



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:59 PM GMT

PDB ID : 3CWG
Title : Unphosphorylated mouse STAT3 core fragment
Authors : Ren, Z.; Mao, X.; Mertens, C.; Krishnaraj, R.; Qin, J.; Mandal, P.K.; Romanowshi, M.J.; McMurray, J.S.
Deposited on : 2008-04-21
Resolution : 3.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

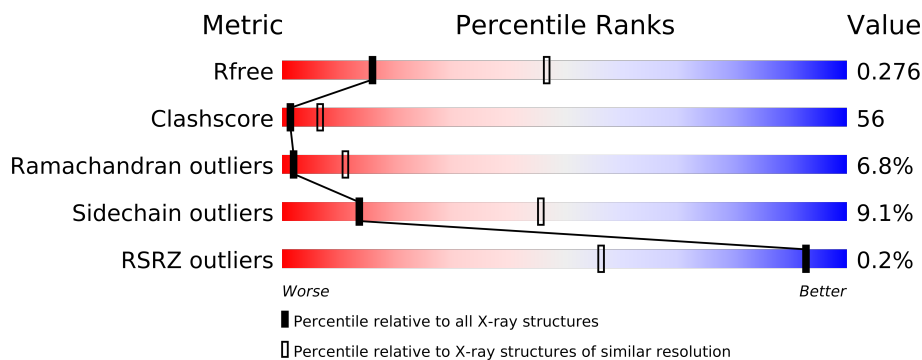
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.05 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 2079 (3.12-3.00) |
| Clashscore | 79885 | 2629 (3.12-3.00) |
| Ramachandran outliers | 78287 | 2536 (3.12-3.00) |
| Sidechain outliers | 78261 | 2539 (3.12-3.00) |
| RSRZ outliers | 66119 | 2081 (3.12-3.00) |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 562 | |
| 1 | B | 562 | |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8215 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Signal transducer and activator of transcription 3.

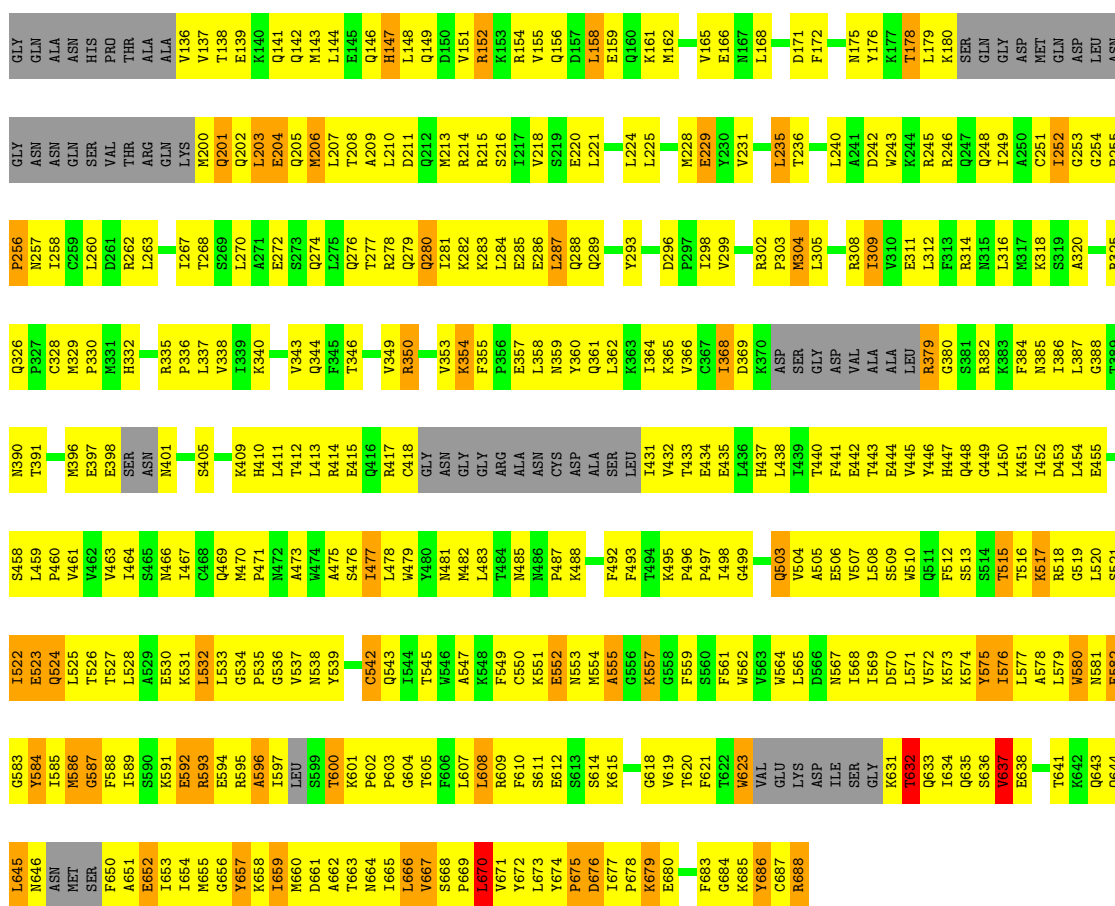
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 501 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4082 | 2615 | 692 | 748 | 27 | | | |
| 1 | B | 507 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4133 | 2645 | 704 | 758 | 26 | | | |

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.

