



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 PM GMT

PDB ID : 4AI6
Title : Dynein Motor Domain - ADP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-08
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

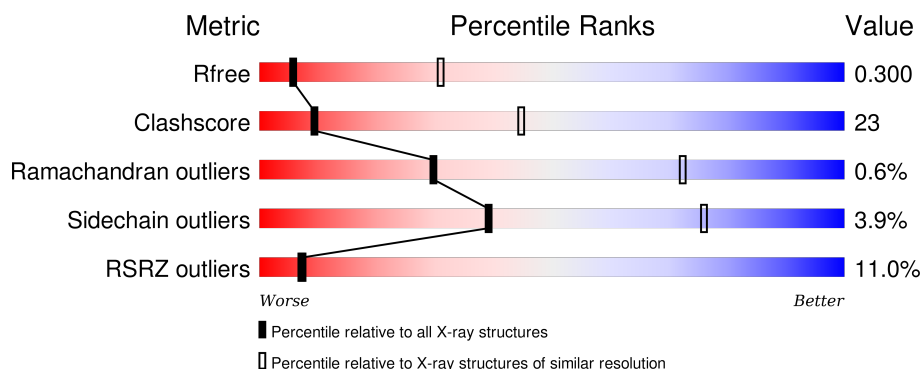
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1476 (3.50-3.30) |
| Clashscore | 102246 | 1611 (3.50-3.30) |
| Ramachandran outliers | 100387 | 1571 (3.50-3.30) |
| Sidechain outliers | 100360 | 1571 (3.50-3.30) |
| RSRZ outliers | 91569 | 1485 (3.50-3.30) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | 2695 | |
| 1 | B | 2695 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | ATP | B | 5400 | - | - | X | - |
| 3 | ADP | A | 5401 | - | - | X | - |
| 3 | ADP | A | 5402 | - | - | X | - |
| 3 | ADP | B | 5402 | - | - | X | - |
| 4 | SO4 | A | 5403 | - | - | X | - |
| 4 | SO4 | B | 5403 | - | - | X | - |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 41678 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.

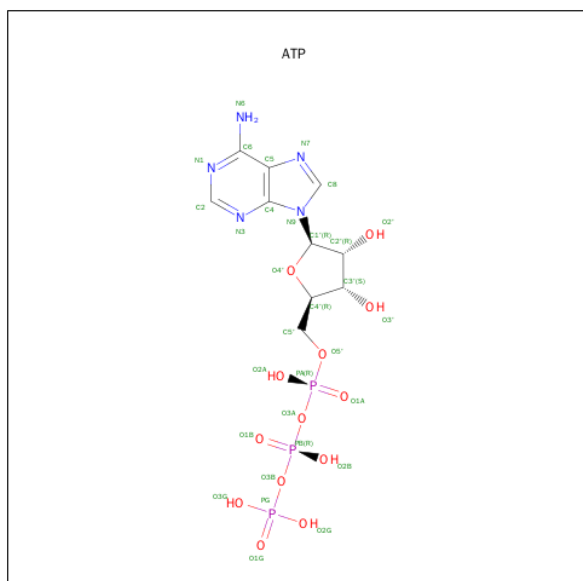
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|---------|-------|
| 1 | A | 2650 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 20748 | 13268 | 3472 | 3915 | 93 | | | |
| 1 | B | 2650 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 20748 | 13268 | 3472 | 3915 | 93 | | | |

There are 4 discrepancies between the modelled and reference sequences:

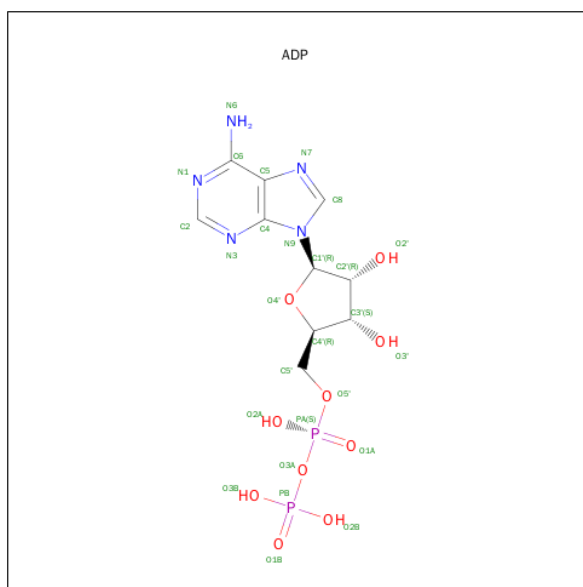
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 1630 | ILE | LEU | CONFLICT | UNP P36022 |
| A | 3782 | ASP | GLU | CONFLICT | UNP P36022 |
| B | 1630 | ILE | LEU | CONFLICT | UNP P36022 |
| B | 3782 | ASP | GLU | CONFLICT | UNP P36022 |

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

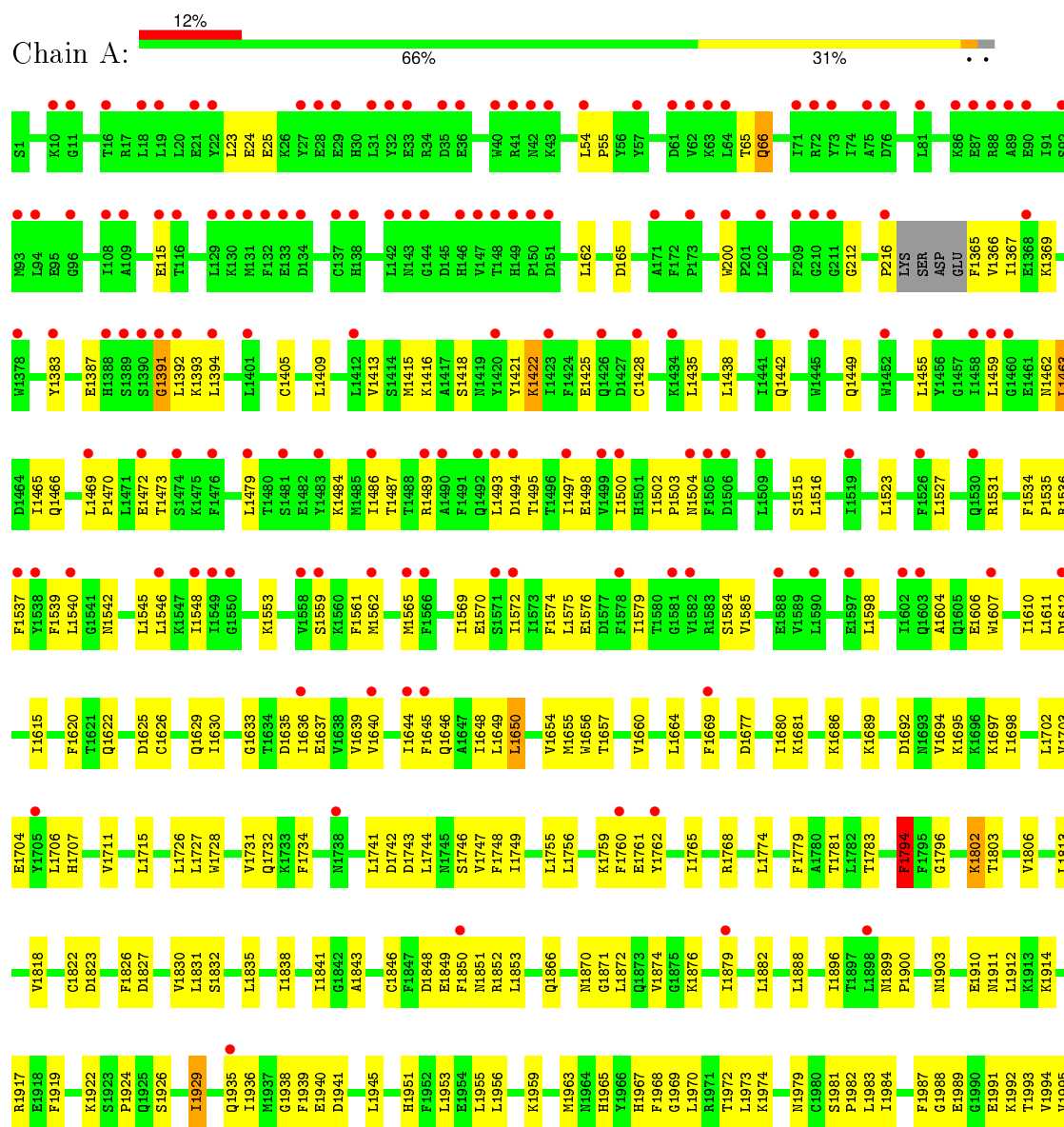
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots

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

- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC







| | | | | | | |
|-------|-------|-------|-------|-------|------|-----|
| L1701 | W1607 | F1505 | M1419 | A184 | I71 | S1 |
| L1702 | I1610 | I1513 | Y1420 | I185 | R72 | P2 |
| L1703 | L1611 | | K1421 | P196 | Y73 | I3 |
| L1704 | D1612 | L1523 | K1422 | Q187 | I74 | L4 |
| L1705 | | S1524 | F1424 | D189 | A75 | G5 |
| L1706 | I1615 | F1525 | E1425 | I190 | G82 | Y6 |
| L1707 | K1616 | F1526 | L1429 | Y191 | G83 | K8 |
| | | L1527 | | K192 | C84 | I9 |
| L1711 | F1620 | R1531 | L1435 | K193 | P85 | K10 |
| | T1621 | | | S194 | K86 | G11 |
| Q1714 | C1626 | F1534 | I1441 | Y197 | E87 | L12 |
| L1715 | P1535 | R1536 | W1445 | I198 | R88 | V13 |
| L1719 | I1630 | F1537 | | A199 | E90 | Q14 |
| T1720 | G1633 | F1538 | Q1449 | W200 | I91 | T16 |
| K1721 | | F1539 | W1452 | L202 | S92 | R17 |
| L1726 | T1636 | L1540 | L1455 | P216 | R93 | L18 |
| L1727 | | L1545 | L1456 | LVS | E95 | L19 |
| W1728 | V1639 | L1546 | SER | ASP | G96 | L23 |
| V1640 | V1640 | K1547 | GLJ | GLJ | A97 | E24 |
| F1734 | Y1643 | I1548 | L1458 | F1365 | V98 | |
| Y1735 | I1644 | I1549 | L1459 | F1366 | M131 | H30 |
| L1741 | F1645 | H1554 | G1460 | I1367 | F132 | L31 |
| D1742 | Q1646 | H1555 | I1465 | E1368 | E133 | Y32 |
| D1743 | | | | K1369 | D134 | R34 |
| L1744 | L1649 | | | M1372 | R135 | D35 |
| F1748 | M1655 | S1559 | L1469 | E1375 | L136 | E36 |
| L1749 | W1656 | M1562 | P1470 | K1376 | C137 | |
| S1750 | T1657 | K1564 | E1472 | K1379 | M143 | K39 |
| | | M1565 | K1475 | F1476 | G144 | W40 |
| L1755 | V1660 | | F1476 | | D145 | R41 |
| | L1664 | I1569 | T1480 | Y1383 | T148 | W42 |
| Y1758 | Q1665 | I1572 | Y1483 | I1386 | F45 | K43 |
| K1759 | F1760 | N1573 | E1485 | E1387 | P150 | K44 |
| E1761 | Q1667 | F1574 | W1485 | G1391 | D151 | E45 |
| L1762 | Q1668 | L1575 | I1486 | L1392 | F152 | L47 |
| L1763 | F1669 | D1577 | F1578 | K1393 | M153 | G48 |
| L1764 | Y1672 | | | L1394 | E154 | L49 |
| L1765 | T1677 | S1584 | | Y1395 | F155 | E50 |
| F1766 | D1677 | Y1589 | F1491 | R1396 | D156 | F51 |
| L1768 | T1680 | L1590 | Q1492 | R1397 | Y162 | P52 |
| L1769 | K1681 | G1682 | L1493 | T1495 | M163 | N53 |
| L1774 | L1683 | N1593 | T1496 | C1405 | D165 | L54 |
| | K1689 | F1594 | I1497 | L1409 | F164 | P55 |
| L1781 | D1692 | K1595 | E1498 | L1412 | G168 | G60 |
| | | I1596 | V1499 | | L169 | D61 |
| F1794 | K1695 | Q1603 | H1501 | L1415 | D170 | V62 |
| F1795 | K1696 | A1604 | I1502 | | F172 | K63 |
| K1802 | K1697 | Q1605 | P1503 | | F173 | L64 |
| L1803 | L1698 | L1603 | | | L175 | |
| L1804 | L1700 | L1701 | | | | Q66 |
| L1805 | L1701 | L1702 | | | | S67 |
| L1806 | L1702 | L1703 | | | | P68 |
| L1807 | L1703 | L1704 | | | | A69 |
| L1808 | L1704 | L1705 | | | | T70 |
| L1809 | L1705 | L1706 | | | | |
| L1810 | L1706 | L1707 | | | | |
| L1811 | L1707 | L1708 | | | | |
| L1812 | L1708 | L1709 | | | | |
| L1813 | L1709 | L1710 | | | | |
| L1814 | L1710 | L1711 | | | | |
| L1815 | L1711 | L1712 | | | | |
| L1816 | L1712 | L1713 | | | | |
| L1817 | L1713 | L1714 | | | | |
| L1818 | L1714 | L1715 | | | | |
| L1819 | L1715 | L1716 | | | | |
| L1820 | L1716 | L1717 | | | | |
| L1821 | L1717 | L1718 | | | | |
| L1822 | L1718 | L1719 | | | | |
| L1823 | L1719 | L1720 | | | | |
| L1824 | L1720 | L1721 | | | | |
| L1825 | L1721 | L1722 | | | | |
| L1826 | L1722 | L1723 | | | | |
| L1827 | L1723 | L1724 | | | | |
| L18 | | | | | | |

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| L3346 | V3347 | L3348 | L3349 | L3350 | L3351 | L3352 | L3353 | L3359 | Y3360 | D3361 | I3367 | V3371 | T3372 | F3390 | L3391 | E3392 | L3393 | S3400 | Q3401 | D3402 | A3403 | F3406 | L3407 | L3408 | D3409 | H3413 | L3414 | L3415 | V3417 | L3429 | R3439 | L3440 | A3443 | F3446 | V3450 | D3459 | F3460 | L3461 | L3462 | S3463 | R3464 | L3465 | S3467 | | | | |
| L3018 | L3019 | G3020 | L2815 | L2816 | L2817 | L2818 | E2819 | L2822 | L2823 | E2824 | L2825 | A2826 | E2829 | L2832 | L2833 | L2834 | L2835 | A2838 | D2842 | L2843 | F2844 | Q2845 | G2846 | Y2849 | L2852 | L2853 | L2856 | T2860 | L2866 | L2867 | E2870 | L2873 | F2877 | V2878 | H2886 | F2889 | S2890 | L2891 | C2892 | L2893 | F2894 | L3010 | L3011 | E3012 | E3341 | R3342 | |
| M2910 | R2911 | C2912 | L2913 | L2914 | L2915 | M2916 | M2920 | T2924 | F2937 | M2938 | T2941 | D2942 | F2943 | I2944 | VAL | PRO | GLU | ASN | VAL | VAL | GLU | VAL | PHE | THR | GLU | PRO | I2960 | L2961 | L2962 | L2963 | A2964 | V2965 | M2967 | F2972 | V2982 | C2983 | S2988 | F2989 | G2990 | K3001 | L3010 | L3011 | E3012 | F3016 | V3017 | | |
| L2712 | V2713 | L2728 | P2731 | L2732 | V2733 | L2734 | S2737 | M2738 | H2741 | L2742 | L2743 | R2744 | L2745 | Q2751 | G2754 | H2755 | M2756 | L2758 | L2759 | G2760 | A2761 | R2762 | R2763 | L2764 | G2765 | G2766 | L2767 | L2768 | L2769 | L2770 | R2771 | L2779 | K2780 | L2781 | V2782 | Q2783 | P2784 | K2785 | L2786 | H2787 | R2788 | L2792 | F2795 | L2799 | R2812 | T2813 | C2814 |
| L2581 | V2582 | R2586 | S2587 | E2590 | P2591 | T2609 | Q2612 | S2613 | R2620 | R2624 | L2625 | V2626 | R2627 | T2631 | M2634 | T2635 | G2636 | P2637 | R2638 | Q2639 | T2640 | L2641 | R2642 | S2643 | R2646 | W2653 | R2654 | K2664 | L2673 | V2677 | L2686 | L2689 | S2690 | S2691 | L2694 | L2695 | L2702 | V2707 | M2708 | K2709 | L2713 | L2714 | C2715 | | | | |
| M2490 | L2491 | P2492 | K2493 | L2494 | D2495 | K2496 | Y2497 | G2498 | S2499 | L2506 | R2507 | Q2508 | K2512 | Q2513 | K2517 | T2518 | P2519 | E2520 | V2524 | T2525 | L2526 | E2527 | R2528 | L2529 | H2530 | L2531 | C2535 | N2536 | G2542 | R2543 | L2544 | R2549 | R2552 | H2553 | L2556 | P2562 | S2563 | S2566 | Y2571 | E2572 | L2573 | Y2574 | Y2575 | L2578 | F2579 | K2580 | |
| L2390 | T2394 | L2395 | L2396 | T2397 | D2406 | N2409 | S2410 | K2411 | R2412 | T2415 | L2416 | Q2417 | P2420 | K2424 | T2425 | M2428 | L2437 | V2440 | P2445 | S2446 | L2447 | D2448 | T2449 | L2455 | L2458 | Y2464 | T2467 | S2468 | L2471 | T2472 | L2473 | L2474 | P2475 | K2476 | S2477 | D2478 | K2480 | L2484 | E2488 | L2489 | | | | | | | |
| R2299 | F2302 | L2305 | D2306 | S2309 | L2310 | D2312 | L2314 | T2315 | L2316 | L2317 | L2318 | K2319 | R2320 | S2321 | L2322 | L2326 | G2332 | Q2335 | R2336 | L2339 | F2346 | S2350 | Q2351 | S2354 | D2355 | Y2356 | S2357 | L2358 | L2359 | V2360 | L2361 | A2362 | N2363 | D2364 | K2365 | L2366 | L2367 | F2368 | V2378 | S2379 | L2380 | E2384 | V2385 | M2386 | R2387 | | |
| F2190 | R2191 | L2192 | L2193 | F2194 | E2195 | T2196 | D2197 | N2198 | L2199 | D2200 | H2201 | T2202 | T2203 | P2204 | A2205 | L2212 | C2220 | S2221 | I2222 | S2223 | S2224 | K2225 | L2229 | L2230 | N2239 | L2249 | L2252 | D2255 | S2256 | F2257 | L2262 | L2265 | H2274 | I2275 | L2276 | R2279 | L2280 | F2281 | N2282 | E2285 | V2288 | H2289 | L2294 | L2295 | | | |
| D2007 | D2008 | E2011 | F2014 | T2021 | F2022 | S2024 | T2027 | F2028 | L2029 | N2030 | S2031 | D2032 | K2033 | L2034 | V2035 | G2042 | D2043 | R2044 | P2049 | R2060 | Y2061 | L2062 | V2063 | Q2064 | L2066 | T2067 | Q2068 | A2069 | L2070 | P2160 | L2071 | E2161 | E2164 | V2169 | T2081 | A2082 | T2083 | K2084 | V2085 | T2086 | V2087 | L2088 | K2091 | L2092 | L2093 | F2094 | D2095 |
| L1813 | C1822 | D1823 | F1826 | D1827 | Y1828 | Q1829 | V1830 | L1831 | S1832 | R1833 | L1834 | L1835 | I1838 | L1841 | G1842 | A1843 | G1845 | E1849 | F1850 | M1851 | R1852 | L1853 | V1857 | M1864 | L1865 | Q1866 | L1870 | G1871 | L1872 | L1882 | L1898 | N1899 | P1900 | R1905 | L1908 | F1909 | E1910 | N1911 | L1912 | R1917 | E1918 | F1919 | S1920 | M1921 | K1922 | | |

| | | | | | |
|-------|-------|-------|-------|-------|-------|
| I4023 | V3923 | Q3842 | L3757 | L3565 | F3470 |
| V4024 | M3924 | M3843 | L3757 | L3566 | M3471 |
| V4027 | S3925 | Q3844 | L3760 | L3567 | E3472 |
| R4028 | V3926 | Q3845 | L3760 | E3568 | A3473 |
| I4029 | Y3927 | M3846 | E3763 | E3569 | R3476 |
| P4030 | Y3927 | L3848 | F3767 | L3570 | V3477 |
| Q4035 | M3934 | S3849 | F3767 | M3571 | T3478 |
| Q4036 | F3935 | W3850 | F3769 | M3572 | |
| Q4037 | T3939 | V3851 | V3769 | S3573 | I3481 |
| S4038 | T3939 | K3852 | V3772 | Q3574 | G3482 |
| E4039 | T3943 | T3853 | K3772 | Q3575 | D3483 |
| E4040 | V3946 | Y3854 | K3773 | M3576 | |
| L4045 | P3947 | L3855 | L3774 | M3577 | V3488 |
| T4052 | H3948 | H3858 | V3777 | L3578 | |
| S4060 | G3949 | V3859 | V3777 | M3580 | S3502 |
| S4061 | F3950 | V3862 | V3778 | D3581 | |
| W4062 | S3951 | T3862 | A3779 | E3582 | I3505 |
| L4065 | Y3955 | A3865 | K3780 | L3583 | L3509 |
| I4070 | F3956 | E3866 | M3784 | M3584 | R3510 |
| E4074 | M3957 | E3867 | Y3785 | T3585 | S3511 |
| Q4077 | D3958 | F3871 | Y3786 | T3586 | R3512 |
| A4078 | C3959 | K3872 | T3787 | L3587 | V3513 |
| S4084 | D3960 | M3873 | R3792 | M3588 | |
| T4085 | F3963 | F3874 | K3799 | I3589 | F3518 |
| L4088 | A3964 | T3875 | K3799 | K3592 | V3519 |
| Q4092 | S3965 | M3876 | L3803 | E3593 | T3520 |
| | L3968 | C3877 | Q3807 | A3594 | N3521 |
| | M3978 | L3884 | K3808 | M3596 | I3525 |
| | N3979 | A3885 | L3811 | E3605 | F3530 |
| | I3980 | P3887 | K3812 | D3612 | D3531 |
| P3981 | P3981 | L3888 | L3813 | M3613 | L3534 |
| W3982 | W3982 | L3889 | L3814 | L3614 | T3535 |
| A3983 | Q3983 | Q3890 | L3815 | V3615 | E3536 |
| Q3984 | Q3984 | R3894 | L3816 | E3616 | E3537 |
| Y3994 | Y3994 | V3895 | G3817 | E3617 | M3538 |
| I3998 | I3998 | V3896 | S3818 | Y3618 | M3541 |
| K4002 | K4002 | Y3897 | L3819 | G3622 | Q3542 |
| D4003 | D4003 | E3898 | E3820 | E3622 | R3543 |
| L4004 | L4004 | D3899 | N3821 | F3629 | K3544 |
| P4005 | P4005 | D3900 | N3822 | S3630 | D3547 |
| V4006 | V4006 | L3904 | N3823 | M3631 | L3548 |
| V4014 | V4014 | T3906 | Q3826 | L3632 | I3549 |
| G4017 | G4017 | W3911 | K3831 | E3633 | K3550 |
| S4018 | S4018 | G3912 | S3832 | F3641 | L3551 |
| D4019 | D4019 | G3915 | K3833 | T3644 | E3554 |
| M4020 | M4020 | F3916 | G3836 | S3645 | Y3555 |
| L4021 | L4021 | F3917 | G3837 | I3646 | K3556 |
| Q4022 | Q4022 | G3918 | K3838 | V3656 | L3557 |
| | | K3919 | L3839 | F3657 | L3562 |
| | | | L3841 | E3563 | R3564 |
| | | | | L3564 | |
| | | | | LYS | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 174.89Å 119.17Å 193.97Å 90.00° 90.18° 90.00° | Depositor |
| Resolution (Å) | 49.29 – 3.40 49.24 – 3.40 | Depositor EDS |
| % Data completeness (in resolution range) | 99.7 (49.29-3.40) 99.9 (49.24-3.40) | Depositor EDS |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.35 (at 3.40Å) | Xtriage |
| Refinement program | REFMAC 5.7.0019 | Depositor |
| R, R_{free} | 0.241 , 0.303 0.236 , 0.300 | Depositor DCC |
| R_{free} test set | 5512 reflections (5.28%) | DCC |
| Wilson B-factor (Å ²) | 133.4 | Xtriage |
| Anisotropy | 0.397 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 132.2 | EDS |
| Estimated twinning fraction | 0.033 for h,-k,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Outliers | 0 of 109869 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 41678 | wwPDB-VP |
| Average B, all atoms (Å ²) | 190.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, SO4, ADP

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 | 0.54 | 0/21146 | 0.77 | 12/28618 (0.0%) |
| 1 | B | 0.52 | 0/21146 | 0.76 | 9/28618 (0.0%) |
| All | All | 0.53 | 0/42292 | 0.77 | 21/57236 (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 | 1 |

There are no bond length outliers.

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|------|------|-----------|-------|------------------------|---------------------|
| 1 | B | 2455 | LEU | CB-CG-CD1 | -8.01 | 97.38 | 111.00 |
| 1 | A | 3650 | LEU | CB-CG-CD1 | -7.07 | 98.98 | 111.00 |
| 1 | A | 1882 | LEU | CA-CB-CG | 6.87 | 131.09 | 115.30 |
| 1 | A | 1463 | LEU | CA-CB-CG | 6.63 | 130.55 | 115.30 |
| 1 | A | 3945 | LEU | CB-CG-CD2 | -6.48 | 99.98 | 111.00 |
| 1 | A | 4021 | LEU | CB-CG-CD2 | -5.99 | 100.81 | 111.00 |
| 1 | A | 4059 | LEU | CB-CG-CD2 | -5.97 | 100.85 | 111.00 |
| 1 | B | 1872 | LEU | CB-CG-CD2 | 5.95 | 121.11 | 111.00 |
| 1 | B | 1882 | LEU | CA-CB-CG | 5.93 | 128.95 | 115.30 |
| 1 | A | 200 | TRP | C-N-CA | 5.77 | 146.22 | 122.00 |
| 1 | B | 200 | TRP | C-N-CA | 5.45 | 144.89 | 122.00 |
| 1 | B | 2158 | LEU | CB-CG-CD2 | -5.42 | 101.79 | 111.00 |
| 1 | A | 4042 | ARG | NE-CZ-NH1 | 5.38 | 122.99 | 120.30 |
| 1 | B | 2471 | LEU | CA-CB-CG | 5.34 | 127.57 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 3726 | LEU | CB-CG-CD1 | -5.33 | 101.93 | 111.00 |
| 1 | A | 4023 | ILE | CG1-CB-CG2 | -5.29 | 99.77 | 111.40 |
| 1 | A | 1794 | PHE | N-CA-CB | 5.27 | 120.09 | 110.60 |
| 1 | B | 2158 | LEU | CA-CB-CG | 5.24 | 127.36 | 115.30 |
| 1 | B | 2279 | ARG | NE-CZ-NH1 | -5.24 | 117.68 | 120.30 |
| 1 | B | 1938 | GLY | N-CA-C | -5.23 | 100.03 | 113.10 |
| 1 | A | 1650 | LEU | CB-CG-CD1 | 5.21 | 119.85 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | A | 3308 | ASN | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 20748 | 0 | 20206 | 934 | 0 |
| 1 | B | 20748 | 0 | 20207 | 930 | 0 |
| 2 | A | 31 | 0 | 12 | 6 | 0 |
| 2 | B | 31 | 0 | 12 | 22 | 0 |
| 3 | A | 54 | 0 | 24 | 28 | 0 |
| 3 | B | 54 | 0 | 24 | 29 | 0 |
| 4 | A | 5 | 0 | 0 | 2 | 0 |
| 4 | B | 5 | 0 | 0 | 2 | 0 |
| 5 | A | 1 | 0 | 0 | 0 | 0 |
| 5 | B | 1 | 0 | 0 | 0 | 0 |
| All | All | 41678 | 0 | 40485 | 1867 | 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 23.

