Full wwPDB EM Validation Report (i)

Nov 23, 2022 – 07:40 AM JST

PDB ID	:	7V1N
EMDB ID	:	EMD-31628
Title	:	Structure of the Clade 2 C. difficile TcdB in complex with its receptor TFPI
Authors	:	Luo, J.; Yang, Q.; Zhang, X.; Zhang, Y.; Wan, L.; Li, Y.; Tao, L.
Deposited on	:	2021-08-05
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

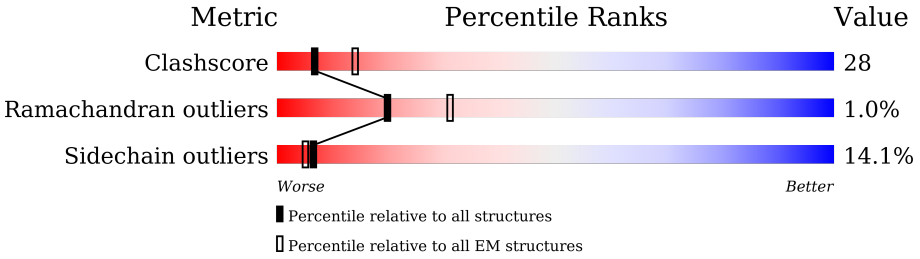
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2375	29%; 47%; 44%; 7% •
2	K	251	11%; 14%; 8% •; 76%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Toxin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2344	18665	11903	2935	3784	43	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	ASP	GLY	conflict	UNP Q9EXR0
A	385	ASN	ASP	conflict	UNP Q9EXR0
A	680	ILE	LEU	conflict	UNP Q9EXR0
A	1211	LYS	GLU	conflict	UNP Q9EXR0
A	1528	LEU	ILE	conflict	UNP Q9EXR0
A	1618	SER	PHE	conflict	UNP Q9EXR0
A	1693	ILE	VAL	conflict	UNP Q9EXR0
A	1697	ASN	GLY	conflict	UNP Q9EXR0
A	1874	ALA	PRO	conflict	UNP Q9EXR0
A	2016	LYS	ARG	conflict	UNP Q9EXR0
A	2229	THR	ALA	conflict	UNP Q9EXR0
A	2368	HIS	-	expression tag	UNP Q9EXR0
A	2369	HIS	-	expression tag	UNP Q9EXR0
A	2370	HIS	-	expression tag	UNP Q9EXR0
A	2371	HIS	-	expression tag	UNP Q9EXR0
A	2372	HIS	-	expression tag	UNP Q9EXR0
A	2373	HIS	-	expression tag	UNP Q9EXR0
A	2374	HIS	-	expression tag	UNP Q9EXR0
A	2375	HIS	-	expression tag	UNP Q9EXR0

- Molecule 2 is a protein called Isoform Beta of Tissue factor pathway inhibitor.

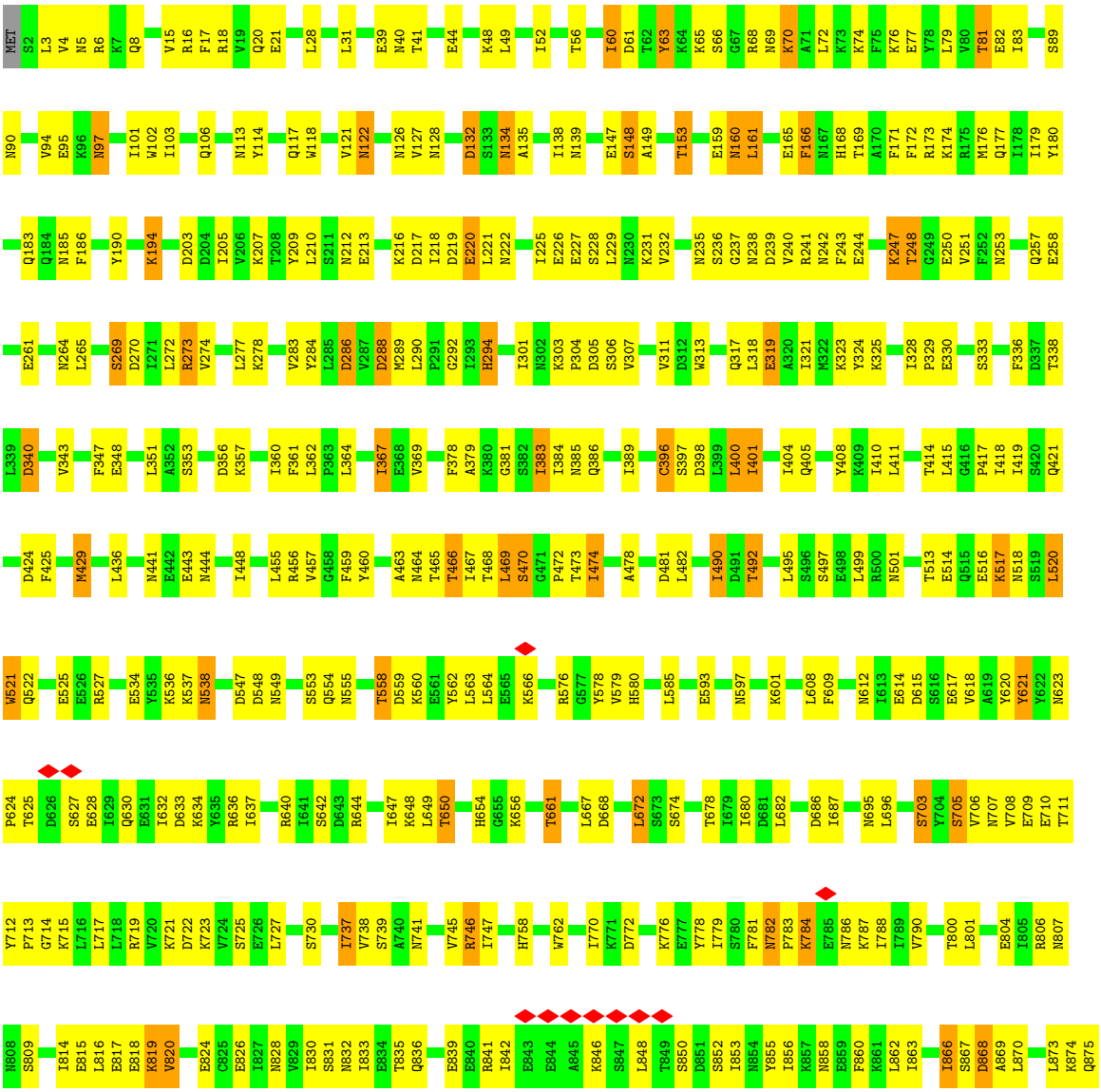
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	59	491	306	81	97	7	1	0

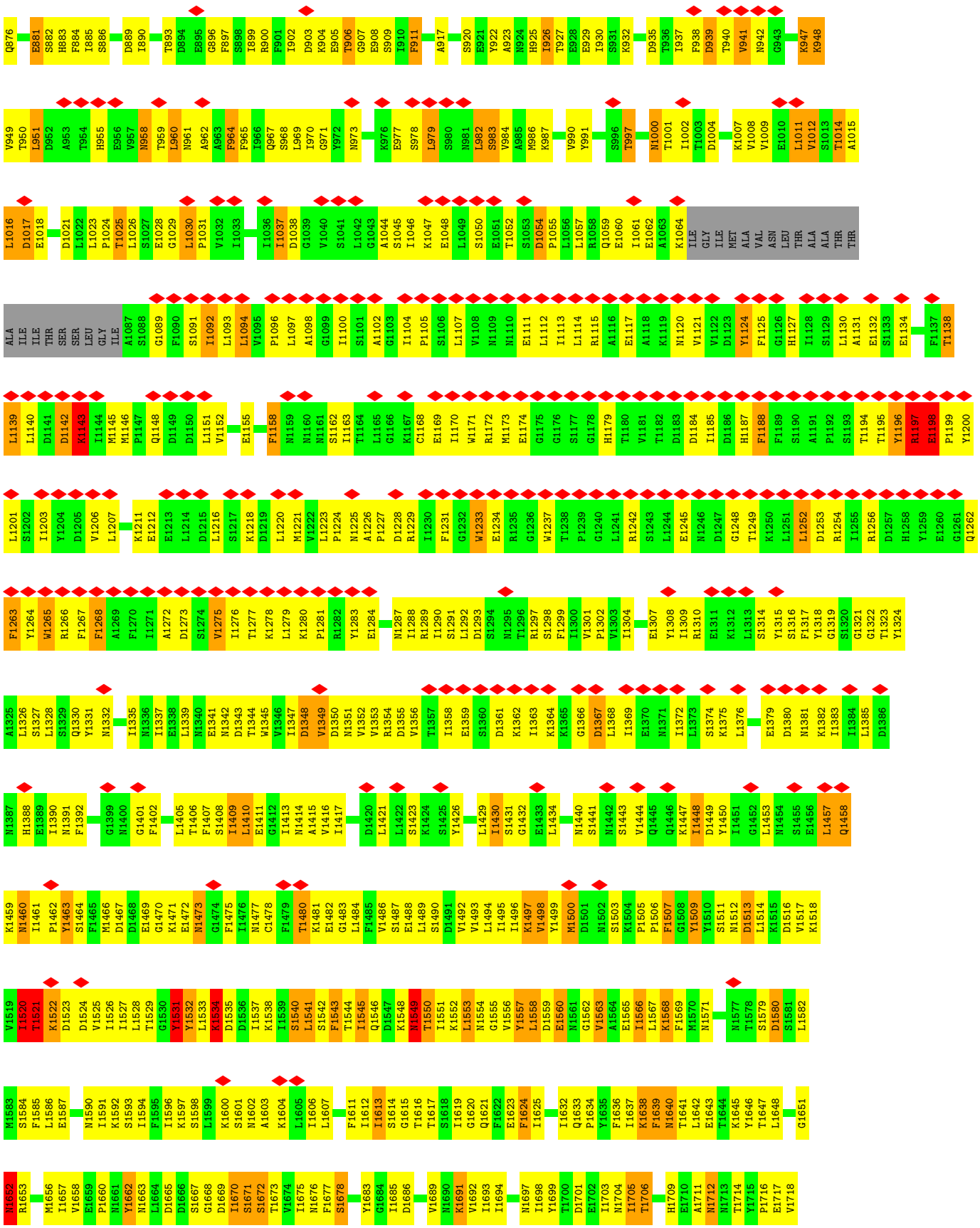
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Toxin B

Chain A: 29% 47% 44% 7%

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V949 T950 L951 D952 A953 T954 H955 E956 V957 N958 T959 L960 N961 A962 A963 F964 F965 I966 Q967 S968 L969 I970 G971 Y972 N973 K976 E977 S978 L979 S980 N981 L982 S983 V984 A985 M986 K987 V990 Y991 S996 T997 N1000 T1001 I1002 T1003 D1004 K1007 V1008 V1009 E1010 L1011 V1012 S1013 T1014 A1015
L1016 D1017 E1018 D1021 L1022 L1023 P1024 T1025 L1026 S1027 E1028 G1029 L1030 P1031 V1032 I1033 I1036 I1037 D1038 G1039 V1040 S1041 L1042 G1043 A1044 S1045 I1046 K1047 E1048 L1049 S1050 E1051 T1052 S1053 D1054 P1055 L1056 L1057 R1058 Q1059 E1060 I1061 E1062 A1063 K1064 ILE GLY ILE MET ALA VAL ASN LEU THR ALA ALA THR THR
ALA ILE ILE THR SER SER LEU GLY ILE A1087 S1088 G1089 F1090 S1091 I1092 L1093 L1094 V1095 P1096 L1097 A1098 G1099 I1100 S1101 A1102 G1103 I1104 P1105 S1106 L1107 V1108 N1109 N1110 E1111 L1112 I1113 L1114 R1115 A1116 E1117 A1118 K1119 N1120 V1121 V1122 D1123 Y1124 F1125 G1126 H1127 I1128 S1129 L1130 A1131 E1132 S1133 E1134 F1137 T1138
L1139 L1140 D1141 D1142 K1143 I1144 M1145 M1146 P1147 Q1148 D1149 D1150 L1151 V1152 E1155 F1158 N1159 N1160 N1161 S1162 I1163 T1164 L1165 G1166 K1167 C1168 E1169 I1170 W1171 R1172 M1173 E1174 G1175 G1176 S1177 G1178 H1179 T1180 V1181 T1182 D1183 D1184 I1185 D1186 H1187 F1188 F1189 S1190 A1191 P1192 S1193 T1194 T1195 Y1196 R1197 E1198 P1199 Y1200
L1201 S1202 I1203 Y1204 D1205 V1206 L1207 K1211 E1212 E1213 L1214 D1215 L1216 S1217 K1218 D1219 L1220 M1221 V1222 L1223 P1224 N1225 A1226 P1227 D1228 R1229 I1230 F1231 G1232 W1233 E1234 R1235 G1236 W1237 T1238 P1239 G1240 L1241 R1242 S1243 L1244 E1245 N1246 D1247 G1248 T1249 K1250 L1251 L1252 D1253 R1254 I1255 R1256 D1257 H1258 Y1259 E1260 G1261 Q1262
F1263 Y1264 W1265 R1266 F1267 F1268 A1269 F1270 I1271 A1272 D1273 S1274 V1275 I1276 T1277 K1278 L1279 K1280 P1281 R1282 Y1283 E1284 N1287 I1288 R1289 I1290 S1291 L1292 D1293 S1294 N1295 T1296 R1297 S1298 F1299 I1300 V1301 P1302 V1303 I1304 E1307 Y1308 I1309 R1310 E1311 K1312 L1313 S1314 Y1315 S1316 F1317 Y1318 G1319 S1320 G1321 G1322 T1323 Y1324
A1325 L1326 S1327 L1328 S1329 Q1330 Y1331 N1332 I1335 N1336 I1337 E1338 L1339 N1340 E1341 N1342 D1343 T1344 W1345 V1346 I1347 D1348 V1349 D1350 N1351 V1352 V1353 R1354 D1355 V1356 T1357 I1358 E1359 S1360 D1361 K1362 I1363 K1364 K1365 G1366 D1367 L1368 I1369 E1370 N1371 I1372 L1373 S1374 K1375 L1376 E1379 D1380 N1381 K1382 I1383 I1384 L1385 D1386
N1387 H1388 E1389 I1390 N1391 F1392 G1399 N1400 G1401 F1402 L1405 T1406 F1407 S1408 I1409 L1410 E1411 G1412 I1413 N1414 A1415 V1416 I1417 D1420 L1421 L1422 S1423 K1424 S1425 Y1426 L1429 I1430 S1431 G1432 E1433 L1434 N1440 S1441 N1442 S1443 V1444 Q1445 Q1446 K1447 I1448 D1449 Y1450 I1451 G1452 L1453 N1454 S1455 E1456 L1457 Q1458
K1459 N1460 I1461 P1462 Y1463 S1464 F1465 M1466 D1467 D1468 E1469 G1470 K1471 E1472 N1473 G1474 F1475 I1476 N1477 C1478 F1479 T1480 K1481 E1482 G1483 L1484 F1485 V1486 S1487 E1488 L1489 S1490 D1491 V1492 V1493 L1494 I1495 I1496 K1497 V1498 Y1499 M1500 D1501 N1502 S1503 K1504 P1505 P1506 F1507 G1508 Y1509 Y1510 S1511 N1512 D1513 L1514 K1515 D1516 V1517 K1518
V1519 I1520 T1521 K1522 D1523 D1524 V1525 I1526 I1527 L1528 I1529 G1530 Y1531 Y1532 L1533 K1534 D1535 D1536 I1537 K1538 I1539 S1540 L1541 S1542 F1543 T1544 I1545 Q1546 D1547 K1548 N1549 T1550 I1551 K1552 L1553 N1554 G1555 V1556 Y1557 L1558 D1559 E1560 N1561 G1562 V1563 A1564 E1565 I1566 L1567 K1568 F1569 M1570 N1571 N1577 T1578 S1579 D1580 S1581 L1582
M1583 S1584 F1585 L1586 E1587 N1590 I1591 K1592 S1593 I1594 F1595 I1596 K1597 S1598 L1599 K1600 S1601 N1602 A1603 K1604 L1605 I1606 L1607 F1611 I1612 I1613 S1614 G1615 T1616 T1617 S1618 I1619 G1620 Q1621 F1622 E1623 F1624 I1625 I1632 Q1633 P1634 Y1635 F1636 I1637 K1638 F1639 N1640 T1641 L1642 E1643 T1644 K1645 Y1646 T1647 L1648 G1651
N1652 R1653 M1656 I1657 V1658 E1659 P1660 N1661 Y1662 N1663 L1664 D1665 D1666 S1667 G1668 D1669 I1670 S1671 S1672 T1673 V1674 I1675 N1676 F1677 S1678 Y1683 G1684 I1685 D1686 V1689 N1690 K1691 V1692 I1693 I1694 N1697 I1698 Y1699 T1700 D1701 E1702 I1703 N1704 I1705 T1706 H1709 E1710 A1711 N1712 N1713 T1714 Y1715 P1716 E1717 V1718

I1719 V1720 Y1725 K1729 I1732 N1733 D1736 L1737 S1738 I1739 R1740 Y1741 V1742 N1745 D1746 G1747 S1748 I1751 L1752 M1753 S1754 T1755 D1756 E1757 E1758 N1759 K1760 V1761 S1762 Q1763 I1766 R1767 F1772 K1773 T1776 I1777 K1780 F1783 D1787 K1788 I1791 N1794 S1798 T1799 F1800

T1801 P1802 Y1805 V1806 E1807 G1808 L1809 L1810 N1811 Y1812 D1813 L1814 I1817 S1818 F1824 Y1825 I1826 N1827 N1828 L1829 M1832 V1833 S1834 G1835 L1836 V1837 Y1838 I1839 N1840 D1841 S1842 L1843 Y1844 Y1845 F1846 K1847 P1848 P1849 I1850 K1851 N1852 F1857 T1858 T1859 I1860 G1861 D1862 D1863 K1864 F1867 N1868 N1871 G1872

G1873 A1874 A1875 S1876 E1879 I1882 D1883 G1884 K1885 N1886 Y1887 Y1888 F1889 S1890 G1893 V1894 L1895 Q1896 T1897 F1900 S1901 T1902 E1903 D1904 K1907 Y1908 F1909 A1910 P1911 A1912 D1913 T1914 L1915 D1916 E1917 N1918 L1919 E1920 G1921 E1922 A1923 I1924 D1925 F1926 T1927 G1928 K1929 L1930 I1931 I1932 D1933 E1934 N1935 V1936 Y1937

Y1938 F1939 G1940 D1941 N1942 Y1943 R1944 A1945 A1946 I1947 E1948 W1949 Q1950 T1951 L1952 D1953 D1954 E1955 V1956 Y1957 Y1958 F1959 S1960 T1961 D1962 T1963 G1964 R1965 A1966 F1967 K1968 G1969 L1970 N1971 Q1972 I1973 G1974 D1975 D1976 K1977 F1978 Y1979 F1980 N1981 S1982 D1983 G1984 I1985 M1986 Q1987 K1988 G1989 F1990 V1991 N1992 I1993 N1994 D1995 K1996 T1997

