:HA	1.66	0.77
1:A:853:PRO:O	1:A:855:SER:N	2.17	0.77
1:A:1285:SER:O	1:A:1341:VAL:CB	2.33	0.77
1:A:1839:GLN:O	1:A:1842:PHE:N	2.18	0.77
1:B:1625:LEU:O	1:B:1628:VAL:N	2.18	0.76
1:A:1794:VAL:CB	1:A:1831:LEU:O	2.33	0.76
1:B:666:ILE:CB	1:B:671:VAL:H	1.99	0.76
1:A:1839:GLN:O	1:A:1842:PHE:CB	2.33	0.76
1:B:2000:CYS:O	1:B:2003:LEU:N	2.17	0.76
1:A:1816:SER:O	1:A:1818:ARG:N	2.19	0.76
1:B:865:GLU:O	1:B:869:LEU:N	2.17	0.76
1:B:2090:ASN:O	1:B:2094:LEU:CB	2.34	0.76
1:A:101:LYS:O	1:A:104:GLU:N	2.19	0.76
1:A:1682:MET:CB	1:A:1686:ARG:CB	2.64	0.76
1:B:1178:GLU:O	1:B:1182:ARG:CB	2.34	0.76
1:B:140:ALA:N	1:B:146:ALA:O	2.19	0.75
1:A:977:ILE:O	1:A:981:ILE:N	2.18	0.75
1:B:1277:PHE:O	1:B:1280:ASN:N	2.20	0.75
1:B:1284:CYS:O	1:B:1286:GLU:N	2.19	0.74
1:B:1631:ARG:O	1:B:1634:LEU:N	2.20	0.74
1:A:1857:LYS:O	1:A:1859:PHE:N	2.20	0.74
1:B:282:TRP:HA	1:B:306:LYS:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:THR:O	1:A:1050:LEU:N	2.20	0.74
1:A:1859:PHE:O	1:A:1862:ARG:N	2.21	0.74
1:B:2040:THR:O	1:B:2044:GLN:CB	2.36	0.74
1:A:781:PHE:O	1:A:784:LEU:N	2.21	0.73
1:B:1286:GLU:O	1:B:1289:GLU:O	2.06	0.73
1:A:573:TYR:O	1:A:577:GLN:N	2.21	0.73
1:A:565:GLN:O	1:A:567:TYR:N	2.21	0.73
1:A:1194:VAL:O	1:A:1197:SER:N	2.22	0.73
1:B:2186:GLU:O	1:B:2189:ALA:N	2.21	0.73
1:B:125:HIS:O	1:B:129:ASN:N	2.21	0.73
1:A:769:SER:CB	1:A:779:ALA:HA	2.19	0.73
1:A:595:ILE:O	1:A:598:LEU:CB	2.37	0.72
1:B:1051:ASP:O	1:B:1055:HIS:N	2.21	0.72
1:A:782:CYS:O	1:A:785:MET:CB	2.37	0.72
1:A:2189:ALA:O	1:A:2191:HIS:N	2.22	0.72
1:B:1632:PRO:O	1:B:1635:LEU:N	2.23	0.72
1:A:1208:MET:O	1:A:1212:ALA:HB2	1.88	0.72
1:A:2003:LEU:O	1:A:2007:ASP:N	2.17	0.72
1:B:2089:ASN:O	1:B:2093:LYS:CB	2.37	0.72
1:A:1802:GLY:O	1:A:1804:SER:N	2.22	0.71
1:B:1115:ILE:O	1:B:1117:GLN:N	2.23	0.71
1:B:684:GLU:O	1:B:687:LEU:N	2.24	0.71
1:B:2151:VAL:O	1:B:2155:ILE:N	2.21	0.71
1:B:1228:THR:HA	1:B:1271:VAL:CB	2.21	0.71
1:A:371:ASP:CB	1:A:389:ARG:O	2.39	0.71
1:B:740:PHE:O	1:B:742:ARG:N	2.24	0.71
1:B:2083:LEU:O	1:B:2086:GLU:N	2.24	0.70
1:B:1129:SER:O	1:B:1133:VAL:N	2.24	0.70
1:A:1118:ASP:O	1:A:1119:LEU:C	2.31	0.69
1:A:203:ASN:O	1:A:205:GLY:N	2.26	0.69
1:B:1850:LYS:O	1:B:1851:LYS:C	2.31	0.69
1:A:830:LYS:O	1:A:833:PHE:N	2.25	0.69
1:A:898:VAL:C	1:A:900:VAL:HA	2.12	0.69
1:B:1632:PRO:O	1:B:1634:LEU:N	2.26	0.69
1:A:2075:PRO:O	1:A:2080:ARG:CB	2.40	0.69
1:B:696:VAL:O	1:B:697:TRP:C	2.31	0.69
1:B:894:ILE:O	1:B:897:CYS:N	2.26	0.69
1:A:719:ALA:HB1	1:A:727:ARG:CB	2.23	0.69
1:A:1796:CYS:O	1:A:1800:LYS:N	2.23	0.68
1:A:783:ARG:O	1:A:784:LEU:C	2.31	0.68
1:B:971:LYS:O	1:B:974:ILE:N	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:VAL:O	1:B:989:ARG:N	2.26	0.68
1:A:1122:LEU:O	1:A:1125:ILE:N	2.26	0.68
1:A:1184:SER:O	1:A:1187:CYS:N	2.27	0.68
1:B:188:ASN:O	1:B:190:GLY:N	2.26	0.68
1:B:653:CYS:O	1:B:656:VAL:CB	2.42	0.68
1:A:852:PHE:O	1:A:856:ASP:CB	2.41	0.68
1:B:2149:ARG:O	1:B:2153:HIS:N	2.27	0.68
1:A:1807:VAL:O	1:A:1809:ASP:N	2.26	0.68
1:B:118:GLY:N	1:B:163:ILE:O	2.23	0.68
1:B:765:LEU:O	1:B:769:SER:N	2.23	0.68
1:B:1387:GLY:O	1:B:1389:ASN:N	2.27	0.68
1:A:725:GLU:O	1:A:729:ILE:N	2.20	0.68
1:A:1682:MET:O	1:A:1686:ARG:N	2.27	0.67
1:B:469:GLU:O	1:B:472:SER:N	2.28	0.67
1:B:1214:VAL:O	1:B:1216:GLU:N	2.28	0.67
1:B:1488:THR:O	1:B:1492:SER:N	2.27	0.67
1:B:1682:MET:O	1:B:1685:ASP:C	2.33	0.67
1:B:1682:MET:O	1:B:1685:ASP:N	2.26	0.67
1:A:975:ILE:O	1:A:979:GLN:CB	2.43	0.67
1:A:1124:SER:O	1:A:1127:GLU:N	2.27	0.67
1:A:985:ARG:O	1:A:989:ARG:CB	2.43	0.67
1:A:840:VAL:O	1:A:843:TYR:N	2.28	0.67
1:A:1378:VAL:O	1:A:1382:ALA:HB2	1.95	0.67
1:B:678:GLU:O	1:B:686:ALA:HB2	1.95	0.67
1:A:386:SER:O	1:A:432:ILE:N	2.17	0.67
1:A:856:ASP:O	1:A:860:ASN:CB	2.43	0.67
1:A:2083:LEU:O	1:A:2087:LEU:CB	2.42	0.66
1:A:565:GLN:C	1:A:567:TYR:H	1.97	0.66
1:A:1076:VAL:O	1:A:1079:ALA:HB3	1.96	0.66
1:A:997:PHE:O	1:A:999:ARG:N	2.27	0.66
1:B:1289:GLU:O	1:B:1291:VAL:N	2.27	0.66
1:B:1650:GLY:O	1:B:1653:CYS:N	2.29	0.66
1:A:1798:LEU:HA	1:A:1802:GLY:HA3	1.78	0.66
1:B:1212:ALA:O	1:B:1216:GLU:CB	2.43	0.66
1:A:125:HIS:O	1:A:129:ASN:CA	2.44	0.66
1:A:682:THR:O	1:A:686:ALA:HB3	1.96	0.66
1:A:2189:ALA:O	1:A:2192:THR:N	2.29	0.66
1:B:628:PRO:O	1:B:632:ASP:N	2.21	0.66
1:B:1635:LEU:O	1:B:1639:ASN:CA	2.43	0.66
1:A:888:THR:O	1:A:891:LEU:CB	2.44	0.66
1:B:1822:GLU:O	1:B:1826:LEU:N	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2194:GLN:O	1:B:2196:GLU:N	2.27	0.66
1:A:1080:LEU:O	1:A:1083:LEU:CB	2.44	0.65
1:A:1623:SER:O	1:A:1626:VAL:N	2.29	0.65
1:A:783:ARG:O	1:A:786:LEU:N	2.29	0.65
1:B:179:GLY:N	1:B:220:ILE:O	2.25	0.65
1:B:11:ILE:N	1:B:113:THR:O	2.25	0.65
1:B:972:LEU:O	1:B:976:GLU:CB	2.44	0.65
1:A:1224:LYS:HA	1:A:1270:ALA:HB3	1.77	0.65
1:A:1969:LEU:O	1:A:1972:LEU:N	2.30	0.65
1:A:1207:ASN:O	1:A:1210:ALA:N	2.29	0.65
1:A:387:TYR:HA	1:A:430:PHE:O	1.97	0.65
1:A:469:GLU:O	1:A:472:SER:N	2.29	0.65
1:A:789:HIS:O	1:A:791:ASP:N	2.29	0.65
1:B:285:GLU:O	1:B:303:PHE:HA	1.97	0.65
1:A:1203:ARG:CB	1:A:1207:ASN:CB	2.74	0.65
1:B:552:ILE:O	1:B:555:LEU:CB	2.45	0.65
1:A:1273:MET:O	1:A:1276:ILE:N	2.31	0.64
1:B:1417:GLU:CB	1:B:1421:ALA:HB2	2.27	0.64
1:B:2188:TYR:O	1:B:2192:THR:CB	2.45	0.64
1:A:2168:GLU:O	1:A:2172:MET:CB	2.45	0.64
1:B:2068:LEU:O	1:B:2071:ASN:O	2.14	0.64
1:A:476:LEU:O	1:A:478:GLU:N	2.29	0.64
1:A:1973:GLN:O	1:A:1976:CYS:N	2.31	0.64
1:B:1635:LEU:HA	1:B:1646:CYS:CB	2.28	0.64
1:A:1208:MET:O	1:A:1212:ALA:HB3	1.96	0.64
1:B:1432:ASP:O	1:B:1493:PRO:C	2.36	0.64
1:A:2114:ASN:O	1:A:2116:ARG:N	2.30	0.64
1:B:1199:LYS:O	1:B:1202:GLN:N	2.31	0.64
1:B:833:PHE:O	1:B:836:THR:N	2.31	0.64
1:A:2189:ALA:O	1:A:2193:ALA:N	2.20	0.64
1:B:766:ARG:O	1:B:768:MET:N	2.31	0.64
1:B:666:ILE:CB	1:B:670:LEU:H	2.10	0.63
1:B:841:GLU:O	1:B:844:LEU:N	2.30	0.63
1:B:1653:CYS:O	1:B:1656:ILE:N	2.31	0.63
1:A:1245:CYS:CB	1:A:1285:SER:O	2.46	0.63
1:B:985:ARG:O	1:B:989:ARG:CB	2.46	0.63
1:A:588:ASP:CB	1:A:591:ALA:HB2	2.28	0.63
1:B:1115:ILE:C	1:B:1117:GLN:H	2.02	0.63
1:B:1634:LEU:O	1:B:1638:GLU:CB	2.47	0.63
1:A:523:LEU:O	1:A:524:GLN:C	2.35	0.63
1:A:1807:VAL:O	1:A:1808:ILE:C	2.37	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:HIS:O	1:A:1240:PHE:N	2.32	0.63
1:A:1859:PHE:O	1:A:1860:TYR:C	2.36	0.63
1:A:844:LEU:O	1:A:847:VAL:CB	2.46	0.63
1:A:968:MET:O	1:A:971:LYS:CB	2.47	0.63
1:A:2119:GLU:O	1:A:2123:VAL:CB	2.47	0.63
1:B:682:THR:O	1:B:686:ALA:HB3	1.98	0.63
1:B:1225:ALA:HB1	1:B:1226:GLU:HA	1.81	0.63
1:B:1668:GLU:O	1:B:1671:CYS:N	2.31	0.63
1:A:707:ILE:O	1:A:709:SER:N	2.32	0.63
1:A:1859:PHE:O	1:A:1861:ASP:N	2.32	0.63
1:A:977:ILE:O	1:A:981:ILE:CB	2.47	0.62
1:B:842:GLU:O	1:B:845:ARG:N	2.32	0.62
1:B:1313:GLN:O	1:B:1316:VAL:N	2.32	0.62
1:B:986:LEU:O	1:B:988:TYR:N	2.32	0.62
1:B:1638:GLU:O	1:B:1640:THR:CA	2.47	0.62
1:B:1849:ASP:O	1:B:1850:LYS:C	2.38	0.62
1:B:2088:LYS:O	1:B:2092:SER:N	2.31	0.62
1:B:2129:MET:O	1:B:2131:GLY:N	2.31	0.62
1:A:844:LEU:O	1:A:847:VAL:CA	2.47	0.62
1:B:1483:MET:CB	1:B:1886:LYS:CB	2.77	0.62
1:A:846:ASP:O	1:A:849:CYS:CB	2.48	0.62
1:A:1245:CYS:CB	1:A:1341:VAL:N	2.62	0.62
1:B:862:LEU:O	1:B:863:THR:C	2.38	0.62
1:A:598:LEU:HA	1:A:602:ASN:CB	2.29	0.62
1:B:1231:GLN:HA	1:B:1275:HIS:CB	2.29	0.62
1:B:856:ASP:O	1:B:857:LYS:O	2.18	0.62
1:B:1086:HIS:O	1:B:1088:SER:N	2.32	0.62
1:B:841:GLU:O	1:B:844:LEU:CB	2.48	0.62
1:A:269:ARG:HG3	2:A:3000:I3P:O4	2.00	0.62
1:A:888:THR:O	1:A:891:LEU:N	2.33	0.62
1:A:1134:TYR:O	1:A:1230:MET:N	2.33	0.62
1:B:680:VAL:C	1:B:682:THR:N	2.51	0.62
1:B:694:GLU:O	1:B:696:VAL:C	2.38	0.62
1:B:1222:TYR:CB	1:B:1272:THR:CB	2.77	0.62
1:B:1846:LEU:O	1:B:1853:GLU:CB	2.47	0.62
1:A:898:VAL:O	1:A:900:VAL:N	2.32	0.61
1:A:981:ILE:O	1:A:985:ARG:CB	2.48	0.61
1:A:866:VAL:O	1:A:869:LEU:CB	2.48	0.61
1:A:1476:LYS:O	1:A:1479:THR:N	2.30	0.61
1:B:743:MET:HA	1:B:744:CYS:CB	2.30	0.61
1:B:1991:ASN:CB	1:B:1998:LEU:HA	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:TYR:O	1:A:1115:ILE:N	2.33	0.61
1:A:1134:TYR:C	1:A:1230:MET:N	2.54	0.61
1:A:1007:GLN:O	1:A:1009:SER:N	2.33	0.61
1:B:567:TYR:CE1	1:B:569:LYS:HB3	2.36	0.61
1:A:437:PRO:O	1:A:440:VAL:CB	2.49	0.61
1:A:1477:TYR:O	1:A:1481:ILE:CB	2.49	0.61
1:B:621:LEU:O	1:B:625:ASN:O	2.19	0.61
1:B:1640:THR:CB	1:B:1646:CYS:CB	2.79	0.61
1:A:1371:LEU:O	1:A:1372:MET:C	2.39	0.61
1:A:1798:LEU:CA	1:A:1802:GLY:HA3	2.31	0.61
1:A:1816:SER:C	1:A:1818:ARG:H	2.04	0.61
1:B:622:VAL:O	1:B:626:ARG:HA	2.00	0.61
1:B:696:VAL:O	1:B:699:PHE:N	2.34	0.61
1:B:2150:ASN:O	1:B:2154:ASN:N	2.34	0.61
1:A:475:LYS:O	1:A:478:GLU:CB	2.48	0.60
1:A:1797:HIS:O	1:A:1798:LEU:C	2.39	0.60
1:A:769:SER:HA	1:A:773:LEU:CB	2.31	0.60
1:B:1631:ARG:O	1:B:1632:PRO:C	2.40	0.60
1:A:833:PHE:O	1:A:836:THR:CB	2.50	0.60
1:A:1422:TYR:O	1:A:1426:LEU:CB	2.49	0.60
1:B:857:LYS:O	1:B:858:GLU:C	2.39	0.60
1:B:2178:GLN:CB	1:B:2183:GLU:CB	2.79	0.60
1:B:2110:ARG:O	1:B:2113:TYR:CB	2.49	0.60
1:A:885:LEU:O	1:A:888:THR:N	2.35	0.60
1:A:1795:GLN:HA	1:A:1798:LEU:CB	2.31	0.60
1:B:1449:LEU:O	1:B:1453:PHE:CB	2.49	0.60
1:B:1813:ASN:C	1:B:1818:ARG:CB	2.70	0.60
1:A:625:ASN:CB	1:A:628:PRO:HA	2.32	0.60
1:A:864:PHE:O	1:A:865:GLU:C	2.36	0.60
1:A:2123:VAL:O	1:A:2127:ALA:HB3	2.02	0.60
1:B:782:CYS:O	1:B:785:MET:CB	2.50	0.60
1:B:1126:VAL:O	1:B:1129:SER:CB	2.49	0.60
1:A:1033:ILE:HA	1:A:1036:GLN:CB	2.32	0.60
1:A:1207:ASN:O	1:A:1209:GLY:N	2.35	0.60
1:A:1252:GLN:O	1:A:1256:HIS:CA	2.49	0.60
1:A:480:LEU:O	1:A:481:VAL:C	2.40	0.60
1:A:1222:TYR:CB	1:A:1272:THR:CB	2.80	0.60
1:B:682:THR:O	1:B:686:ALA:CB	2.50	0.60
1:B:742:ARG:CB	1:B:1040:ILE:CB	2.80	0.60
1:B:961:GLU:O	1:B:965:ILE:CB	2.50	0.60
1:B:982:LEU:O	1:B:984:VAL:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:VAL:O	1:A:899:HIS:C	2.40	0.60
1:B:232:ASP:O	1:B:384:ARG:N	2.29	0.60
1:B:779:ALA:O	1:B:782:CYS:CB	2.50	0.60
1:B:973:LYS:O	1:B:977:ILE:CB	2.50	0.60
1:A:2076:LEU:CA	1:A:2080:ARG:CB	2.80	0.59
1:B:1631:ARG:O	1:B:1632:PRO:O	2.19	0.59
1:B:1798:LEU:HA	1:B:1802:GLY:N	2.17	0.59
1:B:1813:ASN:O	1:B:1815:SER:O	2.20	0.59
1:A:699:PHE:O	1:A:702:ASP:CB	2.50	0.59
1:A:1076:VAL:O	1:A:1080:LEU:N	2.26	0.59
1:B:1214:VAL:O	1:B:1215:LEU:C	2.39	0.59
1:B:1476:LYS:CB	1:B:1953:LYS:HA	2.32	0.59
1:B:893:ALA:O	1:B:896:ASP:N	2.35	0.59
1:A:978:LEU:O	1:A:979:GLN:C	2.36	0.59
1:A:998:LYS:O	1:A:1007:GLN:HA	2.02	0.59
1:A:1376:HIS:O	1:A:1380:LEU:CB	2.50	0.59
1:B:770:ASP:O	1:B:773:LEU:N	2.34	0.59
1:B:1654:LYS:O	1:B:1655:LEU:C	2.41	0.59
1:B:2197:ILE:HA	1:B:2212:PRO:CB	2.32	0.59
1:A:1194:VAL:O	1:A:1197:SER:CB	2.51	0.59
1:A:2114:ASN:C	1:A:2116:ARG:N	2.54	0.59
1:B:242:LEU:O	1:B:251:LEU:N	2.33	0.59
1:A:581:MET:O	1:A:585:ILE:CB	2.50	0.59
1:A:666:ILE:CB	1:A:670:LEU:N	2.66	0.59
1:A:870:ALA:HA	1:A:873:LEU:CB	2.31	0.59
1:A:1294:HIS:O	1:A:1298:CYS:CB	2.50	0.59
1:B:2161:GLN:O	1:B:2168:GLU:CB	2.50	0.59
1:B:595:ILE:O	1:B:596:THR:C	2.39	0.59
1:B:684:GLU:O	1:B:687:LEU:CB	2.51	0.59
1:B:893:ALA:O	1:B:894:ILE:C	2.40	0.59
1:B:185:ASN:HA	1:B:192:PRO:CB	2.32	0.59
1:B:610:ILE:O	1:B:613:ALA:HB3	2.02	0.59
1:B:1289:GLU:C	1:B:1291:VAL:N	2.53	0.59
1:B:1640:THR:CB	1:B:1644:ARG:CB	2.81	0.59
1:B:1649:GLY:O	1:B:1650:GLY:C	2.40	0.59
1:B:2083:LEU:O	1:B:2084:VAL:C	2.40	0.59
1:A:770:ASP:O	1:A:772:ASN:O	2.21	0.59
1:A:1417:GLU:O	1:A:1418:VAL:C	2.40	0.59
1:A:1805:ASN:O	1:A:1808:ILE:N	2.36	0.59
1:B:981:ILE:O	1:B:985:ARG:CB	2.51	0.59
1:A:2032:ILE:O	1:A:2035:THR:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2146:ALA:O	1:A:2148:PRO:N	2.35	0.58
1:A:1862:ARG:O	1:A:1866:ALA:HB2	2.02	0.58
1:B:2202:ARG:CB	1:B:2206:GLN:HA	2.33	0.58
1:B:588:ASP:CB	1:B:591:ALA:H	2.15	0.58
1:B:1850:LYS:O	1:B:1854:LYS:CB	2.52	0.58
1:B:2189:ALA:O	1:B:2193:ALA:HB3	2.04	0.58
1:A:2019:LEU:O	1:A:2021:GLY:N	2.37	0.58
1:B:679:GLY:O	1:B:681:SER:N	2.37	0.58
1:B:982:LEU:O	1:B:985:ARG:N	2.37	0.58
1:A:243:PHE:O	1:A:430:PHE:HA	2.04	0.58
1:A:777:LEU:O	1:A:780:SER:CB	2.51	0.58
1:A:1215:LEU:O	1:A:1217:LEU:N	2.37	0.58
1:A:1251:ASN:CB	1:A:1283:LEU:HA	2.33	0.58
1:A:1860:TYR:O	1:A:1863:MET:N	2.35	0.58
1:B:1636:PHE:O	1:B:1638:GLU:N	2.36	0.58
1:A:867:VAL:O	1:A:868:ASN:C	2.40	0.58
1:A:1813:ASN:CB	1:A:1821:HIS:CB	2.82	0.58
1:B:2185:LEU:HA	1:B:2188:TYR:CB	2.33	0.58
1:A:781:PHE:O	1:A:783:ARG:N	2.36	0.58
1:A:1252:GLN:O	1:A:1256:HIS:CB	2.51	0.58
1:A:1807:VAL:C	1:A:1809:ASP:N	2.54	0.58
1:B:140:ALA:HB3	1:B:143:GLU:O	2.03	0.58
1:B:748:GLN:O	1:B:749:TYR:CB	2.52	0.58
1:B:2087:LEU:O	1:B:2091:ALA:CB	2.51	0.58
1:A:626:ARG:C	1:A:628:PRO:N	2.56	0.57
1:A:676:GLU:O	1:A:679:GLY:N	2.37	0.57
1:B:666:ILE:CB	1:B:670:LEU:N	2.67	0.57
1:B:1093:VAL:HA	1:B:1176:VAL:N	2.19	0.57
1:B:2203:THR:O	1:B:2204:MET:CB	2.51	0.57
1:A:749:TYR:O	1:A:751:ALA:N	2.37	0.57
1:B:985:ARG:O	1:B:989:ARG:N	2.37	0.57
1:A:1076:VAL:HA	1:A:1079:ALA:CB	2.34	0.57
1:A:1197:SER:O	1:A:1200:GLN:N	2.37	0.57
1:A:1833:GLY:C	1:A:1835:ASN:H	2.08	0.57
1:A:2189:ALA:C	1:A:2193:ALA:H	2.07	0.57
1:B:588:ASP:C	1:B:590:LEU:N	2.57	0.57
1:B:680:VAL:C	1:B:682:THR:H	2.06	0.57
1:B:737:LEU:O	1:B:739:LEU:N	2.36	0.57
1:B:2000:CYS:O	1:B:2001:GLU:C	2.42	0.57
1:A:480:LEU:C	1:A:482:TYR:N	2.56	0.57