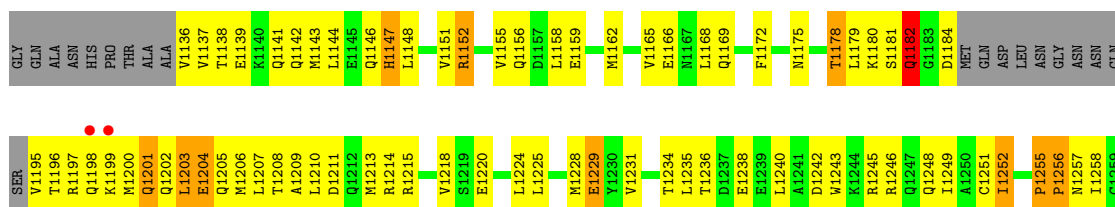
- Molecule 1: Signal transducer and activator of transcription 3

Chain A:



- Molecule 1: Signal transducer and activator of transcription 3

Chain B:



| | | | | | |
|-------|-------|-------|-------|-------|-------|
| G1656 | R1595 | G1534 | M1470 | H1401 | L1260 |
| Y1657 | A1596 | P1535 | P1471 | L1404 | D1261 |
| K1658 | I1597 | G1536 | M1472 | L1432 | L1262 |
| ILE | L1598 | V1537 | A1473 | R1335 | L1263 |
| MET | S1599 | M1538 | W1474 | L1337 | |
| ASP | T1600 | Y1539 | A1475 | V1338 | I1267 |
| ALA | K1601 | S1540 | S1476 | I1339 | T1268 |
| T1663 | P1602 | G1541 | I1477 | K1340 | S1269 |
| M1664 | P1603 | C1542 | L1478 | | A1271 |
| I1665 | G1604 | L1479 | L1413 | V1343 | L1270 |
| L1666 | Q1543 | W1479 | R1414 | Q1344 | E1272 |
| V1667 | T1605 | I1544 | Y1480 | F1345 | S1273 |
| S1668 | M1481 | | M1481 | T1346 | Q1274 |
| P1669 | M1482 | A1547 | M1482 | C1418 | L1275 |
| L1670 | L1483 | K1546 | L1483 | GLY | Q1276 |
| R1609 | T1484 | F1549 | T1484 | ASN | T1277 |
| F1610 | M1485 | C1550 | M1485 | GLY | R1278 |
| S1611 | K1551 | E1552 | N1486 | V1353 | Q1279 |
| E1612 | E1552 | E1552 | P1487 | K1354 | Q1280 |
| S1613 | M1553 | M1553 | K1488 | F1355 | I1281 |
| S1614 | M1554 | M1554 | | F1356 | K1282 |
| K1615 | A1555 | A1555 | F1492 | E1357 | K1283 |
| E1616 | G1556 | G1556 | F1493 | L1358 | L1284 |
| G1617 | K1557 | K1557 | T1494 | N1359 | E1285 |
| G1618 | G1558 | G1558 | K1495 | Y1360 | E1286 |
| V1619 | F1559 | S1560 | P1496 | Q1361 | L1287 |
| T1620 | S1560 | F1561 | P1497 | I1431 | Q1288 |
| F1621 | F1561 | W1562 | I1498 | V1432 | Q1289 |
| T1622 | W1562 | V1563 | G1499 | T1433 | Y1293 |
| W1623 | V1563 | Q1503 | | C1367 | |
| VAL | W1564 | V1504 | H1437 | I1368 | D1296 |
| GLY | L1565 | A1505 | L1438 | D1369 | F1297 |
| LYS | D1566 | E1506 | I1439 | K1370 | I1298 |
| ASP | M1567 | E1506 | T1440 | ASP | V1299 |
| ILE | I1568 | V1507 | F1441 | SER | |
| SER | I1569 | L1508 | E1442 | GLY | R1302 |
| GLY | D1570 | S1509 | T1443 | ASP | P1303 |
| K1631 | L1571 | W1510 | E1444 | VAL | M1304 |
| T1632 | V1572 | Q1511 | V1445 | ALA | |
| Q1633 | K1573 | F1512 | Y1446 | ALA | R1308 |
| I1634 | K1574 | S1513 | H1447 | LEU | E1311 |
| Q1635 | Y1575 | S1514 | Q1448 | G1380 | L1312 |
| S1636 | I1576 | T1515 | G1449 | S1381 | F1313 |
| Y1637 | L1577 | T1516 | L1450 | R1382 | N1315 |
| E1638 | A1578 | K1517 | K1451 | F1384 | L1316 |
| | L1579 | R1518 | I1452 | I1386 | M1317 |
| | W1580 | G1519 | D1453 | L1387 | K1318 |
| K1642 | M1581 | L1520 | L1454 | G1388 | S1319 |
| Q1643 | E1582 | S1521 | E1455 | T1389 | A1320 |
| Q1644 | G1583 | I1522 | | N1390 | R1325 |