All (1867) 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:B:2732:MET:HB2 | 3:B:5402:ADP:C6 | 1.40 | 1.57 |
| 1:B:1365:PHE:CD1 | 1:B:1366:VAL:HG23 | 1.34 | 1.57 |
| 1:A:1365:PHE:CE2 | 1:A:1366:VAL:HG23 | 1.55 | 1.39 |
| 1:A:1365:PHE:CD2 | 1:A:1366:VAL:HG23 | 1.68 | 1.27 |
| 1:B:1365:PHE:CE1 | 1:B:1366:VAL:HG23 | 1.70 | 1.27 |
| 1:A:3777:VAL:HG11 | 1:A:3895:PHE:CE1 | 1.70 | 1.26 |
| 1:B:2386:MET:CG | 1:B:2627:ARG:HD2 | 1.69 | 1.23 |
| 1:B:1620:PHE:HD1 | 1:B:1760:PHE:CZ | 1.60 | 1.19 |
| 1:B:2380:LEU:CD2 | 1:B:2390:ILE:HD11 | 1.71 | 1.19 |
| 1:B:2473:LEU:CD2 | 1:B:2475:PRO:HD3 | 1.72 | 1.18 |
| 1:B:3525:ILE:HD11 | 1:B:3646:ILE:HG22 | 1.22 | 1.18 |
| 1:B:2707:VAL:HB | 1:B:2712:LEU:HD11 | 1.22 | 1.18 |
| 1:B:2732:MET:HB2 | 3:B:5402:ADP:C5 | 1.79 | 1.17 |
| 1:A:1365:PHE:CE2 | 1:A:1366:VAL:CG2 | 2.26 | 1.17 |
| 1:B:2732:MET:HE3 | 1:B:2768:ILE:HG23 | 1.25 | 1.17 |
| 1:A:2517:LYS:HE3 | 1:A:2524:VAL:CG2 | 1.73 | 1.17 |
| 1:A:1983:LEU:HG | 1:A:1993:THR:HG23 | 1.26 | 1.17 |
| 1:A:1620:PHE:HD1 | 1:A:1760:PHE:CZ | 1.62 | 1.15 |
| 1:A:3525:ILE:HD11 | 1:A:3646:ILE:HG22 | 1.23 | 1.15 |
| 1:B:2473:LEU:HD23 | 1:B:2475:PRO:HD3 | 1.17 | 1.15 |
| 1:B:1365:PHE:CD1 | 1:B:1366:VAL:CG2 | 2.30 | 1.15 |
| 1:B:2732:MET:CE | 1:B:2768:ILE:HG21 | 1.78 | 1.14 |
| 1:A:1826:PHE:HE2 | 1:A:1831:LEU:HB2 | 1.13 | 1.14 |
| 1:B:2488:GLU:HB3 | 1:B:2491:LEU:HD12 | 1.17 | 1.13 |
| 1:B:2732:MET:CE | 1:B:2768:ILE:CG2 | 2.26 | 1.13 |
| 1:B:2386:MET:HG2 | 1:B:2627:ARG:HD2 | 1.16 | 1.13 |
| 1:B:3534:LEU:CD1 | 1:B:3618:TYR:HE2 | 1.61 | 1.13 |
| 1:A:1823:ASP:HB2 | 1:A:1852:ARG:O | 1.48 | 1.13 |
| 1:A:2707:VAL:HB | 1:A:2712:LEU:HD11 | 1.13 | 1.12 |
| 1:A:2111:LYS:HD3 | 1:A:2161:GLU:HG3 | 1.22 | 1.12 |
| 1:B:2380:LEU:HD21 | 1:B:2390:ILE:CD1 | 1.78 | 1.11 |
| 1:A:3777:VAL:CG1 | 1:A:3895:PHE:HE1 | 1.61 | 1.11 |
| 1:B:1535:PRO:HB2 | 1:B:1841:ILE:CG1 | 1.81 | 1.11 |
| 1:A:3534:LEU:HD12 | 1:A:3618:TYR:HE2 | 1.15 | 1.11 |
| 1:A:2386:MET:HB2 | 1:A:2627:ARG:HD3 | 1.32 | 1.11 |
| 1:B:3777:VAL:HG11 | 1:B:3895:PHE:HE1 | 1.09 | 1.11 |
| 1:A:3024:LEU:HD11 | 1:A:3303:LYS:HG3 | 1.33 | 1.11 |
| 1:A:4033:LEU:CD1 | 1:A:4035:GLN:HB2 | 1.80 | 1.11 |
| 1:B:2732:MET:HE1 | 1:B:2768:ILE:HG21 | 1.17 | 1.10 |
| 1:B:1992:LYS:HG3 | 1:B:2024:SER:HB2 | 1.30 | 1.10 |
| 1:B:1983:LEU:HG | 1:B:1993:THR:HG23 | 1.14 | 1.10 |
| 1:A:1826:PHE:CE2 | 1:A:1831:LEU:HB2 | 1.86 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2732:MET:CB | 3:B:5402:ADP:C6 | 2.34 | 1.10 |
| 1:B:2732:MET:HE3 | 1:B:2768:ILE:CG2 | 1.80 | 1.10 |
| 1:A:3534:LEU:CD1 | 1:A:3618:TYR:HE2 | 1.64 | 1.10 |
| 1:A:3306:TRP:CH2 | 1:A:3594:ALA:HB3 | 1.86 | 1.09 |
| 1:A:2488:GLU:HB3 | 1:A:2491:LEU:HD12 | 1.15 | 1.09 |
| 1:B:2111:LYS:HD3 | 1:B:2161:GLU:HG3 | 1.20 | 1.09 |
| 1:B:216:PRO:O | 1:B:1365:PHE:HB2 | 1.50 | 1.08 |
| 1:B:2920:TRP:HB2 | 1:B:2989:PRO:HG3 | 1.14 | 1.08 |
| 1:B:1823:ASP:HB2 | 1:B:1852:ARG:O | 1.53 | 1.08 |
| 1:A:2745:ILE:HG23 | 1:A:2756:MET:HE1 | 1.28 | 1.07 |
| 1:B:1822:CYS:HB2 | 1:B:1853:LEU:HD21 | 1.34 | 1.07 |
| 1:B:1421:TYR:O | 1:B:1425:GLU:HB2 | 1.52 | 1.06 |
| 1:B:1409:LEU:HD21 | 1:B:1435:LEU:HB3 | 1.33 | 1.06 |
| 1:B:1645:PHE:HB3 | 1:B:1765:ILE:HG22 | 1.37 | 1.06 |
| 1:A:2107:LYS:HE3 | 1:A:2495:ASP:OD2 | 1.53 | 1.06 |
| 1:B:2473:LEU:HD23 | 1:B:2475:PRO:CD | 1.86 | 1.05 |
| 1:A:2988:SER:HB3 | 1:A:2989:PRO:HD2 | 1.11 | 1.05 |
| 1:B:2785:LYS:HD3 | 1:B:3482:GLY:O | 1.56 | 1.05 |
| 1:B:2473:LEU:CD2 | 1:B:2475:PRO:CD | 2.33 | 1.05 |
| 1:B:1535:PRO:HB2 | 1:B:1841:ILE:HG13 | 1.33 | 1.05 |
| 1:A:1866:GLN:OE1 | 1:A:1911:ASN:HB2 | 1.57 | 1.05 |
| 1:B:2988:SER:HB3 | 1:B:2989:PRO:HD2 | 1.09 | 1.04 |
| 1:B:2386:MET:CB | 1:B:2627:ARG:HD2 | 1.87 | 1.04 |
| 1:B:2378:VAL:HG22 | 1:B:2380:LEU:CD1 | 1.86 | 1.04 |
| 1:A:2707:VAL:CB | 1:A:2712:LEU:HD11 | 1.88 | 1.03 |
| 1:B:2494:LEU:HD13 | 1:B:2498:GLY:HA2 | 1.04 | 1.03 |
| 1:B:2107:LYS:HE3 | 1:B:2495:ASP:OD2 | 1.56 | 1.03 |
| 1:A:1421:TYR:HD1 | 1:A:1425:GLU:HB2 | 1.18 | 1.03 |
| 1:A:2282:ASN:HB3 | 1:A:2552:ARG:HG3 | 1.36 | 1.03 |
| 1:B:3534:LEU:HD12 | 1:B:3618:TYR:HE2 | 1.19 | 1.02 |
| 1:A:2787:HIS:HA | 1:A:3460:PRO:HD2 | 1.38 | 1.02 |
| 1:A:1535:PRO:HB2 | 1:A:1841:ILE:HG13 | 1.39 | 1.02 |
| 1:A:2920:TRP:HB2 | 1:A:2989:PRO:HG3 | 1.02 | 1.02 |
| 1:A:1999:LYS:HG2 | 1:A:2014:PHE:CE1 | 1.95 | 1.01 |
| 1:A:2494:LEU:HD13 | 1:A:2498:GLY:CA | 1.88 | 1.01 |
| 1:A:2494:LEU:CD1 | 1:A:2498:GLY:HA2 | 1.90 | 1.01 |
| 1:B:2732:MET:HB2 | 3:B:5402:ADP:N1 | 1.76 | 1.01 |
| 1:A:3946:VAL:HG12 | 1:A:3950:PHE:O | 1.61 | 1.00 |
| 1:B:2494:LEU:HD13 | 1:B:2498:GLY:CA | 1.91 | 1.00 |
| 1:A:1822:CYS:HB2 | 1:A:1853:LEU:HD21 | 1.38 | 1.00 |
| 1:A:1645:PHE:HB3 | 1:A:1765:ILE:HG22 | 1.41 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3534:LEU:HD12 | 1:B:3618:TYR:CE2 | 1.97 | 1.00 |
| 1:A:2494:LEU:HD13 | 1:A:2498:GLY:HA2 | 1.00 | 1.00 |
| 1:B:2386:MET:HG2 | 1:B:2627:ARG:CD | 1.92 | 0.99 |
| 1:B:3534:LEU:CD1 | 1:B:3618:TYR:CE2 | 2.44 | 0.99 |
| 1:B:1365:PHE:CE1 | 1:B:1366:VAL:CG2 | 2.45 | 0.99 |
| 1:B:1620:PHE:CD1 | 1:B:1760:PHE:CZ | 2.51 | 0.99 |
| 1:B:2494:LEU:CD1 | 1:B:2498:GLY:HA2 | 1.93 | 0.99 |
| 1:B:1365:PHE:HD1 | 1:B:1366:VAL:CG2 | 1.71 | 0.99 |
| 1:B:1645:PHE:HB3 | 1:B:1765:ILE:CG2 | 1.93 | 0.99 |
| 1:A:1992:LYS:CG | 1:A:2024:SER:HB2 | 1.93 | 0.99 |
| 1:B:1421:TYR:CE1 | 1:B:1425:GLU:CG | 2.46 | 0.98 |
| 1:A:1992:LYS:HG3 | 1:A:2024:SER:HB2 | 1.39 | 0.98 |
| 1:A:1620:PHE:HD1 | 1:A:1760:PHE:HZ | 0.98 | 0.98 |
| 1:A:2732:MET:CE | 1:A:2768:ILE:HG21 | 1.94 | 0.98 |
| 1:A:3307:LEU:HD12 | 1:A:3307:LEU:C | 1.82 | 0.97 |
| 1:A:1645:PHE:HB3 | 1:A:1765:ILE:CG2 | 1.93 | 0.97 |
| 1:A:2488:GLU:CB | 1:A:2491:LEU:HD12 | 1.95 | 0.97 |
| 1:A:2920:TRP:HB2 | 1:A:2989:PRO:CG | 1.93 | 0.97 |
| 1:A:3737:THR:HB | 1:A:3740:THR:OG1 | 1.64 | 0.97 |
| 1:B:2137:VAL:O | 1:B:2141:ILE:HG23 | 1.65 | 0.97 |
| 1:B:1620:PHE:HD1 | 1:B:1760:PHE:HZ | 1.02 | 0.97 |
| 1:A:1744:LEU:HA | 1:A:1760:PHE:CE2 | 2.00 | 0.97 |
| 1:B:1535:PRO:CB | 1:B:1841:ILE:HG13 | 1.95 | 0.97 |
| 1:B:1630:ILE:HG22 | 1:B:1655:MET:SD | 2.05 | 0.97 |
| 1:B:3024:LEU:HD11 | 1:B:3303:LYS:HG3 | 1.43 | 0.96 |
| 1:A:3534:LEU:CD1 | 1:A:3618:TYR:CE2 | 2.49 | 0.96 |
| 1:B:3777:VAL:HG11 | 1:B:3895:PHE:CE1 | 2.00 | 0.96 |
| 1:B:2988:SER:HB3 | 1:B:2989:PRO:CD | 1.94 | 0.96 |
| 1:A:2768:ILE:HG22 | 3:A:5402:ADP:O2A | 1.65 | 0.96 |
| 1:A:1421:TYR:O | 1:A:1421:TYR:CD1 | 2.19 | 0.95 |
| 1:B:1649:LEU:HD11 | 1:B:1704:GLU:HG3 | 1.45 | 0.95 |
| 1:A:1620:PHE:CD1 | 1:A:1760:PHE:CZ | 2.53 | 0.95 |
| 1:B:1421:TYR:CE1 | 1:B:1425:GLU:HG3 | 2.02 | 0.95 |
| 1:A:2765:GLY:HA2 | 3:A:5402:ADP:PA | 2.07 | 0.95 |
| 1:A:2407:LEU:HD22 | 1:A:2412:ARG:HH12 | 1.32 | 0.95 |
| 1:B:2412:ARG:NH1 | 1:B:2553:HIS:HA | 1.82 | 0.94 |
| 1:A:3307:LEU:HD12 | 1:A:3307:LEU:O | 1.67 | 0.94 |
| 1:B:2707:VAL:CB | 1:B:2712:LEU:HD11 | 1.96 | 0.94 |
| 1:A:3534:LEU:HD12 | 1:A:3618:TYR:CE2 | 2.02 | 0.94 |
| 1:A:3306:TRP:CZ2 | 1:A:3594:ALA:HB3 | 2.03 | 0.94 |
| 1:B:2080:LYS:HD2 | 1:B:2195:GLU:HB2 | 1.48 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2732:MET:HE3 | 1:A:2768:ILE:HG21 | 1.47 | 0.94 |
| 1:A:1421:TYR:O | 1:A:1425:GLU:HB2 | 1.66 | 0.94 |
| 1:A:2141:ILE:HG22 | 1:A:2145:PHE:HB2 | 1.49 | 0.94 |
| 1:A:1956:LEU:HB3 | 1:A:1968:PHE:CE2 | 2.03 | 0.94 |
| 1:B:3530:PHE:CD1 | 1:B:3618:TYR:HD2 | 1.86 | 0.94 |
| 1:A:2109:LEU:HD11 | 1:A:2129:LEU:HD22 | 1.48 | 0.94 |
| 1:B:2111:LYS:HD3 | 1:B:2161:GLU:CG | 1.98 | 0.94 |
| 1:A:2988:SER:HB3 | 1:A:2989:PRO:CD | 1.96 | 0.94 |
| 1:B:2787:HIS:HA | 1:B:3460:PRO:HD2 | 1.47 | 0.93 |
| 1:A:1409:LEU:HD21 | 1:A:1435:LEU:CB | 1.98 | 0.93 |
| 1:B:1866:GLN:OE1 | 1:B:1911:ASN:HB2 | 1.68 | 0.93 |
| 1:A:2488:GLU:HB3 | 1:A:2491:LEU:CD1 | 1.99 | 0.93 |
| 1:A:3534:LEU:HD11 | 1:A:3614:LEU:HD23 | 1.47 | 0.93 |
| 1:B:2920:TRP:HB2 | 1:B:2989:PRO:CG | 1.97 | 0.93 |
| 1:A:3303:LYS:HD2 | 1:A:3306:TRP:HB2 | 1.51 | 0.93 |
| 1:B:3946:VAL:HG12 | 1:B:3950:PHE:O | 1.69 | 0.93 |
| 1:B:1774:LEU:HD21 | 1:B:1922:LYS:O | 1.67 | 0.93 |
| 1:B:2761:ALA:O | 1:B:2892:CYS:HB3 | 1.69 | 0.93 |
| 1:B:1562:MET:HB3 | 1:B:1569:ILE:HD11 | 1.48 | 0.92 |
| 1:B:3777:VAL:CG1 | 1:B:3895:PHE:HE1 | 1.82 | 0.92 |
| 1:B:1421:TYR:CZ | 1:B:1425:GLU:HG3 | 2.05 | 0.92 |
| 1:B:1645:PHE:CB | 1:B:1765:ILE:HG22 | 1.99 | 0.91 |
| 1:B:1726:LEU:CD1 | 1:B:3984:GLN:HB3 | 2.01 | 0.91 |
| 1:B:1535:PRO:HB2 | 1:B:1841:ILE:CD1 | 2.00 | 0.91 |
| 1:B:3656:VAL:HG13 | 1:B:3677:LEU:HB3 | 1.51 | 0.91 |
| 1:A:1992:LYS:HE2 | 1:A:2024:SER:O | 1.71 | 0.91 |
| 1:A:3777:VAL:HG11 | 1:A:3895:PHE:HE1 | 0.77 | 0.91 |
| 1:B:3303:LYS:HA | 1:B:3306:TRP:CD1 | 2.05 | 0.91 |
| 1:A:3304:GLU:O | 1:A:3307:LEU:HG | 1.68 | 0.90 |
| 1:B:1726:LEU:HD12 | 1:B:3984:GLN:HB3 | 1.50 | 0.90 |
| 1:A:3406:PHE:HB2 | 1:A:3513:VAL:CG1 | 2.01 | 0.90 |
| 1:A:3304:GLU:HG3 | 1:A:3307:LEU:HD23 | 1.51 | 0.90 |
| 1:A:1956:LEU:HB3 | 1:A:1968:PHE:HE2 | 1.36 | 0.90 |
| 1:A:1939:PHE:CD1 | 1:A:1940:GLU:O | 2.24 | 0.90 |
| 1:A:4033:LEU:HD13 | 1:A:4035:GLN:HB2 | 1.53 | 0.90 |
| 1:B:2112:GLU:HB3 | 1:B:2117:SER:HB2 | 1.51 | 0.90 |
| 1:A:2762:SER:O | 1:A:2763:ARG:HB2 | 1.70 | 0.90 |
| 1:A:1421:TYR:CD1 | 1:A:1425:GLU:HB2 | 2.07 | 0.90 |
| 1:B:1802:LYS:HG2 | 1:B:1921:MET:HG3 | 1.52 | 0.89 |
| 1:B:1365:PHE:CD1 | 1:B:1366:VAL:N | 2.40 | 0.89 |
| 1:B:3406:PHE:HB2 | 1:B:3513:VAL:CG1 | 2.03 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2920:TRP:CB | 1:A:2989:PRO:HG3 | 1.98 | 0.89 |
| 1:A:3306:TRP:CH2 | 1:A:3594:ALA:CB | 2.54 | 0.89 |
| 1:B:1940:GLU:HB2 | 1:B:1989:GLU:O | 1.73 | 0.89 |
| 1:A:1604:ALA:HA | 1:A:1607:TRP:CD1 | 2.08 | 0.89 |
| 1:A:2787:HIS:HA | 1:A:3460:PRO:CD | 2.03 | 0.89 |
| 1:A:1940:GLU:HB2 | 1:A:1989:GLU:O | 1.70 | 0.89 |
| 1:B:2732:MET:CB | 3:B:5402:ADP:C5 | 2.56 | 0.88 |
| 1:A:3525:ILE:CD1 | 1:A:3646:ILE:HG22 | 2.03 | 0.88 |
| 1:B:1924:PRO:HB2 | 1:B:1929:ILE:HD11 | 1.53 | 0.88 |
| 1:A:1409:LEU:HD21 | 1:A:1435:LEU:HB3 | 1.53 | 0.88 |
| 1:A:2517:LYS:HE3 | 1:A:2524:VAL:HG22 | 1.54 | 0.88 |
| 1:B:3024:LEU:CD1 | 1:B:3303:LYS:HG3 | 2.03 | 0.88 |
| 1:A:3530:PHE:CD1 | 1:A:3618:TYR:HD2 | 1.91 | 0.88 |
| 1:B:1939:PHE:CD1 | 1:B:1940:GLU:O | 2.26 | 0.88 |
| 1:A:1929:ILE:HD13 | 1:A:1970:LEU:HD11 | 1.56 | 0.88 |
| 1:B:3792:ARG:HB2 | 1:B:3955:TYR:CD1 | 2.09 | 0.88 |
| 1:B:2488:GLU:HB3 | 1:B:2491:LEU:CD1 | 2.03 | 0.88 |
| 1:A:1416:LYS:HA | 1:A:1421:TYR:CZ | 2.09 | 0.88 |
| 1:A:2517:LYS:CE | 1:A:2524:VAL:CG2 | 2.51 | 0.88 |
| 1:A:2111:LYS:HD3 | 1:A:2161:GLU:CG | 2.04 | 0.88 |
| 1:B:1926:SER:CB | 1:B:1970:LEU:HD12 | 2.05 | 0.87 |
| 1:A:2988:SER:CB | 1:A:2989:PRO:HD2 | 2.03 | 0.87 |
| 1:A:2476:LYS:H | 1:A:2476:LYS:CD | 1.86 | 0.87 |
| 1:A:1620:PHE:CD1 | 1:A:1760:PHE:HZ | 1.89 | 0.87 |
| 1:A:2745:ILE:HG23 | 1:A:2756:MET:CE | 2.04 | 0.87 |
| 1:B:2107:LYS:HE2 | 1:B:2499:SER:HB3 | 1.57 | 0.87 |
| 1:A:3656:VAL:HG13 | 1:A:3677:LEU:HB3 | 1.57 | 0.87 |
| 1:B:3737:THR:HB | 1:B:3740:THR:OG1 | 1.74 | 0.87 |
| 1:A:2386:MET:CB | 1:A:2627:ARG:HD3 | 2.04 | 0.86 |
| 1:B:2175:ILE:HG12 | 1:B:2183:ARG:HB3 | 1.56 | 0.86 |
| 1:B:2080:LYS:NZ | 1:B:2549:ARG:NH2 | 2.21 | 0.86 |
| 1:A:2274:HIS:HE1 | 1:A:2326:LEU:O | 1.59 | 0.86 |
| 1:A:2707:VAL:HB | 1:A:2712:LEU:CD1 | 2.01 | 0.86 |
| 1:B:1992:LYS:CG | 1:B:2024:SER:HB2 | 2.04 | 0.86 |
| 1:A:2763:ARG:O | 3:A:5402:ADP:C8 | 2.27 | 0.86 |
| 1:B:2988:SER:CB | 1:B:2989:PRO:HD2 | 2.00 | 0.86 |
| 1:B:2563:SER:HB3 | 1:B:2566:SER:H | 1.39 | 0.86 |
| 1:B:2733:VAL:N | 3:B:5402:ADP:N1 | 2.22 | 0.86 |
| 1:B:2378:VAL:CG2 | 1:B:2380:LEU:CD1 | 2.54 | 0.86 |
| 1:B:3851:VAL:HG13 | 1:B:3855:LEU:HD23 | 1.56 | 0.86 |
| 1:A:4033:LEU:HD11 | 1:A:4035:GLN:HB2 | 1.57 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2080:LYS:HZ2 | 1:B:2549:ARG:NH2 | 1.73 | 0.86 |
| 1:B:1744:LEU:HA | 1:B:1760:PHE:CE2 | 2.11 | 0.85 |
| 1:B:1649:LEU:CD1 | 1:B:1704:GLU:HG3 | 2.06 | 0.85 |
| 1:A:1823:ASP:CB | 1:A:1852:ARG:O | 2.23 | 0.85 |
| 1:A:2362:ALA:HB3 | 1:A:2365:LYS:O | 1.75 | 0.85 |
| 1:A:3792:ARG:HB2 | 1:A:3955:TYR:CD1 | 2.12 | 0.85 |
| 1:A:3024:LEU:CD1 | 1:A:3303:LYS:HG3 | 2.06 | 0.85 |
| 1:B:1823:ASP:CB | 1:B:1852:ARG:O | 2.23 | 0.85 |
| 1:B:1956:LEU:HB3 | 1:B:1968:PHE:CE2 | 2.12 | 0.85 |
| 1:A:3851:VAL:HG13 | 1:A:3855:LEU:HD23 | 1.59 | 0.84 |
| 1:B:1983:LEU:CG | 1:B:1993:THR:HG23 | 2.04 | 0.84 |
| 1:A:1926:SER:CB | 1:A:1970:LEU:HD12 | 2.08 | 0.84 |
| 1:B:2412:ARG:HH11 | 1:B:2553:HIS:HA | 1.35 | 0.84 |
| 1:B:1620:PHE:CD1 | 1:B:1760:PHE:HZ | 1.92 | 0.84 |
| 1:A:2765:GLY:HA2 | 3:A:5402:ADP:O2A | 1.76 | 0.84 |
| 1:B:2225:LYS:HA | 2:B:5400:ATP:C2 | 2.12 | 0.84 |
| 1:B:2003:LEU:HA | 1:B:2006:LEU:HD12 | 1.58 | 0.84 |
| 1:A:1645:PHE:CB | 1:A:1765:ILE:HG22 | 2.08 | 0.84 |
| 1:B:2779:LEU:HD23 | 1:B:2812:ARG:O | 1.78 | 0.84 |
| 1:A:1562:MET:HB3 | 1:A:1569:ILE:HD11 | 1.60 | 0.83 |
| 1:A:1649:LEU:CD1 | 1:A:1704:GLU:HG3 | 2.08 | 0.83 |
| 1:A:2755:HIS:HB2 | 1:A:2911:ARG:O | 1.78 | 0.83 |
| 1:B:2488:GLU:CB | 1:B:2491:LEU:HD12 | 2.04 | 0.83 |
| 1:B:1421:TYR:CE1 | 1:B:1425:GLU:HG2 | 2.10 | 0.83 |
| 1:B:2787:HIS:HA | 1:B:3460:PRO:CD | 2.08 | 0.83 |
| 1:A:1924:PRO:HB2 | 1:A:1929:ILE:HD11 | 1.61 | 0.83 |
| 1:B:1394:LEU:HD22 | 1:B:1449:GLN:HE22 | 1.43 | 0.83 |
| 1:A:2785:LYS:HD2 | 1:A:3482:GLY:O | 1.78 | 0.83 |
| 1:A:2763:ARG:O | 3:A:5402:ADP:H8 | 1.62 | 0.83 |
| 1:B:1392:LEU:HD13 | 1:B:1393:LYS:N | 1.94 | 0.83 |
| 1:A:1574:PHE:HB3 | 1:A:1576:GLU:H | 1.43 | 0.83 |
| 1:B:3923:VAL:HG23 | 1:B:4038:GLU:HA | 1.60 | 0.83 |
| 1:B:2960:THR:HB | 1:B:2963:ASP:HB2 | 1.61 | 0.83 |
| 1:A:2107:LYS:HE2 | 1:A:2499:SER:HB3 | 1.59 | 0.82 |
| 1:B:2131:THR:HG22 | 1:B:2176:LEU:HD21 | 1.61 | 0.82 |
| 1:B:1409:LEU:HD21 | 1:B:1435:LEU:CB | 2.08 | 0.82 |
| 1:A:2173:ASN:HB3 | 1:A:2175:ILE:HG22 | 1.61 | 0.82 |
| 1:A:1640:VAL:HB | 1:A:1686:LYS:HZ1 | 1.42 | 0.82 |
| 1:B:2513:GLN:O | 1:B:2526:ILE:HG13 | 1.79 | 0.82 |
| 1:A:2563:SER:HB3 | 1:A:2566:SER:H | 1.44 | 0.82 |
| 1:B:3919:LYS:HZ3 | 1:B:4038:GLU:CD | 1.83 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3406:PHE:HB2 | 1:A:3513:VAL:HG11 | 1.62 | 0.81 |
| 1:A:2517:LYS:CE | 1:A:2524:VAL:HG21 | 2.11 | 0.81 |
| 1:A:2137:VAL:O | 1:A:2141:ILE:HG23 | 1.78 | 0.81 |
| 1:A:1996:GLU:O | 1:A:2000:ARG:HG3 | 1.78 | 0.81 |
| 1:B:2386:MET:CB | 1:B:2627:ARG:CD | 2.59 | 0.81 |
| 1:A:1965:HIS:HD2 | 1:A:2212:LEU:HD21 | 1.46 | 0.81 |
| 1:B:1421:TYR:O | 1:B:1425:GLU:CB | 2.28 | 0.81 |
| 1:A:1392:LEU:HD13 | 1:A:1393:LYS:N | 1.96 | 0.81 |
| 1:B:3534:LEU:HD11 | 1:B:3614:LEU:HD23 | 1.62 | 0.80 |
| 1:B:1744:LEU:HA | 1:B:1760:PHE:CD2 | 2.16 | 0.80 |
| 1:A:1421:TYR:HE1 | 1:A:1425:GLU:CD | 1.83 | 0.80 |
| 1:A:3816:LEU:HD23 | 1:A:3847:SER:OG | 1.81 | 0.80 |
| 1:A:1535:PRO:C | 1:A:1841:ILE:HD11 | 2.02 | 0.80 |
| 1:A:1983:LEU:CG | 1:A:1993:THR:HG23 | 2.10 | 0.80 |
| 1:B:2332:GLY:HA2 | 1:B:2335:GLN:HB2 | 1.64 | 0.80 |
| 1:B:1387:GLU:HB3 | 1:B:1393:LYS:HG2 | 1.61 | 0.80 |
| 1:A:3979:ASN:O | 1:A:3981:PRO:HD2 | 1.81 | 0.80 |
| 1:B:3946:VAL:CG1 | 1:B:3950:PHE:O | 2.30 | 0.80 |
| 1:A:1983:LEU:HD23 | 1:A:1993:THR:O | 1.81 | 0.79 |
| 1:A:2109:LEU:CD1 | 1:A:2129:LEU:HD22 | 2.12 | 0.79 |
| 1:B:2732:MET:HE1 | 1:B:2768:ILE:CG2 | 1.96 | 0.79 |
| 1:B:1604:ALA:HA | 1:B:1607:TRP:CD1 | 2.17 | 0.79 |
| 1:A:3024:LEU:HD11 | 1:A:3303:LYS:CG | 2.12 | 0.79 |
| 1:A:1999:LYS:HG2 | 1:A:2014:PHE:HE1 | 1.43 | 0.79 |
| 1:A:2175:ILE:HG12 | 1:A:2183:ARG:HB3 | 1.65 | 0.79 |
| 1:A:1706:LEU:HD22 | 1:A:1935:GLN:HG2 | 1.65 | 0.79 |
| 1:B:2472:THR:CG2 | 1:B:2524:VAL:HG22 | 2.12 | 0.79 |
| 1:A:216:PRO:C | 1:A:1365:PHE:HA | 2.04 | 0.78 |
| 1:B:3530:PHE:CD1 | 1:B:3618:TYR:CD2 | 2.71 | 0.78 |
| 1:A:2424:LYS:HZ1 | 3:A:5401:ADP:PB | 2.06 | 0.78 |
| 1:B:2111:LYS:NZ | 1:B:2161:GLU:HG2 | 1.98 | 0.78 |
| 1:A:1462:ASN:HB2 | 1:A:1465:ILE:HG22 | 1.65 | 0.78 |
| 1:B:2080:LYS:HE2 | 2:B:5400:ATP:O1B | 1.84 | 0.78 |
| 1:B:2707:VAL:HB | 1:B:2712:LEU:CD1 | 2.10 | 0.78 |
| 1:A:3618:TYR:CD1 | 1:A:3618:TYR:N | 2.50 | 0.78 |
| 1:B:1992:LYS:HE2 | 1:B:2024:SER:O | 1.84 | 0.78 |
| 1:A:3792:ARG:HB2 | 1:A:3955:TYR:CE1 | 2.19 | 0.78 |
| 1:B:3690:LEU:HD23 | 1:B:3694:PHE:HB3 | 1.66 | 0.78 |
| 1:A:2181:GLY:O | 1:A:2182:GLU:HG3 | 1.84 | 0.77 |
| 1:B:2274:HIS:HE1 | 1:B:2326:LEU:O | 1.67 | 0.77 |
| 1:B:2448:ASP:HB2 | 1:B:2829:GLU:OE1 | 1.83 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4065:LEU:HD11 | 1:B:4070:ILE:HD11 | 1.65 | 0.77 |
| 1:A:1421:TYR:O | 1:A:1425:GLU:CB | 2.31 | 0.77 |
| 1:A:1405:CYS:O | 1:A:1409:LEU:HG | 1.84 | 0.77 |
| 1:A:3530:PHE:CD1 | 1:A:3618:TYR:CD2 | 2.72 | 0.77 |
| 1:B:1425:GLU:OE2 | 1:B:1429:LEU:CG | 2.32 | 0.77 |
| 1:A:2332:GLY:HA2 | 1:A:2335:GLN:HB2 | 1.64 | 0.77 |
| 1:B:2787:HIS:HA | 1:B:3460:PRO:CG | 2.15 | 0.77 |
| 1:B:2446:SER:H | 1:B:2449:THR:HG23 | 1.49 | 0.77 |
| 1:B:1996:GLU:O | 1:B:2000:ARG:HG3 | 1.85 | 0.77 |
| 1:B:3534:LEU:HD13 | 1:B:3618:TYR:HE2 | 1.49 | 0.77 |
| 1:A:2446:SER:H | 1:A:2449:THR:CG2 | 1.97 | 0.77 |
| 1:A:3998:ILE:CG2 | 1:A:4004:LEU:HG | 2.14 | 0.76 |
| 1:A:3306:TRP:CZ2 | 1:A:3594:ALA:CB | 2.69 | 0.76 |
| 1:B:3303:LYS:O | 1:B:3306:TRP:HD1 | 1.68 | 0.76 |
| 1:B:2476:LYS:CD | 1:B:2476:LYS:H | 1.98 | 0.76 |
| 1:A:1495:THR:HG22 | 1:A:1497:ILE:HG22 | 1.67 | 0.76 |
| 1:A:3330:TYR:OH | 1:A:3346:LEU:HD22 | 1.85 | 0.76 |
| 1:A:1983:LEU:CD2 | 1:A:1993:THR:O | 2.34 | 0.76 |
| 1:A:2111:LYS:NZ | 1:A:2161:GLU:HG2 | 2.00 | 0.76 |
| 1:B:1983:LEU:CD2 | 1:B:1993:THR:O | 2.34 | 0.76 |
| 1:B:2517:LYS:HD2 | 1:B:2524:VAL:CG2 | 2.15 | 0.76 |
| 1:B:3774:ILE:O | 1:B:3778:VAL:HG23 | 1.85 | 0.76 |
| 1:A:1802:LYS:HG3 | 4:A:5403:SO4:O2 | 1.86 | 0.76 |
| 1:B:1983:LEU:HG | 1:B:1993:THR:CG2 | 2.07 | 0.76 |
| 1:B:2707:VAL:CG1 | 1:B:2712:LEU:CD1 | 2.64 | 0.76 |
| 1:A:3692:LYS:HE3 | 1:A:3898:GLU:HB3 | 1.68 | 0.76 |
| 1:A:1387:GLU:HB3 | 1:A:1393:LYS:HG2 | 1.68 | 0.76 |
| 1:A:2728:LEU:HD12 | 1:A:2771:ARG:NH2 | 2.00 | 0.76 |
| 1:A:3737:THR:HB | 1:A:3740:THR:CB | 2.15 | 0.75 |
| 1:A:1939:PHE:HD1 | 1:A:1940:GLU:O | 1.69 | 0.75 |
| 1:B:2378:VAL:HG22 | 1:B:2380:LEU:HD12 | 1.66 | 0.75 |
| 1:B:2737:SER:HB2 | 1:B:2924:THR:HG21 | 1.68 | 0.75 |
| 1:B:2473:LEU:HD11 | 1:B:2527:GLU:CG | 2.16 | 0.75 |
| 1:A:2513:GLN:O | 1:A:2526:ILE:HG13 | 1.86 | 0.75 |
| 1:B:3799:LYS:O | 1:B:3803:LEU:HG | 1.87 | 0.75 |
| 1:B:2732:MET:HA | 3:B:5402:ADP:C2 | 2.22 | 0.75 |
| 1:B:2787:HIS:HA | 1:B:3460:PRO:HG2 | 1.68 | 0.75 |
| 1:A:1531:ARG:HG2 | 1:A:1537:PHE:HB3 | 1.68 | 0.74 |
| 1:A:1604:ALA:HA | 1:A:1607:TRP:NE1 | 2.02 | 0.74 |
| 1:A:3785:TYR:HE1 | 1:A:3859:VAL:HG22 | 1.52 | 0.74 |
| 1:A:3700:MET:HB3 | 1:A:4085:THR:HG21 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3923:VAL:HG23 | 1:A:4038:GLU:HA | 1.69 | 0.74 |
| 1:A:2728:LEU:HD12 | 1:A:2771:ARG:CZ | 2.17 | 0.74 |
| 1:A:2336:ARG:HD3 | 1:A:2355:ASP:OD2 | 1.87 | 0.74 |
| 1:B:2473:LEU:CD2 | 1:B:2475:PRO:CG | 2.66 | 0.74 |
| 1:A:1421:TYR:CE1 | 1:A:1425:GLU:CD | 2.61 | 0.74 |
| 1:A:2106:THR:OG1 | 1:A:2154:PHE:HB3 | 1.87 | 0.74 |
| 1:B:2380:LEU:HD21 | 1:B:2390:ILE:HD11 | 0.82 | 0.74 |
| 1:B:2473:LEU:HD22 | 1:B:2475:PRO:HD3 | 1.69 | 0.74 |
| 1:B:1535:PRO:HB2 | 1:B:1841:ILE:HD11 | 1.68 | 0.74 |
| 1:A:2424:LYS:NZ | 3:A:5401:ADP:PB | 2.61 | 0.74 |
| 1:B:2420:PRO:HD3 | 1:B:2536:ASN:HD21 | 1.51 | 0.74 |
| 1:B:1536:ARG:N | 1:B:1841:ILE:HD11 | 2.03 | 0.73 |
| 1:B:1425:GLU:OE2 | 1:B:1429:LEU:HG | 1.87 | 0.73 |
| 1:B:2080:LYS:HG2 | 2:B:5400:ATP:PB | 2.27 | 0.73 |
| 1:B:3330:TYR:OH | 1:B:3346:LEU:HD22 | 1.88 | 0.73 |
| 1:A:3618:TYR:HD1 | 1:A:3618:TYR:N | 1.86 | 0.73 |
| 1:A:2763:ARG:HE | 3:A:5402:ADP:H4' | 1.53 | 0.73 |
| 1:B:1953:LEU:HD11 | 1:B:1973:LEU:HB3 | 1.69 | 0.73 |
| 1:B:2517:LYS:HD2 | 1:B:2524:VAL:HG21 | 1.69 | 0.73 |
| 1:B:1365:PHE:HD1 | 1:B:1366:VAL:H | 1.11 | 0.73 |
| 1:A:3304:GLU:O | 1:A:3307:LEU:CG | 2.37 | 0.73 |
| 1:B:1910:GLU:HB2 | 1:B:3846:MET:CB | 2.18 | 0.73 |
| 1:A:2493:LYS:HG3 | 1:A:2494:LEU:H | 1.53 | 0.73 |
| 1:B:2853:LEU:HD21 | 1:B:2870:GLU:HG3 | 1.69 | 0.73 |
| 1:A:3566:LEU:O | 1:A:3570:LEU:HG | 1.89 | 0.73 |
| 1:B:1826:PHE:CE2 | 1:B:1853:LEU:HD22 | 2.23 | 0.73 |
| 1:B:1574:PHE:HB3 | 1:B:1576:GLU:H | 1.54 | 0.73 |
| 1:B:2112:GLU:HB3 | 1:B:2117:SER:CB | 2.18 | 0.72 |
| 1:A:1929:ILE:HD13 | 1:A:1970:LEU:CD1 | 2.18 | 0.72 |
| 1:A:3679:TYR:HB3 | 1:A:3767:PHE:HE1 | 1.53 | 0.72 |
| 1:B:3839:ILE:HG23 | 1:B:3873:MET:HG3 | 1.71 | 0.72 |
| 1:B:1967:HIS:O | 1:B:1968:PHE:HD1 | 1.72 | 0.72 |
| 1:A:2787:HIS:CA | 1:A:3460:PRO:HD2 | 2.18 | 0.72 |
| 1:A:1649:LEU:HD11 | 1:A:1704:GLU:HG3 | 1.70 | 0.72 |
| 1:A:3799:LYS:O | 1:A:3803:LEU:HG | 1.89 | 0.72 |
| 1:B:3566:LEU:CD1 | 1:B:3570:LEU:HD11 | 2.19 | 0.72 |
| 1:B:1983:LEU:HD21 | 1:B:1993:THR:O | 1.90 | 0.72 |
| 1:B:2446:SER:H | 1:B:2449:THR:CG2 | 2.03 | 0.72 |
| 1:A:2787:HIS:HA | 1:A:3460:PRO:CG | 2.18 | 0.72 |
| 1:A:3848:LEU:HD21 | 1:A:3852:LYS:HE3 | 1.71 | 0.72 |
| 1:A:1981:SER:HB3 | 1:A:1982:PRO:HD3 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2762:SER:C | 1:B:2764:THR:H | 1.94 | 0.72 |
| 1:B:2080:LYS:NZ | 2:B:5400:ATP:O3G | 2.23 | 0.72 |
| 1:B:2755:HIS:HB2 | 1:B:2911:ARG:O | 1.90 | 0.72 |
| 1:B:2425:THR:HB | 3:B:5401:ADP:O2A | 1.90 | 0.72 |
| 1:B:3566:LEU:HA | 1:B:3583:LEU:CD2 | 2.20 | 0.71 |