1:B:1287:ILE:O	1:B:1288:ASN:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PHE:HA	1:A:416:LEU:O	2.05	0.57
1:A:1840:HIS:O	1:A:1841:SER:C	2.43	0.57
1:B:469:GLU:O	1:B:471:ARG:N	2.37	0.57
1:B:593:ASP:O	1:B:594:THR:C	2.43	0.57
1:A:681:SER:O	1:A:682:THR:O	2.23	0.57
1:B:1843:PHE:O	1:B:1846:LEU:N	2.37	0.57
1:B:2129:MET:O	1:B:2130:GLN:C	2.43	0.57
1:B:985:ARG:HA	1:B:989:ARG:CB	2.34	0.57
1:A:503:ASN:O	1:A:507:GLN:HG3	2.04	0.56
1:A:653:CYS:O	1:A:656:VAL:CB	2.53	0.56
1:A:715:LEU:O	1:A:716:ALA:C	2.42	0.56
1:B:775:TYR:O	1:B:776:ASP:CB	2.53	0.56
1:B:974:ILE:O	1:B:978:LEU:CB	2.53	0.56
1:B:1240:PHE:CB	1:B:1244:PHE:O	2.53	0.56
1:B:2193:ALA:O	1:B:2195:ILE:N	2.35	0.56
1:A:978:LEU:O	1:A:982:LEU:CB	2.54	0.56
1:A:1061:LEU:HA	1:A:1101:GLN:CB	2.35	0.56
1:A:1178:GLU:O	1:A:1182:ARG:CB	2.53	0.56
1:B:14:ILE:HA	1:B:58:PHE:O	2.05	0.56
1:B:282:TRP:CA	1:B:306:LYS:O	2.53	0.56
1:B:576:LYS:C	1:B:578:PHE:N	2.58	0.56
1:B:766:ARG:C	1:B:768:MET:N	2.57	0.56
1:B:976:GLU:O	1:B:978:LEU:N	2.38	0.56
1:B:1052:LEU:O	1:B:1057:GLY:N	2.39	0.56
1:B:1653:CYS:O	1:B:1654:LYS:C	2.43	0.56
1:B:1798:LEU:HA	1:B:1802:GLY:CA	2.35	0.56
1:A:708:ARG:H	1:A:711:SER:CB	2.18	0.56
1:A:1842:PHE:O	1:A:1843:PHE:C	2.44	0.56
1:A:1857:LYS:C	1:A:1859:PHE:H	2.08	0.56
1:A:2194:GLN:N	1:A:2216:GLU:CB	2.68	0.56
1:B:753:ASN:O	1:B:756:SER:CB	2.54	0.56
1:B:2111:ILE:O	1:B:2112:LEU:C	2.44	0.56
1:A:1863:MET:O	1:A:1867:GLN:CB	2.54	0.56
1:B:1245:CYS:CB	1:B:1285:SER:CB	2.82	0.56
1:A:704:ASN:C	1:A:706:GLU:H	2.09	0.56
1:A:726:ASP:O	1:A:727:ARG:C	2.44	0.56
1:B:503:ASN:O	1:B:507:GLN:HG3	2.06	0.56
1:A:519:ILE:O	1:A:522:LEU:N	2.34	0.56
1:A:552:ILE:O	1:A:555:LEU:CB	2.54	0.56
1:B:1657:LYS:O	1:B:1660:LYS:N	2.33	0.56
1:A:978:LEU:O	1:A:979:GLN:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:PHE:O	1:A:998:LYS:C	2.45	0.56
1:B:1230:MET:O	1:B:1234:MET:CB	2.54	0.56
1:A:1679:ARG:O	1:A:1682:MET:CB	2.53	0.56
1:A:1998:LEU:O	1:A:2000:CYS:N	2.39	0.56
1:B:743:MET:CA	1:B:744:CYS:CB	2.84	0.56
1:A:15:CYS:CB	1:A:222:LEU:HA	2.36	0.55
1:A:967:VAL:O	1:A:968:MET:C	2.44	0.55
1:A:1081:GLN:O	1:A:1082:LEU:C	2.42	0.55
1:A:1682:MET:HA	1:A:1686:ARG:H	1.71	0.55
1:A:2185:LEU:HA	1:A:2188:TYR:CB	2.36	0.55
1:B:848:VAL:O	1:B:850:GLN:N	2.39	0.55
1:B:1650:GLY:O	1:B:1651:PHE:C	2.45	0.55
1:B:2049:GLU:O	1:B:2053:CYS:CB	2.54	0.55
1:A:1061:LEU:O	1:A:1065:LEU:N	2.31	0.55
1:A:1188:VAL:O	1:A:1191:SER:N	2.39	0.55
1:A:1209:GLY:O	1:A:1213:VAL:CB	2.54	0.55
1:B:982:LEU:O	1:B:983:ASN:C	2.44	0.55
1:A:845:ARG:O	1:A:848:VAL:N	2.39	0.55
1:A:899:HIS:N	1:A:900:VAL:HA	2.21	0.55
1:B:763:LEU:O	1:B:764:ILE:C	2.44	0.55
1:B:849:CYS:O	1:B:850:GLN:C	2.45	0.55
1:B:856:ASP:O	1:B:860:ASN:N	2.29	0.55
1:B:1228:THR:CB	1:B:1271:VAL:CB	2.85	0.55
1:B:1851:LYS:O	1:B:1855:PHE:CB	2.54	0.55
1:B:782:CYS:O	1:B:785:MET:CA	2.54	0.55
1:B:2001:GLU:O	1:B:2004:GLN:N	2.39	0.55
1:B:729:ILE:O	1:B:732:TYR:CB	2.55	0.55
1:B:854:PHE:O	1:B:857:LYS:CB	2.55	0.55
1:A:867:VAL:HA	1:A:870:ALA:HB3	1.89	0.55
1:A:974:ILE:O	1:A:975:ILE:C	2.44	0.55
1:A:1096:ALA:O	1:A:1100:VAL:N	2.39	0.55
1:B:1251:ASN:CB	1:B:1283:LEU:HA	2.37	0.55
1:A:988:TYR:O	1:A:989:ARG:C	2.45	0.55
1:B:1327:GLN:O	1:B:1330:VAL:CB	2.54	0.55
1:A:1116:LYS:O	1:A:1117:GLN:C	2.44	0.55
1:A:2150:ASN:O	1:A:2151:VAL:C	2.44	0.55
1:A:777:LEU:O	1:A:780:SER:N	2.40	0.54
1:A:1335:VAL:O	1:A:1384:CYS:CB	2.55	0.54
1:A:2003:LEU:O	1:A:2007:ASP:CB	2.55	0.54
1:B:567:TYR:CD2	1:B:570:ASN:HB2	2.42	0.54
1:B:2044:GLN:C	1:B:2046:PRO:N	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:HA	1:A:96:ALA:CB	2.36	0.54
1:A:2131:GLY:HA3	1:A:2147:SER:CB	2.37	0.54
1:B:588:ASP:CB	1:B:591:ALA:N	2.71	0.54
1:B:1489:PHE:HA	1:B:1493:PRO:HA	1.89	0.54
1:B:1623:SER:O	1:B:1626:VAL:CB	2.55	0.54
1:A:773:LEU:CB	1:A:778:ARG:CB	2.85	0.54
1:A:1129:SER:CB	1:A:1180:LEU:HA	2.37	0.54
1:A:1345:TYR:O	1:A:1350:SER:CB	2.55	0.54
1:A:1627:ASP:O	1:A:1630:HIS:N	2.41	0.54
1:B:991:SER:O	1:B:994:LEU:CB	2.55	0.54
1:A:992:CYS:O	1:A:993:LEU:C	2.46	0.54
1:A:2122:GLU:O	1:A:2126:LYS:CB	2.55	0.54
1:B:1053:ASP:O	1:B:1057:GLY:HA3	2.08	0.54
1:B:1840:HIS:O	1:B:1841:SER:C	2.43	0.54
1:A:710:LYS:HA	1:A:713:ARG:CB	2.38	0.54
1:A:862:LEU:O	1:A:863:THR:C	2.45	0.54
1:A:976:GLU:HA	1:A:979:GLN:CB	2.37	0.54
1:B:590:LEU:O	1:B:593:ASP:N	2.35	0.54
1:B:2184:ALA:O	1:B:2188:TYR:CB	2.55	0.54
1:A:573:TYR:O	1:A:577:GLN:CB	2.55	0.54
1:A:1954:ASP:O	1:A:1955:ASP:C	2.45	0.54
1:B:2015:GLY:O	1:B:2067:ALA:HB1	2.07	0.54
1:A:980:PHE:O	1:A:981:ILE:C	2.45	0.54
1:B:652:ILE:O	1:B:655:ALA:HB3	2.08	0.54
1:B:786:LEU:O	1:B:789:HIS:N	2.40	0.54
1:B:894:ILE:O	1:B:895:LEU:C	2.45	0.54
1:B:1275:HIS:O	1:B:1279:ASN:CB	2.56	0.54
1:B:1403:ASP:HA	1:B:1406:VAL:CB	2.38	0.54
1:B:1986:PHE:O	1:B:1988:ARG:C	2.46	0.54
1:A:838:GLU:O	1:A:841:GLU:N	2.41	0.54
1:B:510:MET:SD	1:B:515:ILE:CB	2.96	0.54
1:B:707:ILE:CB	1:B:1046:GLU:CB	2.85	0.54
1:B:1625:LEU:O	1:B:1628:VAL:CB	2.56	0.54
1:B:1833:GLY:C	1:B:1835:ASN:H	2.11	0.54
1:A:268:GLY:CA	2:A:3000:I3P:O42	2.55	0.54
1:A:780:SER:O	1:A:783:ARG:CB	2.55	0.54
1:A:1476:LYS:CB	1:A:1883:ASN:HA	2.38	0.54
1:B:666:ILE:CB	1:B:667:GLU:C	2.76	0.54
1:B:1379:GLU:O	1:B:1382:ALA:HB3	2.08	0.54
1:A:1076:VAL:HA	1:A:1079:ALA:HB3	1.89	0.54
1:B:621:LEU:O	1:B:622:VAL:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:GLU:O	1:B:680:VAL:O	2.26	0.54
1:B:998:LYS:O	1:B:999:ARG:CB	2.56	0.54
1:B:1191:SER:CB	1:B:1236:LEU:O	2.56	0.54
1:A:1636:PHE:O	1:A:1638:GLU:N	2.41	0.53
1:A:1679:ARG:HA	1:A:1682:MET:CB	2.38	0.53
1:B:105:THR:O	1:B:106:GLU:C	2.45	0.53
1:B:871:ARG:O	1:B:872:ASN:C	2.47	0.53
1:B:1378:VAL:O	1:B:1382:ALA:HB2	2.08	0.53
1:A:564:GLN:O	1:A:571:GLN:HG3	2.08	0.53
1:A:1972:LEU:O	1:A:1975:LEU:CB	2.56	0.53
1:B:590:LEU:O	1:B:592:GLU:N	2.40	0.53
1:A:1371:LEU:O	1:A:1374:HIS:N	2.41	0.53
1:A:1839:GLN:O	1:A:1840:HIS:C	2.47	0.53
1:B:678:GLU:CB	1:B:686:ALA:HA	2.38	0.53
1:B:769:SER:O	1:B:773:LEU:HA	2.08	0.53
1:B:2190:LYS:O	1:B:2195:ILE:CB	2.56	0.53
1:A:781:PHE:C	1:A:783:ARG:N	2.61	0.53
1:A:1316:VAL:HA	1:A:1319:GLU:CB	2.38	0.53
1:A:1820:PHE:O	1:A:1823:SER:N	2.42	0.53
1:B:1238:HIS:O	1:B:1240:PHE:N	2.42	0.53
1:B:729:ILE:O	1:B:732:TYR:N	2.42	0.53
1:A:682:THR:C	1:A:686:ALA:HB3	2.29	0.53
1:A:1476:LYS:CB	1:A:1884:LYS:HA	2.39	0.53
1:B:188:ASN:C	1:B:190:GLY:N	2.62	0.53
1:B:870:ALA:O	1:B:874:ILE:N	2.37	0.53
1:B:1377:LEU:O	1:B:1381:LEU:CB	2.57	0.53
1:B:594:THR:O	1:B:597:ALA:HB3	2.09	0.53
1:A:860:ASN:O	1:A:861:LYS:C	2.46	0.53
1:A:1654:LYS:O	1:A:1656:ILE:N	2.42	0.53
1:A:1839:GLN:O	1:A:1842:PHE:CA	2.57	0.53
1:A:1842:PHE:O	1:A:1845:ARG:N	2.42	0.53
1:A:1846:LEU:O	1:A:1847:THR:C	2.45	0.53
1:B:681:SER:O	1:B:682:THR:C	2.45	0.53
1:B:1093:VAL:O	1:B:1095:GLN:N	2.42	0.53
1:B:1863:MET:O	1:B:1864:LYS:C	2.46	0.53
1:A:1864:LYS:O	1:A:1865:VAL:C	2.46	0.53
1:A:1998:LEU:C	1:A:2000:CYS:H	2.12	0.53
1:A:1998:LEU:C	1:A:2000:CYS:N	2.60	0.53
1:B:707:ILE:O	1:B:708:ARG:CB	2.57	0.53
1:A:772:ASN:O	1:A:774:PRO:N	2.41	0.53
1:A:863:THR:O	1:A:866:VAL:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1287:ILE:HA	1:A:1344:PHE:CB	2.38	0.53
1:A:1809:ASP:O	1:A:1811:ILE:N	2.42	0.53
1:B:781:PHE:O	1:B:784:LEU:CB	2.57	0.53
1:B:549:PHE:O	1:B:551:HIS:N	2.43	0.52
1:B:1682:MET:C	1:B:1686:ARG:H	2.12	0.52
1:A:1817:ASP:O	1:A:1821:HIS:CB	2.57	0.52
1:A:181:LYS:HA	1:A:218:TRP:O	2.10	0.52
1:A:520:PHE:C	1:A:522:LEU:H	2.12	0.52
1:B:1194:VAL:N	1:B:1197:SER:CB	2.72	0.52
1:B:1289:GLU:O	1:B:1290:ARG:C	2.47	0.52
1:B:2092:SER:O	1:B:2096:LEU:CB	2.57	0.52
1:A:769:SER:O	1:A:773:LEU:CB	2.58	0.52
1:B:1638:GLU:O	1:B:1640:THR:CB	2.58	0.52
1:A:969:ASP:O	1:A:970:THR:C	2.44	0.52
1:A:1245:CYS:CB	1:A:1285:SER:CB	2.88	0.52
1:B:200:LEU:N	1:B:206:CYS:O	2.43	0.52
1:B:1310:LYS:O	1:B:1311:PHE:CB	2.57	0.52
1:B:1827:ALA:O	1:B:1828:ILE:C	2.47	0.52
1:A:769:SER:O	1:A:772:ASN:O	2.27	0.52
1:A:1085:ARG:O	1:A:1087:PHE:N	2.43	0.52
1:A:1654:LYS:C	1:A:1656:ILE:N	2.63	0.52
1:B:870:ALA:O	1:B:873:LEU:CB	2.58	0.52
1:A:1317:LYS:CA	1:A:1323:ILE:CB	2.86	0.52
1:B:106:GLU:O	1:B:109:LYS:N	2.36	0.52
1:B:969:ASP:O	1:B:970:THR:C	2.47	0.52
1:A:830:LYS:O	1:A:833:PHE:CB	2.58	0.52
1:B:869:LEU:O	1:B:870:ALA:C	2.48	0.52
1:B:1682:MET:CB	1:B:1686:ARG:H	2.23	0.52
1:B:2152:GLY:O	1:B:2156:TYR:N	2.41	0.52
1:A:753:ASN:O	1:A:754:GLU:C	2.48	0.52
1:A:770:ASP:O	1:A:771:GLU:C	2.48	0.52
1:B:549:PHE:C	1:B:551:HIS:N	2.63	0.52
1:A:850:GLN:O	1:A:851:ARG:C	2.48	0.52
1:A:1477:TYR:HA	1:A:1881:LEU:C	2.31	0.52
1:A:474:THR:O	1:A:475:LYS:C	2.48	0.51
1:A:768:MET:O	1:A:772:ASN:C	2.48	0.51
1:B:269:ARG:NH2	2:B:3000:I3P:O51	2.34	0.51
1:B:1651:PHE:O	1:B:1652:ILE:C	2.48	0.51
1:B:1815:SER:O	1:B:1816:SER:C	2.49	0.51
1:B:2129:MET:O	1:B:2132:GLU:N	2.42	0.51
1:A:412:LYS:CB	1:A:1257:LYS:CB	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:GLU:O	1:A:689:ALA:C	2.48	0.51
1:A:1791:LEU:O	1:A:1795:GLN:CB	2.58	0.51
1:A:2178:GLN:CB	1:A:2183:GLU:CB	2.88	0.51
1:B:1193:SER:CB	1:B:1197:SER:CB	2.88	0.51
1:B:1682:MET:CB	1:B:1687:GLY:H	2.23	0.51
1:B:2086:GLU:O	1:B:2090:ASN:CB	2.58	0.51
1:A:683:GLY:O	1:A:685:ASN:N	2.44	0.51
1:A:708:ARG:O	1:A:712:VAL:CA	2.58	0.51
1:A:2020:LEU:O	1:A:2024:ILE:CA	2.52	0.51
1:A:2150:ASN:O	1:A:2152:GLY:N	2.44	0.51
1:B:829:ILE:O	1:B:832:ARG:N	2.44	0.51
1:A:588:ASP:C	1:A:590:LEU:N	2.62	0.51
1:A:978:LEU:HA	1:A:981:ILE:CB	2.40	0.51
1:B:568:ARG:O	1:B:572:GLU:HG3	2.11	0.51
1:B:892:LEU:O	1:B:893:ALA:O	2.29	0.51
1:A:475:LYS:O	1:A:476:LEU:C	2.49	0.51
1:A:476:LEU:C	1:A:478:GLU:N	2.58	0.51
1:A:781:PHE:O	1:A:782:CYS:C	2.49	0.51
1:B:986:LEU:C	1:B:988:TYR:N	2.64	0.51
1:B:1246:ALA:O	1:B:1248:ASN:N	2.43	0.51
1:B:1640:THR:CB	1:B:1644:ARG:O	2.59	0.51
1:B:1652:ILE:O	1:B:1653:CYS:C	2.49	0.51
1:A:118:GLY:N	1:A:163:ILE:O	2.42	0.51
1:A:469:GLU:O	1:A:470:ARG:C	2.48	0.51
1:A:683:GLY:O	1:A:684:GLU:C	2.49	0.51
1:A:867:VAL:O	1:A:871:ARG:CB	2.59	0.51
1:A:873:LEU:O	1:A:874:ILE:C	2.49	0.51
1:A:874:ILE:O	1:A:878:PHE:N	2.43	0.51
1:B:101:LYS:O	1:B:104:GLU:N	2.44	0.51
1:B:867:VAL:O	1:B:868:ASN:C	2.48	0.51
1:B:2186:GLU:O	1:B:2189:ALA:HB3	2.11	0.51
1:A:250:PHE:O	1:A:264:LEU:HA	2.11	0.51
1:A:1377:LEU:C	1:A:1381:LEU:H	2.15	0.51
1:B:199:GLN:HA	1:B:206:CYS:O	2.11	0.51
1:B:252:THR:O	1:B:262:VAL:HA	2.10	0.51
1:B:1231:GLN:CB	1:B:1275:HIS:CB	2.89	0.51
1:B:1214:VAL:O	1:B:1217:LEU:N	2.35	0.51
1:B:1489:PHE:HA	1:B:1493:PRO:CA	2.41	0.51
1:B:1682:MET:C	1:B:1686:ARG:N	2.62	0.51
1:A:763:LEU:O	1:A:764:ILE:C	2.49	0.51
1:B:52:LYS:O	1:B:54:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:HIS:O	1:A:129:ASN:HA	2.11	0.50
1:A:970:THR:HA	1:A:973:LYS:CB	2.41	0.50
1:B:750:LEU:O	1:B:751:ALA:C	2.48	0.50
1:A:559:VAL:O	1:A:562:HIS:CB	2.59	0.50
1:A:1213:VAL:HA	1:A:1216:GLU:CB	2.41	0.50
1:A:2060:ASN:O	1:A:2061:GLY:C	2.49	0.50
1:B:615:ILE:O	1:B:616:ASP:C	2.48	0.50
1:B:1813:ASN:O	1:B:1818:ARG:CB	2.58	0.50
1:B:1850:LYS:O	1:B:1852:SER:N	2.44	0.50
1:A:666:ILE:CB	1:A:671:VAL:H	2.25	0.50
1:A:1218:LEU:O	1:A:1221:PRO:O	2.30	0.50
1:B:552:ILE:O	1:B:555:LEU:CA	2.59	0.50
1:B:1190:GLU:O	1:B:1193:SER:CB	2.60	0.50
1:B:1816:SER:O	1:B:1817:ASP:CB	2.59	0.50
1:A:598:LEU:O	1:A:599:LEU:C	2.49	0.50
1:A:650:GLU:O	1:A:651:LEU:C	2.49	0.50
1:A:2035:THR:O	1:A:2039:LEU:CB	2.59	0.50
1:B:1293:GLN:CB	1:B:1345:TYR:O	2.59	0.50
1:B:1650:GLY:O	1:B:1653:CYS:CB	2.59	0.50
1:B:1973:GLN:O	1:B:1976:CYS:N	2.45	0.50
1:B:2014:THR:O	1:B:2067:ALA:HB2	2.11	0.50
1:A:588:ASP:O	1:A:591:ALA:HB3	2.11	0.50
1:B:1966:GLN:C	1:B:1970:ARG:H	2.15	0.50
1:B:2133:VAL:O	1:B:2134:GLU:C	2.47	0.50
1:B:282:TRP:CB	1:B:306:LYS:O	2.60	0.50
1:B:692:ASP:O	1:B:693:GLU:C	2.49	0.50
1:B:842:GLU:O	1:B:843:TYR:C	2.48	0.50
1:B:1293:GLN:HA	1:B:1345:TYR:HA	1.92	0.50
1:A:776:ASP:O	1:A:777:LEU:C	2.49	0.50
1:A:2146:ALA:O	1:A:2150:ASN:CB	2.59	0.50
1:B:666:ILE:CB	1:B:668:THR:N	2.75	0.50
1:B:888:THR:O	1:B:891:LEU:N	2.44	0.50
1:A:660:THR:O	1:A:662:ALA:N	2.45	0.50
1:A:1061:LEU:O	1:A:1064:LEU:CB	2.60	0.50
1:B:1470:ALA:O	1:B:1471:ASP:CB	2.60	0.50
1:B:1986:PHE:O	1:B:1987:LEU:C	2.50	0.50
1:A:628:PRO:O	1:A:631:LEU:CB	2.59	0.49
1:B:188:ASN:C	1:B:190:GLY:H	2.15	0.49
1:B:1682:MET:CA	1:B:1686:ARG:H	2.25	0.49
1:B:1798:LEU:O	1:B:1801:GLU:N	2.45	0.49
1:A:1612:ASP:O	1:A:1615:ARG:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LYS:O	1:B:236:GLY:C	2.50	0.49
1:B:316:ALA:HA	1:B:354:SER:O	2.12	0.49
1:B:666:ILE:CB	1:B:668:THR:C	2.81	0.49
1:B:694:GLU:O	1:B:695:GLU:C	2.50	0.49
1:B:1225:ALA:HA	1:B:1226:GLU:C	2.32	0.49
1:B:1292:VAL:O	1:B:1295:PHE:CB	2.60	0.49
1:B:1459:ARG:C	1:B:1461:CYS:H	2.15	0.49
1:B:1682:MET:C	1:B:1685:ASP:H	2.14	0.49
1:B:1823:SER:O	1:B:1824:ILE:C	2.48	0.49
1:B:2001:GLU:O	1:B:2002:THR:C	2.51	0.49
1:A:117:TYR:HA	1:A:163:ILE:O	2.12	0.49
1:A:392:HIS:O	1:A:396:ASN:N	2.45	0.49
1:A:666:ILE:CB	1:A:667:GLU:C	2.80	0.49
1:A:707:ILE:HA	1:A:710:LYS:CB	2.42	0.49
1:A:783:ARG:C	1:A:785:MET:N	2.63	0.49
1:A:992:CYS:O	1:A:994:LEU:N	2.45	0.49
1:A:1191:SER:CB	1:A:1236:LEU:O	2.61	0.49
1:B:762:ASP:O	1:B:766:ARG:N	2.24	0.49
1:A:748:GLN:CB	1:A:1074:PRO:CB	2.90	0.49
1:A:1605:ASP:O	1:A:1609:ALA:HB2	2.11	0.49