| L1645 | Y1584 | E1523 | S1458 | T1391 | Q1326 |
| M1646 | I1585 | Q1524 | L1459 | M1396 | P1327 |
| ASN | M1586 | L1525 | P1460 | E1397 | C1328 |
| MET | G1587 | T1526 | V1461 | E1398 | M1329 |
| SER | F1588 | T1527 | V1462 | SER | P1330 |
| | I1589 | L1528 | V1463 | ASN | M1331 |
| F1650 | S1590 | A1529 | | | |
| A1651 | K1591 | E1530 | M1466 | | |
| E1652 | E1592 | L1531 | I1467 | | |
| I1653 | R1593 | L1532 | C1468 | | |
| T1654 | E1594 | L1533 | Q1469 | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 31 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 254.78Å 254.78Å 123.78Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 30.00 – 3.05 29.70 – 3.02 | Depositor EDS |
| % Data completeness (in resolution range) | 91.2 (30.00-3.05) 90.1 (29.70-3.02) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.93 (at 3.00Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.250 , 0.269 0.256 , 0.276 | Depositor DCC |
| R_{free} test set | 7413 reflections (10.20%) | DCC |
| Wilson B-factor (Å ²) | 71.6 | Xtriage |
| Anisotropy | 0.491 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 45.6 | EDS |
| Estimated twinning fraction | 0.367 for -h,-k,l | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$ | Xtriage |
| Outliers | 0 of 84177 reflections | Xtriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 8215 | wwPDB-VP |
| Average B, all atoms (Å ²) | 97.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 | 0.47 | 0/4159 | 0.71 | 0/5608 |
| 1 | B | 0.47 | 0/4210 | 0.70 | 0/5675 |
| All | All | 0.47 | 0/8369 | 0.70 | 0/11283 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4082 | 0 | 4139 | 481 | 0 |
| 1 | B | 4133 | 0 | 4195 | 461 | 1 |
| All | All | 8215 | 0 | 8334 | 929 | 1 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 56.

All (929) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|----------------|-------------|----------|
| 1:A:660:MET:HA | 1:A:666:LEU:HA | 1.37 | 1.07 |
| 1:B:1597:ILE:HG13 | 1:B:1598:LEU:H | 1.22 | 1.04 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:650:PHE:HA | 1:A:653:ILE:HD13 | 1.39 | 1.04 |
| 1:B:1605:THR:HG22 | 1:B:1672:TYR:HB2 | 1.42 | 1.01 |
| 1:A:547:ALA:HA | 1:A:551:LYS:HB3 | 1.43 | 1.00 |
| 1:A:517:LYS:HD2 | 1:A:517:LYS:H | 1.28 | 0.99 |
| 1:B:1547:ALA:HA | 1:B:1551:LYS:HB3 | 1.41 | 0.98 |
| 1:B:1470:MET:HB3 | 1:B:1471:PRO:HD3 | 1.46 | 0.98 |
| 1:A:535:PRO:HB2 | 1:B:1596:ALA:HB1 | 1.43 | 0.98 |
| 1:B:1137:VAL:HG22 | 1:B:1262:ARG:HH22 | 1.27 | 0.97 |
| 1:B:1670:LEU:H | 1:B:1670:LEU:HD22 | 1.27 | 0.97 |
| 1:B:1576:ILE:HA | 1:B:1579:LEU:HD13 | 1.45 | 0.97 |
| 1:B:1517:LYS:HD2 | 1:B:1517:LYS:H | 1.30 | 0.95 |
