



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 02:48 PM EDT

PDB ID : 7K17
Title : Re-refined crystal structure of DNA-dependent protein kinase catalytic subunit complexed with Ku80 C-terminal helix
Authors : Chen, X.; Gellert, M.; Yang, W.
Deposited on : 2020-09-07
Resolution : 4.30 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

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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
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

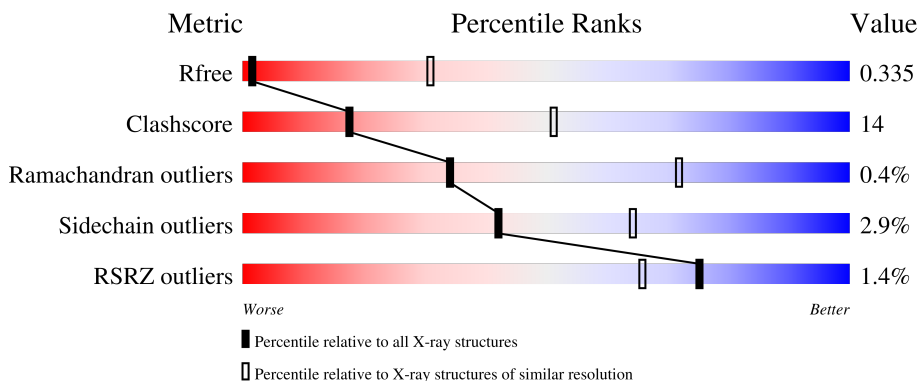
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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 | 1014 (4.80-3.80) |
| Clashscore | 141614 | 1077 (4.80-3.80) |
| Ramachandran outliers | 138981 | 1029 (4.80-3.80) |
| Sidechain outliers | 138945 | 1012 (4.80-3.80) |
| RSRZ outliers | 127900 | 1075 (4.90-3.70) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 3986 | |
| 1 | B | 3986 | |
| 2 | C | 192 | |
| 2 | D | 192 | |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 56895 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------|------------|-----------|-----------|----------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 3629 | Total 28238 | C 18117 | N 4751 | O 5184 | S 186 | 0 | 0 | 0 |
| 1 | B | 3645 | Total 28521 | C 18300 | N 4815 | O 5221 | S 185 | 0 | 0 | 0 |

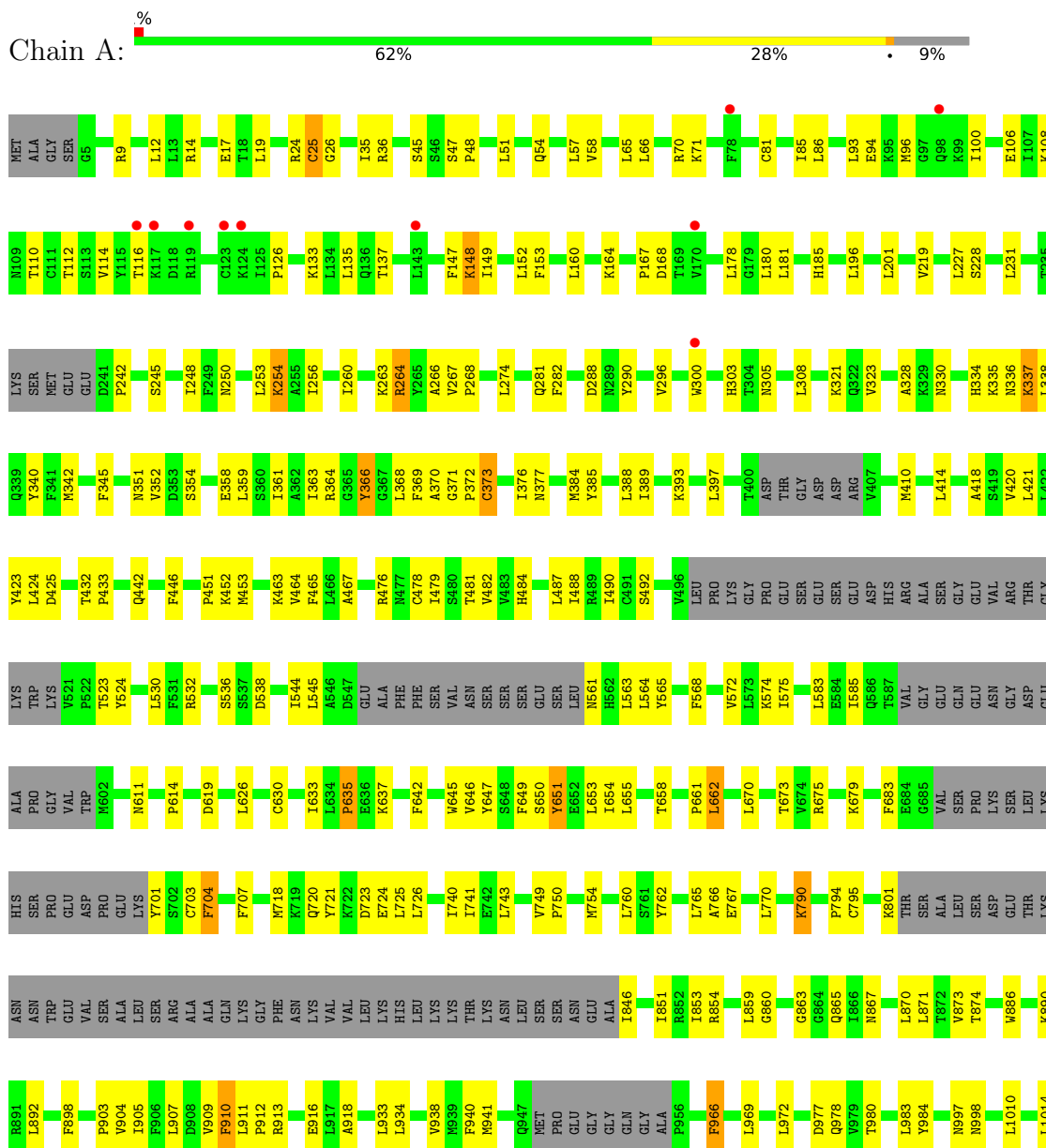
- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | D | 9 | Total 68 | C 43 | N 9 | O 15 | S 1 | 0 | 0 | 0 |
| 2 | C | 9 | Total 68 | C 43 | N 9 | O 15 | S 1 | 0 | 0 | 0 |

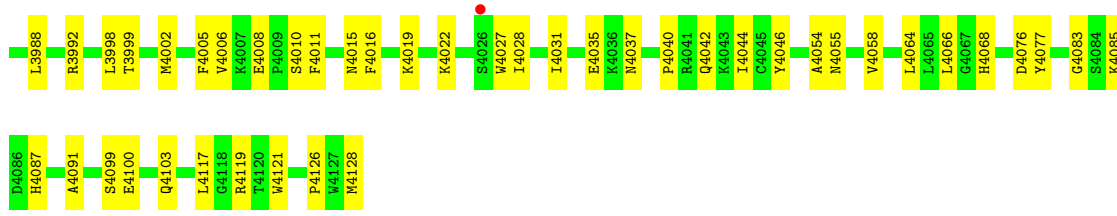
3 Residue-property plots

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.

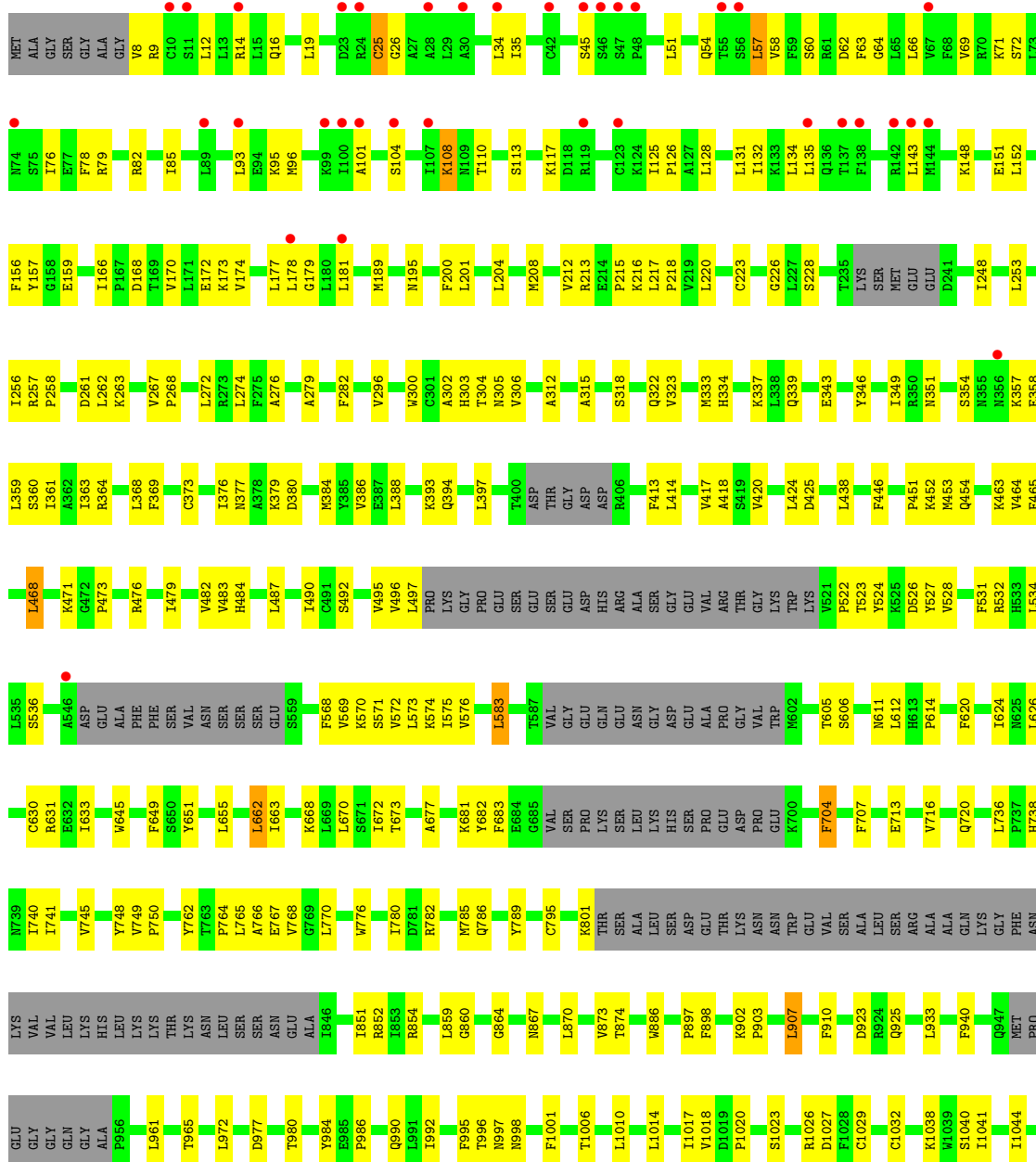
- Molecule 1: DNA-dependent protein kinase catalytic subunit



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| L2237 | R2143 | L2144 | K2148 | L2151 | M2152 | S2250 | L2249 | L2165 | L2168 | N2177 | C2178 | D2269 | I2274 | Q2275 | L2276 | L2277 | V2280 | M2281 | D2284 | L2285 | P2286 | F2287 | D2288 | P2289 | Q2291 | C2292 | G2293 | I2294 | Q2295 | S2296 | V2304 | N2305 | F2309 | Y2312 | V2315 | A2318 | E2321 | V2322 | I2326 | L2327 | | | | | | | | | |
| THR | GLY | PHE | ARG | ARG | ARG | PRO | GLU | GLN | ASP | LEU | LEU | ARG | LYS | GLU | ILE | ILE | ARG | ASN | GLY | ASP | ASP | ASP | GLY | PRO | PRO | GLN | GLY | LEU | S2029 | T2035 | L2036 | G2048 | VAL | GLN | GLN | TVR | TYR | TYR | GLN | ASP | PRO | ARG | ALA | | | | | | |
| G1122 | T1123 | I1124 | Q1125 | L1134 | I1137 | I1138 | E1139 | K1140 | K1141 | K1038 | H1037 | V1143 | M1146 | K1147 | R1151 | F1154 | R1155 | G1156 | F1157 | C1164 | L1165 | L1166 | R1178 | P1179 | Q1180 | T1181 | E1182 | C1183 | R1184 | Y1192 | K1193 | F1194 | V1195 | P1196 | L1197 | S1203 | P1204 | L1208 | L1212 | K1213 | L1220 | F1224 | G1228 | G1229 | L1230 | GLN | | | |
| PRO | SER | GLY | ILE | LEU | ALA | GLN | PRO | THR | LEU | LEU | TYR | ARG | GLY | PRO | LEU | C1251 | C1255 | W1256 | L1257 | D1258 | L1259 | L1260 | L1261 | A1262 | C1266 | T1275 | L1279 | L1282 | G1283 | L1291 | K1292 | K1293 | V1294 | A1295 | S1301 | A1302 | M1303 | HIS | ASP | ILE | ILE | ALA | ALA | GLU | LYS | | | | |
| CYS | PHE | THR | GLY | ALA | ALA | GLY | ASN | THR | S1323 | S1333 | K1334 | C1335 | T1336 | E1430 | V1337 | M1342 | E1343 | F1344 | T1345 | T1346 | L1347 | L1348 | L1349 | S1352 | F1353 | A1354 | G1355 | W1356 | K1357 | L1358 | L1359 | K1361 | D1362 | C1364 | M1365 | H1366 | L1368 | V1371 | L1372 | V1373 | H1382 | V1389 | P1501 | H1394 | L1395 | P1396 | L1402 | | |
| L1406 | Y1411 | L1415 | E1416 | R1420 | K1422 | A1425 | G1426 | S1427 | L1428 | E1429 | E1430 | L1431 | C1432 | A1433 | E1434 | V1434 | M1435 | L1436 | F1439 | D1440 | V1443 | L1448 | H1459 | L1463 | N1466 | D1474 | V1479 | L1483 | V1487 | G1494 | ASP | GLU | ARG | GLN | CYS | LEU | P1501 | S1502 | L1503 | D1504 | C1507 | K1508 | | | | | | | |
| Q1509 | L1510 | L1514 | L1515 | F1519 | A1520 | L1528 | L1533 | M1534 | P1535 | A1536 | V1537 | LEU | SER | THR | ALA | SER | VAL | ILE | HIS | PHE | SER | ASN | THR | SER | Y1560 | S1564 | M1568 | L1572 | M1574 | L1575 | D1576 | L1577 | A1578 | V1579 | L1580 | E1581 | L1582 | M1583 | M1589 | V1593 | G1599 | | | | | | | | |
| H1800 | L1601 | D1602 | Q1603 | S1604 | K1612 | H1613 | K1617 | L1618 | T1621 | H1625 | A1636 | W1633 | D1636 | E1640 | T1641 | K1642 | L1646 | L1653 | S1657 | VAL | VAL | SER | ILE | HIS | PHE | ASN | THR | H1665 | G1666 | S1667 | P1669 | T1674 | V1675 | I1676 | L1679 | A1680 | D1681 | T1682 | K1683 | L1686 | A1692 | L1695 | L1696 | P1697 | F1698 | | | | |
| L1702 | T1703 | L1707 | R1712 | V1713 | Q1716 | L1717 | I1718 | H1721 | F1722 | P1723 | M1724 | Q1725 | P1730 | T1733 | P1734 | R1735 | F1736 | Y1739 | M1743 | L1747 | L1750 | S1753 | Q1754 | S1755 | L1758 | L1759 | E1760 | E1764 | V1765 | L1766 | C1767 | R1768 | E1769 | D1681 | T1682 | K1683 | L1686 | A1692 | L1695 | L1696 | P1697 | R1787 | R1788 | | | | | | |
| G1789 | S1790 | T1793 | Q1794 | L1797 | V1801 | Y1802 | W1820 | D1821 | A1822 | S1823 | L1824 | W1825 | W1829 | H1830 | C1831 | S1832 | L1833 | D1834 | A1835 | L1836 | R1837 | F1840 | I1843 | W1844 | V1845 | I1848 | D1849 | V1850 | L1851 | S1853 | T1856 | K1857 | L1858 | S1861 | S1968 | E1969 | L1976 | I1977 | Y1978 | D1878 | Y1881 | H1890 | A1891 | K1892 | | | | | |
| K1895 | I1896 | V1899 | E1993 | V1994 | T1906 | M1909 | E1910 | L1911 | L1912 | K1913 | L1914 | L1915 | L1916 | A1917 | L1918 | C1919 | Y1920 | F1923 | E1928 | L1933 | E1930 | M1931 | L1934 | R1937 | R1938 | M1946 | C1947 | I1948 | S1950 | V1951 | I1952 | V1955 | F1956 | M1957 | F1967 | S1968 | E1969 | L1976 | I1977 | Y1978 | D1878 | Y1881 | H1890 | A1891 | K1892 | | | | |
| F1990 | V1992 | E1993 | V1994 | E1995 | V1996 | MET | GLU | ASP | ARG | LYS | LYS | LYS | TYR | ILE | GLU | ILE | ARG | LYS | GLU | ASP | ASP | ASP | GLY | PRO | PRO | GLY | PRO | GLN | GLN | S2029 | T2035 | L2036 | G2048 | VAL | GLN | GLN | TVR | SER | TYR | SER | SER | GLN | ASP | PRO | ARG | ALA | | | |
| THR | GLY | PHE | ARG | ARG | ARG | PRO | GLU | GLN | ASP | ASP | VAL | HIS | ASP | ASP | VAL | LEU | E2082 | L2083 | E2084 | M2085 | L2088 | M2089 | R2090 | H2091 | G2092 | C2093 | L2100 | V2101 | H2105 | L2108 | GLY | PRO | PRO | GLN | GLY | GLU | ASP | SER | VAL | R2120 | D2121 | L2122 | G2131 | N2135 | P2136 | I2137 | V2138 | P2139 | L2140 |
| R2143 | L2144 | K2148 | L2151 | M2152 | S2250 | L2249 | L2165 | L2168 | N2177 | C2178 | G2179 | E2180 | G2181 | L2182 | H2183 | Y2184 | W2185 | V2186 | E2187 | I2188 | L2189 | V2190 | A2191 | L2192 | I2193 | D2288 | L2194 | S2195 | W2196 | T2197 | G2198 | L2199 | A2200 | T2203 | D2208 | L2219 | M2220 | V2223 | F2224 | H2225 | P2226 | K2227 | V2230 | F2231 | M2234 | L2327 | | | |
| V1018 | T1123 | I1124 | S1023 | R1026 | C1029 | C1032 | L1037 | K1038 | W1039 | S1040 | L1041 | K1042 | S1052 | N1055 | T1056 | K1057 | A1067 | N1071 | F1072 | K1074 | R1075 | L1076 | G1077 | A1078 | F1082 | I1085 | F1089 | R1090 | V1096 | F1099 | V1100 | F1101 | E1102 | A1103 | L1104 | V1105 | Y1107 | A1114 | D1117 | E1118 | L1121 | | | | | | | | |



• Molecule 1: DNA-dependent protein kinase catalytic subunit



| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| R3992 | P3879 | I3740 | R3630 | Q3494 | PRO | L3298 | L3157 | ARG | D2821 | P2548 | V2461 | Y2329 |
| L3997 | A3680 | R3741 | K3631 | S3497 | A3406 | T3299 | S3047 | LEU | K2822 | K2549 | V2458 | K2334 |
| F4005 | L3881 | G3742 | F3632 | S3497 | A3407 | V3300 | K3048 | PRO | K2823 | L2550 | V2459 | |
| E4008 | L3882 | H3743 | I3633 | M3503 | I3410 | T3303 | L3049 | PRO | K2824 | E2551 | F2461 | |
| F4009 | R3885 | D3744 | F3636 | M3503 | I3411 | T3303 | K3050 | V2920 | T2825 | F2554 | Q2472 | |
| S4010 | V3888 | K3763 | D3641 | L3506 | A3412 | L3307 | L3052 | L2921 | K2829 | L2555 | M2473 | |
| F4011 | G3754 | G3755 | K3642 | D3507 | Y3413 | N3319 | L3053 | R2922 | K2835 | S2556 | | |
| D4012 | L3758 | L3758 | G3645 | Q3510 | D3418 | F3323 | A3057 | E2925 | N2560 | N2560 | I2476 | |
| K4013 | R3769 | R3769 | K3646 | A3511 | D3421 | T3198 | Q3058 | D2925 | N2566 | L2477 | | |
| L4014 | Q3760 | Q3760 | G3647 | V3512 | Q3422 | LEU | Q3059 | D2937 | M2565 | I2480 | | |
| M4015 | G3761 | G3761 | G3648 | A3513 | Q3422 | PRO | S3060 | R2940 | N2568 | E2481 | | |
| F4016 | V3764 | V3764 | L3651 | Q3514 | K3426 | GLU | L3061 | R2940 | M2568 | D2482 | | |
| I4031 | S3778 | S3778 | L3652 | Q3515 | E3427 | ASP | I3065 | T2949 | Y2572 | N2483 | | |
| E4035 | N3772 | N3772 | L3653 | S3517 | E3428 | ASN | Q3066 | K2950 | N2574 | P2373 | | |
| A4047 | L3775 | L3775 | M3654 | S3517 | A3429 | SER | K3067 | Q2951 | N2574 | L2374 | | |
| K4050 | G3779 | G3779 | K3655 | A3528 | ASN | MET | A3068 | I2952 | V2575 | A2375 | | |
| R4054 | R3784 | R3784 | K3655 | A3528 | ASN | ASN | M3069 | S2856 | F2487 | V2485 | | |
| M4055 | A3785 | A3785 | K3656 | I3529 | ALA | VAL | Q3074 | C2857 | F2577 | E2488 | | |
| V4058 | L3786 | L3786 | L3656 | F3542 | SER | ASP | Q3074 | A2956 | R2577 | E2489 | | |
| L4064 | R3789 | R3789 | L3666 | F3542 | SER | ASP | K3075 | L2957 | S2582 | S2489 | | |
| H4068 | S3790 | S3790 | L3667 | H3549 | ILE | GLN | L3078 | L2958 | E2582 | E2490 | | |
| Y4077 | K3669 | K3669 | K3668 | H3549 | ASP | GLY | E3079 | Y2965 | E2583 | T2491 | | |
| R4082 | S3674 | S3674 | K3669 | F3554 | SER | ASP | Y3082 | A2968 | C2584 | D2492 | | |
| G4087 | P3676 | P3676 | K3669 | F3554 | LEU | PRO | S3083 | Q2971 | E2585 | F2387 | | |
| S3943 | E3682 | E3682 | K3669 | I3558 | LEU | ASP | Q3084 | Y2972 | F2586 | T2389 | | |
| A3949 | D3689 | D3689 | K3669 | I3558 | LEU | PRO | E3085 | D2973 | F2586 | L2393 | | |
| V3955 | V3692 | V3692 | L3669 | L3562 | LEU | SER | Y3082 | Q2971 | F2586 | L2398 | | |
| P3956 | E3693 | E3693 | L3669 | L3562 | LEU | ASP | S3083 | Q2972 | T2591 | L2501 | | |
| E3957 | F3694 | F3694 | L3669 | L3562 | LEU | ASP | Q3084 | Y2972 | L2591 | L2501 | | |
| L3958 | L3695 | L3695 | L3669 | L3562 | LEU | GLY | E3085 | D2973 | L2591 | L2501 | | |
| R3962 | R3696 | R3696 | L3669 | L3562 | LEU | GLY | L3086 | E2974 | UNK | V2505 | | |
| Q3966 | M3697 | M3697 | L3669 | L3562 | LEU | GLN | Y3102 | A2975 | X2603 | L2806 | | |
| N3969 | E3682 | E3682 | L3669 | L3562 | LEU | GLN | M3111 | N2977 | X2606 | I2507 | | |
| E3976 | M3682 | M3682 | L3669 | L3562 | LEU | GLY | G3112 | K2978 | X2610 | I2511 | | |
| L3979 | M3820 | M3820 | L3669 | L3562 | LEU | GLY | N3113 | W2981 | X2610 | N2514 | | |
| R3984 | E3824 | E3824 | L3669 | L3562 | LEU | GLY | Y3114 | V2962 | L2780 | L2517 | | |
| M3984 | L3829 | L3829 | L3669 | L3562 | LEU | GLY | S3115 | D2983 | P2781 | Q2518 | | |
| E3987 | R3833 | R3833 | L3669 | L3562 | LEU | GLY | I3117 | E2990 | D2782 | L2519 | | |
| L4116 | V3833 | V3833 | L3669 | L3562 | LEU | GLY | L3120 | S2988 | L2783 | F2524 | | |
| L4117 | V3833 | V3833 | L3669 | L3562 | LEU | GLY | L3120 | S2988 | L2783 | F2524 | | |
| R4119 | V3833 | V3833 | L3669 | L3562 | LEU | GLY | L3120 | S2988 | L2783 | F2524 | | |
| T4120 | V3833 | V3833 | L3669 | L3562 | LEU | GLY | L3120 | S2988 | L2783 | F2524 | | |
| W4121 | V3833 | V3833 | L3669 | L3562 | LEU | GLY | L3120 | S2988 | L2783 | F2524 | | |
| E4125 | V3833 | V3833 | L3669 | L3562 | LEU | GLY | L3120 | S2988 | L2783 | F2524 | | |
| P4126 | V3833 | V3833 | L3669 | L3562 | LEU | GLY | L3120 | S2988 | L2783 | F2524 | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 169.12Å 132.64Å 296.59Å 90.00° 105.53° 90.00° | Depositor |
| Resolution (Å) | 49.92 – 4.30 49.92 – 4.30 | Depositor EDS |
| % Data completeness (in resolution range) | 97.8 (49.92-4.30) 97.6 (49.92-4.30) | Depositor EDS |
| R_{merge} | 0.16 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.33 (at 4.29Å) | Xtrriage |
| Refinement program | PHENIX 1.14_3260 | Depositor |
| R, R_{free} | 0.286 , 0.335 0.286 , 0.335 | Depositor DCC |
| R_{free} test set | 2009 reflections (2.32%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 184.6 | Xtrriage |
| Anisotropy | 0.337 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 157.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtrriage |
| Estimated twinning fraction | 0.019 for h,-k,-h-l | Xtrriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 56895 | wwPDB-VP |
| Average B, all atoms (Å ²) | 217.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality 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 | 0.29 | 0/28603 | 0.52 | 5/38757 (0.0%) |
| 1 | B | 0.29 | 0/28898 | 0.51 | 8/39125 (0.0%) |
| 2 | C | 0.25 | 0/67 | 0.43 | 0/90 |
| 2 | D | 0.28 | 0/67 | 0.50 | 0/90 |
| All | All | 0.29 | 0/57635 | 0.52 | 13/78062 (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 | 2 |
| 1 | B | 0 | 1 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 3652 | LEU | CB-CG-CD2 | -7.00 | 99.10 | 111.00 |
| 1 | A | 2781 | PRO | N-CA-CB | 6.49 | 111.08 | 103.30 |
| 1 | B | 1858 | LEU | CB-CG-CD1 | -6.17 | 100.51 | 111.00 |
| 1 | B | 1752 | LEU | CB-CG-CD1 | -5.72 | 101.27 | 111.00 |
| 1 | B | 1752 | LEU | CB-CG-CD2 | 5.72 | 120.72 | 111.00 |
| 1 | A | 2100 | LEU | CA-CB-CG | 5.71 | 128.43 | 115.30 |
| 1 | A | 1825 | LEU | CB-CG-CD2 | -5.58 | 101.52 | 111.00 |
| 1 | B | 907 | LEU | CB-CG-CD2 | 5.43 | 120.22 | 111.00 |
| 1 | B | 261 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 1 | B | 57 | LEU | CA-CB-CG | 5.18 | 127.22 | 115.30 |
| 1 | B | 2208 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 1 | A | 3259 | LEU | CA-CB-CG | 5.15 | 127.15 | 115.30 |
| 1 | B | 1752 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | A | 1994 | VAL | Peptide |
| 1 | A | 2120 | ARG | Peptide |
| 1 | B | 1202 | ARG | 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 | 28238 | 0 | 27963 | 774 | 0 |
| 1 | B | 28521 | 0 | 28367 | 774 | 0 |
| 2 | C | 68 | 0 | 64 | 1 | 0 |
| 2 | D | 68 | 0 | 64 | 1 | 0 |
| All | All | 56895 | 0 | 56458 | 1550 | 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 14.