F1998 Y1999 F2000 D2001 D2002 S2003 G2004 V2005 M2006 K2007 S2008 G2009 Y2010 T2011 E2012 I2013 D2014 G2015 K2016 Y2017 F2018 Y2019 F2020 A2021 E2022 N2023 G2024 E2025 M2026 Q2027 I2028 G2029 V2030 F2031 M2032 T2033 A2034 D2035 G2036 F2037 K2038 Y2039 F2040 A2041 H2042 H2043 D2044 E2045 D2046 L2047 G2048 N2049 E2050 E2051 G2052 E2053 A2054 L2055 S2056 Y2057

S2058 G2059 I2060 L2061 N2062 F2063 N2064 N2065 K2066 I2067 Y2068 Y2069 F2070 D2071 D2072 S2073 F2074 T2075 A2076 V2077 V2078 G2079 W2080 K2081 D2082 L2083 E2084 D2085 G2086 S2087 K2088 Y2089 Y2090 F2091 D2092 E2093 N2094 T2095 A2096 E2097 A2098 S2099 I2100 G2101 I2102 S2103 I2104 I2105 N2106 D2107 G2108 K2109 Y2110 Y2111 F2112 N2113 D2114 S2115 G2116 I2117

M2118 Q2119 I2120 G2121 F2122 V2123 T2124 I2125 N2126 N2127 E2128 V2129 F2130 Y2131 F2132 S2133 D2134 S2135 G2136 I2137 V2138 E2139 S2140 G2141 M2142 Q2143 N2144 I2145 D2146 D2147 N2148 Y2149 F2150 Y2151 I2152 S2153 E2154 N2155 G2156 L2157 V2158 Q2159 I2160 G2161 V2162 F2163 D2164 T2165 S2166 D2167 G2168 Y2169 K2170 Y2171 F2172 A2173 P2174 A2175 N2176 T2177

V2178 N2179 D2180 N2181 I2182 Y2183 G2184 Q2185 A2186 V2187 E2188 Y2189 S2190 G2191 L2192 V2193 R2194 V2195 N2196 E2197 D2198 V2199 Y2200 S2201 F2202 G2203 E2204 S2205 Y2206 T2207 I2208 E2209 T2210 G2211 W2212 I2213 Y2214 D2215 S2216 E2217 N2218 E2219 S2220 D2221 K2222 Y2223 Y2224 F2225 D2226 P2227 E2228 T2229 K2230 K2231 A2232 Y2233 K2234 G2235 I2236 N2237

V2238 I2239 D2240 D2241 I2242 K2243 Y2244 Y2245 F2246 D2247 E2248 N2249 G2250 I2251 M2252 R2253 T2254 G2255 L2256 I2257 T2258 F2259 E2260 D2261 N2262 H2263 Y2264 Y2265 F2266 N2267 E2268 D2269 G2270 E2271 M2272 Q2273 Y2274 G2275 Y2276 L2277 N2278 I2279 E2280 D2281 K2282 M2283 F2284 Y2285 F2286 S2287 E2288 D2289 G2290 I2291 M2292 Q2293 I2294 G2295 V2296 F2297

N2298 T2299 P2300 D2301 G2302 F2303 K2304 Y2305 F2306 A2307 H2308 Q2309 N2310 T2311 L2312 D2313 E2314 N2315 F2316 E2317 G2318 E2319 S2320 I2321 N2322 Y2323 T2324 G2325 W2326 L2327 D2328 L2329 D2330 E2331 K2332 R2333 Y2334 Y2335 F2336 T2337 D2338 E2339 Y2340 I2341 A2342 A2343 T2344 G2345 S2346 V2347 I2348 I2349 D2350 G2351 E2352 E2353 Y2354 Y2355 F2356 D2357

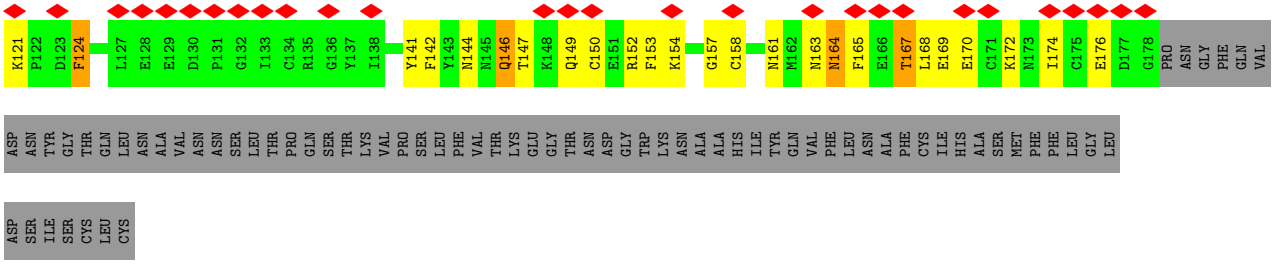
P2358 D2359 T2360 A2361 Q2362 L2363 V2364 I2365 S2366 E2367 HIS HIS HIS HIS HIS HIS HIS

- Molecule 2: Isoform Beta of Tissue factor pathway inhibitor

Chain K: 11% 14% 8% • 76%

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

GLY PRO CYS LYS ALA ILE MET LYS ARG PHE PHE PHE ASN ILE PHE THR ARG GLN CYS GLU GLU PHE ILE TYR GLY GLY CYS GLU GLY ASN GLN ASN ARG PHE GLU SER LEU GLU GLU CYS LYS LYS MET CYS THR ARG ASP ASN ALA ASN ARG ILE ILE LYS THR THR LEU GLN GLN E120


K121 P122 D123 F124 L127 E128 E129 D130 P131 G132 I133 C134 R135 G136 Y137 I138 Y141 F142 Y143 N144 N145 Q146 T147 K148 Q149 C150 E151 R152 F153 K154 G157 C158 N161 M162 N163 N164 F165 E166 T167 L168 E169 E170 C171 K172 N173 I174 C175 E176 D177 G178 PRO ASN GLY PHE GLN VAL
ASP ASN TYR GLY THR GLN LEU ASN ALA VAL ASN ASN SER LEU THR PRO GLN SER THR LYS VAL PRO SER LEU PHE VAL THR LYS GLU GLY THR ASN ASP GLY TRP LYS ASN ALA ALA HIS ILE TYR GLN VAL PHE LEU ASN ALA PHE CYS ILE HIS ALA SER MET PHE PHE LEU GLY LEU
ASP SER ILE SER CYS LEU CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227825	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.190	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.63	1/19027 (0.0%)	0.62	0/25754
2	K	0.43	0/504	0.63	0/674
All	All	0.63	1/19531 (0.0%)	0.62	0/26428