| 1:B:2106:THR:OG1 | 1:B:2154:PHE:HB3 | 1.89 | 0.71 |
| 1:B:2424:LYS:NZ | 3:B:5401:ADP:O2B | 2.23 | 0.71 |
| 1:A:1707:HIS:O | 1:A:1711:VAL:HG23 | 1.89 | 0.71 |
| 1:A:1535:PRO:HB2 | 1:A:1841:ILE:CG1 | 2.18 | 0.71 |
| 1:B:1956:LEU:HB3 | 1:B:1968:PHE:HE2 | 1.50 | 0.71 |
| 1:B:2472:THR:HG21 | 1:B:2524:VAL:HG22 | 1.70 | 0.71 |
| 1:A:3302:GLU:O | 1:A:3305:ARG:HB2 | 1.90 | 0.71 |
| 1:A:3946:VAL:CG1 | 1:A:3950:PHE:O | 2.36 | 0.71 |
| 1:B:3566:LEU:O | 1:B:3570:LEU:HG | 1.90 | 0.71 |
| 1:B:3303:LYS:HA | 1:B:3306:TRP:HD1 | 1.49 | 0.71 |
| 1:B:3406:PHE:HB2 | 1:B:3513:VAL:HG12 | 1.72 | 0.71 |
| 1:A:2315:THR:HG21 | 1:A:2350:SER:HB3 | 1.72 | 0.71 |
| 1:A:2448:ASP:HB2 | 1:A:2829:GLU:OE1 | 1.90 | 0.71 |
| 1:A:2112:GLU:HB3 | 1:A:2117:SER:HB2 | 1.72 | 0.71 |
| 1:A:1849:GLU:HG2 | 1:A:1899:ASN:ND2 | 2.05 | 0.71 |
| 1:B:2761:ALA:O | 1:B:2892:CYS:CB | 2.37 | 0.71 |
| 1:B:1392:LEU:HD13 | 1:B:1392:LEU:C | 2.11 | 0.71 |
| 1:A:2446:SER:H | 1:A:2449:THR:HG23 | 1.56 | 0.71 |
| 1:A:4020:ASN:HB3 | 1:A:4028:ARG:HH21 | 1.56 | 0.71 |
| 1:A:2226:ILE:HG23 | 1:A:2288:VAL:HG21 | 1.71 | 0.71 |
| 1:B:3618:TYR:CD1 | 1:B:3618:TYR:N | 2.57 | 0.71 |
| 1:B:1849:GLU:HG2 | 1:B:1899:ASN:HD22 | 1.54 | 0.71 |
| 1:A:2765:GLY:HA2 | 3:A:5402:ADP:O3A | 1.89 | 0.71 |
| 1:A:1726:LEU:CD1 | 1:A:3984:GLN:HB3 | 2.20 | 0.71 |
| 1:B:2473:LEU:HD11 | 1:B:2527:GLU:HG2 | 1.72 | 0.71 |
| 1:B:1926:SER:HB2 | 1:B:1970:LEU:HD12 | 1.72 | 0.71 |
| 1:A:1995:VAL:HG21 | 1:A:2024:SER:HB3 | 1.72 | 0.71 |
| 1:A:1409:LEU:HD21 | 1:A:1435:LEU:HB2 | 1.72 | 0.71 |
| 1:A:1726:LEU:HD12 | 1:A:3984:GLN:HB3 | 1.72 | 0.71 |
| 1:A:1630:ILE:HG22 | 1:A:1655:MET:SD | 2.31 | 0.71 |
| 1:B:2473:LEU:HD22 | 1:B:2475:PRO:HG3 | 1.73 | 0.70 |
| 1:B:1394:LEU:HD22 | 1:B:1449:GLN:NE2 | 2.05 | 0.70 |
| 1:A:3737:THR:OG1 | 1:A:3740:THR:HB | 1.90 | 0.70 |
| 1:A:3473:ALA:HB3 | 1:A:3476:ARG:O | 1.90 | 0.70 |
| 1:A:2620:ARG:NH2 | 3:A:5401:ADP:PA | 2.64 | 0.70 |
| 1:A:3566:LEU:HA | 1:A:3583:LEU:CD2 | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2779:LEU:HD23 | 1:A:2812:ARG:O | 1.91 | 0.70 |
| 1:B:2631:THR:O | 1:B:2635:THR:HG22 | 1.92 | 0.70 |
| 1:B:2489:ILE:HG22 | 1:B:2535:CYS:HB3 | 1.72 | 0.70 |
| 1:A:2252:LEU:HD21 | 1:A:2310:LEU:HD23 | 1.74 | 0.70 |
| 1:B:3303:LYS:HD2 | 1:B:3306:TRP:CD1 | 2.27 | 0.70 |
| 1:B:2220:CYS:SG | 1:B:2224:SER:HB2 | 2.32 | 0.70 |
| 1:A:4033:LEU:CD1 | 1:A:4035:GLN:CB | 2.65 | 0.70 |
| 1:A:2763:ARG:HE | 3:A:5402:ADP:C4' | 2.04 | 0.70 |
| 1:B:2707:VAL:CG1 | 1:B:2712:LEU:HD12 | 2.21 | 0.70 |
| 1:A:2141:ILE:CG2 | 1:A:2145:PHE:HB2 | 2.19 | 0.70 |
| 1:A:1455:LEU:HD12 | 1:A:1516:LEU:HD23 | 1.74 | 0.70 |
| 1:B:2111:LYS:HZ3 | 1:B:2161:GLU:HG2 | 1.55 | 0.70 |
| 1:A:3304:GLU:O | 1:A:3307:LEU:CB | 2.40 | 0.70 |
| 1:B:1630:ILE:CG2 | 1:B:1655:MET:SD | 2.78 | 0.70 |
| 1:B:3645:SER:HB3 | 1:B:3890:GLN:NE2 | 2.07 | 0.70 |
| 1:A:1540:LEU:CD1 | 1:A:1548:ILE:HD11 | 2.22 | 0.70 |
| 1:B:3409:ASP:HB3 | 1:B:3518:PHE:HB2 | 1.73 | 0.70 |
| 1:B:3845:GLN:OE1 | 1:B:3878:HIS:HB2 | 1.91 | 0.70 |
| 1:B:3737:THR:OG1 | 1:B:3740:THR:HB | 1.92 | 0.70 |
| 1:A:2063:MET:HB3 | 1:A:2070:LEU:HD11 | 1.74 | 0.70 |
| 1:A:3307:LEU:C | 1:A:3307:LEU:CD1 | 2.57 | 0.69 |
| 1:A:3406:PHE:HB2 | 1:A:3513:VAL:HG12 | 1.74 | 0.69 |
| 1:A:2476:LYS:HG2 | 1:A:2478:ASP:O | 1.90 | 0.69 |
| 1:B:1540:LEU:CD1 | 1:B:1548:ILE:CD1 | 2.69 | 0.69 |
| 1:B:2378:VAL:CG2 | 1:B:2380:LEU:HD11 | 2.23 | 0.69 |
| 1:B:3024:LEU:HD11 | 1:B:3303:LYS:CG | 2.19 | 0.69 |
| 1:B:2080:LYS:HE2 | 2:B:5400:ATP:PB | 2.32 | 0.69 |
| 1:A:3777:VAL:CG1 | 1:A:3895:PHE:CE1 | 2.51 | 0.69 |
| 1:B:2728:LEU:HD12 | 1:B:2771:ARG:HH22 | 1.57 | 0.69 |
| 1:A:1744:LEU:HA | 1:A:1760:PHE:CD2 | 2.27 | 0.69 |
| 1:B:3566:LEU:HD13 | 1:B:3570:LEU:HD11 | 1.74 | 0.69 |
| 1:B:1612:ASP:HA | 1:B:1615:ILE:CD1 | 2.22 | 0.69 |
| 1:A:1415:MET:O | 1:A:1421:TYR:CD2 | 2.46 | 0.69 |
| 1:A:2766:LYS:HE2 | 1:A:2890:THR:HB | 1.73 | 0.69 |
| 1:B:2732:MET:CE | 1:B:2768:ILE:HG23 | 1.99 | 0.69 |
| 1:B:2563:SER:HB2 | 1:B:2566:SER:OG | 1.91 | 0.69 |
| 1:A:3534:LEU:HD13 | 1:A:3618:TYR:HE2 | 1.58 | 0.69 |
| 1:B:3777:VAL:CG1 | 1:B:3895:PHE:CE1 | 2.68 | 0.69 |
| 1:B:1995:VAL:HG21 | 1:B:2024:SER:HB3 | 1.75 | 0.69 |
| 1:B:1604:ALA:HA | 1:B:1607:TRP:NE1 | 2.07 | 0.69 |
| 1:B:1365:PHE:HE1 | 1:B:1366:VAL:CG2 | 2.04 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2476:LYS:HD2 | 1:B:2476:LYS:H | 1.57 | 0.68 |
| 1:A:1794:PHE:HD1 | 1:A:1802:LYS:HB3 | 1.56 | 0.68 |
| 1:B:2312:ASP:HB3 | 1:B:2351:GLN:HG3 | 1.76 | 0.68 |
| 1:A:2707:VAL:CG1 | 1:A:2712:LEU:CD1 | 2.71 | 0.68 |
| 1:B:2572:GLU:CD | 1:B:2590:GLU:HG3 | 2.14 | 0.68 |
| 1:A:3534:LEU:HD13 | 1:A:3618:TYR:CE2 | 2.28 | 0.68 |
| 1:B:1366:VAL:HG13 | 1:B:1369:LYS:HE3 | 1.75 | 0.68 |
| 1:A:2282:ASN:CB | 1:A:2552:ARG:HG3 | 2.20 | 0.68 |
| 1:A:2846:GLY:O | 1:A:2849:TYR:HB3 | 1.93 | 0.68 |
| 1:B:1562:MET:CB | 1:B:1569:ILE:HD11 | 2.23 | 0.68 |
| 1:B:1938:GLY:O | 1:B:1989:GLU:HB3 | 1.93 | 0.68 |
| 1:B:1984:ILE:HG21 | 1:B:1989:GLU:HG3 | 1.74 | 0.68 |
| 1:B:3912:GLY:O | 1:B:3915:PHE:CE2 | 2.46 | 0.68 |
| 1:B:3460:PRO:O | 1:B:3463:SER:HB2 | 1.94 | 0.68 |
| 1:B:2476:LYS:HG2 | 1:B:2478:ASP:O | 1.93 | 0.68 |
| 1:B:3473:ALA:HB3 | 1:B:3476:ARG:O | 1.93 | 0.68 |
| 1:A:1612:ASP:HA | 1:A:1615:ILE:CD1 | 2.24 | 0.68 |
| 1:A:1392:LEU:HD13 | 1:A:1392:LEU:C | 2.14 | 0.68 |
| 3:B:5401:ADP:N3 | 3:B:5401:ADP:H2' | 2.09 | 0.68 |
| 1:A:3935:PHE:HB2 | 1:A:4014:VAL:HG11 | 1.76 | 0.68 |
| 1:A:2787:HIS:HA | 1:A:3460:PRO:HG2 | 1.76 | 0.68 |
| 1:B:1569:ILE:HA | 1:B:1584:SER:HA | 1.76 | 0.68 |
| 1:A:1489:ARG:HH12 | 1:A:1503:PRO:HG2 | 1.58 | 0.68 |
| 1:B:2176:LEU:O | 1:B:2183:ARG:HA | 1.94 | 0.67 |
| 1:A:1569:ILE:HA | 1:A:1584:SER:HA | 1.75 | 0.67 |
| 1:A:3979:ASN:C | 1:A:3981:PRO:HD2 | 2.14 | 0.67 |
| 1:B:2386:MET:HB2 | 1:B:2627:ARG:HD2 | 1.75 | 0.67 |
| 1:B:2080:LYS:NZ | 1:B:2549:ARG:CZ | 2.57 | 0.67 |
| 1:A:3509:LEU:CD1 | 1:A:3513:VAL:HG21 | 2.24 | 0.67 |
| 1:A:1926:SER:HA | 1:A:1970:LEU:HD12 | 1.76 | 0.67 |
| 1:B:3566:LEU:HD13 | 1:B:3570:LEU:CD1 | 2.23 | 0.67 |
| 1:A:2763:ARG:NE | 3:A:5402:ADP:H4' | 2.10 | 0.67 |
| 1:B:2220:CYS:SG | 1:B:2224:SER:CB | 2.82 | 0.67 |
| 1:A:2141:ILE:HG22 | 1:A:2145:PHE:CB | 2.22 | 0.67 |
| 1:A:1910:GLU:HB2 | 1:A:3846:MET:CB | 2.23 | 0.67 |
| 1:B:1365:PHE:HD1 | 1:B:1366:VAL:HG23 | 0.91 | 0.67 |
| 1:B:3303:LYS:O | 1:B:3306:TRP:CD1 | 2.48 | 0.67 |
| 1:A:4065:LEU:HD11 | 1:A:4070:ILE:HD11 | 1.76 | 0.67 |
| 1:B:2768:ILE:HG22 | 3:B:5402:ADP:O2A | 1.94 | 0.67 |
| 1:B:2282:ASN:HB3 | 1:B:2552:ARG:HG3 | 1.75 | 0.67 |
| 1:A:3886:ALA:N | 1:A:3887:PRO:HD2 | 2.09 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4021:LEU:HD23 | 1:A:4023:ILE:HG13 | 1.76 | 0.67 |
| 1:B:1827:ASP:HB3 | 1:B:1830:VAL:HG12 | 1.75 | 0.67 |
| 1:B:2080:LYS:HG3 | 1:B:2081:THR:N | 2.10 | 0.67 |
| 1:A:2476:LYS:H | 1:A:2476:LYS:HD2 | 1.60 | 0.67 |
| 1:A:1531:ARG:HG2 | 1:A:1537:PHE:CB | 2.24 | 0.67 |
| 1:A:2941:THR:HG22 | 1:A:2942:ASP:H | 1.59 | 0.67 |
| 1:A:2745:ILE:HG12 | 1:A:2756:MET:HE3 | 1.76 | 0.67 |
| 1:B:3792:ARG:HB2 | 1:B:3955:TYR:CE1 | 2.29 | 0.67 |
| 1:A:3998:ILE:HG21 | 1:A:4004:LEU:HG | 1.77 | 0.67 |
| 1:B:2728:LEU:CD1 | 1:B:2771:ARG:HH22 | 2.08 | 0.67 |
| 1:A:3871:PHE:CZ | 1:A:3873:MET:HB2 | 2.30 | 0.67 |
| 1:B:2745:ILE:HG23 | 1:B:2756:MET:CE | 2.25 | 0.67 |
| 1:B:2762:SER:O | 1:B:2764:THR:N | 2.28 | 0.66 |
| 1:B:1802:LYS:N | 4:B:5403:SO4:O1 | 2.28 | 0.66 |
| 1:A:3322:GLY:HA2 | 1:A:3325:ILE:HD12 | 1.77 | 0.66 |
| 1:A:2707:VAL:CG1 | 1:A:2712:LEU:HD11 | 2.25 | 0.66 |
| 1:B:2080:LYS:CG | 2:B:5400:ATP:O1B | 2.44 | 0.66 |
| 1:A:3566:LEU:HA | 1:A:3583:LEU:HD21 | 1.76 | 0.66 |
| 1:A:2407:LEU:HD22 | 1:A:2412:ARG:NH1 | 2.09 | 0.66 |
| 1:A:2620:ARG:NH2 | 3:A:5401:ADP:O3A | 2.29 | 0.66 |
| 1:B:1612:ASP:HA | 1:B:1615:ILE:HD11 | 1.78 | 0.66 |
| 1:B:2141:ILE:HG22 | 1:B:2145:PHE:HB2 | 1.78 | 0.66 |
| 1:B:3871:PHE:CZ | 1:B:3873:MET:HB2 | 2.31 | 0.66 |
| 1:A:2938:MET:SD | 1:A:3321:ILE:HG21 | 2.35 | 0.66 |
| 1:A:3303:LYS:HD2 | 1:A:3306:TRP:CB | 2.25 | 0.66 |
| 1:B:2044:ARG:HH21 | 1:B:2093:ILE:HD11 | 1.61 | 0.65 |
| 1:A:2241:LEU:HD13 | 1:A:2299:ARG:HH11 | 1.61 | 0.65 |
| 1:B:1409:LEU:CD2 | 1:B:1435:LEU:HB3 | 2.19 | 0.65 |
| 1:A:1645:PHE:CB | 1:A:1765:ILE:CG2 | 2.71 | 0.65 |
| 1:B:3010:LEU:HD21 | 1:B:3317:SER:HB3 | 1.77 | 0.65 |
| 1:B:4017:GLY:HA3 | 1:B:4021:LEU:HD12 | 1.77 | 0.65 |
| 1:A:2476:LYS:NZ | 1:A:2528:ARG:HD2 | 2.11 | 0.65 |
| 1:B:2386:MET:HB3 | 1:B:2627:ARG:HE | 1.60 | 0.65 |
| 1:A:3306:TRP:CE3 | 1:A:3306:TRP:HA | 2.31 | 0.65 |
| 1:A:1421:TYR:CE1 | 1:A:1425:GLU:OE1 | 2.48 | 0.65 |
| 1:A:1967:HIS:C | 1:A:1968:PHE:HD1 | 2.00 | 0.65 |
| 1:A:1394:LEU:HD22 | 1:A:1449:GLN:HE22 | 1.62 | 0.65 |
| 1:A:2517:LYS:HE2 | 1:A:2524:VAL:HG21 | 1.78 | 0.65 |
| 1:B:1939:PHE:HD1 | 1:B:1940:GLU:O | 1.79 | 0.65 |
| 1:A:2476:LYS:H | 1:A:2476:LYS:HD3 | 1.62 | 0.65 |
| 1:B:2458:LEU:HD11 | 1:B:2484:LEU:HD11 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1774:LEU:HD21 | 1:A:1922:LYS:O | 1.96 | 0.65 |
| 1:B:3877:CYS:SG | 1:B:3884:LEU:HD22 | 2.36 | 0.65 |
| 1:B:1929:ILE:HD13 | 1:B:1970:LEU:HD11 | 1.79 | 0.65 |
| 1:B:1822:CYS:SG | 1:B:1849:GLU:O | 2.55 | 0.65 |
| 1:B:3737:THR:HB | 1:B:3740:THR:CB | 2.27 | 0.65 |
| 1:A:2112:GLU:HB3 | 1:A:2117:SER:CB | 2.27 | 0.65 |
| 1:A:1999:LYS:CG | 1:A:2014:PHE:HE1 | 2.10 | 0.65 |
| 1:A:2109:LEU:CD1 | 1:A:2129:LEU:CD2 | 2.74 | 0.65 |
| 1:B:1991:GLU:O | 1:B:1995:VAL:HG23 | 1.97 | 0.64 |
| 1:B:2412:ARG:HH11 | 1:B:2553:HIS:CA | 2.09 | 0.64 |
| 1:B:3837:GLY:O | 1:B:3871:PHE:HD1 | 1.80 | 0.64 |
| 1:B:2728:LEU:HD12 | 1:B:2771:ARG:NH2 | 2.12 | 0.64 |
| 1:A:3810:SER:O | 1:A:3838:TRP:HB2 | 1.97 | 0.64 |
| 1:A:3306:TRP:HE3 | 1:A:3306:TRP:HA | 1.63 | 0.64 |
| 1:B:2080:LYS:HG3 | 1:B:2081:THR:H | 1.60 | 0.64 |
| 1:B:3406:PHE:HB2 | 1:B:3513:VAL:HG11 | 1.79 | 0.64 |
| 1:A:1562:MET:CB | 1:A:1569:ILE:HD11 | 2.26 | 0.64 |
| 1:A:1965:HIS:CD2 | 1:A:2212:LEU:HD21 | 2.32 | 0.64 |
| 1:B:2707:VAL:CG1 | 1:B:2712:LEU:HD11 | 2.26 | 0.64 |
| 1:B:3618:TYR:HD1 | 1:B:3618:TYR:N | 1.94 | 0.64 |
| 1:B:1405:CYS:O | 1:B:1409:LEU:HG | 1.98 | 0.64 |
| 1:A:3787:THR:HG22 | 1:A:3875:MET:HB2 | 1.78 | 0.64 |
| 1:A:2203:THR:HG22 | 1:A:2205:ALA:H | 1.61 | 0.64 |
| 1:A:3440:LEU:CD2 | 1:A:3462:ILE:HD12 | 2.27 | 0.64 |
| 1:B:2411:LYS:HG2 | 1:B:2530:HIS:HE1 | 1.62 | 0.64 |
| 1:A:2765:GLY:CA | 3:A:5402:ADP:O3A | 2.46 | 0.64 |
| 1:A:2421:GLY:N | 3:A:5401:ADP:O2B | 2.29 | 0.64 |
| 1:B:2181:GLY:O | 1:B:2182:GLU:HG3 | 1.97 | 0.64 |
| 1:B:2386:MET:HB3 | 1:B:2627:ARG:NE | 2.13 | 0.64 |
| 1:B:3871:PHE:HZ | 1:B:3873:MET:HB2 | 1.63 | 0.64 |
| 1:A:2151:TRP:HE3 | 1:A:2193:LEU:HD11 | 1.61 | 0.64 |
| 1:A:1917:ARG:HD2 | 1:A:3963:PHE:CZ | 2.33 | 0.64 |
| 1:B:3631:MET:CE | 1:B:3698:MET:HG3 | 2.28 | 0.64 |
| 1:A:1664:LEU:HD23 | 1:A:1669:PHE:HZ | 1.61 | 0.64 |
| 1:A:3010:LEU:HD21 | 1:A:3317:SER:HB3 | 1.79 | 0.64 |
| 1:B:2437:LEU:HA | 1:B:2480:LYS:HD3 | 1.80 | 0.64 |
| 1:B:1489:ARG:HH12 | 1:B:1503:PRO:HG2 | 1.63 | 0.64 |
| 1:A:3833:LYS:HZ3 | 1:A:3862:THR:HG21 | 1.62 | 0.64 |
| 1:B:1681:LYS:HE2 | 1:B:1939:PHE:HZ | 1.62 | 0.64 |
| 1:A:2224:SER:O | 2:A:5400:ATP:H2 | 1.80 | 0.64 |
| 1:B:3688:THR:HG21 | 1:B:3777:VAL:HG21 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3509:LEU:CD1 | 1:B:3513:VAL:HG21 | 2.28 | 0.64 |
| 1:A:1527:LEU:CD2 | 1:A:1545:LEU:HD22 | 2.27 | 0.64 |
| 1:A:3737:THR:CB | 1:A:3740:THR:HB | 2.27 | 0.64 |
| 1:B:2080:LYS:HZ2 | 1:B:2549:ARG:CZ | 2.11 | 0.64 |
| 1:A:2380:LEU:HD12 | 1:A:2577:ALA:HB1 | 1.80 | 0.64 |
| 1:B:3519:VAL:HG13 | 1:B:3521:ASN:ND2 | 2.13 | 0.64 |
| 1:B:1531:ARG:HG2 | 1:B:1537:PHE:HB3 | 1.78 | 0.64 |
| 1:B:1493:LEU:HD23 | 1:B:1498:GLU:HB3 | 1.79 | 0.64 |
| 1:B:1681:LYS:HE2 | 1:B:1939:PHE:CZ | 2.33 | 0.63 |
| 1:A:1527:LEU:HD22 | 1:A:1545:LEU:HD22 | 1.80 | 0.63 |
| 1:B:2787:HIS:CA | 1:B:3460:PRO:HD2 | 2.24 | 0.63 |
| 1:A:3871:PHE:HZ | 1:A:3873:MET:HB2 | 1.63 | 0.63 |
| 1:A:3307:LEU:CD1 | 1:A:3307:LEU:O | 2.44 | 0.63 |
| 1:A:2424:LYS:NZ | 3:A:5401:ADP:O1B | 2.30 | 0.63 |
| 1:A:1536:ARG:N | 1:A:1841:ILE:HD11 | 2.12 | 0.63 |
| 1:A:3566:LEU:CD1 | 1:A:3570:LEU:HD11 | 2.27 | 0.63 |
| 1:A:1612:ASP:HA | 1:A:1615:ILE:HD11 | 1.79 | 0.63 |
| 1:B:2732:MET:HB2 | 3:B:5402:ADP:C2 | 2.32 | 0.63 |
| 1:A:3302:GLU:O | 1:A:3305:ARG:N | 2.31 | 0.63 |
| 1:A:2290:LEU:HD23 | 1:A:2321:SER:HA | 1.80 | 0.63 |
| 1:B:1911:ASN:OD1 | 1:B:1912:LEU:N | 2.31 | 0.63 |
| 1:A:3541:MET:HA | 1:A:3544:LYS:HG2 | 1.81 | 0.63 |
| 1:B:3534:LEU:HD13 | 1:B:3618:TYR:CE2 | 2.27 | 0.63 |
| 1:B:2493:LYS:HG3 | 1:B:2494:LEU:H | 1.63 | 0.63 |
| 1:B:3592:LYS:O | 1:B:3596:ASN:HB2 | 1.99 | 0.63 |
| 1:A:1741:LEU:O | 1:A:1742:ASP:HB2 | 1.98 | 0.63 |
| 1:B:1421:TYR:O | 1:B:1425:GLU:N | 2.32 | 0.63 |
| 1:A:3566:LEU:HD13 | 1:A:3570:LEU:CD1 | 2.29 | 0.63 |
| 1:A:1611:LEU:O | 1:A:1615:ILE:HG23 | 1.98 | 0.63 |
| 1:A:1926:SER:HB2 | 1:A:1970:LEU:HD12 | 1.79 | 0.63 |
| 1:B:3886:ALA:N | 1:B:3887:PRO:HD2 | 2.13 | 0.63 |
| 1:B:2766:LYS:HE2 | 1:B:2890:THR:HB | 1.80 | 0.63 |
| 1:A:1365:PHE:CE2 | 1:A:1366:VAL:HG21 | 2.29 | 0.62 |
| 1:A:1620:PHE:CZ | 1:A:1743:ASP:HB3 | 2.33 | 0.62 |
| 1:A:1967:HIS:O | 1:A:1968:PHE:HD1 | 1.81 | 0.62 |
| 1:A:2176:LEU:O | 1:A:2183:ARG:HA | 1.98 | 0.62 |
| 1:A:2637:PRO:O | 1:A:2639:GLN:NE2 | 2.32 | 0.62 |
| 1:B:2315:THR:HG21 | 1:B:2350:SER:HB3 | 1.81 | 0.62 |
| 1:B:3401:GLN:C | 1:B:3403:ALA:H | 2.00 | 0.62 |
| 1:A:3698:MET:O | 1:A:3702:MET:HG3 | 1.98 | 0.62 |
| 1:A:1822:CYS:SG | 1:A:1849:GLU:O | 2.57 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3303:LYS:CA | 1:B:3306:TRP:HD1 | 2.11 | 0.62 |
| 1:B:2225:LYS:HA | 2:B:5400:ATP:H2 | 1.64 | 0.62 |
| 1:A:1926:SER:CA | 1:A:1970:LEU:HD12 | 2.29 | 0.62 |
| 1:A:2536:ASN:HB2 | 1:A:2543:ARG:HE | 1.64 | 0.62 |
| 1:A:2293:HIS:NE2 | 1:A:2409:ASN:HB3 | 2.14 | 0.62 |
| 1:B:2034:ILE:HD12 | 1:B:2061:TYR:CZ | 2.34 | 0.62 |
| 1:B:2764:THR:O | 3:B:5402:ADP:C8 | 2.52 | 0.62 |
| 1:A:1416:LYS:HA | 1:A:1421:TYR:OH | 1.99 | 0.62 |
| 1:B:4024:VAL:HG23 | 1:B:4027:VAL:H | 1.64 | 0.62 |
| 1:A:2741:HIS:HA | 1:A:2744:ARG:HD2 | 1.81 | 0.62 |
| 1:A:2677:VAL:HG11 | 1:A:2686:LEU:HD21 | 1.81 | 0.62 |
| 1:B:1849:GLU:HG2 | 1:B:1899:ASN:ND2 | 2.14 | 0.62 |
| 1:B:1645:PHE:CB | 1:B:1765:ILE:CG2 | 2.66 | 0.62 |
| 1:B:2637:PRO:O | 1:B:2639:GLN:NE2 | 2.32 | 0.62 |
| 1:A:1999:LYS:CG | 1:A:2014:PHE:CE1 | 2.79 | 0.62 |
| 1:A:1995:VAL:HG22 | 1:A:2022:PHE:CD2 | 2.34 | 0.62 |
| 1:B:2536:ASN:HB2 | 1:B:2543:ARG:HE | 1.64 | 0.62 |
| 1:B:2080:LYS:NZ | 1:B:2549:ARG:HH21 | 1.95 | 0.62 |
| 1:B:1394:LEU:CD2 | 1:B:1449:GLN:HE22 | 2.12 | 0.62 |
| 1:A:1965:HIS:HD2 | 1:A:2212:LEU:CD2 | 2.11 | 0.62 |
| 1:B:3350:LYS:HA | 1:B:3353:LEU:HD12 | 1.82 | 0.62 |
| 1:B:1540:LEU:CD1 | 1:B:1548:ILE:HD11 | 2.29 | 0.62 |
| 1:B:1493:LEU:HD23 | 1:B:1498:GLU:CB | 2.28 | 0.62 |
| 1:A:4033:LEU:HD13 | 1:A:4035:GLN:CB | 2.29 | 0.62 |
| 1:A:1940:GLU:HG3 | 1:A:1941:ASP:H | 1.63 | 0.62 |
| 1:A:3566:LEU:HD13 | 1:A:3570:LEU:HD11 | 1.81 | 0.62 |
| 1:A:2624:ARG:NH2 | 1:A:2910:ASN:O | 2.32 | 0.62 |
| 1:A:1979:ASN:OD1 | 1:A:2066:THR:HG21 | 2.00 | 0.62 |
| 1:B:2920:TRP:CB | 1:B:2989:PRO:HG3 | 2.09 | 0.62 |
| 1:A:1421:TYR:HD1 | 1:A:1425:GLU:CB | 2.05 | 0.62 |
| 1:B:1802:LYS:NZ | 4:B:5403:SO4:S | 2.71 | 0.62 |
| 1:B:2448:ASP:HB2 | 1:B:2829:GLU:CD | 2.18 | 0.62 |
| 1:B:2709:LYS:O | 1:B:2713:VAL:HG23 | 1.99 | 0.62 |
| 1:B:162:LEU:HA | 1:B:165:ASP:O | 1.99 | 0.62 |
| 1:B:2084:TRP:HE3 | 1:B:2088:ILE:HD12 | 1.64 | 0.62 |
| 1:A:1938:GLY:O | 1:A:1989:GLU:HB3 | 2.00 | 0.62 |
| 1:A:2476:LYS:HZ1 | 1:A:2528:ARG:HD2 | 1.64 | 0.62 |
| 1:B:1698:ILE:O | 1:B:1702:LEU:HG | 2.00 | 0.62 |
| 1:B:1620:PHE:HA | 1:B:1760:PHE:CE1 | 2.34 | 0.61 |
| 1:A:1827:ASP:HB3 | 1:A:1830:VAL:HG12 | 1.82 | 0.61 |
| 1:B:1953:LEU:CD1 | 1:B:1973:LEU:HB3 | 2.29 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2081:THR:O | 1:B:2085:LYS:HB2 | 1.99 | 0.61 |
| 1:B:2760:GLY:O | 1:B:2761:ALA:C | 2.38 | 0.61 |
| 1:B:1391:GLY:HA3 | 1:B:1484:LYS:NZ | 2.14 | 0.61 |
| 1:B:3816:LEU:HD23 | 1:B:3847:SER:OG | 2.00 | 0.61 |
| 1:A:1540:LEU:CD1 | 1:A:1548:ILE:CD1 | 2.77 | 0.61 |
| 1:B:2293:HIS:CE1 | 1:B:2409:ASN:HB3 | 2.35 | 0.61 |
| 1:B:2293:HIS:NE2 | 1:B:2409:ASN:HB3 | 2.15 | 0.61 |
| 1:B:3787:THR:HG22 | 1:B:3875:MET:HB2 | 1.81 | 0.61 |
| 1:A:1645:PHE:CG | 1:A:1765:ILE:HG22 | 2.35 | 0.61 |
| 1:B:1967:HIS:C | 1:B:1968:PHE:HD1 | 2.04 | 0.61 |
| 1:B:3017:VAL:HG21 | 1:B:3313:PHE:CE2 | 2.36 | 0.61 |
| 1:A:2034:ILE:HD12 | 1:A:2061:TYR:CZ | 2.35 | 0.61 |
| 1:A:3807:SER:O | 1:A:3808:LYS:HB2 | 2.00 | 0.61 |
| 1:B:2032:LYS:O | 1:B:2035:VAL:HG12 | 1.99 | 0.61 |
| 1:B:3429:LEU:HD21 | 1:B:3439:ARG:HB3 | 1.82 | 0.61 |
| 1:A:2786:ILE:O | 1:A:3460:PRO:HB2 | 2.00 | 0.61 |
| 1:A:1992:LYS:HG2 | 1:A:2024:SER:HB2 | 1.76 | 0.61 |
| 1:B:2131:THR:HG22 | 1:B:2176:LEU:CD2 | 2.30 | 0.61 |
| 1:A:3645:SER:HB3 | 1:A:3890:GLN:NE2 | 2.14 | 0.61 |
| 1:B:216:PRO:O | 1:B:1365:PHE:CB | 2.36 | 0.61 |
| 1:A:1620:PHE:HA | 1:A:1760:PHE:HE1 | 1.64 | 0.61 |
| 1:B:1983:LEU:HD23 | 1:B:1993:THR:O | 2.00 | 0.61 |
| 1:A:1606:GLU:O | 1:A:1610:ILE:HG12 | 2.01 | 0.61 |
| 1:A:1756:LEU:HD13 | 1:A:1813:LEU:HD11 | 1.82 | 0.61 |
| 1:B:3912:GLY:O | 1:B:3915:PHE:CZ | 2.54 | 0.61 |
| 1:A:4022:GLN:HA | 1:A:4027:VAL:O | 2.01 | 0.61 |
| 1:A:1646:GLN:OE1 | 1:A:1762:TYR:HA | 1.99 | 0.61 |
| 1:A:1744:LEU:HA | 1:A:1760:PHE:HE2 | 1.60 | 0.61 |
| 1:A:4033:LEU:HD12 | 1:A:4035:GLN:N | 2.16 | 0.61 |
| 1:A:3459:ASP:OD2 | 1:A:3461:ILE:HG12 | 2.00 | 0.61 |
| 1:A:3737:THR:CB | 1:A:3740:THR:CB | 2.79 | 0.61 |
| 1:A:1626:CYS:SG | 1:A:1639:VAL:HG11 | 2.41 | 0.61 |
| 1:A:1692:ASP:O | 1:A:1695:LYS:HB3 | 2.00 | 0.61 |
| 1:B:3785:TYR:CE1 | 1:B:3859:VAL:HG22 | 2.36 | 0.61 |
| 1:A:3308:ASN:C | 1:A:3310:THR:N | 2.54 | 0.61 |
| 1:A:3303:LYS:CD | 1:A:3306:TRP:HB2 | 2.28 | 0.60 |
| 1:A:1502:ILE:HG23 | 1:A:1503:PRO:HD2 | 1.82 | 0.60 |
| 1:A:2512:LYS:O | 1:A:2513:GLN:HB2 | 2.00 | 0.60 |
| 1:A:1540:LEU:HD12 | 1:A:1548:ILE:CD1 | 2.30 | 0.60 |
| 1:A:2391:VAL:HG23 | 1:A:2426:MET:SD | 2.41 | 0.60 |
| 1:B:2512:LYS:O | 1:B:2513:GLN:HB2 | 1.99 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1645:PHE:CG | 1:B:1765:ILE:HG22 | 2.35 | 0.60 |
| 1:B:4024:VAL:HG11 | 1:B:4062:TRP:CD2 | 2.36 | 0.60 |
| 1:A:1953:LEU:CD1 | 1:A:1973:LEU:HB3 | 2.31 | 0.60 |
| 1:A:2563:SER:HB2 | 1:A:2566:SER:OG | 2.01 | 0.60 |
| 1:A:2620:ARG:NH2 | 3:A:5401:ADP:O1A | 2.34 | 0.60 |
| 1:A:2380:LEU:HD12 | 1:A:2577:ALA:CB | 2.31 | 0.60 |
| 1:A:3982:TRP:CD1 | 1:A:4015:PHE:O | 2.55 | 0.60 |
| 1:A:1425:GLU:HG3 | 1:A:1428:CYS:SG | 2.41 | 0.60 |
| 1:A:1704:GLU:OE2 | 1:A:1768:ARG:NH1 | 2.35 | 0.60 |
| 1:B:2473:LEU:HD23 | 1:B:2474:LEU:N | 2.17 | 0.60 |
| 1:B:1425:GLU:OE2 | 1:B:1429:LEU:HD21 | 2.02 | 0.60 |
| 1:B:2788:ARG:HB2 | 1:B:3459:ASP:HB3 | 1.82 | 0.60 |
| 1:B:2445:PHE:HA | 1:B:2449:THR:HG21 | 1.83 | 0.60 |
| 1:A:2631:THR:O | 1:A:2635:THR:HG22 | 2.00 | 0.60 |
| 1:A:4033:LEU:HD12 | 1:A:4036:GLN:H | 1.67 | 0.60 |
| 1:A:1917:ARG:HD2 | 1:A:3963:PHE:CE2 | 2.36 | 0.60 |
| 1:B:1534:PHE:HD2 | 1:B:1537:PHE:CE2 | 2.20 | 0.60 |
| 1:B:3919:LYS:HZ3 | 1:B:4038:GLU:CG | 2.14 | 0.60 |
| 1:B:3839:ILE:CG2 | 1:B:3873:MET:HG3 | 2.31 | 0.60 |
| 1:A:2081:THR:O | 1:A:2085:LYS:HB2 | 2.01 | 0.60 |
| 1:A:1394:LEU:HD22 | 1:A:1449:GLN:NE2 | 2.16 | 0.60 |
| 1:B:3951:SER:HB2 | 1:B:4002:LYS:HD2 | 1.83 | 0.60 |
| 1:A:2080:LYS:O | 1:A:2084:TRP:CD1 | 2.54 | 0.60 |
| 1:A:3774:ILE:O | 1:A:3778:VAL:HG23 | 2.02 | 0.60 |
| 1:A:2125:TRP:CZ2 | 1:A:2178:LEU:HD13 | 2.37 | 0.60 |
| 1:A:2290:LEU:HD13 | 1:A:2407:LEU:HD23 | 1.84 | 0.59 |
| 1:A:2109:LEU:CD2 | 1:A:2518:THR:HG22 | 2.32 | 0.59 |
| 1:B:1849:GLU:CG | 1:B:1899:ASN:HD22 | 2.15 | 0.59 |
| 1:A:2127:ASP:O | 1:A:2131:THR:OG1 | 2.21 | 0.59 |
| 1:A:2332:GLY:HA2 | 1:A:2335:GLN:CB | 2.32 | 0.59 |
| 1:A:3583:LEU:O | 1:A:3587:LEU:HG | 2.02 | 0.59 |
| 1:B:3700:MET:HB3 | 1:B:4085:THR:HG21 | 1.83 | 0.59 |
| 1:A:2295:ILE:HG12 | 1:A:2314:ILE:HD12 | 1.83 | 0.59 |
| 1:B:3512:ARG:NH2 | 3:B:5402:ADP:O3B | 2.35 | 0.59 |
| 1:B:2764:THR:O | 3:B:5402:ADP:H8 | 1.85 | 0.59 |
| 1:B:1536:ARG:HD2 | 1:B:1565:MET:O | 2.02 | 0.59 |
| 1:A:2002:ILE:HB | 1:A:2014:PHE:HE2 | 1.66 | 0.59 |
| 1:B:2141:ILE:HG22 | 1:B:2145:PHE:CB | 2.32 | 0.59 |
| 1:B:3583:LEU:O | 1:B:3587:LEU:HG | 2.02 | 0.59 |
| 1:B:3817:GLY:H | 1:B:3821:ASN:HB2 | 1.67 | 0.59 |
| 1:A:1779:PHE:O | 1:A:1783:THR:HG22 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2378:VAL:HG22 | 1:B:2380:LEU:HD13 | 1.80 | 0.59 |
| 1:B:2732:MET:CB | 3:B:5402:ADP:N1 | 2.54 | 0.59 |
| 1:B:2473:LEU:CD2 | 1:B:2475:PRO:HG3 | 2.30 | 0.59 |
| 1:B:1534:PHE:CE2 | 1:B:1536:ARG:HB2 | 2.37 | 0.59 |
| 1:A:1849:GLU:OE2 | 1:A:1899:ASN:ND2 | 2.35 | 0.59 |
| 1:A:1409:LEU:CD2 | 1:A:1435:LEU:HB2 | 2.32 | 0.59 |
| 1:B:3017:VAL:HG21 | 1:B:3313:PHE:HE2 | 1.68 | 0.59 |
| 1:B:1781:THR:HG21 | 1:B:1919:PHE:CD1 | 2.37 | 0.59 |
| 1:A:2476:LYS:CD | 1:A:2476:LYS:N | 2.63 | 0.59 |
| 1:B:2428:MET:HE1 | 1:B:2440:VAL:HG21 | 1.84 | 0.59 |
| 1:B:2707:VAL:HG12 | 1:B:2712:LEU:HD12 | 1.84 | 0.59 |
| 1:A:1415:MET:O | 1:A:1421:TYR:CE2 | 2.55 | 0.59 |
| 1:A:1640:VAL:HB | 1:A:1686:LYS:NZ | 2.16 | 0.59 |
| 1:B:3330:TYR:CE1 | 1:B:3334:PHE:CD2 | 2.91 | 0.59 |