1:B:871:ARG:C	1:B:873:LEU:N	2.65	0.49
1:B:873:LEU:O	1:B:874:ILE:C	2.46	0.49
1:B:1215:LEU:O	1:B:1219:GLN:N	2.43	0.49
1:B:2082:ASP:O	1:B:2083:LEU:C	2.48	0.49
1:B:2162:LEU:HA	1:B:2168:GLU:CB	2.42	0.49
1:A:412:LYS:HA	1:A:1257:LYS:CB	2.43	0.49
1:A:742:ARG:O	1:A:743:MET:C	2.50	0.49
1:A:891:LEU:O	1:A:892:LEU:C	2.49	0.49
1:A:1090:ARG:O	1:A:1176:VAL:HA	2.12	0.49
1:A:1657:LYS:O	1:A:1660:LYS:N	2.44	0.49
1:B:473:VAL:O	1:B:474:THR:C	2.47	0.49
1:B:549:PHE:O	1:B:550:ARG:C	2.50	0.49
1:B:769:SER:CB	1:B:779:ALA:HB2	2.43	0.49
1:B:1042:GLY:O	1:B:1043:GLY:C	2.50	0.49
1:B:1064:LEU:O	1:B:1068:THR:N	2.46	0.49
1:B:1810:LEU:O	1:B:1813:ASN:CB	2.60	0.49
1:B:1791:LEU:O	1:B:1795:GLN:CB	2.61	0.49
1:A:1253:ALA:HA	1:A:1256:HIS:CB	2.43	0.49
1:A:2056:THR:O	1:A:2059:SER:N	2.45	0.49
1:B:10:HIS:HA	1:B:114:VAL:HA	1.93	0.49
1:A:388:VAL:N	1:A:430:PHE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:ASN:CB	1:A:1283:LEU:CA	2.90	0.49
1:A:1251:ASN:CB	1:A:1283:LEU:O	2.61	0.49
1:A:2189:ALA:O	1:A:2190:LYS:C	2.51	0.49
1:B:235:LYS:O	1:B:236:GLY:O	2.29	0.49
1:B:1130:GLU:HA	1:B:1133:VAL:O	2.12	0.49
1:A:833:PHE:O	1:A:836:THR:CA	2.61	0.49
1:A:897:CYS:C	1:A:899:HIS:H	2.14	0.49
1:A:1847:THR:O	1:A:1848:GLU:C	2.51	0.49
1:B:962:LYS:O	1:B:966:MET:CB	2.60	0.49
1:B:970:THR:O	1:B:973:LYS:CB	2.61	0.49
1:B:976:GLU:C	1:B:978:LEU:N	2.64	0.49
1:B:1094:LEU:O	1:B:1095:GLN:C	2.50	0.49
1:B:1677:THR:O	1:B:1680:GLU:N	2.39	0.49
1:B:2023:TYR:O	1:B:2025:ASN:N	2.46	0.49
1:A:750:LEU:O	1:A:751:ALA:C	2.51	0.49
1:A:1061:LEU:CB	1:A:1101:GLN:CB	2.91	0.49
1:A:1679:ARG:C	1:A:1682:MET:H	2.16	0.49
1:B:688:GLU:O	1:B:691:GLU:N	2.46	0.49
1:B:695:GLU:O	1:B:696:VAL:O	2.31	0.49
1:A:743:MET:O	1:A:744:CYS:C	2.50	0.48
1:A:838:GLU:O	1:A:840:VAL:N	2.46	0.48
1:B:469:GLU:C	1:B:471:ARG:N	2.65	0.48
1:B:1277:PHE:O	1:B:1278:MET:C	2.51	0.48
1:B:1884:LYS:CB	1:B:1886:LYS:H	2.27	0.48
1:A:1807:VAL:C	1:A:1809:ASP:H	2.16	0.48
1:B:1051:ASP:O	1:B:1055:HIS:CB	2.62	0.48
1:B:1193:SER:C	1:B:1197:SER:CB	2.82	0.48
1:B:1625:LEU:O	1:B:1628:VAL:CA	2.61	0.48
1:B:2088:LYS:O	1:B:2091:ALA:N	2.46	0.48
1:B:2182:ASP:O	1:B:2184:ALA:N	2.47	0.48
1:B:2182:ASP:C	1:B:2184:ALA:N	2.65	0.48
1:A:553:CYS:C	1:A:555:LEU:H	2.16	0.48
1:A:827:ASP:O	1:A:830:LYS:CB	2.61	0.48
1:A:1817:ASP:O	1:A:1818:ARG:C	2.51	0.48
1:B:224:MET:HA	1:B:293:ARG:CB	2.43	0.48
1:B:2111:ILE:C	1:B:2113:TYR:N	2.63	0.48
1:A:779:ALA:O	1:A:782:CYS:N	2.46	0.48
1:B:1290:ARG:O	1:B:1291:VAL:C	2.52	0.48
1:B:1460:ALA:O	1:B:1461:CYS:CB	2.62	0.48
1:A:751:ALA:O	1:A:752:ILE:C	2.52	0.48
1:B:1215:LEU:O	1:B:1219:GLN:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1480:GLU:CB	1:B:1883:ASN:CB	2.92	0.48
1:B:2014:THR:O	1:B:2067:ALA:CB	2.61	0.48
1:A:565:GLN:C	1:A:567:TYR:N	2.65	0.48
1:A:999:ARG:HA	1:A:1007:GLN:HA	1.94	0.48
1:A:1295:PHE:C	1:A:1297:HIS:N	2.65	0.48
1:A:2150:ASN:C	1:A:2152:GLY:N	2.66	0.48
1:B:763:LEU:O	1:B:767:CYS:CB	2.61	0.48
1:A:632:ASP:O	1:A:635:SER:N	2.46	0.48
1:A:1638:GLU:O	1:A:1639:ASN:C	2.52	0.48
1:A:2064:ILE:O	1:A:2067:ALA:N	2.44	0.48
1:A:2185:LEU:O	1:A:2188:TYR:CB	2.61	0.48
1:B:778:ARG:O	1:B:779:ALA:C	2.51	0.48
1:A:38:VAL:HA	1:A:207:ASN:O	2.14	0.48
1:B:111:LEU:C	1:B:113:THR:H	2.18	0.48
1:B:290:ASP:O	1:B:292:CYS:N	2.47	0.48
1:A:645:ILE:O	1:A:646:PRO:C	2.50	0.48
1:A:707:ILE:C	1:A:711:SER:H	2.17	0.48
1:A:724:LYS:C	1:A:726:ASP:H	2.17	0.48
1:A:1800:LYS:O	1:A:1801:GLU:O	2.31	0.48
1:A:1861:ASP:O	1:A:1865:VAL:CB	2.62	0.48
1:B:590:LEU:C	1:B:592:GLU:N	2.67	0.48
1:B:697:TRP:O	1:B:698:LEU:C	2.50	0.48
1:B:2111:ILE:O	1:B:2113:TYR:N	2.47	0.48
1:A:506:ARG:O	1:A:510:MET:HG2	2.14	0.47
1:A:975:ILE:O	1:A:979:GLN:CA	2.62	0.47
1:A:1809:ASP:O	1:A:1810:LEU:C	2.52	0.47
1:A:2167:LYS:O	1:A:2170:GLN:CB	2.62	0.47
1:B:620:SER:O	1:B:621:LEU:C	2.53	0.47
1:B:621:LEU:O	1:B:625:ASN:C	2.52	0.47
1:B:870:ALA:HA	1:B:873:LEU:CB	2.44	0.47
1:A:973:LYS:O	1:A:977:ILE:CB	2.61	0.47
1:A:1868:GLN:O	1:A:1869:GLU:C	2.52	0.47
1:A:2164:ARG:O	1:A:2165:HIS:CB	2.63	0.47
1:A:2184:ALA:HA	1:A:2187:PHE:CB	2.43	0.47
1:B:769:SER:CB	1:B:779:ALA:HA	2.43	0.47
1:B:1850:LYS:O	1:B:1854:LYS:N	2.47	0.47
1:B:2061:GLY:O	1:B:2062:ILE:C	2.52	0.47
1:A:692:ASP:O	1:A:693:GLU:C	2.52	0.47
1:A:761:VAL:O	1:A:764:ILE:CB	2.62	0.47
1:A:1449:LEU:O	1:A:1453:PHE:CB	2.62	0.47
1:A:1859:PHE:C	1:A:1861:ASP:N	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:TYR:O	1:B:577:GLN:N	2.47	0.47
1:B:694:GLU:O	1:B:696:VAL:N	2.48	0.47
1:B:885:LEU:O	1:B:888:THR:CB	2.62	0.47
1:B:1610:LEU:O	1:B:1614:LEU:CB	2.62	0.47
1:A:475:LYS:O	1:A:478:GLU:N	2.47	0.47
1:B:695:GLU:O	1:B:699:PHE:CB	2.61	0.47
1:B:2053:CYS:O	1:B:2054:ILE:C	2.52	0.47
1:A:1612:ASP:O	1:A:1613:ARG:C	2.53	0.47
1:A:1661:GLN:O	1:A:1663:LEU:N	2.48	0.47
1:A:1864:LYS:O	1:A:1866:ALA:N	2.47	0.47
1:A:2058:GLU:O	1:A:2060:ASN:N	2.48	0.47
1:B:126:LEU:O	1:B:129:ASN:N	2.48	0.47
1:B:666:ILE:H	1:B:667:GLU:HA	1.79	0.47
1:B:868:ASN:O	1:B:869:LEU:C	2.53	0.47
1:B:1223:GLU:O	1:B:1270:ALA:C	2.52	0.47
1:B:1632:PRO:O	1:B:1633:GLU:C	2.52	0.47
1:B:2142:GLU:N	1:B:2143:ASP:CB	2.78	0.47
1:A:387:TYR:HA	1:A:431:ALA:HA	1.95	0.47
1:A:598:LEU:O	1:A:602:ASN:N	2.48	0.47
1:A:1251:ASN:O	1:A:1255:LEU:CB	2.62	0.47
1:A:1628:VAL:O	1:A:1629:LEU:C	2.51	0.47
1:A:2044:GLN:HA	1:A:2097:ALA:HB1	1.97	0.47
1:B:785:MET:O	1:B:786:LEU:C	2.52	0.47
1:B:1080:LEU:O	1:B:1084:PHE:N	2.39	0.47
1:B:1867:GLN:O	1:B:1871:LYS:CB	2.62	0.47
1:A:708:ARG:N	1:A:711:SER:H	2.13	0.47
1:A:766:ARG:O	1:A:767:CYS:C	2.52	0.47
1:A:845:ARG:O	1:A:848:VAL:CB	2.62	0.47
1:A:891:LEU:O	1:A:894:ILE:N	2.48	0.47
1:A:979:GLN:O	1:A:980:PHE:C	2.50	0.47
1:A:983:ASN:O	1:A:984:VAL:C	2.53	0.47
1:A:1071:ASP:O	1:A:1072:TYR:C	2.52	0.47
1:A:2177:GLY:O	1:A:2178:GLN:CB	2.62	0.47
1:B:969:ASP:O	1:B:971:LYS:N	2.48	0.47
1:B:1461:CYS:O	1:B:1462:ASN:CB	2.63	0.47
1:B:1821:HIS:O	1:B:1825:LEU:CB	2.63	0.47
1:A:984:VAL:O	1:A:985:ARG:C	2.53	0.47
1:A:2180:ASP:O	1:A:2184:ALA:N	2.48	0.47
1:B:890:ILE:O	1:B:893:ALA:HB3	2.14	0.47
1:B:1238:HIS:CB	1:B:1282:GLN:CB	2.93	0.47
1:A:10:HIS:CB	1:A:112:GLY:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1826:LEU:O	1:B:1827:ALA:C	2.50	0.47
1:A:778:ARG:O	1:A:779:ALA:C	2.49	0.47
1:A:1803:ALA:HB1	1:A:1842:PHE:CB	2.45	0.47
1:A:1816:SER:C	1:A:1818:ARG:N	2.66	0.47
1:B:1093:VAL:O	1:B:1094:LEU:C	2.54	0.47
1:B:1445:HIS:O	1:B:1446:MET:CB	2.63	0.47
1:B:2032:ILE:O	1:B:2035:THR:N	2.48	0.47
1:A:610:ILE:O	1:A:613:ALA:HB3	2.15	0.46
1:A:761:VAL:O	1:A:762:ASP:C	2.53	0.46
1:A:827:ASP:O	1:A:830:LYS:N	2.49	0.46
1:A:1007:GLN:C	1:A:1009:SER:H	2.16	0.46
1:B:885:LEU:C	1:B:888:THR:H	2.16	0.46
1:B:1489:PHE:HA	1:B:1493:PRO:C	2.36	0.46
1:B:1986:PHE:O	1:B:1988:ARG:CA	2.62	0.46
1:B:549:PHE:O	1:B:552:ILE:N	2.48	0.46
1:B:836:THR:O	1:B:839:PHE:N	2.48	0.46
1:B:986:LEU:C	1:B:988:TYR:H	2.19	0.46
1:B:1795:GLN:O	1:B:1799:ASP:N	2.48	0.46
1:A:1095:GLN:O	1:A:1096:ALA:C	2.54	0.46
1:A:1245:CYS:CB	1:A:1341:VAL:H	2.26	0.46
1:A:1463:ASN:O	1:A:1464:THR:CB	2.62	0.46
1:A:1605:ASP:O	1:A:1609:ALA:CB	2.64	0.46
1:B:1210:ALA:O	1:B:1211:HIS:C	2.53	0.46
1:B:1634:LEU:O	1:B:1638:GLU:O	2.33	0.46
1:B:856:ASP:O	1:B:860:ASN:CB	2.64	0.46
1:B:960:PRO:N	1:B:961:GLU:HA	2.30	0.46
1:B:1201:GLN:C	1:B:1203:ARG:H	2.19	0.46
1:B:1630:HIS:O	1:B:1631:ARG:C	2.54	0.46
1:B:1813:ASN:O	1:B:1814:ALA:C	2.54	0.46
1:B:2153:HIS:HA	1:B:2156:TYR:CB	2.45	0.46
1:A:230:LYS:HA	1:A:232:ASP:N	2.30	0.46
1:A:476:LEU:O	1:A:478:GLU:C	2.53	0.46
1:A:883:ASP:C	1:A:885:LEU:N	2.66	0.46
1:A:1214:VAL:O	1:A:1218:LEU:CB	2.64	0.46
1:A:1295:PHE:C	1:A:1297:HIS:H	2.19	0.46
1:A:2150:ASN:C	1:A:2153:HIS:H	2.13	0.46
1:B:576:LYS:C	1:B:578:PHE:H	2.19	0.46
1:B:1293:GLN:CA	1:B:1345:TYR:HA	2.46	0.46
1:B:1315:ILE:O	1:B:1316:VAL:C	2.52	0.46
1:A:476:LEU:O	1:A:477:LEU:C	2.54	0.46
1:A:1223:GLU:CB	1:A:1228:THR:CB	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1461:CYS:CB	1:A:1465:SER:CB	2.93	0.46
1:B:686:ALA:O	1:B:689:ALA:HB3	2.15	0.46
1:B:858:GLU:O	1:B:859:LYS:C	2.52	0.46
1:B:885:LEU:O	1:B:888:THR:CA	2.63	0.46
1:B:1354:LEU:O	1:B:1355:ILE:C	2.54	0.46
1:B:2186:GLU:O	1:B:2187:PHE:C	2.54	0.46
1:A:617:THR:O	1:A:621:LEU:N	2.32	0.46
1:A:829:ILE:O	1:A:830:LYS:C	2.54	0.46
1:A:976:GLU:O	1:A:977:ILE:C	2.52	0.46
1:A:1251:ASN:O	1:A:1255:LEU:N	2.45	0.46
1:B:721:GLU:O	1:B:722:GLY:C	2.53	0.46
1:B:1231:GLN:CA	1:B:1275:HIS:CB	2.93	0.46
1:B:1376:HIS:C	1:B:1378:VAL:H	2.19	0.46
1:B:1459:ARG:O	1:B:1461:CYS:N	2.49	0.46
1:B:1624:VAL:O	1:B:1627:ASP:CB	2.64	0.46
1:A:480:LEU:O	1:A:482:TYR:N	2.49	0.46
1:A:631:LEU:O	1:A:634:LEU:CB	2.64	0.46
1:A:830:LYS:O	1:A:831:GLU:C	2.54	0.46
1:A:2055:ALA:O	1:A:2059:SER:CA	2.64	0.46
1:A:2174:LYS:O	1:A:2177:GLY:O	2.33	0.46
1:B:984:VAL:O	1:B:985:ARG:C	2.53	0.46
1:B:992:CYS:O	1:B:994:LEU:N	2.48	0.46
1:B:1072:TYR:N	1:B:1106:SER:CB	2.79	0.46
1:A:277:SER:O	1:A:280:ALA:N	2.48	0.46
1:A:724:LYS:O	1:A:726:ASP:N	2.45	0.46
1:B:469:GLU:O	1:B:470:ARG:C	2.55	0.46
1:B:841:GLU:O	1:B:842:GLU:C	2.52	0.46
1:B:1200:GLN:O	1:B:1203:ARG:N	2.49	0.46
1:B:1228:THR:CA	1:B:1271:VAL:CB	2.92	0.46
1:A:1223:GLU:O	1:A:1271:VAL:CB	2.63	0.46
1:B:978:LEU:O	1:B:979:GLN:C	2.52	0.46
1:B:1191:SER:O	1:B:1239:GLU:CB	2.63	0.46
1:B:1845:ARG:O	1:B:1848:GLU:N	2.49	0.46
1:A:2173:LEU:O	1:A:2177:GLY:N	2.49	0.45
1:B:1061:LEU:O	1:B:1062:ARG:C	2.53	0.45
1:A:554:ARG:CB	1:A:557:TYR:CB	2.94	0.45
1:A:867:VAL:O	1:A:868:ASN:O	2.34	0.45
1:B:110:LEU:O	1:B:113:THR:CB	2.64	0.45
1:B:857:LYS:O	1:B:858:GLU:O	2.34	0.45
1:B:974:ILE:O	1:B:975:ILE:C	2.53	0.45
1:B:1101:GLN:O	1:B:1102:LEU:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:THR:O	1:A:508:LYS:NZ	2.38	0.45
1:A:653:CYS:O	1:A:657:LEU:N	2.48	0.45
1:A:1476:LYS:C	1:A:1478:VAL:N	2.69	0.45
1:B:611:THR:C	1:B:613:ALA:N	2.69	0.45
1:B:666:ILE:CB	1:B:669:LYS:N	2.79	0.45
1:B:1798:LEU:CA	1:B:1802:GLY:H	2.29	0.45
1:A:894:ILE:O	1:A:898:VAL:N	2.50	0.45
1:A:1848:GLU:C	1:A:1850:LYS:H	2.20	0.45
1:B:754:GLU:O	1:B:758:GLN:N	2.43	0.45
1:B:761:VAL:O	1:B:762:ASP:C	2.55	0.45
1:B:971:LYS:O	1:B:972:LEU:C	2.54	0.45
1:A:411:GLU:O	1:A:412:LYS:CB	2.64	0.45
1:A:649:GLN:O	1:A:652:ILE:CB	2.64	0.45
1:A:1194:VAL:O	1:A:1197:SER:CA	2.63	0.45
1:B:967:VAL:C	1:B:969:ASP:N	2.70	0.45
1:B:1313:GLN:O	1:B:1314:THR:C	2.54	0.45
1:B:1433:THR:HA	1:B:1493:PRO:N	2.32	0.45
1:B:2117:PRO:HA	1:B:2171:THR:CB	2.46	0.45
1:B:263:PHE:CB	1:B:416:LEU:O	2.65	0.45
1:B:766:ARG:C	1:B:768:MET:H	2.19	0.45
1:B:864:PHE:O	1:B:865:GLU:C	2.51	0.45
1:B:992:CYS:O	1:B:993:LEU:C	2.53	0.45
1:B:1096:ALA:O	1:B:1097:PHE:C	2.51	0.45
1:B:1224:LYS:O	1:B:1227:ASP:O	2.35	0.45
1:A:1194:VAL:O	1:A:1195:ARG:C	2.55	0.45
1:A:1270:ALA:HB2	1:A:1319:GLU:CB	2.46	0.45
1:B:271:SER:O	1:B:273:THR:N	2.50	0.45
1:B:832:ARG:O	1:B:833:PHE:C	2.54	0.45
1:A:758:GLN:O	1:A:759:LEU:C	2.54	0.45
1:B:992:CYS:C	1:B:994:LEU:N	2.69	0.45
1:B:1223:GLU:O	1:B:1270:ALA:O	2.34	0.45
1:B:1272:THR:O	1:B:1275:HIS:N	2.49	0.45
1:B:1825:LEU:O	1:B:1826:LEU:C	2.53	0.45
1:B:1854:LYS:O	1:B:1857:LYS:CB	2.65	0.45
1:A:2062:ILE:O	1:A:2063:ASP:C	2.55	0.45
1:A:2062:ILE:O	1:A:2065:ILE:N	2.50	0.45
1:B:885:LEU:O	1:B:886:ARG:C	2.52	0.45
1:A:1280:ASN:O	1:A:1281:PHE:C	2.55	0.45
1:B:654:LYS:O	1:B:658:ASN:N	2.31	0.45
1:B:773:LEU:C	1:B:775:TYR:N	2.70	0.45
1:B:865:GLU:O	1:B:869:LEU:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1640:THR:CB	1:B:1644:ARG:C	2.85	0.45
1:B:314:LEU:O	1:B:366:SER:HA	2.17	0.44
1:B:588:ASP:CB	1:B:591:ALA:HB3	2.47	0.44
1:B:622:VAL:O	1:B:625:ASN:O	2.34	0.44
1:B:1287:ILE:CB	1:B:1341:VAL:CB	2.95	0.44
1:B:2087:LEU:O	1:B:2091:ALA:HB3	2.16	0.44
1:B:131:TYR:O	1:B:151:LEU:HA	2.17	0.44
1:B:504:ARG:HA	1:B:507:GLN:OE1	2.18	0.44
1:B:611:THR:O	1:B:613:ALA:N	2.50	0.44
1:B:829:ILE:O	1:B:832:ARG:CB	2.65	0.44
1:B:1284:CYS:C	1:B:1286:GLU:N	2.70	0.44
1:B:2005:PHE:O	1:B:2008:CYS:N	2.50	0.44
1:B:2153:HIS:O	1:B:2157:ILE:CB	2.65	0.44
1:A:1679:ARG:O	1:A:1682:MET:N	2.51	0.44
1:B:760:ASP:O	1:B:761:VAL:C	2.55	0.44
1:B:780:SER:O	1:B:781:PHE:C	2.53	0.44
1:B:780:SER:O	1:B:783:ARG:CA	2.65	0.44
1:B:997:PHE:O	1:B:998:LYS:C	2.56	0.44
1:B:1630:HIS:O	1:B:1633:GLU:N	2.50	0.44
1:B:2061:GLY:O	1:B:2064:ILE:CA	2.64	0.44
1:B:2151:VAL:C	1:B:2154:ASN:H	2.21	0.44
1:A:398:TRP:O	1:A:399:VAL:C	2.55	0.44
1:A:520:PHE:O	1:A:522:LEU:N	2.51	0.44
1:A:549:PHE:O	1:A:551:HIS:N	2.51	0.44
1:A:606:LEU:O	1:A:607:GLU:C	2.56	0.44
1:A:772:ASN:O	1:A:773:LEU:C	2.55	0.44
1:A:1973:GLN:O	1:A:1974:LEU:C	2.55	0.44
1:A:2120:LEU:O	1:A:2124:ILE:CB	2.65	0.44
1:A:2203:THR:O	1:A:2204:MET:CB	2.65	0.44
1:B:860:ASN:O	1:B:861:LYS:C	2.53	0.44
1:B:976:GLU:O	1:B:977:ILE:C	2.56	0.44
1:A:1488:THR:O	1:A:1490:PHE:N	2.50	0.44
1:A:1677:THR:O	1:A:1680:GLU:N	2.50	0.44
1:A:1847:THR:O	1:A:1850:LYS:N	2.49	0.44
1:A:2064:ILE:O	1:A:2065:ILE:C	2.55	0.44
1:B:104:GLU:O	1:B:105:THR:C	2.55	0.44
1:B:580:PHE:O	1:B:581:MET:C	2.56	0.44
1:B:701:ARG:O	1:B:702:ASP:C	2.56	0.44
1:B:1081:GLN:O	1:B:1082:LEU:C	2.56	0.44
1:B:1285:SER:C	1:B:1287:ILE:H	2.21	0.44
1:A:1371:LEU:CB	1:A:1374:HIS:CB	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:981:ILE:O	1:B:982:LEU:O	2.35	0.44