All (1550) 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:260:ILE:HG22 | 1:A:300:TRP:CZ2 | 1.96 | 1.00 |
| 1:B:3701:ILE:HD12 | 1:B:3740:ILE:HD11 | 1.50 | 0.94 |
| 1:A:645:TRP:O | 1:A:649:PHE:HB2 | 1.71 | 0.91 |
| 1:A:1406:LEU:HB3 | 1:A:1415:LEU:HD11 | 1.51 | 0.89 |
| 1:B:2459:VAL:HB | 1:B:2505:VAL:HG21 | 1.55 | 0.88 |
| 1:A:3028:ASN:HA | 1:A:3031:TRP:HD1 | 1.39 | 0.86 |
| 1:A:385:TYR:CE2 | 1:A:389:ILE:HD11 | 2.10 | 0.86 |
| 1:A:354:SER:HB3 | 1:A:358:GLU:HB2 | 1.62 | 0.82 |
| 1:B:1608:ARG:HA | 1:B:1612:LYS:HB3 | 1.62 | 0.81 |
| 1:A:1676:ILE:O | 1:A:1680:ALA:HB2 | 1.81 | 0.79 |
| 1:A:3545:THR:HG22 | 1:A:3546:SER:H | 1.47 | 0.79 |
| 1:B:1615:GLY:HA3 | 1:B:1655:ILE:HG21 | 1.61 | 0.79 |
| 1:B:3325:ASP:HA | 1:B:3328:ILE:HD12 | 1.65 | 0.79 |
| 1:B:3700:GLU:HA | 1:B:3718:ARG:HA | 1.64 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:260:ILE:HG22 | 1:A:300:TRP:CH2 | 2.19 | 0.78 |
| 1:A:1204:PRO:HB2 | 1:A:1275:THR:HG22 | 1.65 | 0.78 |
| 1:B:583:LEU:HA | 1:B:614:PRO:HA | 1.66 | 0.78 |
| 1:B:1579:VAL:HG21 | 1:B:1621:THR:HG21 | 1.66 | 0.78 |
| 1:A:873:VAL:HG13 | 1:A:874:THR:H | 1.48 | 0.77 |
| 1:B:135:LEU:HD12 | 1:B:177:LEU:HD11 | 1.67 | 0.77 |
| 1:B:1686:LEU:HD11 | 1:B:1721:HIS:HB3 | 1.66 | 0.76 |
| 1:A:3930:VAL:HG12 | 1:A:3937:VAL:HG12 | 1.67 | 0.76 |
| 1:A:1787:ARG:HB3 | 1:A:1831:CYS:HB3 | 1.66 | 0.76 |
| 1:B:873:VAL:HG13 | 1:B:874:THR:H | 1.50 | 0.76 |
| 1:A:801:LYS:HA | 1:A:3115:SER:HB2 | 1.68 | 0.76 |
| 1:A:2825:THR:HG22 | 1:A:2826:LEU:H | 1.51 | 0.76 |
| 1:B:3700:GLU:HG3 | 1:B:3718:ARG:HG2 | 1.66 | 0.75 |
| 1:A:1178:ARG:NH1 | 1:A:1183:CYS:SG | 2.59 | 0.75 |
| 1:B:1068:LEU:HD11 | 1:B:1106:ILE:HG13 | 1.68 | 0.75 |
| 1:B:1076:LEU:HB2 | 1:B:1123:THR:HG22 | 1.68 | 0.75 |
| 1:B:1832:SER:H | 1:B:1883:ARG:HH22 | 1.34 | 0.75 |
| 1:B:2851:PHE:HB3 | 1:B:2854:PHE:HB3 | 1.69 | 0.75 |
| 1:A:363:ILE:HG23 | 1:A:388:LEU:HD11 | 1.69 | 0.74 |
| 1:A:770:LEU:HD23 | 1:A:854:ARG:HD3 | 1.68 | 0.74 |
| 1:B:1090:ARG:HB2 | 1:B:1137:ILE:HG12 | 1.68 | 0.74 |
| 1:B:1406:LEU:HB3 | 1:B:1415:LEU:HD11 | 1.70 | 0.74 |
| 1:B:1727:ARG:HD2 | 1:B:1773:VAL:HG23 | 1.69 | 0.74 |
| 1:A:66:LEU:HD21 | 1:A:106:GLU:HB3 | 1.69 | 0.74 |
| 1:A:1082:PHE:HZ | 1:A:1134:LEU:HG | 1.53 | 0.73 |
| 1:B:1955:VAL:HG13 | 1:B:1956:PHE:H | 1.52 | 0.73 |
| 1:A:14:ARG:HA | 1:A:17:GLU:HG2 | 1.70 | 0.73 |
| 1:B:2965:TYR:HA | 1:B:2968:ALA:HB3 | 1.70 | 0.73 |
| 1:A:35:ILE:HD12 | 1:A:81:CYS:HB2 | 1.70 | 0.73 |
| 1:A:3503:VAL:HG21 | 1:A:3532:PRO:HB2 | 1.71 | 0.73 |
| 1:A:300:TRP:CE3 | 1:A:308:LEU:HD21 | 2.24 | 0.73 |
| 1:B:2451:LEU:HD23 | 1:B:2484:TYR:HE2 | 1.54 | 0.73 |
| 1:A:1697:PRO:HB3 | 1:A:1753:SER:HB3 | 1.71 | 0.73 |
| 1:B:200:PHE:HD1 | 1:B:223:CYS:HG | 1.35 | 0.72 |
| 1:A:3515:GLN:NE2 | 1:A:3551:ASN:OD1 | 2.22 | 0.72 |
| 1:B:4011:PHE:HA | 1:B:4015:ASN:HB2 | 1.70 | 0.72 |
| 1:A:3144:PHE:O | 1:A:3150:ASN:ND2 | 2.22 | 0.72 |
| 1:B:1825:LEU:HD22 | 1:B:1879:VAL:HG21 | 1.70 | 0.72 |
| 1:A:1090:ARG:HB2 | 1:A:1137:ILE:HG12 | 1.70 | 0.72 |
| 1:A:2837:LEU:O | 1:A:2841:ASN:ND2 | 2.21 | 0.72 |
| 1:A:260:ILE:HA | 1:A:300:TRP:CH2 | 2.24 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1991:PRO:HG2 | 1:B:2000:ARG:HH22 | 1.55 | 0.72 |
| 1:B:2823:PHE:HD1 | 1:B:2824:LYS:HG2 | 1.53 | 0.72 |
| 1:A:4011:PHE:HA | 1:A:4015:ASN:HB2 | 1.71 | 0.72 |
| 1:A:4042:GLN:NE2 | 1:A:4046:TYR:CE2 | 2.57 | 0.71 |
| 1:B:424:LEU:O | 1:B:471:LYS:NZ | 2.22 | 0.71 |
| 1:B:3137:GLU:OE1 | 1:B:3164:TRP:NE1 | 2.22 | 0.71 |
| 1:A:228:SER:HA | 1:A:274:LEU:HD13 | 1.71 | 0.71 |
| 1:B:1892:LYS:H | 1:B:1892:LYS:HD2 | 1.55 | 0.71 |
| 1:A:1845:VAL:HA | 1:A:1848:ILE:HG22 | 1.72 | 0.71 |
| 1:A:3695:LEU:HD12 | 1:A:3698:GLU:HG2 | 1.71 | 0.71 |
| 1:B:394:GLN:HB3 | 1:B:1687:HIS:HB2 | 1.72 | 0.71 |
| 1:B:1817:GLN:NE2 | 1:B:1871:MET:SD | 2.64 | 0.71 |
| 1:B:19:LEU:HD22 | 1:B:71:LYS:HG3 | 1.73 | 0.71 |
| 1:B:3833:ARG:HB3 | 1:B:3877:LYS:HE2 | 1.73 | 0.71 |
| 1:A:1373:VAL:HG11 | 1:A:1422:LYS:HE3 | 1.74 | 0.70 |
| 1:B:2148:LYS:O | 1:B:2152:ASN:ND2 | 2.23 | 0.70 |
| 1:A:1955:VAL:HG23 | 1:A:1957:ASN:H | 1.56 | 0.70 |
| 1:B:1257:LEU:HD22 | 1:B:1337:VAL:HG11 | 1.73 | 0.70 |
| 1:A:1406:LEU:HD13 | 1:A:1415:LEU:HD21 | 1.74 | 0.70 |
| 1:B:3549:HIS:HA | 1:B:3552:LYS:HE2 | 1.72 | 0.70 |
| 1:A:762:TYR:HB3 | 1:A:765:LEU:HD22 | 1.72 | 0.69 |
| 1:A:3772:ASN:HA | 1:A:3775:LEU:HB2 | 1.73 | 0.69 |
| 1:B:990:GLN:HG2 | 1:B:2780:LEU:O | 1.90 | 0.69 |
| 1:B:1766:LEU:HG | 1:B:1778:PHE:HD2 | 1.56 | 0.69 |
| 1:B:54:GLN:HA | 1:B:57:LEU:HB3 | 1.73 | 0.69 |
| 1:B:228:SER:HA | 1:B:274:LEU:HD13 | 1.74 | 0.69 |
| 1:B:2880:CYS:HB3 | 1:B:2886:GLN:HA | 1.73 | 0.69 |
| 1:A:2887:PRO:HG2 | 1:A:3895:GLU:HG2 | 1.75 | 0.69 |
| 1:A:1257:LEU:HD22 | 1:A:1337:VAL:HG11 | 1.73 | 0.69 |
| 1:B:859:LEU:HG | 1:B:867:ASN:HD21 | 1.56 | 0.69 |
| 1:A:148:LYS:HD3 | 1:A:148:LYS:H | 1.57 | 0.69 |
| 1:A:4037:ASN:ND2 | 1:A:4066:LEU:O | 2.25 | 0.69 |
| 1:A:160:LEU:HD21 | 1:A:178:LEU:HD12 | 1.76 | 0.68 |
| 1:A:1082:PHE:CZ | 1:A:1134:LEU:HG | 2.29 | 0.68 |
| 1:B:72:SER:O | 1:B:82:ARG:NH1 | 2.26 | 0.68 |
| 1:B:323:VAL:HG13 | 1:B:369:PHE:HZ | 1.59 | 0.68 |
| 1:B:992:ILE:O | 1:B:996:THR:HG22 | 1.94 | 0.68 |
| 1:A:2290:PRO:HD3 | 1:A:2296:SER:HB3 | 1.76 | 0.68 |
| 1:B:2387:PRO:HG3 | 1:B:2418:LYS:HB3 | 1.74 | 0.68 |
| 1:A:1930:GLU:OE1 | 1:A:1937:ARG:NH2 | 2.26 | 0.68 |
| 1:A:2952:ILE:HD13 | 1:A:2975:ALA:HB2 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3949:ALA:HB1 | 1:B:3957:GLU:HG3 | 1.75 | 0.68 |
| 1:A:2140:LEU:HD21 | 1:A:2178:GLY:HA2 | 1.76 | 0.68 |
| 1:B:1896:ILE:HD13 | 1:B:1906:THR:HB | 1.74 | 0.68 |
| 1:A:3545:THR:HG22 | 1:A:3546:SER:N | 2.09 | 0.67 |
| 1:B:2290:PRO:HD3 | 1:B:2296:SER:HB3 | 1.76 | 0.67 |
| 1:A:330:ASN:HB2 | 1:A:334:HIS:CD2 | 2.29 | 0.67 |
| 1:A:3577:GLN:HG3 | 1:A:3630:ARG:HD3 | 1.76 | 0.67 |
| 1:B:339:GLN:NE2 | 1:B:343:GLU:OE2 | 2.28 | 0.67 |
| 1:B:1406:LEU:HD13 | 1:B:1415:LEU:HD21 | 1.76 | 0.67 |
| 1:B:1147:LYS:O | 1:B:1151:ARG:NH2 | 2.27 | 0.67 |
| 1:B:1398:VAL:HA | 1:B:1401:ASN:HB2 | 1.75 | 0.67 |
| 1:A:1686:LEU:HD13 | 1:A:1721:HIS:HB3 | 1.77 | 0.67 |
| 1:A:1560:TYR:OH | 1:A:1568:ASN:ND2 | 2.27 | 0.67 |
| 1:B:1440:ASP:HB2 | 1:B:1443:VAL:HG22 | 1.76 | 0.67 |
| 1:A:3775:LEU:HD11 | 1:A:3910:LEU:HD11 | 1.77 | 0.67 |
| 1:B:1828:LEU:O | 1:B:1883:ARG:NH2 | 2.20 | 0.66 |
| 1:B:1483:LEU:HD22 | 1:B:1514:LEU:HD11 | 1.76 | 0.66 |
| 1:B:3775:LEU:HD11 | 1:B:3910:LEU:HD11 | 1.77 | 0.66 |
| 1:A:3462:ARG:NH1 | 1:A:3497:SER:OG | 2.29 | 0.66 |
| 1:B:2194:LEU:HD11 | 1:B:2241:LEU:HD13 | 1.77 | 0.66 |
| 1:B:3503:VAL:HG21 | 1:B:3532:PRO:HB2 | 1.77 | 0.66 |
| 1:B:3585:PHE:HD2 | 1:B:3667:LEU:HD13 | 1.60 | 0.66 |
| 1:B:3758:LEU:HD12 | 1:B:3801:GLY:HA3 | 1.77 | 0.66 |
| 1:A:2148:LYS:O | 1:A:2152:ASN:ND2 | 2.26 | 0.66 |
| 1:A:2312:TYR:HB3 | 1:A:2315:VAL:HG12 | 1.78 | 0.66 |
| 1:B:1626:TRP:CD1 | 1:B:1671:VAL:HG12 | 2.31 | 0.66 |
| 1:A:3339:ASN:ND2 | 1:A:3422:GLN:OE1 | 2.29 | 0.66 |
| 1:B:1984:LEU:HD11 | 1:B:2139:PRO:HG2 | 1.77 | 0.66 |
| 1:B:1361:LYS:HA | 1:B:1364:CYS:HB2 | 1.78 | 0.65 |
| 1:B:272:LEU:HB3 | 1:B:315:ALA:HB2 | 1.77 | 0.65 |
| 1:A:903:PRO:HG3 | 1:A:2816:ILE:HG12 | 1.77 | 0.65 |
| 1:A:1850:VAL:O | 1:A:1870:LYS:NZ | 2.25 | 0.65 |
| 1:A:4083:GLY:HA3 | 1:A:4091:ALA:HB2 | 1.77 | 0.65 |
| 1:A:328:ALA:HA | 1:A:372:PRO:HB3 | 1.79 | 0.65 |
| 1:A:1052:SER:HB2 | 1:A:1055:ASN:HB2 | 1.77 | 0.65 |
| 1:A:4064:LEU:HD13 | 1:A:4077:TYR:HB3 | 1.76 | 0.65 |
| 1:B:1038:LYS:NZ | 1:B:1088:GLU:OE2 | 2.30 | 0.65 |
| 1:B:1750:LEU:HD13 | 1:B:1758:LEU:HB2 | 1.79 | 0.65 |
| 1:B:3946:PHE:O | 1:B:3948:SER:N | 2.27 | 0.65 |
| 1:B:1345:THR:HG21 | 1:B:1368:LEU:HD21 | 1.78 | 0.65 |
| 1:B:1750:LEU:HG | 1:B:1785:ILE:HD11 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2448:PRO:HB3 | 1:A:2498:ILE:HD13 | 1.79 | 0.64 |
| 1:B:1612:LYS:O | 1:B:1614:GLN:N | 2.29 | 0.64 |
| 1:A:178:LEU:HB3 | 1:A:196:LEU:HD11 | 1.79 | 0.64 |
| 1:A:2286:PRO:HB3 | 1:A:2329:TYR:CE2 | 2.32 | 0.64 |
| 1:A:2458:VAL:HG11 | 1:A:2476:ILE:HD11 | 1.78 | 0.64 |
| 1:A:2856:SER:HA | 1:A:2888:VAL:HG11 | 1.79 | 0.64 |
| 1:B:363:ILE:HG23 | 1:B:388:LEU:HD11 | 1.79 | 0.64 |
| 1:B:1108:MET:HG3 | 1:B:1131:ILE:HG21 | 1.80 | 0.64 |
| 1:B:1969:GLU:HB3 | 1:B:1977:ILE:HG13 | 1.79 | 0.64 |
| 1:A:2181:GLY:O | 1:A:2183:HIS:N | 2.30 | 0.64 |
| 1:A:2409:THR:O | 1:A:2411:LEU:N | 2.31 | 0.64 |
| 1:B:2952:ILE:HD13 | 1:B:2975:ALA:HB2 | 1.80 | 0.64 |
| 1:B:3880:ALA:HB1 | 1:B:3969:ASN:HD22 | 1.62 | 0.64 |
| 1:A:160:LEU:O | 1:A:164:LYS:NZ | 2.22 | 0.64 |
| 1:B:66:LEU:HD11 | 1:B:110:THR:HG21 | 1.79 | 0.64 |
| 1:B:572:VAL:HG23 | 1:B:626:LEU:HD11 | 1.79 | 0.64 |
| 1:B:704:PHE:CE1 | 1:B:741:ILE:HG12 | 2.33 | 0.64 |
| 1:B:2011:ALA:HA | 1:B:2195:SER:HA | 1.80 | 0.64 |
| 1:A:2148:LYS:HA | 1:A:2151:ILE:HD12 | 1.80 | 0.63 |
| 1:B:3005:LEU:HA | 1:B:3254:LEU:HD13 | 1.80 | 0.63 |
| 1:B:35:ILE:HD13 | 1:B:85:ILE:HG13 | 1.79 | 0.63 |
| 1:B:373:CYS:SG | 1:B:376:ILE:HG21 | 2.37 | 0.63 |
| 1:B:3468:LEU:HA | 1:B:3471:ILE:HG22 | 1.79 | 0.63 |
| 1:A:3137:GLU:OE1 | 1:A:3164:TRP:NE1 | 2.32 | 0.63 |
| 1:B:1845:VAL:HA | 1:B:1848:ILE:HG22 | 1.81 | 0.63 |
| 1:B:1877:LEU:O | 1:B:1881:TYR:HB2 | 1.99 | 0.63 |
| 1:B:2133:LEU:HB2 | 1:B:2146:LEU:HD23 | 1.81 | 0.63 |
| 1:A:3587:ASP:OD2 | 1:A:3733:ARG:NH1 | 2.32 | 0.63 |
| 1:B:1623:LEU:HD22 | 1:B:1671:VAL:HG11 | 1.81 | 0.63 |
| 1:B:2148:LYS:HA | 1:B:2151:ILE:HD12 | 1.80 | 0.63 |
| 1:B:359:LEU:O | 1:B:363:ILE:HG12 | 1.99 | 0.63 |
| 1:B:3328:ILE:HD11 | 1:B:3412:ALA:HB2 | 1.81 | 0.63 |
| 1:A:93:LEU:HD12 | 1:A:100:ILE:HD13 | 1.81 | 0.62 |
| 1:B:1525:CYS:SG | 1:B:1574:ASN:ND2 | 2.70 | 0.62 |
| 1:A:1825:LEU:O | 1:A:1829:TRP:HB2 | 1.98 | 0.62 |
| 1:B:3027:LEU:HG | 1:B:3067:LYS:HD2 | 1.81 | 0.62 |
| 1:A:3813:LYS:HB2 | 1:A:3925:LEU:HB3 | 1.81 | 0.62 |
| 1:B:3879:PRO:O | 1:B:3966:GLN:NE2 | 2.31 | 0.62 |
| 1:A:3468:LEU:HA | 1:A:3471:ILE:HG22 | 1.80 | 0.62 |
| 1:B:148:LYS:HB3 | 1:B:151:GLU:HB2 | 1.80 | 0.62 |
| 1:A:1582:LEU:HG | 1:A:1593:VAL:HG23 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1992:VAL:HG12 | 1:B:2183:HIS:CD2 | 2.35 | 0.62 |
| 1:A:1346:THR:HG22 | 1:A:1402:LEU:HA | 1.82 | 0.62 |
| 1:A:2375:ALA:HB3 | 1:A:2404:ARG:HG2 | 1.82 | 0.62 |
| 1:B:1658:SER:HB3 | 1:B:1661:PHE:HE1 | 1.64 | 0.62 |
| 1:B:2085:MET:HA | 1:B:2089:ASN:HB2 | 1.82 | 0.62 |
| 1:B:451:PRO:O | 1:B:452:LYS:HG2 | 1.99 | 0.62 |
| 1:B:704:PHE:HE1 | 1:B:741:ILE:HG12 | 1.64 | 0.62 |
| 1:B:1612:LYS:C | 1:B:1614:GLN:H | 2.02 | 0.62 |
| 1:B:4117:LEU:HB3 | 1:B:4126:PRO:HB2 | 1.80 | 0.62 |
| 1:B:2458:VAL:HG11 | 1:B:2476:ILE:HD11 | 1.81 | 0.61 |
| 1:B:1820:VAL:O | 1:B:1825:LEU:HG | 2.00 | 0.61 |
| 1:A:1833:LEU:HG | 1:A:1835:ALA:H | 1.65 | 0.61 |
| 1:B:2538:ARG:NE | 1:B:2565:MET:SD | 2.73 | 0.61 |
| 1:A:1181:THR:HG22 | 1:A:1184:ARG:HH12 | 1.66 | 0.61 |
| 1:B:16:GLN:NE2 | 1:B:62:ASP:O | 2.33 | 0.61 |
| 1:A:1166:LEU:H | 1:A:1166:LEU:HD12 | 1.65 | 0.61 |
| 1:A:1106:ILE:HD11 | 1:A:1155:ARG:H | 1.65 | 0.61 |
| 1:B:1992:VAL:HG23 | 1:B:1993:GLU:H | 1.65 | 0.61 |
| 1:B:3630:ARG:O | 1:B:3633:ILE:HG12 | 2.01 | 0.61 |
| 1:B:333:MET:SD | 1:B:333:MET:N | 2.72 | 0.61 |
| 1:B:1121:LEU:HD22 | 1:B:1123:THR:HG23 | 1.81 | 0.61 |
| 1:A:1448:LEU:HD23 | 1:A:1510:LEU:HD21 | 1.81 | 0.61 |
| 1:B:770:LEU:HD23 | 1:B:854:ARG:HD2 | 1.82 | 0.61 |
| 1:B:1143:VAL:HA | 1:B:1197:LEU:HD21 | 1.82 | 0.61 |
| 1:A:3174:ASP:O | 1:A:3249:GLN:NE2 | 2.30 | 0.61 |
| 1:A:4064:LEU:O | 1:A:4068:HIS:HB2 | 2.01 | 0.61 |
| 1:A:1533:LEU:HD22 | 1:A:1589:ASN:HB2 | 1.83 | 0.60 |
| 1:B:376:ILE:HG13 | 1:B:377:ASN:H | 1.65 | 0.60 |
| 1:A:1733:THR:HB | 1:A:1736:PHE:H | 1.66 | 0.60 |
| 1:A:2588:GLU:HG3 | 1:A:2785:ILE:HD11 | 1.83 | 0.60 |
| 1:A:2940:ARG:HG3 | 1:A:2957:LEU:HD22 | 1.81 | 0.60 |
| 1:B:864:GLY:HA2 | 1:B:867:ASN:HB2 | 1.83 | 0.60 |
| 1:A:1579:VAL:HG21 | 1:A:1621:THR:HG21 | 1.82 | 0.60 |
| 1:B:12:LEU:HD23 | 1:B:64:GLY:HA2 | 1.83 | 0.60 |
| 1:B:358:GLU:O | 1:B:361:ILE:HG12 | 2.01 | 0.60 |
| 1:B:2178:GLY:O | 1:B:2182:ILE:HB | 2.00 | 0.60 |
| 1:A:3955:VAL:HG11 | 1:A:4121:TRP:CE3 | 2.37 | 0.60 |
| 1:B:1425:ALA:O | 1:B:1429:GLU:HG2 | 2.01 | 0.60 |
| 1:B:394:GLN:HE22 | 1:B:1688:LEU:HD23 | 1.67 | 0.60 |
| 1:B:3031:TRP:HZ2 | 1:B:3068:ALA:HB1 | 1.66 | 0.60 |
| 1:A:704:PHE:CE1 | 1:A:741:ILE:HG12 | 2.37 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1212:LEU:HD13 | 1:B:1220:LEU:HD22 | 1.84 | 0.60 |
| 1:B:2234:ASN:HA | 1:B:2237:ILE:HD12 | 1.83 | 0.60 |
| 1:A:300:TRP:HE3 | 1:A:308:LEU:HD21 | 1.67 | 0.60 |
| 1:A:647:TYR:HD1 | 1:A:703:CYS:HB3 | 1.67 | 0.60 |
| 1:A:2546:TYR:CE2 | 1:A:2548:PRO:HB3 | 2.36 | 0.60 |
| 1:A:2575:PRO:HB3 | 1:A:2787:HIS:NE2 | 2.17 | 0.60 |
| 1:A:2841:ASN:O | 1:A:2845:ASN:ND2 | 2.29 | 0.60 |
| 1:B:4058:VAL:HG21 | 1:B:4095:GLU:HB3 | 1.84 | 0.60 |
| 1:A:321:LYS:HA | 1:A:368:LEU:HD21 | 1.83 | 0.59 |
| 1:A:1574:ASN:HB3 | 1:A:1577:LEU:HD21 | 1.83 | 0.59 |
| 1:B:3079:GLU:HB2 | 1:B:3102:TYR:HE1 | 1.67 | 0.59 |
| 1:B:3842:TRP:HH2 | 1:B:3867:THR:HG22 | 1.66 | 0.59 |
| 1:A:54:GLN:HA | 1:A:57:LEU:HB3 | 1.85 | 0.59 |
| 1:A:1892:LYS:H | 1:A:1892:LYS:HD3 | 1.67 | 0.59 |
| 1:B:3733:ARG:NH2 | 1:B:3755:GLY:O | 2.35 | 0.59 |
| 1:B:3028:ASN:HA | 1:B:3031:TRP:HD1 | 1.66 | 0.59 |
| 1:A:1255:CYS:SG | 1:A:3695:LEU:HD23 | 2.42 | 0.59 |
| 1:A:1676:ILE:O | 1:A:1680:ALA:CB | 2.50 | 0.59 |
| 1:A:3309:GLU:HG2 | 1:A:3310:ASN:H | 1.66 | 0.59 |
| 1:A:3789:ARG:HG2 | 1:A:3938:ILE:HD12 | 1.82 | 0.59 |
| 1:B:903:PRO:HG3 | 1:B:2816:ILE:HG12 | 1.84 | 0.59 |
| 1:B:1302:ALA:HA | 1:B:1382:ILE:HA | 1.83 | 0.59 |
| 1:B:1828:LEU:HB3 | 1:B:1879:VAL:HG11 | 1.84 | 0.59 |
| 1:B:3484:THR:HG22 | 1:B:3513:ALA:HA | 1.83 | 0.59 |
| 1:A:487:LEU:HD21 | 1:A:568:PHE:HE1 | 1.68 | 0.59 |
| 1:A:3696:ARG:HD2 | 1:A:3697:ASN:H | 1.67 | 0.59 |
| 1:B:156:PHE:HA | 1:B:159:GLU:HB2 | 1.85 | 0.59 |
| 1:B:473:PRO:HA | 1:B:476:ARG:HG2 | 1.83 | 0.59 |
| 1:A:366:TYR:CE2 | 1:A:384:MET:HG2 | 2.37 | 0.59 |
| 1:A:2373:PRO:HA | 1:A:2404:ARG:HE | 1.67 | 0.59 |
| 1:B:166:ILE:HG22 | 1:B:168:ASP:H | 1.68 | 0.59 |
| 1:B:1612:LYS:HG3 | 1:B:1613:HIS:H | 1.68 | 0.59 |
| 1:A:1686:LEU:H | 1:A:1686:LEU:HD23 | 1.68 | 0.59 |
| 1:A:3795:PRO:HA | 1:A:3801:GLY:HA2 | 1.85 | 0.59 |
| 1:A:572:VAL:HG23 | 1:A:626:LEU:HD21 | 1.83 | 0.59 |
| 1:A:260:ILE:CG2 | 1:A:300:TRP:CZ2 | 2.81 | 0.58 |
| 1:A:1743:MET:HG3 | 1:A:1774:MET:HE1 | 1.85 | 0.58 |
| 1:B:1138:ILE:HG21 | 1:B:1194:PHE:CE1 | 2.39 | 0.58 |
| 1:B:1881:TYR:CE1 | 1:B:1889:VAL:HG21 | 2.38 | 0.58 |
| 1:B:3130:GLN:HB3 | 1:B:3178:ILE:HG12 | 1.84 | 0.58 |
| 1:A:1483:LEU:HD22 | 1:A:1514:LEU:HD11 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3110:PHE:HD1 | 1:A:3128:LYS:HD2 | 1.68 | 0.58 |
| 1:B:1362:ASP:O | 1:B:1367:HIS:ND1 | 2.21 | 0.58 |
| 1:A:1783:ARG:HB3 | 1:A:1830:HIS:CD2 | 2.38 | 0.58 |
| 1:B:1427:SER:HA | 1:B:1430:GLU:HG2 | 1.84 | 0.58 |
| 1:B:1582:LEU:HG | 1:B:1593:VAL:HG23 | 1.86 | 0.58 |
| 1:A:1675:TYR:O | 1:A:1679:LEU:HD23 | 2.04 | 0.58 |
| 1:A:2249:LEU:O | 1:A:2251:ILE:N | 2.36 | 0.58 |
| 1:A:3121:LEU:O | 1:A:3124:SER:OG | 2.21 | 0.58 |
| 1:A:3962:ARG:NH1 | 1:A:4128:MET:O | 2.35 | 0.58 |
| 1:B:3514:VAL:HG23 | 1:B:3517:SER:HB2 | 1.85 | 0.58 |
| 1:A:260:ILE:HG22 | 1:A:300:TRP:CE2 | 2.39 | 0.58 |
| 1:A:670:LEU:HA | 1:A:673:THR:HG22 | 1.85 | 0.58 |
| 1:A:2522:ARG:HG3 | 1:A:2561:PHE:HE1 | 1.68 | 0.58 |
| 1:A:3630:ARG:O | 1:A:3633:ILE:HG12 | 2.02 | 0.58 |
| 1:B:1801:VAL:HB | 1:B:1824:LEU:HD12 | 1.86 | 0.58 |
| 1:A:4005:PHE:O | 1:A:4011:PHE:HZ | 1.86 | 0.58 |
| 1:A:3587:ASP:HB3 | 1:A:4022:LYS:HE2 | 1.85 | 0.58 |
| 1:A:4042:GLN:HE21 | 1:A:4046:TYR:HE2 | 1.50 | 0.58 |
| 1:B:859:LEU:O | 1:B:867:ASN:ND2 | 2.36 | 0.58 |
| 1:B:1831:CYS:HA | 1:B:1883:ARG:HH12 | 1.69 | 0.58 |
| 1:B:2490:GLU:OE1 | 1:B:2496:GLN:NE2 | 2.37 | 0.58 |
| 1:B:3421:ASP:OD1 | 1:B:3467:ARG:NE | 2.37 | 0.58 |
| 1:A:260:ILE:HA | 1:A:300:TRP:HH2 | 1.67 | 0.58 |
| 1:A:2234:ASN:HA | 1:A:2237:ILE:HD12 | 1.86 | 0.58 |
| 1:B:2201:THR:HB | 1:B:2205:VAL:H | 1.68 | 0.58 |
| 1:B:3407:ALA:HA | 1:B:3410:ILE:HG12 | 1.86 | 0.58 |
| 1:B:4055:ASN:HB2 | 1:B:4095:GLU:HA | 1.86 | 0.58 |
| 1:A:3696:ARG:HD2 | 1:A:3697:ASN:N | 2.18 | 0.57 |
| 1:B:2459:VAL:HG21 | 1:B:2501:LEU:HD11 | 1.86 | 0.57 |
| 1:B:3462:ARG:HG3 | 1:B:3494:GLN:HB3 | 1.85 | 0.57 |
| 1:A:2255:LEU:HD23 | 1:A:2256:ILE:H | 1.69 | 0.57 |
| 1:B:2150:VAL:HG13 | 1:B:2157:PHE:CD2 | 2.39 | 0.57 |
| 1:B:1279:LEU:H | 1:B:1279:LEU:HD23 | 1.69 | 0.57 |
| 1:B:1930:GLU:HB3 | 1:B:1937:ARG:HH12 | 1.68 | 0.57 |
| 1:A:25:CYS:SG | 1:A:26:GLY:N | 2.77 | 0.57 |
| 1:A:724:GLU:HG2 | 1:A:725:LEU:N | 2.18 | 0.57 |
| 1:A:1023:SER:HA | 1:A:1026:ARG:HE | 1.69 | 0.57 |
| 1:A:1976:LEU:HD22 | 1:A:1979:GLU:HG3 | 1.87 | 0.57 |
| 1:A:3549:HIS:HA | 1:A:3552:LYS:HE2 | 1.85 | 0.57 |
| 1:B:1605:PHE:CE1 | 1:B:1608:ARG:HD3 | 2.40 | 0.57 |
| 1:A:1103:ALA:HB1 | 1:A:1106:ILE:HB | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2294:ILE:HG22 | 1:A:2295:GLN:H | 1.70 | 0.57 |
| 1:A:3946:PHE:O | 1:A:3948:SER:N | 2.30 | 0.57 |
| 1:B:1619:ALA:HB1 | 1:B:1652:ILE:HG23 | 1.85 | 0.57 |
| 1:A:892:LEU:HB3 | 1:A:940:PHE:HE2 | 1.70 | 0.57 |
| 1:B:2119:PRO:N | 1:B:2163:HIS:HE2 | 2.02 | 0.57 |
| 1:B:3789:ARG:HG2 | 1:B:3938:ILE:HD12 | 1.85 | 0.57 |
| 1:A:760:LEU:HD13 | 1:A:760:LEU:O | 2.05 | 0.57 |
| 1:A:2084:GLU:O | 1:A:2089:ASN:ND2 | 2.38 | 0.57 |
| 1:A:2610:UNK:O | 1:A:2614:UNK:CB | 2.52 | 0.57 |
| 1:A:2894:GLU:OE2 | 1:A:3901:ARG:NH2 | 2.37 | 0.57 |
| 1:B:1298:LEU:HB3 | 1:B:1367:HIS:HB3 | 1.86 | 0.57 |