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1198	GLU	C-N	8.49	1.50	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	18665	0	17845	1015	0
2	K	491	0	443	19	0
All	All	19156	0	18288	1032	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1032) 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:1541:LEU:CD1	1:A:1556:VAL:HA	1.55	1.36
1:A:1619:ILE:HG21	1:A:1641:THR:CG2	1.63	1.27
1:A:1541:LEU:CG	1:A:1556:VAL:HA	1.74	1.16
1:A:1031:PRO:HG2	1:A:1542:SER:HB2	1.14	1.13
1:A:1541:LEU:HD12	1:A:1556:VAL:HA	1.35	1.09
1:A:1541:LEU:CD1	1:A:1556:VAL:CA	2.33	1.07
1:A:1139:LEU:HD11	1:A:1218:LYS:NZ	1.70	1.05
1:A:1541:LEU:HG	1:A:1556:VAL:HA	1.37	1.05
1:A:1619:ILE:HG21	1:A:1641:THR:HG22	1.36	1.05
1:A:1541:LEU:HB3	1:A:1555:GLY:O	1.57	1.04
1:A:1541:LEU:HD12	1:A:1556:VAL:CA	1.87	1.03
1:A:1527:ILE:HG22	1:A:1542:SER:HB3	1.34	1.03
1:A:1031:PRO:HG2	1:A:1542:SER:CB	1.90	1.00
1:A:1619:ILE:HG21	1:A:1641:THR:HG23	1.41	0.98
1:A:1415:ALA:HA	1:A:1430:ILE:HA	1.46	0.97
1:A:1541:LEU:CB	1:A:1555:GLY:O	2.13	0.97
1:A:960:LEU:HD21	1:A:1651:GLY:HA2	1.45	0.95
1:A:708:VAL:O	1:A:711:THR:HG22	1.69	0.92
1:A:1376:LEU:HD13	1:A:1385:LEU:HB3	1.49	0.92
1:A:2098:ALA:O	1:A:2100:ILE:HG12	1.68	0.92
1:A:1061:ILE:CG1	1:A:1522:LYS:HE3	2.01	0.90
1:A:960:LEU:CD2	1:A:1651:GLY:HA2	2.00	0.90
1:A:1031:PRO:HB2	1:A:1527:ILE:HG21	1.52	0.90
1:A:1619:ILE:CG2	1:A:1641:THR:HG22	2.02	0.89
1:A:1197:ARG:HH21	1:A:1197:ARG:HG2	1.34	0.89
1:A:1527:ILE:CG2	1:A:1542:SER:HB3	2.05	0.86
1:A:1139:LEU:HD11	1:A:1218:LYS:CE	2.05	0.86
2:K:169:GLU:HA	2:K:172:LYS:HD3	1.58	0.85
1:A:1414:ASN:O	1:A:1431:SER:N	2.08	0.85
1:A:1619:ILE:CG2	1:A:1641:THR:CG2	2.53	0.85
1:A:278:LYS:NZ	1:A:398:ASP:OD1	2.09	0.85
1:A:2102:ILE:HD11	1:A:2110:TYR:O	1.75	0.85
1:A:902:ILE:HG22	1:A:903:ASP:H	1.41	0.84
1:A:1030:LEU:HD21	1:A:1612:ILE:HG12	1.60	0.84
1:A:1061:ILE:HG13	1:A:1522:LYS:HE3	1.59	0.83
1:A:1545:ILE:HG22	1:A:1551:ILE:HG13	1.60	0.83
1:A:2181:ASN:HD22	1:A:2187:VAL:HG11	1.44	0.83
1:A:1541:LEU:HD12	1:A:1556:VAL:C	1.98	0.83
1:A:1541:LEU:HD11	1:A:1557:TYR:N	1.93	0.83
1:A:1031:PRO:CG	1:A:1542:SER:HB2	2.05	0.82
1:A:881:GLU:HG2	1:A:905:GLU:HB3	1.60	0.82
1:A:1430:ILE:HG12	1:A:1463:TYR:CG	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:ND2	1:A:44:GLU:OE1	2.10	0.82
1:A:935:ASP:O	1:A:938:PHE:CE2	2.32	0.82
1:A:1541:LEU:CD1	1:A:1557:TYR:N	2.42	0.82
1:A:1171:TRP:CD2	1:A:1195:THR:HG22	2.15	0.81
1:A:547:ASP:OD2	1:A:654:HIS:ND1	2.13	0.81
1:A:1738:SER:O	1:A:1738:SER:OG	1.97	0.81
1:A:106:GLN:HA	1:A:228:SER:OG	1.81	0.80
1:A:1484:LEU:HD11	1:A:1545:ILE:HD11	1.63	0.80
1:A:2033:THR:HG22	1:A:2035:ASP:H	1.45	0.80
1:A:969:LEU:HD23	1:A:986:MET:HG3	1.62	0.80
1:A:1354:ARG:NH2	1:A:1409:ILE:O	2.13	0.80
1:A:2102:ILE:CD1	1:A:2110:TYR:O	2.29	0.80
1:A:628:GLU:OE2	1:A:630:GLN:NE2	2.16	0.80
1:A:324:TYR:HB2	1:A:351:LEU:HD13	1.64	0.79
1:A:2344:THR:HB	1:A:2358:PRO:HA	1.64	0.79
1:A:1139:LEU:HD11	1:A:1218:LYS:HZ3	1.44	0.79
1:A:218:ILE:O	1:A:222:ASN:ND2	2.16	0.79
1:A:1449:ASP:OD2	1:A:1481:LYS:NZ	2.16	0.79
1:A:1115:ARG:HD2	1:A:1120:ASN:HB3	1.65	0.78
1:A:786:ASN:OD1	1:A:787:LYS:N	2.15	0.78
1:A:1663:ASN:HA	1:A:1671:SER:HB2	1.66	0.78
1:A:2049:ASN:HB2	1:A:2053:GLU:HB3	1.66	0.78
1:A:1354:ARG:NH1	1:A:1366:GLY:O	2.17	0.77
1:A:1185:ILE:HG23	1:A:1266:ARG:HG2	1.67	0.77
1:A:2130:PHE:HA	1:A:2158:VAL:HG23	1.65	0.77
1:A:1094:LEU:O	1:A:1362:LYS:NZ	2.18	0.77
1:A:1520:ILE:CG1	1:A:1527:ILE:H	1.98	0.77
1:A:1988:LYS:HA	1:A:2000:PHE:HB2	1.65	0.77
1:A:1134:GLU:OE1	1:A:1148:GLN:NE2	2.18	0.77
1:A:1227:PRO:HG3	1:A:1309:ILE:HG12	1.67	0.77
1:A:1408:SER:HA	1:A:1414:ASN:HA	1.65	0.77
1:A:973:ASN:OD1	1:A:977:GLU:N	2.18	0.76
1:A:1170:ILE:HG22	1:A:1201:LEU:HB2	1.65	0.76
1:A:623:ASN:ND2	1:A:630:GLN:OE1	2.14	0.76
1:A:1171:TRP:CG	1:A:1195:THR:HG22	2.19	0.76
1:A:1473:ASN:HB3	1:A:1518:LYS:HA	1.67	0.76
1:A:1104:ILE:HG13	1:A:1105:PRO:HD2	1.69	0.75
1:A:1523:ASP:C	1:A:1525:VAL:H	1.88	0.75
1:A:1030:LEU:HB2	1:A:1037:ILE:HA	1.67	0.75
1:A:1328:LEU:HD21	1:A:1390:ILE:HD11	1.66	0.75
1:A:1867:PHE:O	1:A:1873:GLY:HA2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1541:LEU:N	1:A:1541:LEU:HD22	2.00	0.75
1:A:2049:ASN:HD22	1:A:2055:LEU:HD11	1.52	0.75
1:A:1094:LEU:HD22	1:A:1363:ILE:HB	1.69	0.74
1:A:948:LYS:HE3	1:A:949:VAL:H	1.53	0.74
2:K:153:PHE:HZ	2:K:164:ASN:HD22	1.35	0.74
1:A:303:LYS:NZ	1:A:307:VAL:O	2.20	0.74
1:A:250:GLU:OE2	1:A:405:GLN:NE2	2.21	0.73
1:A:1061:ILE:HG13	1:A:1522:LYS:CE	2.18	0.73
1:A:1523:ASP:O	1:A:1525:VAL:N	2.21	0.73
1:A:1155:GLU:HG2	1:A:1289:ARG:HB3	1.70	0.73
1:A:1197:ARG:HG2	1:A:1197:ARG:NH2	2.04	0.73
1:A:938:PHE:H	1:A:948:LYS:HG2	1.54	0.73
1:A:1538:LYS:NZ	1:A:1540:SER:HB3	2.04	0.73
1:A:134:ASN:HD21	1:A:241:ARG:HG3	1.54	0.72
1:A:534:GLU:O	1:A:538:ASN:ND2	2.22	0.72
1:A:922:TYR:CZ	1:A:926:ILE:HG13	2.25	0.72
1:A:1359:GLU:HB2	1:A:1364:LYS:HD3	1.71	0.72
1:A:1520:ILE:HG23	1:A:1526:ILE:HG23	1.72	0.72
1:A:1407:PHE:O	1:A:1415:ALA:N	2.16	0.72
1:A:218:ILE:HA	1:A:221:LEU:HD12	1.72	0.72
1:A:1002:ILE:HG21	1:A:1007:LYS:O	1.90	0.72
1:A:1475:PHE:CZ	1:A:1521:THR:HB	2.25	0.72
1:A:960:LEU:HD21	1:A:1651:GLY:CA	2.19	0.72
1:A:1061:ILE:HG12	1:A:1522:LYS:HE3	1.71	0.72
1:A:1171:TRP:CE2	1:A:1195:THR:CG2	2.73	0.72
1:A:2049:ASN:HB3	1:A:2055:LEU:HD21	1.71	0.71
1:A:1902:THR:HG22	1:A:1903:GLU:H	1.54	0.71
1:A:1677:PHE:HD2	1:A:1705:ILE:HG22	1.56	0.71
1:A:1466:MET:HA	1:A:1471:LYS:HG2	1.73	0.70
1:A:126:ASN:OD1	1:A:127:VAL:N	2.23	0.70
1:A:1857:PHE:HE1	1:A:1864:LYS:HB3	1.57	0.70
1:A:1287:ASN:OD1	1:A:1288:ILE:N	2.23	0.70
1:A:514:GLU:O	1:A:518:ASN:ND2	2.24	0.70
1:A:1430:ILE:H	1:A:1463:TYR:HB3	1.57	0.70
1:A:1130:LEU:HG	1:A:1134:GLU:HG3	1.73	0.70
1:A:95:GLU:N	1:A:95:GLU:OE1	2.25	0.69
1:A:1048:GLU:OE2	1:A:1052:THR:OG1	2.09	0.69
1:A:1520:ILE:HG13	1:A:1527:ILE:H	1.55	0.69
1:A:2299:THR:HG21	1:A:2304:LYS:HE2	1.73	0.69
1:A:1932:ILE:HG13	1:A:1935:ASN:HB2	1.75	0.69
1:A:424:ASP:OD1	1:A:424:ASP:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1464:SER:OG	1:A:1473:ASN:ND2	2.25	0.69
1:A:712:TYR:HB3	1:A:713:PRO:HD3	1.74	0.69
1:A:1620:GLY:HA3	1:A:1639:PHE:HA	1.74	0.69
1:A:1663:ASN:CG	1:A:1670:ILE:O	2.31	0.69
1:A:782:ASN:HB3	1:A:786:ASN:HB3	1.75	0.69
1:A:973:ASN:O	1:A:987:LYS:NZ	2.25	0.69
1:A:1725:TYR:O	1:A:1780:LYS:NZ	2.25	0.69
1:A:239:ASP:OD1	1:A:240:VAL:N	2.25	0.69
1:A:364:LEU:HD22	1:A:367:ILE:HD11	1.75	0.69
1:A:1541:LEU:HG	1:A:1556:VAL:CA	2.18	0.69
1:A:340:ASP:OD2	1:A:340:ASP:N	2.26	0.68
1:A:1000:ASN:OD1	1:A:1000:ASN:N	2.17	0.68
1:A:1686:ASP:O	1:A:1714:THR:OG1	2.10	0.68
1:A:1656:MET:O	1:A:1693:ILE:N	2.25	0.68
1:A:1799:THR:O	1:A:1800:PHE:HD1	1.77	0.68
1:A:1802:PRO:O	1:A:1828:ASN:ND2	2.25	0.68
1:A:65:LYS:O	1:A:1669:ASP:HA	1.93	0.68
1:A:168:HIS:NE2	1:A:525:GLU:OE1	2.23	0.68
1:A:708:VAL:O	1:A:711:THR:CG2	2.41	0.68
1:A:1061:ILE:CG1	1:A:1522:LYS:CE	2.72	0.68
1:A:1718:VAL:HB	1:A:1766:ILE:HG23	1.75	0.68
1:A:232:VAL:O	1:A:237:GLY:N	2.27	0.67
1:A:950:THR:OG1	1:A:951:LEU:N	2.25	0.67
1:A:1520:ILE:HD12	1:A:1520:ILE:C	2.14	0.67
1:A:1591:ILE:HA	1:A:1594:ILE:HD11	1.75	0.67
1:A:1612:ILE:HG22	1:A:1625:ILE:HG22	1.74	0.67
1:A:2102:ILE:HD11	1:A:2110:TYR:C	2.14	0.67
1:A:2315:ASN:ND2	1:A:2316:PHE:O	2.27	0.67
1:A:1062:GLU:O	1:A:1064:LYS:N	2.28	0.67
1:A:580:HIS:HE2	1:A:650:THR:HG1	1.41	0.67
1:A:1538:LYS:HZ1	1:A:1540:SER:HB3	1.57	0.67
1:A:1597:LYS:N	1:A:1601:SER:O	2.19	0.67
1:A:890:ILE:HD12	1:A:899:ILE:HG22	1.77	0.67
1:A:1171:TRP:CE2	1:A:1195:THR:HG21	2.30	0.67
1:A:580:HIS:NE2	1:A:650:THR:OG1	2.25	0.67
1:A:1900:PHE:HB2	1:A:1909:PHE:HE2	1.60	0.67
1:A:903:ASP:HB3	1:A:907:GLY:HA2	1.76	0.67
1:A:1958:TYR:HB3	1:A:1980:PHE:HE2	1.60	0.67
1:A:1301:VAL:HG21	1:A:1328:LEU:HA	1.75	0.67
1:A:1488:GLU:HB2	1:A:1493:VAL:HG23	1.74	0.67
1:A:1580:ASP:O	1:A:1584:SER:OG	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:ASN:O	1:A:1798:SER:OG	2.11	0.67
1:A:396:CYS:O	1:A:400:LEU:HB2	1.95	0.67
1:A:1111:GLU:HG3	1:A:1280:LYS:HD2	1.76	0.67
1:A:1656:MET:HB3	1:A:1692:VAL:HG22	1.76	0.66
1:A:1061:ILE:O	1:A:1522:LYS:HE3	1.94	0.66
1:A:1541:LEU:CD1	1:A:1556:VAL:C	2.61	0.66
1:A:1283:TYR:HB2	1:A:1308:TYR:HE2	1.60	0.66
1:A:1511:SER:OG	1:A:1514:LEU:HB2	1.96	0.66
1:A:1860:ILE:O	1:A:1863:ASP:N	2.28	0.66
1:A:1904:ASP:O	1:A:1944:ARG:NH1	2.29	0.66
1:A:1935:ASN:HD22	1:A:1965:ARG:HD3	1.59	0.66
1:A:770:ILE:HD13	1:A:801:LEU:HD22	1.77	0.66
1:A:89:SER:OG	1:A:90:ASN:ND2	2.29	0.66
1:A:1625:ILE:O	1:A:1633:GLN:N	2.24	0.66
1:A:1171:TRP:CD2	1:A:1195:THR:CG2	2.79	0.66
1:A:1405:LEU:O	1:A:1417:ILE:N	2.28	0.66
1:A:1571:ASN:ND2	1:A:1711:ALA:O	2.29	0.66
1:A:1697:ASN:OD1	1:A:1699:TYR:N	2.27	0.66
1:A:1330:GLN:O	1:A:1388:HIS:NE2	2.28	0.66
1:A:207:LYS:HG3	1:A:221:LEU:HD13	1.78	0.66
1:A:356:ASP:OD1	1:A:357:LYS:N	2.23	0.65
1:A:1590:ASN:OD1	1:A:1593:SER:OG	2.11	0.65
1:A:2223:TYR:HB3	1:A:2252:MET:H	1.61	0.65
1:A:856:ILE:HG23	1:A:965:PHE:HZ	1.61	0.65
1:A:283:VAL:HG22	1:A:389:ILE:HG12	1.78	0.65
1:A:614:GLU:OE1	1:A:614:GLU:N	2.24	0.65
1:A:1513:ASP:OD1	1:A:1513:ASP:N	2.29	0.65
1:A:978:SER:HB3	1:A:983:SER:HA	1.79	0.65
1:A:1343:ASP:HB2	1:A:1345:TRP:HE1	1.61	0.65
1:A:1670:ILE:HD13	1:A:1699:TYR:CD1	2.32	0.65
1:A:278:LYS:HB3	1:A:397:SER:HB2	1.77	0.64
1:A:1050:SER:HB2	1:A:1402:PHE:HE2	1.62	0.64
1:A:578:TYR:HD1	1:A:644:ARG:HH21	1.42	0.64
1:A:1171:TRP:CE2	1:A:1195:THR:HG22	2.32	0.64
1:A:1955:GLU:HG2	1:A:1985:ILE:HG23	1.79	0.64
1:A:1349:VAL:HG23	1:A:1407:PHE:HD1	1.63	0.64
1:A:1592:LYS:NZ	1:A:1603:ALA:O	2.20	0.64
1:A:514:GLU:HG2	1:A:518:ASN:HD21	1.61	0.64
1:A:722:ASP:O	1:A:725:SER:OG	2.16	0.64
1:A:1223:LEU:HD11	1:A:1299:PHE:HD2	1.61	0.64
1:A:1566:ILE:HD13	1:A:1613:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1859:THR:HG22	1:A:1864:LYS:HE3	1.80	0.64
1:A:2016:LYS:HE3	1:A:2017:TYR:H	1.63	0.64
2:K:141:TYR:N	2:K:165:PHE:O	2.30	0.64
2:K:141:TYR:O	2:K:165:PHE:N	2.30	0.64
1:A:102:TRP:NE1	1:A:106:GLN:O	2.31	0.63
1:A:1541:LEU:HD11	1:A:1557:TYR:H	1.59	0.63
1:A:1543:PHE:HB3	1:A:1553:LEU:HA	1.78	0.63
1:A:467:ILE:HG23	1:A:472:PRO:HD2	1.79	0.63
1:A:964:PHE:CZ	1:A:1657:ILE:HG12	2.33	0.63
1:A:1016:LEU:C	1:A:1016:LEU:HD23	2.18	0.63
1:A:562:TYR:HA	1:A:566:LYS:HE2	1.81	0.63
1:A:705:SER:O	1:A:705:SER:OG	2.15	0.63
1:A:1486:VAL:HG12	1:A:1495:ILE:HG23	1.79	0.63
1:A:1758:GLU:OE1	1:A:1818:SER:OG	2.16	0.63
1:A:1864:LYS:HB2	1:A:1895:LEU:HB3	1.80	0.63
1:A:1184:ASP:OD2	1:A:1266:ARG:NH2	2.32	0.63
1:A:1330:GLN:OE1	1:A:1351:ASN:ND2	2.31	0.63
1:A:1637:ILE:HD13	1:A:1685:ILE:HD13	1.81	0.63
1:A:1714:THR:HA	1:A:1761:VAL:O	1.99	0.63
1:A:737:ILE:HD12	1:A:778:TYR:HB3	1.81	0.62
1:A:492:THR:O	1:A:492:THR:OG1	2.13	0.62
1:A:601:LYS:NZ	1:A:745:VAL:O	2.25	0.62
1:A:2279:ILE:HG21	1:A:2284:PHE:HE2	1.64	0.62
1:A:2333:ARG:HB2	1:A:2363:LEU:HD13	1.80	0.62
2:K:144:ASN:HB2	2:K:147:THR:HG22	1.81	0.62
1:A:1914:THR:HB	1:A:1918:ASN:HD21	1.62	0.62
1:A:625:THR:HB	1:A:628:GLU:HG3	1.80	0.62
1:A:1520:ILE:HG12	1:A:1527:ILE:H	1.65	0.62
1:A:562:TYR:OH	1:A:593:GLU:OE1	2.18	0.62
1:A:1330:GLN:HB3	1:A:1351:ASN:OD1	2.00	0.62
1:A:160:ASN:OD1	1:A:160:ASN:N	2.32	0.61
1:A:1145:MET:HE1	1:A:1216:LEU:HD12	1.82	0.61
1:A:1514:LEU:HD23	1:A:1532:TYR:HB3	1.81	0.61
1:A:417:PRO:O	1:A:421:GLN:NE2	2.26	0.61
1:A:1220:LEU:HD12	1:A:1220:LEU:H	1.65	0.61
1:A:1523:ASP:C	1:A:1525:VAL:N	2.53	0.61
1:A:1613:ILE:HG23	1:A:1624:PHE:HB2	1.83	0.61
1:A:1638:LYS:O	1:A:1638:LYS:HG2	1.99	0.61
1:A:1897:THR:OG1	1:A:1909:PHE:O	2.18	0.61
1:A:114:TYR:CE2	1:A:290:LEU:HG	2.36	0.61
1:A:269:SER:O	1:A:269:SER:OG	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ILE:HD13	1:A:1829:LEU:HD13	1.82	0.61
1:A:113:ASN:HB3	1:A:328:ILE:HG23	1.82	0.61
1:A:1565:GLU:O	1:A:1568:LYS:N	2.29	0.61
1:A:1100:ILE:HD12	1:A:1100:ILE:H	1.66	0.61
1:A:534:GLU:HG2	1:A:538:ASN:HD21	1.66	0.61
1:A:826:GLU:O	1:A:830:ILE:HG13	1.99	0.61