| 1:A:670:LEU:HD22 | 1:A:670:LEU:H | 1.26 | 0.95 |
| 1:A:470:MET:HB3 | 1:A:471:PRO:HD3 | 1.46 | 0.95 |
| 1:A:221:LEU:HD13 | 1:A:281:ILE:HD13 | 1.47 | 0.95 |
| 1:B:1595:ARG:NH1 | 1:B:1634:ILE:HD13 | 1.82 | 0.94 |
| 1:A:576:ILE:HA | 1:A:579:LEU:HD13 | 1.47 | 0.94 |
| 1:B:1280:GLN:HE21 | 1:B:1280:GLN:HA | 1.34 | 0.93 |
| 1:A:280:GLN:HE21 | 1:A:280:GLN:HA | 1.34 | 0.92 |
| 1:A:137:VAL:HG22 | 1:A:262:ARG:HH22 | 1.33 | 0.92 |
| 1:A:537:VAL:HG11 | 1:B:1523:GLU:HG2 | 1.53 | 0.89 |
| 1:B:1595:ARG:HH11 | 1:B:1634:ILE:HD13 | 1.34 | 0.89 |
| 1:A:235:LEU:HD13 | 1:A:267:ILE:HD13 | 1.52 | 0.89 |
| 1:A:605:THR:HG22 | 1:A:672:TYR:HB2 | 1.55 | 0.88 |
| 1:B:1598:LEU:HD11 | 1:B:1604:GLY:H | 1.37 | 0.88 |
| 1:B:1379:ARG:HD3 | 1:B:1380:GLY:N | 1.89 | 0.88 |
| 1:A:512:PHE:HB2 | 1:A:519:GLY:HA2 | 1.58 | 0.85 |
| 1:B:1201:GLN:HA | 1:B:1204:GLU:CD | 1.97 | 0.85 |
| 1:A:246:ARG:HG2 | 1:A:258:ILE:HG22 | 1.59 | 0.84 |
| 1:A:201:GLN:HA | 1:A:204:GLU:CD | 1.97 | 0.84 |
| 1:B:1512:PHE:HB2 | 1:B:1519:GLY:HA2 | 1.60 | 0.84 |
| 1:A:591:LYS:HE2 | 1:A:609:ARG:NH2 | 1.93 | 0.83 |
| 1:B:1633:GLN:HG2 | 1:B:1634:ILE:N | 1.93 | 0.83 |
| 1:B:1633:GLN:CG | 1:B:1634:ILE:N | 2.38 | 0.83 |
| 1:A:658:LYS:O | 1:A:667:VAL:HG23 | 1.80 | 0.82 |
| 1:A:314:ARG:HA | 1:A:452:ILE:HD11 | 1.59 | 0.82 |
| 1:B:1597:ILE:HG13 | 1:B:1598:LEU:N | 1.92 | 0.82 |
| 1:B:1229:GLU:HG3 | 1:B:1312:LEU:HD21 | 1.61 | 0.82 |
| 1:A:535:PRO:CB | 1:B:1596:ALA:HB1 | 2.10 | 0.82 |
| 1:A:139:GLU:HA | 1:A:142:GLN:HG2 | 1.62 | 0.81 |
| 1:A:663:THR:O | 1:A:665:ILE:HG12 | 1.80 | 0.81 |
| 1:A:138:THR:HG23 | 1:A:141:GLN:NE2 | 1.94 | 0.81 |
| 1:B:1346:THR:HG22 | 1:B:1409:LYS:HA | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1246:ARG:HG2 | 1:B:1258:ILE:HG22 | 1.61 | 0.81 |
| 1:A:229:GLU:HG3 | 1:A:312:LEU:HD21 | 1.61 | 0.80 |
| 1:B:1601:LYS:HB3 | 1:B:1602:PRO:HD2 | 1.64 | 0.80 |
| 1:A:603:PRO:HB3 | 1:A:632:THR:HG21 | 1.63 | 0.80 |
| 1:B:1314:ARG:HA | 1:B:1452:ILE:HD11 | 1.64 | 0.80 |
| 1:B:1379:ARG:HH11 | 1:B:1380:GLY:H | 1.29 | 0.80 |
| 1:B:1565:LEU:HA | 1:B:1568:ILE:CD1 | 2.11 | 0.80 |
| 1:A:670:LEU:CD2 | 1:A:670:LEU:H | 1.94 | 0.80 |
| 1:A:601:LYS:HB3 | 1:A:602:PRO:HD2 | 1.64 | 0.79 |
| 1:A:660:MET:HB2 | 1:A:666:LEU:HG | 1.63 | 0.79 |
| 1:B:1565:LEU:HA | 1:B:1568:ILE:HD12 | 1.64 | 0.79 |
| 1:B:1670:LEU:H | 1:B:1670:LEU:CD2 | 1.95 | 0.79 |
| 1:B:1195:VAL:HG12 | 1:B:1196:THR:H | 1.47 | 0.79 |
| 1:A:539:TYR:HA | 1:A:542:CYS:SG | 2.23 | 0.78 |
| 1:A:607:LEU:O | 1:A:608:LEU:HG | 1.84 | 0.78 |
| 1:B:1498:ILE:HG21 | 1:B:1543:GLN:HB3 | 1.65 | 0.78 |
| 1:B:1607:LEU:O | 1:B:1608:LEU:HG | 1.82 | 0.78 |
| 1:A:338:VAL:HG11 | 1:A:470:MET:HE3 | 1.64 | 0.78 |