| 1:B:1837:ARG:HH11 | 1:B:1884:LEU:HD21 | 1.69 | 0.57 |
| 1:B:3698:GLU:HG3 | 1:B:3718:ARG:HD2 | 1.87 | 0.57 |
| 1:A:1212:LEU:HD13 | 1:A:1220:LEU:HD22 | 1.86 | 0.57 |
| 1:B:583:LEU:HD12 | 1:B:611:ASN:ND2 | 2.20 | 0.57 |
| 1:A:3640:PHE:CZ | 1:A:3670:MET:HG3 | 2.39 | 0.57 |
| 1:A:108:LYS:HE3 | 1:A:152:LEU:HD22 | 1.87 | 0.57 |
| 1:A:2591:ILE:HD13 | 1:A:2796:ALA:HB2 | 1.86 | 0.57 |
| 1:B:2528:GLU:O | 1:B:2529:THR:HG22 | 2.05 | 0.57 |
| 1:B:3577:GLN:HG3 | 1:B:3630:ARG:HD3 | 1.85 | 0.57 |
| 1:A:662:LEU:HD23 | 1:A:662:LEU:H | 1.70 | 0.56 |
| 1:A:1990:PHE:CZ | 1:A:2144:LEU:HD21 | 2.40 | 0.56 |
| 1:A:3590:ASN:HA | 1:A:3593:ARG:HG2 | 1.87 | 0.56 |
| 1:A:3820:MET:HB3 | 1:A:3824:GLU:HG3 | 1.86 | 0.56 |
| 1:B:3008:TRP:HB2 | 1:B:3051:LEU:HD13 | 1.87 | 0.56 |
| 1:B:3842:TRP:CH2 | 1:B:3867:THR:HG22 | 2.40 | 0.56 |
| 1:A:1076:LEU:HB2 | 1:A:1123:THR:HG22 | 1.88 | 0.56 |
| 1:A:2251:ILE:HD11 | 1:A:2288:TYR:CZ | 2.40 | 0.56 |
| 1:A:2591:ILE:HD11 | 1:A:2792:THR:HB | 1.88 | 0.56 |
| 1:A:3244:ASP:OD1 | 1:A:3247:ARG:NH1 | 2.37 | 0.56 |
| 1:A:3327:ASN:HB3 | 1:A:3384:HIS:O | 2.06 | 0.56 |
| 1:A:3662:ILE:HA | 1:A:3665:MET:HE2 | 1.86 | 0.56 |
| 1:B:414:LEU:HD12 | 1:B:464:VAL:HG21 | 1.86 | 0.56 |
| 1:B:2359:LYS:H | 1:B:2359:LYS:HD2 | 1.71 | 0.56 |
| 1:B:2797:VAL:HG13 | 1:B:2804:ILE:HG21 | 1.87 | 0.56 |
| 1:B:2877:SER:HB2 | 1:B:2925:GLU:HB3 | 1.86 | 0.56 |
| 1:B:3480:LEU:HD11 | 1:B:3510:GLN:OE1 | 2.05 | 0.56 |
| 1:B:3617:LEU:HD13 | 1:B:3636:PHE:CD2 | 2.41 | 0.56 |
| 1:B:3630:ARG:HG2 | 1:B:3632:PHE:H | 1.70 | 0.56 |
| 1:A:2528:GLU:O | 1:A:2529:THR:HG22 | 2.06 | 0.56 |
| 1:A:2826:LEU:HA | 1:A:2829:LYS:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2923:TRP:CE3 | 1:A:2946:GLU:HG3 | 2.41 | 0.56 |
| 1:B:3588:TRP:HH2 | 1:B:3651:LEU:HD21 | 1.70 | 0.56 |
| 1:B:3631:LYS:HD3 | 1:B:3682:GLU:HB3 | 1.87 | 0.56 |
| 1:A:2083:LEU:H | 1:A:2083:LEU:HD12 | 1.70 | 0.56 |
| 1:A:3514:VAL:HG23 | 1:A:3517:SER:HB2 | 1.85 | 0.56 |
| 1:A:3918:LEU:O | 1:A:3920:ILE:HG13 | 2.05 | 0.56 |
| 1:B:181:LEU:HB3 | 1:B:189:MET:HE1 | 1.88 | 0.56 |
| 1:B:2409:THR:HG23 | 1:B:2410:GLU:H | 1.71 | 0.56 |
| 1:A:1504:ASP:HB3 | 1:A:1507:CYS:HB3 | 1.87 | 0.56 |
| 1:B:2225:HIS:O | 1:B:2227:LYS:N | 2.39 | 0.56 |
| 1:B:2940:ARG:HG3 | 1:B:2957:LEU:HD22 | 1.86 | 0.56 |
| 1:B:3918:LEU:O | 1:B:3920:ILE:HG13 | 2.06 | 0.56 |
| 1:A:724:GLU:HG3 | 1:A:2743:UNK:O | 2.06 | 0.56 |
| 1:A:354:SER:CB | 1:A:358:GLU:HB2 | 2.36 | 0.56 |
| 1:A:2137:ILE:HG13 | 1:A:2138:VAL:H | 1.71 | 0.56 |
| 1:A:385:TYR:CZ | 1:A:389:ILE:HD11 | 2.41 | 0.56 |
| 1:A:704:PHE:HE1 | 1:A:741:ILE:HG12 | 1.71 | 0.56 |
| 1:A:2446:LEU:O | 1:A:2451:LEU:HB2 | 2.06 | 0.56 |
| 1:A:3278:GLN:HG2 | 1:A:3329:LEU:HD21 | 1.87 | 0.56 |
| 1:A:242:PRO:HA | 1:A:245:SER:HB3 | 1.88 | 0.55 |
| 1:A:2131:GLY:O | 1:A:2135:ASN:ND2 | 2.38 | 0.55 |
| 1:B:996:THR:OG1 | 1:B:1040:SER:HA | 2.06 | 0.55 |
| 1:B:1155:ARG:HH21 | 1:B:3689:ASP:HB3 | 1.70 | 0.55 |
| 1:B:1686:LEU:HD11 | 1:B:1721:HIS:CB | 2.36 | 0.55 |
| 1:B:2824:LYS:O | 1:B:2829:LYS:HG3 | 2.05 | 0.55 |
| 1:B:3297:VAL:HA | 1:B:3300:VAL:HG22 | 1.87 | 0.55 |
| 1:A:3138:ILE:HG12 | 1:A:3189:PHE:HZ | 1.71 | 0.55 |
| 1:A:3285:HIS:NE2 | 1:A:3333:THR:OG1 | 2.35 | 0.55 |
| 1:A:3463:LEU:HD13 | 1:A:3498:TRP:HZ2 | 1.71 | 0.55 |
| 1:B:864:GLY:HA2 | 1:B:867:ASN:CB | 2.36 | 0.55 |
| 1:B:1271:ILE:HD13 | 1:B:1348:LEU:HD13 | 1.89 | 0.55 |
| 1:B:1993:GLU:OE2 | 1:B:2230:VAL:HB | 2.06 | 0.55 |
| 1:B:2480:ILE:O | 1:B:2484:TYR:HB2 | 2.06 | 0.55 |
| 1:A:4006:VAL:HG21 | 1:A:4044:ILE:HG12 | 1.88 | 0.55 |
| 1:B:1096:VAL:HB | 1:B:1101:PHE:HE2 | 1.69 | 0.55 |
| 1:B:1563:PHE:HB2 | 1:B:1567:ILE:HG13 | 1.88 | 0.55 |
| 1:B:2519:LEU:HD22 | 1:B:2606:UNK:O | 2.07 | 0.55 |
| 1:A:305:ASN:HB2 | 1:A:308:LEU:HB3 | 1.87 | 0.55 |
| 1:A:1750:LEU:HD13 | 1:A:1758:LEU:HB2 | 1.87 | 0.55 |
| 1:B:1752:LEU:HD12 | 1:B:1753:SER:N | 2.21 | 0.55 |
| 1:A:2088:LEU:HD11 | 1:A:2144:LEU:HD23 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2547:SER:O | 1:B:2549:LYS:N | 2.40 | 0.55 |
| 1:B:3244:ASP:OD1 | 1:B:3247:ARG:NH1 | 2.39 | 0.55 |
| 1:A:478:CYS:HA | 1:A:481:THR:HG22 | 1.88 | 0.55 |
| 1:A:1037:LEU:O | 1:A:1040:SER:OG | 2.21 | 0.55 |
| 1:A:2823:PHE:HD1 | 1:A:2824:LYS:HG2 | 1.71 | 0.55 |
| 1:A:2978:LYS:HG3 | 1:A:2981:TRP:CD2 | 2.41 | 0.55 |
| 1:B:446:PHE:CZ | 1:B:454:GLN:HG2 | 2.41 | 0.55 |
| 1:A:3727:THR:OG1 | 1:A:3737:ARG:HB3 | 2.07 | 0.55 |
| 1:B:78:PHE:O | 1:B:82:ARG:NH1 | 2.39 | 0.55 |
| 1:B:2949:THR:OG1 | 1:B:2990:GLU:OE2 | 2.23 | 0.55 |
| 1:A:1769:GLU:O | 1:A:1822:ARG:NH1 | 2.40 | 0.55 |
| 1:B:483:VAL:HG23 | 1:B:571:SER:HB2 | 1.89 | 0.55 |
| 1:A:35:ILE:HD13 | 1:A:85:ILE:HG13 | 1.89 | 0.55 |
| 1:B:1040:SER:O | 1:B:1049:GLN:NE2 | 2.39 | 0.55 |
| 1:A:2246:LYS:NZ | 1:A:2284:ASP:OD2 | 2.38 | 0.55 |
| 1:A:2590:THR:HG22 | 1:A:2591:ILE:H | 1.72 | 0.55 |
| 1:A:3888:VAL:HA | 1:A:3891:SER:HB2 | 1.88 | 0.55 |
| 1:B:801:LYS:HA | 1:B:3115:SER:HB2 | 1.88 | 0.55 |
| 1:B:1538:LEU:O | 1:B:1553:PHE:N | 2.40 | 0.55 |
| 1:B:1802:TYR:CZ | 1:B:1843:ILE:HD11 | 2.42 | 0.55 |
| 1:B:2856:SER:HA | 1:B:2888:VAL:HG11 | 1.89 | 0.55 |
| 1:B:3121:LEU:O | 1:B:3124:SER:OG | 2.25 | 0.55 |
| 1:A:1298:LEU:HB3 | 1:A:1367:HIS:HB3 | 1.88 | 0.54 |
| 1:A:1668:PHE:HZ | 1:A:1702:LEU:HD22 | 1.72 | 0.54 |
| 1:B:2133:LEU:HD13 | 1:B:2146:LEU:HB3 | 1.88 | 0.54 |
| 1:A:351:ASN:OD1 | 1:A:352:VAL:N | 2.39 | 0.54 |
| 1:A:1881:TYR:CE1 | 1:A:1951:VAL:HG23 | 2.42 | 0.54 |
| 1:A:3522:THR:HG23 | 1:A:3562:LEU:HD13 | 1.89 | 0.54 |
| 1:B:1090:ARG:HH11 | 1:B:1137:ILE:HD13 | 1.71 | 0.54 |
| 1:B:2255:LEU:HD23 | 1:B:2256:ILE:H | 1.71 | 0.54 |
| 1:A:3527:GLN:HG2 | 1:A:3700:GLU:HB3 | 1.89 | 0.54 |
| 1:A:3760:GLN:OE1 | 1:A:4019:LYS:NZ | 2.27 | 0.54 |
| 1:B:201:LEU:HD21 | 1:B:248:ILE:HG12 | 1.88 | 0.54 |
| 1:B:583:LEU:HD12 | 1:B:611:ASN:HD22 | 1.72 | 0.54 |
| 1:A:359:LEU:O | 1:A:363:ILE:HG12 | 2.08 | 0.54 |
| 1:A:1147:LYS:O | 1:A:1151:ARG:NH2 | 2.41 | 0.54 |
| 1:A:3811:THR:OG1 | 1:A:3814:ASP:OD1 | 2.25 | 0.54 |
| 1:B:1104:LEU:HD12 | 1:B:1134:LEU:HD23 | 1.89 | 0.54 |
| 1:B:1368:LEU:HA | 1:B:1371:VAL:HG22 | 1.88 | 0.54 |
| 1:B:3692:VAL:HA | 1:B:3696:ARG:NH1 | 2.22 | 0.54 |
| 1:A:651:TYR:CE1 | 1:A:655:LEU:HD21 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2931:ARG:NH2 | 1:A:3043:TYR:OH | 2.41 | 0.54 |
| 1:B:25:CYS:SG | 1:B:26:GLY:N | 2.81 | 0.54 |
| 1:B:1367:HIS:O | 1:B:1371:VAL:HG13 | 2.08 | 0.54 |
| 1:B:2560:ASN:ND2 | 1:B:2799:GLN:OE1 | 2.35 | 0.54 |
| 1:B:2584:CYS:SG | 1:B:2783:ILE:HG12 | 2.48 | 0.54 |
| 1:A:1228:GLY:HA3 | 1:A:1259:LEU:HD13 | 1.89 | 0.54 |
| 1:A:2614:UNK:HA | 1:A:2795:GLN:OE1 | 2.08 | 0.54 |
| 1:A:3422:GLN:HE22 | 1:A:3423:GLN:HE21 | 1.55 | 0.54 |
| 1:A:4117:LEU:HB3 | 1:A:4126:PRO:HB2 | 1.90 | 0.54 |
| 1:B:334:HIS:HB3 | 1:B:337:LYS:HD2 | 1.89 | 0.54 |
| 1:B:522:PRO:HB3 | 1:B:526:ASP:CG | 2.28 | 0.54 |
| 1:B:1206:LEU:O | 1:B:1210:ASP:HB2 | 2.08 | 0.54 |
| 1:B:2140:LEU:HD21 | 1:B:2178:GLY:HA2 | 1.90 | 0.54 |
| 1:A:12:LEU:HD21 | 1:A:58:VAL:HG12 | 1.89 | 0.54 |
| 1:A:1760:GLU:O | 1:A:1764:GLU:HG2 | 2.07 | 0.54 |
| 1:A:1896:ILE:HG22 | 1:A:1911:LEU:H | 1.71 | 0.54 |
| 1:B:346:TYR:HA | 1:B:349:ILE:HG22 | 1.89 | 0.54 |
| 1:B:1967:PHE:CE1 | 1:B:2129:LEU:HD11 | 2.41 | 0.54 |
| 1:B:2409:THR:O | 1:B:2411:LEU:N | 2.40 | 0.54 |
| 1:B:3443:PRO:HA | 1:B:3471:ILE:HD11 | 1.89 | 0.54 |
| 1:A:201:LEU:HD21 | 1:A:248:ILE:HG12 | 1.88 | 0.54 |
| 1:A:1101:PHE:CE1 | 1:A:1138:ILE:HG12 | 2.43 | 0.54 |
| 1:B:1802:TYR:CE1 | 1:B:1843:ILE:HD11 | 2.43 | 0.54 |
| 1:B:2582:SER:HB2 | 1:B:2781:PRO:HD2 | 1.90 | 0.54 |
| 1:A:3949:ALA:HB1 | 1:A:3957:GLU:HG3 | 1.89 | 0.54 |
| 1:B:860:GLY:HA3 | 1:B:3136:THR:OG1 | 2.08 | 0.54 |
| 1:B:1504:ASP:HB3 | 1:B:1507:CYS:HB3 | 1.89 | 0.54 |
| 1:B:1881:TYR:CE1 | 1:B:1951:VAL:HG23 | 2.43 | 0.54 |
| 1:A:2165:LEU:HD21 | 1:A:2208:ASP:OD2 | 2.08 | 0.54 |
| 1:B:204:LEU:O | 1:B:208:MET:HB2 | 2.08 | 0.54 |
| 1:B:662:LEU:H | 1:B:662:LEU:HD23 | 1.73 | 0.54 |
| 1:A:860:GLY:HA2 | 1:A:3132:VAL:HG23 | 1.89 | 0.53 |
| 1:A:2091:HIS:O | 1:A:2092:GLU:HG2 | 2.08 | 0.53 |
| 1:A:2188:GLU:O | 1:A:2192:THR:HG22 | 2.08 | 0.53 |
| 1:B:645:TRP:O | 1:B:649:PHE:HB2 | 2.08 | 0.53 |
| 1:A:2996:LEU:HD13 | 1:A:3039:THR:HB | 1.90 | 0.53 |
| 1:B:1575:LEU:HD23 | 1:B:1617:LYS:HG2 | 1.91 | 0.53 |
| 1:B:1758:LEU:O | 1:B:1762:MET:HB2 | 2.08 | 0.53 |
| 1:B:2546:TYR:CE2 | 1:B:2548:PRO:HB3 | 2.43 | 0.53 |
| 1:B:3133:GLN:O | 1:B:3137:GLU:HG2 | 2.08 | 0.53 |
| 1:A:1090:ARG:HH11 | 1:A:1137:ILE:HD13 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1633:TRP:CZ2 | 1:A:1674:THR:HG22 | 2.44 | 0.53 |
| 1:A:2464:HIS:ND1 | 1:A:2465:PRO:O | 2.41 | 0.53 |
| 1:A:3057:ALA:C | 1:A:3059:GLN:H | 2.12 | 0.53 |
| 1:B:464:VAL:O | 1:B:468:LEU:HD23 | 2.09 | 0.53 |
| 1:B:1825:LEU:HD11 | 1:B:1875:LYS:HB3 | 1.90 | 0.53 |
| 1:B:2190:VAL:HA | 1:B:2193:ILE:HG22 | 1.90 | 0.53 |
| 1:B:2234:ASN:O | 1:B:2238:ILE:HG13 | 2.08 | 0.53 |
| 1:A:1089:PHE:CE1 | 1:A:1096:VAL:HA | 2.44 | 0.53 |
| 1:A:3243:ILE:HD13 | 1:A:3259:LEU:HD13 | 1.91 | 0.53 |
| 1:A:3328:ILE:HD11 | 1:A:3412:ALA:HB2 | 1.91 | 0.53 |
| 1:B:859:LEU:HD21 | 1:B:870:LEU:HD13 | 1.91 | 0.53 |
| 1:B:1153:LEU:HD12 | 1:B:1154:PRO:HD2 | 1.90 | 0.53 |
| 1:B:1291:LEU:HD12 | 1:B:1291:LEU:H | 1.74 | 0.53 |
| 1:B:1503:LEU:HD12 | 1:B:1508:LYS:HE2 | 1.89 | 0.53 |
| 1:B:2894:GLU:OE2 | 1:B:3901:ARG:NH2 | 2.31 | 0.53 |
| 1:A:544:ILE:HG13 | 1:A:545:LEU:HG | 1.90 | 0.53 |
| 1:A:1718:ILE:HG23 | 1:A:1722:PHE:CD2 | 2.44 | 0.53 |
| 1:A:2877:SER:HB2 | 1:A:2925:GLU:HB3 | 1.91 | 0.53 |
| 1:A:3411:ASP:N | 1:A:3411:ASP:OD1 | 2.41 | 0.53 |
| 1:B:8:VAL:HG12 | 1:B:9:ARG:H | 1.73 | 0.53 |
| 1:B:1195:VAL:HG23 | 1:B:1196:PRO:HD3 | 1.89 | 0.53 |
| 1:B:1854:ARG:O | 1:B:1866:GLN:NE2 | 2.41 | 0.53 |
| 1:A:418:ALA:HB2 | 1:A:464:VAL:HG23 | 1.91 | 0.53 |
| 1:A:451:PRO:O | 1:A:452:LYS:HG2 | 2.09 | 0.53 |
| 1:A:654:ILE:O | 1:A:658:THR:OG1 | 2.26 | 0.53 |
| 1:A:1195:VAL:HG23 | 1:A:1196:PRO:HD3 | 1.91 | 0.53 |
| 1:A:1297:PHE:CZ | 1:A:1301:ILE:HD13 | 2.44 | 0.53 |
| 1:B:279:ALA:HB1 | 1:B:322:GLN:HG3 | 1.90 | 0.53 |
| 1:A:966:PHE:CE1 | 1:A:969:LEU:HD12 | 2.43 | 0.53 |
| 1:A:1463:LEU:HG | 1:A:1466:ASN:HB2 | 1.90 | 0.53 |
| 1:A:2492:ASP:HB3 | 1:A:2495:SER:H | 1.74 | 0.53 |
| 1:B:2182:ILE:HD11 | 1:B:2185:MET:HB3 | 1.90 | 0.53 |
| 1:A:410:MET:HG2 | 1:A:442:GLN:HB2 | 1.90 | 0.53 |
| 1:B:1884:LEU:HD23 | 1:B:1885:PRO:HD2 | 1.91 | 0.53 |
| 1:A:1368:LEU:HA | 1:A:1371:VAL:HG22 | 1.91 | 0.52 |
| 1:A:3975:LYS:HB2 | 1:A:3977:THR:HG22 | 1.91 | 0.52 |
| 1:A:342:MET:HE3 | 1:A:345:PHE:HD2 | 1.74 | 0.52 |
| 1:A:2304:VAL:HG11 | 1:A:2344:LEU:HG | 1.90 | 0.52 |
| 1:A:3325:ASP:HA | 1:A:3328:ILE:HD12 | 1.91 | 0.52 |
| 1:B:157:TYR:OH | 1:B:195:ASN:HB3 | 2.09 | 0.52 |
| 1:A:1955:VAL:O | 1:A:1957:ASN:ND2 | 2.35 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3786:LEU:HD21 | 1:A:3983:ILE:HD12 | 1.92 | 0.52 |
| 1:B:531:PHE:HA | 1:B:534:LEU:HD12 | 1.90 | 0.52 |
| 1:B:1346:THR:HG23 | 1:B:1405:ALA:HB2 | 1.91 | 0.52 |
| 1:B:2532:PRO:HB2 | 1:B:2537:ASP:HB2 | 1.90 | 0.52 |
| 1:B:3360:LEU:HG | 1:B:3373:VAL:HG21 | 1.91 | 0.52 |
| 1:A:1104:LEU:HD12 | 1:A:1134:LEU:HB3 | 1.92 | 0.52 |
| 1:A:1134:LEU:O | 1:A:1138:ILE:HG13 | 2.10 | 0.52 |
| 1:A:1990:PHE:HE2 | 1:A:2144:LEU:HD11 | 1.74 | 0.52 |
| 1:A:3535:ILE:HD12 | 1:A:3759:ARG:CZ | 2.40 | 0.52 |
| 1:B:1297:PHE:CZ | 1:B:1301:ILE:HD13 | 2.45 | 0.52 |
| 1:B:3319:ASN:O | 1:B:3323:PHE:HB2 | 2.10 | 0.52 |
| 1:A:765:LEU:HD23 | 1:A:766:ALA:H | 1.73 | 0.52 |
| 1:A:1279:LEU:HD23 | 1:A:1279:LEU:H | 1.74 | 0.52 |
| 1:A:2546:TYR:HH | 1:A:2854:PHE:HE2 | 1.58 | 0.52 |
| 1:B:1962:TYR:O | 1:B:1967:PHE:HD2 | 1.92 | 0.52 |
| 1:B:2188:GLU:O | 1:B:2191:ALA:HB3 | 2.08 | 0.52 |
| 1:B:113:SER:O | 1:B:117:LYS:HG2 | 2.10 | 0.52 |
| 1:B:3341:LEU:HD13 | 1:B:3374:ILE:HG12 | 1.92 | 0.52 |
| 1:A:9:ARG:HB2 | 1:A:57:LEU:HD11 | 1.92 | 0.52 |
| 1:A:3330:LEU:HD13 | 1:A:3384:HIS:CE1 | 2.44 | 0.52 |
| 1:A:3654:MET:HG2 | 1:A:3656:LEU:HB2 | 1.92 | 0.52 |
| 1:A:3667:LEU:HA | 1:A:3670:MET:HE3 | 1.91 | 0.52 |
| 1:A:96:MET:SD | 1:A:96:MET:N | 2.83 | 0.52 |
| 1:A:655:LEU:HD22 | 1:A:1389:VAL:HG12 | 1.91 | 0.52 |
| 1:A:3761:ASP:HA | 1:A:3764:VAL:HG22 | 1.92 | 0.52 |
| 1:B:1765:VAL:HA | 1:B:1768:ARG:HB2 | 1.91 | 0.52 |
| 1:B:1481:THR:HG22 | 1:B:1524:LEU:HD11 | 1.91 | 0.52 |
| 1:B:1948:ALA:O | 1:B:1952:ILE:HG13 | 2.10 | 0.52 |
| 1:B:2402:LEU:O | 1:B:2405:VAL:HG23 | 2.10 | 0.52 |
| 1:B:3913:ILE:HB | 1:B:3984:MET:HG2 | 1.91 | 0.52 |
| 1:A:19:LEU:CD2 | 1:A:71:LYS:HG3 | 2.39 | 0.52 |
| 1:A:749:VAL:N | 1:A:750:PRO:HD2 | 2.25 | 0.52 |
| 1:A:794:PRO:CG | 1:A:873:VAL:HB | 2.41 | 0.52 |
| 1:A:3028:ASN:HA | 1:A:3031:TRP:CD1 | 2.31 | 0.52 |
| 1:A:3617:LEU:HD22 | 1:A:3636:PHE:CE2 | 2.45 | 0.52 |
| 1:B:3786:LEU:HD21 | 1:B:3983:ILE:HD12 | 1.91 | 0.52 |
| 1:A:898:PHE:HD2 | 1:A:903:PRO:HD2 | 1.75 | 0.51 |
| 1:A:1283:GLY:HA2 | 1:A:1358:LEU:CD1 | 2.40 | 0.51 |
| 1:A:1572:LEU:HD11 | 1:A:1604:SER:HB3 | 1.92 | 0.51 |
| 1:A:3567:VAL:HG11 | 1:A:3697:ASN:HB3 | 1.90 | 0.51 |
| 1:A:3588:TRP:HH2 | 1:A:3651:LEU:HD21 | 1.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:738:HIS:NE2 | 1:B:745:VAL:HG23 | 2.24 | 0.51 |
| 1:B:3586:LYS:HD3 | 1:B:3667:LEU:HD21 | 1.91 | 0.51 |
| 1:A:86:LEU:HB2 | 1:A:126:PRO:HB2 | 1.92 | 0.51 |
| 1:A:1071:ASN:HD21 | 1:A:1073:PHE:HB2 | 1.75 | 0.51 |
| 1:B:1142:HIS:CE1 | 1:B:1146:ASN:HA | 2.45 | 0.51 |
| 1:A:1427:SER:HA | 1:A:1430:GLU:HG2 | 1.92 | 0.51 |
| 1:B:496:VAL:HG12 | 1:B:497:LEU:H | 1.75 | 0.51 |
| 1:B:683:PHE:O | 1:B:740:ILE:HG12 | 2.10 | 0.51 |
| 1:B:996:THR:HA | 1:B:1001:PHE:HD1 | 1.74 | 0.51 |
| 1:A:323:VAL:HG13 | 1:A:369:PHE:HZ | 1.75 | 0.51 |
| 1:A:414:LEU:HG | 1:A:464:VAL:HG21 | 1.92 | 0.51 |
| 1:A:890:LYS:HD3 | 1:A:909:VAL:HG13 | 1.93 | 0.51 |
| 1:A:1724:MET:SD | 1:A:1724:MET:N | 2.81 | 0.51 |
| 1:A:1783:ARG:HD2 | 1:A:1830:HIS:ND1 | 2.24 | 0.51 |
| 1:A:1896:ILE:HD13 | 1:A:1906:THR:O | 2.11 | 0.51 |
| 1:A:3144:PHE:HE1 | 1:A:3156:PRO:HB2 | 1.75 | 0.51 |
| 1:B:178:LEU:HD23 | 1:B:181:LEU:HD12 | 1.92 | 0.51 |
| 1:A:1082:PHE:HA | 1:A:1085:ILE:HG12 | 1.93 | 0.51 |
| 1:B:1142:HIS:ND1 | 1:B:1145:LEU:O | 2.44 | 0.51 |
| 1:B:1633:TRP:CZ2 | 1:B:1674:THR:HG22 | 2.46 | 0.51 |
| 1:B:2461:PHE:HB2 | 1:B:2473:MET:HG3 | 1.92 | 0.51 |
| 1:B:3506:LEU:HA | 1:B:3511:ALA:HB1 | 1.91 | 0.51 |
| 1:A:2251:ILE:HD12 | 1:A:2253:TYR:CE2 | 2.46 | 0.51 |
| 1:B:1851:LEU:O | 1:B:1870:LYS:NZ | 2.38 | 0.51 |
| 1:A:1686:LEU:HD22 | 1:A:1721:HIS:CD2 | 2.46 | 0.51 |
| 1:A:2886:GLN:N | 1:A:2887:PRO:HD3 | 2.25 | 0.51 |
| 1:A:3258:LEU:HA | 1:A:3261:GLU:HG2 | 1.91 | 0.51 |
| 1:B:1020:PRO:HA | 1:B:1073:PHE:CE1 | 2.45 | 0.51 |
| 1:B:1102:GLU:O | 1:B:1154:PRO:HB3 | 2.11 | 0.51 |
| 1:B:1575:LEU:HG | 1:B:1576:ASP:H | 1.76 | 0.51 |
| 1:A:2223:VAL:HG23 | 1:A:2234:ASN:HB3 | 1.93 | 0.51 |
| 1:A:2575:PRO:HB3 | 1:A:2787:HIS:CE1 | 2.46 | 0.51 |
| 1:B:1055:ASN:O | 1:B:1058:SER:OG | 2.22 | 0.51 |
| 1:B:2101:VAL:HG12 | 1:B:2156:VAL:HG21 | 1.92 | 0.51 |
| 1:B:3718:ARG:H | 1:B:3743:HIS:CE1 | 2.28 | 0.51 |
| 1:B:354:SER:HB2 | 1:B:359:LEU:CB | 2.41 | 0.51 |
| 1:B:1947:CYS:O | 1:B:1951:VAL:HG12 | 2.11 | 0.51 |
| 1:B:4008:GLU:O | 1:B:4010:SER:N | 2.44 | 0.51 |
| 1:A:661:PRO:HD2 | 1:A:662:LEU:HD23 | 1.93 | 0.51 |
| 1:A:718:MET:HA | 1:A:721:TYR:CD2 | 2.46 | 0.51 |
| 1:A:2288:TYR:HD1 | 1:A:2291:GLN:HB2 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3506:LEU:HD22 | 1:A:3555:VAL:HG22 | 1.93 | 0.51 |
| 1:A:3545:THR:CG2 | 1:A:3546:SER:H | 2.22 | 0.51 |
| 1:A:3585:PHE:HD2 | 1:A:3667:LEU:HD13 | 1.75 | 0.51 |
| 1:B:532:ARG:O | 1:B:536:SER:HB3 | 2.10 | 0.51 |
| 1:B:3958:LEU:HB2 | 1:B:4116:ILE:HG23 | 1.93 | 0.51 |
| 1:A:1766:LEU:HG | 1:A:1778:PHE:HD2 | 1.76 | 0.50 |
| 1:A:3842:TRP:CZ2 | 1:A:3867:THR:HG22 | 2.46 | 0.50 |
| 1:B:60:SER:HB2 | 1:B:63:PHE:O | 2.11 | 0.50 |
| 1:B:782:ARG:O | 1:B:786:GLN:HG3 | 2.11 | 0.50 |
| 1:B:1027:ASP:OD1 | 1:B:1027:ASP:N | 2.43 | 0.50 |
| 1:B:3271:ASP:HA | 1:B:3274:VAL:HG12 | 1.93 | 0.50 |
| 1:A:2472:GLN:O | 1:A:2476:ILE:HG23 | 2.12 | 0.50 |
| 1:A:3354:ASP:O | 1:A:3358:ARG:HG2 | 2.11 | 0.50 |
| 1:B:1766:LEU:HG | 1:B:1778:PHE:CD2 | 2.44 | 0.50 |
| 1:B:3717:VAL:HA | 1:B:3743:HIS:HE1 | 1.76 | 0.50 |
| 1:A:1038:LYS:HD3 | 1:A:1042:LYS:HE3 | 1.94 | 0.50 |
| 1:A:3630:ARG:HG2 | 1:A:3632:PHE:H | 1.76 | 0.50 |
| 1:B:495:VAL:HG12 | 1:B:496:VAL:H | 1.76 | 0.50 |
| 1:B:2004:TYR:CZ | 1:B:2187:VAL:HG11 | 2.46 | 0.50 |
| 1:B:2249:LEU:HG | 1:B:2285:LEU:HD13 | 1.94 | 0.50 |
| 1:B:3542:PHE:CG | 1:B:3552:LYS:HG2 | 2.47 | 0.50 |
| 1:A:1104:LEU:HD13 | 1:A:1138:ILE:HD11 | 1.92 | 0.50 |
| 1:A:1653:LEU:HB3 | 1:A:1698:PHE:CD1 | 2.47 | 0.50 |
| 1:A:2409:THR:O | 1:A:2411:LEU:HB2 | 2.11 | 0.50 |
| 1:A:3619:ASP:HB2 | 1:A:3622:ALA:HB2 | 1.93 | 0.50 |
| 1:B:1693:VAL:O | 1:B:1696:LEU:HD23 | 2.12 | 0.50 |
| 1:B:2887:PRO:HB3 | 1:B:3898:LEU:HD22 | 1.94 | 0.50 |
| 1:B:3065:ILE:HG23 | 1:B:3078:LEU:HD21 | 1.94 | 0.50 |
| 1:B:3648:GLY:O | 1:B:3652:LEU:HD12 | 2.11 | 0.50 |
| 1:A:487:LEU:HA | 1:A:490:ILE:HG12 | 1.94 | 0.50 |
| 1:A:1848:ILE:O | 1:A:1852:LYS:HB2 | 2.12 | 0.50 |
| 1:A:1861:SER:O | 1:A:1865:THR:OG1 | 2.24 | 0.50 |
| 1:A:2138:VAL:HG12 | 1:A:2143:ARG:HB2 | 1.92 | 0.50 |
| 1:B:479:ILE:HA | 1:B:482:VAL:HG12 | 1.93 | 0.50 |
| 1:B:487:LEU:HD21 | 1:B:568:PHE:HE1 | 1.77 | 0.50 |
| 1:B:780:ILE:HG21 | 1:B:785:MET:SD | 2.52 | 0.50 |
| 1:B:786:GLN:HA | 1:B:789:TYR:CD2 | 2.46 | 0.50 |
| 1:B:2419:ASP:HB2 | 1:B:2422:GLN:HB2 | 1.94 | 0.50 |