1:A:2181:ASN:OD1	1:A:2181:ASN:N	2.32	0.61
1:A:1472:GLU:HA	1:A:1487:SER:HA	1.83	0.60
1:A:1552:LYS:HG2	1:A:1606:ILE:HD11	1.82	0.60
1:A:2092:ASP:OD2	1:A:2099:SER:HB2	2.01	0.60
1:A:1453:LEU:HD13	1:A:1461:ILE:HD11	1.83	0.60
1:A:1541:LEU:HD11	1:A:1556:VAL:HA	1.75	0.60
1:A:1646:TYR:OH	1:A:1677:PHE:HA	2.01	0.60
1:A:1405:LEU:N	1:A:1417:ILE:O	2.35	0.60
1:A:1541:LEU:HD11	1:A:1556:VAL:CA	2.30	0.60
1:A:1559:ASP:CG	1:A:1560:GLU:H	2.05	0.60
1:A:1972:GLN:HA	1:A:1977:LYS:HA	1.81	0.60
1:A:2152:ILE:HG13	1:A:2158:VAL:HA	1.84	0.60
1:A:886:SER:HB3	1:A:902:ILE:HG13	1.83	0.60
1:A:890:ILE:HG23	1:A:899:ILE:HG22	1.83	0.60
1:A:1008:VAL:HG12	1:A:1008:VAL:O	2.01	0.60
1:A:1677:PHE:CD2	1:A:1705:ILE:HG22	2.35	0.60
1:A:1107:LEU:HB3	1:A:1112:LEU:HD23	1.83	0.60
1:A:1326:LEU:HD12	1:A:1327:SER:H	1.66	0.60
1:A:2013:ILE:N	1:A:2016:LYS:O	2.30	0.60
1:A:667:LEU:HD12	1:A:672:LEU:HD22	1.82	0.59
1:A:900:ARG:HH21	1:A:909:SER:HB3	1.67	0.59
1:A:1868:ASN:ND2	1:A:1876:SER:OG	2.35	0.59
1:A:1354:ARG:NE	1:A:1408:SER:O	2.34	0.59
1:A:2104:ILE:HG22	1:A:2104:ILE:O	2.02	0.59
1:A:1462:PRO:HB3	1:A:1475:PHE:CZ	2.38	0.59
1:A:1520:ILE:HG23	1:A:1526:ILE:CG2	2.31	0.59
1:A:1114:LEU:O	1:A:1115:ARG:HD3	2.02	0.59
1:A:251:VAL:HG21	1:A:401:ILE:CD1	2.33	0.59
1:A:881:GLU:OE2	1:A:904:LYS:N	2.35	0.59
1:A:1121:VAL:HG22	1:A:1279:LEU:HD13	1.85	0.59
1:A:1319:GLY:HA3	1:A:1343:ASP:OD1	2.02	0.59
1:A:77:GLU:O	1:A:81:THR:HG23	2.02	0.58
1:A:106:GLN:HE21	1:A:231:LYS:HD2	1.67	0.58
1:A:1171:TRP:CD1	1:A:1195:THR:HG22	2.37	0.58
1:A:1500:MET:O	1:A:1503:SER:OG	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1586:LEU:HB3	1:A:1591:ILE:HG21	1.85	0.58
1:A:1983:ASP:OD1	1:A:1985:ILE:HG13	2.03	0.58
1:A:1252:LEU:HD21	1:A:1265:TRP:CD1	2.38	0.58
1:A:60:ILE:HD13	1:A:69:ASN:ND2	2.18	0.58
1:A:219:ASP:HA	1:A:222:ASN:HD22	1.69	0.58
1:A:1475:PHE:CE2	1:A:1521:THR:HB	2.38	0.58
1:A:1552:LYS:CG	1:A:1606:ILE:HD11	2.33	0.58
1:A:1537:ILE:HD13	1:A:1562:GLY:HA2	1.85	0.58
1:A:468:THR:HA	1:A:473:THR:OG1	2.03	0.58
1:A:210:LEU:HD22	1:A:216:LYS:HD2	1.85	0.58
1:A:939:ASP:N	1:A:948:LYS:HD3	2.18	0.58
1:A:1355:ASP:N	1:A:1367:ASP:O	2.27	0.58
1:A:815:GLU:HB2	1:A:818:GLU:OE1	2.03	0.58
1:A:960:LEU:CD2	1:A:1651:GLY:CA	2.77	0.58
1:A:1265:TRP:CE2	1:A:1266:ARG:HB2	2.39	0.57
1:A:1709:HIS:HB3	1:A:1712:ASN:HD21	1.68	0.57
1:A:1245:GLU:OE2	1:A:1266:ARG:NH2	2.37	0.57
1:A:1548:LYS:O	1:A:1550:THR:N	2.33	0.57
1:A:1639:PHE:N	1:A:1639:PHE:CD2	2.73	0.57
1:A:3:LEU:HD11	1:A:79:LEU:HD23	1.86	0.57
1:A:1444:VAL:O	1:A:1448:ILE:HG23	2.04	0.57
1:A:1694:ILE:HB	1:A:1720:VAL:HG22	1.86	0.57
1:A:1358:ILE:HG13	1:A:1358:ILE:O	2.03	0.57
1:A:1486:VAL:HG11	1:A:1528:LEU:HD13	1.87	0.57
1:A:168:HIS:HE2	1:A:525:GLU:CD	2.07	0.57
1:A:1410:LEU:HB2	1:A:1413:ILE:HD12	1.86	0.57
1:A:313:TRP:O	1:A:317:GLN:HG3	2.04	0.57
1:A:1347:ILE:O	1:A:1406:THR:HG22	2.05	0.57
1:A:1480:THR:OG1	1:A:1482:GLU:OE2	2.22	0.57
1:A:2033:THR:HG21	1:A:2038:LYS:HE2	1.86	0.57
1:A:2105:ILE:HG22	1:A:2106:ASN:H	1.69	0.57
1:A:932:LYS:NZ	1:A:959:THR:HG21	2.19	0.57
1:A:1252:LEU:HD21	1:A:1265:TRP:CG	2.39	0.57
1:A:1484:LEU:HD11	1:A:1545:ILE:CD1	2.35	0.57
1:A:1526:ILE:O	1:A:1544:THR:OG1	2.17	0.57
1:A:534:GLU:HA	1:A:537:LYS:HD3	1.86	0.57
1:A:1265:TRP:O	1:A:1275:VAL:HA	2.05	0.57
1:A:1634:PRO:HB3	1:A:1637:ILE:HD12	1.87	0.57
1:A:2103:SER:O	1:A:2103:SER:OG	2.22	0.57
1:A:1234:GLU:HG2	1:A:1278:LYS:HB2	1.87	0.57
1:A:2092:ASP:N	1:A:2097:GLU:O	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:HG3	1:A:247:LYS:HD2	1.87	0.56
1:A:863:ILE:HA	1:A:866:ILE:HD11	1.87	0.56
1:A:1517:VAL:HG12	1:A:1529:THR:O	2.05	0.56
1:A:180:TYR:HE1	1:A:455:LEU:HD13	1.70	0.56
1:A:1004:ASP:HB2	1:A:1007:LYS:HB2	1.88	0.56
1:A:1488:GLU:HG3	1:A:1493:VAL:HB	1.88	0.56
1:A:1981:ASN:OD1	1:A:1982:SER:N	2.39	0.56
1:A:1115:ARG:HG2	1:A:1124:TYR:HD1	1.70	0.56
1:A:1117:GLU:O	1:A:1121:VAL:HG23	2.04	0.56
1:A:1409:ILE:HD11	1:A:1430:ILE:HD12	1.86	0.56
1:A:1514:LEU:CD2	1:A:1532:TYR:HB3	2.36	0.56
1:A:1660:PRO:HD3	1:A:1675:ILE:HD11	1.88	0.56
1:A:258:GLU:OE2	1:A:408:TYR:OH	2.23	0.56
1:A:997:THR:HB	1:A:1001:THR:HG21	1.88	0.56
1:A:1349:VAL:HG22	1:A:1406:THR:H	1.70	0.56
1:A:903:ASP:CB	1:A:907:GLY:HA2	2.36	0.56
1:A:1031:PRO:HB3	1:A:1554:ASN:HB2	1.88	0.56
1:A:2236:ILE:HG23	1:A:2245:TYR:HD2	1.70	0.56
1:A:49:LEU:HD22	1:A:79:LEU:HD22	1.87	0.56
1:A:856:ILE:HD11	1:A:1652:ASN:HB3	1.88	0.56
1:A:850:SER:HB3	1:A:853:ILE:HB	1.87	0.56
1:A:1245:GLU:HB2	1:A:1249:THR:OG1	2.05	0.56
1:A:1494:LEU:HD13	2:K:157:GLY:HA3	1.88	0.56
1:A:1757:GLU:HG3	1:A:1763:GLN:HB3	1.87	0.56
1:A:2102:ILE:HD13	1:A:2110:TYR:O	2.06	0.56
1:A:425:PHE:O	1:A:429:MET:HB2	2.05	0.56
1:A:521:TRP:CH2	1:A:707:ASN:HB2	2.41	0.56
1:A:1837:VAL:HG12	1:A:1839:ILE:HG13	1.87	0.56
1:A:647:ILE:HD11	1:A:687:ILE:HD13	1.87	0.56
1:A:917:ALA:O	1:A:920:SER:OG	2.21	0.56
1:A:1673:THR:OG1	1:A:1701:ASP:OD1	2.22	0.56
1:A:1754:SER:OG	1:A:1755:THR:N	2.39	0.56
1:A:2016:LYS:HE2	1:A:2053:GLU:HG2	1.88	0.56
1:A:1140:LEU:HB2	1:A:1146:MET:SD	2.46	0.55
1:A:1415:ALA:HA	1:A:1430:ILE:CA	2.30	0.55
1:A:1951:THR:HG22	1:A:1956:VAL:HA	1.88	0.55
1:A:882:SER:HA	1:A:902:ILE:O	2.06	0.55
1:A:1423:SER:O	1:A:1423:SER:OG	2.23	0.55
1:A:1788:LYS:HD2	1:A:1841:ASP:O	2.06	0.55
1:A:301:ILE:HG21	1:A:347:PHE:CE1	2.40	0.55
1:A:1612:ILE:HD12	1:A:1623:GLU:CD	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:PHE:HA	1:A:1273:ASP:HA	1.89	0.55
1:A:3:LEU:HB2	1:A:82:GLU:HG3	1.89	0.55
1:A:1745:ASN:HB2	1:A:1772:PHE:HE2	1.70	0.55
1:A:1224:PRO:O	1:A:1315:TYR:OH	2.23	0.55
1:A:1636:PHE:CZ	1:A:1638:LYS:HD2	2.41	0.55
1:A:94:VAL:HG22	1:A:369:VAL:HG22	1.88	0.55
1:A:1841:ASP:O	1:A:1842:SER:OG	2.18	0.55
1:A:1967:PHE:O	1:A:1980:PHE:HB2	2.07	0.55
1:A:1447:LYS:O	1:A:1450:TYR:N	2.40	0.55
1:A:179:ILE:HD13	1:A:459:PHE:CD1	2.42	0.55
1:A:172:PHE:O	1:A:460:TYR:CE1	2.59	0.54
1:A:674:SER:O	1:A:678:THR:HG23	2.07	0.54
1:A:1562:GLY:O	1:A:1565:GLU:HB2	2.06	0.54
1:A:1871:ASN:OD1	1:A:1871:ASN:N	2.40	0.54
1:A:1173:MET:HB3	1:A:1262:GLN:HA	1.89	0.54
1:A:1552:LYS:HG2	1:A:1606:ILE:CD1	2.37	0.54
1:A:70:LYS:O	1:A:70:LYS:NZ	2.27	0.54
1:A:1140:LEU:HB2	1:A:1146:MET:CE	2.38	0.54
1:A:1885:LYS:NZ	1:A:1922:GLU:OE2	2.30	0.54
1:A:1579:SER:OG	1:A:1580:ASP:OD1	2.25	0.54
1:A:1172:ARG:HD2	1:A:1199:PRO:O	2.08	0.54
1:A:1429:LEU:HD12	1:A:1462:PRO:HG2	1.90	0.54
1:A:1846:PHE:HA	1:A:1852:ASN:O	2.08	0.54
1:A:2239:ILE:HD12	1:A:2244:TYR:HB2	1.88	0.54
1:A:1369:ILE:O	1:A:1372:ILE:HG13	2.07	0.54
1:A:1847:LYS:O	1:A:1851:LYS:HA	2.08	0.54
1:A:1868:ASN:HB3	1:A:1871:ASN:OD1	2.07	0.54
1:A:74:LYS:NZ	1:A:77:GLU:OE1	2.39	0.53
1:A:1703:ILE:HB	1:A:1732:ILE:HD13	1.90	0.53
1:A:2296:VAL:HG22	1:A:2303:PHE:HB3	1.90	0.53
1:A:623:ASN:O	1:A:625:THR:N	2.36	0.53
1:A:937:ILE:HA	1:A:948:LYS:HG2	1.90	0.53
1:A:1038:ASP:O	1:A:1062:GLU:HB3	2.07	0.53
1:A:1663:ASN:HA	1:A:1670:ILE:O	2.08	0.53
1:A:117:GLN:OE1	1:A:357:LYS:NZ	2.41	0.53
1:A:1367:ASP:OD1	1:A:1367:ASP:N	2.41	0.53
1:A:1550:THR:HA	1:A:1604:LYS:O	2.08	0.53
1:A:1440:ASN:HB3	1:A:1443:SER:OG	2.09	0.53
1:A:1689:VAL:O	1:A:1689:VAL:HG12	2.08	0.53
1:A:1494:LEU:HB2	1:A:1496:ILE:HD11	1.90	0.53
1:A:153:THR:O	1:A:153:THR:OG1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:O	1:A:235:ASN:ND2	2.42	0.53
1:A:1169:GLU:HB3	1:A:1200:TYR:HB3	1.90	0.53
1:A:1337:ILE:HD13	1:A:1390:ILE:HG23	1.91	0.53
1:A:1751:ILE:HD11	1:A:1767:ARG:NH1	2.24	0.53
1:A:2057:TYR:CZ	1:A:2061:LEU:HD13	2.43	0.53
1:A:1315:TYR:HB3	1:A:1317:PHE:CE2	2.43	0.53
1:A:2273:GLN:HG3	1:A:2274:TYR:H	1.73	0.53
1:A:176:MET:SD	1:A:456:ARG:HG2	2.49	0.53
1:A:520:LEU:O	1:A:706:VAL:HG21	2.08	0.53
1:A:1701:ASP:OD1	1:A:1701:ASP:N	2.39	0.53
1:A:21:GLU:OE1	1:A:21:GLU:N	2.38	0.53
1:A:1514:LEU:HA	1:A:1531:TYR:O	2.09	0.53
1:A:1541:LEU:CG	1:A:1555:GLY:O	2.56	0.53
1:A:1647:THR:O	1:A:1656:MET:HA	2.08	0.53
1:A:970:ILE:HG13	1:A:971:GLY:H	1.73	0.53
1:A:1469:GLU:O	1:A:1490:SER:N	2.42	0.53
1:A:2033:THR:HB	1:A:2036:GLY:O	2.08	0.53
1:A:695:ASN:OD1	1:A:696:LEU:N	2.42	0.52
1:A:977:GLU:O	1:A:979:LEU:HD22	2.08	0.52
1:A:1413:ILE:HA	1:A:1432:GLY:HA3	1.89	0.52
1:A:2030:VAL:HB	1:A:2039:TYR:HB2	1.91	0.52
1:A:2059:GLY:O	1:A:2070:PHE:N	2.36	0.52
1:A:868:ASP:OD1	1:A:868:ASP:N	2.42	0.52
1:A:1709:HIS:HB3	1:A:1712:ASN:ND2	2.24	0.52
1:A:305:ASP:O	1:A:306:SER:OG	2.16	0.52
1:A:521:TRP:HA	1:A:521:TRP:CE3	2.44	0.52
1:A:741:ASN:HD21	1:A:776:LYS:NZ	2.07	0.52
1:A:855:TYR:HE1	1:A:962:ALA:HB2	1.73	0.52
1:A:1353:VAL:HG21	1:A:1407:PHE:CD2	2.45	0.52
1:A:1520:ILE:HG12	1:A:1527:ILE:O	2.10	0.52
1:A:578:TYR:HD1	1:A:644:ARG:NH2	2.07	0.52
1:A:642:SER:O	1:A:642:SER:OG	2.22	0.52
1:A:770:ILE:CD1	1:A:801:LEU:HD22	2.40	0.52
1:A:866:ILE:O	1:A:870:LEU:HG	2.09	0.52
1:A:902:ILE:HG22	1:A:903:ASP:N	2.18	0.52
1:A:1288:ILE:HG22	1:A:1290:ILE:HD11	1.91	0.52
1:A:1327:SER:HA	1:A:1348:ASP:HB2	1.91	0.52
1:A:882:SER:O	1:A:884:PHE:N	2.43	0.52
1:A:1372:ILE:O	1:A:1374:SER:N	2.42	0.52
1:A:717:LEU:O	1:A:721:LYS:HB2	2.09	0.52
1:A:1173:MET:HG2	1:A:1174:GLU:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1642:LEU:O	1:A:1676:ASN:ND2	2.42	0.52
1:A:935:ASP:O	1:A:938:PHE:CZ	2.63	0.52
1:A:938:PHE:H	1:A:948:LYS:CG	2.22	0.52
1:A:1002:ILE:HD13	1:A:1007:LYS:O	2.08	0.52
1:A:1030:LEU:N	1:A:1031:PRO:HD3	2.24	0.52
1:A:1256:ARG:HG3	1:A:1263:PHE:O	2.10	0.52
1:A:1356:VAL:HA	1:A:1364:LYS:O	2.10	0.52
1:A:1534:LYS:HD2	1:A:1537:ILE:HB	1.91	0.52
1:A:2113:ASN:OD1	1:A:2119:GLN:NE2	2.42	0.52
1:A:621:TYR:HD1	1:A:621:TYR:H	1.58	0.52
1:A:881:GLU:OE2	1:A:905:GLU:N	2.27	0.52
1:A:1936:VAL:O	1:A:1965:ARG:HA	2.10	0.52
1:A:938:PHE:H	1:A:948:LYS:HD3	1.74	0.52
1:A:1061:ILE:HG12	1:A:1522:LYS:CE	2.39	0.52
1:A:1843:LEU:HB3	1:A:1875:ALA:HB3	1.92	0.52
1:A:304:PRO:HG2	1:A:307:VAL:HG22	1.91	0.52
1:A:881:GLU:CD	1:A:906:THR:H	2.13	0.52
1:A:1139:LEU:HD11	1:A:1218:LYS:HE2	1.89	0.52
1:A:1613:ILE:CG2	1:A:1624:PHE:HB2	2.40	0.52
1:A:113:ASN:O	1:A:117:GLN:NE2	2.43	0.51
1:A:265:LEU:O	1:A:269:SER:HB3	2.10	0.51
1:A:1055:PRO:HB2	1:A:1057:LEU:HD13	1.91	0.51
1:A:1636:PHE:O	1:A:1637:ILE:HG13	2.10	0.51
1:A:1918:ASN:HD22	1:A:1924:ILE:HG21	1.75	0.51
1:A:816:LEU:HA	1:A:819:LYS:HD2	1.91	0.51
1:A:1315:TYR:HB3	1:A:1317:PHE:HE2	1.75	0.51
1:A:1689:VAL:HG11	1:A:1716:PRO:HG3	1.92	0.51
1:A:1748:SER:HA	1:A:1772:PHE:HB2	1.92	0.51
1:A:1494:LEU:HD22	2:K:158:CYS:SG	2.50	0.51
1:A:633:ASP:OD1	1:A:633:ASP:N	2.36	0.51
1:A:856:ILE:HG23	1:A:965:PHE:CZ	2.42	0.51
1:A:1223:LEU:HD11	1:A:1299:PHE:CD2	2.44	0.51
1:A:1636:PHE:CE2	1:A:1638:LYS:HD2	2.45	0.51
1:A:2258:THR:HA	1:A:2263:HIS:HA	1.91	0.51
1:A:212:ASN:OD1	1:A:213:GLU:HG2	2.10	0.51
1:A:1541:LEU:HD12	1:A:1557:TYR:N	2.19	0.51
1:A:2145:ILE:HB	1:A:2150:PHE:HE1	1.74	0.51
1:A:970:ILE:HG21	1:A:990:VAL:HG21	1.93	0.51
1:A:1353:VAL:HG21	1:A:1407:PHE:CG	2.45	0.51
1:A:2245:TYR:H	1:A:2266:PHE:HE2	1.57	0.51
2:K:167:THR:OG1	2:K:168:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:TRP:HB2	1:A:1233:TRP:CD1	2.46	0.51
1:A:1495:ILE:C	1:A:1496:ILE:HD13	2.31	0.51
1:A:1651:GLY:C	1:A:1653:ARG:H	2.14	0.51
1:A:251:VAL:CG2	1:A:401:ILE:CD1	2.89	0.51
1:A:1293:ASP:O	1:A:1324:TYR:OH	2.27	0.51
1:A:1658:VAL:N	1:A:1693:ILE:O	2.41	0.51
1:A:1879:GLU:HB2	1:A:1888:TYR:HD1	1.75	0.51
1:A:2060:ILE:HG22	1:A:2069:TYR:HD1	1.76	0.51
1:A:1168:CYS:O	1:A:1203:ILE:N	2.43	0.51
1:A:1242:ARG:NE	1:A:1266:ARG:HD2	2.25	0.51
1:A:893:THR:HG23	1:A:896:GLY:O	2.11	0.51
1:A:967:GLN:NE2	1:A:1021:ASP:OD1	2.44	0.51
1:A:1028:GLU:OE1	1:A:1044:ALA:N	2.41	0.51
1:A:1407:PHE:CE2	1:A:1415:ALA:HB3	2.46	0.51
1:A:2019:TYR:CZ	1:A:2031:PHE:HB2	2.46	0.51
1:A:656:LYS:O	1:A:661:THR:OG1	2.28	0.50
1:A:1196:TYR:N	1:A:1196:TYR:CD2	2.77	0.50
1:A:1533:LEU:HD13	1:A:1533:LEU:C	2.31	0.50
1:A:1739:ILE:HD12	1:A:1844:TYR:CE2	2.46	0.50
1:A:719:ARG:O	1:A:723:LYS:HE3	2.11	0.50
1:A:637:ILE:HB	1:A:686:ASP:HB3	1.93	0.50