| 1:B:2654:ARG:HH22 | 1:B:2691:SER:HB2 | 1.67 | 0.59 |
| 1:B:1495:THR:HG22 | 1:B:1497:ILE:HG22 | 1.84 | 0.59 |
| 1:B:2677:VAL:HG11 | 1:B:2686:LEU:HD21 | 1.85 | 0.59 |
| 1:A:3530:PHE:HD1 | 1:A:3618:TYR:CD2 | 2.20 | 0.58 |
| 1:B:3919:LYS:NZ | 1:B:4038:GLU:CD | 2.56 | 0.58 |
| 1:B:2476:LYS:NZ | 1:B:2528:ARG:HD2 | 2.17 | 0.58 |
| 1:A:2293:HIS:CE1 | 1:A:2409:ASN:HB3 | 2.38 | 0.58 |
| 1:A:1466:GLN:CB | 1:A:1473:THR:HG21 | 2.33 | 0.58 |
| 1:B:3819:ILE:O | 1:B:3823:ASN:HB2 | 2.02 | 0.58 |
| 1:A:2111:LYS:CD | 1:A:2161:GLU:HG3 | 2.16 | 0.58 |
| 1:B:2080:LYS:HG2 | 2:B:5400:ATP:O2B | 2.03 | 0.58 |
| 1:B:3737:THR:CB | 1:B:3740:THR:HB | 2.34 | 0.58 |
| 1:A:3308:ASN:O | 1:A:3310:THR:N | 2.36 | 0.58 |
| 1:B:2513:GLN:O | 1:B:2526:ILE:CG1 | 2.52 | 0.58 |
| 1:A:2286:THR:HA | 1:A:2412:ARG:NE | 2.18 | 0.58 |
| 1:B:4060:SER:HB3 | 1:B:4070:ILE:HG13 | 1.84 | 0.58 |
| 1:B:1418:SER:HB2 | 1:B:3446:PHE:HB3 | 1.83 | 0.58 |
| 1:A:2356:TYR:CE1 | 1:A:2395:ILE:HG22 | 2.39 | 0.58 |
| 1:A:3641:PHE:HA | 1:A:3889:LEU:HD21 | 1.85 | 0.58 |
| 1:A:1657:THR:HG21 | 1:A:1734:PHE:O | 2.04 | 0.58 |
| 1:B:1852:ARG:HG3 | 1:B:1852:ARG:O | 2.03 | 0.58 |
| 1:B:2107:LYS:CE | 1:B:2499:SER:HB3 | 2.31 | 0.58 |
| 1:A:1999:LYS:HG2 | 1:A:2014:PHE:CZ | 2.38 | 0.58 |
| 1:A:3837:GLY:O | 1:A:3871:PHE:HD1 | 1.87 | 0.58 |
| 1:B:3998:ILE:CG2 | 1:B:4004:LEU:HG | 2.33 | 0.58 |
| 1:A:2032:LYS:O | 1:A:2035:VAL:HG12 | 2.04 | 0.58 |
| 1:B:1620:PHE:HA | 1:B:1760:PHE:HE1 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1392:LEU:HD13 | 1:A:1393:LYS:C | 2.24 | 0.58 |
| 1:A:4065:LEU:O | 1:A:4065:LEU:HD12 | 2.03 | 0.58 |
| 1:B:1502:ILE:HG23 | 1:B:1503:PRO:HD2 | 1.83 | 0.58 |
| 1:B:1493:LEU:CD2 | 1:B:1498:GLU:HB3 | 2.33 | 0.58 |
| 1:B:2336:ARG:HD3 | 1:B:2355:ASP:OD2 | 2.03 | 0.58 |
| 1:A:2095:ASP:CG | 1:A:2149:ARG:NH2 | 2.57 | 0.58 |
| 1:A:1650:LEU:O | 1:A:1654:VAL:HG23 | 2.03 | 0.58 |
| 1:A:2795:PHE:CE2 | 1:A:2799:LEU:HD11 | 2.38 | 0.58 |
| 1:B:3461:ILE:C | 1:B:3463:SER:H | 2.07 | 0.58 |
| 1:B:2127:ASP:O | 1:B:2131:THR:OG1 | 2.21 | 0.58 |
| 1:A:2080:LYS:NZ | 2:A:5400:ATP:O3G | 2.37 | 0.58 |
| 1:A:2654:ARG:HH22 | 1:A:2691:SER:HB2 | 1.68 | 0.58 |
| 1:B:1372:ASN:O | 1:B:1376:LYS:HG3 | 2.03 | 0.58 |
| 1:B:1826:PHE:HE2 | 1:B:1853:LEU:HD22 | 1.66 | 0.58 |
| 1:A:1991:GLU:O | 1:A:1995:VAL:HG23 | 2.04 | 0.58 |
| 1:A:2084:TRP:HE3 | 1:A:2088:ILE:HD12 | 1.67 | 0.58 |
| 1:B:2276:LEU:HD23 | 1:B:2556:ILE:HD13 | 1.86 | 0.58 |
| 1:A:2111:LYS:HZ3 | 1:A:2161:GLU:HG2 | 1.69 | 0.58 |
| 1:B:1822:CYS:HB2 | 1:B:1853:LEU:CD2 | 2.24 | 0.58 |
| 1:B:1425:GLU:OE2 | 1:B:1429:LEU:CD2 | 2.52 | 0.58 |
| 1:A:3406:PHE:CZ | 1:A:3505:ILE:HG21 | 2.39 | 0.58 |
| 1:B:2177:THR:HG22 | 1:B:2183:ARG:HG2 | 1.85 | 0.58 |
| 1:A:1637:GLU:O | 1:A:1686:LYS:NZ | 2.31 | 0.58 |
| 1:B:2472:THR:HG22 | 1:B:2524:VAL:HG13 | 1.86 | 0.58 |
| 1:A:4021:LEU:HD23 | 1:A:4023:ILE:CG1 | 2.34 | 0.58 |
| 1:A:1394:LEU:CD2 | 1:A:1449:GLN:HE22 | 2.16 | 0.58 |
| 1:A:3889:LEU:HG | 1:A:3894:ARG:HD3 | 1.85 | 0.58 |
| 1:A:1620:PHE:HA | 1:A:1760:PHE:CE1 | 2.39 | 0.57 |
| 1:B:1849:GLU:OE2 | 1:B:1899:ASN:ND2 | 2.35 | 0.57 |
| 1:B:3566:LEU:HA | 1:B:3583:LEU:HD21 | 1.86 | 0.57 |
| 1:A:2076:ALA:HB2 | 1:A:2549:ARG:HG2 | 1.86 | 0.57 |
| 1:B:2201:HIS:NE2 | 1:B:2497:TYR:O | 2.37 | 0.57 |
| 1:A:2960:THR:HB | 1:A:2963:ASP:HB2 | 1.84 | 0.57 |
| 1:B:2763:ARG:O | 3:B:5402:ADP:O4' | 2.22 | 0.57 |
| 1:A:1421:TYR:CG | 1:A:1421:TYR:O | 2.58 | 0.57 |
| 1:B:2042:GLY:HA3 | 1:B:2049:MET:CE | 2.33 | 0.57 |
| 1:A:2768:ILE:CG2 | 3:A:5402:ADP:O2A | 2.47 | 0.57 |
| 1:A:2109:LEU:HD23 | 1:A:2518:THR:HG22 | 1.86 | 0.57 |
| 1:A:3631:MET:CE | 1:A:3698:MET:HG3 | 2.33 | 0.57 |
| 1:A:4020:ASN:HB3 | 1:A:4028:ARG:NH2 | 2.18 | 0.57 |
| 1:B:2745:ILE:HG23 | 1:B:2756:MET:HE3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1995:VAL:HG22 | 1:A:2022:PHE:CE2 | 2.39 | 0.57 |
| 1:A:3845:GLN:OE1 | 1:A:3878:HIS:HB2 | 2.04 | 0.57 |
| 1:A:2386:MET:HB2 | 1:A:2627:ARG:CD | 2.22 | 0.57 |
| 1:B:2437:LEU:H | 1:B:2437:LEU:HD12 | 1.70 | 0.57 |
| 1:A:1536:ARG:HD2 | 1:A:1565:MET:O | 2.04 | 0.57 |
| 1:A:2002:ILE:HB | 1:A:2014:PHE:CE2 | 2.40 | 0.57 |
| 1:B:2095:ASP:CG | 1:B:2149:ARG:NH2 | 2.58 | 0.57 |
| 1:B:2563:SER:CB | 1:B:2566:SER:OG | 2.53 | 0.57 |
| 1:A:1462:ASN:CB | 1:A:1465:ILE:HG22 | 2.35 | 0.57 |
| 1:A:2336:ARG:HA | 1:A:2339:ILE:HD12 | 1.86 | 0.57 |
| 1:B:1940:GLU:CB | 1:B:1989:GLU:O | 2.51 | 0.57 |
| 1:A:1611:LEU:O | 1:A:1615:ILE:HG12 | 2.05 | 0.56 |
| 1:A:3964:ALA:HB2 | 1:A:3993:VAL:HG11 | 1.87 | 0.56 |
| 1:A:2783:GLN:HG2 | 1:A:2816:ILE:HB | 1.86 | 0.56 |
| 1:B:1741:LEU:O | 1:B:1742:ASP:HB2 | 2.04 | 0.56 |
| 1:A:2111:LYS:HZ2 | 1:A:2161:GLU:HG2 | 1.68 | 0.56 |
| 1:B:2517:LYS:CE | 1:B:2520:GLU:OE1 | 2.53 | 0.56 |
| 1:A:2513:GLN:O | 1:A:2526:ILE:CG1 | 2.52 | 0.56 |
| 1:A:2314:ILE:HG22 | 1:A:2318:ILE:HD12 | 1.87 | 0.56 |
| 1:A:2737:SER:HB2 | 1:A:2924:THR:HG21 | 1.88 | 0.56 |
| 1:A:1826:PHE:CZ | 1:A:1831:LEU:HB2 | 2.37 | 0.56 |
| 1:A:2495:ASP:O | 1:A:2498:GLY:N | 2.38 | 0.56 |
| 1:B:1425:GLU:OE2 | 1:B:1429:LEU:HD11 | 2.05 | 0.56 |
| 1:B:2225:LYS:HA | 2:B:5400:ATP:N3 | 2.20 | 0.56 |
| 1:B:2387:ARG:O | 1:B:2390:ILE:HG22 | 2.05 | 0.56 |
| 1:B:1926:SER:HA | 1:B:1970:LEU:HD12 | 1.88 | 0.56 |
| 1:B:2081:THR:HB | 2:B:5400:ATP:PA | 2.45 | 0.56 |
| 1:A:1493:LEU:HD23 | 1:A:1498:GLU:CB | 2.36 | 0.56 |
| 1:A:4065:LEU:HD12 | 1:A:4065:LEU:C | 2.26 | 0.56 |
| 1:A:2420:PRO:HG2 | 1:A:2616:LEU:HD21 | 1.88 | 0.56 |
| 1:A:1796:GLY:O | 1:A:1900:PRO:HD3 | 2.05 | 0.56 |
| 1:B:2203:THR:HG22 | 1:B:2205:ALA:H | 1.70 | 0.56 |
| 1:A:1850:PHE:HB2 | 1:A:1896:ILE:HG23 | 1.88 | 0.56 |
| 1:B:1683:LEU:HB3 | 1:B:1702:LEU:HD21 | 1.88 | 0.56 |
| 1:A:1366:VAL:HG13 | 1:A:1369:LYS:HE3 | 1.88 | 0.56 |
| 1:B:3525:ILE:HD11 | 1:B:3646:ILE:CG2 | 2.14 | 0.56 |
| 1:B:1970:LEU:CD2 | 1:B:1974:LYS:HE2 | 2.36 | 0.56 |
| 1:A:2732:MET:HA | 3:A:5402:ADP:C2 | 2.40 | 0.56 |
| 1:A:2982:VAL:HG12 | 1:A:2983:GLY:N | 2.21 | 0.56 |
| 1:A:2385:VAL:O | 1:A:2574:TYR:HE1 | 1.88 | 0.56 |
| 1:A:2201:HIS:NE2 | 1:A:2497:TYR:O | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3656:VAL:CG1 | 1:B:3677:LEU:HB3 | 2.31 | 0.56 |
| 1:B:1984:ILE:CG2 | 1:B:1989:GLU:HG3 | 2.36 | 0.56 |
| 1:A:3785:TYR:CE1 | 1:A:3859:VAL:HG22 | 2.37 | 0.56 |
| 1:B:2517:LYS:HE2 | 1:B:2520:GLU:OE1 | 2.04 | 0.56 |
| 1:A:162:LEU:HA | 1:A:165:ASP:O | 2.06 | 0.56 |
| 1:A:3683:TYR:O | 1:A:3687:SER:HB2 | 2.06 | 0.56 |
| 1:B:2763:ARG:HG3 | 1:B:2990:GLY:HA3 | 1.87 | 0.56 |
| 1:A:3302:GLU:O | 1:A:3305:ARG:CB | 2.53 | 0.56 |
| 1:A:2107:LYS:CE | 1:A:2499:SER:HB3 | 2.34 | 0.56 |
| 1:B:2728:LEU:HD12 | 1:B:2771:ARG:HH12 | 1.71 | 0.56 |
| 1:A:3308:ASN:O | 1:A:3311:LYS:N | 2.38 | 0.56 |
| 1:A:1851:ASN:HD21 | 1:A:1899:ASN:HB2 | 1.70 | 0.55 |
| 1:B:2141:ILE:CG2 | 1:B:2145:PHE:HB2 | 2.36 | 0.55 |
| 1:A:1911:ASN:OD1 | 1:A:1912:LEU:N | 2.39 | 0.55 |
| 1:B:1392:LEU:HD13 | 1:B:1393:LYS:C | 2.26 | 0.55 |
| 1:A:2386:MET:CB | 1:A:2627:ARG:CD | 2.82 | 0.55 |
| 1:B:1939:PHE:H | 1:B:1939:PHE:HD2 | 1.55 | 0.55 |
| 1:B:2745:ILE:HG23 | 1:B:2756:MET:HE1 | 1.87 | 0.55 |
| 1:A:3017:VAL:HG21 | 1:A:3313:PHE:CE2 | 2.41 | 0.55 |
| 1:B:1527:LEU:CD2 | 1:B:1545:LEU:HD22 | 2.36 | 0.55 |
| 1:B:3530:PHE:HD1 | 1:B:3618:TYR:HD2 | 1.49 | 0.55 |
| 1:A:2842:ASP:O | 1:A:2845:GLN:HG2 | 2.07 | 0.55 |
| 1:B:1707:HIS:O | 1:B:1711:VAL:HG23 | 2.06 | 0.55 |
| 1:A:1637:GLU:HA | 1:A:1686:LYS:HZ3 | 1.72 | 0.55 |
| 1:A:1459:LEU:HD22 | 1:A:1473:THR:CG2 | 2.36 | 0.55 |
| 1:B:2380:LEU:CD2 | 1:B:2390:ILE:CD1 | 2.57 | 0.55 |
| 1:A:3530:PHE:CE1 | 1:A:3618:TYR:CD2 | 2.95 | 0.55 |
| 1:A:2763:ARG:HA | 3:A:5402:ADP:C5' | 2.37 | 0.55 |
| 1:A:1939:PHE:O | 1:A:1940:GLU:HB3 | 2.07 | 0.55 |
| 1:B:2473:LEU:HD23 | 1:B:2475:PRO:N | 2.20 | 0.55 |
| 1:A:3592:LYS:O | 1:A:3596:ASN:HB2 | 2.06 | 0.55 |
| 1:B:3305:ARG:O | 1:B:3307:LEU:N | 2.36 | 0.55 |
| 1:B:2252:LEU:HD21 | 1:B:2310:LEU:HD23 | 1.88 | 0.55 |
| 1:A:1645:PHE:HB2 | 1:A:1697:LYS:HG3 | 1.88 | 0.55 |
| 1:B:2201:HIS:CE1 | 1:B:2497:TYR:HA | 2.40 | 0.55 |
| 1:B:1469:LEU:HB3 | 1:B:1472:GLU:HB2 | 1.88 | 0.55 |
| 1:B:3555:TYR:HE1 | 1:B:3593:GLU:HG2 | 1.71 | 0.55 |
| 1:B:3692:LYS:HE3 | 1:B:3898:GLU:HB3 | 1.88 | 0.55 |
| 1:B:2732:MET:CB | 3:B:5402:ADP:C2 | 2.90 | 0.55 |
| 1:A:3998:ILE:HG22 | 1:A:4004:LEU:HG | 1.87 | 0.55 |
| 1:B:2620:ARG:HH21 | 3:B:5401:ADP:PB | 2.29 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1620:PHE:HB2 | 1:A:1760:PHE:CE1 | 2.42 | 0.55 |
| 1:A:1939:PHE:HD2 | 1:A:1939:PHE:H | 1.55 | 0.55 |
| 1:A:3566:LEU:CA | 1:A:3583:LEU:HD21 | 2.37 | 0.55 |
| 1:B:2489:ILE:HD11 | 1:B:2506:LEU:HD13 | 1.89 | 0.55 |
| 1:B:2728:LEU:HD12 | 1:B:2771:ARG:NH1 | 2.22 | 0.55 |
| 1:A:2074:GLY:O | 1:A:2197:ASP:HA | 2.07 | 0.55 |
| 1:A:1998:LEU:CD1 | 1:A:2022:PHE:HZ | 2.20 | 0.54 |
| 1:B:3303:LYS:C | 1:B:3306:TRP:HD1 | 2.09 | 0.54 |
| 1:B:2293:HIS:CE1 | 1:B:2409:ASN:CB | 2.89 | 0.54 |
| 1:B:2653:TRP:HB3 | 1:B:2654:ARG:NH1 | 2.22 | 0.54 |
| 1:A:2860:THR:HG22 | 1:A:2865:LEU:O | 2.07 | 0.54 |
| 1:B:2960:THR:HG22 | 1:B:2961:ILE:N | 2.21 | 0.54 |
| 1:A:1910:GLU:HB2 | 1:A:3846:MET:HB2 | 1.89 | 0.54 |
| 1:B:3401:GLN:C | 1:B:3403:ALA:N | 2.61 | 0.54 |
| 3:B:5401:ADP:N3 | 3:B:5401:ADP:C2' | 2.70 | 0.54 |
| 1:B:2305:LEU:HB3 | 1:B:2310:LEU:HD12 | 1.90 | 0.54 |
| 1:A:1852:ARG:HG3 | 1:A:1852:ARG:O | 2.08 | 0.54 |
| 1:A:2763:ARG:HD2 | 3:A:5402:ADP:H4' | 1.90 | 0.54 |
| 1:A:1469:LEU:HB3 | 1:A:1472:GLU:HB2 | 1.89 | 0.54 |
| 1:A:1983:LEU:HD21 | 1:A:1996:GLU:HB2 | 1.88 | 0.54 |
| 1:A:2266:PHE:HD1 | 1:A:2326:LEU:HD21 | 1.72 | 0.54 |
| 1:B:3330:TYR:CD1 | 1:B:3334:PHE:CD2 | 2.95 | 0.54 |
| 1:A:4037:SER:HB3 | 1:A:4040:GLU:HB2 | 1.90 | 0.54 |
| 1:B:1835:LEU:O | 1:B:1838:ILE:HG22 | 2.08 | 0.54 |
| 1:B:3440:LEU:CD2 | 1:B:3462:ILE:HD12 | 2.37 | 0.54 |
| 1:B:1425:GLU:OE2 | 1:B:1429:LEU:CD1 | 2.55 | 0.54 |
| 1:A:2446:SER:H | 1:A:2449:THR:HG21 | 1.72 | 0.54 |
| 1:A:2838:ALA:HB3 | 1:A:2878:VAL:HG13 | 1.89 | 0.54 |
| 1:B:1926:SER:CA | 1:B:1970:LEU:HD12 | 2.36 | 0.54 |
| 1:B:3460:PRO:O | 1:B:3463:SER:CB | 2.55 | 0.54 |
| 1:B:4023:ILE:HD12 | 1:B:4029:ILE:HD11 | 1.90 | 0.54 |
| 1:A:1630:ILE:CG2 | 1:A:1655:MET:SD | 2.96 | 0.54 |
| 1:A:2385:VAL:HG23 | 1:A:2574:TYR:HD1 | 1.73 | 0.54 |
| 1:A:3671:VAL:O | 1:A:3674:ILE:HG22 | 2.07 | 0.54 |
| 1:B:2860:THR:HG21 | 1:B:2867:LEU:HD12 | 1.89 | 0.54 |
| 1:B:3459:ASP:OD2 | 1:B:3461:ILE:HG12 | 2.08 | 0.54 |
| 1:A:2835:LEU:HD23 | 1:A:2911:ARG:HB2 | 1.89 | 0.54 |
| 1:A:2220:CYS:SG | 1:A:2224:SER:CB | 2.96 | 0.54 |
| 1:A:2382:ALA:O | 1:A:2385:VAL:HG12 | 2.08 | 0.54 |
| 1:B:3541:MET:HA | 1:B:3544:LYS:HG2 | 1.90 | 0.54 |
| 1:A:2517:LYS:HE3 | 1:A:2524:VAL:HG23 | 1.81 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1951:HIS:O | 1:A:1955:LEU:HB2 | 2.08 | 0.54 |
| 1:A:3855:LEU:HD12 | 1:A:3859:VAL:HG23 | 1.88 | 0.54 |
| 1:B:3538:ASN:HB3 | 1:B:3541:MET:HG2 | 1.89 | 0.54 |
| 1:B:1795:PHE:HE2 | 1:B:1918:GLU:HB3 | 1.73 | 0.54 |
| 1:A:1570:GLU:HB2 | 1:A:1585:VAL:HA | 1.90 | 0.54 |
| 1:A:3304:GLU:CG | 1:A:3307:LEU:HD23 | 2.33 | 0.53 |
| 1:A:3979:ASN:C | 1:A:3981:PRO:CD | 2.76 | 0.53 |
| 1:B:1898:LEU:HD11 | 1:B:1908:LEU:HD23 | 1.90 | 0.53 |
| 1:B:3671:VAL:O | 1:B:3674:ILE:HG22 | 2.07 | 0.53 |
| 1:A:3784:ASN:ND2 | 1:A:3865:ALA:O | 2.41 | 0.53 |
| 1:B:1365:PHE:C | 1:B:1367:ILE:N | 2.59 | 0.53 |
| 1:B:3618:TYR:O | 1:B:3622:GLY:N | 2.40 | 0.53 |
| 1:B:1531:ARG:HG2 | 1:B:1537:PHE:CB | 2.37 | 0.53 |
| 1:A:3330:TYR:CE1 | 1:A:3334:PHE:CD2 | 2.96 | 0.53 |
| 1:B:3566:LEU:HD11 | 1:B:3570:LEU:HD11 | 1.90 | 0.53 |
| 1:B:1677:ASP:HA | 1:B:1680:ILE:HD12 | 1.91 | 0.53 |
| 1:B:1540:LEU:HD12 | 1:B:1548:ILE:CD1 | 2.39 | 0.53 |
| 1:B:2732:MET:CA | 3:B:5402:ADP:N1 | 2.72 | 0.53 |
| 1:B:2474:LEU:HB3 | 1:B:2526:ILE:HG22 | 1.91 | 0.53 |
| 1:A:1983:LEU:HD21 | 1:A:1993:THR:O | 2.09 | 0.53 |
| 1:B:1645:PHE:CZ | 1:B:1649:LEU:HD22 | 2.42 | 0.53 |
| 1:A:2763:ARG:CD | 3:A:5402:ADP:H4' | 2.38 | 0.53 |
| 1:A:3989:ILE:HD13 | 1:A:4015:PHE:CZ | 2.43 | 0.53 |
| 1:B:2428:MET:HE1 | 1:B:2440:VAL:CG2 | 2.38 | 0.53 |
| 1:A:3323:ASN:HD21 | 1:A:3361:ASP:H | 1.55 | 0.53 |
| 1:B:2354:SER:OG | 1:B:2357:SER:HB2 | 2.08 | 0.53 |
| 1:A:2222:ILE:HG23 | 1:A:2284:LEU:HD11 | 1.90 | 0.53 |
| 1:B:3641:PHE:HA | 1:B:3889:LEU:HD21 | 1.88 | 0.53 |
| 1:A:1677:ASP:HA | 1:A:1680:ILE:HD12 | 1.89 | 0.53 |
| 1:A:2786:ILE:HD12 | 1:A:3460:PRO:HG2 | 1.91 | 0.53 |
| 1:B:1726:LEU:HD13 | 1:B:3984:GLN:HB3 | 1.87 | 0.53 |
| 1:A:1872:LEU:HG | 1:A:1888:LEU:HD21 | 1.90 | 0.53 |
| 1:A:3555:TYR:HE1 | 1:A:3593:GLU:HG2 | 1.73 | 0.53 |
| 1:A:1835:LEU:O | 1:A:1838:ILE:HG22 | 2.08 | 0.53 |
| 1:B:2582:VAL:HG23 | 1:B:2582:VAL:O | 2.08 | 0.53 |
| 1:A:2563:SER:CB | 1:A:2566:SER:OG | 2.57 | 0.53 |
| 1:A:2448:ASP:HB2 | 1:A:2829:GLU:CD | 2.29 | 0.53 |
| 1:A:1749:ILE:HD13 | 1:A:1813:LEU:HD22 | 1.90 | 0.53 |
| 1:B:3924:TRP:O | 1:B:3927:TYR:HB3 | 2.08 | 0.53 |
| 1:A:3819:ILE:O | 1:A:3823:ASN:HB2 | 2.09 | 0.53 |
| 1:A:3367:ILE:O | 1:A:3371:VAL:HG22 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1826:PHE:CZ | 1:A:1830:VAL:HG13 | 2.44 | 0.53 |
| 1:B:3530:PHE:CE1 | 1:B:3618:TYR:CD2 | 2.96 | 0.53 |
| 1:A:1418:SER:O | 1:A:1421:TYR:CE2 | 2.62 | 0.53 |
| 1:A:3330:TYR:CE2 | 1:A:3346:LEU:HD13 | 2.43 | 0.53 |
| 1:B:3308:ASN:O | 1:B:3312:GLN:HB2 | 2.09 | 0.53 |
| 1:A:1698:ILE:O | 1:A:1702:LEU:HG | 2.08 | 0.53 |
| 1:B:3342:ARG:NH1 | 1:B:3393:ASN:OD1 | 2.38 | 0.53 |
| 1:B:3760:LEU:HD21 | 1:B:4078:ALA:HA | 1.91 | 0.53 |
| 1:B:3612:ASP:O | 1:B:3615:VAL:HG22 | 2.09 | 0.53 |
| 1:A:1645:PHE:HZ | 1:A:1768:ARG:HD2 | 1.73 | 0.53 |
| 1:B:2112:GLU:CB | 1:B:2117:SER:HB2 | 2.32 | 0.53 |
| 1:A:1493:LEU:CD2 | 1:A:1498:GLU:HB3 | 2.39 | 0.53 |
| 1:A:1794:PHE:CD1 | 1:A:1802:LYS:HB3 | 2.41 | 0.53 |
| 1:A:2220:CYS:SG | 1:A:2221:SER:N | 2.82 | 0.53 |
| 1:B:3998:ILE:HG21 | 1:B:4004:LEU:HG | 1.91 | 0.53 |
| 1:B:1770:ILE:HD11 | 1:B:1936:ILE:HD11 | 1.90 | 0.53 |
| 1:A:2410:SER:C | 1:A:2411:LYS:HG3 | 2.29 | 0.53 |
| 1:A:2707:VAL:CG1 | 1:A:2712:LEU:HD12 | 2.38 | 0.53 |
| 1:A:2476:LYS:HZ2 | 1:A:2528:ARG:HB2 | 1.74 | 0.53 |
| 1:A:3978:ASN:O | 1:A:3981:PRO:HD3 | 2.08 | 0.53 |
| 1:A:1540:LEU:HD11 | 1:A:1561:PHE:HB3 | 1.90 | 0.53 |
| 1:A:2380:LEU:CD1 | 1:A:2577:ALA:CB | 2.86 | 0.53 |
| 1:B:3978:ASN:O | 1:B:3981:PRO:CD | 2.57 | 0.53 |
| 1:A:1534:PHE:CE2 | 1:A:1536:ARG:HB2 | 2.43 | 0.52 |
| 1:B:2080:LYS:HZ1 | 1:B:2549:ARG:NE | 2.07 | 0.52 |
| 1:A:3509:LEU:HD12 | 1:A:3513:VAL:CG2 | 2.39 | 0.52 |
| 1:B:3737:THR:CB | 1:B:3740:THR:CB | 2.87 | 0.52 |
| 1:A:2151:TRP:CE3 | 1:A:2193:LEU:HD11 | 2.44 | 0.52 |
| 1:B:3862:THR:HB | 1:B:3865:ALA:HB2 | 1.91 | 0.52 |
| 1:B:2842:ASP:O | 1:B:2845:GLN:HG2 | 2.09 | 0.52 |
| 1:A:1929:ILE:HD12 | 1:A:1929:ILE:H | 1.74 | 0.52 |
| 1:B:3889:LEU:HG | 1:B:3894:ARG:HD3 | 1.90 | 0.52 |
| 1:A:1731:VAL:HG12 | 1:A:1732:GLN:N | 2.24 | 0.52 |
| 1:A:3547:ASP:HA | 1:A:3550:LYS:HB3 | 1.90 | 0.52 |
| 1:B:2081:THR:HB | 2:B:5400:ATP:O1A | 2.09 | 0.52 |
| 1:B:2151:TRP:HE3 | 1:B:2193:LEU:HD11 | 1.73 | 0.52 |
| 1:B:1866:GLN:O | 1:B:1870:ASN:HB2 | 2.08 | 0.52 |
| 1:B:2563:SER:CB | 1:B:2566:SER:H | 2.16 | 0.52 |
| 1:B:1575:LEU:O | 1:B:1576:GLU:HB3 | 2.10 | 0.52 |
| 1:A:2941:THR:HG22 | 1:A:2942:ASP:N | 2.22 | 0.52 |
| 1:A:4024:VAL:CG2 | 1:A:4027:VAL:HB | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2891:ILE:HD11 | 1:B:2903:ILE:HD11 | 1.90 | 0.52 |
| 1:B:2074:GLY:O | 1:B:2197:ASP:HA | 2.10 | 0.52 |
| 1:B:2784:PRO:HG2 | 1:B:2817:ILE:HD13 | 1.91 | 0.52 |
| 1:A:1416:LYS:O | 1:A:1421:TYR:OH | 2.25 | 0.52 |
| 1:A:2003:LEU:HA | 1:A:2006:LEU:HD12 | 1.91 | 0.52 |
| 1:A:2137:VAL:O | 1:A:2141:ILE:CG2 | 2.54 | 0.52 |
| 1:B:3737:THR:HB | 1:B:3740:THR:HG1 | 1.74 | 0.52 |
| 1:A:3701:THR:OG1 | 1:A:4085:THR:HG22 | 2.08 | 0.52 |
| 1:B:3330:TYR:CE2 | 1:B:3346:LEU:HD13 | 2.45 | 0.52 |
| 1:B:3935:PHE:HB2 | 1:B:4014:VAL:HG11 | 1.92 | 0.52 |
| 1:B:2107:LYS:CE | 1:B:2495:ASP:OD2 | 2.44 | 0.52 |
| 1:A:2473:LEU:HD22 | 1:A:2527:GLU:HG2 | 1.91 | 0.52 |
| 1:A:3530:PHE:HD1 | 1:A:3618:TYR:HD2 | 1.50 | 0.52 |
| 1:A:1416:LYS:O | 1:A:1421:TYR:CE2 | 2.63 | 0.52 |
| 1:A:1645:PHE:CD2 | 1:A:1765:ILE:HG22 | 2.44 | 0.52 |
| 1:A:3304:GLU:O | 1:A:3307:LEU:HB3 | 2.10 | 0.52 |
| 1:A:3538:ASN:HB3 | 1:A:3541:MET:HG2 | 1.91 | 0.52 |
| 1:B:3934:TRP:CB | 1:B:4023:ILE:HD13 | 2.40 | 0.52 |
| 1:B:2624:ARG:NH2 | 1:B:2910:ASN:O | 2.43 | 0.52 |
| 1:A:2488:GLU:CD | 1:A:2491:LEU:HD11 | 2.30 | 0.52 |
| 1:A:2318:ILE:O | 1:A:2322:LEU:HB2 | 2.10 | 0.52 |
| 1:A:2201:HIS:CE1 | 1:A:2497:TYR:HA | 2.44 | 0.52 |
| 1:B:1703:VAL:HG13 | 1:B:1770:ILE:HD13 | 1.90 | 0.52 |
| 1:A:2280:THR:HA | 1:A:2283:LYS:HD2 | 1.91 | 0.52 |
| 1:A:1970:LEU:CD2 | 1:A:1974:LYS:HE2 | 2.40 | 0.52 |
| 1:A:2220:CYS:SG | 1:A:2224:SER:HB2 | 2.50 | 0.52 |
| 1:B:2073:VAL:HG21 | 1:B:2199:LEU:HD11 | 1.92 | 0.52 |
| 1:B:23:LEU:O | 1:B:24:GLU:CB | 2.57 | 0.52 |
| 1:A:1956:LEU:CB | 1:A:1968:PHE:CE2 | 2.87 | 0.52 |
| 1:A:1910:GLU:HB2 | 1:A:3846:MET:HA | 1.91 | 0.52 |
| 1:B:2044:ARG:NH2 | 1:B:2093:ILE:HD11 | 2.24 | 0.52 |
| 1:B:1822:CYS:SG | 1:B:1850:PHE:HA | 2.50 | 0.52 |
| 1:A:3304:GLU:HG3 | 1:A:3307:LEU:CD2 | 2.32 | 0.52 |
| 1:A:1706:LEU:HD22 | 1:A:1935:GLN:CG | 2.38 | 0.52 |
| 1:A:2336:ARG:CD | 1:A:2355:ASP:OD2 | 2.57 | 0.52 |
| 1:B:2728:LEU:CG | 1:B:2771:ARG:HH22 | 2.22 | 0.52 |
| 1:A:1527:LEU:HD21 | 1:A:1546:LEU:HD21 | 1.91 | 0.52 |
| 1:A:2076:ALA:CB | 1:A:2549:ARG:HG2 | 2.40 | 0.52 |
| 1:B:2080:LYS:HG2 | 2:B:5400:ATP:O1B | 2.07 | 0.51 |
| 1:B:1692:ASP:O | 1:B:1695:LYS:HB3 | 2.09 | 0.51 |
| 1:B:1409:LEU:CD2 | 1:B:1435:LEU:CB | 2.86 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2421:GLY:H | 3:A:5401:ADP:PB | 2.33 | 0.51 |
| 1:B:2386:MET:HB2 | 1:B:2627:ARG:CD | 2.37 | 0.51 |
| 1:B:3537:GLU:OE1 | 1:B:3618:TYR:OH | 2.29 | 0.51 |
| 1:B:2080:LYS:HG3 | 2:B:5400:ATP:O1B | 2.11 | 0.51 |
| 1:B:2080:LYS:HG3 | 1:B:2195:GLU:OE1 | 2.10 | 0.51 |
| 1:B:3934:TRP:HB3 | 1:B:4023:ILE:HD13 | 1.93 | 0.51 |
| 1:B:3979:ASN:O | 1:B:3981:PRO:HD2 | 2.11 | 0.51 |
| 1:A:1781:THR:HG21 | 1:A:1919:PHE:CD1 | 2.46 | 0.51 |
| 1:B:1822:CYS:SG | 1:B:1849:GLU:C | 2.89 | 0.51 |
| 1:B:2173:ASN:HB3 | 1:B:2175:ILE:HG22 | 1.92 | 0.51 |
| 1:B:3551:LEU:HA | 1:B:3554:GLU:HB3 | 1.92 | 0.51 |
| 1:A:2633:ILE:HD11 | 1:A:2644:LEU:CD2 | 2.41 | 0.51 |
| 1:A:2489:ILE:HG22 | 1:A:2535:CYS:HB3 | 1.92 | 0.51 |
| 1:A:2517:LYS:HG3 | 1:A:2524:VAL:HG23 | 1.93 | 0.51 |
| 1:A:3303:LYS:HA | 1:A:3306:TRP:HB2 | 1.92 | 0.51 |
| 1:B:1929:ILE:HD13 | 1:B:1970:LEU:CD1 | 2.40 | 0.51 |
| 1:B:3911:TRP:HH2 | 1:B:3926:VAL:HG13 | 1.76 | 0.51 |
| 1:B:2257:PHE:HD1 | 1:B:2262:LEU:HD11 | 1.75 | 0.51 |
| 1:A:3460:PRO:O | 1:A:3463:SER:CB | 2.59 | 0.51 |
| 1:B:2788:ARG:HG3 | 1:B:3459:ASP:HA | 1.92 | 0.51 |
| 1:B:2786:ILE:HD12 | 1:B:3460:PRO:HG2 | 1.92 | 0.51 |
| 1:B:1910:GLU:CB | 1:B:3846:MET:HB3 | 2.41 | 0.51 |
| 1:B:2506:LEU:HD22 | 1:B:2531:ILE:HD12 | 1.91 | 0.51 |
| 1:B:3979:ASN:C | 1:B:3981:PRO:HD2 | 2.30 | 0.51 |
| 1:B:3547:ASP:HA | 1:B:3550:LYS:HB3 | 1.91 | 0.51 |
| 1:A:2154:PHE:CD1 | 1:A:2154:PHE:N | 2.79 | 0.51 |
| 1:A:2112:GLU:HB3 | 1:A:2117:SER:OG | 2.11 | 0.51 |
| 1:B:2336:ARG:HA | 1:B:2339:ILE:HD12 | 1.93 | 0.51 |
| 1:B:3978:ASN:O | 1:B:3981:PRO:HD3 | 2.11 | 0.51 |
| 1:B:2105:ASP:OD2 | 1:B:2508:GLN:HB2 | 2.11 | 0.51 |
| 1:B:1949:ILE:HD11 | 1:B:1994:VAL:HG11 | 1.93 | 0.51 |
| 1:A:2494:LEU:HB2 | 1:A:2499:SER:N | 2.26 | 0.51 |
| 1:A:2788:ARG:HG3 | 1:A:3459:ASP:HA | 1.92 | 0.51 |
| 1:A:2002:ILE:HG22 | 1:A:2006:LEU:HD11 | 1.92 | 0.51 |
| 1:B:1911:ASN:OD1 | 1:B:1912:LEU:HG | 2.11 | 0.51 |
| 1:A:2563:SER:CB | 1:A:2566:SER:H | 2.22 | 0.51 |
| 1:B:3566:LEU:HD23 | 1:B:3587:LEU:HD11 | 1.92 | 0.51 |
| 1:A:3989:ILE:HD13 | 1:A:4015:PHE:CE2 | 2.46 | 0.51 |
| 1:B:3815:PRO:O | 1:B:3821:ASN:HB3 | 2.11 | 0.51 |
| 1:B:3784:ASN:ND2 | 1:B:3865:ALA:O | 2.44 | 0.51 |
| 1:B:2262:LEU:HA | 1:B:2265:ILE:HD12 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3342:ARG:NH1 | 1:A:3393:ASN:OD1 | 2.40 | 0.51 |
| 1:B:1626:CYS:SG | 1:B:1639:VAL:HG11 | 2.51 | 0.51 |
| 1:B:2476:LYS:N | 1:B:2476:LYS:CD | 2.71 | 0.51 |
| 1:B:2410:SER:O | 1:B:2411:LYS:HB2 | 2.11 | 0.51 |
| 1:A:1748:PHE:CD2 | 1:A:1755:LEU:HD22 | 2.46 | 0.51 |
| 1:B:1559:SER:HB3 | 1:B:1572:ILE:HG22 | 1.93 | 0.51 |
| 1:B:1762:TYR:CZ | 1:B:1764:GLY:HA2 | 2.46 | 0.51 |
| 1:B:1365:PHE:CG | 1:B:1366:VAL:N | 2.76 | 0.50 |
| 1:B:2473:LEU:HD22 | 1:B:2475:PRO:CG | 2.32 | 0.50 |
| 1:B:2224:SER:O | 2:B:5400:ATP:H2 | 1.93 | 0.50 |
| 1:A:3785:TYR:CE1 | 1:A:3859:VAL:HG13 | 2.46 | 0.50 |
| 1:B:2380:LEU:HG | 1:B:2384:GLU:OE1 | 2.11 | 0.50 |
| 1:A:1418:SER:HB2 | 1:A:3446:PHE:HB3 | 1.91 | 0.50 |
| 1:A:1849:GLU:CG | 1:A:1899:ASN:ND2 | 2.74 | 0.50 |
| 1:B:2081:THR:OG1 | 2:B:5400:ATP:O1B | 2.26 | 0.50 |
| 1:A:2048:SER:H | 2:A:5400:ATP:N6 | 2.08 | 0.50 |
| 1:A:3308:ASN:C | 1:A:3310:THR:H | 2.12 | 0.50 |
| 1:B:2571:TYR:HD1 | 1:B:2626:VAL:HG21 | 1.75 | 0.50 |
| 1:B:2473:LEU:HD21 | 1:B:2527:GLU:HB2 | 1.94 | 0.50 |
| 1:A:2282:ASN:ND2 | 1:A:2552:ARG:HD2 | 2.26 | 0.50 |
| 1:B:2080:LYS:CG | 1:B:2081:THR:H | 2.25 | 0.50 |
| 1:A:1493:LEU:HD23 | 1:A:1498:GLU:HB3 | 1.93 | 0.50 |
| 1:A:3350:LYS:HA | 1:A:3353:LEU:HD12 | 1.92 | 0.50 |