1:A:966:MET:O	1:A:967:VAL:C	2.55	0.44
1:A:1001:PHE:O	1:A:1003:GLU:N	2.48	0.44
1:A:1434:GLU:O	1:A:1492:SER:CB	2.65	0.44
1:B:1213:VAL:O	1:B:1214:VAL:O	2.35	0.44
1:A:519:ILE:O	1:A:520:PHE:C	2.56	0.44
1:A:2201:ASP:O	1:A:2202:ARG:CB	2.66	0.44
1:B:1432:ASP:C	1:B:1493:PRO:CB	2.86	0.44
1:A:993:LEU:O	1:A:994:LEU:C	2.56	0.44
1:A:1116:LYS:O	1:A:1119:LEU:CB	2.66	0.44
1:A:1362:ARG:O	1:A:1363:ASP:C	2.56	0.44
1:A:1654:LYS:O	1:A:1657:LYS:N	2.51	0.44
1:A:1792:ALA:CB	1:B:1792:ALA:CB	2.96	0.44
1:A:2103:HIS:O	1:A:2104:ASP:CB	2.66	0.44
1:B:745:LEU:O	1:B:1075:LEU:CB	2.66	0.44
1:A:2088:LYS:O	1:A:2092:SER:CB	2.66	0.43
1:B:769:SER:O	1:B:772:ASN:O	2.36	0.43
1:B:971:LYS:C	1:B:973:LYS:N	2.71	0.43
1:A:1378:VAL:O	1:A:1382:ALA:CB	2.65	0.43
1:B:91:LYS:O	1:B:94:HIS:N	2.51	0.43
1:B:1432:ASP:O	1:B:1493:PRO:O	2.36	0.43
1:B:1484:SER:N	1:B:1884:LYS:O	2.51	0.43
1:B:1682:MET:O	1:B:1686:ARG:CA	2.63	0.43
1:B:2087:LEU:O	1:B:2091:ALA:HB2	2.17	0.43
1:A:1049:PRO:O	1:A:1050:LEU:C	2.55	0.43
1:A:1375:ILE:HA	1:A:1378:VAL:H	1.84	0.43
1:A:1417:GLU:O	1:A:1420:ILE:N	2.52	0.43
1:A:1653:CYS:O	1:A:1656:ILE:CB	2.66	0.43
1:A:2020:LEU:O	1:A:2024:ILE:CB	2.66	0.43
1:B:568:ARG:NH1	1:B:572:GLU:OE1	2.51	0.43
1:B:1285:SER:O	1:B:1287:ILE:N	2.46	0.43
1:A:68:ALA:HB1	1:A:95:ALA:HB1	2.00	0.43
1:A:680:VAL:C	1:A:682:THR:H	2.22	0.43
1:A:898:VAL:C	1:A:900:VAL:CA	2.85	0.43
1:A:2094:LEU:O	1:A:2095:LEU:C	2.55	0.43
1:B:597:ALA:O	1:B:598:LEU:C	2.55	0.43
1:B:679:GLY:O	1:B:680:VAL:C	2.55	0.43
1:B:967:VAL:C	1:B:969:ASP:H	2.21	0.43
1:B:1286:GLU:CB	1:B:1289:GLU:CB	2.96	0.43
1:A:1841:SER:O	1:A:1842:PHE:O	2.36	0.43
1:A:1966:GLN:HA	1:A:1969:LEU:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2026:GLU:O	1:A:2027:LYS:C	2.57	0.43
1:B:307:HIS:O	1:B:308:LEU:C	2.57	0.43
1:B:693:GLU:O	1:B:697:TRP:CB	2.67	0.43
1:B:1665:GLU:O	1:B:1666:ASN:C	2.57	0.43
1:A:989:ARG:O	1:A:990:ILE:CB	2.67	0.43
1:A:1215:LEU:C	1:A:1217:LEU:N	2.71	0.43
1:A:1488:THR:O	1:A:1489:PHE:C	2.56	0.43
1:B:560:LEU:O	1:B:562:HIS:N	2.52	0.43
1:B:1246:ALA:C	1:B:1248:ASN:N	2.71	0.43
1:B:1963:THR:HA	1:B:1966:GLN:CB	2.48	0.43
1:A:267:THR:OG1	1:A:275:ALA:HB2	2.18	0.43
1:A:520:PHE:C	1:A:522:LEU:N	2.72	0.43
1:A:982:LEU:O	1:A:983:ASN:C	2.55	0.43
1:A:1477:TYR:CB	1:A:1881:LEU:CB	2.96	0.43
1:B:504:ARG:O	1:B:507:GLN:N	2.51	0.43
1:B:621:LEU:O	1:B:625:ASN:CA	2.65	0.43
1:B:685:ASN:O	1:B:686:ALA:C	2.53	0.43
1:B:831:GLU:O	1:B:832:ARG:C	2.56	0.43
1:B:855:SER:O	1:B:856:ASP:C	2.54	0.43
1:B:1839:GLN:O	1:B:1842:PHE:CB	2.67	0.43
1:A:199:GLN:HA	1:A:206:CYS:O	2.18	0.43
1:A:479:ASP:O	1:A:482:TYR:CB	2.67	0.43
1:A:1201:GLN:O	1:A:1202:GLN:C	2.57	0.43
1:A:1295:PHE:O	1:A:1297:HIS:N	2.51	0.43
1:A:1341:VAL:O	1:A:1344:PHE:N	2.52	0.43
1:B:729:ILE:O	1:B:730:LEU:C	2.56	0.43
1:B:786:LEU:O	1:B:790:VAL:N	2.44	0.43
1:B:853:PRO:O	1:B:855:SER:N	2.51	0.43
1:B:1629:LEU:O	1:B:1632:PRO:CB	2.66	0.43
1:A:11:ILE:CB	1:A:110:LEU:O	2.66	0.43
1:A:560:LEU:O	1:A:561:ARG:C	2.57	0.43
1:A:834:ALA:O	1:A:835:GLN:C	2.55	0.43
1:A:1197:SER:O	1:A:1198:ARG:C	2.57	0.43
1:A:1207:ASN:C	1:A:1209:GLY:N	2.72	0.43
1:A:1952:ALA:O	1:A:1954:ASP:N	2.52	0.43
1:A:2123:VAL:O	1:A:2127:ALA:CB	2.67	0.43
1:B:32:LEU:CB	1:B:445:PHE:HA	2.49	0.43
1:B:769:SER:O	1:B:773:LEU:CA	2.66	0.43
1:B:1796:CYS:O	1:B:1797:HIS:C	2.56	0.43
1:B:1991:ASN:O	1:B:1992:ASN:O	2.36	0.43
1:B:2044:GLN:O	1:B:2046:PRO:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ALA:O	1:A:439:GLU:C	2.55	0.43
1:A:567:TYR:O	1:A:571:GLN:HG3	2.18	0.43
1:A:1420:ILE:C	1:A:1424:ASN:H	2.22	0.43
1:A:1654:LYS:O	1:A:1655:LEU:C	2.57	0.43
1:B:696:VAL:O	1:B:698:LEU:N	2.52	0.43
1:B:863:THR:O	1:B:867:VAL:CB	2.67	0.43
1:B:1986:PHE:C	1:B:1988:ARG:N	2.69	0.43
1:B:2061:GLY:O	1:B:2063:ASP:N	2.52	0.43
1:A:12:GLY:O	1:A:226:TRP:HA	2.19	0.42
1:A:841:GLU:O	1:A:844:LEU:CB	2.67	0.42
1:A:965:ILE:O	1:A:968:MET:CB	2.67	0.42
1:A:984:VAL:O	1:A:988:TYR:CB	2.67	0.42
1:A:1623:SER:O	1:A:1626:VAL:CB	2.67	0.42
1:A:2192:THR:O	1:A:2216:GLU:O	2.37	0.42
1:B:830:LYS:O	1:B:831:GLU:C	2.56	0.42
1:B:833:PHE:O	1:B:836:THR:CB	2.66	0.42
1:B:896:ASP:O	1:B:899:HIS:N	2.52	0.42
1:B:2164:ARG:O	1:B:2165:HIS:CB	2.67	0.42
1:A:480:LEU:O	1:A:483:PHE:N	2.53	0.42
1:A:899:HIS:N	1:A:900:VAL:CA	2.81	0.42
1:A:2192:THR:O	1:A:2216:GLU:CB	2.67	0.42
1:B:769:SER:CB	1:B:779:ALA:CA	2.97	0.42
1:B:1315:ILE:O	1:B:1318:ALA:N	2.51	0.42
1:B:1635:LEU:CA	1:B:1646:CYS:CB	2.96	0.42
1:A:38:VAL:CA	1:A:207:ASN:O	2.67	0.42
1:A:689:ALA:O	1:A:691:GLU:N	2.52	0.42
1:A:729:ILE:O	1:A:732:TYR:CB	2.67	0.42
1:A:871:ARG:O	1:A:872:ASN:C	2.54	0.42
1:A:1083:LEU:O	1:A:1084:PHE:C	2.57	0.42
1:A:2026:GLU:O	1:A:2028:ASN:N	2.51	0.42
1:B:10:HIS:CB	1:B:112:GLY:O	2.68	0.42
1:B:575:ALA:O	1:B:578:PHE:CB	2.67	0.42
1:B:753:ASN:O	1:B:757:GLY:N	2.42	0.42
1:A:888:THR:O	1:A:891:LEU:CA	2.68	0.42
1:A:1294:HIS:O	1:A:1298:CYS:CA	2.67	0.42
1:A:1631:ARG:O	1:A:1632:PRO:C	2.58	0.42
1:A:1640:THR:CB	1:A:1644:ARG:CB	2.97	0.42
1:B:1026:GLY:CA	1:B:1594:ARG:CB	2.98	0.42
1:B:1211:HIS:O	1:B:1214:VAL:CA	2.65	0.42
1:B:1240:PHE:CB	1:B:1245:CYS:HA	2.49	0.42
1:B:1350:SER:O	1:B:1351:PHE:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1383:VAL:O	1:B:1386:GLU:N	2.52	0.42
1:B:1459:ARG:C	1:B:1461:CYS:N	2.73	0.42
1:B:1593:SER:O	1:B:1597:ARG:N	2.42	0.42
1:A:842:GLU:O	1:A:844:LEU:N	2.52	0.42
1:A:846:ASP:O	1:A:849:CYS:N	2.52	0.42
1:A:1112:TYR:HA	1:A:1115:ILE:CB	2.50	0.42
1:A:1634:LEU:CB	1:A:1646:CYS:CA	2.97	0.42
1:A:2179:VAL:O	1:A:2180:ASP:C	2.58	0.42
1:B:2197:ILE:HA	1:B:2212:PRO:N	2.35	0.42
1:A:1037:ALA:C	1:A:1039:GLY:N	2.73	0.42
1:A:2150:ASN:O	1:A:2153:HIS:CA	2.65	0.42
1:B:315:ALA:HB2	1:B:366:SER:HA	2.01	0.42
1:B:684:GLU:O	1:B:687:LEU:CA	2.67	0.42
1:A:666:ILE:CB	1:A:669:LYS:C	2.88	0.42
1:A:1998:LEU:O	1:A:1999:VAL:C	2.55	0.42
1:B:642:ASN:O	1:B:643:LYS:C	2.58	0.42
1:B:732:TYR:O	1:B:733:TYR:C	2.58	0.42
1:B:869:LEU:O	1:B:871:ARG:N	2.53	0.42
1:B:1086:HIS:C	1:B:1088:SER:H	2.22	0.42
1:B:1128:LYS:O	1:B:1132:TRP:CB	2.67	0.42
1:B:2026:GLU:O	1:B:2027:LYS:C	2.57	0.42
1:B:2036:LEU:O	1:B:2040:THR:CB	2.68	0.42
1:A:610:ILE:O	1:A:613:ALA:CB	2.67	0.42
1:A:2061:GLY:O	1:A:2062:ILE:C	2.58	0.42
1:B:103:ASN:O	1:B:104:GLU:C	2.58	0.42
1:B:641:MET:O	1:B:642:ASN:C	2.58	0.42
1:B:1872:ALA:C	1:B:1874:VAL:H	2.23	0.42
1:B:2151:VAL:HA	1:B:2154:ASN:CB	2.50	0.42
1:A:10:HIS:HA	1:A:113:THR:O	2.19	0.42
1:A:749:TYR:C	1:A:751:ALA:N	2.71	0.42
1:A:1849:ASP:O	1:A:1850:LYS:C	2.58	0.42
1:A:2200:LEU:CB	1:A:2209:PHE:O	2.67	0.42
1:B:1312:LEU:O	1:B:1313:GLN:C	2.57	0.42
1:B:1483:MET:HA	1:B:1486:VAL:CB	2.50	0.42
1:A:15:CYS:HA	1:A:223:PHE:H	1.84	0.42
1:A:972:LEU:O	1:A:974:ILE:N	2.52	0.42
1:A:992:CYS:C	1:A:994:LEU:N	2.72	0.42
1:A:1953:LYS:O	1:A:1954:ASP:C	2.57	0.42
1:A:2043:CYS:C	1:A:2097:ALA:HB1	2.40	0.42
1:B:48:ASN:O	1:B:49:PRO:C	2.58	0.42
1:B:645:ILE:O	1:B:646:PRO:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:LEU:O	1:B:866:VAL:N	2.48	0.42
1:B:976:GLU:C	1:B:978:LEU:H	2.23	0.42
1:B:2032:ILE:O	1:B:2035:THR:CB	2.68	0.42
1:A:549:PHE:O	1:A:552:ILE:N	2.40	0.41
1:A:1821:HIS:HA	1:A:1824:ILE:CB	2.50	0.41
1:A:1864:LYS:O	1:A:1866:ALA:C	2.53	0.41
1:B:181:LYS:HA	1:B:218:TRP:O	2.20	0.41
1:B:708:ARG:O	1:B:709:SER:C	2.59	0.41
1:B:742:ARG:CB	1:B:1040:ILE:CA	2.98	0.41
1:B:1118:ASP:O	1:B:1119:LEU:C	2.56	0.41
1:B:1619:GLN:O	1:B:1622:LEU:CB	2.68	0.41
1:A:1070:HIS:O	1:A:1071:ASP:C	2.59	0.41
1:A:1338:GLY:O	1:A:1342:LEU:CB	2.68	0.41
1:A:1363:ASP:O	1:A:1366:ASP:CB	2.68	0.41
1:B:669:LYS:O	1:B:672:LEU:CB	2.68	0.41
1:B:742:ARG:CB	1:B:1040:ILE:HA	2.50	0.41
1:B:882:SER:O	1:B:886:ARG:N	2.46	0.41
1:B:990:ILE:O	1:B:993:LEU:N	2.53	0.41
1:B:1355:ILE:O	1:B:1356:GLN:CB	2.68	0.41
1:A:606:LEU:O	1:A:608:LYS:N	2.53	0.41
1:A:701:ARG:O	1:A:703:SER:O	2.38	0.41
1:A:842:GLU:O	1:A:843:TYR:C	2.59	0.41
1:A:868:ASN:O	1:A:869:LEU:C	2.56	0.41
1:A:1379:GLU:HA	1:A:1382:ALA:CB	2.40	0.41
1:A:1793:GLU:HA	1:A:1796:CYS:CB	2.50	0.41
1:B:111:LEU:O	1:B:113:THR:N	2.53	0.41
1:B:173:GLY:O	1:B:174:ASP:C	2.58	0.41
1:B:969:ASP:C	1:B:971:LYS:N	2.71	0.41
1:B:980:PHE:O	1:B:981:ILE:C	2.59	0.41
1:A:768:MET:O	1:A:769:SER:C	2.59	0.41
1:A:772:ASN:C	1:A:774:PRO:N	2.74	0.41
1:A:1040:ILE:O	1:A:1043:GLY:N	2.52	0.41
1:A:1477:TYR:HA	1:A:1881:LEU:O	2.20	0.41
1:A:1843:PHE:O	1:A:1844:CYS:C	2.58	0.41
1:A:1857:LYS:C	1:A:1859:PHE:N	2.70	0.41
1:A:2032:ILE:O	1:A:2033:ASN:C	2.58	0.41
1:B:439:GLU:O	1:B:442:ASP:N	2.53	0.41
1:B:769:SER:O	1:B:772:ASN:C	2.58	0.41
1:A:689:ALA:O	1:A:690:GLY:C	2.59	0.41
1:A:786:LEU:O	1:A:789:HIS:N	2.53	0.41
1:A:1062:ARG:O	1:A:1063:VAL:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1991:ASN:O	1:A:1992:ASN:O	2.38	0.41
1:A:2006:LEU:O	1:A:2007:ASP:C	2.58	0.41
1:A:2010:CYS:O	1:A:2012:SER:N	2.53	0.41
1:B:883:ASP:HA	1:B:886:ARG:CB	2.50	0.41
1:B:1193:SER:O	1:B:1194:VAL:O	2.39	0.41
1:A:1190:GLU:O	1:A:1193:SER:CB	2.69	0.41
1:A:1855:PHE:O	1:A:1857:LYS:N	2.54	0.41
1:A:2047:CYS:CB	1:A:2050:ASN:CB	2.99	0.41
1:B:560:LEU:C	1:B:562:HIS:N	2.73	0.41
1:B:882:SER:O	1:B:885:LEU:CB	2.68	0.41
1:B:888:THR:C	1:B:891:LEU:H	2.24	0.41
1:B:1988:ARG:C	1:B:1990:GLN:H	2.23	0.41
1:A:446:ALA:O	1:A:447:ASN:C	2.57	0.41
1:A:1298:CYS:O	1:A:1299:ILE:CB	2.68	0.41
1:A:1477:TYR:HA	1:A:1881:LEU:CB	2.50	0.41
1:B:18:TYR:HA	1:B:25:GLY:O	2.21	0.41
1:B:856:ASP:O	1:B:857:LYS:C	2.57	0.41
1:B:1059:THR:O	1:B:1060:PHE:C	2.56	0.41
1:B:1086:HIS:C	1:B:1088:SER:N	2.74	0.41
1:A:316:ALA:HA	1:A:354:SER:O	2.20	0.41
1:A:883:ASP:O	1:A:884:LEU:C	2.57	0.41
1:A:1100:VAL:O	1:A:1101:GLN:C	2.57	0.41
1:B:439:GLU:O	1:B:442:ASP:CB	2.68	0.41
1:B:664:ILE:O	1:B:665:LEU:CB	2.68	0.41
1:B:712:VAL:O	1:B:713:ARG:C	2.59	0.41
1:B:1288:ASN:O	1:B:1290:ARG:N	2.53	0.41
1:B:1594:ARG:HA	1:B:1597:ARG:CB	2.50	0.41
1:B:1952:ALA:O	1:B:1953:LYS:CB	2.69	0.41
1:B:2197:ILE:HA	1:B:2212:PRO:CA	2.50	0.41
1:A:69:GLN:HA	1:A:96:ALA:HB2	2.03	0.41
1:A:398:TRP:O	1:A:399:VAL:O	2.39	0.41
1:A:743:MET:O	1:A:744:CYS:O	2.39	0.41
1:A:833:PHE:O	1:A:834:ALA:C	2.60	0.41
1:A:844:LEU:O	1:A:845:ARG:C	2.57	0.41
1:A:981:ILE:O	1:A:982:LEU:C	2.59	0.41
1:A:1001:PHE:O	1:A:1002:ASP:CB	2.67	0.41
1:A:1355:ILE:O	1:A:1356:GLN:CB	2.69	0.41
1:A:1477:TYR:CA	1:A:1881:LEU:CB	2.99	0.41
1:B:692:ASP:O	1:B:696:VAL:CB	2.69	0.41
1:B:752:ILE:O	1:B:753:ASN:C	2.59	0.41
1:B:776:ASP:O	1:B:778:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1059:THR:C	1:B:1061:LEU:N	2.73	0.41
1:B:1301:THR:O	1:B:1304:ARG:CB	2.69	0.41
1:B:1822:GLU:O	1:B:1825:LEU:CB	2.69	0.41
1:B:2147:SER:O	1:B:2151:VAL:CB	2.69	0.41
1:B:2181:GLY:O	1:B:2184:ALA:HB3	2.21	0.41
1:A:140:ALA:HB3	1:A:143:GLU:O	2.20	0.41
1:A:253:CYS:HA	1:A:262:VAL:HA	2.03	0.41
1:A:773:LEU:CB	1:A:779:ALA:HB2	2.51	0.41
1:A:1661:GLN:C	1:A:1663:LEU:N	2.74	0.41
1:A:1812:MET:O	1:A:1814:ALA:N	2.53	0.41
1:B:52:LYS:C	1:B:54:ARG:H	2.24	0.41
1:B:105:THR:O	1:B:108:ARG:N	2.49	0.41
1:B:266:THR:HG21	1:B:1257:LYS:CB	2.51	0.41
1:B:549:PHE:C	1:B:551:HIS:H	2.24	0.41
1:B:967:VAL:O	1:B:970:THR:N	2.54	0.41
1:B:989:ARG:O	1:B:990:ILE:CB	2.69	0.41
1:A:439:GLU:O	1:A:440:VAL:C	2.59	0.40
1:A:523:LEU:O	1:A:524:GLN:O	2.37	0.40
1:A:886:ARG:O	1:A:889:LYS:N	2.54	0.40
1:A:1201:GLN:O	1:A:1203:ARG:N	2.54	0.40
1:A:1855:PHE:C	1:A:1857:LYS:N	2.74	0.40
1:B:1679:ARG:O	1:B:1687:GLY:C	2.60	0.40
1:B:2157:ILE:O	1:B:2161:GLN:CB	2.68	0.40
1:A:257:ARG:C	1:A:259:LYS:N	2.74	0.40
1:A:1203:ARG:O	1:A:1207:ASN:N	2.45	0.40
1:A:1207:ASN:C	1:A:1209:GLY:H	2.24	0.40
1:A:1285:SER:C	1:A:1341:VAL:CB	2.89	0.40
1:A:1303:GLY:O	1:A:1304:ARG:C	2.59	0.40
1:A:1634:LEU:CB	1:A:1646:CYS:O	2.69	0.40
1:B:1849:ASP:CB	1:B:1853:GLU:H	2.34	0.40
1:B:1976:CYS:O	1:B:1977:GLU:C	2.59	0.40
1:B:2116:ARG:O	1:B:2117:PRO:CB	2.67	0.40
1:B:1682:MET:O	1:B:1683:THR:C	2.57	0.40
1:B:1850:LYS:C	1:B:1854:LYS:CB	2.90	0.40
1:B:1966:GLN:HA	1:B:1969:LEU:CB	2.50	0.40
1:A:101:LYS:O	1:A:102:GLN:C	2.58	0.40
1:A:224:MET:HA	1:A:293:ARG:CB	2.52	0.40
1:A:269:ARG:CZ	2:A:3000:I3P:O52	2.68	0.40
1:A:832:ARG:O	1:A:833:PHE:C	2.59	0.40
1:A:842:GLU:C	1:A:844:LEU:N	2.74	0.40
1:A:888:THR:O	1:A:889:LYS:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:VAL:HA	1:A:1381:LEU:CB	2.51	0.40
1:A:1435:VAL:CB	1:A:1492:SER:CB	3.00	0.40
1:B:606:LEU:O	1:B:607:GLU:C	2.59	0.40
1:B:1194:VAL:C	1:B:1197:SER:H	2.25	0.40
1:B:1836:THR:O	1:B:1839:GLN:CB	2.69	0.40
1:B:1836:THR:CB	1:B:1984:GLN:CB	3.00	0.40
1:B:1886:LYS:O	1:B:1887:ASP:O	2.39	0.40
1:B:2169:LEU:O	1:B:2170:GLN:C	2.58	0.40
1:A:93:HIS:O	1:A:94:HIS:C	2.60	0.40
1:A:838:GLU:C	1:A:840:VAL:N	2.75	0.40
1:B:110:LEU:O	1:B:111:LEU:C	2.58	0.40
1:B:611:THR:C	1:B:613:ALA:H	2.25	0.40
1:B:855:SER:C	1:B:857:LYS:N	2.74	0.40
1:B:1080:LEU:O	1:B:1083:LEU:CB	2.69	0.40
1:B:1179:ILE:O	1:B:1183:LEU:CB	2.69	0.40
1:B:1238:HIS:O	1:B:1239:GLU:C	2.60	0.40
1:B:1246:ALA:C	1:B:1248:ASN:H	2.24	0.40
1:B:2003:LEU:O	1:B:2004:GLN:C	2.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1689/2217 (76%)	1219 (72%)	330 (20%)	140 (8%)	1 12
1	B	1688/2217 (76%)	1173 (70%)	350 (21%)	165 (10%)	0 9
All	All	3377/4434 (76%)	2392 (71%)	680 (20%)	305 (9%)	1 11