| 1:B:1539:TYR:HA | 1:B:1542:CYS:SG | 2.22 | 0.78 |
| 1:A:604:GLY:O | 1:A:670:LEU:HB3 | 1.83 | 0.78 |
| 1:B:1278:ARG:HD3 | 1:B:1448:GLN:OE1 | 1.84 | 0.78 |
| 1:B:1633:GLN:HG3 | 1:B:1634:ILE:H | 1.49 | 0.77 |
| 1:A:498:ILE:HG21 | 1:A:543:GLN:HB3 | 1.66 | 0.77 |
| 1:B:1547:ALA:HA | 1:B:1551:LYS:CB | 2.14 | 0.77 |
| 1:A:547:ALA:HA | 1:A:551:LYS:CB | 2.15 | 0.77 |
| 1:B:1685:LYS:HE3 | 1:B:1686:TYR:CE1 | 2.20 | 0.77 |
| 1:A:325:ARG:NH1 | 1:A:325:ARG:HB3 | 2.00 | 0.76 |
| 1:B:1605:THR:HG22 | 1:B:1672:TYR:CB | 2.14 | 0.76 |
| 1:A:346:THR:HG22 | 1:A:409:LYS:HA | 1.66 | 0.76 |
| 1:B:1198:GLN:HG3 | 1:B:1201:GLN:OE1 | 1.84 | 0.76 |
| 1:B:1633:GLN:CG | 1:B:1634:ILE:H | 1.96 | 0.76 |
| 1:A:221:LEU:HD13 | 1:A:281:ILE:CD1 | 2.16 | 0.76 |
| 1:B:1338:VAL:HG11 | 1:B:1470:MET:HE3 | 1.68 | 0.76 |
| 1:A:568:ILE:O | 1:A:572:VAL:HG23 | 1.86 | 0.76 |
| 1:B:1296:ASP:O | 1:B:1299:VAL:HG22 | 1.86 | 0.75 |
| 1:B:1139:GLU:HA | 1:B:1142:GLN:HG2 | 1.67 | 0.75 |
| 1:B:1658:LYS:HA | 1:B:1658:LYS:HE2 | 1.69 | 0.75 |
| 1:A:536:GLY:O | 1:B:1593:ARG:NH2 | 2.19 | 0.75 |
| 1:A:296:ASP:O | 1:A:299:VAL:HG22 | 1.87 | 0.75 |
| 1:A:658:LYS:HA | 1:A:658:LYS:HE2 | 1.69 | 0.74 |
| 1:B:1365:LYS:HG3 | 1:B:1391:THR:HG22 | 1.69 | 0.74 |
| 1:B:1325:ARG:HB3 | 1:B:1325:ARG:NH1 | 2.01 | 0.74 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1568:ILE:O | 1:B:1572:VAL:HG23 | 1.86 | 0.74 |
| 1:A:325:ARG:HH11 | 1:A:325:ARG:HB3 | 1.52 | 0.74 |
| 1:A:573:LYS:HA | 1:A:577:LEU:HD13 | 1.68 | 0.74 |
| 1:A:268:THR:O | 1:A:272:GLU:HG3 | 1.87 | 0.74 |
| 1:B:1268:THR:O | 1:B:1272:GLU:HG3 | 1.88 | 0.74 |
| 1:A:522:ILE:H | 1:A:522:ILE:HD13 | 1.51 | 0.73 |
| 1:B:1179:LEU:HD12 | 1:B:1182:GLN:OE1 | 1.88 | 0.73 |
| 1:B:1573:LYS:HA | 1:B:1577:LEU:HD13 | 1.69 | 0.73 |
| 1:A:654:ILE:HG21 | 1:A:683:PHE:CE1 | 2.23 | 0.73 |
| 1:B:1597:ILE:HA | 1:B:1674:TYR:HE1 | 1.53 | 0.73 |
| 1:A:344:GLN:HG2 | 1:A:410:HIS:HA | 1.71 | 0.72 |
| 1:A:623:TRP:CH2 | 1:A:659:ILE:HD13 | 2.25 | 0.72 |
| 1:B:1475:ALA:HB2 | 1:B:1562:TRP:CD1 | 2.25 | 0.72 |
| 1:A:475:ALA:HB2 | 1:A:562:TRP:CD1 | 2.24 | 0.72 |
| 1:B:1325:ARG:HB3 | 1:B:1325:ARG:HH11 | 1.53 | 0.71 |
| 1:B:1641:THR:HG23 | 1:B:1644:GLN:HE21 | 1.55 | 0.71 |
| 1:A:504:VAL:HG12 | 1:A:508:LEU:HD11 | 1.73 | 0.71 |
| 1:B:1355:PHE:HB2 | 1:B:1358:LEU:HD12 | 1.73 | 0.71 |
| 1:A:503:GLN:O | 1:A:507:VAL:HG23 | 1.90 | 0.71 |
| 1:A:641:THR:HG23 | 1:A:644:GLN:HE21 | 1.55 | 0.71 |
| 1:B:1148:LEU:HD12 | 1:B:1231:VAL:HG11 | 1.73 | 0.71 |
| 1:A:661:ASP:HB2 | 1:A:667:VAL:HG13 | 1.71 | 0.71 |
| 1:B:1576:ILE:CA | 1:B:1579:LEU:HD13 | 2.20 | 0.71 |
| 1:B:1619:VAL:HG23 | 1:B:1650:PHE:CE1 | 2.26 | 0.71 |
| 1:A:475:ALA:HB2 | 1:A:562:TRP:NE1 | 2.06 | 0.71 |