1:A:1354:ARG:HG2	1:A:1368:LEU:HD23	1.92	0.50
1:A:1982:SER:O	1:A:1982:SER:OG	2.26	0.50
2:K:124:PHE:HD1	2:K:124:PHE:H	1.59	0.50
1:A:294:HIS:HB2	1:A:360:ILE:O	2.11	0.50
1:A:866:ILE:HD13	1:A:982:LEU:HD11	1.94	0.50
1:A:1168:CYS:O	1:A:1203:ILE:HG13	2.11	0.50
1:A:1513:ASP:O	1:A:1532:TYR:HB2	2.11	0.50
1:A:1024:PRO:HG2	1:A:1636:PHE:CG	2.47	0.50
1:A:964:PHE:HB2	1:A:1023:LEU:HD21	1.94	0.50
1:A:1002:ILE:CG2	1:A:1007:LYS:O	2.59	0.50
1:A:1310:ARG:HH21	1:A:1332:ASN:H	1.58	0.50
1:A:1867:PHE:O	1:A:1873:GLY:CA	2.59	0.50
1:A:2038:LYS:HE3	1:A:2040:PHE:HE1	1.77	0.50
1:A:418:ILE:HA	1:A:421:GLN:NE2	2.26	0.50
1:A:1549:ASN:HD22	1:A:1597:LYS:NZ	2.10	0.50
2:K:161:ASN:OD1	2:K:163:ASN:N	2.31	0.50
1:A:1900:PHE:HB2	1:A:1909:PHE:CE2	2.43	0.49
1:A:970:ILE:HG13	1:A:971:GLY:N	2.26	0.49
1:A:1127:HIS:O	1:A:1131:ALA:N	2.44	0.49
1:A:881:GLU:OE1	1:A:907:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:GLN:HB2	1:A:1151:LEU:HG	1.94	0.49
1:A:711:THR:HG23	1:A:714:GLY:H	1.78	0.49
1:A:1322:GLY:O	1:A:1343:ASP:HA	2.13	0.49
1:A:1541:LEU:HD22	1:A:1541:LEU:H	1.76	0.49
1:A:2008:SER:HA	1:A:2020:PHE:HB2	1.95	0.49
1:A:2018:PHE:HB3	1:A:2026:MET:SD	2.53	0.49
1:A:2213:ILE:HB	1:A:2224:TYR:HB2	1.94	0.49
1:A:1566:ILE:HD13	1:A:1613:ILE:CD1	2.42	0.49
1:A:2259:PHE:N	1:A:2262:ASN:O	2.42	0.49
1:A:2283:MET:SD	1:A:2304:LYS:NZ	2.86	0.49
2:K:124:PHE:HZ	2:K:174:ILE:HG12	1.78	0.49
1:A:333:SER:OG	1:A:336:PHE:HB3	2.12	0.49
1:A:396:CYS:SG	1:A:482:LEU:HD22	2.53	0.49
1:A:807:ASN:OD1	1:A:1838:TYR:HB2	2.11	0.49
1:A:1441:SER:HA	1:A:1444:VAL:HB	1.93	0.49
1:A:1484:LEU:O	1:A:1486:VAL:HG13	2.13	0.49
1:A:1697:ASN:OD1	1:A:1698:ILE:N	2.46	0.49
1:A:2181:ASN:ND2	1:A:2187:VAL:HG11	2.22	0.49
1:A:708:VAL:HG11	1:A:788:ILE:HG21	1.93	0.49
1:A:1139:LEU:CD1	1:A:1218:LYS:HE2	2.43	0.49
1:A:1430:ILE:HG12	1:A:1463:TYR:CD2	2.47	0.49
1:A:2039:TYR:CZ	1:A:2041:ALA:HA	2.47	0.49
1:A:329:PRO:O	1:A:330:GLU:HB2	2.13	0.49
1:A:1350:ASP:OD1	1:A:1351:ASN:N	2.45	0.49
1:A:2366:SER:OG	1:A:2367:GLU:N	2.45	0.49
1:A:717:LEU:HD22	1:A:779:ILE:HG13	1.94	0.49
1:A:1125:PHE:HE2	1:A:1279:LEU:HD21	1.78	0.49
1:A:1955:GLU:HG2	1:A:1985:ILE:HA	1.94	0.49
1:A:118:TRP:O	1:A:122:ASN:ND2	2.45	0.48
1:A:632:ILE:HD11	1:A:636:ARG:NH1	2.28	0.48
1:A:1304:ILE:N	1:A:1331:TYR:HD2	2.11	0.48
1:A:1310:ARG:NH2	1:A:1332:ASN:H	2.11	0.48
1:A:2265:TYR:CE1	1:A:2279:ILE:HD12	2.48	0.48
1:A:547:ASP:HB3	1:A:758:HIS:CE1	2.47	0.48
1:A:947:LYS:O	1:A:948:LYS:HB2	2.12	0.48
1:A:1335:ILE:HG22	1:A:1337:ILE:HD11	1.96	0.48
2:K:154:LYS:N	2:K:154:LYS:HD2	2.29	0.48
1:A:1231:PHE:CD1	1:A:1281:PRO:HB3	2.48	0.48
1:A:1115:ARG:HB2	1:A:1279:LEU:HB2	1.95	0.48
1:A:1172:ARG:HH21	1:A:1201:LEU:HD21	1.77	0.48
1:A:1385:LEU:O	1:A:1388:HIS:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:THR:HG23	1:A:171:PHE:CE1	2.49	0.48
1:A:248:THR:O	1:A:248:THR:OG1	2.32	0.48
1:A:961:ASN:HD22	1:A:1653:ARG:HH12	1.61	0.48
1:A:1317:PHE:HB2	1:A:1337:ILE:HA	1.95	0.48
1:A:1676:ASN:HA	1:A:1704:ASN:HB2	1.93	0.48
1:A:2233:TYR:HB2	1:A:2246:PHE:CE2	2.48	0.48
1:A:190:TYR:HD1	1:A:205:ILE:HG21	1.79	0.48
1:A:831:SER:O	1:A:835:THR:HG23	2.14	0.48
1:A:869:ALA:O	1:A:873:LEU:HD13	2.12	0.48
1:A:1168:CYS:SG	1:A:1229:ARG:HD2	2.53	0.48
1:A:1172:ARG:HD3	1:A:1198:GLU:HB2	1.96	0.48
1:A:1886:ASN:HB2	1:A:1923:ALA:HB3	1.94	0.48
1:A:2236:ILE:HG23	1:A:2245:TYR:CD2	2.48	0.48
1:A:2329:LEU:HB3	1:A:2334:TYR:CE2	2.48	0.48
1:A:128:ASN:HB3	1:A:238:ASN:HB2	1.94	0.48
1:A:148:SER:O	1:A:148:SER:OG	2.31	0.48
1:A:1030:LEU:HG	1:A:1612:ILE:HD11	1.95	0.48
1:A:1113:ILE:HA	1:A:1280:LYS:HD3	1.96	0.48
1:A:1302:PRO:HB2	1:A:1304:ILE:HG13	1.96	0.48
1:A:1541:LEU:HG	1:A:1555:GLY:O	2.13	0.48
1:A:1592:LYS:HG3	1:A:1602:ASN:HD22	1.78	0.48
1:A:1925:ASP:HB2	1:A:1943:TYR:CD1	2.49	0.48
1:A:2060:ILE:HA	1:A:2069:TYR:HA	1.95	0.48
1:A:127:VAL:HG12	1:A:236:SER:OG	2.13	0.48
1:A:1441:SER:OG	1:A:1499:TYR:O	2.31	0.48
1:A:1619:ILE:CG2	1:A:1641:THR:HG23	2.26	0.48
1:A:1783:PHE:N	1:A:1791:ILE:O	2.38	0.48
1:A:1928:GLY:O	1:A:1939:PHE:N	2.45	0.48
1:A:1990:PHE:HA	1:A:1998:PHE:O	2.13	0.48
1:A:961:ASN:ND2	1:A:1653:ARG:HH12	2.11	0.48
1:A:1220:LEU:HA	1:A:1298:SER:O	2.14	0.48
1:A:2016:LYS:NZ	1:A:2054:ALA:HB3	2.28	0.48
1:A:2025:GLU:OE2	1:A:2025:GLU:N	2.46	0.48
1:A:2063:PHE:O	1:A:2066:LYS:HD2	2.13	0.48
1:A:2329:LEU:HB3	1:A:2334:TYR:HE2	1.78	0.48
1:A:122:ASN:OD1	1:A:364:LEU:HB2	2.13	0.47
1:A:1691:LYS:HG3	1:A:1717:GLU:O	2.13	0.47
1:A:2047:LEU:HD12	1:A:2055:LEU:HD13	1.95	0.47
1:A:404:ILE:O	1:A:408:TYR:HD1	1.97	0.47
1:A:1569:PHE:CD2	1:A:1585:PHE:HB2	2.48	0.47
1:A:2288:GLU:N	1:A:2288:GLU:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:GLU:O	1:A:820:VAL:HG13	2.14	0.47
1:A:1004:ASP:CB	1:A:1007:LYS:HB2	2.44	0.47
1:A:1252:LEU:HD23	1:A:1253:ASP:N	2.28	0.47
1:A:1379:GLU:HB2	1:A:1382:LYS:O	2.14	0.47
1:A:1857:PHE:CE1	1:A:1864:LYS:HE2	2.49	0.47
1:A:2150:PHE:HA	1:A:2184:GLY:O	2.14	0.47
1:A:194:LYS:HD2	1:A:194:LYS:HA	1.75	0.47
1:A:1125:PHE:HB3	1:A:1248:GLY:HA3	1.97	0.47
1:A:1509:TYR:OH	1:A:1548:LYS:O	2.32	0.47
1:A:2227:PRO:HG3	1:A:2233:TYR:CE1	2.50	0.47
1:A:174:LYS:HD3	1:A:177:GLN:NE2	2.29	0.47
1:A:1909:PHE:HA	1:A:1922:GLU:O	2.15	0.47
1:A:2347:VAL:HG22	1:A:2354:TYR:HB2	1.95	0.47
1:A:186:PHE:HB2	1:A:209:TYR:CE2	2.49	0.47
1:A:547:ASP:HB3	1:A:758:HIS:ND1	2.30	0.47
1:A:319:GLU:HG2	1:A:333:SER:HA	1.97	0.47
1:A:1139:LEU:HD11	1:A:1218:LYS:HZ1	1.70	0.47
1:A:1322:GLY:H	1:A:1324:TYR:HE2	1.63	0.47
1:A:1477:ASN:OD1	1:A:1478:CYS:N	2.46	0.47
1:A:1876:SER:O	1:A:1893:GLY:HA2	2.15	0.47
1:A:1968:LYS:HE2	1:A:1983:ASP:HA	1.97	0.47
1:A:2070:PHE:HA	1:A:2075:THR:O	2.14	0.47
1:A:889:ASP:OD1	1:A:889:ASP:N	2.48	0.47
1:A:1343:ASP:OD2	1:A:1343:ASP:N	2.40	0.47
1:A:1614:SER:OG	1:A:1615:GLY:N	2.47	0.47
1:A:1847:LYS:HG3	1:A:1849:PRO:HD2	1.97	0.47
1:A:1968:LYS:HD2	1:A:1982:SER:C	2.35	0.47
1:A:415:LEU:HG	1:A:419:ILE:HD11	1.95	0.47
1:A:560:LYS:O	1:A:564:LEU:HB2	2.14	0.47
1:A:881:GLU:HG2	1:A:905:GLU:CB	2.39	0.47
1:A:1140:LEU:C	1:A:1142:ASP:H	2.18	0.47
1:A:1297:ARG:HB2	1:A:1324:TYR:HA	1.97	0.47
1:A:2193:VAL:HG12	1:A:2195:VAL:HG22	1.97	0.47
1:A:180:TYR:CE1	1:A:455:LEU:HD13	2.50	0.47
1:A:251:VAL:HG22	1:A:401:ILE:HD12	1.97	0.47
1:A:608:LEU:HD12	1:A:609:PHE:N	2.30	0.47
1:A:1811:ASN:OD1	1:A:1812:TYR:N	2.48	0.47
1:A:1287:ASN:OD1	1:A:1316:SER:HB2	2.15	0.46
1:A:1600:LYS:HD2	1:A:1600:LYS:HA	1.65	0.46
1:A:1996:LYS:HG2	1:A:2025:GLU:HB2	1.96	0.46
1:A:1227:PRO:HG2	1:A:1283:TYR:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1549:ASN:HB3	1:A:1597:LYS:NZ	2.30	0.46
1:A:2043:HIS:HB2	1:A:2051:GLU:HG2	1.97	0.46
1:A:6:ARG:NH1	1:A:28:LEU:O	2.47	0.46
1:A:149:ALA:O	1:A:153:THR:HG22	2.15	0.46
1:A:218:ILE:O	1:A:218:ILE:HG22	2.15	0.46
1:A:465:THR:HG22	1:A:469:LEU:HD22	1.96	0.46
1:A:1566:ILE:HG13	1:A:1566:ILE:O	2.15	0.46
1:A:1882:ILE:HB	1:A:1887:TYR:HE2	1.80	0.46
1:A:114:TYR:CD2	1:A:290:LEU:HG	2.50	0.46
1:A:286:ASP:O	1:A:288:ASP:N	2.48	0.46
1:A:948:LYS:HD2	1:A:948:LYS:HA	1.46	0.46
1:A:1514:LEU:HD23	1:A:1532:TYR:CB	2.45	0.46
1:A:1229:ARG:HD3	1:A:1231:PHE:CE1	2.51	0.46
1:A:1587:GLU:HA	1:A:1591:ILE:HG22	1.98	0.46
1:A:183:GLN:NE2	1:A:261:GLU:O	2.44	0.46
1:A:553:SER:O	1:A:555:ASN:N	2.49	0.46
1:A:703:SER:O	1:A:703:SER:OG	2.30	0.46
1:A:721:LYS:HE3	1:A:721:LYS:HB3	1.55	0.46
1:A:1139:LEU:CD1	1:A:1218:LYS:CE	2.85	0.46
1:A:1908:TYR:CZ	1:A:1910:ALA:HB2	2.51	0.46
1:A:1979:TYR:HD2	1:A:1987:GLN:HB2	1.81	0.46
1:A:40:ASN:OD1	1:A:41:THR:N	2.47	0.46
1:A:270:ASP:OD2	1:A:385:ASN:ND2	2.49	0.46
1:A:608:LEU:HD12	1:A:609:PHE:H	1.80	0.46
1:A:668:ASP:OD2	1:A:668:ASP:N	2.45	0.46
1:A:1390:ILE:HG22	1:A:1392:PHE:CE2	2.51	0.46
1:A:2213:ILE:HD13	1:A:2213:ILE:HA	1.79	0.46
1:A:939:ASP:HB3	1:A:948:LYS:HD2	1.98	0.46
1:A:1496:ILE:HG22	1:A:1497:LYS:H	1.80	0.46
1:A:1686:ASP:OD1	1:A:1712:ASN:HB3	2.16	0.46
2:K:153:PHE:HZ	2:K:164:ASN:ND2	2.08	0.46
1:A:991:TYR:O	1:A:1011:LEU:HD11	2.15	0.46
1:A:1197:ARG:NH2	1:A:1197:ARG:CG	2.73	0.46
1:A:1625:ILE:N	1:A:1633:GLN:O	2.45	0.46
1:A:1825:TYR:O	1:A:1833:VAL:HG23	2.16	0.46
1:A:1930:LEU:N	1:A:1937:TYR:O	2.46	0.46
1:A:1981:ASN:N	1:A:1985:ILE:O	2.44	0.46
1:A:1045:SER:O	1:A:1047:LYS:N	2.44	0.46
1:A:1321:GLY:HA3	1:A:1341:GLU:CD	2.36	0.46
1:A:1341:GLU:HG2	1:A:1342:ASN:H	1.81	0.46
1:A:1930:LEU:HB2	1:A:1939:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2245:TYR:HE1	1:A:2257:ILE:HG12	1.81	0.46
1:A:576:ARG:HG3	1:A:578:TYR:CZ	2.51	0.45
1:A:597:ASN:ND2	1:A:762:TRP:HH2	2.14	0.45
1:A:1152:VAL:HG22	1:A:1226:ALA:HB1	1.97	0.45
1:A:1162:SER:HA	1:A:1212:GLU:HG3	1.98	0.45
1:A:1171:TRP:CZ2	1:A:1195:THR:HG21	2.51	0.45
1:A:4:VAL:HB	1:A:8:GLN:HB3	1.97	0.45
1:A:1532:TYR:O	1:A:1532:TYR:CG	2.69	0.45
1:A:1885:LYS:HB3	1:A:1922:GLU:HG3	1.98	0.45
1:A:436:LEU:HD22	1:A:448:ILE:HG23	1.98	0.45
1:A:1955:GLU:OE1	1:A:1956:VAL:N	2.49	0.45
1:A:2030:VAL:HG11	1:A:2068:TYR:CE1	2.52	0.45
1:A:2308:HIS:CG	1:A:2309:GLN:N	2.85	0.45
1:A:2321:ILE:HB	1:A:2323:TYR:CZ	2.50	0.45
1:A:63:TYR:N	1:A:63:TYR:CD1	2.84	0.45
1:A:106:GLN:NE2	1:A:227:GLU:O	2.49	0.45
1:A:410:ILE:HD12	1:A:490:ILE:HD13	1.97	0.45
1:A:634:LYS:HE3	1:A:634:LYS:HB2	1.58	0.45
1:A:1532:TYR:O	1:A:1532:TYR:CD2	2.70	0.45
1:A:1667:SER:O	1:A:1667:SER:OG	2.26	0.45
1:A:1712:ASN:O	1:A:1760:LYS:HE3	2.16	0.45
1:A:2049:ASN:ND2	1:A:2055:LEU:HD11	2.26	0.45
1:A:6:ARG:HA	1:A:31:LEU:HD23	1.99	0.45
1:A:400:LEU:HD12	1:A:478:ALA:CB	2.47	0.45
1:A:521:TRP:HA	1:A:521:TRP:HE3	1.81	0.45
1:A:1096:PRO:HB2	1:A:1100:ILE:HG12	1.99	0.45
1:A:1228:ASP:O	1:A:1284:GLU:N	2.40	0.45
1:A:1289:ARG:HH21	1:A:1318:TYR:HD1	1.64	0.45
1:A:1380:ASP:O	1:A:1381:ASN:ND2	2.49	0.45
1:A:1381:ASN:O	1:A:1391:ASN:HA	2.17	0.45
1:A:1382:LYS:HE3	1:A:1382:LYS:HB3	1.57	0.45
1:A:1545:ILE:HG12	1:A:1545:ILE:O	2.16	0.45
1:A:132:ASP:HB3	1:A:135:ALA:HB3	1.98	0.45
1:A:138:ILE:HG21	1:A:265:LEU:HD21	1.99	0.45
1:A:217:ASP:OD1	1:A:218:ILE:N	2.50	0.45
1:A:311:VAL:HG12	1:A:311:VAL:O	2.17	0.45
1:A:612:ASN:OD1	1:A:612:ASN:N	2.29	0.45
1:A:870:LEU:N	1:A:870:LEU:HD23	2.31	0.45
1:A:2067:ILE:HD12	1:A:2114:ASP:O	2.15	0.45
1:A:2130:PHE:HB3	1:A:2157:LEU:HA	1.98	0.45
1:A:278:LYS:HE3	1:A:278:LYS:HB2	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:O	1:A:338:THR:OG1	2.27	0.45
1:A:746:ARG:HG2	1:A:762:TRP:CE3	2.52	0.45
1:A:1131:ALA:HA	1:A:1148:GLN:NE2	2.32	0.45
1:A:1483:GLY:HA3	1:A:1498:VAL:HG12	1.99	0.45
1:A:2037:PHE:CG	1:A:2096:ALA:HB2	2.52	0.45
1:A:166:PHE:CG	1:A:166:PHE:O	2.70	0.45
1:A:800:THR:O	1:A:804:GLU:HG3	2.17	0.45
1:A:1434:LEU:HD22	1:A:1487:SER:HB2	1.98	0.45
1:A:251:VAL:CG2	1:A:401:ILE:HD12	2.47	0.45
1:A:1121:VAL:HG13	1:A:1279:LEU:HD21	1.99	0.45
1:A:1132:GLU:HG2	1:A:1207:LEU:HD11	1.98	0.45
1:A:1375:LYS:O	1:A:1385:LEU:HA	2.17	0.45
1:A:226:GLU:O	1:A:228:SER:N	2.49	0.45
1:A:559:ASP:OD1	1:A:560:LYS:N	2.50	0.45
1:A:1548:LYS:HD3	1:A:1548:LYS:HA	1.63	0.45
1:A:1689:VAL:CG1	1:A:1716:PRO:HG3	2.46	0.45
1:A:1738:SER:HB3	1:A:1787:ASP:OD2	2.17	0.45
1:A:2182:ILE:HB	1:A:2185:GLN:HB2	1.99	0.45
2:K:169:GLU:OE1	2:K:169:GLU:N	2.45	0.45
1:A:247:LYS:HB3	1:A:247:LYS:HE3	1.47	0.44
1:A:264:ASN:HD21	1:A:466:THR:HG21	1.81	0.44
1:A:623:ASN:OD1	1:A:624:PRO:HD2	2.17	0.44
1:A:881:GLU:O	1:A:903:ASP:HA	2.17	0.44
1:A:1012:VAL:C	1:A:1014:THR:H	2.19	0.44
1:A:1092:ILE:H	1:A:1092:ILE:HG13	1.52	0.44
1:A:1227:PRO:HG2	1:A:1283:TYR:CD1	2.52	0.44
1:A:1507:PHE:CD1	1:A:1507:PHE:N	2.84	0.44
1:A:1994:ASN:N	1:A:1994:ASN:OD1	2.50	0.44
1:A:470:SER:HA	1:A:474:ILE:HG21	1.99	0.44
1:A:959:THR:HG22	1:A:959:THR:O	2.18	0.44
1:A:1179:HIS:HD1	1:A:1188:PHE:HD1	1.64	0.44
1:A:1401:GLY:HA2	1:A:1421:LEU:HD12	1.99	0.44
1:A:1495:ILE:O	1:A:1496:ILE:HD13	2.17	0.44
1:A:1962:ASP:OD1	1:A:1963:THR:N	2.50	0.44
1:A:2044:ASP:HB3	1:A:2046:ASP:OD2	2.16	0.44
1:A:220:GLU:H	1:A:220:GLU:HG2	1.25	0.44
1:A:288:ASP:HB2	1:A:516:GLU:HG2	1.98	0.44