All (305) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	LEU
1	A	628	PRO
1	A	659	PRO
1	A	666	ILE
1	A	669	LYS
1	A	682	THR
1	A	725	GLU
1	A	744	CYS
1	A	764	ILE
1	A	854	PHE
1	A	986	LEU
1	A	990	ILE
1	A	1119	LEU
1	A	1202	GLN
1	A	1239	GLU
1	A	1264	ASN
1	A	1288	ASN
1	A	1346	ASN
1	A	1370	PRO
1	A	1400	LEU
1	A	1418	VAL
1	A	1458	CYS
1	A	1464	THR
1	A	1637	PRO
1	A	1654	LYS
1	A	1803	ALA
1	A	1842	PHE
1	A	1859	PHE
1	A	1864	LYS
1	A	1865	VAL
1	A	1887	ASP
1	A	1993	LYS
1	A	2011	GLY
1	A	2013	THR
1	A	2046	PRO
1	A	2143	ASP
1	A	2148	PRO
1	A	2178	GLN
1	A	2190	LYS
1	A	2204	MET
1	A	2210	PRO
1	A	2215	CYS
1	B	48	ASN

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Mol	Chain	Res	Type
1	B	591	ALA
1	B	628	PRO
1	B	659	PRO
1	B	665	LEU
1	B	666	ILE
1	B	694	GLU
1	B	696	VAL
1	B	697	TRP
1	B	741	ALA
1	B	744	CYS
1	B	773	LEU
1	B	774	PRO
1	B	776	ASP
1	B	849	CYS
1	B	854	PHE
1	B	857	LYS
1	B	893	ALA
1	B	894	ILE
1	B	968	MET
1	B	982	LEU
1	B	983	ASN
1	B	990	ILE
1	B	999	ARG
1	B	1008	SER
1	B	1107	GLN
1	B	1214	VAL
1	B	1215	LEU
1	B	1220	ILE
1	B	1285	SER
1	B	1288	ASN
1	B	1300	GLU
1	B	1311	PHE
1	B	1400	LEU
1	B	1462	ASN
1	B	1463	ASN
1	B	1492	SER
1	B	1632	PRO
1	B	1637	PRO
1	B	1639	ASN
1	B	1642	ALA
1	B	1801	GLU
1	B	1850	LYS