| 1:A:2375:ALA:O | 1:A:2379:MET:N | 2.44 | 0.50 |
| 1:A:3772:ASN:HD21 | 1:A:3790:THR:HG23 | 1.76 | 0.50 |
| 1:A:3992:ARG:HD3 | 1:A:4100:GLU:HG3 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:897:PRO:HA | 1:B:902:LYS:HG3 | 1.93 | 0.50 |
| 1:B:898:PHE:HD2 | 1:B:903:PRO:HD2 | 1.75 | 0.50 |
| 1:B:1554:SER:OG | 1:B:1557:GLU:HB2 | 2.12 | 0.50 |
| 1:B:1934:LEU:H | 1:B:1934:LEU:HD23 | 1.75 | 0.50 |
| 1:B:2263:LYS:HA | 1:B:2309:PHE:CE2 | 2.46 | 0.50 |
| 1:B:3674:SER:O | 1:B:3676:PRO:HD3 | 2.12 | 0.50 |
| 1:A:1681:ASP:O | 1:A:1683:LYS:N | 2.37 | 0.50 |
| 1:A:2281:MET:SD | 1:A:2287:PRO:HD3 | 2.51 | 0.50 |
| 1:A:2402:LEU:HD13 | 1:A:2434:VAL:HG23 | 1.94 | 0.50 |
| 1:A:3533:PHE:HE2 | 1:A:3559:LYS:HD3 | 1.76 | 0.50 |
| 1:B:1335:CYS:HB3 | 1:B:1384:PHE:CE1 | 2.47 | 0.50 |
| 1:B:1566:THR:O | 1:B:1570:GLU:HG2 | 2.12 | 0.50 |
| 1:B:1602:ASP:HA | 1:B:2045:PHE:HE2 | 1.77 | 0.50 |
| 1:B:3462:ARG:NH1 | 1:B:3497:SER:OG | 2.45 | 0.50 |
| 1:B:3881:ASP:OD1 | 1:B:3881:ASP:N | 2.43 | 0.50 |
| 1:A:94:GLU:OE1 | 1:A:133:LYS:HD2 | 2.11 | 0.50 |
| 1:A:1154:PRO:HG2 | 1:A:1157:PHE:HB2 | 1.93 | 0.50 |
| 1:A:1579:VAL:O | 1:A:1583:MET:HG2 | 2.12 | 0.50 |
| 1:B:388:LEU:HD23 | 1:B:420:VAL:HG11 | 1.93 | 0.50 |
| 1:B:1837:ARG:HG3 | 1:B:1884:LEU:HD11 | 1.94 | 0.50 |
| 1:B:3992:ARG:NH1 | 1:B:4103:GLN:OE1 | 2.44 | 0.50 |
| 1:A:385:TYR:CZ | 1:A:389:ILE:CD1 | 2.95 | 0.50 |
| 1:A:865:GLN:HG2 | 1:A:3170:ASP:HB3 | 1.94 | 0.50 |
| 1:A:2182:ILE:HG23 | 1:A:2186:VAL:HG21 | 1.93 | 0.50 |
| 1:A:2359:LYS:H | 1:A:2359:LYS:HD2 | 1.77 | 0.50 |
| 1:B:108:LYS:HG2 | 1:B:131:LEU:HD11 | 1.94 | 0.50 |
| 1:B:670:LEU:HA | 1:B:673:THR:HG22 | 1.93 | 0.50 |
| 1:B:1833:LEU:HG | 1:B:1835:ALA:H | 1.77 | 0.50 |
| 1:B:3586:LYS:HG2 | 1:B:3667:LEU:HD11 | 1.94 | 0.50 |
| 1:A:997:ASN:OD1 | 1:A:998:ASN:N | 2.44 | 0.49 |
| 1:A:1362:ASP:OD1 | 1:A:1362:ASP:N | 2.45 | 0.49 |
| 1:B:200:PHE:HD1 | 1:B:223:CYS:SG | 2.34 | 0.49 |
| 1:B:933:LEU:HB2 | 1:B:2793:PRO:HB2 | 1.94 | 0.49 |
| 1:B:1082:PHE:HA | 1:B:1085:ILE:HG12 | 1.92 | 0.49 |
| 1:B:3532:PRO:HA | 1:B:3535:ILE:HG12 | 1.93 | 0.49 |
| 1:A:2393:LEU:HA | 1:A:2396:LEU:HD12 | 1.94 | 0.49 |
| 1:A:3422:GLN:HE21 | 1:A:3423:GLN:HG2 | 1.77 | 0.49 |
| 1:B:898:PHE:CD2 | 1:B:903:PRO:HD2 | 2.47 | 0.49 |
| 1:B:1923:PHE:HA | 1:B:1941:HIS:CG | 2.46 | 0.49 |
| 1:A:393:LYS:HA | 1:A:397:LEU:HD12 | 1.94 | 0.49 |
| 1:A:3421:ASP:OD1 | 1:A:3467:ARG:NE | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1099:PHE:CZ | 1:B:1152:ARG:HD2 | 2.47 | 0.49 |
| 1:B:1611:GLN:O | 1:B:1611:GLN:HG2 | 2.12 | 0.49 |
| 1:A:3049:LEU:HD22 | 1:A:3085:GLU:HG3 | 1.94 | 0.49 |
| 1:A:3259:LEU:HD12 | 1:A:3276:TRP:NE1 | 2.27 | 0.49 |
| 1:B:1612:LYS:C | 1:B:1614:GLN:N | 2.65 | 0.49 |
| 1:B:3798:SER:O | 1:B:3799:ARG:HG2 | 2.12 | 0.49 |
| 1:A:683:PHE:HB3 | 1:A:740:ILE:HG13 | 1.93 | 0.49 |
| 1:A:863:GLY:O | 1:A:867:ASN:HB2 | 2.13 | 0.49 |
| 1:A:1783:ARG:HB3 | 1:A:1830:HIS:CG | 2.47 | 0.49 |
| 1:B:1406:LEU:CB | 1:B:1415:LEU:HD11 | 2.41 | 0.49 |
| 1:B:3867:THR:HG21 | 1:B:4119:ARG:CZ | 2.43 | 0.49 |
| 1:A:476:ARG:NH2 | 1:A:1503:LEU:HD22 | 2.28 | 0.49 |
| 1:A:1342:MET:O | 1:A:1346:THR:HG23 | 2.11 | 0.49 |
| 1:A:1612:LYS:O | 1:A:1613:HIS:ND1 | 2.45 | 0.49 |
| 1:A:3065:ILE:HG23 | 1:A:3078:LEU:HD21 | 1.94 | 0.49 |
| 1:A:538:ASP:OD2 | 1:A:561:ASN:N | 2.45 | 0.49 |
| 1:A:767:GLU:HG2 | 1:A:851:ILE:HD11 | 1.94 | 0.49 |
| 1:B:305:ASN:OD1 | 1:B:306:VAL:N | 2.46 | 0.49 |
| 1:B:2310:VAL:HG12 | 1:B:2316:TYR:CG | 2.47 | 0.49 |
| 1:A:476:ARG:HH22 | 1:A:1503:LEU:HD22 | 1.78 | 0.49 |
| 1:A:619:ASP:OD2 | 1:A:2035:THR:HB | 2.13 | 0.49 |
| 1:A:3082:TYR:HB3 | 1:A:3085:GLU:OE1 | 2.13 | 0.49 |
| 1:B:1206:LEU:O | 1:B:1210:ASP:CB | 2.59 | 0.49 |
| 1:A:532:ARG:HG2 | 1:A:637:LYS:HE2 | 1.94 | 0.49 |
| 1:A:1895:LYS:O | 1:A:1899:VAL:HG23 | 2.12 | 0.49 |
| 1:A:2250:SER:O | 1:A:2252:PRO:HD3 | 2.13 | 0.49 |
| 1:A:3095:ASP:OD1 | 1:A:3098:ARG:HB2 | 2.13 | 0.49 |
| 1:B:631:ARG:HH21 | 1:B:668:LYS:HD3 | 1.78 | 0.49 |
| 1:B:997:ASN:OD1 | 1:B:998:ASN:N | 2.45 | 0.49 |
| 1:B:1334:LYS:O | 1:B:1337:VAL:HG22 | 2.12 | 0.49 |
| 1:B:1747:LEU:HD12 | 1:B:1781:SER:HB2 | 1.95 | 0.49 |
| 1:B:1900:PHE:HB3 | 1:B:1904:CYS:SG | 2.53 | 0.49 |
| 1:A:110:THR:O | 1:A:114:VAL:HG23 | 2.13 | 0.49 |
| 1:A:1425:ALA:HA | 1:A:1428:ILE:HD12 | 1.95 | 0.49 |
| 1:A:2219:LEU:O | 1:A:2223:VAL:HB | 2.13 | 0.49 |
| 1:A:2459:VAL:HB | 1:A:2505:VAL:HG21 | 1.95 | 0.49 |
| 1:B:339:GLN:O | 1:B:343:GLU:HG2 | 2.12 | 0.49 |
| 1:B:4054:ALA:HA | 1:B:4096:SER:HA | 1.95 | 0.49 |
| 1:A:370:ALA:HB1 | 1:A:420:VAL:HG23 | 1.94 | 0.48 |
| 1:A:938:VAL:HA | 1:A:941:MET:HG2 | 1.95 | 0.48 |
| 1:A:2887:PRO:CG | 1:A:3895:GLU:HG2 | 2.42 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3120:LEU:HD11 | 1:A:3896:ALA:HA | 1.95 | 0.48 |
| 1:A:3937:VAL:C | 1:A:3938:ILE:HD13 | 2.32 | 0.48 |
| 1:B:1204:PRO:HG2 | 1:B:1205:ASN:ND2 | 2.28 | 0.48 |
| 1:B:1730:PRO:HG2 | 1:B:1733:THR:HG21 | 1.95 | 0.48 |
| 1:B:3444:ALA:HA | 1:B:3479:THR:HG21 | 1.95 | 0.48 |
| 1:A:264:ARG:O | 1:A:266:ALA:N | 2.46 | 0.48 |
| 1:A:538:ASP:HB2 | 1:A:561:ASN:OD1 | 2.14 | 0.48 |
| 1:A:718:MET:HE2 | 1:A:726:LEU:HG | 1.96 | 0.48 |
| 1:A:1096:VAL:HB | 1:A:1101:PHE:HE2 | 1.78 | 0.48 |
| 1:A:3778:ASP:OD1 | 1:A:3779:SER:N | 2.46 | 0.48 |
| 1:B:1606:ARG:HG2 | 1:B:2042:GLN:OE1 | 2.12 | 0.48 |
| 1:B:1668:PHE:O | 1:B:1671:VAL:HG22 | 2.13 | 0.48 |
| 1:B:2249:LEU:O | 1:B:2251:ILE:N | 2.46 | 0.48 |
| 2:D:728:LEU:O | 2:D:731:MET:HB2 | 2.12 | 0.48 |
| 1:A:479:ILE:HA | 1:A:482:VAL:HG12 | 1.96 | 0.48 |
| 1:B:267:VAL:HG23 | 1:B:268:PRO:HD3 | 1.94 | 0.48 |
| 1:B:1739:TYR:O | 1:B:1743:MET:HG2 | 2.14 | 0.48 |
| 1:B:2294:ILE:HG22 | 1:B:2295:GLN:H | 1.77 | 0.48 |
| 1:B:3937:VAL:C | 1:B:3938:ILE:HD13 | 2.33 | 0.48 |
| 1:A:1853:SER:OG | 1:A:1870:LYS:NZ | 2.42 | 0.48 |
| 1:A:1984:LEU:HD11 | 1:A:2139:PRO:HG2 | 1.95 | 0.48 |
| 1:A:1992:VAL:HG23 | 1:A:1993:GLU:H | 1.77 | 0.48 |
| 1:A:2182:ILE:HG12 | 1:A:2186:VAL:HG23 | 1.94 | 0.48 |
| 1:A:2411:LEU:HG | 1:A:2415:LEU:HD13 | 1.94 | 0.48 |
| 1:A:2885:GLN:C | 1:A:2887:PRO:HD3 | 2.33 | 0.48 |
| 1:B:620:PHE:O | 1:B:624:ILE:HG12 | 2.14 | 0.48 |
| 1:B:972:LEU:HD13 | 1:B:984:TYR:CE2 | 2.49 | 0.48 |
| 1:B:1103:ALA:HB1 | 1:B:1106:ILE:HB | 1.94 | 0.48 |
| 1:A:720:GLN:OE1 | 1:A:1026:ARG:NH2 | 2.47 | 0.48 |
| 1:A:1071:ASN:OD1 | 1:A:1072:ALA:N | 2.47 | 0.48 |
| 1:A:1459:HIS:CG | 1:A:1520:ALA:HB1 | 2.48 | 0.48 |
| 1:A:2085:MET:HA | 1:A:2089:ASN:HB2 | 1.95 | 0.48 |
| 1:A:3050:LYS:NZ | 1:A:3181:ASP:OD1 | 2.34 | 0.48 |
| 1:A:3448:GLU:HG2 | 1:A:3482:LEU:HD11 | 1.95 | 0.48 |
| 1:A:3760:GLN:O | 1:A:3764:VAL:HG13 | 2.14 | 0.48 |
| 1:B:256:ILE:HB | 1:B:300:TRP:HZ3 | 1.77 | 0.48 |
| 1:B:1328:GLU:N | 1:B:1328:GLU:OE1 | 2.45 | 0.48 |
| 1:B:2301:GLN:HA | 1:B:2344:LEU:HD21 | 1.95 | 0.48 |
| 1:B:3413:TYR:CD1 | 1:B:3449:LYS:HG3 | 2.49 | 0.48 |
| 1:A:421:LEU:HB3 | 1:A:467:ALA:HB1 | 1.95 | 0.48 |
| 1:A:421:LEU:HD22 | 1:A:424:LEU:HD23 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1753:SER:O | 1:A:1755:SER:N | 2.46 | 0.48 |
| 1:A:3307:LEU:HD22 | 1:A:3330:LEU:HD21 | 1.96 | 0.48 |
| 1:B:570:LYS:O | 1:B:574:LYS:HB2 | 2.12 | 0.48 |
| 1:B:1626:TRP:CE3 | 1:B:1674:THR:HG21 | 2.48 | 0.48 |
| 1:B:2245:TRP:O | 1:B:2247:ASP:N | 2.46 | 0.48 |
| 1:A:108:LYS:NZ | 1:A:147:PHE:HB3 | 2.28 | 0.48 |
| 1:A:2257:PHE:HA | 1:A:2260:PHE:CE2 | 2.49 | 0.48 |
| 1:B:272:LEU:HD13 | 1:B:312:ALA:HA | 1.94 | 0.48 |
| 1:B:1124:ILE:HD12 | 1:B:1124:ILE:H | 1.79 | 0.48 |
| 1:A:135:LEU:HB2 | 1:A:180:LEU:HD21 | 1.95 | 0.48 |
| 1:A:572:VAL:HA | 1:A:575:ILE:HD12 | 1.96 | 0.48 |
| 1:A:2852:PRO:HG2 | 1:A:2853:PRO:HD3 | 1.96 | 0.48 |
| 1:A:3701:ILE:HD12 | 1:A:3740:ILE:HD11 | 1.96 | 0.48 |
| 1:B:1926:ASN:HB3 | 1:B:1974:ASN:O | 2.14 | 0.48 |
| 1:B:1956:PHE:HB2 | 1:B:1961:PHE:HE2 | 1.79 | 0.48 |
| 1:B:3069:MET:SD | 1:B:3075:LYS:HG3 | 2.54 | 0.48 |
| 1:A:2934:GLY:HA2 | 1:A:2936:TYR:CE2 | 2.49 | 0.48 |
| 1:A:3778:ASP:HB3 | 1:A:3781:CYS:HB2 | 1.95 | 0.48 |
| 1:B:3300:VAL:HG11 | 1:B:3336:ILE:HG21 | 1.96 | 0.48 |
| 1:A:296:VAL:O | 1:A:300:TRP:HD1 | 1.97 | 0.48 |
| 1:A:726:LEU:HD21 | 1:A:754:MET:HG2 | 1.95 | 0.48 |
| 1:A:2168:LEU:HB3 | 1:A:2189:ILE:HG23 | 1.95 | 0.48 |
| 1:A:2277:LEU:HA | 1:A:2280:VAL:HG12 | 1.96 | 0.48 |
| 1:B:2320:ALA:O | 1:B:2367:VAL:HG22 | 2.14 | 0.48 |
| 1:B:3407:ALA:H | 1:B:3410:ILE:HG23 | 1.78 | 0.48 |
| 1:A:366:TYR:CZ | 1:A:384:MET:HG2 | 2.49 | 0.47 |
| 1:A:977:ASP:OD1 | 1:A:978:GLN:N | 2.47 | 0.47 |
| 1:A:2251:ILE:HD12 | 1:A:2253:TYR:HE2 | 1.79 | 0.47 |
| 1:A:3171:ALA:HB1 | 1:A:3248:LYS:HD2 | 1.96 | 0.47 |
| 1:A:3413:TYR:CE1 | 1:A:3449:LYS:HG3 | 2.48 | 0.47 |
| 1:B:1029:CYS:O | 1:B:1032:CYS:HB2 | 2.14 | 0.47 |
| 1:B:1875:LYS:O | 1:B:1878:ASP:HB2 | 2.14 | 0.47 |
| 1:B:3596:LEU:HD22 | 1:B:3606:ILE:HD12 | 1.96 | 0.47 |
| 1:A:2190:VAL:HA | 1:A:2193:ILE:HG22 | 1.95 | 0.47 |
| 1:B:215:PRO:O | 1:B:216:LYS:HG2 | 2.14 | 0.47 |
| 1:B:1586:SER:OG | 1:B:1628:LYS:O | 2.29 | 0.47 |
| 1:B:2572:TYR:N | 1:B:2573:PRO:HD3 | 2.29 | 0.47 |
| 1:B:2937:ASP:OD1 | 1:B:3784:ARG:NH2 | 2.47 | 0.47 |
| 1:B:3772:ASN:HD21 | 1:B:3790:THR:HG23 | 1.78 | 0.47 |
| 1:A:153:PHE:HE1 | 1:A:196:LEU:HD13 | 1.79 | 0.47 |
| 1:A:565:TYR:HE1 | 1:A:642:PHE:HD1 | 1.61 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1102:GLU:O | 1:A:1105:VAL:HG22 | 2.14 | 0.47 |
| 1:A:1203:SER:HB3 | 1:A:1204:PRO:HD2 | 1.95 | 0.47 |
| 1:A:1977:ILE:O | 1:A:1981:LEU:HB2 | 2.15 | 0.47 |
| 1:B:3083:SER:HA | 1:B:3086:LEU:HD12 | 1.96 | 0.47 |
| 1:A:1361:LYS:O | 1:A:1365:ASN:HB2 | 2.15 | 0.47 |
| 1:A:2393:LEU:H | 1:A:2393:LEU:HD12 | 1.78 | 0.47 |
| 1:A:3599:THR:HG23 | 1:A:3601:VAL:HG12 | 1.96 | 0.47 |
| 1:B:446:PHE:CE1 | 1:B:454:GLN:HG2 | 2.49 | 0.47 |
| 1:B:2004:TYR:HB3 | 1:B:2233:HIS:CE1 | 2.49 | 0.47 |
| 1:B:3307:LEU:HD12 | 1:B:3307:LEU:HA | 1.68 | 0.47 |
| 1:B:3487:ILE:HG23 | 1:B:3516:HIS:NE2 | 2.29 | 0.47 |
| 1:A:790:LYS:H | 1:A:790:LYS:HD3 | 1.79 | 0.47 |
| 1:A:3049:LEU:HD21 | 1:A:3088:LEU:HD12 | 1.97 | 0.47 |
| 1:B:995:PHE:HB3 | 1:B:1006:THR:HG22 | 1.97 | 0.47 |
| 1:B:2106:ARG:NH2 | 1:B:2155:GLU:OE1 | 2.47 | 0.47 |
| 1:B:2873:PRO:HB3 | 1:B:2922:ARG:HA | 1.97 | 0.47 |
| 1:A:646:VAL:O | 1:A:650:SER:OG | 2.28 | 0.47 |
| 1:A:1519:PHE:CZ | 1:A:1528:LEU:HD22 | 2.49 | 0.47 |
| 1:A:1787:ARG:O | 1:A:1787:ARG:HG2 | 2.15 | 0.47 |
| 1:A:3659:PHE:CE2 | 1:A:3661:ASP:HB3 | 2.50 | 0.47 |
| 1:B:606:SER:OG | 1:B:1023:SER:HB2 | 2.15 | 0.47 |
| 1:B:1658:SER:HB3 | 1:B:1661:PHE:CE1 | 2.47 | 0.47 |
| 1:B:2574:ASN:C | 1:B:2576:MET:H | 2.16 | 0.47 |
| 1:A:373:CYS:HA | 1:A:376:ILE:CG2 | 2.45 | 0.47 |
| 1:A:425:ASP:N | 1:A:425:ASP:OD1 | 2.48 | 0.47 |
| 1:A:1124:ILE:H | 1:A:1124:ILE:HD12 | 1.79 | 0.47 |
| 1:A:1359:LEU:HB3 | 1:A:1363:LEU:HD11 | 1.96 | 0.47 |
| 1:A:1433:ALA:HB3 | 1:A:1436:LEU:HG | 1.97 | 0.47 |
| 1:A:1725:GLN:O | 1:A:1772:HIS:ND1 | 2.45 | 0.47 |
| 1:A:3544:ASP:OD1 | 1:A:3549:HIS:NE2 | 2.47 | 0.47 |
| 1:A:3693:GLU:HG2 | 1:A:3694:PHE:H | 1.80 | 0.47 |
| 1:A:3860:LYS:HB3 | 1:A:4076:ASP:OD2 | 2.14 | 0.47 |
| 1:B:125:ILE:HB | 1:B:126:PRO:HD3 | 1.96 | 0.47 |
| 1:B:786:GLN:HA | 1:B:789:TYR:HD2 | 1.79 | 0.47 |
| 1:B:859:LEU:HG | 1:B:867:ASN:ND2 | 2.25 | 0.47 |
| 1:B:986:PRO:O | 1:B:990:GLN:HG3 | 2.14 | 0.47 |
| 1:B:1202:ARG:O | 1:B:1207:TRP:HB2 | 2.15 | 0.47 |
| 1:B:1426:GLN:HG2 | 1:B:1427:SER:N | 2.30 | 0.47 |
| 1:B:3955:VAL:HG11 | 1:B:4121:TRP:CE3 | 2.50 | 0.47 |
| 1:A:305:ASN:HB2 | 1:A:308:LEU:CB | 2.45 | 0.47 |
| 1:A:1448:LEU:HG | 1:A:1510:LEU:HD11 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1765:VAL:HG23 | 1:A:1768:ARG:CZ | 2.45 | 0.47 |
| 1:A:1949:ILE:HG12 | 1:A:2100:LEU:HD23 | 1.97 | 0.47 |
| 1:A:2036:LEU:HD23 | 1:A:2036:LEU:HA | 1.67 | 0.47 |
| 1:B:14:ARG:HH12 | 1:B:34:LEU:HD21 | 1.80 | 0.47 |
| 1:B:620:PHE:HZ | 1:B:663:ILE:HD12 | 1.80 | 0.47 |
| 1:B:1265:GLU:OE2 | 1:B:1340:ARG:HD2 | 2.15 | 0.47 |
| 1:B:1372:LEU:HD12 | 1:B:1402:LEU:HD23 | 1.97 | 0.47 |
| 1:B:1400:VAL:HG13 | 1:B:1461:ALA:HB2 | 1.96 | 0.47 |
| 1:B:2286:PRO:HB3 | 1:B:2329:TYR:CE2 | 2.50 | 0.47 |
| 1:B:3528:ALA:HB2 | 1:B:3705:TYR:CG | 2.50 | 0.47 |
| 1:A:2184:TYR:H | 1:A:2187:VAL:HG23 | 1.80 | 0.47 |
| 1:A:2556:SER:HB2 | 1:A:2799:GLN:HA | 1.97 | 0.47 |
| 1:B:923:ASP:OD2 | 1:B:925:GLN:HB2 | 2.15 | 0.47 |
| 1:B:996:THR:HA | 1:B:1001:PHE:CD1 | 2.49 | 0.47 |
| 1:B:1992:VAL:HG23 | 1:B:1994:VAL:HG23 | 1.97 | 0.47 |
| 1:B:3479:THR:HB | 1:B:3482:LEU:HD23 | 1.97 | 0.47 |
| 1:B:4126:PRO:HD2 | 1:B:4127:TRP:CE3 | 2.50 | 0.47 |
| 1:A:1934:LEU:HD23 | 1:A:1934:LEU:H | 1.80 | 0.47 |
| 1:A:2893:LEU:HD13 | 1:A:2926:LEU:HB2 | 1.97 | 0.47 |
| 1:A:3418:ASP:OD2 | 1:A:3464:LYS:NZ | 2.38 | 0.47 |
| 1:B:256:ILE:O | 1:B:296:VAL:HG21 | 2.15 | 0.47 |
| 1:B:465:PHE:HE1 | 1:B:482:VAL:HG11 | 1.80 | 0.47 |
| 1:B:1135:CYS:O | 1:B:1138:ILE:HG22 | 2.15 | 0.47 |
| 1:B:2556:SER:HB2 | 1:B:2799:GLN:HG2 | 1.97 | 0.47 |
| 1:B:3130:GLN:NE2 | 1:B:3174:ASP:OD1 | 2.48 | 0.47 |
| 1:B:3885:ARG:HA | 1:B:3888:VAL:HG12 | 1.97 | 0.47 |
| 1:A:358:GLU:O | 1:A:361:ILE:HG12 | 2.15 | 0.46 |
| 1:A:1121:LEU:HD22 | 1:A:1123:THR:HG23 | 1.97 | 0.46 |
| 1:A:1146:ASN:OD1 | 1:A:1164:CYS:HB3 | 2.14 | 0.46 |
| 1:A:2753:UNK:O | 1:A:2757:UNK:CB | 2.63 | 0.46 |
| 1:A:2967:GLU:O | 1:A:2971:GLN:HG2 | 2.15 | 0.46 |
| 1:B:487:LEU:HD21 | 1:B:568:PHE:CE1 | 2.49 | 0.46 |
| 1:B:2409:THR:O | 1:B:2411:LEU:HB2 | 2.14 | 0.46 |
| 1:B:2472:GLN:O | 1:B:2476:ILE:HG23 | 2.14 | 0.46 |
| 1:B:2973:ASP:O | 1:B:2977:ASN:ND2 | 2.48 | 0.46 |
| 1:A:933:LEU:HD22 | 1:A:2797:VAL:HG11 | 1.96 | 0.46 |
| 1:A:2194:LEU:HD11 | 1:A:2241:LEU:HD13 | 1.96 | 0.46 |
| 1:A:2563:LEU:HD21 | 1:A:2812:LEU:HD11 | 1.97 | 0.46 |
| 1:A:3085:GLU:OE1 | 1:A:3085:GLU:N | 2.34 | 0.46 |
| 1:A:4042:GLN:NE2 | 1:A:4046:TYR:HE2 | 2.08 | 0.46 |
| 1:B:253:LEU:HD11 | 1:B:257:ARG:HD2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:852:ARG:HD3 | 1:B:3111:MET:SD | 2.55 | 0.46 |
| 1:B:1653:LEU:HB3 | 1:B:1698:PHE:CD1 | 2.50 | 0.46 |
| 1:B:2458:VAL:HG13 | 1:B:2473:MET:HG2 | 1.96 | 0.46 |
| 1:B:3120:LEU:HD23 | 1:B:3120:LEU:H | 1.79 | 0.46 |
| 1:B:3129:LEU:O | 1:B:3132:VAL:HG22 | 2.16 | 0.46 |
| 1:B:3389:VAL:HG21 | 1:B:3449:LYS:HE2 | 1.96 | 0.46 |
| 1:A:1890:HIS:ND1 | 1:A:1912:THR:HG21 | 2.30 | 0.46 |
| 1:B:1783:ARG:HD2 | 1:B:1830:HIS:ND1 | 2.30 | 0.46 |
| 1:B:3701:ILE:HD12 | 1:B:3740:ILE:CD1 | 2.34 | 0.46 |
| 1:A:2105:HIS:ND1 | 1:A:2156:VAL:HG13 | 2.30 | 0.46 |
| 1:B:2971:GLN:HA | 1:B:2974:GLU:HB2 | 1.96 | 0.46 |
| 1:B:3913:ILE:O | 1:B:3917:ILE:HG12 | 2.16 | 0.46 |
| 1:A:335:LYS:HB2 | 1:A:376:ILE:HD11 | 1.98 | 0.46 |
| 1:A:1416:GLU:O | 1:A:1420:ARG:HG3 | 2.16 | 0.46 |
| 1:B:256:ILE:C | 1:B:258:PRO:HD3 | 2.36 | 0.46 |
| 1:B:767:GLU:HG2 | 1:B:851:ILE:HD11 | 1.97 | 0.46 |
| 1:B:1562:LEU:HD23 | 1:B:1562:LEU:HA | 1.75 | 0.46 |
| 1:B:2169:LEU:HD11 | 1:B:2212:ALA:HA | 1.98 | 0.46 |
| 1:B:2591:ILE:HD11 | 1:B:2792:THR:CB | 2.45 | 0.46 |
| 1:A:133:LYS:O | 1:A:137:THR:HG22 | 2.15 | 0.46 |
| 1:A:3324:ARG:O | 1:A:3328:ILE:HG13 | 2.16 | 0.46 |
| 1:B:425:ASP:OD1 | 1:B:425:ASP:N | 2.46 | 0.46 |
| 1:B:677:ALA:HB1 | 1:B:683:PHE:HE2 | 1.80 | 0.46 |
| 1:B:1224:PHE:HD1 | 1:B:1266:CYS:SG | 2.39 | 0.46 |
| 1:B:2482:ASP:OD2 | 1:B:2530:ARG:NH1 | 2.49 | 0.46 |
| 1:B:2950:LYS:HA | 1:B:2950:LYS:HD3 | 1.64 | 0.46 |
| 1:B:3554:PHE:CE2 | 1:B:3558:ILE:HD11 | 2.51 | 0.46 |
| 1:B:3879:PRO:HG2 | 1:B:3882:LEU:HD22 | 1.98 | 0.46 |
| 1:B:4054:ALA:H | 1:B:4103:GLN:NE2 | 2.14 | 0.46 |
| 1:A:418:ALA:HB1 | 1:A:463:LYS:HG3 | 1.96 | 0.46 |
| 1:A:2921:LEU:H | 1:A:2921:LEU:HD23 | 1.81 | 0.46 |
| 1:A:3487:ILE:HG23 | 1:A:3516:HIS:NE2 | 2.31 | 0.46 |
| 1:A:3545:THR:CG2 | 1:A:3546:SER:N | 2.78 | 0.46 |
| 1:B:451:PRO:C | 1:B:453:MET:H | 2.19 | 0.46 |
| 1:B:749:VAL:N | 1:B:750:PRO:HD2 | 2.30 | 0.46 |
| 1:B:1601:LEU:HD22 | 1:B:1618:LEU:HD21 | 1.96 | 0.46 |
| 1:B:2288:TYR:CD2 | 1:B:2291:GLN:HB2 | 2.51 | 0.46 |
| 1:B:2412:TYR:OH | 1:B:2453:GLU:HG2 | 2.16 | 0.46 |
| 1:A:1343:GLU:O | 1:A:1346:THR:OG1 | 2.26 | 0.46 |
| 1:A:1713:VAL:O | 1:A:1716:GLN:HB2 | 2.14 | 0.46 |
| 1:B:131:LEU:HD22 | 1:B:177:LEU:HD21 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1166:LEU:HD12 | 1:B:1166:LEU:H | 1.81 | 0.46 |
| 1:B:1697:PRO:HG2 | 1:B:1752:LEU:HD11 | 1.98 | 0.46 |
| 1:B:2402:LEU:HD13 | 1:B:2434:VAL:HG23 | 1.97 | 0.46 |
| 1:B:2591:ILE:HD12 | 1:B:2591:ILE:H | 1.81 | 0.46 |
| 1:B:3303:THR:O | 1:B:3303:THR:OG1 | 2.32 | 0.46 |
| 1:B:3502:MET:SD | 1:B:3514:VAL:HG21 | 2.56 | 0.46 |
| 1:A:3419:PHE:O | 1:A:3422:GLN:HG3 | 2.16 | 0.46 |
| 1:B:323:VAL:HG13 | 1:B:369:PHE:CZ | 2.46 | 0.46 |
| 1:B:364:ARG:HH21 | 1:B:368:LEU:HB2 | 1.80 | 0.46 |
| 1:B:1733:THR:O | 1:B:1737:ASN:HB2 | 2.16 | 0.46 |
| 1:B:2393:LEU:HD12 | 1:B:2393:LEU:H | 1.81 | 0.46 |
| 1:A:338:LEU:HD21 | 1:A:376:ILE:HG21 | 1.98 | 0.46 |
| 1:A:647:TYR:O | 1:A:651:TYR:HB2 | 2.16 | 0.46 |
| 1:A:1075:ARG:NH2 | 1:A:1117:ASP:OD1 | 2.49 | 0.46 |
| 1:A:1100:VAL:HG12 | 1:A:1134:LEU:HD11 | 1.98 | 0.46 |
| 1:A:1139:GLU:OE1 | 1:A:1193:LYS:HE2 | 2.16 | 0.46 |
| 1:A:1352:SER:O | 1:A:1354:GLU:N | 2.42 | 0.46 |
| 1:A:1640:GLU:C | 1:A:1642:LYS:H | 2.19 | 0.46 |
| 1:A:1754:GLN:HB2 | 1:A:1797:LEU:HD11 | 1.96 | 0.46 |
| 1:A:1981:LEU:O | 1:A:1981:LEU:HD23 | 2.16 | 0.46 |
| 1:A:2551:GLU:HG3 | 1:A:2849:SER:HB2 | 1.99 | 0.46 |
| 1:B:96:MET:SD | 1:B:96:MET:N | 2.89 | 0.46 |
| 1:B:762:TYR:CE1 | 1:B:764:PRO:HD2 | 2.51 | 0.46 |
| 1:B:1797:LEU:O | 1:B:1801:VAL:HG23 | 2.16 | 0.46 |