1:A:1736:ASP:OD2	1:A:1740:ARG:NH1	2.50	0.44
1:A:1980:PHE:CD1	1:A:1986:MET:HA	2.53	0.44
1:A:2275:GLY:N	1:A:2286:PHE:O	2.28	0.44
1:A:830:ILE:O	1:A:833:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:PHE:CE1	1:A:1281:PRO:HB3	2.52	0.44
1:A:2098:ALA:O	1:A:2100:ILE:CG1	2.54	0.44
2:K:141:TYR:CE1	2:K:152:ARG:HB3	2.52	0.44
1:A:923:ALA:O	1:A:927:THR:OG1	2.18	0.44
1:A:1317:PHE:HD1	1:A:1345:TRP:CZ3	2.35	0.44
1:A:1486:VAL:O	1:A:1486:VAL:HG23	2.18	0.44
1:A:2037:PHE:CD2	1:A:2096:ALA:HB2	2.52	0.44
1:A:95:GLU:HB3	1:A:97:ASN:HD21	1.82	0.44
1:A:236:SER:OG	1:A:236:SER:O	2.25	0.44
1:A:958:ASN:C	1:A:960:LEU:H	2.21	0.44
1:A:1011:LEU:O	1:A:1015:ALA:CB	2.66	0.44
1:A:1102:ALA:HB1	1:A:1124:TYR:CE2	2.51	0.44
1:A:1291:SER:HA	1:A:1318:TYR:CD2	2.53	0.44
1:A:1929:LYS:HD3	1:A:1952:LEU:HD21	2.00	0.44
1:A:273:ARG:HE	1:A:273:ARG:HB3	1.57	0.44
1:A:378:PHE:HZ	1:A:499:LEU:O	2.00	0.44
1:A:495:LEU:HD23	1:A:495:LEU:H	1.82	0.44
1:A:870:LEU:HD22	1:A:885:ILE:HD11	1.99	0.44
1:A:1289:ARG:NH1	1:A:1316:SER:HB3	2.32	0.44
1:A:1908:TYR:O	1:A:1923:ALA:HA	2.18	0.44
1:A:841:ARG:O	1:A:842:ILE:HD13	2.17	0.44
1:A:941:VAL:HG13	1:A:941:VAL:O	2.18	0.44
1:A:1289:ARG:HH11	1:A:1316:SER:HB3	1.83	0.44
1:A:1606:ILE:O	1:A:1607:LEU:HD13	2.18	0.44
1:A:48:LYS:O	1:A:52:ILE:HG13	2.18	0.44
1:A:101:ILE:HD12	1:A:284:TYR:CE1	2.52	0.44
1:A:166:PHE:O	1:A:166:PHE:CD2	2.70	0.44
1:A:415:LEU:O	1:A:419:ILE:HG13	2.18	0.44
1:A:578:TYR:HB3	1:A:644:ARG:CB	2.48	0.44
1:A:1242:ARG:HE	1:A:1266:ARG:HH11	1.66	0.44
1:A:1440:ASN:O	1:A:1443:SER:OG	2.28	0.44
1:A:1523:ASP:O	1:A:1525:VAL:HG23	2.18	0.44
1:A:1652:ASN:ND2	1:A:1657:ILE:CD1	2.81	0.44
1:A:1930:LEU:O	1:A:1936:VAL:HA	2.18	0.44
1:A:1930:LEU:HD21	1:A:1932:ILE:HG23	2.00	0.44
1:A:2235:GLY:HA2	1:A:2245:TYR:CE2	2.53	0.44
1:A:2306:PHE:CD1	1:A:2320:SER:HB2	2.53	0.44
1:A:548:ASP:OD2	1:A:549:ASN:N	2.50	0.43
1:A:900:ARG:HG2	1:A:911:PHE:HA	2.00	0.43
1:A:1458:GLN:HG3	1:A:1461:ILE:HG12	2.00	0.43
1:A:1950:GLN:O	1:A:1957:TYR:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2092:ASP:CG	1:A:2099:SER:HB2	2.39	0.43
1:A:222:ASN:HA	1:A:225:ILE:HD12	2.00	0.43
1:A:317:GLN:O	1:A:321:ILE:HG13	2.18	0.43
1:A:680:ILE:HG22	1:A:727:LEU:HD23	1.99	0.43
1:A:986:MET:HE3	1:A:990:VAL:HG23	2.00	0.43
1:A:1493:VAL:HG12	1:A:1511:SER:HG	1.83	0.43
1:A:1652:ASN:OD1	1:A:1652:ASN:N	2.51	0.43
1:A:1683:TYR:HE1	1:A:1711:ALA:HB1	1.83	0.43
1:A:1206:VAL:O	1:A:1254:ARG:NH2	2.52	0.43
1:A:1541:LEU:CD1	1:A:1557:TYR:CB	2.96	0.43
1:A:1541:LEU:HD13	1:A:1557:TYR:HB3	1.99	0.43
1:A:2102:ILE:CD1	1:A:2110:TYR:C	2.83	0.43
1:A:806:ARG:O	1:A:809:SER:N	2.50	0.43
1:A:1543:PHE:HA	1:A:1554:ASN:OD1	2.18	0.43
1:A:2102:ILE:HD11	1:A:2109:LYS:O	2.18	0.43
1:A:2169:TYR:CE1	1:A:2230:LYS:HE2	2.53	0.43
1:A:2216:SER:HB2	1:A:2220:SER:HA	2.01	0.43
1:A:2225:PHE:CE1	1:A:2227:PRO:HB3	2.52	0.43
1:A:384:ILE:HG12	1:A:386:GLN:HG3	2.00	0.43
1:A:617:GLU:OE1	1:A:634:LYS:HA	2.19	0.43
1:A:705:SER:HB2	1:A:790:VAL:HG11	1.99	0.43
1:A:1172:ARG:HE	1:A:1201:LEU:HG	1.83	0.43
1:A:1484:LEU:CD2	1:A:1528:LEU:HD21	2.49	0.43
1:A:1788:LYS:HB3	1:A:1791:ILE:HD11	2.00	0.43
1:A:2265:TYR:HE1	1:A:2279:ILE:HD12	1.82	0.43
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.79	0.43
1:A:385:ASN:OD1	1:A:385:ASN:N	2.41	0.43
1:A:1289:ARG:HA	1:A:1289:ARG:HD2	1.76	0.43
1:A:2013:ILE:HD12	1:A:2018:PHE:HD2	1.83	0.43
1:A:313:TRP:HA	1:A:313:TRP:CE3	2.54	0.43
1:A:648:LYS:HG3	1:A:649:LEU:N	2.33	0.43
1:A:848:LEU:HD21	1:A:1807:GLU:HB3	1.99	0.43
1:A:929:GLU:OE1	1:A:962:ALA:HB3	2.18	0.43
1:A:1094:LEU:HB2	1:A:1362:LYS:NZ	2.33	0.43
1:A:1187:HIS:HA	1:A:1267:PHE:HB2	2.00	0.43
1:A:1416:VAL:HB	1:A:1429:LEU:HD23	2.00	0.43
1:A:1470:GLY:HA3	1:A:1489:LEU:HA	1.99	0.43
1:A:1646:TYR:O	1:A:1647:THR:OG1	2.32	0.43
1:A:1806:VAL:C	1:A:1808:GLY:H	2.21	0.43
1:A:1810:LEU:O	1:A:1810:LEU:HG	2.19	0.43
1:A:1879:GLU:OE1	1:A:1909:PHE:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1913:ASP:HA	1:A:1917:GLU:HA	1.99	0.43
1:A:56:THR:CG2	1:A:72:LEU:HB3	2.49	0.43
1:A:2000:PHE:HA	1:A:2005:VAL:O	2.19	0.43
1:A:558:THR:HG21	1:A:620:TYR:CE1	2.53	0.43
1:A:922:TYR:O	1:A:926:ILE:HB	2.19	0.43
1:A:1061:ILE:O	1:A:1522:LYS:CE	2.64	0.43
1:A:1115:ARG:HG2	1:A:1124:TYR:CD1	2.50	0.43
1:A:1807:GLU:H	1:A:1807:GLU:HG3	1.48	0.43
1:A:2169:TYR:CZ	1:A:2230:LYS:HE2	2.54	0.43
1:A:527:ARG:O	1:A:527:ARG:HD3	2.19	0.43
1:A:832:ASN:O	1:A:836:GLN:HG2	2.19	0.43
1:A:1025:THR:HA	1:A:1621:GLN:HE22	1.84	0.43
1:A:1158:PHE:HB2	1:A:1292:LEU:HA	2.00	0.43
1:A:1237:TRP:CD1	1:A:1272:ALA:HB3	2.53	0.43
1:A:1383:ILE:HD11	1:A:1421:LEU:HD21	2.00	0.43
1:A:1457:LEU:HD22	1:A:1457:LEU:HA	1.80	0.43
1:A:1533:LEU:HD13	1:A:1534:LYS:N	2.34	0.43
1:A:1582:LEU:HA	1:A:1632:ILE:HD11	2.01	0.43
1:A:2011:THR:O	1:A:2017:TYR:HA	2.19	0.43
1:A:2273:GLN:HG3	1:A:2274:TYR:N	2.34	0.43
1:A:161:LEU:HD23	1:A:161:LEU:O	2.18	0.42
1:A:217:ASP:HB3	1:A:220:GLU:CG	2.49	0.42
1:A:457:VAL:HG22	1:A:463:ALA:O	2.19	0.42
1:A:979:LEU:HD23	1:A:1662:TYR:CE2	2.54	0.42
1:A:1029:GLY:C	1:A:1031:PRO:HD3	2.40	0.42
1:A:1505:PRO:HA	1:A:1506:PRO:HD3	1.86	0.42
1:A:1996:LYS:HE2	1:A:2025:GLU:O	2.19	0.42
1:A:48:LYS:HA	1:A:48:LYS:HD2	1.75	0.42
1:A:1163:ILE:HD11	1:A:1211:LYS:O	2.18	0.42
1:A:1594:ILE:H	1:A:1594:ILE:HG13	1.57	0.42
1:A:1729:LYS:HD3	1:A:1729:LYS:HA	1.83	0.42
1:A:1882:ILE:HB	1:A:1887:TYR:CE2	2.54	0.42
1:A:654:HIS:CE1	1:A:758:HIS:CE1	3.07	0.42
1:A:784:LYS:HE2	1:A:784:LYS:HB2	1.76	0.42
1:A:1001:THR:HG23	1:A:1002:ILE:N	2.34	0.42
1:A:1857:PHE:HZ	1:A:1895:LEU:HD22	1.84	0.42
1:A:926:ILE:O	1:A:930:ILE:HG13	2.19	0.42
1:A:1089:GLY:C	1:A:1091:SER:H	2.23	0.42
1:A:1054:ASP:N	1:A:1055:PRO:HD2	2.34	0.42
1:A:1273:ASP:OD2	1:A:1275:VAL:HG13	2.20	0.42
1:A:1752:LEU:HD23	1:A:1752:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:CYS:SG	1:A:1203:ILE:HB	2.59	0.42
1:A:1826:ILE:HG22	1:A:1832:MET:HA	2.01	0.42
1:A:1648:LEU:HB2	1:A:1656:MET:SD	2.59	0.42
1:A:2040:PHE:HB3	1:A:2052:GLY:O	2.19	0.42
1:A:2094:ASN:OD1	1:A:2094:ASN:N	2.52	0.42
1:A:2328:ASP:HA	1:A:2332:LYS:O	2.20	0.42
2:K:167:THR:HG23	2:K:170:GLU:HG2	2.01	0.42
1:A:121:VAL:HG11	1:A:362:LEU:O	2.20	0.42
1:A:925:HIS:O	1:A:929:GLU:HG2	2.19	0.42
1:A:1567:LEU:HD23	1:A:1683:TYR:HD2	1.85	0.42
1:A:1645:LYS:O	1:A:1658:VAL:HA	2.20	0.42
1:A:1946:ALA:HB3	1:A:1950:GLN:NE2	2.35	0.42
1:A:1973:ILE:HD11	1:A:1978:PHE:HB2	2.02	0.42
1:A:2102:ILE:HD13	1:A:2102:ILE:HA	1.67	0.42
1:A:781:PHE:HE2	1:A:783:PRO:HA	1.85	0.42
1:A:1317:PHE:CD1	1:A:1345:TRP:HZ3	2.38	0.42
1:A:1520:ILE:CG2	1:A:1526:ILE:CG2	2.97	0.42
1:A:1579:SER:OG	1:A:1580:ASP:N	2.53	0.42
1:A:1625:ILE:HG13	1:A:1633:GLN:HB3	2.01	0.42
1:A:2092:ASP:OD2	1:A:2099:SER:N	2.38	0.42
1:A:2125:ILE:HG22	1:A:2126:ASN:H	1.85	0.42
1:A:301:ILE:HG21	1:A:347:PHE:HE1	1.83	0.42
1:A:1233:TRP:CD1	1:A:1233:TRP:N	2.88	0.42
1:A:1459:LYS:O	1:A:1460:ASN:ND2	2.52	0.42
1:A:2276:TYR:CE1	1:A:2300:PRO:HD2	2.55	0.42
1:A:15:VAL:HG12	1:A:16:ARG:O	2.20	0.41
1:A:251:VAL:HG23	1:A:251:VAL:O	2.20	0.41
1:A:481:ASP:N	1:A:481:ASP:OD1	2.53	0.41
1:A:809:SER:O	1:A:814:ILE:HD13	2.20	0.41
1:A:1016:LEU:HD23	1:A:1017:ASP:N	2.35	0.41
1:A:1139:LEU:HD22	1:A:1139:LEU:HA	1.88	0.41
1:A:1170:ILE:HB	1:A:1203:ILE:HD11	2.02	0.41
1:A:1256:ARG:NH2	1:A:1264:TYR:HE1	2.17	0.41
1:A:1705:ILE:HG12	1:A:1733:ASN:O	2.20	0.41
1:A:1776:THR:OG1	1:A:1777:ILE:N	2.53	0.41
1:A:18:ARG:NH1	1:A:1668:GLY:O	2.53	0.41
1:A:292:GLY:O	1:A:361:PHE:HD1	2.03	0.41
1:A:867:SER:OG	1:A:982:LEU:HD12	2.20	0.41
1:A:1430:ILE:HG12	1:A:1463:TYR:CB	2.50	0.41
1:A:1810:LEU:HA	1:A:1812:TYR:CE2	2.55	0.41
1:A:1837:VAL:CG1	1:A:1839:ILE:HG13	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2005:VAL:HG22	1:A:2006:MET:H	1.85	0.41
1:A:1494:LEU:HD12	1:A:1496:ILE:HD11	2.02	0.41
1:A:1531:TYR:CD1	1:A:1531:TYR:C	2.94	0.41
1:A:2057:TYR:O	1:A:2074:PHE:HD1	2.02	0.41
1:A:5:ASN:O	1:A:8:GLN:N	2.44	0.41
1:A:89:SER:OG	1:A:90:ASN:N	2.53	0.41
1:A:1223:LEU:HB3	1:A:1224:PRO:HD2	2.03	0.41
1:A:1559:ASP:CG	1:A:1560:GLU:N	2.72	0.41
1:A:1597:LYS:HB2	1:A:1597:LYS:HE3	1.58	0.41
1:A:1697:ASN:OD1	1:A:1697:ASN:C	2.58	0.41
1:A:101:ILE:HD12	1:A:284:TYR:HE1	1.85	0.41
1:A:325:LYS:HG2	1:A:351:LEU:HD22	2.03	0.41
1:A:627:SER:C	1:A:628:GLU:HG2	2.41	0.41
1:A:1104:ILE:HG13	1:A:1105:PRO:CD	2.44	0.41
1:A:1143:LYS:HA	1:A:1143:LYS:HD3	1.72	0.41
1:A:1458:GLN:NE2	1:A:1458:GLN:HA	2.36	0.41
1:A:1918:ASN:HD22	1:A:1924:ILE:HD13	1.86	0.41
1:A:2304:LYS:HE3	1:A:2320:SER:OG	2.20	0.41
1:A:991:TYR:CB	1:A:1015:ALA:HB1	2.51	0.41
1:A:1059:GLN:HG3	1:A:1060:GLU:H	1.86	0.41
1:A:1288:ILE:HG22	1:A:1290:ILE:CD1	2.50	0.41
1:A:1492:VAL:HG23	1:A:1512:ASN:HA	2.03	0.41
1:A:1558:LEU:HG	1:A:1562:GLY:O	2.20	0.41
1:A:1663:ASN:CA	1:A:1671:SER:HB2	2.45	0.41
1:A:1971:ASN:O	1:A:1978:PHE:N	2.36	0.41
1:A:2105:ILE:HG22	1:A:2106:ASN:N	2.35	0.41
1:A:2148:ASN:HB3	1:A:2185:GLN:HG3	2.03	0.41
1:A:2227:PRO:HD3	1:A:2232:ALA:HA	2.02	0.41
2:K:124:PHE:HD1	2:K:124:PHE:N	2.19	0.41
1:A:5:ASN:OD1	1:A:5:ASN:N	2.52	0.41
1:A:95:GLU:HB3	1:A:97:ASN:ND2	2.36	0.41
1:A:1307:GLU:HA	1:A:1310:ARG:HD3	2.01	0.41
1:A:1549:ASN:HD22	1:A:1597:LYS:HZ2	1.67	0.41
1:A:1563:VAL:HA	1:A:1566:ILE:HG22	2.02	0.41
1:A:1586:LEU:HB3	1:A:1591:ILE:CG2	2.50	0.41
1:A:1845:TYR:HB2	1:A:1867:PHE:CZ	2.56	0.41
1:A:2049:ASN:HA	1:A:2053:GLU:OE1	2.19	0.41
2:K:149:GLN:HG2	2:K:150:CYS:N	2.34	0.41
1:A:441:ASN:OD1	1:A:443:GLU:N	2.44	0.41
1:A:517:LYS:HE3	1:A:517:LYS:HB2	1.73	0.41
1:A:1321:GLY:CA	1:A:1341:GLU:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1981:ASN:HB3	1:A:1983:ASP:OD1	2.20	0.41
1:A:226:GLU:O	1:A:229:LEU:N	2.47	0.41
1:A:875:GLN:OE1	1:A:876:GLN:HG2	2.21	0.41
1:A:1343:ASP:HB2	1:A:1345:TRP:NE1	2.33	0.41
1:A:1817:ILE:HG12	1:A:1824:PHE:O	2.21	0.41
1:A:1907:LYS:HE2	1:A:1907:LYS:HB3	1.88	0.41
1:A:1928:GLY:H	1:A:1939:PHE:HB2	1.86	0.41
2:K:146[A]:GLN:HE21	2:K:146[A]:GLN:HB3	1.70	0.41
1:A:1198:GLU:HA	1:A:1199:PRO:HD3	1.64	0.41
1:A:1462:PRO:HB3	1:A:1475:PHE:CE1	2.56	0.41
1:A:1604:LYS:HB2	1:A:1604:LYS:HE3	1.71	0.41
1:A:788:ILE:H	1:A:788:ILE:HG12	1.61	0.40
1:A:1170:ILE:HD13	1:A:1263:PHE:CZ	2.56	0.40
1:A:1464:SER:HB2	1:A:1473:ASN:OD1	2.21	0.40
1:A:1484:LEU:HD23	1:A:1528:LEU:HD21	2.03	0.40
1:A:1558:LEU:HG	1:A:1562:GLY:C	2.42	0.40
1:A:1739:ILE:O	1:A:1739:ILE:HG12	2.21	0.40
1:A:1938:TYR:CG	1:A:1939:PHE:N	2.89	0.40
1:A:18:ARG:NH2	1:A:66:SER:HB3	2.36	0.40
1:A:257:GLN:HE21	1:A:257:GLN:HB2	1.71	0.40
1:A:383:ILE:HD13	1:A:383:ILE:HG21	1.78	0.40
1:A:682:LEU:HD23	1:A:682:LEU:HA	1.93	0.40
1:A:710:GLU:HA	1:A:715:LYS:HE3	2.01	0.40
1:A:1096:PRO:HB2	1:A:1100:ILE:CD1	2.51	0.40
1:A:1134:GLU:HB3	1:A:1138:THR:HG22	2.03	0.40
1:A:1509:TYR:CD2	1:A:1509:TYR:N	2.89	0.40
1:A:1678:SER:HA	1:A:1706:THR:HG23	2.03	0.40
1:A:890:ILE:HG22	1:A:890:ILE:O	2.21	0.40
1:A:1016:LEU:HG	1:A:1016:LEU:O	2.21	0.40
1:A:1492:VAL:HA	1:A:1512:ASN:HA	2.03	0.40
1:A:1624:PHE:CD2	1:A:1624:PHE:N	2.89	0.40
1:A:1949:TRP:HA	1:A:1957:TYR:O	2.22	0.40
1:A:1980:PHE:HB3	1:A:1984:GLY:HA2	2.02	0.40
1:A:2019:TYR:CE1	1:A:2031:PHE:HB2	2.57	0.40
1:A:741:ASN:HD21	1:A:776:LYS:HZ2	1.70	0.40
1:A:1098:ALA:HA	1:A:1225:ASN:ND2	2.37	0.40
1:A:1293:ASP:OD1	1:A:1293:ASP:N	2.46	0.40
1:A:1314:SER:O	1:A:1316:SER:N	2.55	0.40
1:A:1683:TYR:CE1	1:A:1711:ALA:HB1	2.56	0.40
1:A:2016:LYS:HE2	1:A:2053:GLU:CG	2.52	0.40
1:A:68:ARG:O	1:A:72:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ALA:O	1:A:381:GLY:N	2.51	0.40
1:A:444:ASN:O	1:A:448:ILE:HG12	2.22	0.40
1:A:1290:ILE:HG22	1:A:1292:LEU:HD21	2.04	0.40
1:A:1354:ARG:O	1:A:1356:VAL:HG23	2.21	0.40
1:A:1471:LYS:HE3	1:A:1471:LYS:HB2	1.77	0.40
1:A:1637:ILE:HD13	1:A:1685:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2340/2375 (98%)	1845 (79%)	471 (20%)	24 (1%)	15 54
2	K	58/251 (23%)	47 (81%)	11 (19%)	0	100 100
All	All	2398/2626 (91%)	1892 (79%)	482 (20%)	24 (1%)	20 54