| 1:B:1749:ILE:HD13 | 1:B:1813:LEU:HD22 | 1.92 | 0.50 |
| 1:B:2137:VAL:O | 1:B:2141:ILE:CG2 | 2.49 | 0.50 |
| 1:A:1926:SER:HA | 1:A:1970:LEU:CD1 | 2.40 | 0.50 |
| 1:A:1493:LEU:HD22 | 1:A:1502:ILE:HD11 | 1.93 | 0.50 |
| 1:B:1493:LEU:O | 1:B:1494:ASP:HB2 | 2.11 | 0.50 |
| 1:B:3401:GLN:O | 1:B:3403:ALA:N | 2.44 | 0.50 |
| 1:A:2083:THR:O | 1:A:2087:VAL:HG23 | 2.12 | 0.50 |
| 1:B:3530:PHE:HD1 | 1:B:3618:TYR:CD2 | 2.26 | 0.50 |
| 1:B:3461:ILE:C | 1:B:3463:SER:N | 2.65 | 0.50 |
| 1:A:1387:GLU:HA | 1:A:1393:LYS:HA | 1.93 | 0.50 |
| 1:A:2984:VAL:C | 1:A:2986:PRO:HD3 | 2.32 | 0.50 |
| 1:A:2762:SER:O | 1:A:2763:ARG:CB | 2.47 | 0.50 |
| 1:A:2364:ASP:O | 1:A:2365:LYS:HG3 | 2.11 | 0.50 |
| 1:A:2081:THR:HA | 1:A:2084:TRP:NE1 | 2.27 | 0.50 |
| 1:B:1917:ARG:HD2 | 1:B:3963:PHE:CE2 | 2.47 | 0.50 |
| 1:A:2181:GLY:O | 1:A:2182:GLU:CG | 2.58 | 0.50 |
| 1:B:3965:SER:HA | 1:B:3968:LEU:HD12 | 1.92 | 0.50 |
| 1:B:2080:LYS:HE2 | 2:B:5400:ATP:PG | 2.52 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3919:LYS:NZ | 1:B:4038:GLU:CG | 2.74 | 0.50 |
| 1:A:1438:LEU:O | 1:A:1442:GLN:HB2 | 2.12 | 0.50 |
| 1:B:3323:ASN:HD21 | 1:B:3361:ASP:H | 1.60 | 0.50 |
| 1:A:2780:LYS:HB3 | 1:A:2813:THR:HG22 | 1.94 | 0.50 |
| 1:A:3725:VAL:HG22 | 1:A:3731:ASP:HA | 1.93 | 0.50 |
| 1:A:3461:ILE:C | 1:A:3463:SER:H | 2.16 | 0.50 |
| 1:A:1409:LEU:CD2 | 1:A:1435:LEU:CB | 2.82 | 0.50 |
| 1:A:2424:LYS:NZ | 3:A:5401:ADP:O2B | 2.32 | 0.50 |
| 1:A:1493:LEU:O | 1:A:1494:ASP:HB2 | 2.11 | 0.50 |
| 1:A:1802:LYS:NZ | 4:A:5403:SO4:O2 | 2.32 | 0.50 |
| 1:A:3817:GLY:H | 1:A:3821:ASN:HB2 | 1.77 | 0.50 |
| 1:A:3854:TYR:O | 1:A:3858:HIS:HB2 | 2.12 | 0.50 |
| 1:B:2362:ALA:HB3 | 1:B:2365:LYS:O | 2.12 | 0.50 |
| 1:B:3848:LEU:HD21 | 1:B:3852:LYS:HE3 | 1.94 | 0.50 |
| 1:B:2741:HIS:HA | 1:B:2744:ARG:HD2 | 1.93 | 0.50 |
| 1:B:2732:MET:HB2 | 3:B:5402:ADP:C4 | 2.41 | 0.49 |
| 1:B:1973:LEU:O | 1:B:1977:LEU:HG | 2.12 | 0.49 |
| 1:B:1645:PHE:CD2 | 1:B:1765:ILE:HG22 | 2.47 | 0.49 |
| 1:B:1681:LYS:CE | 1:B:1939:PHE:HZ | 2.24 | 0.49 |
| 1:B:3855:LEU:HD12 | 1:B:3859:VAL:HG23 | 1.94 | 0.49 |
| 1:A:2941:THR:CG2 | 1:A:2942:ASP:H | 2.25 | 0.49 |
| 1:A:2394:THR:H | 1:A:2397:THR:HB | 1.76 | 0.49 |
| 1:B:1469:LEU:HD13 | 1:B:1523:LEU:CD2 | 2.42 | 0.49 |
| 1:B:1554:HIS:O | 1:B:1555:HIS:HB2 | 2.11 | 0.49 |
| 1:B:2318:ILE:O | 1:B:2322:LEU:HB2 | 2.11 | 0.49 |
| 1:B:3509:LEU:HD12 | 1:B:3513:VAL:CG2 | 2.42 | 0.49 |
| 1:A:2293:HIS:CE1 | 1:A:2409:ASN:CB | 2.96 | 0.49 |
| 1:A:2170:LEU:HB3 | 1:A:2209:ARG:HD3 | 1.92 | 0.49 |
| 1:A:1926:SER:HB2 | 1:A:1973:LEU:HD21 | 1.93 | 0.49 |
| 1:A:1495:THR:CG2 | 1:A:1497:ILE:HG22 | 2.40 | 0.49 |
| 1:A:1802:LYS:O | 1:A:1806:VAL:HG23 | 2.12 | 0.49 |
| 1:A:2104:ILE:O | 1:A:2154:PHE:HA | 2.12 | 0.49 |
| 1:B:1794:PHE:HB3 | 1:B:1919:PHE:HB3 | 1.95 | 0.49 |
| 1:B:3481:ILE:O | 1:B:3483:ASP:N | 2.45 | 0.49 |
| 1:A:1850:PHE:CB | 1:A:1896:ILE:HG23 | 2.42 | 0.49 |
| 1:A:1940:GLU:HG3 | 1:A:1941:ASP:N | 2.27 | 0.49 |
| 1:A:1970:LEU:CD2 | 1:A:1974:LYS:CE | 2.90 | 0.49 |
| 1:A:2829:GLU:HA | 1:A:2832:ASN:HD22 | 1.76 | 0.49 |
| 1:A:3631:MET:HE3 | 1:A:3698:MET:HG3 | 1.93 | 0.49 |
| 1:B:2354:SER:H | 1:B:2357:SER:HB2 | 1.77 | 0.49 |
| 1:B:1981:SER:HB3 | 1:B:1982:PRO:HD3 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3537:GLU:OE1 | 1:A:3618:TYR:OH | 2.31 | 0.49 |
| 1:A:1870:ASN:O | 1:A:1874:VAL:HG23 | 2.13 | 0.49 |
| 1:B:3306:TRP:CH2 | 1:B:3594:ALA:HB1 | 2.48 | 0.49 |
| 1:B:2755:HIS:NE2 | 1:B:2835:LEU:HG | 2.26 | 0.49 |
| 1:B:4022:GLN:HG2 | 1:B:4022:GLN:O | 2.13 | 0.49 |
| 1:B:2063:MET:HB3 | 1:B:2070:LEU:HD11 | 1.93 | 0.49 |
| 1:A:1822:CYS:HB2 | 1:A:1853:LEU:CD2 | 2.26 | 0.49 |
| 1:A:1637:GLU:HA | 1:A:1686:LYS:NZ | 2.27 | 0.49 |
| 1:A:1910:GLU:HB2 | 1:A:3846:MET:CA | 2.42 | 0.49 |
| 1:B:2580:LYS:HG2 | 1:B:2586:ARG:HH22 | 1.77 | 0.49 |
| 1:B:3338:ASN:HD22 | 1:B:3341:GLU:HG2 | 1.77 | 0.49 |
| 1:B:2732:MET:CA | 3:B:5402:ADP:C2 | 2.93 | 0.49 |
| 1:B:3505:ILE:O | 1:B:3510:ARG:NH1 | 2.46 | 0.49 |
| 1:B:1795:PHE:CE2 | 1:B:1918:GLU:HB3 | 2.48 | 0.49 |
| 1:A:1838:ILE:HG13 | 1:A:1843:ALA:HB3 | 1.93 | 0.49 |
| 1:B:2758:LEU:HD23 | 1:B:2915:ASN:HB3 | 1.95 | 0.49 |
| 1:B:3702:MET:HB3 | 1:B:3767:PHE:HZ | 1.77 | 0.49 |
| 1:A:1656:TRP:O | 1:A:1660:VAL:HG12 | 2.11 | 0.49 |
| 1:B:2229:LEU:HB3 | 1:B:2288:VAL:HG11 | 1.94 | 0.49 |
| 1:B:1929:ILE:HD12 | 1:B:1929:ILE:H | 1.78 | 0.49 |
| 1:B:2080:LYS:CG | 1:B:2081:THR:N | 2.76 | 0.49 |
| 1:A:2274:HIS:CE1 | 1:A:2326:LEU:O | 2.51 | 0.49 |
| 1:B:2305:LEU:HD11 | 1:B:2368:PHE:HB3 | 1.94 | 0.49 |
| 1:B:1838:ILE:CD1 | 1:B:1845:GLY:HA3 | 2.43 | 0.49 |
| 1:A:2489:ILE:HD11 | 1:A:2506:LEU:HD13 | 1.94 | 0.49 |
| 1:A:1803:THR:HG21 | 1:A:1848:ASP:CG | 2.33 | 0.49 |
| 1:B:2792:LEU:HD13 | 1:B:2826:ALA:HB3 | 1.95 | 0.49 |
| 1:B:3330:TYR:CE1 | 1:B:3334:PHE:CE2 | 3.01 | 0.49 |
| 1:A:3010:LEU:CD2 | 1:A:3317:SER:HB3 | 2.41 | 0.49 |
| 1:A:3989:ILE:HA | 1:A:3993:VAL:HB | 1.95 | 0.49 |
| 1:A:3612:ASP:O | 1:A:3615:VAL:HG22 | 2.13 | 0.49 |
| 1:B:1995:VAL:HG22 | 1:B:2022:PHE:CE2 | 2.48 | 0.49 |
| 1:B:3946:VAL:HA | 1:B:3947:PRO:C | 2.32 | 0.49 |
| 1:B:1657:THR:HG21 | 1:B:1734:PHE:O | 2.12 | 0.49 |
| 1:B:2002:ILE:HG22 | 1:B:2006:LEU:HD11 | 1.95 | 0.48 |
| 1:B:1748:PHE:HD2 | 1:B:1755:LEU:HD22 | 1.78 | 0.48 |
| 1:B:3319:GLU:HA | 1:B:3359:LYS:O | 2.13 | 0.48 |
| 1:B:2473:LEU:CD2 | 1:B:2475:PRO:N | 2.76 | 0.48 |
| 1:B:3688:THR:HG21 | 1:B:3777:VAL:CG2 | 2.42 | 0.48 |
| 1:A:3737:THR:HB | 1:A:3740:THR:HB | 1.90 | 0.48 |
| 1:B:3785:TYR:HE1 | 1:B:3859:VAL:HG22 | 1.74 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1391:GLY:HA3 | 1:A:1484:LYS:NZ | 2.27 | 0.48 |
| 1:B:2316:LEU:HD13 | 1:B:2351:GLN:HB3 | 1.95 | 0.48 |
| 1:B:3817:GLY:H | 1:B:3821:ASN:CB | 2.27 | 0.48 |
| 1:B:1527:LEU:HD22 | 1:B:1545:LEU:HD22 | 1.94 | 0.48 |
| 1:B:2257:PHE:CD1 | 1:B:2262:LEU:HD11 | 2.48 | 0.48 |
| 1:B:1606:GLU:O | 1:B:1610:ILE:HG12 | 2.13 | 0.48 |
| 1:A:3971:VAL:O | 1:A:3975:ASN:HB2 | 2.13 | 0.48 |
| 1:A:2027:THR:HA | 1:A:2028:PRO:HD3 | 1.62 | 0.48 |
| 1:A:2401:GLU:HG2 | 1:A:2431:ALA:HB2 | 1.94 | 0.48 |
| 1:A:2131:THR:HG22 | 1:A:2176:LEU:HD21 | 1.94 | 0.48 |
| 1:A:1466:GLN:HB3 | 1:A:1473:THR:HG21 | 1.94 | 0.48 |
| 1:A:3440:LEU:HD22 | 1:A:3462:ILE:HD12 | 1.95 | 0.48 |
| 1:B:3592:LYS:O | 1:B:3596:ASN:N | 2.46 | 0.48 |
| 1:A:2985:ASN:N | 1:A:2986:PRO:HD3 | 2.28 | 0.48 |
| 1:B:1917:ARG:HD2 | 1:B:3963:PHE:CZ | 2.48 | 0.48 |
| 1:B:3807:SER:O | 1:B:3808:LYS:HB2 | 2.14 | 0.48 |
| 1:A:1953:LEU:HD11 | 1:A:1973:LEU:HB3 | 1.94 | 0.48 |
| 1:B:1781:THR:HG21 | 1:B:1919:PHE:CE1 | 2.48 | 0.48 |
| 1:A:65:THR:O | 1:A:66:GLN:CB | 2.60 | 0.48 |
| 1:B:1531:ARG:HD3 | 1:B:1537:PHE:O | 2.14 | 0.48 |
| 1:A:1984:ILE:HG21 | 1:A:1989:GLU:HG3 | 1.95 | 0.48 |
| 1:B:1940:GLU:HG3 | 1:B:1941:ASP:H | 1.79 | 0.48 |
| 1:B:1392:LEU:C | 1:B:1392:LEU:CD1 | 2.80 | 0.48 |
| 1:A:3330:TYR:CD1 | 1:A:3334:PHE:CD2 | 3.02 | 0.48 |
| 1:A:3833:LYS:NZ | 1:A:3862:THR:HG21 | 2.27 | 0.48 |
| 1:A:2394:THR:HG22 | 1:A:2395:ILE:H | 1.78 | 0.48 |
| 1:A:2571:TYR:HA | 1:A:2574:TYR:HB2 | 1.95 | 0.48 |
| 1:B:4020:ASN:HB3 | 1:B:4028:ARG:HH21 | 1.77 | 0.48 |
| 1:A:4074:GLU:HA | 1:A:4077:GLN:HE21 | 1.78 | 0.48 |
| 1:B:1535:PRO:C | 1:B:1841:ILE:HD11 | 2.33 | 0.48 |
| 1:A:2302:PHE:HA | 1:A:2310:LEU:HD11 | 1.95 | 0.48 |
| 1:A:1803:THR:HG21 | 1:A:1848:ASP:OD1 | 2.14 | 0.48 |
| 1:B:3854:TYR:O | 1:B:3858:HIS:HB2 | 2.14 | 0.48 |
| 1:A:3409:ASP:HB3 | 1:A:3518:PHE:HB2 | 1.96 | 0.48 |
| 1:A:1559:SER:HB3 | 1:A:1572:ILE:HG22 | 1.96 | 0.48 |
| 1:A:1911:ASN:OD1 | 1:A:1912:LEU:HG | 2.14 | 0.48 |
| 1:A:2079:GLY:HA2 | 2:A:5400:ATP:H5'2 | 1.96 | 0.48 |
| 1:A:1749:ILE:O | 1:A:1755:LEU:HA | 2.13 | 0.48 |
| 1:B:3306:TRP:HH2 | 1:B:3594:ALA:HB1 | 1.77 | 0.48 |
| 1:A:1604:ALA:HA | 1:A:1607:TRP:HE1 | 1.78 | 0.48 |
| 1:A:2728:LEU:HD12 | 1:A:2771:ARG:NH1 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2982:VAL:CG1 | 1:A:2983:GLY:N | 2.77 | 0.48 |
| 1:B:2642:ARG:O | 1:B:2646:ARG:HG3 | 2.14 | 0.48 |
| 1:B:1714:GLN:HB3 | 1:B:1727:LEU:HD11 | 1.96 | 0.48 |
| 1:B:1386:ILE:HG22 | 1:B:1396:ARG:HG2 | 1.95 | 0.48 |
| 1:A:3797:THR:O | 1:A:3801:ILE:HG12 | 2.13 | 0.48 |
| 1:B:1823:ASP:HB2 | 1:B:1853:LEU:HD23 | 1.96 | 0.48 |
| 1:B:1967:HIS:C | 1:B:1968:PHE:CD1 | 2.85 | 0.48 |
| 1:A:1455:LEU:HD12 | 1:A:1516:LEU:CD2 | 2.41 | 0.48 |
| 1:A:2463:ASN:O | 1:A:2475:PRO:HD2 | 2.13 | 0.48 |
| 1:B:2787:HIS:CA | 1:B:3460:PRO:HG2 | 2.43 | 0.48 |
| 1:A:2771:ARG:HG2 | 1:A:2781:ILE:HG21 | 1.96 | 0.48 |
| 1:B:2295:ILE:HG12 | 1:B:2314:ILE:HD12 | 1.96 | 0.48 |
| 1:B:1838:ILE:HG13 | 1:B:1843:ALA:HB3 | 1.96 | 0.48 |
| 1:A:1969:GLY:O | 1:A:1972:THR:HB | 2.14 | 0.48 |
| 1:B:2707:VAL:HG12 | 1:B:2712:LEU:CD1 | 2.39 | 0.47 |
| 1:A:1941:ASP:O | 1:A:1945:LEU:HG | 2.13 | 0.47 |
| 1:B:1910:GLU:HB2 | 1:B:3846:MET:HB3 | 1.91 | 0.47 |
| 1:B:2754:GLY:HA3 | 1:B:2886:HIS:CE1 | 2.49 | 0.47 |
| 1:A:1620:PHE:CA | 1:A:1760:PHE:CE1 | 2.97 | 0.47 |
| 1:B:1392:LEU:N | 1:B:1484:LYS:HE2 | 2.29 | 0.47 |
| 1:B:2728:LEU:HD12 | 1:B:2771:ARG:CZ | 2.44 | 0.47 |
| 1:A:2839:ASP:HB3 | 1:A:2878:VAL:HG22 | 1.94 | 0.47 |
| 1:B:1748:PHE:CD2 | 1:B:1755:LEU:HD22 | 2.49 | 0.47 |
| 1:B:2467:THR:HG22 | 1:B:2468:SER:N | 2.28 | 0.47 |
| 1:B:2220:CYS:SG | 2:B:5400:ATP:C6 | 3.07 | 0.47 |
| 1:B:1392:LEU:HD23 | 1:B:1484:LYS:HA | 1.96 | 0.47 |
| 1:B:1611:LEU:O | 1:B:1615:ILE:HG12 | 2.14 | 0.47 |
| 1:A:2201:HIS:CE1 | 1:A:2497:TYR:HB3 | 2.48 | 0.47 |
| 1:B:3772:TRP:HZ3 | 1:B:3780:ASN:HD22 | 1.63 | 0.47 |
| 1:A:3628:ILE:HG22 | 1:A:3649:PHE:CE2 | 2.49 | 0.47 |
| 1:B:2122:THR:O | 1:B:2123:LEU:C | 2.53 | 0.47 |
| 1:B:2732:MET:CB | 3:B:5402:ADP:C4 | 2.97 | 0.47 |
| 1:A:3460:PRO:O | 1:A:3463:SER:HB3 | 2.14 | 0.47 |
| 1:B:3459:ASP:OD2 | 1:B:3461:ILE:CG1 | 2.62 | 0.47 |
| 1:A:2034:ILE:CD1 | 1:A:2061:TYR:CZ | 2.97 | 0.47 |
| 1:A:3628:ILE:HG22 | 1:A:3649:PHE:HE2 | 1.80 | 0.47 |
| 1:B:2106:THR:H | 1:B:2156:SER:HB2 | 1.79 | 0.47 |
| 1:B:1979:ASN:OD1 | 1:B:2066:THR:HG21 | 2.15 | 0.47 |
| 1:A:3940:THR:O | 1:A:3943:THR:HB | 2.14 | 0.47 |
| 1:B:2846:GLY:O | 1:B:2849:TYR:HB3 | 2.14 | 0.47 |
| 1:B:2757:MET:HG2 | 1:B:2914:ILE:HG13 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2889:PHE:CD1 | 1:A:2902:MET:HE1 | 2.50 | 0.47 |
| 1:B:2473:LEU:HD23 | 1:B:2473:LEU:C | 2.34 | 0.47 |
| 1:A:1938:GLY:HA3 | 1:A:1989:GLU:HG2 | 1.96 | 0.47 |
| 1:A:3979:ASN:O | 1:A:3981:PRO:CD | 2.57 | 0.47 |
| 1:B:2002:ILE:HB | 1:B:2014:PHE:CE2 | 2.49 | 0.47 |
| 1:B:2891:ILE:CD1 | 1:B:2903:ILE:HD11 | 2.44 | 0.47 |
| 1:B:1750:SER:HB2 | 1:B:1755:LEU:CD2 | 2.45 | 0.47 |
| 1:B:1715:LEU:HG | 1:B:1727:LEU:HD22 | 1.97 | 0.47 |
| 1:B:3897:TYR:CZ | 1:B:3899:ASP:HB3 | 2.50 | 0.47 |
| 1:B:1534:PHE:CD2 | 1:B:1537:PHE:CE2 | 3.02 | 0.47 |
| 1:A:1992:LYS:HG2 | 1:A:2024:SER:CB | 2.43 | 0.47 |
| 1:A:2368:PHE:O | 1:A:2369:SER:CB | 2.62 | 0.47 |
| 1:B:2361:ILE:HG22 | 1:B:2367:SER:O | 2.15 | 0.47 |
| 1:A:2578:ILE:HG21 | 1:A:2630:TYR:HB2 | 1.97 | 0.47 |
| 1:B:2941:THR:HG22 | 1:B:2942:ASP:N | 2.30 | 0.47 |
| 1:A:1422:LYS:HA | 1:A:1422:LYS:HD3 | 1.63 | 0.47 |
| 1:B:2734:ILE:HD12 | 1:B:2734:ILE:H | 1.80 | 0.47 |
| 1:A:1998:LEU:HD11 | 1:A:2022:PHE:HZ | 1.79 | 0.47 |
| 1:B:2420:PRO:HD3 | 1:B:2536:ASN:ND2 | 2.25 | 0.47 |
| 1:B:2424:LYS:N | 3:B:5401:ADP:O1B | 2.48 | 0.47 |
| 1:B:3994:TYR:O | 1:B:3998:ILE:HD12 | 2.15 | 0.47 |
| 1:B:3326:ILE:HA | 1:B:3349:LEU:HD21 | 1.96 | 0.47 |
| 1:B:2707:VAL:HG11 | 1:B:2712:LEU:HD12 | 1.97 | 0.47 |
| 1:A:3302:GLU:O | 1:A:3305:ARG:CA | 2.63 | 0.47 |
| 1:B:2111:LYS:HZ2 | 1:B:2161:GLU:HG2 | 1.79 | 0.47 |
| 1:B:1849:GLU:CD | 1:B:1899:ASN:HD22 | 2.18 | 0.47 |
| 1:B:1910:GLU:HB2 | 1:B:3846:MET:HB2 | 1.97 | 0.47 |
| 1:B:1540:LEU:HD11 | 1:B:1548:ILE:HD11 | 1.96 | 0.47 |
| 1:A:2420:PRO:HD3 | 1:A:2536:ASN:HD21 | 1.80 | 0.47 |
| 1:B:2354:SER:OG | 1:B:2357:SER:CB | 2.63 | 0.47 |
| 1:B:2169:VAL:HG13 | 1:B:2186:ILE:HG12 | 1.96 | 0.47 |
| 1:B:4037:SER:HB3 | 1:B:4040:GLU:HB2 | 1.97 | 0.47 |
| 1:A:3718:ALA:O | 1:A:3721:THR:HG22 | 2.15 | 0.47 |
| 1:A:1970:LEU:HD23 | 1:A:1974:LYS:HE3 | 1.97 | 0.46 |
| 1:B:2252:LEU:HD22 | 1:B:2314:ILE:HG13 | 1.97 | 0.46 |
| 1:B:1706:LEU:HD22 | 1:B:1935:GLN:CG | 2.45 | 0.46 |
| 1:B:2819:GLU:O | 1:B:2822:ILE:HG13 | 2.15 | 0.46 |
| 1:A:3956:PHE:CD1 | 1:A:3994:TYR:HD1 | 2.33 | 0.46 |
| 1:B:1620:PHE:CA | 1:B:1760:PHE:CE1 | 2.97 | 0.46 |
| 1:B:2152:VAL:HG12 | 1:B:2154:PHE:CE1 | 2.50 | 0.46 |
| 1:B:4074:GLU:HA | 1:B:4077:GLN:HE21 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1828:TYR:HB2 | 1:B:1857:VAL:HG13 | 1.98 | 0.46 |
| 1:A:3304:GLU:O | 1:A:3307:LEU:N | 2.48 | 0.46 |
| 1:B:2080:LYS:CE | 1:B:2549:ARG:HH21 | 2.28 | 0.46 |
| 1:B:1563:LYS:HA | 1:B:1569:ILE:O | 2.15 | 0.46 |
| 1:A:3509:LEU:O | 1:A:3513:VAL:HG23 | 2.16 | 0.46 |
| 1:A:3844:ILE:HG12 | 1:A:3851:VAL:HG21 | 1.97 | 0.46 |
| 1:B:1611:LEU:O | 1:B:1615:ILE:HG23 | 2.15 | 0.46 |
| 1:A:3945:LEU:HD21 | 1:A:4070:ILE:CD1 | 2.45 | 0.46 |
| 1:B:4023:ILE:CD1 | 1:B:4029:ILE:HD11 | 2.45 | 0.46 |
| 1:A:3624:HIS:ND1 | 1:A:3675:LEU:HD11 | 2.30 | 0.46 |
| 1:A:2856:LEU:HD21 | 1:A:2877:PHE:HB2 | 1.97 | 0.46 |
| 1:B:1646:GLN:OE1 | 1:B:1763:ILE:HG12 | 2.15 | 0.46 |
| 1:B:2732:MET:SD | 3:B:5402:ADP:N7 | 2.89 | 0.46 |
| 1:B:2081:THR:HG22 | 1:B:2085:LYS:HD2 | 1.97 | 0.46 |
| 1:B:2786:ILE:HD12 | 1:B:3460:PRO:CG | 2.46 | 0.46 |
| 1:A:1970:LEU:HD21 | 1:A:1974:LYS:HE2 | 1.97 | 0.46 |
| 1:B:2961:ILE:O | 1:B:2965:VAL:HG23 | 2.14 | 0.46 |
| 1:B:3911:TRP:HH2 | 1:B:3926:VAL:CG1 | 2.28 | 0.46 |
| 1:B:1386:ILE:CG2 | 1:B:1396:ARG:HG2 | 2.46 | 0.46 |
| 1:B:2824:GLU:HG2 | 1:B:2825:THR:H | 1.80 | 0.46 |
| 1:A:3990:ALA:HB2 | 1:A:4011:CYS:SG | 2.56 | 0.46 |
| 1:B:1826:PHE:O | 1:B:1826:PHE:CG | 2.68 | 0.46 |
| 3:A:5401:ADP:H2' | 3:A:5401:ADP:N3 | 2.31 | 0.46 |
| 1:B:2424:LYS:HE2 | 1:B:2424:LYS:HB2 | 1.55 | 0.46 |
| 1:B:2064:GLN:OE1 | 1:B:2065:LYS:HG3 | 2.15 | 0.46 |
| 1:A:2655:ILE:HD11 | 1:A:2747:ARG:HH22 | 1.81 | 0.46 |
| 1:A:2068:GLN:HE22 | 1:A:2188:PRO:HA | 1.81 | 0.46 |
| 1:A:3912:GLY:O | 1:A:3915:PHE:CZ | 2.69 | 0.46 |
| 1:A:4019:ASP:H | 1:A:4031:GLN:HE21 | 1.64 | 0.46 |
| 1:B:1620:PHE:CZ | 1:B:1743:ASP:HB3 | 2.50 | 0.46 |
| 1:B:2220:CYS:SG | 1:B:2224:SER:HB3 | 2.55 | 0.46 |
| 1:B:3737:THR:OG1 | 1:B:3740:THR:CB | 2.63 | 0.46 |
| 1:A:2339:ILE:HG23 | 1:A:2353:LEU:HB3 | 1.97 | 0.46 |
| 1:A:2999:LEU:HD11 | 1:A:3325:ILE:HG12 | 1.97 | 0.46 |
| 1:A:2938:MET:SD | 1:A:3321:ILE:CG2 | 3.03 | 0.46 |
| 1:A:2420:PRO:CG | 1:A:2616:LEU:HD21 | 2.45 | 0.46 |
| 1:B:2302:PHE:HA | 1:B:2310:LEU:HD11 | 1.98 | 0.46 |
| 1:B:3911:TRP:CH2 | 1:B:3926:VAL:HG13 | 2.51 | 0.46 |
| 1:A:1418:SER:O | 1:A:1421:TYR:CD2 | 2.68 | 0.46 |
| 1:A:3566:LEU:CD2 | 1:A:3587:LEU:HD11 | 2.45 | 0.46 |
| 1:A:3839:ILE:HG23 | 1:A:3873:MET:HG3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2219:VAL:HG21 | 2:A:5400:ATP:N7 | 2.31 | 0.46 |
| 1:B:3701:THR:OG1 | 1:B:4085:THR:HG22 | 2.15 | 0.46 |
| 1:A:2581:LEU:HD13 | 1:A:2633:ILE:HG22 | 1.96 | 0.46 |
| 1:B:2081:THR:HB | 2:B:5400:ATP:O2A | 2.15 | 0.46 |
| 1:B:3725:VAL:HG22 | 1:B:3731:ASP:HA | 1.96 | 0.46 |
| 1:B:2080:LYS:HZ1 | 1:B:2549:ARG:CZ | 2.26 | 0.46 |
| 1:B:3367:ILE:O | 1:B:3371:VAL:HG22 | 2.16 | 0.46 |
| 1:A:3728:GLU:CG | 1:A:4079:LYS:HE2 | 2.46 | 0.46 |
| 1:A:1636:ILE:O | 1:A:1640:VAL:HG23 | 2.16 | 0.46 |
| 1:B:1838:ILE:HD11 | 1:B:1845:GLY:CA | 2.46 | 0.46 |
| 1:A:3471:ASN:HB2 | 1:A:3478:THR:HG23 | 1.97 | 0.46 |
| 1:A:23:LEU:O | 1:A:25:GLU:N | 2.49 | 0.46 |
| 1:B:2394:THR:H | 1:B:2397:THR:HB | 1.81 | 0.46 |
| 1:A:1759:LYS:HE3 | 1:A:1761:GLU:OE2 | 2.16 | 0.46 |
| 1:A:2754:GLY:HA3 | 1:A:2886:HIS:CE1 | 2.51 | 0.46 |
| 1:A:2336:ARG:HG2 | 1:A:2355:ASP:OD1 | 2.16 | 0.45 |
| 1:B:1706:LEU:HD11 | 1:B:1936:ILE:HG12 | 1.97 | 0.45 |
| 1:B:2358:THR:HG22 | 1:B:2359:ILE:N | 2.31 | 0.45 |
| 1:A:1644:ILE:O | 1:A:1648:ILE:HG22 | 2.16 | 0.45 |
| 1:B:1366:VAL:CG1 | 1:B:1369:LYS:HE3 | 2.45 | 0.45 |
| 1:A:3459:ASP:OD2 | 1:A:3461:ILE:CG1 | 2.64 | 0.45 |
| 1:A:2763:ARG:HA | 3:A:5402:ADP:C4' | 2.47 | 0.45 |
| 1:B:2856:LEU:HD21 | 1:B:2877:PHE:HB2 | 1.98 | 0.45 |
| 1:B:2473:LEU:HD21 | 1:B:2475:PRO:CG | 2.47 | 0.45 |
| 1:B:2088:ILE:HG12 | 1:B:2151:TRP:CZ2 | 2.51 | 0.45 |
| 1:B:1391:GLY:HA3 | 1:B:1484:LYS:HZ1 | 1.81 | 0.45 |
| 1:B:2336:ARG:CD | 1:B:2355:ASP:OD2 | 2.63 | 0.45 |
| 1:A:2761:ALA:O | 1:A:2892:CYS:HB3 | 2.16 | 0.45 |
| 1:A:2072:LEU:HB3 | 1:A:2215:PHE:HE1 | 1.80 | 0.45 |
| 1:B:65:THR:O | 1:B:66:GLN:CB | 2.64 | 0.45 |
| 1:A:3373:LEU:HD13 | 1:A:3557:LEU:CD1 | 2.47 | 0.45 |
| 1:B:1620:PHE:HB2 | 1:B:1760:PHE:CE1 | 2.51 | 0.45 |
| 1:A:1968:PHE:CD1 | 1:A:1968:PHE:N | 2.84 | 0.45 |
| 1:A:1392:LEU:CD1 | 1:A:1392:LEU:C | 2.84 | 0.45 |
| 1:B:3683:TYR:O | 1:B:3687:SER:HB2 | 2.16 | 0.45 |
| 1:B:216:PRO:HA | 1:B:1365:PHE:HA | 1.98 | 0.45 |
| 1:B:1998:LEU:CD1 | 1:B:2022:PHE:HZ | 2.29 | 0.45 |
| 1:B:2332:GLY:HA2 | 1:B:2335:GLN:CB | 2.38 | 0.45 |
| 1:A:2445:PHE:HA | 1:A:2449:THR:HG21 | 1.97 | 0.45 |
| 1:B:2068:GLN:HA | 1:B:2191:ARG:HG2 | 1.98 | 0.45 |
| 1:A:2893:ASP:HA | 1:A:2894:PRO:HD2 | 1.89 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2008:ASP:HA | 1:B:2011:GLU:HB2 | 1.99 | 0.45 |
| 1:A:2853:LEU:HD21 | 1:A:2870:GLU:HG3 | 1.98 | 0.45 |
| 1:B:40:TRP:O | 1:B:44:LYS:N | 2.50 | 0.45 |
| 1:A:3636:GLY:CA | 1:A:3642:TYR:O | 2.64 | 0.45 |
| 1:B:3525:ILE:CD1 | 1:B:3646:ILE:HG22 | 2.16 | 0.45 |
| 1:A:2788:ARG:HB2 | 1:A:3459:ASP:HB3 | 1.99 | 0.45 |
| 1:A:2786:ILE:HD12 | 1:A:3460:PRO:CG | 2.47 | 0.45 |
| 1:A:3509:LEU:CD1 | 1:A:3513:VAL:CG2 | 2.94 | 0.45 |
| 1:B:2034:ILE:CD1 | 1:B:2061:TYR:CE2 | 3.00 | 0.45 |
| 1:A:2982:VAL:CG1 | 1:A:2983:GLY:H | 2.29 | 0.45 |
| 1:B:2249:LEU:HA | 1:B:2252:LEU:HD12 | 1.99 | 0.45 |
| 1:B:2230:LEU:HD23 | 1:B:2288:VAL:HG13 | 1.98 | 0.45 |
| 1:B:2467:THR:O | 1:B:2471:LEU:N | 2.48 | 0.45 |
| 1:B:4084:SER:O | 1:B:4088:LEU:HG | 2.17 | 0.45 |
| 1:A:2039:LYS:HG2 | 1:A:2049:MET:HG3 | 1.98 | 0.45 |
| 1:A:1995:VAL:HG22 | 1:A:2022:PHE:HD2 | 1.80 | 0.45 |
| 1:B:3509:LEU:HD12 | 1:B:3513:VAL:HG21 | 1.98 | 0.45 |
| 1:B:2476:LYS:HE3 | 1:B:2528:ARG:CB | 2.47 | 0.45 |
| 1:A:1540:LEU:HD23 | 1:A:1540:LEU:HA | 1.73 | 0.45 |
| 1:B:2745:ILE:HG12 | 1:B:2756:MET:HE3 | 1.97 | 0.45 |
| 1:B:2181:GLY:C | 1:B:2182:GLU:HG3 | 2.36 | 0.45 |
| 1:B:3631:MET:HE1 | 1:B:3698:MET:HG3 | 1.99 | 0.45 |
| 1:A:2034:ILE:CD1 | 1:A:2061:TYR:CE2 | 2.99 | 0.45 |
| 1:A:2708:ASN:O | 1:A:2712:LEU:HD13 | 2.17 | 0.45 |
| 1:A:3306:TRP:CH2 | 1:A:3594:ALA:HB1 | 2.45 | 0.45 |
| 1:A:1956:LEU:HB3 | 1:A:1968:PHE:CD2 | 2.51 | 0.45 |
| 1:A:2241:LEU:HD21 | 1:A:2249:LEU:HD12 | 1.99 | 0.45 |
| 1:A:2034:ILE:HD12 | 1:A:2061:TYR:CE2 | 2.52 | 0.45 |
| 1:B:2941:THR:CG2 | 1:B:2942:ASP:H | 2.29 | 0.45 |
| 1:B:2941:THR:HG22 | 1:B:2942:ASP:H | 1.81 | 0.45 |
| 1:B:2609:THR:HA | 1:B:2612:GLN:O | 2.17 | 0.45 |
| 1:B:3470:PHE:CE1 | 1:B:3488:VAL:HG21 | 2.52 | 0.45 |
| 1:B:2695:LEU:HD23 | 1:B:2743:LEU:HD11 | 1.99 | 0.45 |
| 1:B:2795:PHE:CE2 | 1:B:2799:LEU:HD11 | 2.51 | 0.45 |
| 1:B:1536:ARG:HD3 | 1:B:1841:ILE:HD13 | 1.98 | 0.45 |
| 1:A:1416:LYS:CA | 1:A:1421:TYR:OH | 2.65 | 0.45 |
| 1:B:2285:GLU:HB2 | 1:B:2412:ARG:NH2 | 2.32 | 0.45 |
| 1:B:2786:ILE:O | 1:B:3460:PRO:HB2 | 2.17 | 0.45 |
| 1:A:3505:ILE:O | 1:A:3510:ARG:NH1 | 2.50 | 0.45 |
| 1:A:2152:VAL:HG12 | 1:A:2154:PHE:CE1 | 2.51 | 0.45 |
| 1:A:1646:GLN:OE1 | 1:A:1762:TYR:HD1 | 2.00 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2653:TRP:HB3 | 1:A:2654:ARG:NH1 | 2.31 | 0.45 |
| 1:A:3592:LYS:O | 1:A:3596:ASN:N | 2.50 | 0.45 |
| 1:B:2780:LYS:HD3 | 1:B:2813:THR:HG22 | 1.99 | 0.45 |
| 1:B:4018:SER:O | 1:B:4019:ASP:HB2 | 2.17 | 0.45 |
| 1:B:2091:MET:CE | 1:B:2149:ARG:NH1 | 2.80 | 0.45 |
| 1:B:2960:THR:CG2 | 1:B:2961:ILE:N | 2.80 | 0.45 |
| 1:B:3330:TYR:OH | 1:B:3346:LEU:HD13 | 2.16 | 0.45 |
| 1:B:2822:ILE:O | 1:B:2822:ILE:HG13 | 2.17 | 0.45 |
| 1:A:3002:LEU:HD21 | 1:A:3370:LEU:HD11 | 1.99 | 0.45 |
| 1:A:4033:LEU:HD12 | 1:A:4035:GLN:H | 1.82 | 0.44 |
| 1:B:1945:LEU:HD13 | 1:B:1994:VAL:HG21 | 1.99 | 0.44 |
| 1:B:1421:TYR:O | 1:B:1425:GLU:CA | 2.65 | 0.44 |
| 1:B:1967:HIS:NE2 | 1:B:2204:PRO:HB3 | 2.31 | 0.44 |
| 1:A:3671:VAL:HA | 1:A:3674:ILE:HG22 | 1.99 | 0.44 |
| 1:A:2764:THR:HG21 | 1:A:2917:MET:HB3 | 1.99 | 0.44 |
| 1:B:1660:VAL:HG13 | 1:B:1728:TRP:CH2 | 2.51 | 0.44 |
| 1:A:3338:ASN:HB2 | 1:A:3341:GLU:HG2 | 1.99 | 0.44 |
| 1:A:3737:THR:OG1 | 1:A:3740:THR:CB | 2.63 | 0.44 |
| 1:A:2635:THR:O | 1:A:2704:PHE:N | 2.40 | 0.44 |
| 1:B:1527:LEU:HD21 | 1:B:1546:LEU:HD21 | 1.98 | 0.44 |
| 1:B:2757:MET:HB2 | 1:B:2889:PHE:HB2 | 1.98 | 0.44 |
| 1:A:2042:GLY:HA3 | 1:A:2049:MET:CE | 2.46 | 0.44 |
| 1:B:3632:LEU:HD13 | 1:B:3644:ILE:HD13 | 1.98 | 0.44 |
| 1:B:2838:ALA:HB3 | 1:B:2878:VAL:HG13 | 1.99 | 0.44 |
| 1:A:2565:LYS:O | 1:A:2569:GLN:HG3 | 2.16 | 0.44 |
| 1:B:1365:PHE:HE1 | 1:B:1366:VAL:HG21 | 1.81 | 0.44 |
| 1:B:1421:TYR:CD1 | 1:B:1425:GLU:CG | 2.99 | 0.44 |
| 1:B:2517:LYS:NZ | 1:B:2520:GLU:OE1 | 2.50 | 0.44 |
| 1:A:2048:SER:O | 2:A:5400:ATP:N6 | 2.45 | 0.44 |
| 1:A:1748:PHE:CE2 | 1:A:1755:LEU:HD22 | 2.52 | 0.44 |
| 1:B:4020:ASN:HD22 | 1:B:4028:ARG:HB3 | 1.82 | 0.44 |
| 1:B:1646:GLN:NE2 | 1:B:1758:TYR:OH | 2.50 | 0.44 |