| 1:A:977:ASP:HB3 | 1:A:980:THR:HG22 | 1.98 | 0.45 |
| 1:A:1425:ALA:O | 1:A:1429:GLU:HG2 | 2.16 | 0.45 |
| 1:A:2165:LEU:HD12 | 1:A:2200:ALA:HB1 | 1.97 | 0.45 |
| 1:A:3295:GLU:HA | 1:A:3298:LEU:HD12 | 1.99 | 0.45 |
| 1:A:3607:GLU:OE2 | 1:A:3655:LYS:NZ | 2.48 | 0.45 |
| 1:A:3694:PHE:O | 1:A:3696:ARG:N | 2.47 | 0.45 |
| 1:B:1479:VAL:O | 1:B:1483:LEU:HG | 2.16 | 0.45 |
| 1:B:1684:LEU:HD23 | 1:B:1684:LEU:HA | 1.77 | 0.45 |
| 1:B:2224:PHE:CE2 | 1:B:2226:PRO:HG3 | 2.51 | 0.45 |
| 1:B:4090:ARG:NH1 | 1:B:4113:ASP:OD2 | 2.39 | 0.45 |
| 1:A:918:ALA:O | 1:A:972:LEU:HD21 | 2.16 | 0.45 |
| 1:A:2394:LYS:O | 1:A:2398:LEU:HG | 2.16 | 0.45 |
| 1:A:3658:ASP:OD1 | 1:A:3659:PHE:N | 2.49 | 0.45 |
| 1:B:216:LYS:O | 1:B:220:LEU:HD13 | 2.16 | 0.45 |
| 1:B:397:LEU:HD11 | 1:B:438:LEU:HD13 | 1.97 | 0.45 |
| 1:B:1779:GLN:NE2 | 1:B:1822:ARG:O | 2.47 | 0.45 |
| 1:B:3082:TYR:C | 1:B:3084:GLN:H | 2.19 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:651:TYR:O | 1:A:655:LEU:HG | 2.17 | 0.45 |
| 1:A:907:LEU:HA | 1:A:910:PHE:CZ | 2.51 | 0.45 |
| 1:A:1881:TYR:CD1 | 1:A:1951:VAL:HG23 | 2.51 | 0.45 |
| 1:A:2281:MET:HE1 | 1:A:2326:ILE:HG23 | 1.97 | 0.45 |
| 1:A:3133:GLN:O | 1:A:3137:GLU:HG2 | 2.17 | 0.45 |
| 1:A:4006:VAL:HB | 1:A:4040:PRO:HB3 | 1.99 | 0.45 |
| 1:A:4008:GLU:O | 1:A:4010:SER:N | 2.48 | 0.45 |
| 1:B:1423:ILE:HD12 | 1:B:1458:LEU:HD11 | 1.99 | 0.45 |
| 1:B:1529:VAL:HA | 1:B:1532:LEU:HD12 | 1.97 | 0.45 |
| 1:B:1840:PHE:O | 1:B:1843:ILE:HG22 | 2.16 | 0.45 |
| 1:B:2524:PHE:O | 1:B:2530:ARG:HG2 | 2.16 | 0.45 |
| 1:B:2841:ASN:O | 1:B:2845:ASN:ND2 | 2.37 | 0.45 |
| 1:B:3694:PHE:O | 1:B:3696:ARG:HG3 | 2.15 | 0.45 |
| 2:C:729:LEU:O | 2:C:732:ILE:HB | 2.16 | 0.45 |
| 1:A:574:LYS:HA | 1:A:574:LYS:HD2 | 1.71 | 0.45 |
| 1:A:1224:PHE:HD1 | 1:A:1266:CYS:SG | 2.39 | 0.45 |
| 1:A:3575:LEU:HB3 | 1:A:3800:LEU:HD21 | 1.98 | 0.45 |
| 1:B:907:LEU:CD2 | 1:B:940:PHE:CD2 | 2.99 | 0.45 |
| 1:B:2486:ASP:O | 1:B:2488:GLU:N | 2.50 | 0.45 |
| 1:B:3659:PHE:HD2 | 1:B:3662:ILE:HG12 | 1.80 | 0.45 |
| 1:B:4013:TRP:HA | 1:B:4016:PHE:HB3 | 1.98 | 0.45 |
| 1:A:743:LEU:HD12 | 1:A:743:LEU:O | 2.16 | 0.45 |
| 1:A:2973:ASP:O | 1:A:2977:ASN:ND2 | 2.47 | 0.45 |
| 1:A:3335:ARG:NH1 | 1:A:3422:GLN:HG2 | 2.31 | 0.45 |
| 1:B:148:LYS:O | 1:B:152:LEU:HB2 | 2.16 | 0.45 |
| 1:B:1832:SER:OG | 1:B:1833:LEU:N | 2.50 | 0.45 |
| 1:B:3288:SER:HB2 | 1:B:3296:GLN:HG3 | 1.99 | 0.45 |
| 1:B:3354:ASP:OD1 | 1:B:3354:ASP:N | 2.46 | 0.45 |
| 1:B:3862:ALA:HB3 | 1:B:4119:ARG:HH12 | 1.81 | 0.45 |
| 1:B:4047:ALA:HA | 1:B:4050:LYS:HG2 | 1.98 | 0.45 |
| 1:A:1920:TYR:HA | 1:A:1923:PHE:CZ | 2.52 | 0.45 |
| 1:A:2787:HIS:O | 1:A:2790:LEU:HG | 2.17 | 0.45 |
| 1:A:3506:LEU:HA | 1:A:3511:ALA:HB1 | 1.98 | 0.45 |
| 1:B:3455:LYS:HE2 | 1:B:3489:SER:O | 2.17 | 0.45 |
| 1:A:19:LEU:O | 1:A:24:ARG:NH1 | 2.50 | 0.45 |
| 1:A:253:LEU:HA | 1:A:256:ILE:HG12 | 1.98 | 0.45 |
| 1:A:1427:SER:O | 1:A:1431:LEU:HG | 2.16 | 0.45 |
| 1:A:1646:LEU:HD13 | 1:A:1692:ALA:HB2 | 1.98 | 0.45 |
| 1:B:2004:TYR:O | 1:B:2007:ILE:HB | 2.17 | 0.45 |
| 1:A:376:ILE:HG23 | 1:A:377:ASN:H | 1.82 | 0.45 |
| 1:A:1181:THR:HG22 | 1:A:1184:ARG:NH1 | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1580:LEU:HG | 1:A:1625:HIS:NE2 | 2.31 | 0.45 |
| 1:A:2538:ARG:O | 1:A:2542:LEU:HG | 2.17 | 0.45 |
| 1:A:3120:LEU:H | 1:A:3120:LEU:HD23 | 1.81 | 0.45 |
| 1:A:3885:ARG:HA | 1:A:3888:VAL:HG12 | 1.99 | 0.45 |
| 1:B:3061:LEU:O | 1:B:3065:ILE:HG12 | 2.16 | 0.45 |
| 1:A:288:ASP:OD1 | 1:A:288:ASP:N | 2.50 | 0.45 |
| 1:A:371:GLY:HA2 | 1:A:423:TYR:CD2 | 2.52 | 0.45 |
| 1:A:1143:VAL:HG23 | 1:A:1197:LEU:HD22 | 1.98 | 0.45 |
| 1:A:3948:SER:HB3 | 1:A:4016:PHE:HZ | 1.82 | 0.45 |
| 1:B:1205:ASN:HA | 1:B:1275:THR:HA | 1.99 | 0.45 |
| 1:B:1941:HIS:HB3 | 1:B:1981:LEU:HD23 | 1.98 | 0.45 |
| 1:B:2277:LEU:HD21 | 1:B:2326:ILE:HD11 | 1.99 | 0.45 |
| 1:B:3493:TRP:CE3 | 1:B:3494:GLN:HG3 | 2.52 | 0.45 |
| 1:B:3563:ASP:CG | 1:B:3568:ILE:H | 2.21 | 0.45 |
| 1:B:3988:LEU:O | 1:B:3992:ARG:HG2 | 2.17 | 0.45 |
| 1:A:583:LEU:HA | 1:A:614:PRO:HA | 1.99 | 0.45 |
| 1:A:2420:PHE:HE1 | 1:A:2435:CYS:HB2 | 1.82 | 0.45 |
| 1:A:2572:TYR:HA | 1:A:2787:HIS:CD2 | 2.52 | 0.45 |
| 1:A:3476:PRO:HA | 1:A:3480:LEU:HD13 | 1.99 | 0.45 |
| 1:B:12:LEU:HD21 | 1:B:58:VAL:HA | 1.99 | 0.45 |
| 1:B:1362:ASP:OD1 | 1:B:1362:ASP:N | 2.50 | 0.45 |
| 1:B:1872:GLY:O | 1:B:1876:ILE:HG13 | 2.17 | 0.45 |
| 1:B:1877:LEU:HD13 | 1:B:1915:LEU:HD11 | 1.98 | 0.45 |
| 1:B:1906:THR:HG22 | 1:B:1906:THR:O | 2.16 | 0.45 |
| 1:B:2172:ALA:HB2 | 1:B:2189:ILE:HG21 | 1.99 | 0.45 |
| 1:B:4005:PHE:O | 1:B:4011:PHE:HZ | 1.99 | 0.45 |
| 1:A:3813:LYS:HB2 | 1:A:3925:LEU:CB | 2.47 | 0.44 |
| 1:B:487:LEU:HA | 1:B:490:ILE:HG12 | 2.00 | 0.44 |
| 1:B:1006:THR:OG1 | 1:B:1054:VAL:HG21 | 2.17 | 0.44 |
| 1:B:1190:LEU:HD23 | 1:B:1190:LEU:HA | 1.80 | 0.44 |
| 1:B:3082:TYR:HB3 | 1:B:3085:GLU:OE1 | 2.17 | 0.44 |
| 1:B:3962:ARG:NH1 | 1:B:4125:GLU:O | 2.29 | 0.44 |
| 1:A:1878:ASP:OD2 | 1:A:1946:ASN:HB3 | 2.17 | 0.44 |
| 1:A:2249:LEU:O | 1:A:2251:ILE:HG23 | 2.17 | 0.44 |
| 1:A:3091:LEU:O | 1:A:3192:LYS:HE2 | 2.16 | 0.44 |
| 1:A:3257:LYS:HG3 | 1:A:3258:LEU:N | 2.31 | 0.44 |
| 1:B:569:VAL:HG12 | 1:B:573:LEU:HD23 | 1.99 | 0.44 |
| 1:B:1072:ALA:HA | 1:B:1075:ARG:NH2 | 2.32 | 0.44 |
| 1:B:1508:LYS:HZ2 | 1:B:1562:LEU:HD22 | 1.82 | 0.44 |
| 1:B:1727:ARG:HH21 | 1:B:1773:VAL:HG23 | 1.83 | 0.44 |
| 1:B:3113:ASN:O | 1:B:3117:ILE:HG13 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3450:MET:HB3 | 1:B:3468:LEU:HD11 | 1.98 | 0.44 |
| 1:B:3733:ARG:HD3 | 1:B:3753:LYS:HG2 | 1.98 | 0.44 |
| 1:B:3811:THR:HG21 | 1:B:3926:ASN:ND2 | 2.32 | 0.44 |
| 1:B:4064:LEU:HD13 | 1:B:4077:TYR:HB3 | 1.98 | 0.44 |
| 1:A:1633:TRP:CD1 | 1:A:1633:TRP:N | 2.85 | 0.44 |
| 1:B:303:HIS:O | 1:B:305:ASN:N | 2.44 | 0.44 |
| 1:B:1143:VAL:HG23 | 1:B:1197:LEU:HG | 1.99 | 0.44 |
| 1:B:2168:LEU:HB2 | 1:B:2193:ILE:HD12 | 1.99 | 0.44 |
| 1:B:2436:LEU:HD23 | 1:B:2472:GLN:HB3 | 1.99 | 0.44 |
| 1:B:3295:GLU:HA | 1:B:3298:LEU:HD12 | 1.99 | 0.44 |
| 1:A:19:LEU:HD21 | 1:A:71:LYS:HG3 | 1.98 | 0.44 |
| 1:A:635:PRO:O | 1:A:679:LYS:NZ | 2.44 | 0.44 |
| 1:A:870:LEU:HB3 | 1:A:3129:LEU:HD11 | 1.99 | 0.44 |
| 1:A:1730:PRO:HG2 | 1:A:1733:THR:OG1 | 2.16 | 0.44 |
| 1:A:2531:LEU:HD22 | 1:A:2541:ALA:HB1 | 2.00 | 0.44 |
| 1:A:2801:ASP:HB3 | 1:A:2804:ILE:HG22 | 1.99 | 0.44 |
| 1:A:3385:LEU:HD22 | 1:A:3416:LEU:HB2 | 2.00 | 0.44 |
| 1:B:377:ASN:HB3 | 1:B:380:ASP:H | 1.83 | 0.44 |
| 1:B:1298:LEU:CB | 1:B:1367:HIS:HB3 | 2.47 | 0.44 |
| 1:B:2894:GLU:O | 1:B:2896:ALA:N | 2.44 | 0.44 |
| 1:B:3659:PHE:CE2 | 1:B:3662:ILE:HG23 | 2.53 | 0.44 |
| 1:A:2473:MET:O | 1:A:2476:ILE:HG12 | 2.17 | 0.44 |
| 1:A:2813:PHE:CD2 | 1:A:2861:ILE:HB | 2.53 | 0.44 |
| 1:A:2870:SER:HB2 | 1:A:2922:ARG:HH22 | 1.81 | 0.44 |
| 1:B:720:GLN:OE1 | 1:B:1026:ARG:NH2 | 2.50 | 0.44 |
| 1:B:1690:GLY:O | 1:B:1693:VAL:HG12 | 2.18 | 0.44 |
| 1:B:3057:ALA:C | 1:B:3059:GLN:H | 2.19 | 0.44 |
| 1:A:267:VAL:HG23 | 1:A:268:PRO:HD3 | 2.00 | 0.44 |
| 1:A:859:LEU:HD21 | 1:A:870:LEU:HD13 | 1.99 | 0.44 |
| 1:A:2389:PHE:CE1 | 1:A:2393:LEU:HD22 | 2.53 | 0.44 |
| 1:A:3833:ARG:HB3 | 1:A:3877:LYS:HE2 | 2.00 | 0.44 |
| 1:B:605:THR:OG1 | 1:B:1027:ASP:HB3 | 2.18 | 0.44 |
| 1:B:1070:PRO:HA | 1:B:1113:LEU:HD21 | 1.99 | 0.44 |
| 1:B:1900:PHE:CE2 | 1:B:1906:THR:OG1 | 2.71 | 0.44 |
| 1:B:2404:ARG:HD2 | 1:B:2404:ARG:HA | 1.64 | 0.44 |
| 1:A:359:LEU:HD23 | 1:A:359:LEU:H | 1.81 | 0.44 |
| 1:A:563:LEU:HD13 | 1:A:563:LEU:HA | 1.84 | 0.44 |
| 1:A:1010:LEU:O | 1:A:1014:LEU:HD13 | 2.18 | 0.44 |
| 1:A:2122:LEU:HA | 1:A:2122:LEU:HD23 | 1.66 | 0.44 |
| 1:A:2572:TYR:N | 1:A:2573:PRO:HD3 | 2.32 | 0.44 |
| 1:B:364:ARG:HH22 | 1:B:368:LEU:HD13 | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1041:ILE:HG22 | 1:B:1049:GLN:HE22 | 1.83 | 0.44 |
| 1:B:2972:TYR:HB3 | 1:B:2998:SER:OG | 2.17 | 0.44 |
| 1:B:3326:GLN:O | 1:B:3329:LEU:HG | 2.16 | 0.44 |
| 1:A:250:ASN:O | 1:A:254:LYS:HE2 | 2.17 | 0.44 |
| 1:A:336:ASN:OD1 | 1:A:337:LYS:HD2 | 2.18 | 0.44 |
| 1:A:1633:TRP:CH2 | 1:A:1674:THR:HG22 | 2.53 | 0.44 |
| 1:A:1951:VAL:O | 1:A:1955:VAL:HG13 | 2.18 | 0.44 |
| 1:A:1990:PHE:HZ | 1:A:2144:LEU:HD21 | 1.83 | 0.44 |
| 1:A:2785:ILE:HG12 | 1:A:2786:LYS:HB2 | 1.99 | 0.44 |
| 1:A:3094:ASP:OD1 | 1:A:3196:LYS:NZ | 2.43 | 0.44 |
| 1:A:3846:MET:HG2 | 1:A:3862:ALA:HB2 | 2.00 | 0.44 |
| 1:B:263:LYS:HA | 1:B:263:LYS:HD3 | 1.82 | 0.44 |
| 1:B:1089:PHE:CE1 | 1:B:1096:VAL:HA | 2.53 | 0.44 |
| 1:B:1787:ARG:HB3 | 1:B:1831:CYS:HB3 | 1.98 | 0.44 |
| 1:B:3629:ARG:HD2 | 1:B:3633:ILE:HD11 | 2.00 | 0.44 |
| 1:B:3666:LEU:HA | 1:B:3669:LYS:HG2 | 2.00 | 0.44 |
| 1:A:1483:LEU:O | 1:A:1487:VAL:HG23 | 2.18 | 0.44 |
| 1:A:1712:ARG:O | 1:A:1716:GLN:HG2 | 2.18 | 0.44 |
| 1:A:3422:GLN:HE22 | 1:A:3423:GLN:NE2 | 2.15 | 0.44 |
| 1:B:1563:PHE:C | 1:B:1565:GLU:H | 2.21 | 0.44 |
| 1:B:1813:SER:HB3 | 1:B:1936:ARG:NH2 | 2.32 | 0.44 |
| 1:B:1861:SER:O | 1:B:1865:THR:OG1 | 2.25 | 0.44 |
| 1:B:2870:SER:HB2 | 1:B:2922:ARG:HH22 | 1.83 | 0.44 |
| 1:B:3085:GLU:OE1 | 1:B:3085:GLU:N | 2.40 | 0.44 |
| 1:B:3307:LEU:HD21 | 1:B:3326:GLN:OE1 | 2.17 | 0.44 |
| 1:A:388:LEU:HD12 | 1:A:388:LEU:HA | 1.86 | 0.43 |
| 1:A:642:PHE:HE2 | 1:A:673:THR:HG1 | 1.66 | 0.43 |
| 1:A:765:LEU:HD23 | 1:A:766:ALA:N | 2.32 | 0.43 |
| 1:A:1948:ALA:O | 1:A:1952:ILE:HG13 | 2.18 | 0.43 |
| 1:A:2572:TYR:CD2 | 1:A:2787:HIS:HB2 | 2.53 | 0.43 |
| 1:A:2863:CYS:HB2 | 1:A:2892:LEU:HD13 | 1.99 | 0.43 |
| 1:B:16:GLN:NE2 | 1:B:63:PHE:HA | 2.33 | 0.43 |
| 1:B:1563:PHE:HD1 | 1:B:1567:ILE:HD11 | 1.83 | 0.43 |
| 1:B:2146:LEU:HD12 | 1:B:2146:LEU:HA | 1.87 | 0.43 |
| 1:B:2538:ARG:O | 1:B:2542:LEU:HG | 2.17 | 0.43 |
| 1:A:1029:CYS:O | 1:A:1032:CYS:HB2 | 2.18 | 0.43 |
| 1:A:1067:ALA:O | 1:A:1075:ARG:HB2 | 2.18 | 0.43 |
| 1:A:1075:ARG:NE | 1:A:1114:ALA:HB2 | 2.34 | 0.43 |
| 1:A:1282:LEU:HD13 | 1:A:1291:LEU:HD21 | 1.99 | 0.43 |
| 1:A:1361:LYS:HA | 1:A:1364:CYS:HB2 | 2.00 | 0.43 |
| 1:A:1802:TYR:CZ | 1:A:1843:ILE:HD11 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3662:ILE:HA | 1:A:3665:MET:CE | 2.48 | 0.43 |
| 1:A:3835:PRO:O | 1:A:3839:TYR:HB2 | 2.17 | 0.43 |
| 1:B:713:GLU:O | 1:B:716:VAL:HG12 | 2.19 | 0.43 |
| 1:B:1787:ARG:O | 1:B:1787:ARG:HG2 | 2.18 | 0.43 |
| 1:B:2084:GLU:O | 1:B:2089:ASN:ND2 | 2.49 | 0.43 |
| 1:B:2239:LYS:HG3 | 1:B:2279:ILE:HG23 | 2.00 | 0.43 |
| 1:B:2264:ASP:O | 1:B:2266:ASN:N | 2.49 | 0.43 |
| 1:A:1723:PRO:HD2 | 1:A:1739:TYR:CD1 | 2.53 | 0.43 |
| 1:A:1790:SER:O | 1:A:1793:THR:HG22 | 2.18 | 0.43 |
| 1:B:1672:PHE:HE2 | 1:B:1702:LEU:HD21 | 1.84 | 0.43 |
| 1:B:1848:ILE:HD12 | 1:B:1848:ILE:HA | 1.85 | 0.43 |
| 1:B:2958:LEU:HG | 1:B:4101:GLU:HG2 | 2.00 | 0.43 |
| 1:B:3386:SER:O | 1:B:3389:VAL:HG22 | 2.18 | 0.43 |
| 1:B:3778:ASP:OD1 | 1:B:3779:SER:N | 2.50 | 0.43 |
| 1:A:583:LEU:HD23 | 1:A:583:LEU:H | 1.83 | 0.43 |
| 1:A:585:ILE:HA | 1:A:611:ASN:OD1 | 2.18 | 0.43 |
| 1:A:4099:SER:O | 1:A:4103:GLN:HB2 | 2.18 | 0.43 |
| 1:B:414:LEU:HD13 | 1:B:414:LEU:HA | 1.87 | 0.43 |
| 1:B:1186:LYS:HA | 1:B:1186:LYS:HD3 | 1.82 | 0.43 |
| 1:B:1463:LEU:HG | 1:B:1466:ASN:HB2 | 2.00 | 0.43 |
| 1:B:2372:PRO:HG2 | 1:B:2373:PRO:HD3 | 2.01 | 0.43 |
| 1:B:3659:PHE:CE2 | 1:B:3661:ASP:HB3 | 2.53 | 0.43 |
| 1:B:3910:LEU:HD12 | 1:B:3910:LEU:HA | 1.84 | 0.43 |
| 1:A:227:LEU:O | 1:A:231:LEU:HB2 | 2.18 | 0.43 |
| 1:A:432:THR:N | 1:A:433:PRO:HD2 | 2.33 | 0.43 |
| 1:A:561:ASN:HA | 1:A:564:LEU:HD12 | 2.00 | 0.43 |
| 1:A:1294:VAL:O | 1:A:1298:LEU:HD13 | 2.18 | 0.43 |
| 1:A:1479:VAL:O | 1:A:1483:LEU:HG | 2.17 | 0.43 |
| 1:A:1666:GLY:C | 1:A:1669:PRO:HD2 | 2.39 | 0.43 |
| 1:A:2091:HIS:O | 1:A:2093:CYS:N | 2.52 | 0.43 |
| 1:A:2281:MET:HG2 | 1:A:2326:ILE:HG12 | 2.01 | 0.43 |
| 1:A:3623:PRO:HG2 | 1:A:3633:ILE:HD12 | 2.00 | 0.43 |
| 1:B:1017:ILE:HG23 | 1:B:1018:VAL:HG13 | 2.01 | 0.43 |
| 1:B:1023:SER:HA | 1:B:1026:ARG:HE | 1.83 | 0.43 |
| 1:B:1747:LEU:HD12 | 1:B:1781:SER:CB | 2.48 | 0.43 |
| 1:B:1790:SER:O | 1:B:1793:THR:HG22 | 2.18 | 0.43 |
| 1:B:1832:SER:N | 1:B:1883:ARG:HH22 | 2.11 | 0.43 |
| 1:B:2375:ALA:O | 1:B:2379:MET:N | 2.51 | 0.43 |
| 1:B:2439:ILE:O | 1:B:2443:MET:HG3 | 2.19 | 0.43 |
| 1:B:2950:LYS:HE3 | 1:B:2981:TRP:CE3 | 2.54 | 0.43 |
| 1:B:3068:ALA:O | 1:B:3074:GLN:HB3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3979:LEU:O | 1:B:3983:ILE:HG12 | 2.19 | 0.43 |
| 1:A:1208:LEU:HD12 | 1:A:1208:LEU:HA | 1.81 | 0.43 |
| 1:A:1575:LEU:HD23 | 1:A:1617:LYS:HG2 | 2.00 | 0.43 |
| 1:A:3077:ILE:HG23 | 1:A:3081:HIS:CE1 | 2.52 | 0.43 |
| 1:A:3992:ARG:NH1 | 1:A:4103:GLN:OE1 | 2.51 | 0.43 |
| 1:A:3999:THR:HA | 1:A:4002:MET:CE | 2.49 | 0.43 |
| 1:B:765:LEU:HA | 1:B:768:VAL:HG12 | 2.01 | 0.43 |
| 1:B:1361:LYS:HA | 1:B:1361:LYS:HD2 | 1.88 | 0.43 |
| 1:B:1626:TRP:CZ3 | 1:B:1674:THR:HG21 | 2.54 | 0.43 |
| 1:B:2398:LEU:O | 1:B:2401:VAL:HG12 | 2.19 | 0.43 |
| 1:A:1718:ILE:HG12 | 1:A:1722:PHE:CE2 | 2.54 | 0.43 |
| 1:A:2327:LEU:HD13 | 1:A:2371:PHE:CD2 | 2.54 | 0.43 |
| 1:A:2419:ASP:HB2 | 1:A:2422:GLN:HB2 | 2.00 | 0.43 |
| 1:A:3268:THR:HG23 | 1:A:3269:ARG:H | 1.84 | 0.43 |
| 1:B:418:ALA:CB | 1:B:463:LYS:HG3 | 2.49 | 0.43 |
| 1:B:977:ASP:O | 1:B:980:THR:HG22 | 2.18 | 0.43 |
| 1:B:1839:PHE:HA | 1:B:1842:THR:HG22 | 2.00 | 0.43 |
| 1:B:2551:GLU:HA | 1:B:2554:PHE:HB2 | 2.00 | 0.43 |
| 1:B:3829:LEU:HD23 | 1:B:3829:LEU:HA | 1.87 | 0.43 |
| 1:B:3988:LEU:HD21 | 1:B:4103:GLN:OE1 | 2.19 | 0.43 |
| 1:B:4126:PRO:HD2 | 1:B:4127:TRP:CZ3 | 2.53 | 0.43 |
| 1:A:3596:LEU:HD22 | 1:A:3606:ILE:HD12 | 2.01 | 0.43 |
| 1:A:3670:MET:HE2 | 1:A:3670:MET:HB2 | 1.78 | 0.43 |
| 1:A:3798:SER:O | 1:A:3799:ARG:HG2 | 2.19 | 0.43 |
| 1:A:3867:THR:HG21 | 1:A:4119:ARG:CZ | 2.49 | 0.43 |
| 1:B:484:HIS:CE1 | 1:B:575:ILE:HG13 | 2.53 | 0.43 |
| 1:B:2511:ILE:HG12 | 1:B:2550:ILE:HG22 | 2.01 | 0.43 |
| 1:B:2548:PRO:HG3 | 1:B:2846:THR:HB | 2.01 | 0.43 |
| 1:B:3418:ASP:OD2 | 1:B:3464:LYS:NZ | 2.31 | 0.43 |
| 1:A:647:TYR:CD1 | 1:A:703:CYS:HB3 | 2.51 | 0.43 |
| 1:A:873:VAL:HG13 | 1:A:874:THR:N | 2.26 | 0.43 |
| 1:A:3019:ILE:HG21 | 1:A:3029:LYS:HB3 | 2.01 | 0.43 |
| 1:A:3301:LEU:HD11 | 1:A:3359:ILE:HD11 | 2.01 | 0.43 |
| 1:A:3669:LYS:HE2 | 1:A:3669:LYS:HB2 | 1.92 | 0.43 |
| 1:B:276:ALA:HA | 1:B:318:SER:CB | 2.49 | 0.43 |
| 1:B:1346:THR:HG23 | 1:B:1405:ALA:CB | 2.49 | 0.43 |
| 1:B:2451:LEU:HD12 | 1:B:2451:LEU:HA | 1.78 | 0.43 |
| 1:B:2492:ASP:HB3 | 1:B:2495:SER:H | 1.84 | 0.43 |
| 1:B:3411:ASP:OD1 | 1:B:3411:ASP:N | 2.46 | 0.43 |
| 1:B:3742:GLY:C | 1:B:3744:ASP:H | 2.22 | 0.43 |
| 1:A:112:THR:O | 1:A:116:THR:OG1 | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:149:ILE:HB | 1:A:185:HIS:ND1 | 2.34 | 0.43 |
| 1:A:633:ILE:C | 1:A:635:PRO:HD3 | 2.39 | 0.43 |
| 1:A:723:ASP:OD1 | 1:A:723:ASP:N | 2.52 | 0.43 |
| 1:A:912:PRO:O | 1:A:916:GLU:HB2 | 2.19 | 0.43 |
| 1:A:1122:GLY:HA2 | 1:A:1125:GLN:OE1 | 2.19 | 0.43 |
| 1:A:1962:TYR:O | 1:A:1967:PHE:HD2 | 2.02 | 0.43 |
| 1:A:2225:HIS:CE1 | 1:A:2230:VAL:HG21 | 2.54 | 0.43 |
| 1:A:3489:SER:O | 1:A:3490:VAL:HG23 | 2.19 | 0.43 |
| 1:A:4044:ILE:HD13 | 1:A:4044:ILE:HA | 1.72 | 0.43 |
| 1:A:4054:ALA:H | 1:A:4103:GLN:NE2 | 2.16 | 0.43 |
| 1:B:1001:PHE:CE1 | 1:B:1044:ILE:HD11 | 2.54 | 0.43 |
| 1:B:1859:ASN:HB3 | 1:B:1862:THR:HG22 | 2.01 | 0.43 |
| 1:B:3820:MET:HB3 | 1:B:3824:GLU:HG3 | 2.00 | 0.43 |
| 1:A:1348:LEU:HG | 1:A:1359:LEU:HD21 | 2.01 | 0.42 |
| 1:A:1411:TYR:O | 1:A:1415:LEU:HG | 2.19 | 0.42 |
| 1:A:1440:ASP:OD1 | 1:A:1440:ASP:N | 2.52 | 0.42 |
| 1:A:1858:LEU:HD23 | 1:A:1858:LEU:HA | 1.88 | 0.42 |
| 1:A:3661:ASP:O | 1:A:3665:MET:HG3 | 2.18 | 0.42 |
| 1:B:487:LEU:HD22 | 1:B:571:SER:OG | 2.19 | 0.42 |
| 1:B:523:THR:OG1 | 1:B:524:TYR:N | 2.52 | 0.42 |
| 1:B:2219:LEU:O | 1:B:2223:VAL:HB | 2.19 | 0.42 |
| 1:B:3324:ARG:O | 1:B:3328:ILE:HG13 | 2.18 | 0.42 |
| 1:B:3872:ARG:HA | 1:B:3875:GLU:HG2 | 2.01 | 0.42 |
| 1:A:465:PHE:HE1 | 1:A:482:VAL:HG11 | 1.84 | 0.42 |
| 1:A:969:LEU:HD23 | 1:A:969:LEU:HA | 1.79 | 0.42 |
| 1:A:1057:LYS:HE3 | 1:A:1099:PHE:HB2 | 2.01 | 0.42 |
| 1:A:1134:LEU:HD23 | 1:A:1134:LEU:HA | 1.83 | 0.42 |
| 1:A:1263:ALA:HA | 1:A:1266:CYS:HG | 1.84 | 0.42 |
| 1:A:2896:ALA:O | 1:A:2899:ARG:NE | 2.47 | 0.42 |
| 1:B:527:TYR:O | 1:B:531:PHE:HD1 | 2.02 | 0.42 |
| 1:B:961:LEU:O | 1:B:965:THR:OG1 | 2.21 | 0.42 |
| 1:B:1579:VAL:O | 1:B:1583:MET:HG2 | 2.19 | 0.42 |
| 1:B:1648:LEU:O | 1:B:1652:ILE:HG12 | 2.20 | 0.42 |
| 1:B:1984:LEU:O | 1:B:1984:LEU:HD23 | 2.19 | 0.42 |
| 1:B:3114:TYR:CE2 | 1:B:3125:ARG:HB3 | 2.54 | 0.42 |
| 1:A:168:ASP:OD1 | 1:A:219:VAL:HG23 | 2.19 | 0.42 |
| 1:A:767:GLU:OE1 | 1:A:854:ARG:NH1 | 2.52 | 0.42 |
| 1:A:1801:VAL:HB | 1:A:1824:LEU:HD12 | 2.01 | 0.42 |
| 1:A:1856:THR:HG22 | 1:A:1858:LEU:HB2 | 2.00 | 0.42 |
| 1:A:2477:LEU:HB3 | 1:A:2506:LEU:HG | 2.02 | 0.42 |
| 1:A:2881:LEU:HD23 | 1:A:2886:GLN:HE21 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3118:ASP:OD2 | 1:A:3895:GLU:HB3 | 2.19 | 0.42 |
| 1:A:4027:TRP:O | 1:A:4028:ILE:HG23 | 2.18 | 0.42 |
| 1:A:4085:LYS:H | 1:A:4091:ALA:HB3 | 1.84 | 0.42 |
| 1:B:128:LEU:HD23 | 1:B:128:LEU:HA | 1.86 | 0.42 |
| 1:A:1333:SER:O | 1:A:1336:THR:HG22 | 2.20 | 0.42 |
| 1:A:1342:MET:HA | 1:A:1345:THR:HG22 | 2.02 | 0.42 |
| 1:A:1515:LEU:HD21 | 1:A:1519:PHE:CE2 | 2.54 | 0.42 |
| 1:A:1820:VAL:O | 1:A:1825:LEU:HG | 2.19 | 0.42 |
| 1:A:1851:LEU:HB3 | 1:A:1918:LEU:HD13 | 2.01 | 0.42 |
| 1:A:2225:HIS:O | 1:A:2227:LYS:N | 2.52 | 0.42 |
| 1:A:2288:TYR:CD1 | 1:A:2291:GLN:HB2 | 2.54 | 0.42 |