| 1:B:1332:HIS:CE1 | 1:B:1467:ILE:HD11 | 2.26 | 0.70 |
| 1:B:1475:ALA:HB2 | 1:B:1562:TRP:NE1 | 2.06 | 0.70 |
| 1:B:1151:VAL:O | 1:B:1155:VAL:HG23 | 1.91 | 0.70 |
| 1:B:1483:LEU:HD13 | 1:B:1497:PRO:HB2 | 1.73 | 0.70 |
| 1:A:547:ALA:HB1 | 1:A:552:GLU:OE1 | 1.92 | 0.70 |
| 1:B:1152:ARG:HH22 | 1:B:1272:GLU:HB2 | 1.56 | 0.70 |
| 1:A:248:GLN:HE22 | 1:A:485:ASN:HA | 1.55 | 0.70 |
| 1:A:576:ILE:CA | 1:A:579:LEU:HD13 | 2.21 | 0.70 |
| 1:A:252:ILE:CG2 | 1:A:481:ASN:HD22 | 2.05 | 0.70 |
| 1:A:162:MET:O | 1:A:166:GLU:HG3 | 1.92 | 0.70 |
| 1:A:604:GLY:HA2 | 1:A:670:LEU:HD12 | 1.72 | 0.70 |
| 1:B:1530:GLU:HG3 | 1:B:1534:GLY:O | 1.91 | 0.70 |
| 1:A:637:VAL:HG13 | 1:A:638:GLU:N | 2.07 | 0.70 |
| 1:B:1162:MET:O | 1:B:1166:GLU:HG3 | 1.92 | 0.70 |
| 1:A:530:GLU:HG3 | 1:A:534:GLY:O | 1.92 | 0.70 |
| 1:B:1504:VAL:HG12 | 1:B:1508:LEU:HD11 | 1.73 | 0.70 |
| 1:B:1283:LYS:HA | 1:B:1286:GLU:HG3 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1685:LYS:HE3 | 1:B:1686:TYR:HE1 | 1.57 | 0.70 |
| 1:A:483:LEU:HD13 | 1:A:497:PRO:HB2 | 1.74 | 0.70 |
| 1:A:288:GLN:OE1 | 1:A:302:ARG:NH2 | 2.23 | 0.69 |
| 1:B:1386:ILE:O | 1:B:1387:LEU:HD23 | 1.92 | 0.69 |
| 1:B:1531:LYS:HZ1 | 1:B:1612:GLU:HB3 | 1.57 | 0.69 |
| 1:B:1470:MET:CB | 1:B:1471:PRO:HD3 | 2.22 | 0.69 |
| 1:B:1498:ILE:HD12 | 1:B:1498:ILE:H | 1.56 | 0.69 |
| 1:B:1288:GLN:OE1 | 1:B:1302:ARG:NH2 | 2.25 | 0.69 |
| 1:A:287:LEU:C | 1:A:289:GLN:H | 1.95 | 0.69 |
| 1:B:1503:GLN:O | 1:B:1507:VAL:HG23 | 1.92 | 0.69 |
| 1:B:1547:ALA:HB1 | 1:B:1552:GLU:OE1 | 1.91 | 0.69 |
| 1:A:252:ILE:HB | 1:A:478:LEU:HD23 | 1.74 | 0.69 |
| 1:B:1637:VAL:HG13 | 1:B:1638:GLU:N | 2.07 | 0.69 |
| 1:A:151:VAL:O | 1:A:155:VAL:HG23 | 1.93 | 0.69 |
| 1:B:1531:LYS:NZ | 1:B:1612:GLU:HB3 | 2.08 | 0.69 |
| 1:A:379:ARG:HD3 | 1:A:380:GLY:N | 2.07 | 0.69 |
| 1:B:1287:LEU:C | 1:B:1289:GLN:H | 1.95 | 0.69 |
| 1:B:1554:MET:HB2 | 1:B:1557:LYS:HB2 | 1.75 | 0.69 |
| 1:A:386:ILE:HG22 | 1:A:411:LEU:HD22 | 1.74 | 0.69 |
| 1:A:596:ALA:HB1 | 1:B:1535:PRO:HB2 | 1.74 | 0.69 |
| 1:A:535:PRO:HG3 | 1:B:1600:THR:HB | 1.75 | 0.69 |
| 1:A:644:GLN:C | 1:A:646:ASN:H | 1.97 | 0.68 |
| 1:B:1337:LEU:HA | 1:B:1461:VAL:HG22 | 1.74 | 0.68 |
| 1:A:386:ILE:O | 1:A:387:LEU:HD23 | 1.93 | 0.68 |
| 1:B:1598:LEU:HD22 | 1:B:1623:TRP:C | 2.14 | 0.68 |
| 1:A:493:PHE:HA | 1:A:496:PRO:HG3 | 1.75 | 0.68 |
| 1:B:1493:PHE:HA | 1:B:1496:PRO:HG3 | 1.75 | 0.68 |
| 1:A:596:ALA:HB1 | 1:B:1535:PRO:CB | 2.24 | 0.68 |
| 1:A:470:MET:CB | 1:A:471:PRO:HD3 | 2.22 | 0.68 |
| 1:A:355:PHE:HB2 | 1:A:358:LEU:HD12 | 1.76 | 0.68 |
| 1:B:1137:VAL:HG22 | 1:B:1262:ARG:NH2 | 2.07 | 0.68 |
| 1:A:446:TYR:HA | 1:A:450:LEU:O | 1.94 | 0.68 |
| 1:B:1583:GLY:O | 1:B:1585:ILE:N | 2.27 | 0.67 |