| 1:A:1416:LYS:O | 1:A:1421:TYR:HE2 | 2.01 | 0.44 |
| 1:A:1995:VAL:HG21 | 1:A:2024:SER:CB | 2.44 | 0.44 |
| 1:B:3946:VAL:HB | 1:B:3947:PRO:HA | 2.00 | 0.44 |
| 1:A:2839:ASP:O | 1:A:2841:PRO:HD3 | 2.17 | 0.44 |
| 1:B:3979:ASN:C | 1:B:3981:PRO:CD | 2.85 | 0.44 |
| 1:A:1620:PHE:CB | 1:A:1760:PHE:CE1 | 3.00 | 0.44 |
| 1:A:1575:LEU:O | 1:A:1576:GLU:HB3 | 2.16 | 0.44 |
| 1:A:1392:LEU:HD13 | 1:A:1393:LYS:CA | 2.48 | 0.44 |
| 1:A:2623:THR:HG21 | 3:A:5401:ADP:O2' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2728:LEU:HG | 1:B:2771:ARG:HH22 | 1.81 | 0.44 |
| 1:B:3631:MET:HE3 | 1:B:3698:MET:HG3 | 1.98 | 0.44 |
| 1:B:2385:VAL:HG23 | 1:B:2574:TYR:HD1 | 1.82 | 0.44 |
| 1:B:1735:TYR:HB2 | 1:B:1748:PHE:CZ | 2.53 | 0.44 |
| 1:A:2761:ALA:O | 1:A:2892:CYS:SG | 2.75 | 0.44 |
| 1:A:2354:SER:OG | 1:A:2357:SER:HB2 | 2.17 | 0.44 |
| 1:B:2640:THR:HG23 | 1:B:2643:SER:H | 1.83 | 0.44 |
| 1:A:2122:THR:O | 1:A:2123:LEU:C | 2.55 | 0.44 |
| 1:B:3348:ILE:HA | 1:B:3351:ARG:HG2 | 1.99 | 0.44 |
| 1:B:3708:PHE:HZ | 1:B:3720:LEU:HD21 | 1.82 | 0.44 |
| 1:A:3919:LYS:HG3 | 1:A:3919:LYS:O | 2.18 | 0.44 |
| 1:B:2733:VAL:H | 3:B:5402:ADP:N6 | 2.16 | 0.44 |
| 1:A:3305:ARG:HD3 | 1:A:3305:ARG:HA | 1.42 | 0.44 |
| 1:B:1980:CYS:O | 1:B:1983:LEU:HB3 | 2.17 | 0.44 |
| 1:A:2745:ILE:HG12 | 1:A:2756:MET:CE | 2.44 | 0.44 |
| 1:B:3407:LEU:HD23 | 1:B:3518:PHE:CE2 | 2.52 | 0.44 |
| 1:A:4024:VAL:HG23 | 1:A:4027:VAL:HB | 2.00 | 0.44 |
| 1:B:1969:GLY:O | 1:B:1972:THR:HB | 2.17 | 0.44 |
| 1:A:3772:TRP:HZ3 | 1:A:3780:ASN:HD22 | 1.66 | 0.44 |
| 1:A:2111:LYS:CD | 1:A:2161:GLU:CG | 2.87 | 0.44 |
| 1:A:1849:GLU:CD | 1:A:1899:ASN:ND2 | 2.70 | 0.44 |
| 1:B:2786:ILE:HD13 | 1:B:2823:LEU:HD11 | 1.98 | 0.44 |
| 1:A:1681:LYS:HE2 | 1:A:1939:PHE:CZ | 2.53 | 0.44 |
| 1:A:2936:ILE:HG22 | 1:A:2962:ARG:HD3 | 1.99 | 0.44 |
| 1:A:3785:TYR:CD2 | 1:A:3785:TYR:N | 2.85 | 0.44 |
| 1:A:2099:ASN:HD22 | 1:A:2151:TRP:HE1 | 1.66 | 0.44 |
| 1:B:1900:PRO:HB3 | 1:B:1905:ARG:HA | 1.99 | 0.44 |
| 1:A:3703:PHE:CE1 | 1:A:3766:GLU:HG2 | 2.53 | 0.44 |
| 1:B:1365:PHE:O | 1:B:1366:VAL:C | 2.56 | 0.44 |
| 1:B:1536:ARG:HD3 | 1:B:1536:ARG:HA | 1.78 | 0.44 |
| 1:B:1926:SER:HA | 1:B:1970:LEU:CD1 | 2.48 | 0.44 |
| 1:B:2080:LYS:HZ1 | 1:B:2549:ARG:HE | 1.65 | 0.44 |
| 1:A:1806:VAL:HG11 | 1:A:1846:CYS:HB2 | 1.99 | 0.44 |
| 1:A:1650:LEU:HD11 | 1:A:1747:VAL:HG11 | 1.99 | 0.44 |
| 1:A:2654:ARG:NH1 | 1:A:2658:ASP:OD1 | 2.51 | 0.44 |
| 1:B:4022:GLN:HA | 1:B:4028:ARG:HA | 2.00 | 0.44 |
| 1:B:2673:LEU:HD23 | 1:B:2689:ILE:HG23 | 2.00 | 0.44 |
| 1:B:2473:LEU:HD11 | 1:B:2527:GLU:HG3 | 1.98 | 0.43 |
| 1:B:2707:VAL:HG11 | 1:B:2712:LEU:CD1 | 2.46 | 0.43 |
| 1:A:1983:LEU:HD13 | 1:A:2000:ARG:HE | 1.82 | 0.43 |
| 1:B:1645:PHE:HZ | 1:B:1768:ARG:HD2 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3461:ILE:C | 1:A:3463:SER:N | 2.71 | 0.43 |
| 1:A:2177:THR:HG22 | 1:A:2183:ARG:HG2 | 1.99 | 0.43 |
| 1:B:3407:LEU:HD23 | 1:B:3518:PHE:HE2 | 1.83 | 0.43 |
| 1:A:2084:TRP:CH2 | 1:A:2153:VAL:HG21 | 2.53 | 0.43 |
| 1:A:2039:LYS:O | 1:A:2043:GLN:HG2 | 2.17 | 0.43 |
| 1:B:2738:MET:HG2 | 1:B:2769:LEU:HD21 | 1.99 | 0.43 |
| 1:B:3443:ALA:HB1 | 1:B:3450:VAL:CG2 | 2.48 | 0.43 |
| 1:B:3024:LEU:HD13 | 1:B:3303:LYS:HG3 | 1.91 | 0.43 |
| 1:A:1459:LEU:HD23 | 1:A:1465:ILE:HG13 | 1.99 | 0.43 |
| 1:B:3566:LEU:CA | 1:B:3583:LEU:HD21 | 2.48 | 0.43 |
| 1:A:2201:HIS:CE1 | 1:A:2497:TYR:CA | 3.01 | 0.43 |
| 1:A:1963:MET:HG2 | 1:A:1965:HIS:CE1 | 2.53 | 0.43 |
| 1:B:2476:LYS:HZ1 | 1:B:2528:ARG:HD2 | 1.81 | 0.43 |
| 1:A:3407:LEU:HD23 | 1:A:3518:PHE:CE2 | 2.53 | 0.43 |
| 1:B:2754:GLY:HA3 | 1:B:2886:HIS:ND1 | 2.32 | 0.43 |
| 1:B:3579:GLU:O | 1:B:3582:GLU:N | 2.44 | 0.43 |
| 1:B:2473:LEU:HD22 | 1:B:2475:PRO:CD | 2.30 | 0.43 |
| 1:B:3303:LYS:CA | 1:B:3306:TRP:CD1 | 2.86 | 0.43 |
| 1:A:1497:ILE:O | 1:A:1500:ILE:HG12 | 2.18 | 0.43 |
| 1:B:3544:LYS:O | 1:B:3548:LEU:HB2 | 2.17 | 0.43 |
| 1:B:2571:TYR:HA | 1:B:2574:TYR:HB2 | 1.99 | 0.43 |
| 1:B:2060:PHE:HD2 | 1:B:2087:VAL:HG11 | 1.83 | 0.43 |
| 1:A:2225:LYS:HD2 | 1:A:2281:PHE:CZ | 2.54 | 0.43 |
| 1:B:2027:THR:HA | 1:B:2028:PRO:HD3 | 1.76 | 0.43 |
| 1:B:1636:ILE:O | 1:B:1640:VAL:HG23 | 2.19 | 0.43 |
| 1:A:1866:GLN:O | 1:A:1870:ASN:HB2 | 2.18 | 0.43 |
| 1:B:2084:TRP:CZ3 | 1:B:2085:LYS:HG3 | 2.53 | 0.43 |
| 1:B:2080:LYS:HZ1 | 1:B:2549:ARG:NH2 | 2.11 | 0.43 |
| 1:A:3815:PRO:O | 1:A:3821:ASN:HB3 | 2.17 | 0.43 |
| 1:A:2761:ALA:O | 1:A:2892:CYS:CB | 2.66 | 0.43 |
| 1:B:1616:LYS:HE3 | 1:B:1761:GLU:HG3 | 2.01 | 0.43 |
| 1:B:1924:PRO:CB | 1:B:1929:ILE:HD11 | 2.37 | 0.43 |
| 1:A:1991:GLU:O | 1:A:1994:VAL:HB | 2.19 | 0.43 |
| 1:A:1392:LEU:N | 1:A:1484:LYS:HE2 | 2.33 | 0.43 |
| 1:B:3330:TYR:CZ | 1:B:3346:LEU:HD13 | 2.54 | 0.43 |
| 1:A:3877:CYS:SG | 1:A:3884:LEU:HD22 | 2.59 | 0.43 |
| 1:A:3544:LYS:HE3 | 1:A:3607:PHE:CD1 | 2.54 | 0.43 |
| 1:A:1469:LEU:HD13 | 1:A:1523:LEU:CD2 | 2.49 | 0.43 |
| 1:A:2581:LEU:HD11 | 1:A:2634:ASN:HD22 | 1.84 | 0.43 |
| 1:A:1987:PHE:HB3 | 1:A:1988:GLY:H | 1.69 | 0.43 |
| 1:B:2733:VAL:N | 3:B:5402:ADP:C6 | 2.80 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1926:SER:HB2 | 1:B:1973:LEU:HD21 | 2.00 | 0.43 |
| 1:B:1898:LEU:HD11 | 1:B:1908:LEU:CD2 | 2.49 | 0.43 |
| 1:B:2780:LYS:HB3 | 1:B:2813:THR:HG22 | 2.00 | 0.43 |
| 1:A:3911:TRP:HH2 | 1:A:3926:VAL:CG1 | 2.32 | 0.43 |
| 1:B:2160:PRO:O | 1:B:2164:GLU:HG3 | 2.18 | 0.43 |
| 1:A:3696:MET:SD | 1:A:3760:LEU:HB3 | 2.58 | 0.43 |
| 1:B:1945:LEU:HD21 | 1:B:1991:GLU:CB | 2.49 | 0.43 |
| 1:B:2581:LEU:HD11 | 1:B:2634:ASN:HD22 | 1.82 | 0.43 |
| 1:A:1689:LYS:HG3 | 1:A:1689:LYS:O | 2.19 | 0.43 |
| 1:B:1365:PHE:O | 1:B:1367:ILE:N | 2.52 | 0.43 |
| 1:B:2464:TYR:CE2 | 1:B:2474:LEU:HD12 | 2.54 | 0.43 |
| 1:A:2707:VAL:HG12 | 1:A:2712:LEU:CD1 | 2.49 | 0.43 |
| 1:A:4033:LEU:CD1 | 1:A:4036:GLN:H | 2.32 | 0.43 |
| 1:A:1998:LEU:CD1 | 1:A:2022:PHE:CZ | 3.02 | 0.43 |
| 1:B:2154:PHE:CD1 | 1:B:2154:PHE:N | 2.86 | 0.43 |
| 1:A:3934:TRP:CB | 1:A:4023:ILE:HD13 | 2.49 | 0.43 |
| 1:A:2356:TYR:O | 1:A:2372:CYS:HB2 | 2.19 | 0.43 |
| 1:B:3978:ASN:ND2 | 1:B:3980:ILE:HG22 | 2.34 | 0.43 |
| 1:A:2354:SER:OG | 1:A:2357:SER:CB | 2.67 | 0.43 |
| 1:B:2759:ILE:HG21 | 1:B:2916:TRP:CZ2 | 2.54 | 0.43 |
| 1:A:1871:GLY:HA3 | 1:A:1879:ILE:HG21 | 2.01 | 0.43 |
| 1:A:3618:TYR:O | 1:A:3622:GLY:N | 2.51 | 0.43 |
| 1:B:1704:GLU:OE2 | 1:B:1768:ARG:NH1 | 2.52 | 0.43 |
| 1:B:2080:LYS:CE | 2:B:5400:ATP:O1B | 2.60 | 0.43 |
| 1:B:1910:GLU:HB2 | 1:B:3846:MET:CA | 2.48 | 0.43 |
| 1:B:3833:LYS:NZ | 1:B:3862:THR:HG21 | 2.34 | 0.43 |
| 1:A:3924:TRP:O | 1:A:3927:TYR:HB3 | 2.18 | 0.43 |
| 1:A:2437:LEU:HD12 | 1:A:2437:LEU:H | 1.84 | 0.43 |
| 1:A:2514:GLY:HA3 | 1:A:2525:THR:HA | 2.01 | 0.43 |
| 1:A:1744:LEU:HD22 | 1:A:1760:PHE:CG | 2.54 | 0.42 |
| 1:A:2763:ARG:HA | 1:A:2763:ARG:HD2 | 1.55 | 0.42 |
| 1:A:2141:ILE:HG22 | 1:A:2145:PHE:CG | 2.54 | 0.42 |
| 1:A:1574:PHE:HB3 | 1:A:1576:GLU:N | 2.24 | 0.42 |
| 1:A:2506:LEU:HA | 1:A:2509:LEU:HD12 | 2.01 | 0.42 |
| 1:B:3848:LEU:O | 1:B:3849:SER:C | 2.57 | 0.42 |
| 1:B:2764:THR:HG22 | 1:B:2765:GLY:N | 2.34 | 0.42 |
| 1:A:1365:PHE:CG | 1:A:1366:VAL:N | 2.86 | 0.42 |
| 1:B:2707:VAL:CB | 1:B:2712:LEU:CD1 | 2.76 | 0.42 |
| 1:B:1770:ILE:HD13 | 1:B:1770:ILE:HA | 1.93 | 0.42 |
| 1:B:2783:GLN:HG2 | 1:B:2816:ILE:HB | 2.01 | 0.42 |
| 1:A:1826:PHE:CE1 | 1:A:1830:VAL:HG13 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1940:GLU:HG3 | 1:B:1941:ASP:N | 2.33 | 0.42 |
| 1:A:3978:ASN:O | 1:A:3981:PRO:CD | 2.67 | 0.42 |
| 1:A:1539:PHE:N | 1:A:1539:PHE:CD1 | 2.87 | 0.42 |
| 1:A:1367:ILE:H | 1:A:1367:ILE:HD12 | 1.83 | 0.42 |
| 1:B:2021:ILE:HG22 | 1:B:2022:PHE:HD1 | 1.83 | 0.42 |
| 1:B:2111:LYS:CD | 1:B:2161:GLU:CG | 2.85 | 0.42 |
| 1:A:1421:TYR:HE1 | 1:A:1425:GLU:OE2 | 2.02 | 0.42 |
| 1:B:1939:PHE:CD2 | 1:B:1939:PHE:N | 2.87 | 0.42 |
| 1:A:2106:THR:H | 1:A:2156:SER:HB2 | 1.84 | 0.42 |
| 1:A:1981:SER:CB | 1:A:1982:PRO:HD3 | 2.45 | 0.42 |
| 1:B:2889:PHE:CD1 | 1:B:2902:MET:HE1 | 2.54 | 0.42 |
| 1:A:2507:ARG:HB2 | 1:A:2550:PHE:HB2 | 2.01 | 0.42 |
| 1:B:1977:LEU:O | 1:B:1980:CYS:HB3 | 2.20 | 0.42 |
| 1:A:3946:VAL:HA | 1:A:3947:PRO:C | 2.39 | 0.42 |
| 1:A:2021:ILE:HG22 | 1:A:2022:PHE:HD1 | 1.84 | 0.42 |
| 1:B:3584:MET:HA | 1:B:3587:LEU:HB2 | 1.99 | 0.42 |
| 1:A:3810:SER:HB3 | 1:A:3837:GLY:HA2 | 2.02 | 0.42 |
| 1:B:1497:ILE:O | 1:B:1500:ILE:HG12 | 2.20 | 0.42 |
| 1:B:2158:LEU:HD13 | 1:B:2202:THR:HB | 2.02 | 0.42 |
| 1:B:2386:MET:HB3 | 1:B:2627:ARG:CD | 2.39 | 0.42 |
| 1:A:1743:ASP:HA | 1:A:1746:SER:HB3 | 2.00 | 0.42 |
| 1:A:1421:TYR:O | 1:A:1425:GLU:HB3 | 2.18 | 0.42 |
| 1:B:2080:LYS:CE | 2:B:5400:ATP:O3G | 2.67 | 0.42 |
| 1:B:2099:ASN:HA | 1:B:2149:ARG:O | 2.20 | 0.42 |
| 1:B:3846:MET:HG3 | 1:B:3847:SER:N | 2.34 | 0.42 |
| 1:B:3519:VAL:CG1 | 1:B:3521:ASN:ND2 | 2.82 | 0.42 |
| 1:B:3671:VAL:HA | 1:B:3674:ILE:HG22 | 2.01 | 0.42 |
| 1:B:3612:ASP:O | 1:B:3615:VAL:CG2 | 2.67 | 0.42 |
| 1:A:2109:LEU:HD12 | 1:A:2129:LEU:HD23 | 2.01 | 0.42 |
| 1:A:2512:LYS:O | 1:A:2513:GLN:CB | 2.68 | 0.42 |
| 1:A:3934:TRP:HB3 | 1:A:4023:ILE:HD13 | 2.01 | 0.42 |
| 1:A:3321:ILE:HD12 | 1:A:3321:ILE:H | 1.84 | 0.42 |
| 1:B:2159:ASP:HB2 | 1:B:2160:PRO:HD2 | 2.01 | 0.42 |
| 1:B:2893:ASP:HA | 1:B:2894:PRO:HD2 | 1.96 | 0.42 |
| 1:A:2707:VAL:HG12 | 1:A:2712:LEU:HD12 | 2.02 | 0.42 |
| 1:A:1681:LYS:HE2 | 1:A:1939:PHE:HZ | 1.84 | 0.42 |
| 1:A:2476:LYS:N | 1:A:2476:LYS:HD3 | 2.31 | 0.42 |
| 1:A:2175:ILE:HG13 | 1:A:2184:LEU:C | 2.39 | 0.42 |
| 1:B:3843:ASN:O | 1:B:3846:MET:HG2 | 2.19 | 0.42 |
| 1:A:3799:LYS:HG3 | 1:A:3803:LEU:HD11 | 2.02 | 0.42 |
| 1:A:2060:PHE:CZ | 1:A:2193:LEU:HD21 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2356:TYR:CE1 | 1:A:2399:LYS:HD2 | 2.54 | 0.42 |
| 1:A:3353:LEU:HD23 | 1:A:3358:VAL:HG11 | 2.02 | 0.42 |
| 1:A:3968:LEU:HA | 1:A:3971:VAL:HG12 | 2.02 | 0.42 |
| 1:A:1914:LYS:HD3 | 1:A:3959:CYS:SG | 2.60 | 0.42 |
| 1:A:216:PRO:CB | 1:A:1365:PHE:N | 2.83 | 0.42 |
| 1:B:2787:HIS:HB3 | 1:B:3461:ILE:HG23 | 2.01 | 0.42 |
| 1:B:2034:ILE:HD12 | 1:B:2061:TYR:CE2 | 2.54 | 0.42 |
| 1:A:1622:GLN:HE22 | 1:A:1644:ILE:H | 1.67 | 0.42 |
| 1:B:2071:ILE:HB | 1:B:2212:LEU:HD12 | 2.01 | 0.42 |
| 1:A:2582:VAL:O | 1:A:2582:VAL:HG23 | 2.20 | 0.42 |
| 1:A:2707:VAL:CB | 1:A:2712:LEU:CD1 | 2.72 | 0.42 |
| 1:A:3302:GLU:O | 1:A:3306:TRP:N | 2.49 | 0.42 |
| 1:B:1645:PHE:HB2 | 1:B:1697:LYS:HG3 | 2.02 | 0.42 |
| 1:A:1874:VAL:HG21 | 1:A:1876:LYS:NZ | 2.34 | 0.42 |
| 1:A:2412:ARG:HH11 | 1:A:2555:ALA:HB2 | 1.85 | 0.42 |
| 1:B:2082:ALA:N | 2:B:5400:ATP:O2A | 2.53 | 0.42 |
| 1:A:4023:ILE:HD12 | 1:A:4029:ILE:HD11 | 2.01 | 0.42 |
| 1:A:3839:ILE:HG22 | 1:A:3873:MET:HA | 2.02 | 0.42 |
| 1:B:2178:LEU:HD12 | 1:B:2182:GLU:HB2 | 2.02 | 0.42 |
| 1:A:3830:SER:HA | 1:A:3833:LYS:HE3 | 2.02 | 0.42 |
| 1:A:2081:THR:HG22 | 1:A:2085:LYS:HD2 | 2.01 | 0.42 |
| 1:B:2415:ILE:O | 1:B:2556:ILE:HA | 2.20 | 0.42 |
| 1:A:3636:GLY:HA2 | 1:A:3642:TYR:O | 2.20 | 0.42 |
| 1:A:2847:GLU:HG3 | 1:A:2848:GLU:N | 2.34 | 0.42 |
| 1:A:3327:SER:O | 1:A:3331:GLU:HG3 | 2.20 | 0.42 |
| 1:A:3566:LEU:HD11 | 1:A:3570:LEU:HD11 | 1.99 | 0.41 |
| 1:A:3555:TYR:HB3 | 1:A:3597:ILE:HD11 | 2.02 | 0.41 |
| 1:B:2852:LEU:O | 1:B:2856:LEU:HB2 | 2.20 | 0.41 |
| 1:B:4019:ASP:O | 1:B:4030:PRO:HA | 2.19 | 0.41 |
| 1:B:1664:LEU:O | 1:B:1721:LYS:HE3 | 2.19 | 0.41 |
| 1:A:1625:ASP:O | 1:A:1629:GLN:HG3 | 2.19 | 0.41 |
| 1:B:3413:HIS:O | 1:B:3417:VAL:HG23 | 2.20 | 0.41 |
| 1:A:3903:ILE:O | 1:A:3907:VAL:HG23 | 2.20 | 0.41 |
| 1:B:2222:ILE:H | 1:B:2222:ILE:HG13 | 1.67 | 0.41 |
| 1:A:2701:SER:HB2 | 1:A:2703:ASP:O | 2.20 | 0.41 |
| 1:B:1531:ARG:CD | 1:B:1538:TYR:HA | 2.50 | 0.41 |
| 1:B:1534:PHE:HD2 | 1:B:1537:PHE:CD2 | 2.38 | 0.41 |
| 1:B:3466:ILE:HD13 | 1:B:3509:LEU:HD13 | 2.02 | 0.41 |
| 1:B:1392:LEU:HD13 | 1:B:1393:LYS:CA | 2.49 | 0.41 |
| 1:A:1542:ASN:O | 1:A:1546:LEU:HG | 2.20 | 0.41 |
| 1:A:4024:VAL:HG11 | 1:A:4062:TRP:CD2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2197:ASP:HB3 | 1:A:2549:ARG:HD2 | 2.02 | 0.41 |
| 1:A:3850:TRP:NE1 | 1:A:3854:TYR:HB3 | 2.35 | 0.41 |
| 1:A:2575:TYR:HD1 | 1:A:2578:ILE:HD11 | 1.85 | 0.41 |
| 1:B:3471:ASN:HB2 | 1:B:3478:THR:HG23 | 2.01 | 0.41 |
| 1:A:2828:LEU:HD11 | 1:A:2908:LEU:HD11 | 2.01 | 0.41 |
| 1:A:3319:GLU:HA | 1:A:3359:LYS:O | 2.20 | 0.41 |
| 1:B:2091:MET:HE3 | 1:B:2149:ARG:NH1 | 2.35 | 0.41 |
| 1:A:1956:LEU:CB | 1:A:1968:PHE:CD2 | 3.04 | 0.41 |
| 1:A:1967:HIS:C | 1:A:1968:PHE:CD1 | 2.87 | 0.41 |
| 1:A:1392:LEU:HD22 | 1:A:1393:LYS:H | 1.86 | 0.41 |
| 1:A:3330:TYR:CE1 | 1:A:3334:PHE:CE2 | 3.08 | 0.41 |
| 1:B:3645:SER:CB | 1:B:3890:GLN:NE2 | 2.80 | 0.41 |
| 1:A:4023:ILE:HD13 | 1:A:4023:ILE:HG21 | 1.70 | 0.41 |
| 1:A:3631:MET:HE2 | 1:A:3632:LEU:HG | 2.02 | 0.41 |
| 1:B:2493:LYS:HD2 | 1:B:2493:LYS:HA | 1.81 | 0.41 |
| 1:A:1534:PHE:HD2 | 1:A:1537:PHE:CE2 | 2.38 | 0.41 |
| 1:B:2220:CYS:SG | 2:B:5400:ATP:N1 | 2.89 | 0.41 |
| 1:A:2339:ILE:HG23 | 1:A:2353:LEU:HD23 | 2.03 | 0.41 |
| 1:B:3519:VAL:CG1 | 1:B:3521:ASN:HD21 | 2.33 | 0.41 |
| 1:A:2095:ASP:CG | 1:A:2149:ARG:HH21 | 2.23 | 0.41 |
| 1:A:3612:ASP:C | 1:A:3615:VAL:HG22 | 2.41 | 0.41 |
| 1:B:3464:ARG:O | 1:B:3467:SER:O | 2.37 | 0.41 |
| 1:A:2929:ALA:O | 1:A:2933:VAL:HG22 | 2.21 | 0.41 |
| 1:A:54:LEU:HA | 1:A:55:PRO:HA | 1.83 | 0.41 |
| 1:A:3951:SER:HB2 | 1:A:4002:LYS:HD2 | 2.02 | 0.41 |
| 1:A:1744:LEU:HD22 | 1:A:1760:PHE:CD2 | 2.54 | 0.41 |
| 1:A:1826:PHE:HE2 | 1:A:1831:LEU:CB | 2.05 | 0.41 |
| 1:A:1951:HIS:HD2 | 1:A:2021:ILE:HD12 | 1.84 | 0.41 |
| 1:B:3939:ILE:HG23 | 1:B:3950:PHE:HE2 | 1.86 | 0.41 |
| 1:A:3995:GLY:HA2 | 1:A:3998:ILE:CD1 | 2.50 | 0.41 |
| 1:A:2474:LEU:HB3 | 1:A:2526:ILE:HG22 | 2.01 | 0.41 |
| 1:B:1469:LEU:HD13 | 1:B:1523:LEU:HD21 | 2.01 | 0.41 |
| 1:B:1838:ILE:HD11 | 1:B:1845:GLY:N | 2.35 | 0.41 |
| 1:B:2866:LEU:HD12 | 1:B:2867:LEU:H | 1.84 | 0.41 |
| 1:A:1727:LEU:O | 1:A:1731:VAL:HG23 | 2.20 | 0.41 |
| 1:A:1660:VAL:HG13 | 1:A:1728:TRP:CH2 | 2.55 | 0.41 |
| 1:A:2754:GLY:HA3 | 1:A:2886:HIS:ND1 | 2.36 | 0.41 |
| 1:B:1593:ASN:HD21 | 1:B:1621:THR:CB | 2.31 | 0.41 |
| 1:B:3832:SER:O | 1:B:3836:GLY:N | 2.49 | 0.41 |
| 1:A:2378:VAL:HG11 | 1:A:2392:ILE:HD12 | 2.02 | 0.41 |
| 1:B:3311:LYS:HG2 | 1:B:3315:LYS:NZ | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2476:LYS:HB3 | 1:A:2482:LEU:HB2 | 2.02 | 0.41 |
| 1:A:1495:THR:HB | 1:A:1498:GLU:HB2 | 2.01 | 0.41 |
| 1:A:3692:LYS:HG3 | 1:A:3898:GLU:HG3 | 2.02 | 0.41 |
| 1:A:1726:LEU:HD13 | 1:A:3984:GLN:HB3 | 2.01 | 0.41 |
| 1:B:3896:VAL:HG12 | 1:B:3898:GLU:HG2 | 2.02 | 0.41 |
| 1:B:1626:CYS:HB2 | 1:B:1643:TYR:CD2 | 2.56 | 0.41 |
| 1:B:2982:VAL:HG12 | 1:B:2983:GLY:N | 2.35 | 0.41 |
| 1:A:2821:ASN:O | 1:A:2823:LEU:HD13 | 2.21 | 0.41 |
| 1:A:2640:THR:HG23 | 1:A:2643:SER:H | 1.85 | 0.41 |
| 1:A:3786:PHE:CD1 | 1:A:3893:ASP:HB2 | 2.56 | 0.41 |
| 1:A:1579:ILE:HG13 | 1:A:1598:LEU:HD11 | 2.02 | 0.41 |
| 1:B:1375:LYS:O | 1:B:1379:LYS:HG2 | 2.21 | 0.41 |
| 1:B:2732:MET:CG | 3:B:5402:ADP:C6 | 3.02 | 0.41 |
| 1:A:2765:GLY:CA | 3:A:5402:ADP:O2A | 2.59 | 0.41 |
| 1:B:2285:GLU:CB | 1:B:2412:ARG:NH2 | 2.83 | 0.41 |
| 1:B:2788:ARG:H | 1:B:3459:ASP:HB2 | 1.85 | 0.41 |
| 1:B:3950:PHE:HE1 | 1:B:4006:VAL:HB | 1.86 | 0.41 |
| 1:A:3886:ALA:N | 1:A:3887:PRO:CD | 2.81 | 0.41 |
| 1:B:1706:LEU:CD1 | 1:B:1936:ILE:HG12 | 2.51 | 0.41 |
| 1:B:1578:PHE:HB3 | 1:B:1595:LYS:HB2 | 2.02 | 0.41 |
| 1:A:1744:LEU:CD2 | 1:A:1760:PHE:CD2 | 3.03 | 0.41 |
| 1:B:1926:SER:HB3 | 1:B:1970:LEU:HD12 | 1.97 | 0.41 |
| 1:B:1697:LYS:O | 1:B:1701:LEU:HG | 2.20 | 0.41 |
| 1:A:1409:LEU:O | 1:A:1413:VAL:HG23 | 2.20 | 0.41 |
| 1:A:2131:THR:HG22 | 1:A:2176:LEU:CD2 | 2.50 | 0.41 |
| 1:A:2728:LEU:HB2 | 1:A:2771:ARG:HH12 | 1.86 | 0.41 |
| 1:B:3409:ASP:HB3 | 1:B:3518:PHE:CB | 2.47 | 0.41 |
| 1:A:2982:VAL:HG12 | 1:A:2983:GLY:H | 1.85 | 0.41 |
| 1:B:3304:GLU:O | 1:B:3305:ARG:C | 2.59 | 0.41 |
| 1:A:3971:VAL:HA | 1:A:3974:THR:HG22 | 2.03 | 0.41 |
| 1:B:3826:GLN:HB2 | 1:B:3854:TYR:CZ | 2.56 | 0.41 |
| 1:B:3757:ILE:HD11 | 1:B:4074:GLU:HG2 | 2.02 | 0.41 |
| 1:A:2488:GLU:CG | 1:A:2491:LEU:HD12 | 2.48 | 0.41 |
| 1:A:1822:CYS:SG | 1:A:1850:PHE:HA | 2.61 | 0.41 |
| 1:B:2099:ASN:HD22 | 1:B:2151:TRP:HE1 | 1.68 | 0.41 |
| 1:A:1462:ASN:HB2 | 1:A:1465:ILE:CG2 | 2.42 | 0.41 |
| 1:B:4065:LEU:HD11 | 1:B:4070:ILE:CD1 | 2.45 | 0.41 |
| 1:A:3566:LEU:HD23 | 1:A:3587:LEU:HD11 | 2.02 | 0.41 |
| 1:A:2226:ILE:HG23 | 1:A:2288:VAL:CG2 | 2.46 | 0.41 |
| 1:A:1540:LEU:HD11 | 1:A:1548:ILE:HD11 | 1.99 | 0.41 |
| 1:B:1612:ASP:HA | 1:B:1615:ILE:HG12 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2590:GLU:N | 1:B:2591:PRO:HD2 | 2.36 | 0.41 |
| 1:B:1830:VAL:HG23 | 1:B:1833:ARG:NH2 | 2.36 | 0.41 |
| 1:A:2084:TRP:CZ3 | 1:A:2085:LYS:HG3 | 2.56 | 0.41 |
| 1:A:3544:LYS:O | 1:A:3548:LEU:HB2 | 2.21 | 0.41 |
| 1:A:3645:SER:HB3 | 1:A:3890:GLN:HE21 | 1.86 | 0.41 |
| 1:B:1838:ILE:HD11 | 1:B:1845:GLY:HA3 | 2.03 | 0.41 |
| 1:A:3338:ASN:H | 1:A:3341:GLU:HB2 | 1.83 | 0.41 |
| 1:A:3703:PHE:HE2 | 1:A:3719:VAL:HG21 | 1.86 | 0.41 |
| 1:A:3948:HIS:NE2 | 1:A:4072:ASN:CG | 2.74 | 0.41 |
| 1:A:3464:ARG:O | 1:A:3467:SER:O | 2.38 | 0.41 |
| 1:A:2485:PHE:CZ | 1:A:2534:ALA:HB2 | 2.56 | 0.41 |
| 1:B:2782:VAL:HB | 1:B:2815:LEU:HD12 | 2.02 | 0.41 |
| 1:A:3528:ARG:HH11 | 1:A:3650:LEU:HD11 | 1.86 | 0.41 |
| 1:A:2266:PHE:CD1 | 1:A:2326:LEU:HD21 | 2.53 | 0.41 |
| 1:A:1664:LEU:HD21 | 1:A:1715:LEU:HD22 | 2.03 | 0.41 |
| 1:A:2985:ASN:N | 1:A:2986:PRO:CD | 2.84 | 0.41 |
| 1:A:3817:GLY:H | 1:A:3821:ASN:CB | 2.34 | 0.41 |
| 1:A:2408:LEU:HD13 | 1:A:2432:LEU:HD21 | 2.03 | 0.41 |
| 1:B:2225:LYS:HD2 | 1:B:2281:PHE:CZ | 2.55 | 0.40 |
| 1:A:2332:GLY:HA2 | 1:A:2335:GLN:CG | 2.50 | 0.40 |
| 1:B:3839:ILE:HG22 | 1:B:3871:PHE:HE1 | 1.86 | 0.40 |
| 1:B:2766:LYS:HD2 | 1:B:2890:THR:HG22 | 2.02 | 0.40 |
| 1:B:2299:ARG:HA | 1:B:2302:PHE:CD2 | 2.56 | 0.40 |
| 1:B:3833:LYS:HZ3 | 1:B:3862:THR:HG21 | 1.85 | 0.40 |
| 1:A:2819:GLU:HB3 | 1:A:2891:ILE:HG22 | 2.03 | 0.40 |
| 1:B:2320:ARG:NH1 | 1:B:2406:ASP:OD2 | 2.40 | 0.40 |
| 1:B:3629:PHE:O | 1:B:3633:GLU:HB2 | 2.20 | 0.40 |
| 1:A:2257:PHE:CD1 | 1:A:2262:LEU:HD11 | 2.56 | 0.40 |
| 1:A:3946:VAL:HB | 1:A:3947:PRO:HA | 2.03 | 0.40 |
| 1:B:2151:TRP:CE3 | 1:B:2193:LEU:HD11 | 2.54 | 0.40 |
| 1:B:1939:PHE:O | 1:B:1940:GLU:HB3 | 2.21 | 0.40 |
| 1:A:3844:ILE:HD11 | 1:A:3855:LEU:HD22 | 2.03 | 0.40 |
| 1:A:1392:LEU:HD21 | 1:A:1487:THR:HG21 | 2.02 | 0.40 |
| 1:A:2060:PHE:HZ | 1:A:2193:LEU:HD21 | 1.86 | 0.40 |
| 1:A:2380:LEU:HD12 | 1:A:2380:LEU:C | 2.42 | 0.40 |
| 1:A:1702:LEU:HD23 | 1:A:1702:LEU:HA | 1.91 | 0.40 |
| 1:A:1479:LEU:HD11 | 1:A:1515:SER:HB3 | 2.02 | 0.40 |
| 1:A:3458:PHE:HD2 | 1:A:3506:PRO:HG2 | 1.86 | 0.40 |
| 1:B:2494:LEU:HB2 | 1:B:2499:SER:N | 2.37 | 0.40 |
| 1:A:1637:GLU:C | 1:A:1686:LYS:HZ2 | 2.20 | 0.40 |
| 1:A:3566:LEU:HD13 | 1:A:3570:LEU:HD12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3767:PHE:HB3 | 1:B:3769:VAL:HG23 | 2.03 | 0.40 |
| 1:B:2757:MET:CB | 1:B:2889:PHE:HB2 | 2.52 | 0.40 |
| 1:B:2575:TYR:HD1 | 1:B:2578:ILE:HD11 | 1.85 | 0.40 |
| 1:B:2306:ASP:HB2 | 1:B:2309:SER:HB3 | 2.03 | 0.40 |
| 1:A:1703:VAL:HG21 | 1:A:1768:ARG:HB2 | 2.03 | 0.40 |
| 1:B:3939:ILE:HG22 | 1:B:3956:PHE:CE2 | 2.57 | 0.40 |
| 1:A:3509:LEU:HD12 | 1:A:3513:VAL:HG21 | 1.97 | 0.40 |
| 1:B:2755:HIS:HB3 | 1:B:2912:CYS:SG | 2.62 | 0.40 |
| 1:B:2572:GLU:CG | 1:B:2590:GLU:HG3 | 2.51 | 0.40 |
| 1:B:2751:GLN:H | 1:B:2751:GLN:HG2 | 1.74 | 0.40 |
| 1:B:2972:PHE:CE2 | 1:B:3329:ILE:HG12 | 2.57 | 0.40 |
| 1:B:3406:PHE:CZ | 1:B:3505:ILE:HG21 | 2.57 | 0.40 |
| 1:A:3570:LEU:HD23 | 1:A:3580:ASN:CG | 2.42 | 0.40 |
| 1:A:3848:LEU:HD12 | 1:A:3884:LEU:HD12 | 2.04 | 0.40 |
| 1:B:1495:THR:HB | 1:B:1498:GLU:CG | 2.51 | 0.40 |
| 1:B:2276:LEU:HD13 | 1:B:2417:CYS:SG | 2.62 | 0.40 |
| 1:B:3772:TRP:HZ3 | 1:B:3780:ASN:ND2 | 2.18 | 0.40 |
| 1:A:3528:ARG:HD2 | 1:A:3650:LEU:HD11 | 2.03 | 0.40 |
| 1:B:2542:GLY:O | 1:B:2544:ILE:HD12 | 2.21 | 0.40 |
| 1:B:2832:ASN:OD1 | 1:B:2907:ALA:HB3 | 2.21 | 0.40 |
| 1:A:3519:VAL:HG13 | 1:A:3521:ASN:ND2 | 2.35 | 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 | 2640/2695 (98%) | 2503 (95%) | 121 (5%) | 16 (1%) | 30 | 72 |
| 1 | B | 2640/2695 (98%) | 2506 (95%) | 116 (4%) | 18 (1%) | 26 | 70 |
| All | All | 5280/5390 (98%) | 5009 (95%) | 237 (4%) | 34 (1%) | 30 | 72 |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 24 | GLU |
| 1 | A | 1391 | GLY |
| 1 | A | 2369 | SER |
| 1 | A | 3309 | THR |
| 1 | B | 1391 | GLY |
| 1 | B | 2761 | ALA |
| 1 | B | 3306 | TRP |
| 1 | A | 212 | GLY |
| 1 | A | 1633 | GLY |
| 1 | B | 2763 | ARG |
| 1 | B | 2764 | THR |
| 1 | B | 2990 | GLY |
| 1 | B | 3482 | GLY |
| 1 | A | 2562 | PRO |
| 1 | A | 2990 | GLY |
| 1 | A | 3980 | ILE |
| 1 | A | 115 | GLU |
| 1 | A | 2513 | GLN |
| 1 | A | 2519 | PRO |
| 1 | A | 3809 | GLU |
| 1 | B | 66 | GLN |
| 1 | B | 2519 | PRO |
| 1 | B | 3402 | ASP |
| 1 | A | 66 | GLN |
| 1 | B | 2562 | PRO |
| 1 | A | 3482 | GLY |
| 1 | B | 1366 | VAL |
| 1 | B | 3462 | ILE |
| 1 | B | 3980 | ILE |
| 1 | B | 1633 | GLY |
| 1 | B | 2028 | PRO |
| 1 | B | 1470 | PRO |
| 1 | B | 2141 | ILE |
| 1 | A | 1470 | PRO |