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Mol	Chain	Res	Type
1	B	1887	ASP
1	B	1967	PRO
1	B	1986	PHE
1	B	1987	LEU
1	B	1992	ASN
1	B	2046	PRO
1	B	2075	PRO
1	B	2117	PRO
1	B	2129	MET
1	B	2194	GLN
1	B	2209	PHE
1	B	2210	PRO
1	A	225	LYS
1	A	399	VAL
1	A	412	LYS
1	A	477	LEU
1	A	550	ARG
1	A	566	ASP
1	A	578	PHE
1	A	708	ARG
1	A	726	ASP
1	A	739	LEU
1	A	858	GLU
1	A	899	HIS
1	A	983	ASN
1	A	1008	SER
1	A	1083	LEU
1	A	1208	MET
1	A	1267	ILE
1	A	1299	ILE
1	A	1347	ASP
1	A	1461	CYS
1	A	1612	ASP
1	A	1817	ASP
1	A	1820	PHE
1	A	1844	CYS
1	A	1885	LYS
1	A	1966	GLN
1	A	1984	GLN
1	A	2020	LEU
1	A	2054	ILE
1	A	2060	ASN

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Mol	Chain	Res	Type
1	A	2104	ASP
1	A	2115	MET
1	A	2146	ALA
1	B	189	ALA
1	B	236	GLY
1	B	269	ARG
1	B	552	ILE
1	B	589	VAL
1	B	612	ALA
1	B	680	VAL
1	B	681	SER
1	B	682	THR
1	B	695	GLU
1	B	703	SER
1	B	708	ARG
1	B	767	CYS
1	B	790	VAL
1	B	853	PRO
1	B	869	LEU
1	B	980	PHE
1	B	987	ASP
1	B	989	ARG
1	B	1002	ASP
1	B	1095	GLN
1	B	1116	LYS
1	B	1129	SER
1	B	1130	GLU
1	B	1239	GLU
1	B	1289	GLU
1	B	1290	ARG
1	B	1291	VAL
1	B	1388	LYS
1	B	1461	CYS
1	B	1471	ASP
1	B	1633	GLU
1	B	1817	ASP
1	B	1828	ILE
1	B	1966	GLN
1	B	2029	VAL
1	B	2178	GLN
1	B	2195	ILE
1	B	2197	ILE