| 1:A:2368:THR:HA | 1:A:2371:PHE:O | 2.20 | 0.42 |
| 1:A:3020:ASP:O | 1:A:3024:PRO:HB3 | 2.18 | 0.42 |
| 1:A:3274:VAL:O | 1:A:3278:GLN:HG3 | 2.19 | 0.42 |
| 1:A:4055:ASN:HB3 | 1:A:4058:VAL:HG23 | 2.00 | 0.42 |
| 1:B:51:LEU:HD11 | 1:B:95:LYS:HD3 | 2.01 | 0.42 |
| 1:B:101:ALA:HB1 | 1:B:143:LEU:HD11 | 2.02 | 0.42 |
| 1:B:104:SER:HB3 | 1:B:134:LEU:HD11 | 2.01 | 0.42 |
| 1:B:302:ALA:HB2 | 1:B:358:GLU:OE2 | 2.20 | 0.42 |
| 1:B:651:TYR:CE1 | 1:B:655:LEU:HD11 | 2.53 | 0.42 |
| 1:B:1927:MET:HE3 | 1:B:1927:MET:HB2 | 1.90 | 0.42 |
| 1:A:767:GLU:HG3 | 1:A:846:ILE:HD13 | 2.01 | 0.42 |
| 1:A:983:LEU:O | 1:A:984:TYR:HB2 | 2.19 | 0.42 |
| 1:A:1873:TYR:HD1 | 1:A:1873:TYR:HA | 1.78 | 0.42 |
| 1:A:1990:PHE:HB2 | 1:A:2179:GLY:HA3 | 2.01 | 0.42 |
| 1:A:2350:LYS:HG2 | 1:A:2378:PHE:HE1 | 1.84 | 0.42 |
| 1:A:3535:ILE:HD12 | 1:A:3759:ARG:NH1 | 2.33 | 0.42 |
| 1:B:354:SER:HA | 1:B:358:GLU:HB2 | 2.00 | 0.42 |
| 1:B:3049:LEU:O | 1:B:3053:LEU:HG | 2.18 | 0.42 |
| 1:B:3654:MET:HG2 | 1:B:3656:LEU:HB2 | 2.02 | 0.42 |
| 1:B:3891:SER:C | 1:B:3893:SER:H | 2.22 | 0.42 |
| 1:A:1788:ARG:H | 1:A:1794:GLN:HE21 | 1.67 | 0.42 |
| 1:A:1840:PHE:O | 1:A:1843:ILE:HG22 | 2.19 | 0.42 |
| 1:A:2193:ILE:O | 1:A:2196:TRP:NE1 | 2.52 | 0.42 |
| 1:A:2514:ASN:O | 1:A:2517:LEU:HB3 | 2.18 | 0.42 |
| 1:A:3450:MET:HB2 | 1:A:3450:MET:HE2 | 1.92 | 0.42 |
| 1:A:3998:LEU:O | 1:A:4002:MET:HG3 | 2.19 | 0.42 |
| 1:B:413:PHE:O | 1:B:417:VAL:HG23 | 2.19 | 0.42 |
| 1:B:1254:LEU:H | 1:B:1254:LEU:HD22 | 1.84 | 0.42 |
| 1:B:1264:LEU:HD21 | 1:B:1341:ILE:HG13 | 2.01 | 0.42 |
| 1:B:2556:SER:HB2 | 1:B:2799:GLN:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3558:ILE:O | 1:B:3562:LEU:HB2 | 2.20 | 0.42 |
| 1:A:71:LYS:O | 1:A:71:LYS:HD3 | 2.20 | 0.42 |
| 1:A:1909:ASN:HB2 | 1:A:1913:LYS:HB2 | 2.01 | 0.42 |
| 1:A:2101:VAL:HG12 | 1:A:2156:VAL:HG21 | 2.01 | 0.42 |
| 1:A:2436:LEU:O | 1:A:2439:ILE:HG22 | 2.19 | 0.42 |
| 1:A:3144:PHE:CE2 | 1:A:3157:LEU:HD13 | 2.55 | 0.42 |
| 1:B:1010:LEU:O | 1:B:1014:LEU:HD13 | 2.20 | 0.42 |
| 1:B:1519:PHE:CE2 | 1:B:1528:LEU:HD22 | 2.54 | 0.42 |
| 1:B:2312:TYR:O | 1:B:2315:VAL:HG12 | 2.19 | 0.42 |
| 1:B:2921:LEU:O | 1:B:2925:GLU:HG2 | 2.20 | 0.42 |
| 1:A:178:LEU:HD23 | 1:A:181:LEU:HD12 | 2.01 | 0.42 |
| 1:A:1395:LEU:HB3 | 1:A:1396:PRO:HD3 | 2.02 | 0.42 |
| 1:A:1703:THR:O | 1:A:1707:LEU:HB2 | 2.19 | 0.42 |
| 1:A:2105:HIS:CG | 1:A:2156:VAL:HG13 | 2.55 | 0.42 |
| 1:A:3502:MET:SD | 1:A:3514:VAL:HG21 | 2.59 | 0.42 |
| 1:B:93:LEU:HD21 | 1:B:134:LEU:HD12 | 2.01 | 0.42 |
| 1:B:528:VAL:HA | 1:B:633:ILE:HD11 | 2.02 | 0.42 |
| 1:B:2288:TYR:HD2 | 1:B:2291:GLN:HB2 | 1.85 | 0.42 |
| 1:B:2586:PHE:N | 1:B:2783:ILE:HD11 | 2.34 | 0.42 |
| 1:B:3006:ALA:O | 1:B:3257:LYS:HE3 | 2.20 | 0.42 |
| 1:B:3760:GLN:O | 1:B:3764:VAL:HG13 | 2.20 | 0.42 |
| 1:A:268:PRO:HB2 | 1:A:308:LEU:HD11 | 2.01 | 0.42 |
| 1:A:484:HIS:CE1 | 1:A:488:ILE:HD11 | 2.55 | 0.42 |
| 1:A:1601:LEU:HD22 | 1:A:1618:LEU:HD21 | 2.02 | 0.42 |
| 1:A:1952:ILE:O | 1:A:1955:VAL:HG22 | 2.20 | 0.42 |
| 1:A:2255:LEU:HD23 | 1:A:2256:ILE:HG13 | 2.01 | 0.42 |
| 1:B:736:LEU:HD22 | 1:B:741:ILE:HD12 | 2.01 | 0.42 |
| 1:B:2128:PHE:CZ | 1:B:2132:LYS:HD2 | 2.55 | 0.42 |
| 1:B:2251:ILE:HD12 | 1:B:2253:TYR:CE2 | 2.55 | 0.42 |
| 1:B:3464:LYS:HE3 | 1:B:3997:LEU:HD23 | 2.01 | 0.42 |
| 1:A:465:PHE:CE1 | 1:A:482:VAL:HG11 | 2.55 | 0.42 |
| 1:A:966:PHE:HE1 | 1:A:969:LEU:HD12 | 1.83 | 0.42 |
| 1:A:1018:VAL:CG1 | 1:A:1074:LYS:HA | 2.50 | 0.42 |
| 1:A:1283:GLY:HA2 | 1:A:1358:LEU:HD11 | 2.02 | 0.42 |
| 1:A:1991:PRO:O | 1:A:2184:TYR:HB2 | 2.20 | 0.42 |
| 1:A:3110:PHE:CD1 | 1:A:3128:LYS:HD2 | 2.52 | 0.42 |
| 1:A:3511:ALA:HB3 | 1:A:3551:ASN:ND2 | 2.34 | 0.42 |
| 1:A:3554:PHE:CE2 | 1:A:3558:ILE:HD11 | 2.54 | 0.42 |
| 1:A:3629:ARG:NH2 | 1:A:3634:GLN:HB2 | 2.35 | 0.42 |
| 1:A:3868:VAL:O | 1:A:3872:ARG:HG2 | 2.19 | 0.42 |
| 1:B:573:LEU:HA | 1:B:576:VAL:HG12 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:631:ARG:HG3 | 1:B:672:ILE:HD11 | 2.01 | 0.42 |
| 1:B:2255:LEU:HD23 | 1:B:2256:ILE:HG13 | 2.02 | 0.42 |
| 1:B:2304:VAL:HG21 | 1:B:2344:LEU:HG | 2.02 | 0.42 |
| 1:B:2334:LYS:HE3 | 1:B:2334:LYS:HB2 | 1.90 | 0.42 |
| 1:B:2458:VAL:CG1 | 1:B:2476:ILE:HD11 | 2.50 | 0.42 |
| 1:B:2855:VAL:HA | 1:B:2858:ILE:HG12 | 2.02 | 0.42 |
| 1:B:3654:MET:HE2 | 1:B:3656:LEU:HB2 | 2.02 | 0.42 |
| 1:A:227:LEU:HD21 | 1:A:248:ILE:HD13 | 2.01 | 0.41 |
| 1:A:1982:ILE:HG22 | 1:A:1983:ASP:H | 1.85 | 0.41 |
| 1:A:2801:ASP:O | 1:A:2804:ILE:HG22 | 2.20 | 0.41 |
| 1:A:3326:GLN:O | 1:A:3329:LEU:HG | 2.20 | 0.41 |
| 1:B:1455:CYS:HA | 1:B:1458:LEU:HD12 | 2.01 | 0.41 |
| 1:B:1623:LEU:HD23 | 1:B:1623:LEU:HA | 1.87 | 0.41 |
| 1:B:1828:LEU:HD23 | 1:B:1828:LEU:HA | 1.90 | 0.41 |
| 1:B:3144:PHE:CZ | 1:B:3157:LEU:HD13 | 2.55 | 0.41 |
| 1:B:4055:ASN:HB3 | 1:B:4058:VAL:HG23 | 2.02 | 0.41 |
| 1:B:4082:ARG:HH12 | 1:B:4091:ALA:HA | 1.85 | 0.41 |
| 1:A:934:LEU:HB3 | 1:A:984:TYR:OH | 2.20 | 0.41 |
| 1:A:1916:ILE:HD13 | 1:A:1916:ILE:HA | 1.91 | 0.41 |
| 1:A:1947:CYS:O | 1:A:1951:VAL:HG12 | 2.20 | 0.41 |
| 1:A:2389:PHE:HB3 | 1:A:2393:LEU:HB2 | 2.02 | 0.41 |
| 1:B:69:VAL:HG22 | 1:B:82:ARG:HG3 | 2.02 | 0.41 |
| 1:B:132:ILE:HD12 | 1:B:173:LYS:HD2 | 2.01 | 0.41 |
| 1:B:217:LEU:HB3 | 1:B:218:PRO:HD3 | 2.02 | 0.41 |
| 1:B:873:VAL:HG13 | 1:B:874:THR:N | 2.28 | 0.41 |
| 1:B:1083:ASN:OD1 | 1:B:1126:GLN:HG3 | 2.19 | 0.41 |
| 1:B:1361:LYS:O | 1:B:1365:ASN:HB2 | 2.20 | 0.41 |
| 1:B:1837:ARG:HD3 | 1:B:1837:ARG:N | 2.34 | 0.41 |
| 1:B:1956:PHE:O | 1:B:1958:GLU:HG3 | 2.20 | 0.41 |
| 1:B:2151:ILE:HD13 | 1:B:2188:GLU:HB3 | 2.01 | 0.41 |
| 1:B:3268:THR:HG23 | 1:B:3269:ARG:H | 1.85 | 0.41 |
| 1:B:3339:ASN:OD1 | 1:B:3426:LYS:NZ | 2.37 | 0.41 |
| 1:B:3413:TYR:HB3 | 1:B:3449:LYS:O | 2.21 | 0.41 |
| 1:B:3761:ASP:HA | 1:B:3764:VAL:HG22 | 2.02 | 0.41 |
| 1:A:303:HIS:ND1 | 1:A:305:ASN:OD1 | 2.41 | 0.41 |
| 1:A:1579:VAL:H | 1:A:1579:VAL:HG22 | 1.66 | 0.41 |
| 1:A:2220:MET:HG2 | 1:A:2276:LEU:HD11 | 2.02 | 0.41 |
| 1:A:2274:ILE:HD12 | 1:A:2318:ALA:HB3 | 2.02 | 0.41 |
| 1:A:2402:LEU:CD1 | 1:A:2437:ASP:HB3 | 2.50 | 0.41 |
| 1:A:2887:PRO:HD2 | 1:A:2888:VAL:H | 1.84 | 0.41 |
| 1:A:2923:TRP:CD2 | 1:A:2946:GLU:HG3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1225:GLU:OE2 | 1:B:1288:SER:OG | 2.38 | 0.41 |
| 1:B:2003:LYS:HD3 | 1:B:2184:TYR:HE1 | 1.85 | 0.41 |
| 1:B:2519:LEU:HD13 | 1:B:2610:UNK:CA | 2.50 | 0.41 |
| 1:B:2528:GLU:OE2 | 1:B:2533:SER:HB3 | 2.21 | 0.41 |
| 1:A:1096:VAL:HB | 1:A:1101:PHE:CE2 | 2.55 | 0.41 |
| 1:A:1599:GLY:HA2 | 1:A:1602:ASP:OD1 | 2.21 | 0.41 |
| 1:A:2338:GLU:HA | 1:A:2341:LEU:HD21 | 2.02 | 0.41 |
| 1:A:3463:LEU:HD13 | 1:A:3498:TRP:CZ2 | 2.52 | 0.41 |
| 1:A:3652:LEU:HB3 | 1:A:3653:ARG:HE | 1.86 | 0.41 |
| 1:A:3708:ARG:HA | 1:A:3708:ARG:HD2 | 1.85 | 0.41 |
| 1:B:1096:VAL:HB | 1:B:1101:PHE:CE2 | 2.53 | 0.41 |
| 1:B:1261:LEU:HD21 | 1:B:1337:VAL:HA | 2.02 | 0.41 |
| 1:B:1825:LEU:O | 1:B:1829:TRP:HB2 | 2.21 | 0.41 |
| 1:B:2590:THR:OG1 | 1:B:2591:ILE:N | 2.53 | 0.41 |
| 1:B:3701:ILE:HB | 1:B:3719:ILE:HB | 2.02 | 0.41 |
| 1:B:3924:HIS:CD2 | 1:B:3924:HIS:H | 2.37 | 0.41 |
| 1:A:263:LYS:O | 1:A:264:ARG:HG2 | 2.21 | 0.41 |
| 1:A:1141:LYS:HA | 1:A:1141:LYS:HD2 | 1.80 | 0.41 |
| 1:A:1389:VAL:O | 1:A:1393:ALA:HB3 | 2.21 | 0.41 |
| 1:A:1440:ASP:HB2 | 1:A:1443:VAL:HG22 | 2.02 | 0.41 |
| 1:A:1474:ASP:OD1 | 1:A:1474:ASP:N | 2.54 | 0.41 |
| 1:A:1646:LEU:HD23 | 1:A:1646:LEU:HA | 1.87 | 0.41 |
| 1:B:170:VAL:O | 1:B:174:VAL:HG23 | 2.19 | 0.41 |
| 1:B:2379:MET:HG3 | 1:B:2383:PHE:CE2 | 2.55 | 0.41 |
| 1:B:3562:LEU:HD12 | 1:B:3562:LEU:HA | 1.88 | 0.41 |
| 1:B:3652:LEU:HB3 | 1:B:3653:ARG:HE | 1.86 | 0.41 |
| 1:B:3802:LEU:HD12 | 1:B:3802:LEU:HA | 1.96 | 0.41 |
| 1:B:3944:HIS:HB3 | 1:B:3948:SER:HB2 | 2.02 | 0.41 |
| 1:A:653:LEU:HD13 | 1:A:670:LEU:HG | 2.03 | 0.41 |
| 1:A:983:LEU:HD12 | 1:A:983:LEU:HA | 1.90 | 0.41 |
| 1:A:1117:ASP:O | 1:A:1118:GLU:HG2 | 2.20 | 0.41 |
| 1:A:1747:LEU:HD21 | 1:A:1778:PHE:CE1 | 2.55 | 0.41 |
| 1:A:3881:ASP:OD1 | 1:A:3881:ASP:N | 2.48 | 0.41 |
| 1:B:569:VAL:HA | 1:B:572:VAL:HG12 | 2.01 | 0.41 |
| 1:B:1448:LEU:HD23 | 1:B:1510:LEU:HD11 | 2.02 | 0.41 |
| 1:B:1949:ILE:HD11 | 1:B:2097:LEU:HD23 | 2.02 | 0.41 |
| 1:B:2477:LEU:HB3 | 1:B:2506:LEU:HG | 2.02 | 0.41 |
| 1:B:2507:ILE:HG22 | 1:B:2550:ILE:HD11 | 2.02 | 0.41 |
| 1:B:3082:TYR:O | 1:B:3084:GLN:N | 2.54 | 0.41 |
| 1:B:3554:PHE:O | 1:B:3558:ILE:HG13 | 2.20 | 0.41 |
| 1:B:3647:GLY:O | 1:B:3651:LEU:HB3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:385:TYR:CD2 | 1:A:389:ILE:HD11 | 2.50 | 0.41 |
| 1:A:446:PHE:CD1 | 1:A:530:LEU:HD22 | 2.55 | 0.41 |
| 1:A:871:LEU:H | 1:A:871:LEU:HD23 | 1.84 | 0.41 |
| 1:A:913:ARG:HA | 1:A:913:ARG:HD2 | 1.88 | 0.41 |
| 1:A:1117:ASP:OD2 | 1:A:1123:THR:OG1 | 2.25 | 0.41 |
| 1:A:1349:LEU:HD21 | 1:A:1356:TRP:HA | 2.02 | 0.41 |
| 1:A:1717:LEU:O | 1:A:1721:HIS:HB2 | 2.20 | 0.41 |
| 1:A:2289:ASP:O | 1:A:2291:GLN:N | 2.53 | 0.41 |
| 1:A:2436:LEU:HD22 | 1:A:2469:CYS:SG | 2.61 | 0.41 |
| 1:A:3167:ARG:O | 1:A:3186:ARG:NH2 | 2.52 | 0.41 |
| 1:A:3462:ARG:NH1 | 1:A:3707:GLY:HA3 | 2.35 | 0.41 |
| 1:A:3802:LEU:HA | 1:A:3802:LEU:HD12 | 1.86 | 0.41 |
| 1:B:1052:SER:HB3 | 1:B:1055:ASN:HB2 | 2.02 | 0.41 |
| 1:B:1601:LEU:HD13 | 1:B:1601:LEU:HA | 1.95 | 0.41 |
| 1:B:2256:ILE:H | 1:B:2256:ILE:HG13 | 1.56 | 0.41 |
| 1:B:2366:LYS:HA | 1:B:2366:LYS:HD3 | 1.84 | 0.41 |
| 1:B:2591:ILE:HD11 | 1:B:2792:THR:OG1 | 2.21 | 0.41 |
| 1:B:3465:PHE:HB3 | 1:B:3466:PRO:HD3 | 2.03 | 0.41 |
| 1:B:3598:LYS:NZ | 1:B:4031:ILE:HD13 | 2.36 | 0.41 |
| 1:A:414:LEU:HG | 1:A:464:VAL:CG2 | 2.51 | 0.41 |
| 1:A:451:PRO:C | 1:A:453:MET:H | 2.24 | 0.41 |
| 1:A:1134:LEU:O | 1:A:1137:ILE:HG22 | 2.19 | 0.41 |
| 1:A:1334:LYS:O | 1:A:1337:VAL:HG22 | 2.21 | 0.41 |
| 1:A:1969:GLU:HB3 | 1:A:1977:ILE:HG13 | 2.03 | 0.41 |
| 1:A:3061:LEU:HD12 | 1:A:3061:LEU:HA | 1.88 | 0.41 |
| 1:B:738:HIS:ND1 | 1:B:741:ILE:O | 2.54 | 0.41 |
| 1:B:1586:SER:HA | 1:B:1593:VAL:HG11 | 2.01 | 0.41 |
| 1:B:1969:GLU:HB2 | 1:B:1975:LEU:O | 2.21 | 0.41 |
| 1:B:2825:THR:O | 1:B:2829:LYS:N | 2.40 | 0.41 |
| 1:B:3641:ASP:O | 1:B:3645:GLY:N | 2.53 | 0.41 |
| 1:A:385:TYR:O | 1:A:389:ILE:HG13 | 2.21 | 0.41 |
| 1:A:904:VAL:O | 1:A:905:ILE:HD13 | 2.21 | 0.41 |
| 1:A:1534:ASN:HA | 1:A:1535:PRO:HD3 | 1.87 | 0.41 |
| 1:A:1733:THR:HG22 | 1:A:1735:ARG:H | 1.84 | 0.41 |
| 1:A:1779:GLN:O | 1:A:1783:ARG:HG3 | 2.20 | 0.41 |
| 1:A:1832:SER:OG | 1:A:1833:LEU:N | 2.52 | 0.41 |
| 1:A:1982:ILE:HG22 | 1:A:1983:ASP:N | 2.36 | 0.41 |
| 1:A:1990:PHE:CE2 | 1:A:2144:LEU:HD11 | 2.55 | 0.41 |
| 1:A:2203:THR:OG1 | 1:A:2247:ASP:HB2 | 2.21 | 0.41 |
| 1:A:2284:ASP:HB3 | 1:A:2285:LEU:HG | 2.03 | 0.41 |
| 1:A:2322:VAL:O | 1:A:2326:ILE:HG13 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2447:LYS:O | 1:A:2449:VAL:N | 2.50 | 0.41 |
| 1:A:2792:THR:N | 1:A:2793:PRO:HD2 | 2.36 | 0.41 |
| 1:A:3542:PHE:HZ | 1:A:3555:VAL:HG21 | 1.86 | 0.41 |
| 1:A:3924:HIS:H | 1:A:3924:HIS:CD2 | 2.39 | 0.41 |
| 1:B:212:VAL:HG22 | 1:B:213:ARG:H | 1.86 | 0.41 |
| 1:B:354:SER:CB | 1:B:359:LEU:H | 2.33 | 0.41 |
| 1:B:393:LYS:HA | 1:B:397:LEU:HD13 | 2.03 | 0.41 |
| 1:B:612:LEU:HA | 1:B:612:LEU:HD23 | 1.82 | 0.41 |
| 1:B:683:PHE:HB3 | 1:B:740:ILE:HD13 | 2.03 | 0.41 |
| 1:B:776:TRP:O | 1:B:780:ILE:HG22 | 2.20 | 0.41 |
| 1:B:1433:ALA:O | 1:B:1436:LEU:HD23 | 2.21 | 0.41 |
| 1:B:1617:LYS:HB2 | 1:B:1617:LYS:HE3 | 1.89 | 0.41 |
| 1:B:1696:LEU:N | 1:B:1697:PRO:CD | 2.84 | 0.41 |
| 1:B:1848:ILE:HD11 | 1:B:1918:LEU:HD21 | 2.01 | 0.41 |
| 1:B:1930:GLU:HB3 | 1:B:1937:ARG:NH1 | 2.36 | 0.41 |
| 1:B:2268:LYS:HD3 | 1:B:2314:GLU:OE2 | 2.21 | 0.41 |
| 1:B:2586:PHE:H | 1:B:2783:ILE:HD11 | 1.85 | 0.41 |
| 1:B:2814:SER:HA | 1:B:2865:HIS:NE2 | 2.36 | 0.41 |
| 1:B:3577:GLN:HA | 1:B:3630:ARG:HH11 | 1.85 | 0.41 |
| 1:B:4064:LEU:O | 1:B:4068:HIS:HB2 | 2.21 | 0.41 |
| 1:A:290:TYR:HE2 | 1:A:340:TYR:CD2 | 2.39 | 0.41 |
| 1:A:655:LEU:HD22 | 1:A:1389:VAL:CG1 | 2.51 | 0.41 |
| 1:A:873:VAL:CG1 | 1:A:874:THR:H | 2.27 | 0.41 |
| 1:A:1564:SER:O | 1:A:1603:GLN:HG3 | 2.21 | 0.41 |
| 1:A:1914:THR:O | 1:A:1918:LEU:HG | 2.20 | 0.41 |
| 1:A:1978:PHE:O | 1:A:1982:ILE:HG12 | 2.21 | 0.41 |
| 1:A:2351:GLN:O | 1:A:2355:THR:HG22 | 2.21 | 0.41 |
| 1:A:2942:ILE:H | 1:A:2942:ILE:HG12 | 1.75 | 0.41 |
| 1:A:3386:SER:O | 1:A:3389:VAL:HG22 | 2.21 | 0.41 |
| 1:A:3988:LEU:O | 1:A:3992:ARG:HG2 | 2.21 | 0.41 |
| 1:A:4031:ILE:HG13 | 1:A:4035:GLU:HB2 | 2.03 | 0.41 |
| 1:B:1267:TYR:HB3 | 1:B:1344:PHE:CE1 | 2.56 | 0.41 |
| 1:B:1419:LEU:HD13 | 1:B:1467:ILE:HD11 | 2.03 | 0.41 |
| 1:B:2091:HIS:O | 1:B:2093:CYS:N | 2.54 | 0.41 |
| 1:B:2140:LEU:HD21 | 1:B:2179:GLY:H | 1.84 | 0.41 |
| 1:B:3480:LEU:HD12 | 1:B:3480:LEU:HA | 1.86 | 0.41 |
| 1:A:9:ARG:HA | 1:A:12:LEU:HD13 | 2.04 | 0.40 |
| 1:A:523:THR:OG1 | 1:A:524:TYR:N | 2.53 | 0.40 |
| 1:A:1938:ARG:HH21 | 1:A:1983:ASP:HA | 1.86 | 0.40 |
| 1:A:2366:LYS:HD3 | 1:A:2366:LYS:HA | 1.86 | 0.40 |
| 1:A:3666:LEU:HA | 1:A:3669:LYS:HG2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3719:ILE:HD12 | 1:A:3740:ILE:HD12 | 2.02 | 0.40 |
| 1:B:620:PHE:CZ | 1:B:663:ILE:HD12 | 2.56 | 0.40 |
| 1:B:1197:LEU:O | 1:B:1197:LEU:HD23 | 2.21 | 0.40 |
| 1:B:1334:LYS:NZ | 1:B:1383:GLY:HA3 | 2.35 | 0.40 |
| 1:B:1344:PHE:O | 1:B:1347:THR:HG22 | 2.21 | 0.40 |
| 1:B:1372:LEU:O | 1:B:1375:THR:OG1 | 2.32 | 0.40 |
| 1:B:2097:LEU:HB3 | 1:B:2149:LEU:HD11 | 2.03 | 0.40 |
| 1:B:2164:TRP:O | 1:B:2196:TRP:HZ3 | 2.04 | 0.40 |
| 1:B:2263:LYS:HA | 1:B:2309:PHE:HE2 | 1.86 | 0.40 |
| 1:B:3129:LEU:HD23 | 1:B:3129:LEU:HA | 1.92 | 0.40 |
| 1:A:1372:LEU:HD12 | 1:A:1402:LEU:HD23 | 2.02 | 0.40 |
| 1:A:2253:TYR:HD2 | 1:A:2292:CYS:HB2 | 1.87 | 0.40 |
| 1:A:2306:ASN:O | 1:A:2309:PHE:HB2 | 2.21 | 0.40 |
| 1:B:1263:ALA:HA | 1:B:1266:CYS:SG | 2.62 | 0.40 |
| 1:B:1627:LYS:HE2 | 1:B:1627:LYS:HB2 | 1.80 | 0.40 |
| 1:B:1832:SER:H | 1:B:1883:ARG:NH2 | 2.10 | 0.40 |
| 1:B:1894:SER:HA | 1:B:1897:ASN:HB2 | 2.03 | 0.40 |
| 1:B:2514:ASN:O | 1:B:2517:LEU:HB3 | 2.21 | 0.40 |
| 1:B:2884:LEU:HD23 | 1:B:2884:LEU:HA | 1.97 | 0.40 |
| 1:A:853:ILE:HD11 | 1:A:3108:GLN:OE1 | 2.21 | 0.40 |
| 1:A:1178:ARG:HG2 | 1:A:1180:GLN:H | 1.86 | 0.40 |
| 1:A:2294:ILE:HG22 | 1:A:2295:GLN:N | 2.35 | 0.40 |
| 1:A:2551:GLU:HG3 | 1:A:2849:SER:CB | 2.50 | 0.40 |
| 1:A:3053:LEU:HD11 | 1:A:3088:LEU:HD13 | 2.03 | 0.40 |
| 1:A:3674:SER:O | 1:A:3676:PRO:HD3 | 2.21 | 0.40 |
| 1:B:179:GLY:HA3 | 1:B:226:GLY:HA2 | 2.04 | 0.40 |
| 1:B:357:LYS:O | 1:B:360:SER:HB3 | 2.21 | 0.40 |
| 1:B:681:LYS:O | 1:B:683:PHE:N | 2.54 | 0.40 |
| 1:B:738:HIS:HE1 | 1:B:748:TYR:CE1 | 2.39 | 0.40 |
| 1:B:765:LEU:HD23 | 1:B:766:ALA:H | 1.85 | 0.40 |
| 1:B:1101:PHE:CE1 | 1:B:1138:ILE:HD13 | 2.56 | 0.40 |
| 1:B:1423:ILE:HD11 | 1:B:1467:ILE:HD13 | 2.03 | 0.40 |
| 1:B:1831:CYS:HA | 1:B:1883:ARG:NH1 | 2.36 | 0.40 |
| 1:B:2956:ALA:HB1 | 1:B:2972:TYR:CZ | 2.56 | 0.40 |
| 1:B:3011:LEU:HD23 | 1:B:3047:SER:HB3 | 2.03 | 0.40 |
| 1:B:3389:VAL:HB | 1:B:3413:TYR:HE1 | 1.85 | 0.40 |
| 1:A:47:SER:N | 1:A:48:PRO:HD2 | 2.36 | 0.40 |
| 1:A:1503:LEU:HD12 | 1:A:1508:LYS:HE2 | 2.03 | 0.40 |
| 1:A:1515:LEU:CD2 | 1:A:1519:PHE:CE2 | 3.04 | 0.40 |
| 1:A:3059:GLN:HE21 | 1:A:3063:THR:HG23 | 1.86 | 0.40 |
| 1:A:3896:ALA:O | 1:A:3900:LEU:HD13 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:384:MET:C | 1:B:386:VAL:H | 2.24 | 0.40 |
| 1:B:1436:LEU:HD13 | 1:B:1444:ASP:HB3 | 2.03 | 0.40 |
| 1:B:1832:SER:O | 1:B:1833:LEU:HB2 | 2.21 | 0.40 |
| 1:B:3530:VAL:HA | 1:B:3562:LEU:HD21 | 2.04 | 0.40 |
| 1:A:45:SER:HB3 | 1:A:51:LEU:HD22 | 2.04 | 0.40 |
| 1:A:886:TRP:CZ3 | 1:A:911:LEU:HG | 2.56 | 0.40 |
| 1:A:1078:ALA:O | 1:A:1107:TYR:OH | 2.38 | 0.40 |
| 1:A:1261:LEU:HD21 | 1:A:1337:VAL:HG12 | 2.03 | 0.40 |
| 1:A:2549:LYS:HD3 | 1:A:2549:LYS:HA | 1.96 | 0.40 |
| 1:A:3462:ARG:HG3 | 1:A:3494:GLN:HB3 | 2.02 | 0.40 |
| 1:A:3858:MET:HE2 | 1:A:3858:MET:HB3 | 1.92 | 0.40 |
| 1:B:9:ARG:HA | 1:B:12:LEU:HD13 | 2.03 | 0.40 |
| 1:B:76:ILE:O | 1:B:79:ARG:NH1 | 2.54 | 0.40 |
| 1:B:172:GLU:HB2 | 1:B:218:PRO:O | 2.21 | 0.40 |
| 1:B:476:ARG:NH2 | 1:B:1503:LEU:HD22 | 2.36 | 0.40 |
| 1:B:1333:SER:O | 1:B:1337:VAL:HG13 | 2.21 | 0.40 |
| 1:B:1754:GLN:HB2 | 1:B:1797:LEU:HD11 | 2.03 | 0.40 |
| 1:B:1982:ILE:HG22 | 1:B:1983:ASP:N | 2.36 | 0.40 |
| 1:B:2310:VAL:HG12 | 1:B:2316:TYR:CD2 | 2.56 | 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 | 3544/3986 (89%) | 3047 (86%) | 482 (14%) | 15 (0%) | 34 | 72 |
| 1 | B | 3559/3986 (89%) | 3069 (86%) | 475 (13%) | 15 (0%) | 34 | 72 |
| 2 | C | 7/192 (4%) | 7 (100%) | 0 | 0 | 100 | 100 |
| 2 | D | 7/192 (4%) | 7 (100%) | 0 | 0 | 100 | 100 |
| All | All | 7117/8356 (85%) | 6130 (86%) | 957 (13%) | 30 (0%) | 34 | 72 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2182 | ILE |
| 1 | A | 2250 | SER |
| 1 | A | 2410 | GLU |
| 1 | A | 2781 | PRO |
| 1 | B | 1613 | HIS |
| 1 | B | 2250 | SER |
| 1 | B | 2410 | GLU |
| 1 | A | 1681 | ASP |
| 1 | B | 2246 | LYS |
| 1 | B | 3059 | GLN |
| 1 | B | 2206 | PRO |
| 1 | B | 2406 | GLU |
| 1 | B | 2407 | GLY |
| 1 | A | 167 | PRO |
| 1 | A | 2577 | PHE |
| 1 | A | 3059 | GLN |
| 1 | A | 1682 | THR |
| 1 | A | 1956 | PHE |
| 1 | A | 2886 | GLN |
| 1 | A | 2121 | ASP |
| 1 | A | 2177 | ASN |
| 1 | B | 304 | THR |
| 1 | B | 682 | TYR |
| 1 | B | 2577 | PHE |
| 1 | A | 635 | PRO |
| 1 | A | 2783 | ILE |
| 1 | B | 1992 | VAL |
| 1 | B | 2226 | PRO |
| 1 | B | 2573 | PRO |
| 1 | B | 2781 | PRO |