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 2218/2453 (90%) | 2128 (96%) | 90 (4%) | 37 | 75 |
| 1 | B | 2218/2453 (90%) | 2133 (96%) | 85 (4%) | 40 | 76 |
| All | All | 4436/4906 (90%) | 4261 (96%) | 175 (4%) | 39 | 76 |

All (175) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1383 | TYR |
| 1 | A | 1422 | LYS |
| 1 | A | 1463 | LEU |
| 1 | A | 1486 | ILE |
| 1 | A | 1504 | ASN |
| 1 | A | 1553 | LYS |
| 1 | A | 1635 | ASP |
| 1 | A | 1694 | VAL |
| 1 | A | 1794 | PHE |
| 1 | A | 1802 | LYS |
| 1 | A | 1818 | VAL |
| 1 | A | 1832 | SER |
| 1 | A | 1903 | ASN |
| 1 | A | 1929 | ILE |
| 1 | A | 1936 | ILE |
| 1 | A | 1959 | LYS |
| 1 | A | 2064 | GLN |
| 1 | A | 2075 | LYS |
| 1 | A | 2078 | CYS |
| 1 | A | 2080 | LYS |
| 1 | A | 2122 | THR |
| 1 | A | 2154 | PHE |
| 1 | A | 2155 | ASP |
| 1 | A | 2202 | THR |
| 1 | A | 2239 | ASN |
| 1 | A | 2246 | LEU |
| 1 | A | 2276 | LEU |
| 1 | A | 2285 | GLU |
| 1 | A | 2323 | LEU |
| 1 | A | 2346 | PHE |
| 1 | A | 2428 | MET |
| 1 | A | 2472 | THR |
| 1 | A | 2474 | LEU |
| 1 | A | 2476 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2566 | SER |
| 1 | A | 2681 | LEU |
| 1 | A | 2694 | LEU |
| 1 | A | 2785 | LYS |
| 1 | A | 2829 | GLU |
| 1 | A | 2843 | LEU |
| 1 | A | 2856 | LEU |
| 1 | A | 2865 | LEU |
| 1 | A | 2873 | LEU |
| 1 | A | 2961 | ILE |
| 1 | A | 3023 | LYS |
| 1 | A | 3304 | GLU |
| 1 | A | 3305 | ARG |
| 1 | A | 3306 | TRP |
| 1 | A | 3307 | LEU |
| 1 | A | 3312 | GLN |
| 1 | A | 3316 | THR |
| 1 | A | 3355 | LYS |
| 1 | A | 3372 | THR |
| 1 | A | 3386 | LYS |
| 1 | A | 3391 | LEU |
| 1 | A | 3400 | SER |
| 1 | A | 3439 | ARG |
| 1 | A | 3483 | ASP |
| 1 | A | 3534 | LEU |
| 1 | A | 3536 | GLU |
| 1 | A | 3538 | ASN |
| 1 | A | 3557 | LEU |
| 1 | A | 3559 | LEU |
| 1 | A | 3567 | LEU |
| 1 | A | 3578 | LEU |
| 1 | A | 3598 | GLU |
| 1 | A | 3601 | LEU |
| 1 | A | 3673 | GLU |
| 1 | A | 3717 | GLU |
| 1 | A | 3729 | SER |
| 1 | A | 3737 | THR |
| 1 | A | 3794 | VAL |
| 1 | A | 3799 | LYS |
| 1 | A | 3802 | GLU |
| 1 | A | 3805 | LYS |
| 1 | A | 3811 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 3844 | ILE |
| 1 | A | 3871 | PHE |
| 1 | A | 3899 | ASP |
| 1 | A | 3900 | ILE |
| 1 | A | 3906 | THR |
| 1 | A | 3940 | THR |
| 1 | A | 3943 | THR |
| 1 | A | 3952 | LYS |
| 1 | A | 3960 | ASP |
| 1 | A | 3980 | ILE |
| 1 | A | 3982 | TRP |
| 1 | A | 4040 | GLU |
| 1 | A | 4064 | GLN |
| 1 | A | 4068 | GLU |
| 1 | B | 1399 | ASP |
| 1 | B | 1421 | TYR |
| 1 | B | 1455 | LEU |
| 1 | B | 1475 | LYS |
| 1 | B | 1486 | ILE |
| 1 | B | 1491 | PHE |
| 1 | B | 1493 | LEU |
| 1 | B | 1525 | THR |
| 1 | B | 1689 | LYS |
| 1 | B | 1794 | PHE |
| 1 | B | 1832 | SER |
| 1 | B | 1936 | ILE |
| 1 | B | 1939 | PHE |
| 1 | B | 1971 | ARG |
| 1 | B | 2003 | LEU |
| 1 | B | 2035 | VAL |
| 1 | B | 2064 | GLN |
| 1 | B | 2109 | LEU |
| 1 | B | 2155 | ASP |
| 1 | B | 2202 | THR |
| 1 | B | 2222 | ILE |
| 1 | B | 2239 | ASN |
| 1 | B | 2255 | ASP |
| 1 | B | 2295 | ILE |
| 1 | B | 2310 | LEU |
| 1 | B | 2346 | PHE |
| 1 | B | 2351 | GLN |
| 1 | B | 2357 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 2387 | ARG |
| 1 | B | 2395 | ILE |
| 1 | B | 2428 | MET |
| 1 | B | 2476 | LYS |
| 1 | B | 2563 | SER |
| 1 | B | 2566 | SER |
| 1 | B | 2574 | TYR |
| 1 | B | 2587 | SER |
| 1 | B | 2613 | SER |
| 1 | B | 2664 | LYS |
| 1 | B | 2689 | ILE |
| 1 | B | 2694 | LEU |
| 1 | B | 2702 | LEU |
| 1 | B | 2757 | MET |
| 1 | B | 2829 | GLU |
| 1 | B | 2833 | THR |
| 1 | B | 2843 | LEU |
| 1 | B | 2853 | LEU |
| 1 | B | 2873 | LEU |
| 1 | B | 2967 | ASN |
| 1 | B | 3001 | LYS |
| 1 | B | 3012 | GLU |
| 1 | B | 3329 | ILE |
| 1 | B | 3360 | TYR |
| 1 | B | 3372 | THR |
| 1 | B | 3391 | LEU |
| 1 | B | 3400 | SER |
| 1 | B | 3401 | GLN |
| 1 | B | 3502 | SER |
| 1 | B | 3510 | ARG |
| 1 | B | 3531 | ASP |
| 1 | B | 3534 | LEU |
| 1 | B | 3536 | GLU |
| 1 | B | 3538 | ASN |
| 1 | B | 3565 | ARG |
| 1 | B | 3567 | LEU |
| 1 | B | 3605 | GLU |
| 1 | B | 3618 | TYR |
| 1 | B | 3729 | SER |
| 1 | B | 3737 | THR |
| 1 | B | 3744 | LEU |
| 1 | B | 3811 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 3813 | ILE |
| 1 | B | 3831 | LYS |
| 1 | B | 3871 | PHE |
| 1 | B | 3876 | THR |
| 1 | B | 3899 | ASP |
| 1 | B | 3906 | THR |
| 1 | B | 3917 | THR |
| 1 | B | 3943 | THR |
| 1 | B | 3958 | ASP |
| 1 | B | 3960 | ASP |
| 1 | B | 3980 | ILE |
| 1 | B | 3982 | TRP |
| 1 | B | 4004 | LEU |
| 1 | B | 4021 | LEU |
| 1 | B | 4040 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1533 | GLN |
| 1 | A | 1605 | GLN |
| 1 | A | 1622 | GLN |
| 1 | A | 1745 | ASN |
| 1 | A | 1851 | ASN |
| 1 | A | 1864 | ASN |
| 1 | A | 1873 | GLN |
| 1 | A | 1899 | ASN |
| 1 | A | 1951 | HIS |
| 1 | A | 1965 | HIS |
| 1 | A | 2068 | GLN |
| 1 | A | 2099 | ASN |
| 1 | A | 2228 | HIS |
| 1 | A | 2274 | HIS |
| 1 | A | 2282 | ASN |
| 1 | A | 2335 | GLN |
| 1 | A | 2383 | HIS |
| 1 | A | 2409 | ASN |
| 1 | A | 2536 | ASN |
| 1 | A | 2598 | HIS |
| 1 | A | 2634 | ASN |
| 1 | A | 2683 | ASN |
| 1 | A | 2688 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2753 | GLN |
| 1 | A | 3323 | ASN |
| 1 | A | 3338 | ASN |
| 1 | A | 3420 | ASN |
| 1 | A | 3521 | ASN |
| 1 | A | 3588 | ASN |
| 1 | A | 3685 | GLN |
| 1 | A | 3780 | ASN |
| 1 | A | 3890 | GLN |
| 1 | A | 4020 | ASN |
| 1 | A | 4031 | GLN |
| 1 | A | 4077 | GLN |
| 1 | B | 1449 | GLN |
| 1 | B | 1501 | HIS |
| 1 | B | 1622 | GLN |
| 1 | B | 1646 | GLN |
| 1 | B | 1736 | GLN |
| 1 | B | 1899 | ASN |
| 1 | B | 1951 | HIS |
| 1 | B | 2068 | GLN |
| 1 | B | 2099 | ASN |
| 1 | B | 2228 | HIS |
| 1 | B | 2282 | ASN |
| 1 | B | 2293 | HIS |
| 1 | B | 2383 | HIS |
| 1 | B | 2409 | ASN |
| 1 | B | 2536 | ASN |
| 1 | B | 2601 | ASN |
| 1 | B | 2634 | ASN |
| 1 | B | 2688 | ASN |
| 1 | B | 2753 | GLN |
| 1 | B | 3323 | ASN |
| 1 | B | 3338 | ASN |
| 1 | B | 3497 | HIS |
| 1 | B | 3521 | ASN |
| 1 | B | 3624 | HIS |
| 1 | B | 3780 | ASN |
| 1 | B | 3783 | ASN |
| 1 | B | 3868 | HIS |
| 1 | B | 3890 | GLN |
| 1 | B | 4020 | ASN |
| 1 | B | 4077 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 2 | ATP | A | 5400 | 5 | 24,33,33 | 1.02 | 1 (4%) | 31,52,52 | 1.97 | 6 (19%) |
| 3 | ADP | A | 5401 | - | 22,29,29 | 1.26 | 3 (13%) | 27,45,45 | 1.72 | 4 (14%) |
| 3 | ADP | A | 5402 | - | 22,29,29 | 1.01 | 1 (4%) | 27,45,45 | 2.11 | 6 (22%) |
| 4 | SO4 | A | 5403 | - | 4,4,4 | 0.69 | 0 | 6,6,6 | 0.63 | 0 |
| 2 | ATP | B | 5400 | 5 | 24,33,33 | 1.04 | 1 (4%) | 31,52,52 | 1.97 | 6 (19%) |
| 3 | ADP | B | 5401 | - | 22,29,29 | 1.23 | 1 (4%) | 27,45,45 | 2.29 | 7 (25%) |
| 3 | ADP | B | 5402 | - | 22,29,29 | 1.02 | 1 (4%) | 27,45,45 | 1.99 | 5 (18%) |
| 4 | SO4 | B | 5403 | - | 4,4,4 | 0.48 | 0 | 6,6,6 | 0.42 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | ATP | A | 5400 | 5 | - | 0/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 3 | ADP | A | 5401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 3 | ADP | A | 5402 | - | - | 0/12/32/32 | 0/3/3/3 |
| 4 | SO4 | A | 5403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | ATP | B | 5400 | 5 | - | 0/18/38/38 | 0/3/3/3 |
| 3 | ADP | B | 5401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 3 | ADP | B | 5402 | - | - | 0/12/32/32 | 0/3/3/3 |
| 4 | SO4 | B | 5403 | - | - | 0/0/0/0 | 0/0/0/0 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3 | A | 5401 | ADP | O4'-C1' | 2.06 | 1.43 | 1.41 |
| 3 | A | 5401 | ADP | C2-N3 | 2.39 | 1.36 | 1.32 |
| 2 | A | 5400 | ATP | C5-C4 | 2.99 | 1.47 | 1.40 |
| 3 | A | 5402 | ADP | C5-C4 | 3.03 | 1.47 | 1.40 |
| 2 | B | 5400 | ATP | C5-C4 | 3.07 | 1.47 | 1.40 |
| 3 | B | 5402 | ADP | C5-C4 | 3.24 | 1.47 | 1.40 |
| 3 | B | 5401 | ADP | C5-C4 | 3.27 | 1.47 | 1.40 |
| 3 | A | 5401 | ADP | C5-C4 | 3.60 | 1.48 | 1.40 |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3 | A | 5402 | ADP | N3-C2-N1 | -8.20 | 122.61 | 128.89 |
| 3 | B | 5401 | ADP | N3-C2-N1 | -7.88 | 122.86 | 128.89 |
| 3 | B | 5402 | ADP | N3-C2-N1 | -7.33 | 123.28 | 128.89 |
| 2 | B | 5400 | ATP | N3-C2-N1 | -6.69 | 123.77 | 128.89 |
| 2 | A | 5400 | ATP | N3-C2-N1 | -6.65 | 123.80 | 128.89 |
| 3 | A | 5401 | ADP | N3-C2-N1 | -5.68 | 124.55 | 128.89 |
| 2 | A | 5400 | ATP | PA-O3A-PB | -4.26 | 120.76 | 132.73 |
| 2 | B | 5400 | ATP | PA-O3A-PB | -4.03 | 121.41 | 132.73 |
| 3 | B | 5401 | ADP | O3A-PA-O5' | -3.94 | 92.48 | 102.94 |
| 3 | B | 5401 | ADP | PA-O3A-PB | -3.78 | 119.99 | 132.67 |
| 3 | B | 5402 | ADP | PA-O3A-PB | -3.60 | 120.58 | 132.67 |
| 2 | A | 5400 | ATP | PB-O3B-PG | -3.59 | 120.64 | 132.67 |
| 2 | B | 5400 | ATP | PB-O3B-PG | -3.54 | 120.80 | 132.67 |
| 3 | A | 5402 | ADP | PA-O3A-PB | -3.25 | 121.78 | 132.67 |
| 3 | A | 5402 | ADP | C4-C5-N7 | -3.21 | 106.53 | 109.48 |
| 2 | A | 5400 | ATP | C4-C5-N7 | -3.16 | 106.58 | 109.48 |
| 2 | B | 5400 | ATP | C4-C5-N7 | -3.14 | 106.59 | 109.48 |
| 2 | B | 5400 | ATP | C2'-C1'-N9 | -3.11 | 109.54 | 114.29 |
| 2 | A | 5400 | ATP | C2'-C1'-N9 | -3.06 | 109.62 | 114.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3 | A | 5401 | ADP | PA-O3A-PB | -2.90 | 122.95 | 132.67 |
| 3 | B | 5401 | ADP | C2'-C1'-N9 | -2.88 | 109.89 | 114.29 |
| 3 | B | 5402 | ADP | C2'-C1'-N9 | -2.78 | 110.05 | 114.29 |
| 3 | B | 5402 | ADP | C4-C5-N7 | -2.73 | 106.97 | 109.48 |
| 3 | B | 5401 | ADP | C4-C5-N7 | -2.50 | 107.18 | 109.48 |
| 3 | A | 5401 | ADP | C4-C5-N7 | -2.44 | 107.23 | 109.48 |
| 3 | A | 5402 | ADP | C2'-C1'-N9 | -2.31 | 110.77 | 114.29 |
| 3 | B | 5401 | ADP | O4'-C1'-N9 | 2.02 | 112.34 | 108.10 |
| 2 | A | 5400 | ATP | O3G-PG-O2G | 2.09 | 115.34 | 107.38 |
| 3 | A | 5402 | ADP | O3B-PB-O2B | 2.12 | 115.44 | 107.38 |
| 3 | B | 5401 | ADP | C4'-O4'-C1' | 2.17 | 112.10 | 109.72 |
| 2 | B | 5400 | ATP | O3G-PG-O2G | 2.33 | 116.24 | 107.38 |
| 3 | A | 5401 | ADP | C2'-C3'-C4' | 2.34 | 107.43 | 102.61 |
| 3 | B | 5402 | ADP | O3B-PB-O2B | 2.35 | 116.31 | 107.38 |
| 3 | A | 5402 | ADP | C4'-O4'-C1' | 2.64 | 112.62 | 109.72 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 89 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | A | 5400 | ATP | 6 | 0 |
| 3 | A | 5401 | ADP | 11 | 0 |
| 3 | A | 5402 | ADP | 17 | 0 |
| 4 | A | 5403 | SO4 | 2 | 0 |
| 2 | B | 5400 | ATP | 22 | 0 |
| 3 | B | 5401 | ADP | 6 | 0 |
| 3 | B | 5402 | ADP | 23 | 0 |
| 4 | B | 5403 | SO4 | 2 | 0 |