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Mol	Chain	Res	Type
1	B	2204	MET
1	A	180	ASP
1	A	521	LYS
1	A	727	ARG
1	A	773	LEU
1	A	973	LYS
1	A	984	VAL
1	A	994	LEU
1	A	1028	LEU
1	A	1049	PRO
1	A	1090	ARG
1	A	1216	GLU
1	A	1349	ALA
1	A	1394	ILE
1	A	1801	GLU
1	A	1881	LEU
1	A	1992	ASN
1	A	1999	VAL
1	A	2056	THR
1	A	2062	ILE
1	A	2147	SER
1	A	2165	HIS
1	A	2189	ALA
1	A	2202	ARG
1	B	50	PRO
1	B	53	PHE
1	B	396	ASN
1	B	595	ILE
1	B	604	LYS
1	B	699	PHE
1	B	971	LYS
1	B	978	LEU
1	B	1082	LEU
1	B	1088	SER
1	B	1241	LEU
1	B	1244	PHE
1	B	1258	HIS
1	B	1405	ILE
1	B	1435	VAL
1	B	1460	ALA
1	B	1814	ALA
1	B	2012	SER

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Mol	Chain	Res	Type
1	B	2024	ILE
1	B	2045	GLY
1	B	2060	ASN
1	B	2112	LEU
1	B	2130	GLN
1	B	2146	ALA
1	B	2196	GLU
1	B	2207	ILE
1	A	606	LEU
1	A	607	GLU
1	A	685	ASN
1	A	704	ASN
1	A	719	ALA
1	A	790	VAL
1	A	1095	GLN
1	A	1630	HIS
1	A	1639	ASN
1	A	1860	TYR
1	A	1967	PRO
1	A	2150	ASN
1	B	383	PRO
1	B	640	SER
1	B	785	MET
1	B	899	HIS
1	B	993	LEU
1	B	1083	LEU
1	B	1087	PHE
1	B	1243	ASN
1	B	1268	LEU
1	B	1363	ASP
1	B	1397	ASN
1	B	1651	PHE
1	B	1953	LYS
1	B	2183	GLU
1	B	2205	GLU
1	A	383	PRO
1	A	573	TYR
1	A	661	ASN
1	A	750	LEU
1	A	763	LEU
1	A	864	PHE
1	A	871	ARG

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Mol	Chain	Res	Type
1	A	1006	SER
1	A	1311	PHE
1	A	1414	CYS
1	A	1463	ASN
1	A	1655	LEU
1	A	1662	LEU
1	A	1805	ASN
1	B	291	PRO
1	B	761	VAL
1	B	766	ARG
1	B	858	GLU
1	B	984	VAL
1	B	1247	GLY
1	B	1277	PHE
1	B	1347	ASP
1	B	1355	ILE
1	B	1356	GLN
1	B	1480	GLU
1	B	2165	HIS
1	B	2202	ARG
1	A	236	GLY
1	A	572	GLU
1	A	600	HIS
1	A	707	ILE
1	A	752	ILE
1	A	993	LEU
1	A	998	LYS
1	B	126	LEU
1	B	683	GLY
1	B	698	LEU
1	B	700	TRP
1	B	1098	LYS
1	B	1202	GLN
1	B	1286	GLU
1	B	2054	ILE
1	A	291	PRO
1	A	1109	VAL
1	A	1834	GLY
1	A	1858	VAL
1	A	1833	GLY
1	B	722	GLY
1	B	1194	VAL

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Mol	Chain	Res	Type
1	B	2176	GLY
1	A	852	PHE
1	B	413	PRO
1	B	414	VAL
1	B	627	GLU
1	B	1650	GLY
1	B	2084	VAL
1	A	645	ILE
1	A	840	VAL
1	A	2207	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	26/1980 (1%)	26 (100%)	0	100	100
1	B	26/1980 (1%)	26 (100%)	0	100	100
All	All	52/3960 (1%)	52 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	I3P	A	3000	-	24,24,24	1.13	1 (4%)	36,39,39	1.08	3 (8%)
2	I3P	B	3000	-	24,24,24	1.15	2 (8%)	36,39,39	1.09	4 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	I3P	A	3000	-	-	0/15/39/39	0/1/1/1
2	I3P	B	3000	-	-	0/15/39/39	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3000	I3P	P5-O53	-2.23	1.46	1.54
2	A	3000	I3P	P4-O42	-2.15	1.46	1.54
2	B	3000	I3P	P1-O13	-2.12	1.46	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3000	I3P	O13-P1-O12	2.51	117.24	107.64
2	B	3000	I3P	O43-P4-O42	2.38	116.74	107.64
2	A	3000	I3P	O53-P5-O52	2.27	116.32	107.64
2	A	3000	I3P	O1-P1-O11	-2.26	100.67	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3000	I3P	O1-C1-C2	2.12	113.60	108.66
2	A	3000	I3P	O1-C1-C2	2.07	113.49	108.66
2	B	3000	I3P	O53-P5-O52	2.07	115.55	107.64

There are no chirality outliers.

There are no torsion outliers.

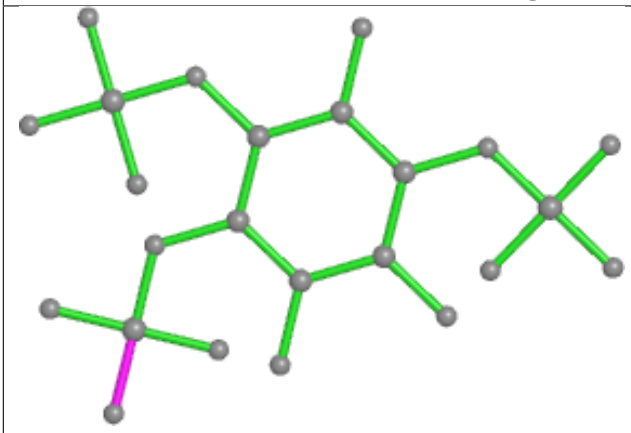
There are no ring outliers.

2 monomers are involved in 7 short contacts:

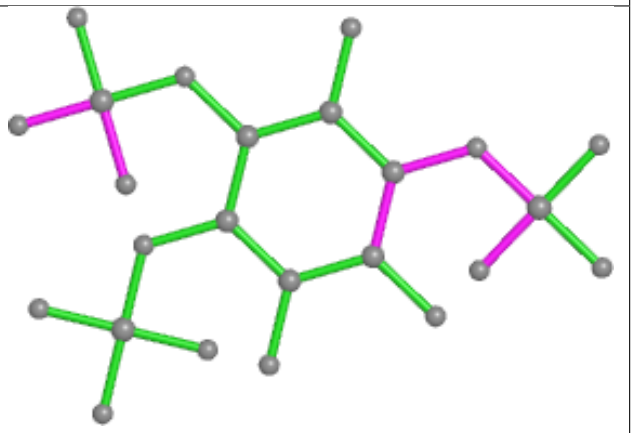
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3000	I3P	6	0
2	B	3000	I3P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