| 1:A:337:LEU:HA | 1:A:461:VAL:HG22 | 1.76 | 0.67 |
| 1:A:211:ASP:O | 1:A:215:ARG:HG3 | 1.94 | 0.67 |
| 1:A:573:LYS:O | 1:A:577:LEU:HD22 | 1.94 | 0.67 |
| 1:A:593:ARG:NH2 | 1:B:1536:GLY:O | 2.26 | 0.67 |
| 1:B:1532:LEU:HD12 | 1:B:1561:PHE:CE2 | 2.30 | 0.67 |
| 1:B:1517:LYS:N | 1:B:1517:LYS:HD2 | 2.08 | 0.67 |
| 1:B:1573:LYS:O | 1:B:1577:LEU:HD22 | 1.94 | 0.67 |
| 1:A:417:ARG:HG2 | 1:A:418:CYS:H | 1.59 | 0.67 |
| 1:B:1644:GLN:C | 1:B:1646:ASN:H | 1.98 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1631:LYS:O | 1:B:1632:THR:C | 2.34 | 0.66 |
| 1:B:1284:LEU:HD22 | 1:B:1298:ILE:CD1 | 2.26 | 0.66 |
| 1:A:554:MET:HB2 | 1:A:557:LYS:HB2 | 1.76 | 0.66 |
| 1:B:1564:TRP:CD2 | 1:B:1568:ILE:HD11 | 2.30 | 0.66 |
| 1:B:1196:THR:HB | 1:B:1199:LYS:HB2 | 1.78 | 0.66 |
| 1:B:1267:ILE:HG23 | 1:B:1316:LEU:HD11 | 1.78 | 0.66 |
| 1:A:283:LYS:HA | 1:A:286:GLU:HG3 | 1.76 | 0.66 |
| 1:B:1288:GLN:HE21 | 1:B:1298:ILE:HG22 | 1.61 | 0.66 |
| 1:B:1211:ASP:O | 1:B:1215:ARG:HG3 | 1.95 | 0.66 |
| 1:B:1675:PRO:HB2 | 1:B:1677:ILE:HG13 | 1.77 | 0.66 |
| 1:A:532:LEU:HD12 | 1:A:561:PHE:CE2 | 2.30 | 0.66 |
| 1:B:1591:LYS:HE2 | 1:B:1609:ARG:NH2 | 2.10 | 0.66 |
| 1:A:515:THR:HG21 | 1:A:573:LYS:HG3 | 1.78 | 0.66 |
| 1:B:1446:TYR:HA | 1:B:1450:LEU:O | 1.96 | 0.66 |
| 1:B:1444:GLU:OE1 | 1:B:1451:LYS:HE3 | 1.95 | 0.66 |
| 1:B:1583:GLY:C | 1:B:1585:ILE:H | 1.99 | 0.66 |
| 1:B:1252:ILE:CG2 | 1:B:1481:ASN:HD22 | 2.09 | 0.66 |
| 1:A:479:TRP:HD1 | 1:A:492:PHE:HE1 | 1.44 | 0.65 |
| 1:B:1252:ILE:HB | 1:B:1478:LEU:HD23 | 1.77 | 0.65 |
| 1:A:523:GLU:HG2 | 1:B:1537:VAL:HG11 | 1.78 | 0.65 |
| 1:A:686:TYR:H | 1:A:686:TYR:HD2 | 1.44 | 0.65 |
| 1:A:633:GLN:HG3 | 1:A:634:ILE:N | 2.12 | 0.65 |
| 1:A:498:ILE:HD12 | 1:A:545:THR:HG22 | 1.78 | 0.65 |
| 1:B:1344:GLN:HG2 | 1:B:1410:HIS:HA | 1.77 | 0.65 |
| 1:A:611:SER:HB3 | 1:A:614:SER:OG | 1.97 | 0.65 |
| 1:A:267:ILE:HG23 | 1:A:316:LEU:HD11 | 1.78 | 0.65 |
| 1:A:309:ILE:O | 1:A:309:ILE:HD13 | 1.97 | 0.65 |
| 1:B:1515:THR:HG21 | 1:B:1573:LYS:HG3 | 1.77 | 0.65 |
| 1:A:246:ARG:HG2 | 1:A:258:ILE:CG2 | 2.27 | 0.65 |
| 1:A:444:GLU:OE1 | 1:A:451:LYS:HE3 | 1.96 | 0.65 |
| 1:B:1248:GLN:HE22 | 1:B:1485:ASN:HA | 1.61 | 0.64 |
| 1:A:657:TYR:CE2 | 1:A:659:ILE:HG12 | 2.33 | 0.64 |
| 1:A:517:LYS:HD2 | 1:A:517:LYS:N | 2.06 | 0.64 |
| 1:A:512:PHE:HB3 | 1:A:518:ARG:O | 1.97 | 0.64 |
| 1:A:338:VAL:HG11 | 1:A:470:MET:CE | 2.26 | 0.64 |
| 1:A:460:PRO:HD3 | 1:A:487:PRO:O | 1.98 | 0.64 |
| 1:A:583:GLY:C | 1:A:585:ILE:H | 2.01 | 0.64 |
| 1:A:252:ILE:HG23 | 1:A:481:ASN:HD22 | 1.62 | 0.64 |
| 1:A:379:ARG:HH11 | 1:A:380:GLY:H | 1.45 | 0.64 |
| 1:B:1479:TRP:HD1 | 1:B:1492:PHE:HE1 | 1.45 | 0.64 |