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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 | 2650/2695 (98%) | 0.64 | 314 (11%) 6 6 | 88, 185, 310, 500 | 1 (0%) |
| 1 | B | 2650/2695 (98%) | 0.74 | 271 (10%) 9 9 | 96, 180, 317, 500 | 1 (0%) |
| All | All | 5300/5390 (98%) | 0.69 | 585 (11%) 7 7 | 88, 183, 311, 500 | 2 (0%) |

All (585) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 49 | LEU | 36.5 |
| 1 | B | 33 | GLU | 30.3 |
| 1 | B | 83 | GLY | 27.7 |
| 1 | B | 69 | ALA | 27.3 |
| 1 | A | 131 | MET | 25.7 |
| 1 | B | 91 | ILE | 24.5 |
| 1 | B | 199 | ALA | 24.3 |
| 1 | B | 198 | ILE | 24.0 |
| 1 | B | 66 | GLN | 23.6 |
| 1 | B | 84 | CYS | 22.7 |
| 1 | B | 16 | THR | 22.1 |
| 1 | B | 92 | SER | 20.1 |
| 1 | B | 52 | PRO | 19.7 |
| 1 | A | 1460 | GLY | 19.4 |
| 1 | B | 15 | PRO | 19.0 |
| 1 | B | 35 | ASP | 18.2 |
| 1 | B | 4 | LEU | 16.0 |
| 1 | B | 155 | TYR | 15.9 |
| 1 | B | 34 | ARG | 15.6 |
| 1 | B | 200 | TRP | 15.6 |
| 1 | A | 132 | PHE | 15.6 |
| 1 | B | 189 | ASP | 15.1 |
| 1 | B | 152 | PHE | 14.6 |
| 1 | B | 50 | GLU | 14.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 95 | GLU | 13.9 |
| 1 | B | 68 | MET | 13.5 |
| 1 | B | 14 | GLN | 13.4 |
| 1 | A | 1459 | LEU | 13.3 |
| 1 | B | 32 | TYR | 12.9 |
| 1 | B | 17 | ARG | 12.7 |
| 1 | B | 186 | PRO | 12.4 |
| 1 | B | 88 | ARG | 12.1 |
| 1 | B | 87 | GLU | 11.7 |
| 1 | B | 89 | ALA | 11.7 |
| 1 | B | 18 | LEU | 11.3 |
| 1 | A | 27 | TYR | 10.9 |
| 1 | B | 48 | GLY | 10.8 |
| 1 | A | 143 | ASN | 10.4 |
| 1 | B | 149 | HIS | 10.2 |
| 1 | B | 65 | THR | 10.1 |
| 1 | B | 5 | GLY | 10.0 |
| 1 | B | 151 | ASP | 9.9 |
| 1 | A | 31 | LEU | 9.7 |
| 1 | B | 90 | GLU | 9.5 |
| 1 | A | 3580 | ASN | 9.4 |
| 1 | A | 1483 | TYR | 9.0 |
| 1 | B | 171 | ALA | 8.8 |
| 1 | B | 1483 | TYR | 8.8 |
| 1 | B | 194 | SER | 8.4 |
| 1 | A | 42 | ASN | 8.4 |
| 1 | A | 108 | ILE | 8.3 |
| 1 | B | 168 | CYS | 8.3 |
| 1 | B | 36 | GLU | 8.3 |
| 1 | A | 3575 | GLY | 8.2 |
| 1 | B | 45 | PHE | 8.0 |
| 1 | B | 73 | TYR | 7.9 |
| 1 | A | 3581 | ASP | 7.9 |
| 1 | B | 193 | LYS | 7.7 |
| 1 | B | 70 | ILE | 7.7 |
| 1 | A | 115 | GLU | 7.6 |
| 1 | B | 53 | ASN | 7.6 |
| 1 | A | 28 | GLU | 7.6 |
| 1 | B | 6 | TYR | 7.6 |
| 1 | A | 210 | GLY | 7.5 |
| 1 | A | 202 | LEU | 7.5 |
| 1 | B | 11 | GLY | 7.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 40 | TRP | 7.4 |
| 1 | B | 19 | LEU | 7.3 |
| 1 | B | 8 | LYS | 7.3 |
| 1 | B | 96 | GLY | 7.2 |
| 1 | B | 3580 | ASN | 7.2 |
| 1 | A | 35 | ASP | 7.2 |
| 1 | A | 3578 | LEU | 7.0 |
| 1 | A | 148 | THR | 6.9 |
| 1 | B | 3 | ILE | 6.8 |
| 1 | A | 3979 | ASN | 6.8 |
| 1 | A | 1549 | ILE | 6.8 |
| 1 | A | 2364 | ASP | 6.6 |
| 1 | B | 72 | ARG | 6.5 |
| 1 | A | 1500 | ILE | 6.4 |
| 1 | A | 2687 | GLY | 6.4 |
| 1 | A | 134 | ASP | 6.4 |
| 1 | B | 143 | ASN | 6.4 |
| 1 | B | 174 | LYS | 6.3 |
| 1 | B | 2941 | THR | 6.2 |
| 1 | A | 173 | PRO | 6.2 |
| 1 | A | 2362 | ALA | 6.1 |
| 1 | A | 2942 | ASP | 6.1 |
| 1 | B | 94 | LEU | 6.1 |
| 1 | B | 3567 | LEU | 6.1 |
| 1 | A | 1445 | TRP | 6.1 |
| 1 | A | 29 | GLU | 6.1 |
| 1 | A | 1458 | ILE | 6.0 |
| 1 | A | 1504 | ASN | 6.0 |
| 1 | B | 3300 | THR | 6.0 |
| 1 | B | 55 | PRO | 6.0 |
| 1 | B | 172 | PHE | 6.0 |
| 1 | A | 1390 | SER | 5.9 |
| 1 | B | 190 | LYS | 5.9 |
| 1 | A | 1490 | ALA | 5.9 |
| 1 | A | 150 | PRO | 5.9 |
| 1 | A | 130 | LYS | 5.8 |
| 1 | B | 2938 | MET | 5.8 |
| 1 | A | 3306 | TRP | 5.7 |
| 1 | B | 169 | LEU | 5.7 |
| 1 | A | 1548 | ILE | 5.7 |
| 1 | B | 1669 | PHE | 5.7 |
| 1 | A | 54 | LEU | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 13 | VAL | 5.6 |
| 1 | B | 1459 | LEU | 5.6 |
| 1 | B | 3575 | GLY | 5.5 |
| 1 | B | 61 | ASP | 5.5 |
| 1 | A | 1392 | LEU | 5.5 |
| 1 | B | 2368 | PHE | 5.5 |
| 1 | B | 3735 | LYS | 5.4 |
| 1 | A | 3579 | GLU | 5.4 |
| 1 | A | 3577 | MET | 5.4 |
| 1 | B | 30 | HIS | 5.3 |
| 1 | A | 2302 | PHE | 5.2 |
| 1 | B | 98 | VAL | 5.2 |
| 1 | A | 41 | ARG | 5.2 |
| 1 | B | 7 | TRP | 5.2 |
| 1 | A | 1368 | GLU | 5.1 |
| 1 | A | 1389 | SER | 5.1 |
| 1 | B | 85 | PRO | 5.1 |
| 1 | B | 10 | LYS | 5.1 |
| 1 | B | 2 | PRO | 5.0 |
| 1 | A | 1383 | TYR | 5.0 |
| 1 | A | 1558 | VAL | 5.0 |
| 1 | A | 3980 | ILE | 4.9 |
| 1 | A | 2363 | ASN | 4.9 |
| 1 | B | 39 | LYS | 4.9 |
| 1 | A | 1434 | LYS | 4.9 |
| 1 | B | 184 | ALA | 4.8 |
| 1 | A | 64 | LEU | 4.8 |
| 1 | A | 2248 | LYS | 4.7 |
| 1 | B | 137 | CYS | 4.7 |
| 1 | A | 2808 | LEU | 4.7 |
| 1 | A | 3562 | LEU | 4.7 |
| 1 | B | 134 | ASP | 4.7 |
| 1 | A | 89 | ALA | 4.7 |
| 1 | B | 3741 | ASN | 4.7 |
| 1 | A | 116 | THR | 4.7 |
| 1 | A | 3555 | TYR | 4.6 |
| 1 | A | 63 | LYS | 4.6 |
| 1 | A | 3576 | ASN | 4.6 |
| 1 | B | 2121 | ALA | 4.6 |
| 1 | A | 1879 | ILE | 4.6 |
| 1 | A | 90 | GLU | 4.5 |
| 1 | B | 187 | GLN | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 81 | LEU | 4.5 |
| 1 | B | 3024 | LEU | 4.5 |
| 1 | A | 1388 | HIS | 4.5 |
| 1 | A | 133 | GLU | 4.5 |
| 1 | A | 144 | GLY | 4.4 |
| 1 | A | 216 | PRO | 4.4 |
| 1 | B | 74 | ILE | 4.4 |
| 1 | A | 32 | TYR | 4.4 |
| 1 | B | 67 | SER | 4.3 |
| 1 | A | 129 | LEU | 4.3 |
| 1 | B | 1394 | LEU | 4.3 |
| 1 | B | 3734 | PRO | 4.2 |
| 1 | B | 154 | LEU | 4.2 |
| 1 | B | 3542 | GLN | 4.2 |
| 1 | B | 1458 | ILE | 4.2 |
| 1 | B | 153 | MET | 4.2 |
| 1 | B | 3016 | PHE | 4.2 |
| 1 | A | 3301 | PHE | 4.2 |
| 1 | B | 86 | LYS | 4.2 |
| 1 | A | 1493 | LEU | 4.1 |
| 1 | A | 2854 | ASN | 4.1 |
| 1 | B | 1485 | MET | 4.1 |
| 1 | B | 192 | LEU | 4.1 |
| 1 | A | 75 | ALA | 4.1 |
| 1 | A | 3583 | LEU | 4.1 |
| 1 | B | 1727 | LEU | 4.1 |
| 1 | B | 24 | GLU | 4.1 |
| 1 | A | 209 | PHE | 4.1 |
| 1 | B | 3304 | GLU | 4.1 |
| 1 | B | 3573 | SER | 4.1 |
| 1 | B | 3763 | PHE | 4.1 |
| 1 | A | 1452 | TRP | 4.0 |
| 1 | B | 145 | ASP | 4.0 |
| 1 | B | 3303 | LYS | 4.0 |
| 1 | A | 3739 | ASP | 4.0 |
| 1 | A | 1492 | GLN | 4.0 |
| 1 | A | 3017 | VAL | 4.0 |
| 1 | B | 202 | LEU | 4.0 |
| 1 | A | 2941 | THR | 4.0 |
| 1 | A | 1546 | LEU | 3.9 |
| 1 | B | 3585 | VAL | 3.9 |
| 1 | A | 1479 | LEU | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 3564 | LYS | 3.9 |
| 1 | B | 4035 | GLN | 3.9 |
| 1 | B | 31 | LEU | 3.9 |
| 1 | B | 1945 | LEU | 3.9 |
| 1 | B | 64 | LEU | 3.9 |
| 1 | B | 1 | SER | 3.9 |
| 1 | B | 42 | ASN | 3.8 |
| 1 | A | 4034 | LEU | 3.8 |
| 1 | A | 1644 | ILE | 3.8 |
| 1 | B | 2172 | ASP | 3.8 |
| 1 | A | 1394 | LEU | 3.8 |
| 1 | B | 9 | ILE | 3.8 |
| 1 | B | 3703 | PHE | 3.8 |
| 1 | A | 142 | LEU | 3.8 |
| 1 | A | 3591 | LYS | 3.8 |
| 1 | A | 1572 | ILE | 3.8 |
| 1 | A | 86 | LYS | 3.8 |
| 1 | B | 1383 | TYR | 3.8 |
| 1 | B | 1502 | ILE | 3.8 |
| 1 | A | 2852 | LEU | 3.7 |
| 1 | A | 1378 | TRP | 3.7 |
| 1 | B | 1705 | TYR | 3.7 |
| 1 | A | 19 | LEU | 3.7 |
| 1 | B | 1762 | TYR | 3.7 |
| 1 | A | 147 | VAL | 3.7 |
| 1 | A | 1602 | ILE | 3.7 |
| 1 | A | 2916 | TRP | 3.7 |
| 1 | A | 2676 | THR | 3.6 |
| 1 | A | 2965 | VAL | 3.6 |
| 1 | A | 1530 | GLN | 3.6 |
| 1 | B | 1456 | TYR | 3.6 |
| 1 | A | 3024 | LEU | 3.6 |
| 1 | B | 3020 | GLY | 3.6 |
| 1 | B | 2364 | ASP | 3.6 |
| 1 | A | 211 | GLY | 3.6 |
| 1 | B | 3617 | GLU | 3.6 |
| 1 | B | 63 | LYS | 3.6 |
| 1 | A | 3920 | ILE | 3.6 |
| 1 | A | 2937 | PRO | 3.6 |
| 1 | A | 1550 | GLY | 3.5 |
| 1 | A | 2574 | TYR | 3.5 |
| 1 | A | 3589 | ASN | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 135 | ARG | 3.5 |
| 1 | A | 138 | HIS | 3.5 |
| 1 | A | 1401 | LEU | 3.5 |
| 1 | A | 1738 | ASN | 3.5 |
| 1 | A | 72 | ARG | 3.5 |
| 1 | A | 3570 | LEU | 3.5 |
| 1 | A | 1489 | ARG | 3.5 |
| 1 | A | 1391 | GLY | 3.5 |
| 1 | A | 2371 | PHE | 3.4 |
| 1 | B | 3569 | GLU | 3.4 |
| 1 | B | 44 | LYS | 3.4 |
| 1 | A | 151 | ASP | 3.4 |
| 1 | B | 3919 | LYS | 3.4 |
| 1 | A | 1472 | GLU | 3.4 |
| 1 | A | 171 | ALA | 3.4 |
| 1 | B | 3579 | GLU | 3.4 |
| 1 | B | 3571 | ASN | 3.4 |
| 1 | A | 18 | LEU | 3.4 |
| 1 | A | 2611 | LEU | 3.4 |
| 1 | B | 148 | THR | 3.3 |
| 1 | B | 1445 | TRP | 3.3 |
| 1 | A | 2029 | LEU | 3.3 |
| 1 | B | 3543 | ARG | 3.3 |
| 1 | A | 2870 | GLU | 3.3 |
| 1 | A | 1441 | ILE | 3.3 |
| 1 | B | 131 | MET | 3.3 |
| 1 | B | 3566 | LEU | 3.3 |
| 1 | A | 16 | THR | 3.3 |
| 1 | B | 3984 | GLN | 3.3 |
| 1 | A | 87 | GLU | 3.3 |
| 1 | A | 1565 | MET | 3.3 |
| 1 | A | 1607 | TRP | 3.2 |
| 1 | A | 3551 | LEU | 3.2 |
| 1 | A | 3561 | ASN | 3.2 |
| 1 | B | 23 | LEU | 3.2 |
| 1 | A | 57 | TYR | 3.2 |
| 1 | B | 3572 | ASN | 3.2 |
| 1 | A | 3584 | MET | 3.2 |
| 1 | A | 88 | ARG | 3.2 |
| 1 | B | 4052 | THR | 3.2 |
| 1 | A | 1597 | GLU | 3.2 |
| 1 | A | 1581 | GLY | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2918 | GLY | 3.2 |
| 1 | A | 109 | ALA | 3.2 |
| 1 | A | 1636 | ILE | 3.1 |
| 1 | B | 3028 | VAL | 3.1 |
| 1 | A | 2368 | PHE | 3.1 |
| 1 | B | 1767 | GLU | 3.1 |
| 1 | B | 3873 | MET | 3.1 |
| 1 | A | 137 | CYS | 3.1 |
| 1 | B | 1898 | LEU | 3.1 |
| 1 | A | 3019 | VAL | 3.1 |
| 1 | B | 2942 | ASP | 3.1 |
| 1 | B | 51 | PHE | 3.0 |
| 1 | B | 132 | PHE | 3.0 |
| 1 | A | 2179 | PRO | 3.0 |
| 1 | A | 2303 | GLN | 3.0 |
| 1 | B | 3568 | GLU | 3.0 |
| 1 | B | 1590 | LEU | 3.0 |
| 1 | B | 3715 | TYR | 3.0 |
| 1 | A | 3425 | LYS | 3.0 |
| 1 | A | 33 | GLU | 3.0 |
| 1 | A | 1578 | PHE | 3.0 |
| 1 | B | 3577 | MET | 3.0 |
| 1 | B | 2173 | ASN | 3.0 |
| 1 | A | 4029 | ILE | 3.0 |
| 1 | B | 3927 | TYR | 3.0 |
| 1 | B | 1549 | ILE | 3.0 |
| 1 | A | 2130 | PHE | 3.0 |
| 1 | A | 3436 | PHE | 3.0 |
| 1 | A | 1486 | ILE | 3.0 |
| 1 | A | 2582 | VAL | 3.0 |
| 1 | A | 2359 | ILE | 3.0 |
| 1 | B | 185 | ILE | 3.0 |
| 1 | B | 1460 | GLY | 2.9 |
| 1 | B | 1486 | ILE | 2.9 |
| 1 | B | 1513 | ILE | 2.9 |
| 1 | B | 82 | GLY | 2.9 |
| 1 | B | 1449 | GLN | 2.9 |
| 1 | B | 1441 | ILE | 2.9 |
| 1 | B | 1452 | TRP | 2.9 |
| 1 | B | 3564 | LYS | 2.9 |
| 1 | A | 2361 | ILE | 2.9 |
| 1 | A | 2943 | PHE | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 2022 | PHE | 2.9 |
| 1 | A | 3554 | GLU | 2.9 |
| 1 | A | 2091 | MET | 2.9 |
| 1 | B | 1937 | MET | 2.9 |
| 1 | A | 3484 | HIS | 2.9 |
| 1 | A | 3309 | THR | 2.9 |
| 1 | A | 3020 | GLY | 2.9 |
| 1 | A | 1562 | MET | 2.8 |
| 1 | A | 3594 | ALA | 2.8 |
| 1 | A | 2249 | LEU | 2.8 |
| 1 | A | 1519 | ILE | 2.8 |
| 1 | B | 60 | GLY | 2.8 |
| 1 | A | 1526 | PHE | 2.8 |
| 1 | A | 1760 | PHE | 2.8 |
| 1 | A | 3868 | HIS | 2.8 |
| 1 | A | 2938 | MET | 2.8 |
| 1 | A | 4033 | LEU | 2.8 |
| 1 | B | 3744 | LEU | 2.8 |
| 1 | B | 188 | ILE | 2.8 |
| 1 | A | 3313 | PHE | 2.8 |
| 1 | A | 92 | SER | 2.8 |
| 1 | A | 3026 | GLU | 2.8 |
| 1 | A | 4036 | GLN | 2.8 |
| 1 | A | 2689 | ILE | 2.8 |
| 1 | A | 1505 | PHE | 2.8 |
| 1 | A | 3446 | PHE | 2.8 |
| 1 | B | 3934 | TRP | 2.8 |
| 1 | B | 3025 | ASN | 2.8 |
| 1 | B | 3853 | THR | 2.8 |
| 1 | B | 1719 | SER | 2.8 |
| 1 | B | 3747 | LEU | 2.8 |
| 1 | B | 3017 | VAL | 2.8 |
| 1 | B | 3581 | ASP | 2.7 |
| 1 | A | 2190 | PHE | 2.7 |
| 1 | A | 1456 | TYR | 2.7 |
| 1 | A | 94 | LEU | 2.7 |
| 1 | B | 1683 | LEU | 2.7 |
| 1 | B | 75 | ALA | 2.7 |
| 1 | B | 144 | GLY | 2.7 |
| 1 | B | 1476 | PHE | 2.7 |
| 1 | B | 1596 | ILE | 2.7 |
| 1 | A | 3025 | ASN | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1905 | ARG | 2.7 |
| 1 | A | 3567 | LEU | 2.7 |
| 1 | B | 191 | TYR | 2.7 |
| 1 | B | 1952 | PHE | 2.7 |
| 1 | A | 76 | ASP | 2.7 |
| 1 | B | 3618 | TYR | 2.6 |
| 1 | A | 3865 | ALA | 2.6 |
| 1 | B | 3867 | GLU | 2.6 |
| 1 | A | 1497 | ILE | 2.6 |
| 1 | A | 3873 | MET | 2.6 |
| 1 | A | 2838 | ALA | 2.6 |
| 1 | B | 1480 | THR | 2.6 |
| 1 | A | 2739 | VAL | 2.6 |
| 1 | B | 1505 | PHE | 2.6 |
| 1 | B | 3582 | GLU | 2.6 |
| 1 | B | 1415 | MET | 2.6 |
| 1 | B | 2024 | SER | 2.6 |
| 1 | A | 1476 | PHE | 2.6 |
| 1 | A | 2682 | PRO | 2.6 |
| 1 | B | 3576 | ASN | 2.6 |
| 1 | A | 1469 | LEU | 2.6 |
| 1 | A | 2681 | LEU | 2.6 |
| 1 | B | 3726 | LEU | 2.6 |
| 1 | B | 3904 | LEU | 2.6 |
| 1 | A | 2121 | ALA | 2.6 |
| 1 | A | 2607 | TYR | 2.6 |
| 1 | A | 3305 | ARG | 2.6 |
| 1 | A | 2581 | LEU | 2.6 |
| 1 | A | 2853 | LEU | 2.6 |
| 1 | B | 3686 | PHE | 2.6 |
| 1 | A | 1590 | LEU | 2.6 |
| 1 | B | 3026 | GLU | 2.6 |
| 1 | B | 3557 | LEU | 2.6 |
| 1 | A | 1506 | ASP | 2.5 |
| 1 | A | 36 | GLU | 2.5 |
| 1 | A | 1559 | SER | 2.5 |
| 1 | A | 3847 | SER | 2.5 |
| 1 | B | 3587 | LEU | 2.5 |
| 1 | A | 146 | HIS | 2.5 |
| 1 | A | 4035 | GLN | 2.5 |
| 1 | A | 1705 | TYR | 2.5 |
| 1 | B | 1672 | TYR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 3019 | VAL | 2.5 |
| 1 | A | 96 | GLY | 2.5 |
| 1 | A | 200 | TRP | 2.5 |
| 1 | B | 1864 | ASN | 2.5 |
| 1 | B | 1760 | PHE | 2.5 |
| 1 | A | 62 | VAL | 2.5 |
| 1 | A | 1669 | PHE | 2.5 |
| 1 | A | 1898 | LEU | 2.5 |
| 1 | B | 3555 | TYR | 2.5 |
| 1 | A | 11 | GLY | 2.5 |
| 1 | A | 3014 | GLN | 2.5 |
| 1 | A | 3028 | VAL | 2.5 |
| 1 | B | 156 | ASP | 2.5 |
| 1 | B | 2943 | PHE | 2.5 |
| 1 | B | 3565 | ARG | 2.5 |
| 1 | B | 197 | TYR | 2.5 |
| 1 | A | 2656 | PHE | 2.5 |
| 1 | A | 2844 | PHE | 2.5 |
| 1 | B | 175 | LEU | 2.5 |
| 1 | A | 2876 | TRP | 2.5 |
| 1 | A | 3007 | TYR | 2.5 |
| 1 | A | 1423 | ILE | 2.5 |
| 1 | A | 3415 | ILE | 2.5 |
| 1 | A | 2129 | LEU | 2.5 |
| 1 | A | 2782 | VAL | 2.5 |
| 1 | A | 1494 | ASP | 2.5 |
| 1 | A | 2024 | SER | 2.5 |
| 1 | A | 1640 | VAL | 2.5 |
| 1 | A | 10 | LYS | 2.5 |
| 1 | B | 1850 | PHE | 2.5 |
| 1 | A | 3357 | ALA | 2.4 |
| 1 | A | 22 | TYR | 2.4 |
| 1 | A | 3875 | MET | 2.4 |
| 1 | B | 4092 | MET | 2.4 |
| 1 | A | 2038 | LEU | 2.4 |
| 1 | A | 93 | MET | 2.4 |
| 1 | B | 2014 | PHE | 2.4 |
| 1 | A | 1426 | GLN | 2.4 |
| 1 | B | 1572 | ILE | 2.4 |
| 1 | B | 47 | LEU | 2.4 |
| 1 | A | 3326 | ILE | 2.4 |
| 1 | B | 1589 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 2302 | PHE | 2.4 |
| 1 | A | 73 | TYR | 2.4 |
| 1 | B | 1953 | LEU | 2.4 |
| 1 | A | 3559 | LEU | 2.4 |
| 1 | A | 2444 | ASN | 2.4 |
| 1 | A | 3593 | GLU | 2.4 |
| 1 | A | 2385 | VAL | 2.4 |
| 1 | A | 2977 | TYR | 2.4 |
| 1 | B | 3768 | PHE | 2.4 |
| 1 | B | 1423 | ILE | 2.4 |
| 1 | B | 2962 | ARG | 2.4 |
| 1 | A | 2912 | CYS | 2.3 |
| 1 | A | 71 | ILE | 2.3 |
| 1 | A | 3021 | LEU | 2.3 |
| 1 | B | 1664 | LEU | 2.3 |
| 1 | B | 3562 | LEU | 2.3 |
| 1 | B | 2122 | THR | 2.3 |
| 1 | A | 2856 | LEU | 2.3 |
| 1 | A | 2874 | TYR | 2.3 |
| 1 | A | 1588 | GLU | 2.3 |
| 1 | A | 2367 | SER | 2.3 |
| 1 | A | 1762 | TYR | 2.3 |
| 1 | A | 3542 | GLN | 2.3 |
| 1 | A | 2470 | GLY | 2.3 |
| 1 | A | 2022 | PHE | 2.3 |
| 1 | A | 2784 | PRO | 2.3 |
| 1 | B | 3839 | ILE | 2.3 |
| 1 | A | 3563 | GLU | 2.3 |
| 1 | A | 3590 | LEU | 2.3 |
| 1 | B | 1942 | SER | 2.3 |
| 1 | A | 1540 | LEU | 2.3 |
| 1 | A | 2366 | LEU | 2.3 |
| 1 | B | 2990 | GLY | 2.3 |
| 1 | A | 61 | ASP | 2.3 |
| 1 | B | 1666 | THR | 2.3 |
| 1 | B | 3847 | SER | 2.3 |
| 1 | A | 2314 | ILE | 2.3 |
| 1 | A | 2686 | LEU | 2.3 |
| 1 | A | 2940 | PHE | 2.3 |
| 1 | A | 2150 | ILE | 2.3 |
| 1 | A | 2962 | ARG | 2.3 |
| 1 | A | 2310 | LEU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 3884 | LEU | 2.3 |
| 1 | B | 2795 | PHE | 2.3 |
| 1 | B | 3415 | ILE | 2.3 |
| 1 | B | 3841 | LEU | 2.3 |
| 1 | B | 3725 | VAL | 2.3 |
| 1 | B | 2021 | ILE | 2.2 |
| 1 | A | 2603 | CYS | 2.2 |
| 1 | A | 1537 | PHE | 2.2 |
| 1 | B | 3948 | HIS | 2.2 |
| 1 | A | 1509 | LEU | 2.2 |
| 1 | B | 1546 | LEU | 2.2 |
| 1 | B | 2006 | LEU | 2.2 |
| 1 | B | 2190 | PHE | 2.2 |
| 1 | A | 3899 | ASP | 2.2 |
| 1 | A | 1474 | SER | 2.2 |
| 1 | A | 3994 | TYR | 2.2 |
| 1 | B | 3589 | ASN | 2.2 |
| 1 | A | 1428 | CYS | 2.2 |
| 1 | B | 4045 | LEU | 2.2 |
| 1 | A | 3869 | GLU | 2.2 |
| 1 | B | 1605 | GLN | 2.2 |
| 1 | B | 1668 | GLN | 2.2 |
| 1 | A | 3557 | LEU | 2.2 |
| 1 | B | 1420 | TYR | 2.2 |
| 1 | B | 3923 | VAL | 2.2 |
| 1 | A | 3426 | THR | 2.2 |
| 1 | B | 1603 | GLN | 2.2 |
| 1 | A | 149 | HIS | 2.2 |
| 1 | A | 4019 | ASP | 2.2 |
| 1 | A | 1935 | GLN | 2.2 |
| 1 | A | 43 | LYS | 2.2 |
| 1 | B | 3390 | PHE | 2.2 |
| 1 | B | 3958 | ASP | 2.2 |
| 1 | B | 1500 | ILE | 2.2 |
| 1 | B | 1828 | TYR | 2.2 |
| 1 | A | 1603 | GLN | 2.2 |
| 1 | A | 2106 | THR | 2.2 |
| 1 | A | 2252 | LEU | 2.2 |
| 1 | B | 2295 | ILE | 2.2 |
| 1 | A | 2673 | LEU | 2.2 |
| 1 | B | 3027 | SER | 2.2 |
| 1 | A | 2292 | VAL | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1538 | TYR | 2.1 |
| 1 | A | 2474 | LEU | 2.1 |
| 1 | A | 2999 | LEU | 2.1 |
| 1 | B | 3657 | PHE | 2.1 |
| 1 | A | 3480 | GLU | 2.1 |
| 1 | A | 1412 | LEU | 2.1 |
| 1 | A | 2170 | LEU | 2.1 |
| 1 | A | 1571 | SER | 2.1 |
| 1 | A | 1566 | PHE | 2.1 |
| 1 | B | 3895 | PHE | 2.1 |
| 1 | B | 2989 | PRO | 2.1 |
| 1 | A | 2237 | LEU | 2.1 |
| 1 | A | 2257 | PHE | 2.1 |
| 1 | A | 1612 | ASP | 2.1 |
| 1 | B | 1412 | LEU | 2.1 |
| 1 | A | 1645 | PHE | 2.1 |
| 1 | A | 3448 | SER | 2.1 |
| 1 | A | 2599 | LEU | 2.1 |
| 1 | B | 3767 | PHE | 2.1 |
| 1 | B | 3816 | LEU | 2.1 |
| 1 | B | 1386 | ILE | 2.1 |
| 1 | A | 2592 | PHE | 2.1 |
| 1 | A | 1582 | VAL | 2.1 |
| 1 | A | 1481 | SER | 2.1 |
| 1 | A | 2316 | LEU | 2.1 |
| 1 | B | 3406 | PHE | 2.1 |
| 1 | B | 1595 | LYS | 2.1 |
| 1 | A | 2304 | ASN | 2.1 |
| 1 | A | 2464 | TYR | 2.1 |
| 1 | B | 164 | MET | 2.1 |
| 1 | B | 3328 | SER | 2.1 |
| 1 | A | 2298 | TYR | 2.1 |
| 1 | A | 1850 | PHE | 2.0 |
| 1 | A | 2868 | ASP | 2.0 |
| 1 | A | 2873 | LEU | 2.0 |
| 1 | B | 1812 | ASN | 2.0 |
| 1 | A | 21 | GLU | 2.0 |
| 1 | B | 2464 | TYR | 2.0 |
| 1 | B | 2731 | PRO | 2.0 |
| 1 | A | 3325 | ILE | 2.0 |
| 1 | A | 3786 | PHE | 2.0 |
| 1 | A | 2809 | LYS | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 3568 | GLU | 2.0 |
| 1 | A | 1499 | VAL | 2.0 |
| 1 | A | 2034 | ILE | 2.0 |
| 1 | B | 1465 | ILE | 2.0 |
| 1 | B | 2937 | PRO | 2.0 |
| 1 | B | 43 | LYS | 2.0 |
| 1 | B | 2130 | PHE | 2.0 |
| 1 | B | 2030 | ASN | 2.0 |
| 1 | B | 2062 | TYR | 2.0 |
| 1 | B | 4027 | VAL | 2.0 |
| 1 | A | 2178 | LEU | 2.0 |
| 1 | B | 3874 | PHE | 2.0 |
| 1 | A | 2736 | GLU | 2.0 |
| 1 | A | 1420 | TYR | 2.0 |
| 1 | A | 2866 | LEU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 5 | MG | B | 5404 | 1/1 | 0.90 | 0.30 | 1.51 | 107,107,107,107 | 0 |
| 2 | ATP | A | 5400 | 31/31 | 0.94 | 0.31 | 1.08 | 122,147,224,246 | 0 |
| 4 | SO4 | A | 5403 | 5/5 | 0.92 | 0.23 | 0.70 | 101,136,142,145 | 0 |
| 2 | ATP | B | 5400 | 31/31 | 0.91 | 0.27 | 0.62 | 124,160,195,221 | 0 |
| 3 | ADP | B | 5401 | 27/27 | 0.94 | 0.27 | 0.39 | 98,121,138,153 | 0 |
| 3 | ADP | B | 5402 | 27/27 | 0.87 | 0.33 | 0.34 | 108,145,183,194 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 3 | ADP | A | 5401 | 27/27 | 0.89 | 0.28 | -0.18 | 126,146,191,198 | 0 |
| 3 | ADP | A | 5402 | 27/27 | 0.93 | 0.25 | -0.69 | 134,176,208,218 | 0 |
| 4 | SO4 | B | 5403 | 5/5 | 0.91 | 0.16 | -0.78 | 139,143,171,171 | 0 |
| 5 | MG | A | 5404 | 1/1 | 0.77 | 0.17 | -2.20 | 97,97,97,97 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.