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1197	ARG
1	A	1524	ASP
1	A	1670	ILE
1	A	1520	ILE
1	A	1640	ASN
1	A	1810	LEU
1	A	1531	TYR
1	A	1549	ASN
1	A	1652	ASN
1	A	1671	SER
1	A	2099	SER
1	A	940	THR

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Mol	Chain	Res	Type
1	A	1143	LYS
1	A	1672	SER
1	A	1872	GLY
1	A	1009	VAL
1	A	1534	LYS
1	A	2102	ILE
1	A	1521	THR
1	A	941	VAL
1	A	1046	ILE
1	A	579	VAL
1	A	1012	VAL
1	A	1037	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2054/2140 (96%)	1764 (86%)	290 (14%)	3 16
2	K	54/222 (24%)	46 (85%)	8 (15%)	3 14
All	All	2108/2362 (89%)	1810 (86%)	298 (14%)	6 16

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	20	GLN
1	A	39	GLU
1	A	60	ILE
1	A	61	ASP
1	A	63	TYR
1	A	70	LYS
1	A	76	LYS
1	A	81	THR
1	A	83	ILE
1	A	97	ASN

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Mol	Chain	Res	Type
1	A	103	ILE
1	A	122	ASN
1	A	132	ASP
1	A	134	ASN
1	A	139	ASN
1	A	147	GLU
1	A	148	SER
1	A	153	THR
1	A	159	GLU
1	A	160	ASN
1	A	161	LEU
1	A	165	GLU
1	A	166	PHE
1	A	169	THR
1	A	173	ARG
1	A	185	ASN
1	A	194	LYS
1	A	203	ASP
1	A	220	GLU
1	A	242	ASN
1	A	243	PHE
1	A	247	LYS
1	A	248	THR
1	A	253	ASN
1	A	269	SER
1	A	272	LEU
1	A	273	ARG
1	A	274	VAL
1	A	277	LEU
1	A	286	ASP
1	A	288	ASP
1	A	289	MET
1	A	294	HIS
1	A	318	LEU
1	A	319	GLU
1	A	323	LYS
1	A	340	ASP
1	A	343	VAL
1	A	348	GLU
1	A	353	SER
1	A	367	ILE
1	A	383	ILE

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Mol	Chain	Res	Type
1	A	396	CYS
1	A	400	LEU
1	A	401	ILE
1	A	411	LEU
1	A	414	THR
1	A	429	MET
1	A	464	ASN
1	A	466	THR
1	A	469	LEU
1	A	470	SER
1	A	474	ILE
1	A	490	ILE
1	A	492	THR
1	A	497	SER
1	A	501	ASN
1	A	513	THR
1	A	517	LYS
1	A	520	LEU
1	A	521	TRP
1	A	522	GLN
1	A	536	LYS
1	A	538	ASN
1	A	554	GLN
1	A	558	THR
1	A	563	LEU
1	A	585	LEU
1	A	615	ASP
1	A	618	VAL
1	A	621	TYR
1	A	640	ARG
1	A	650	THR
1	A	661	THR
1	A	672	LEU
1	A	703	SER
1	A	705	SER
1	A	709	GLU
1	A	730	SER
1	A	737	ILE
1	A	738	VAL
1	A	739	SER
1	A	746	ARG
1	A	772	ASP

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Mol	Chain	Res	Type
1	A	782	ASN
1	A	784	LYS
1	A	819	LYS
1	A	820	VAL
1	A	824	GLU
1	A	828	ASN
1	A	839	GLU
1	A	846	LYS
1	A	852	SER
1	A	858	ASN
1	A	860	PHE
1	A	862	LEU
1	A	866	ILE
1	A	868	ASP
1	A	874	LYS
1	A	881	GLU
1	A	883	HIS
1	A	897	PHE
1	A	906	THR
1	A	908	GLU
1	A	911	PHE
1	A	926	ILE
1	A	939	ASP
1	A	942	ASN
1	A	947	LYS
1	A	948	LYS
1	A	951	LEU
1	A	955	HIS
1	A	958	ASN
1	A	960	LEU
1	A	964	PHE
1	A	968	SER
1	A	979	LEU
1	A	982	LEU
1	A	983	SER
1	A	984	VAL
1	A	997	THR
1	A	1000	ASN
1	A	1011	LEU
1	A	1014	THR
1	A	1016	LEU
1	A	1017	ASP

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Mol	Chain	Res	Type
1	A	1018	GLU
1	A	1025	THR
1	A	1026	LEU
1	A	1030	LEU
1	A	1054	ASP
1	A	1092	ILE
1	A	1093	LEU
1	A	1094	LEU
1	A	1097	LEU
1	A	1124	TYR
1	A	1138	THR
1	A	1139	LEU
1	A	1142	ASP
1	A	1143	LYS
1	A	1158	PHE
1	A	1188	PHE
1	A	1194	THR
1	A	1196	TYR
1	A	1197	ARG
1	A	1198	GLU
1	A	1221	MET
1	A	1233	TRP
1	A	1252	LEU
1	A	1263	PHE
1	A	1265	TRP
1	A	1268	PHE
1	A	1275	VAL
1	A	1276	ILE
1	A	1277	THR
1	A	1323	THR
1	A	1339	LEU
1	A	1344	THR
1	A	1348	ASP
1	A	1349	VAL
1	A	1352	VAL
1	A	1361	ASP
1	A	1367	ASP
1	A	1409	ILE
1	A	1410	LEU
1	A	1411	GLU
1	A	1426	TYR
1	A	1430	ILE

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Mol	Chain	Res	Type
1	A	1448	ILE
1	A	1457	LEU
1	A	1458	GLN
1	A	1460	ASN
1	A	1463	TYR
1	A	1467	ASP
1	A	1473	ASN
1	A	1480	THR
1	A	1497	LYS
1	A	1498	VAL
1	A	1500	MET
1	A	1507	PHE
1	A	1509	TYR
1	A	1513	ASP
1	A	1516	ASP
1	A	1520	ILE
1	A	1521	THR
1	A	1522	LYS
1	A	1531	TYR
1	A	1532	TYR
1	A	1534	LYS
1	A	1535	ASP
1	A	1540	SER
1	A	1541	LEU
1	A	1543	PHE
1	A	1545	ILE
1	A	1546	GLN
1	A	1549	ASN
1	A	1550	THR
1	A	1553	LEU
1	A	1557	TYR
1	A	1558	LEU
1	A	1560	GLU
1	A	1563	VAL
1	A	1566	ILE
1	A	1568	LYS
1	A	1580	ASP
1	A	1596	ILE
1	A	1598	SER
1	A	1611	PHE
1	A	1613	ILE
1	A	1616	THR

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Mol	Chain	Res	Type
1	A	1617	THR
1	A	1624	PHE
1	A	1638	LYS
1	A	1639	PHE
1	A	1640	ASN
1	A	1643	GLU
1	A	1652	ASN
1	A	1662	TYR
1	A	1665	ASP
1	A	1672	SER
1	A	1678	SER
1	A	1691	LYS
1	A	1705	ILE
1	A	1706	THR
1	A	1712	ASN
1	A	1738	SER
1	A	1742	VAL
1	A	1745	ASN
1	A	1746	ASP
1	A	1753	MET
1	A	1773	LYS
1	A	1780	LYS
1	A	1798	SER
1	A	1800	PHE
1	A	1805	TYR
1	A	1807	GLU
1	A	1809	LEU
1	A	1812	TYR
1	A	1814	LEU
1	A	1817	ILE
1	A	1824	PHE
1	A	1834	SER
1	A	1836	LEU
1	A	1838	TYR
1	A	1852	ASN
1	A	1857	PHE
1	A	1871	ASN
1	A	1876	SER
1	A	1883	ASP
1	A	1890	SER
1	A	1916	ASP
1	A	1944	ARG

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Mol	Chain	Res	Type
1	A	1959	PHE
1	A	1960	SER
1	A	1975	ASP
1	A	2051	GLU
1	A	2087	SER
1	A	2100	ILE
1	A	2102	ILE
1	A	2104	ILE
1	A	2111	TYR
1	A	2122	PHE
1	A	2130	PHE
1	A	2143	GLN
1	A	2154	GLU
1	A	2165	THR
1	A	2181	ASN
1	A	2202	PHE
1	A	2205	SER
1	A	2212	TRP
1	A	2214	TYR
1	A	2221	ASP
1	A	2231	LYS
1	A	2247	ASP
1	A	2254	THR
1	A	2259	PHE
1	A	2263	HIS
1	A	2337	THR
1	A	2363	LEU
2	K	121	LYS
2	K	124	PHE
2	K	142	PHE
2	K	146[A]	GLN
2	K	146[B]	GLN
2	K	164	ASN
2	K	167	THR
2	K	176	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	53	ASN
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	97	ASN
1	A	106	GLN
1	A	134	ASN
1	A	139	ASN
1	A	162	ASN
1	A	167	ASN
1	A	222	ASN
1	A	257	GLN
1	A	344	GLN
1	A	386	GLN
1	A	412	ASN
1	A	426	ASN
1	A	464	ASN
1	A	518	ASN
1	A	538	ASN
1	A	597	ASN
1	A	741	ASN
1	A	758	HIS
1	A	782	ASN
1	A	803	GLN
1	A	925	HIS
1	A	958	ASN
1	A	961	ASN
1	A	993	GLN
1	A	1127	HIS
1	A	1381	ASN
1	A	1400	ASN
1	A	1446	GLN
1	A	1473	ASN
1	A	1502	ASN
1	A	1549	ASN
1	A	1621	GLN
1	A	1709	HIS
1	A	1712	ASN
1	A	1828	ASN
1	A	1868	ASN
1	A	1886	ASN
1	A	1935	ASN
1	A	2148	ASN
1	A	2176	ASN
1	A	2298	ASN
1	A	2310	ASN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

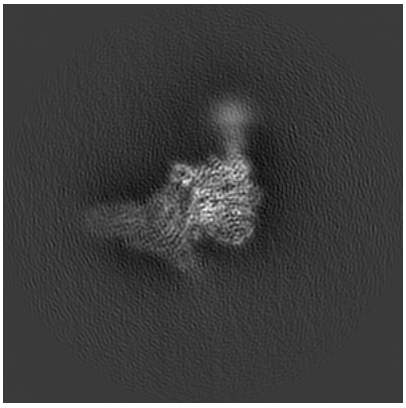
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31628. These allow visual inspection of the internal detail of the map and identification of artifacts.

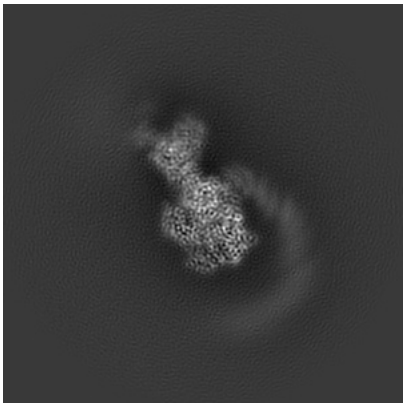
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

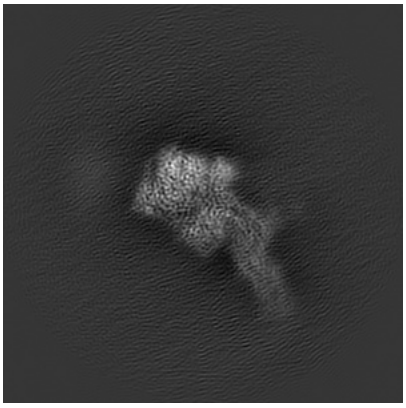
6.1.1 Primary map



X



Y

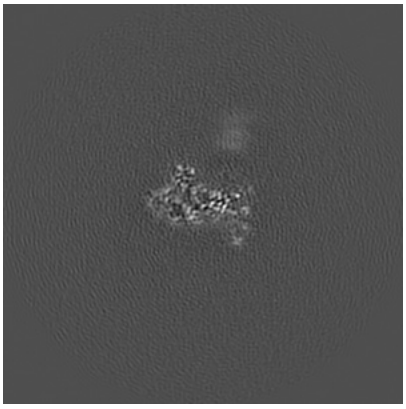


Z

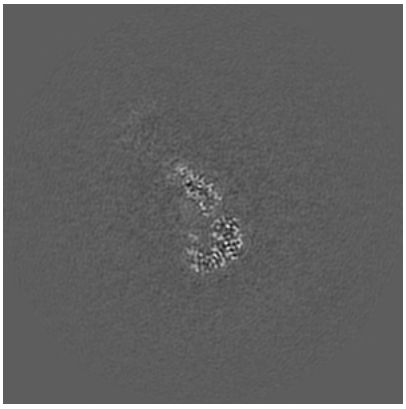
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

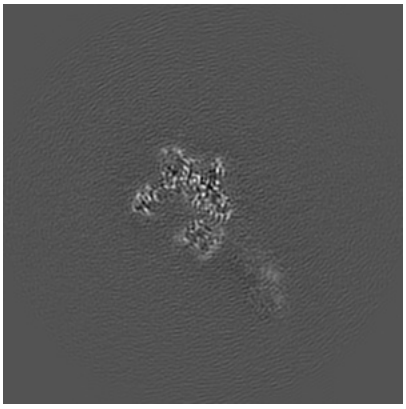
6.2.1 Primary map



X Index: 160



Y Index: 160

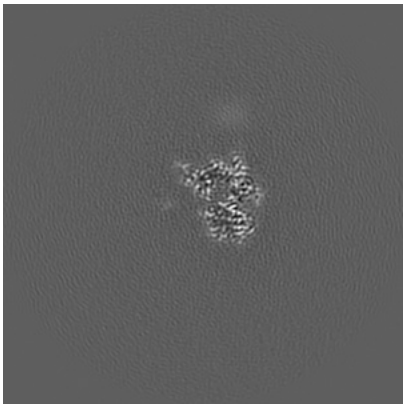


Z Index: 160

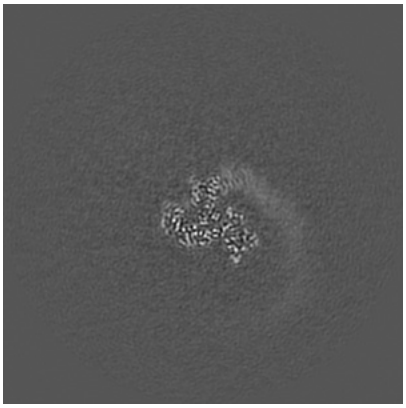
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

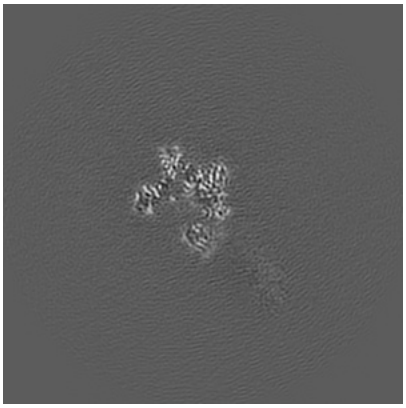
6.3.1 Primary map



X Index: 136



Y Index: 184



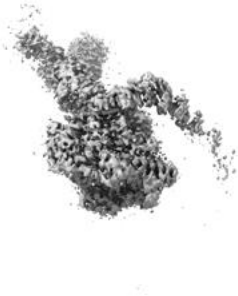
Z Index: 164

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

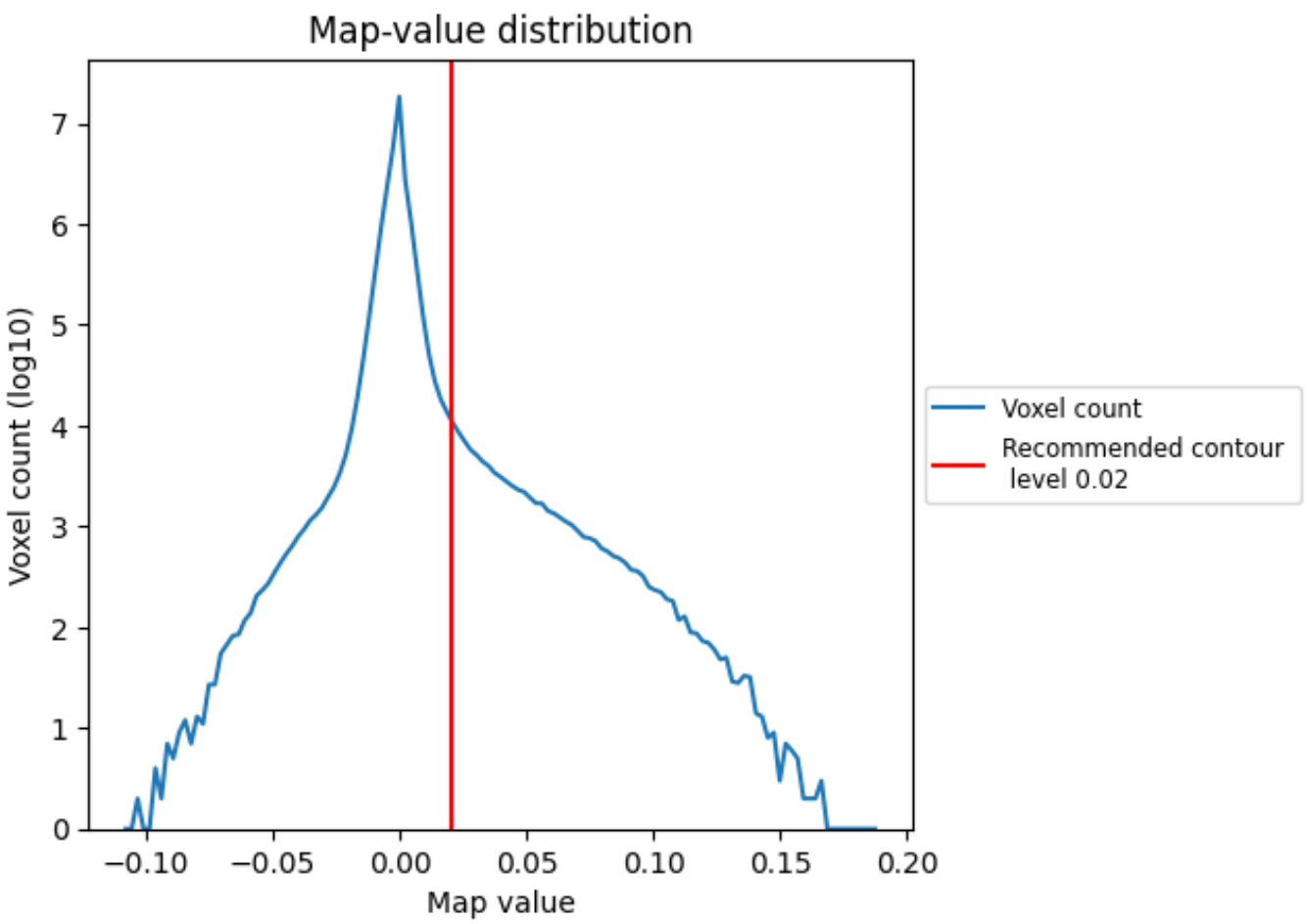
6.5 Mask visualisation (i)