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.

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | A | 3046/3515 (87%) | 2953 (97%) | 93 (3%) | 40 | 63 |
| 1 | B | 3093/3515 (88%) | 3005 (97%) | 88 (3%) | 43 | 65 |
| 2 | C | 8/165 (5%) | 8 (100%) | 0 | 100 | 100 |
| 2 | D | 8/165 (5%) | 8 (100%) | 0 | 100 | 100 |
| All | All | 6155/7360 (84%) | 5974 (97%) | 181 (3%) | 42 | 64 |

All (181) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 25 | CYS |
| 1 | A | 36 | ARG |
| 1 | A | 65 | LEU |
| 1 | A | 70 | ARG |
| 1 | A | 148 | LYS |
| 1 | A | 254 | LYS |
| 1 | A | 264 | ARG |
| 1 | A | 281 | GLN |
| 1 | A | 282 | PHE |
| 1 | A | 337 | LYS |
| 1 | A | 364 | ARG |
| 1 | A | 366 | TYR |
| 1 | A | 373 | CYS |
| 1 | A | 492 | SER |
| 1 | A | 536 | SER |
| 1 | A | 630 | CYS |
| 1 | A | 651 | TYR |
| 1 | A | 662 | LEU |
| 1 | A | 675 | ARG |
| 1 | A | 701 | TYR |
| 1 | A | 704 | PHE |
| 1 | A | 707 | PHE |
| 1 | A | 790 | LYS |
| 1 | A | 795 | CYS |
| 1 | A | 910 | PHE |
| 1 | A | 966 | PHE |
| 1 | A | 1099 | PHE |
| 1 | A | 1107 | TYR |
| 1 | A | 1192 | TYR |
| 1 | A | 1213 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1229 | CYS |
| 1 | A | 1296 | PHE |
| 1 | A | 1507 | CYS |
| 1 | A | 1613 | HIS |
| 1 | A | 1633 | TRP |
| 1 | A | 1636 | ASP |
| 1 | A | 1679 | LEU |
| 1 | A | 1695 | LEU |
| 1 | A | 1787 | ARG |
| 1 | A | 1829 | TRP |
| 1 | A | 1837 | ARG |
| 1 | A | 1881 | TYR |
| 1 | A | 1910 | GLU |
| 1 | A | 1931 | ASN |
| 1 | A | 1979 | GLU |
| 1 | A | 1987 | ARG |
| 1 | A | 2029 | SER |
| 1 | A | 2154 | GLU |
| 1 | A | 2184 | TYR |
| 1 | A | 2196 | TRP |
| 1 | A | 2231 | PHE |
| 1 | A | 2248 | CYS |
| 1 | A | 2254 | ARG |
| 1 | A | 2269 | ASP |
| 1 | A | 2275 | GLN |
| 1 | A | 2306 | ASN |
| 1 | A | 2312 | TYR |
| 1 | A | 2321 | GLU |
| 1 | A | 2341 | LEU |
| 1 | A | 2342 | CYS |
| 1 | A | 2357 | GLU |
| 1 | A | 2389 | PHE |
| 1 | A | 2408 | MET |
| 1 | A | 2425 | ARG |
| 1 | A | 2489 | SER |
| 1 | A | 2527 | HIS |
| 1 | A | 2574 | ASN |
| 1 | A | 2577 | PHE |
| 1 | A | 2579 | HIS |
| 1 | A | 2809 | PHE |
| 1 | A | 2821 | ASP |
| 1 | A | 2851 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 2931 | ARG |
| 1 | A | 2978 | LYS |
| 1 | A | 3005 | LEU |
| 1 | A | 3120 | LEU |
| 1 | A | 3122 | HIS |
| 1 | A | 3159 | ARG |
| 1 | A | 3244 | ASP |
| 1 | A | 3425 | ARG |
| 1 | A | 3428 | GLU |
| 1 | A | 3442 | TYR |
| 1 | A | 3570 | ASP |
| 1 | A | 3629 | ARG |
| 1 | A | 3632 | PHE |
| 1 | A | 3642 | LYS |
| 1 | A | 3659 | PHE |
| 1 | A | 3690 | PHE |
| 1 | A | 3694 | PHE |
| 1 | A | 3696 | ARG |
| 1 | A | 3775 | LEU |
| 1 | A | 3784 | ARG |
| 1 | A | 4087 | HIS |
| 1 | B | 25 | CYS |
| 1 | B | 45 | SER |
| 1 | B | 108 | LYS |
| 1 | B | 262 | LEU |
| 1 | B | 282 | PHE |
| 1 | B | 351 | ASN |
| 1 | B | 379 | LYS |
| 1 | B | 468 | LEU |
| 1 | B | 492 | SER |
| 1 | B | 583 | LEU |
| 1 | B | 630 | CYS |
| 1 | B | 662 | LEU |
| 1 | B | 704 | PHE |
| 1 | B | 707 | PHE |
| 1 | B | 795 | CYS |
| 1 | B | 886 | TRP |
| 1 | B | 910 | PHE |
| 1 | B | 1099 | PHE |
| 1 | B | 1107 | TYR |
| 1 | B | 1127 | CYS |
| 1 | B | 1167 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 1205 | ASN |
| 1 | B | 1213 | LYS |
| 1 | B | 1229 | CYS |
| 1 | B | 1279 | LEU |
| 1 | B | 1370 | ARG |
| 1 | B | 1409 | SER |
| 1 | B | 1507 | CYS |
| 1 | B | 1558 | TYR |
| 1 | B | 1588 | ASP |
| 1 | B | 1667 | SER |
| 1 | B | 1695 | LEU |
| 1 | B | 1727 | ARG |
| 1 | B | 1762 | MET |
| 1 | B | 1787 | ARG |
| 1 | B | 1788 | ARG |
| 1 | B | 1813 | SER |
| 1 | B | 1829 | TRP |
| 1 | B | 1837 | ARG |
| 1 | B | 1864 | ASP |
| 1 | B | 1881 | TYR |
| 1 | B | 1910 | GLU |
| 1 | B | 1990 | PHE |
| 1 | B | 2083 | LEU |
| 1 | B | 2085 | MET |
| 1 | B | 2154 | GLU |
| 1 | B | 2184 | TYR |
| 1 | B | 2195 | SER |
| 1 | B | 2231 | PHE |
| 1 | B | 2233 | HIS |
| 1 | B | 2269 | ASP |
| 1 | B | 2306 | ASN |
| 1 | B | 2321 | GLU |
| 1 | B | 2334 | LYS |
| 1 | B | 2341 | LEU |
| 1 | B | 2342 | CYS |
| 1 | B | 2389 | PHE |
| 1 | B | 2404 | ARG |
| 1 | B | 2489 | SER |
| 1 | B | 2492 | ASP |
| 1 | B | 2527 | HIS |
| 1 | B | 2568 | MET |
| 1 | B | 2577 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 2585 | GLU |
| 1 | B | 2800 | ARG |
| 1 | B | 2809 | PHE |
| 1 | B | 2821 | ASP |
| 1 | B | 2835 | LYS |
| 1 | B | 2851 | PHE |
| 1 | B | 2978 | LYS |
| 1 | B | 3005 | LEU |
| 1 | B | 3014 | CYS |
| 1 | B | 3120 | LEU |
| 1 | B | 3168 | TYR |
| 1 | B | 3244 | ASP |
| 1 | B | 3323 | PHE |
| 1 | B | 3378 | TYR |
| 1 | B | 3422 | GLN |
| 1 | B | 3428 | GLU |
| 1 | B | 3507 | ASP |
| 1 | B | 3570 | ASP |
| 1 | B | 3629 | ARG |
| 1 | B | 3642 | LYS |
| 1 | B | 3689 | ASP |
| 1 | B | 3694 | PHE |
| 1 | B | 3696 | ARG |
| 1 | B | 3716 | HIS |
| 1 | B | 4087 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 322 | GLN |
| 1 | A | 1721 | HIS |
| 1 | A | 3059 | GLN |
| 1 | A | 3423 | GLN |
| 1 | A | 3924 | HIS |
| 1 | A | 4015 | ASN |
| 1 | B | 484 | HIS |
| 1 | B | 1048 | GLN |
| 1 | B | 1049 | GLN |
| 1 | B | 3130 | GLN |
| 1 | B | 3278 | GLN |
| 1 | B | 3743 | HIS |
| 1 | B | 3969 | 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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | B | 2 |
| 1 | A | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | B | 2614:UNK | C | 2740:UNK | N | 43.02 |
| 1 | A | 2614:UNK | C | 2739:UNK | N | 37.67 |
| 1 | B | 2765:UNK | C | 2779:ASP | N | 14.02 |
| 1 | A | 2765:UNK | C | 2779:ASP | N | 13.16 |