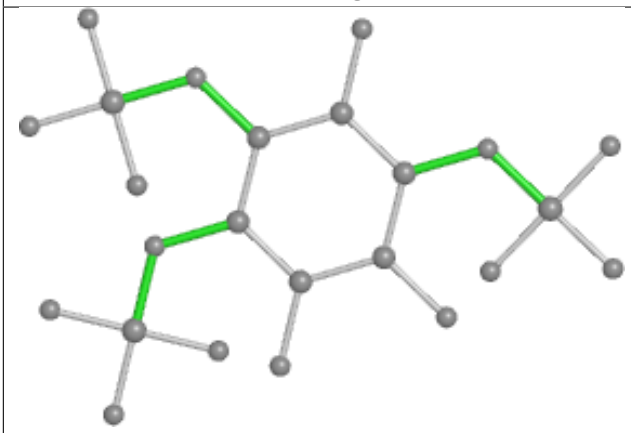
Ligand I3P A 3000



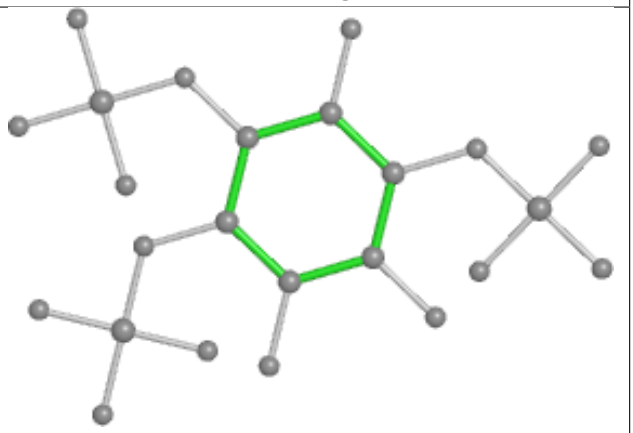
Bond lengths



Bond angles

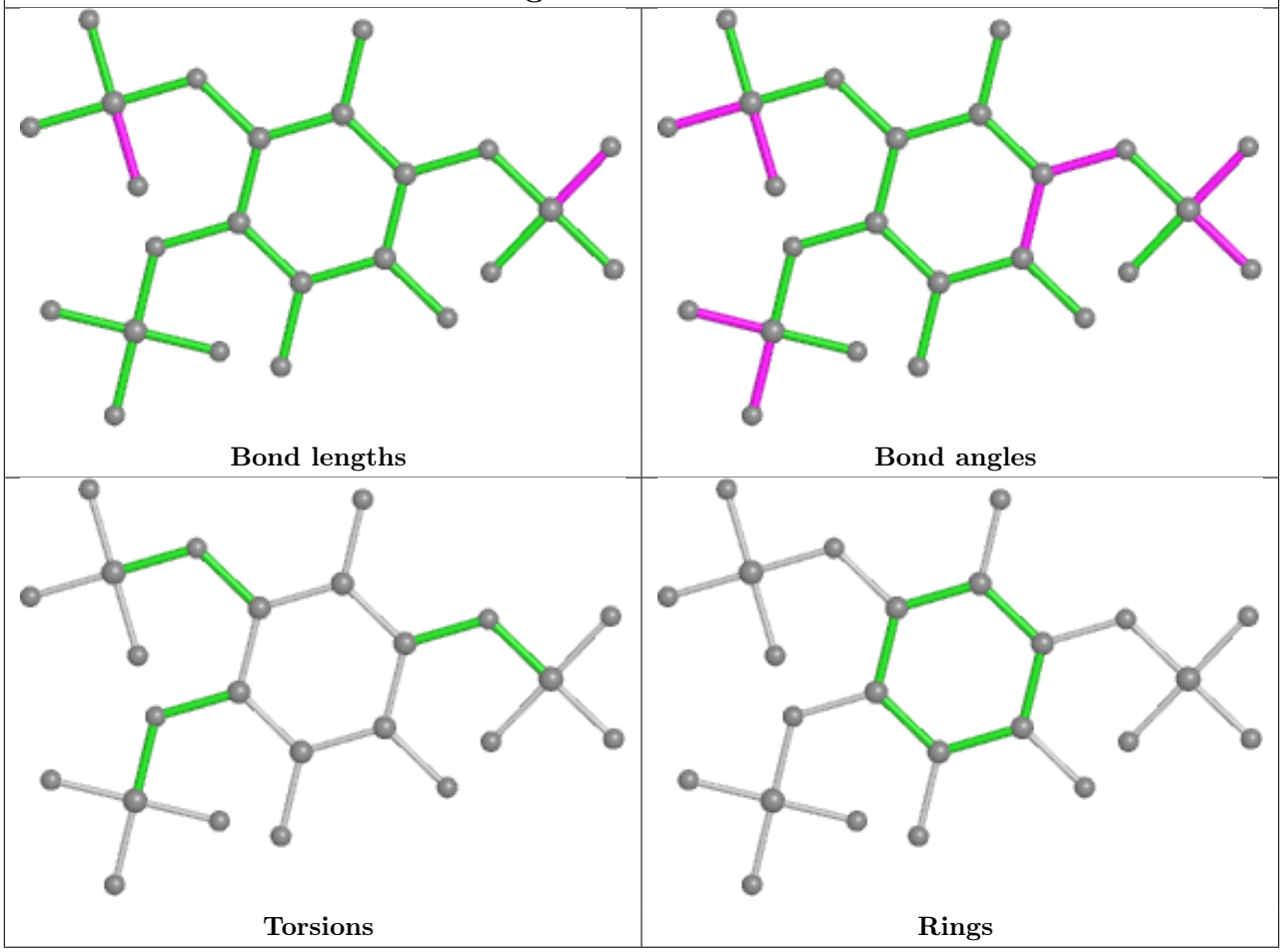


Torsions



Rings

Ligand I3P B 3000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1721/2217 (77%)	0.15	126 (7%)	15	16	135, 166, 176, 187	0
1	B	1720/2217 (77%)	0.10	117 (6%)	17	18	145, 165, 178, 192	0
All	All	3441/4434 (77%)	0.12	243 (7%)	16	16	135, 166, 177, 192	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1436	GLU	7.8
1	B	401	SER	7.8
1	A	1468	LYS	7.3
1	B	1437	MET	6.8
1	A	1368	ASN	6.3
1	B	419	GLY	6.3
1	B	400	HIS	6.2
1	B	1438	LYS	6.0
1	A	1469	HIS	5.8
1	B	402	THR	5.8
1	B	418	ILE	5.7
1	B	1370	PRO	5.7
1	B	6	SER	5.3
1	B	420	THR	5.3
1	A	1388	LYS	5.0
1	A	1387	GLY	5.0
1	B	1435	VAL	5.0
1	B	195	ALA	5.0
1	B	194	HIS	5.0
1	B	25	GLY	4.9
1	B	403	ASN	4.9
1	B	1369	SER	4.8
1	B	586	GLY	4.7
1	B	1443	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	267	THR	4.4
1	A	548	PRO	4.3
1	B	301	SER	4.3
1	A	1398	SER	4.3
1	A	1096	ALA	4.3
1	B	2018	GLY	4.3
1	B	639	VAL	4.2
1	A	1095	GLN	4.2
1	A	1467	ARG	4.2
1	A	2106	GLU	4.2
1	A	1434	GLU	4.1
1	B	1444	ASN	4.1
1	B	587	TYR	4.1
1	A	1369	SER	4.0
1	B	405	PRO	4.0
1	B	1456	ASP	4.0
1	A	1433	THR	4.0
1	A	156	ASN	3.9
1	B	24	ASN	3.9
1	B	302	LEU	3.9
1	A	1989	CYS	3.8
1	B	640	SER	3.8
1	A	195	ALA	3.8
1	A	1458	CYS	3.8
1	A	63	MET	3.7
1	A	155	GLY	3.7
1	A	1982	ASP	3.7
1	B	266	THR	3.6
1	B	2019	LEU	3.6
1	A	1386	GLU	3.6
1	B	7	SER	3.5
1	A	2140	ASN	3.5
1	B	1177	LYS	3.5
1	A	82	SER	3.4
1	A	238	ASP	3.4
1	B	638	CYS	3.4
1	B	1439	GLU	3.4
1	B	399	VAL	3.4
1	B	2074	ASN	3.3
1	A	1029	ASP	3.3
1	A	1027	ALA	3.3
1	A	724	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	67	SER	3.3
1	B	2047	CYS	3.3
1	A	1300	GLU	3.3
1	B	2138	GLY	3.2
1	B	2075	PRO	3.2
1	A	1301	THR	3.2
1	B	216	THR	3.2
1	B	355	LEU	3.2
1	A	1384	CYS	3.1
1	B	1429	CYS	3.1
1	A	1414	CYS	3.1
1	B	704	ASN	3.1
1	B	2048	HIS	3.1
1	B	84	THR	3.0
1	A	154	ALA	3.0
1	B	354	SER	3.0
1	B	404	ILE	3.0
1	A	83	THR	3.0
1	A	1132	TRP	3.0
1	A	217	SER	3.0
1	A	1459	ARG	3.0
1	A	66	TYR	3.0
1	A	157	GLU	3.0
1	B	2160	HIS	3.0
1	A	2144	GLY	2.9
1	B	1431	VAL	2.9
1	A	2109	GLU	2.9
1	B	1834	GLY	2.9
1	B	1434	GLU	2.9
1	A	2042	TYR	2.9
1	A	53	PHE	2.9
1	A	2210	PRO	2.9
1	B	417	LYS	2.9
1	A	1026	GLY	2.8
1	B	779	ALA	2.8
1	B	1428	HIS	2.8
1	A	1367	GLU	2.8
1	B	2163	ALA	2.8
1	A	1432	ASP	2.8
1	B	2137	ASP	2.8
1	B	265	ARG	2.8
1	B	19	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1985	ASN	2.8
1	A	52	LYS	2.8
1	B	1414	CYS	2.8
1	A	2196	GLU	2.8
1	B	2076	LEU	2.8
1	A	351	MET	2.8
1	B	2046	PRO	2.8
1	A	401	SER	2.7
1	A	1435	VAL	2.7
1	B	414	VAL	2.7
1	B	2020	LEU	2.7
1	A	196	SER	2.7
1	A	64	ASN	2.7
1	A	6	SER	2.7
1	A	1046	GLU	2.7
1	B	193	LEU	2.7
1	A	309	ALA	2.6
1	B	776	ASP	2.6
1	B	1442	THR	2.6
1	B	351	MET	2.6
1	B	1347	ASP	2.6
1	A	1997	ASN	2.6
1	B	154	ALA	2.6
1	A	314	LEU	2.6
1	A	2101	SER	2.6
1	A	54	ARG	2.6
1	A	1097	PHE	2.6
1	A	236	GLY	2.6
1	A	2203	THR	2.6
1	A	2099	MET	2.6
1	A	2199	ARG	2.6
1	A	2107	ASN	2.5
1	B	960	PRO	2.5
1	A	304	ARG	2.5
1	B	415	MET	2.5
1	A	237	GLY	2.5
1	A	28	SER	2.5
1	A	216	THR	2.5
1	B	1427	ASN	2.5
1	B	2159	ALA	2.5
1	A	84	THR	2.5
1	B	1368	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1009	SER	2.5
1	B	413	PRO	2.5
1	A	2160	HIS	2.5
1	B	210	ASN	2.5
1	B	2203	THR	2.5
1	A	1133	VAL	2.4
1	A	1981	ARG	2.4
1	A	252	THR	2.4
1	B	2216	GLU	2.4
1	B	1327	GLN	2.4
1	A	1389	ASN	2.4
1	A	284	VAL	2.4
1	B	159	SER	2.4
1	A	2050	ASN	2.4
1	A	1178	GLU	2.4
1	A	1385	THR	2.4
1	A	1366	ASP	2.4
1	B	83	THR	2.4
1	A	218	TRP	2.4
1	B	2144	GLY	2.4
1	A	62	PRO	2.4
1	B	26	PHE	2.4
1	A	1471	ASP	2.3
1	A	1094	LEU	2.3
1	A	27	ILE	2.3
1	A	1470	ALA	2.3
1	B	1326	CYS	2.3
1	A	503	ASN	2.3
1	B	289	HIS	2.3
1	B	156	ASN	2.3
1	A	2212	PRO	2.3
1	B	2139	GLU	2.3
1	B	157	GLU	2.3
1	A	55	ASP	2.3
1	A	2043	CYS	2.3
1	B	300	ASN	2.3
1	A	316	ALA	2.3
1	B	778	ARG	2.3
1	A	283	GLU	2.3
1	A	1299	ILE	2.3
1	A	502	PRO	2.3
1	A	22	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	197	SER	2.2
1	A	2105	SER	2.2
1	A	2110	ARG	2.2
1	A	199	GLN	2.2
1	B	1348	ARG	2.2
1	B	2045	GLY	2.2
1	A	352	VAL	2.2
1	B	2077	GLY	2.2
1	A	2209	PHE	2.2
1	B	2193	ALA	2.2
1	B	23	THR	2.2
1	A	500	SER	2.2
1	A	2082	ASP	2.2
1	B	2101	SER	2.2
1	B	211	SER	2.2
1	A	723	GLN	2.2
1	A	1427	ASN	2.2
1	A	2045	GLY	2.2
1	B	1108	ASP	2.2
1	B	1432	ASP	2.2
1	B	268	GLY	2.2
1	A	310	THR	2.1
1	A	2141	GLY	2.1
1	B	45	ASP	2.1
1	A	305	PHE	2.1
1	A	127	LYS	2.1
1	B	303	PHE	2.1
1	B	1978	ASN	2.1
1	B	2002	THR	2.1
1	B	563	SER	2.1
1	A	1438	LYS	2.1
1	A	1028	LEU	2.1
1	A	2047	CYS	2.1
1	A	2100	GLU	2.1
1	B	368	PHE	2.1
1	B	1371	LEU	2.1
1	A	1442	THR	2.1
1	A	900	VAL	2.1
1	B	510	MET	2.1
1	A	235	LYS	2.1
1	B	1415	ILE	2.0
1	A	1487	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	2021	GLY	2.0
1	B	1008	SER	2.0
1	A	661	ASN	2.0
1	A	1889	GLU	2.0
1	B	465	ILE	2.0
1	B	1430	TYR	2.0
1	B	1472	SER	2.0
1	A	403	ASN	2.0
1	A	1441	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

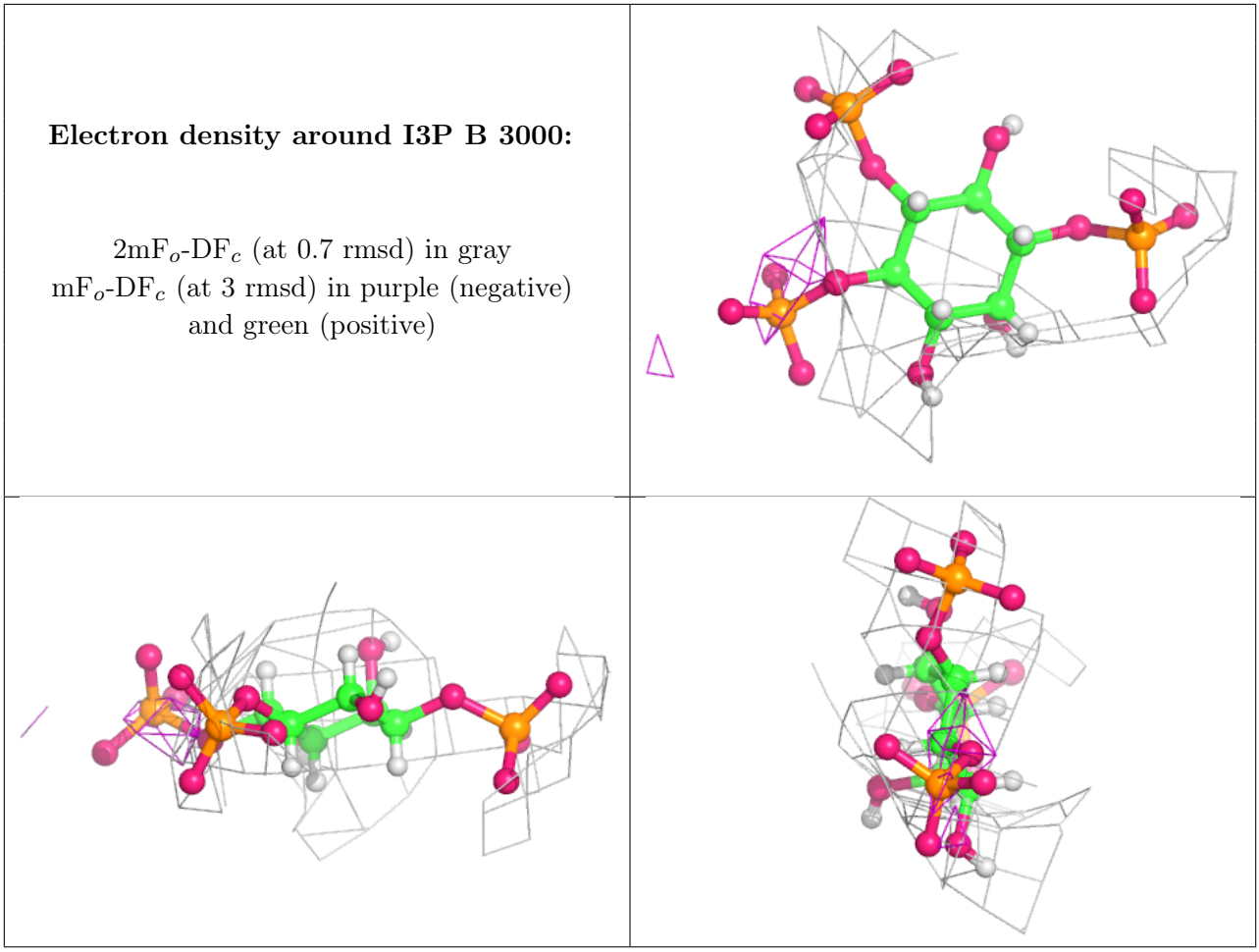
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	I3P	B	3000	24/24	0.57	0.70	199,199,203,203	0
2	I3P	A	3000	24/24	0.59	0.35	169,172,172,172	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

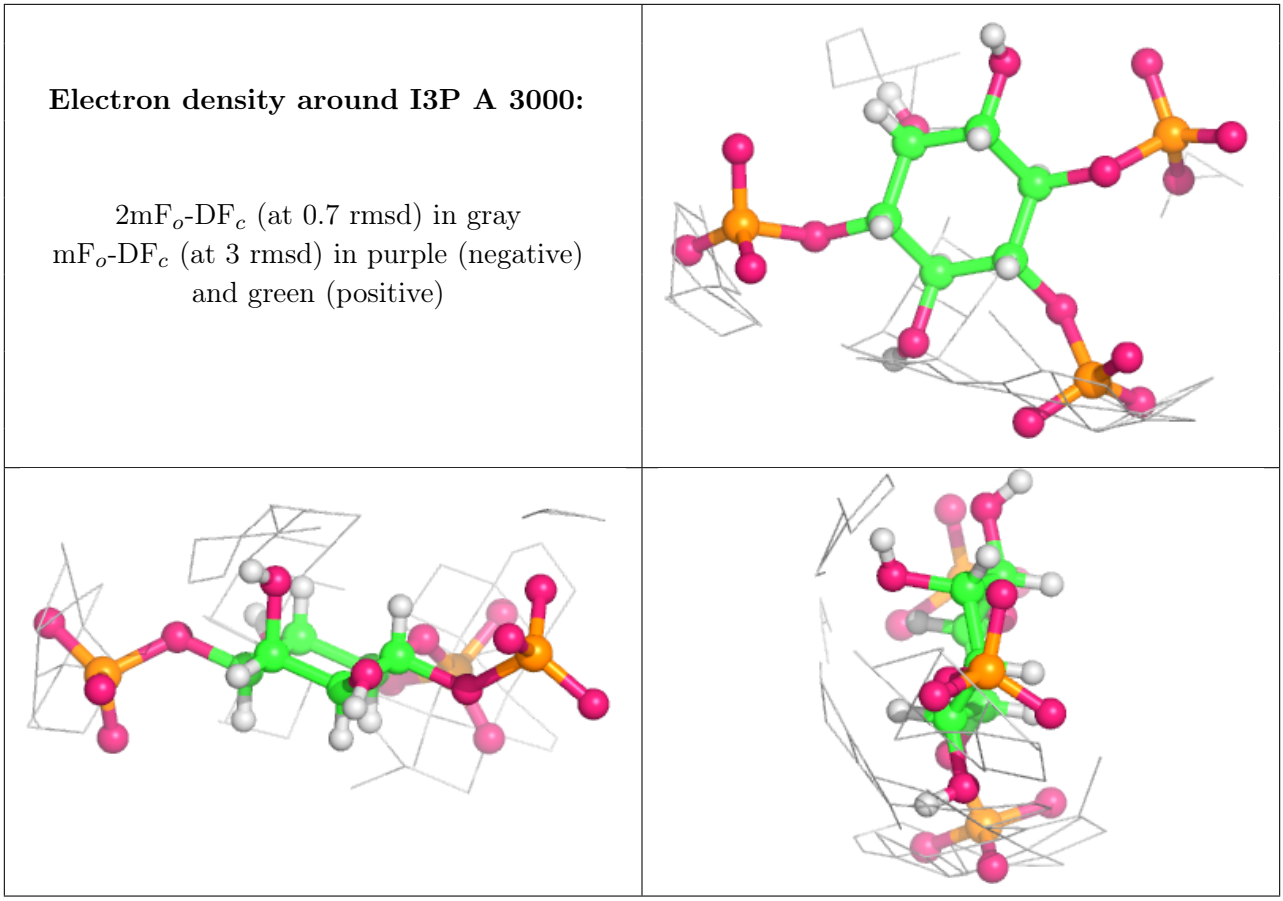
Electron density around I3P B 3000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around I3P A 3000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.