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

7 Map analysis (i)

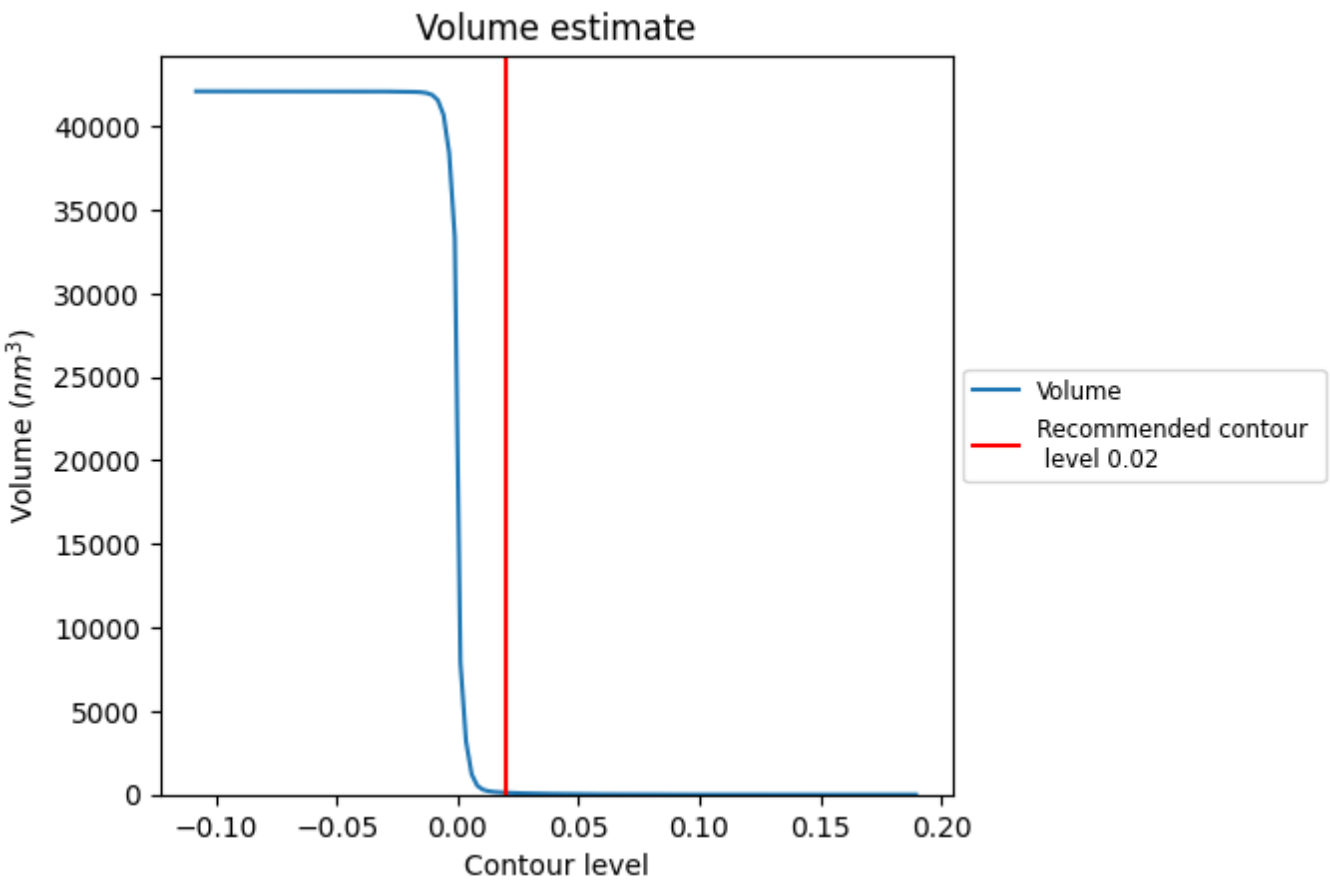
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

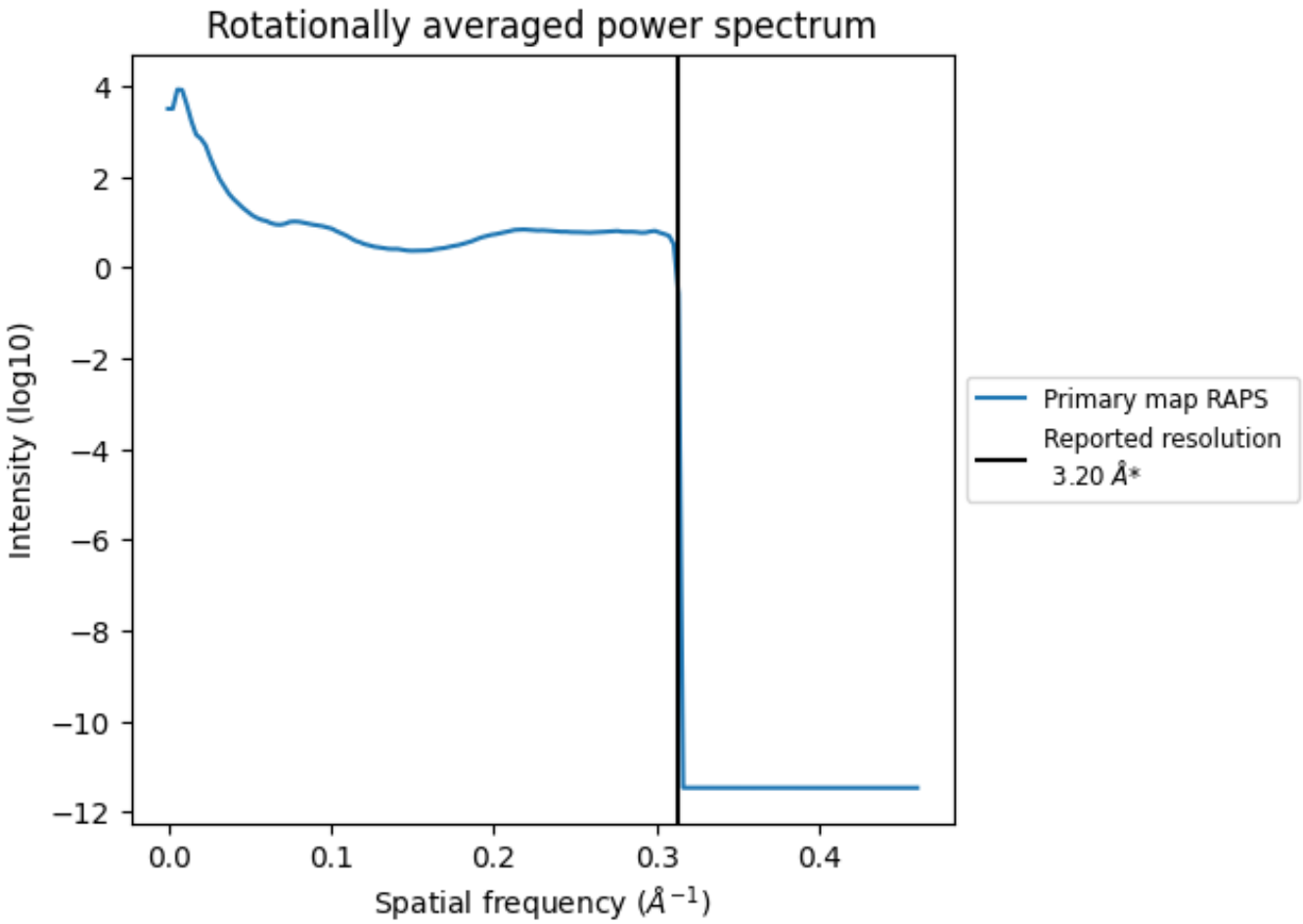
7.2 Volume estimate (i)



The volume at the recommended contour level is 111 nm^3; this corresponds to an approximate mass of 101 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

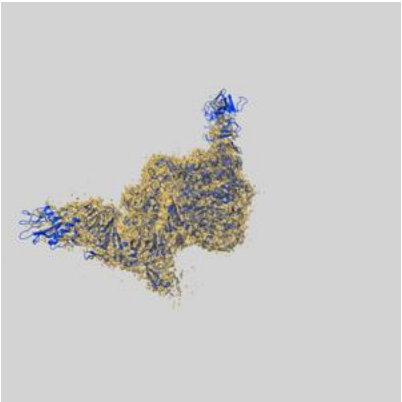
8 Fourier-Shell correlation (i)

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

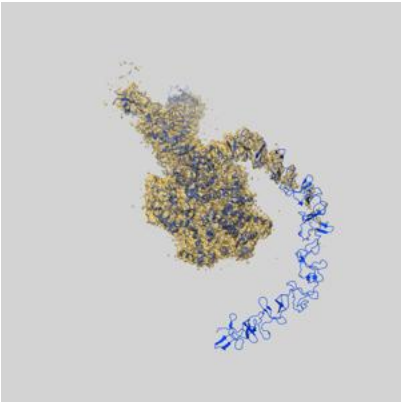
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31628 and PDB model 7V1N. Per-residue inclusion information can be found in section 3 on page 4.

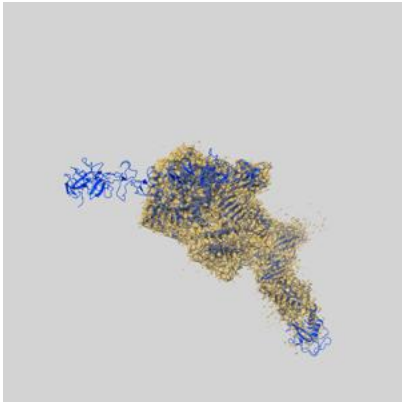
9.1 Map-model overlay (i)



X



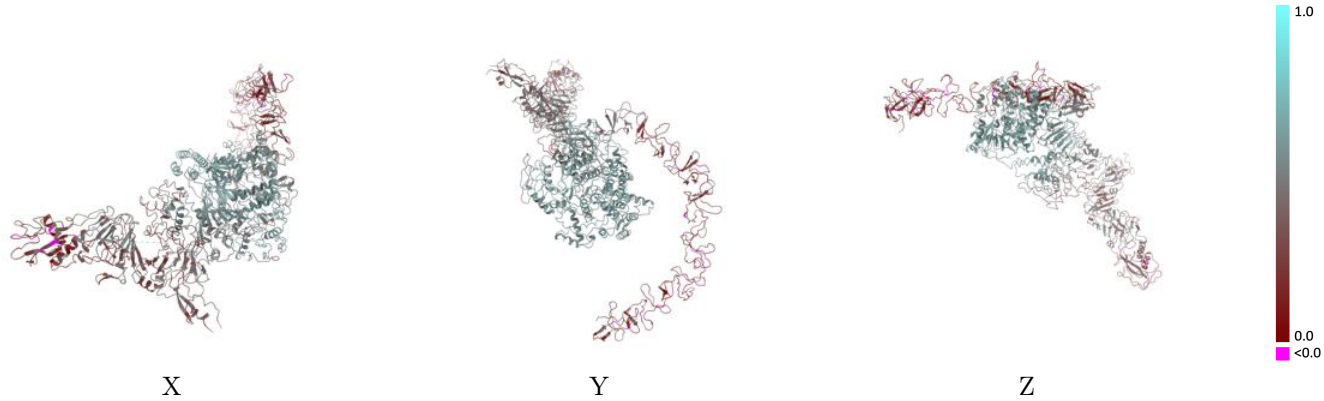
Y



Z

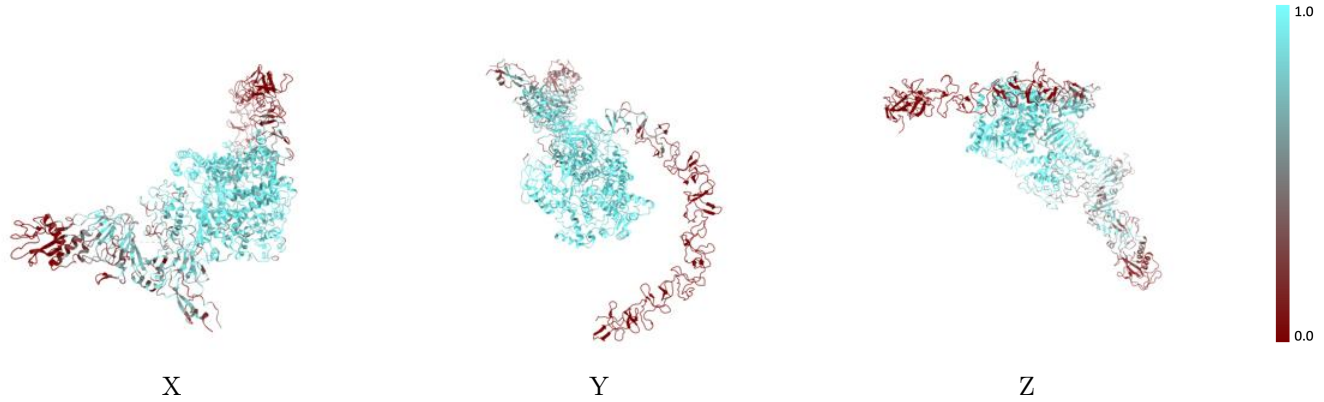
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



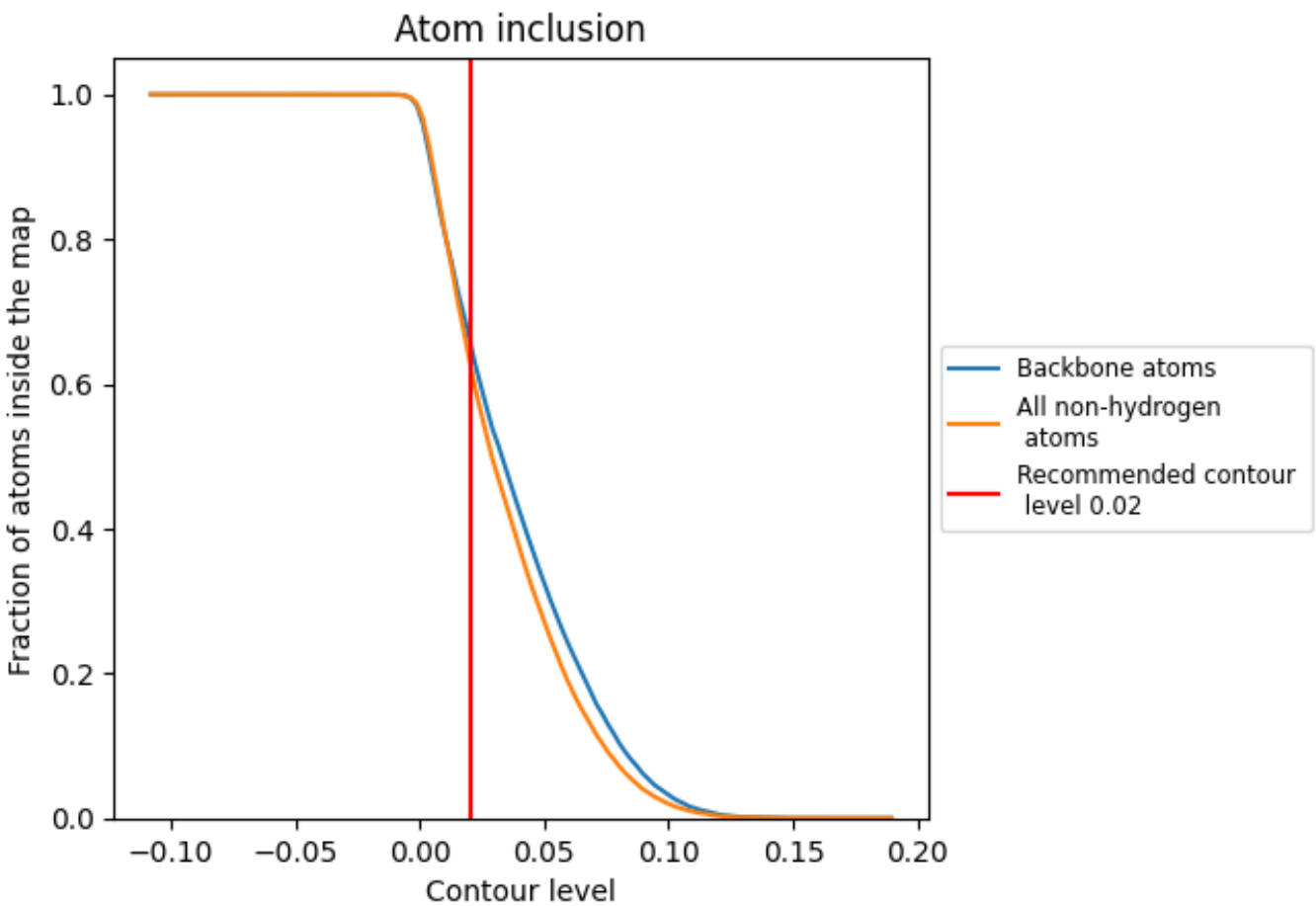
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6310	0.4410
A	0.6361	0.4430
K	0.4316	0.3700