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | A | 3590/3986 (90%) | -0.14 | 46 (1%) 77 68 | 144, 217, 281, 339 | 0 |
| 1 | B | 3607/3986 (90%) | -0.11 | 55 (1%) 73 64 | 148, 210, 309, 413 | 0 |
| 2 | C | 9/192 (4%) | -0.39 | 0 100 100 | 217, 221, 227, 228 | 0 |
| 2 | D | 9/192 (4%) | -0.53 | 0 100 100 | 160, 169, 180, 182 | 0 |
| All | All | 7215/8356 (86%) | -0.13 | 101 (1%) 75 66 | 144, 213, 288, 413 | 0 |

All (101) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 47 | SER | 5.7 |
| 1 | B | 46 | SER | 5.2 |
| 1 | A | 3310 | ASN | 5.0 |
| 1 | B | 55 | THR | 4.6 |
| 1 | B | 1994 | VAL | 4.3 |
| 1 | A | 3316 | LEU | 4.2 |
| 1 | B | 100 | ILE | 4.2 |
| 1 | A | 2986 | PRO | 4.0 |
| 1 | B | 11 | SER | 4.0 |
| 1 | A | 1993 | GLU | 4.0 |
| 1 | B | 30 | ALA | 3.8 |
| 1 | A | 1435 | ASN | 3.7 |
| 1 | A | 3311 | ASN | 3.7 |
| 1 | B | 3025 | PRO | 3.6 |
| 1 | A | 2985 | GLU | 3.6 |
| 1 | B | 1993 | GLU | 3.5 |
| 1 | B | 143 | LEU | 3.4 |
| 1 | B | 74 | ASN | 3.3 |
| 1 | B | 99 | LYS | 3.3 |
| 1 | A | 123 | CYS | 3.2 |
| 1 | B | 45 | SER | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 4026 | SER | 3.1 |
| 1 | B | 546 | ALA | 3.1 |
| 1 | B | 10 | CYS | 3.1 |
| 1 | B | 56 | SER | 3.0 |
| 1 | B | 142 | ARG | 2.9 |
| 1 | A | 3312 | VAL | 2.9 |
| 1 | B | 3502 | MET | 2.9 |
| 1 | B | 119 | ARG | 2.9 |
| 1 | A | 3642 | LYS | 2.9 |
| 1 | A | 3007 | GLU | 2.9 |
| 1 | B | 93 | LEU | 2.8 |
| 1 | A | 170 | VAL | 2.8 |
| 1 | B | 23 | ASP | 2.8 |
| 1 | B | 28 | ALA | 2.8 |
| 1 | A | 116 | THR | 2.8 |
| 1 | A | 3277 | VAL | 2.8 |
| 1 | B | 1047 | GLN | 2.7 |
| 1 | A | 3270 | ASP | 2.7 |
| 1 | A | 1439 | PRO | 2.6 |
| 1 | A | 3292 | GLY | 2.6 |
| 1 | B | 24 | ARG | 2.6 |
| 1 | B | 2983 | ASP | 2.6 |
| 1 | B | 3506 | LEU | 2.6 |
| 1 | B | 138 | PHE | 2.6 |
| 1 | B | 356 | ASN | 2.6 |
| 1 | B | 67 | VAL | 2.6 |
| 1 | A | 3449 | LYS | 2.5 |
| 1 | B | 42 | CYS | 2.4 |
| 1 | B | 3861 | GLY | 2.4 |
| 1 | A | 3319 | ASN | 2.4 |
| 1 | A | 2919 | ASP | 2.4 |
| 1 | A | 3643 | HIS | 2.3 |
| 1 | B | 3026 | ASP | 2.3 |
| 1 | A | 3280 | TYR | 2.3 |
| 1 | A | 300 | TRP | 2.3 |
| 1 | A | 1292 | LYS | 2.3 |
| 1 | A | 3447 | VAL | 2.3 |
| 1 | A | 119 | ARG | 2.3 |
| 1 | A | 3301 | LEU | 2.3 |
| 1 | A | 3304 | VAL | 2.3 |
| 1 | A | 2895 | GLU | 2.3 |
| 1 | B | 144 | MET | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 4035 | GLU | 2.3 |
| 1 | B | 89 | LEU | 2.3 |
| 1 | B | 14 | ARG | 2.3 |
| 1 | B | 181 | LEU | 2.2 |
| 1 | B | 1271 | ILE | 2.2 |
| 1 | B | 3028 | ASN | 2.2 |
| 1 | A | 78 | PHE | 2.2 |
| 1 | B | 2002 | LYS | 2.2 |
| 1 | A | 143 | LEU | 2.2 |
| 1 | A | 3451 | LEU | 2.2 |
| 1 | B | 2010 | GLU | 2.2 |
| 1 | B | 107 | ILE | 2.2 |
| 1 | A | 2484 | TYR | 2.2 |
| 1 | A | 2984 | GLY | 2.2 |
| 1 | A | 3291 | GLN | 2.2 |
| 1 | B | 101 | ALA | 2.2 |
| 1 | B | 178 | LEU | 2.2 |
| 1 | A | 2489 | SER | 2.1 |
| 1 | B | 123 | CYS | 2.1 |
| 1 | A | 3139 | GLN | 2.1 |
| 1 | A | 124 | LYS | 2.1 |
| 1 | A | 3314 | SER | 2.1 |
| 1 | B | 1287 | GLN | 2.1 |
| 1 | B | 48 | PRO | 2.1 |
| 1 | B | 3440 | GLN | 2.1 |
| 1 | A | 2198 | GLY | 2.1 |
| 1 | A | 3072 | GLU | 2.1 |
| 1 | B | 34 | LEU | 2.1 |
| 1 | A | 3273 | LEU | 2.1 |
| 1 | A | 98 | GLN | 2.0 |
| 1 | A | 117 | LYS | 2.0 |
| 1 | B | 1284 | THR | 2.0 |
| 1 | B | 4128 | MET | 2.0 |
| 1 | B | 137 | THR | 2.0 |
| 1 | B | 104 | SER | 2.0 |
| 1 | B | 135 | LEU | 2.0 |
| 1 | B | 3976 | GLU | 2.0 |
| 1 | A | 1382 | ILE | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.