| 1:A:675:PRO:HB2 | 1:A:677:ILE:HG13 | 1.79 | 0.64 |
| 1:B:1609:ARG:HH11 | 1:B:1620:THR:HG21 | 1.63 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1263:LEU:O | 1:B:1267:ILE:HG13 | 1.98 | 0.63 |
| 1:B:1460:PRO:HD3 | 1:B:1487:PRO:O | 1.98 | 0.63 |
| 1:B:1582:GLU:CD | 1:B:1582:GLU:H | 2.02 | 0.63 |
| 1:A:609:ARG:HH11 | 1:A:620:THR:HG21 | 1.64 | 0.63 |
| 1:B:1288:GLN:HB2 | 1:B:1298:ILE:HG21 | 1.80 | 0.63 |
| 1:A:623:TRP:CB | 1:A:670:LEU:HG | 2.29 | 0.63 |
| 1:B:1335:ARG:HG3 | 1:B:1470:MET:SD | 2.38 | 0.63 |
| 1:A:583:GLY:O | 1:A:585:ILE:N | 2.29 | 0.62 |
| 1:B:1493:PHE:HD1 | 1:B:1496:PRO:HG3 | 1.63 | 0.62 |
| 1:A:650:PHE:CA | 1:A:653:ILE:HD13 | 2.23 | 0.62 |
| 1:A:288:GLN:HB2 | 1:A:298:ILE:HG21 | 1.82 | 0.62 |
| 1:A:148:LEU:HD12 | 1:A:231:VAL:HG11 | 1.81 | 0.62 |
| 1:B:1512:PHE:HB3 | 1:B:1518:ARG:O | 1.99 | 0.62 |
| 1:A:582:GLU:CD | 1:A:582:GLU:H | 2.03 | 0.62 |
| 1:B:1686:TYR:N | 1:B:1686:TYR:CD1 | 2.68 | 0.62 |
| 1:A:493:PHE:HD1 | 1:A:496:PRO:HG3 | 1.64 | 0.62 |
| 1:B:1320:ALA:CB | 1:B:1353:VAL:HG23 | 2.29 | 0.62 |
| 1:A:597:ILE:HD11 | 1:A:634:ILE:HD12 | 1.80 | 0.62 |
| 1:A:143:MET:O | 1:A:146:GLN:HB3 | 2.00 | 0.62 |
| 1:A:602:PRO:HG2 | 1:A:605:THR:HG23 | 1.82 | 0.62 |
| 1:A:210:LEU:O | 1:A:214:ARG:HG3 | 2.00 | 0.62 |
| 1:B:1368:ILE:CG2 | 1:B:1386:ILE:HG13 | 2.30 | 0.62 |
| 1:B:1672:TYR:HA | 1:B:1677:ILE:O | 2.00 | 0.62 |
| 1:A:576:ILE:CD1 | 1:A:645:LEU:HD13 | 2.30 | 0.62 |
| 1:A:320:ALA:CB | 1:A:353:VAL:HG23 | 2.30 | 0.62 |
| 1:A:537:VAL:CG1 | 1:B:1523:GLU:HG2 | 2.27 | 0.61 |
| 1:B:1246:ARG:HG2 | 1:B:1258:ILE:CG2 | 2.28 | 0.61 |
| 1:A:235:LEU:HD13 | 1:A:267:ILE:CD1 | 2.25 | 0.61 |
| 1:B:1287:LEU:C | 1:B:1289:GLN:N | 2.53 | 0.61 |
| 1:A:654:ILE:HG21 | 1:A:683:PHE:CD1 | 2.36 | 0.61 |
| 1:A:571:LEU:O | 1:A:575:TYR:O | 2.18 | 0.61 |
| 1:B:1143:MET:O | 1:B:1146:GLN:HB3 | 1.99 | 0.61 |
| 1:A:445:VAL:HB | 1:A:452:ILE:HG22 | 1.82 | 0.61 |
| 1:A:531:LYS:HZ1 | 1:A:612:GLU:HB3 | 1.65 | 0.61 |
| 1:A:270:LEU:O | 1:A:274:GLN:HG3 | 2.01 | 0.61 |
| 1:A:631:LYS:O | 1:A:632:THR:C | 2.39 | 0.61 |
| 1:B:1651:ALA:HB3 | 1:B:1688:ARG:HH22 | 1.66 | 0.61 |
| 1:A:287:LEU:C | 1:A:289:GLN:N | 2.54 | 0.61 |
| 1:A:245:ARG:HE | 1:A:249:ILE:HD11 | 1.66 | 0.61 |
| 1:B:1595:ARG:O | 1:B:1599:SER:HB2 | 2.01 | 0.61 |
| 1:B:1195:VAL:HG21 | 1:B:1200:MET:CE | 2.31 | 0.61 |
| 1:B:1611:SER:HB3 | 1:B:1614:SER:OG | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1602:PRO:HG2 | 1:B:1605:THR:HG23 | 1.81 | 0.61 |
| 1:B:1283:LYS:O | 1:B:1287:LEU:HD13 | 2.01 | 0.61 |
| 1:A:576:ILE:HD11 | 1:A:645:LEU:HD13 | 1.83 | 0.60 |
| 1:B:1210:LEU:O | 1:B:1214:ARG:HG3 | 2.01 | 0.60 |
| 1:A:288:GLN:HE21 | 1:A:298:ILE:HG22 | 1.64 | 0.60 |
| 1:A:304:MET:HA | 1:A:304:MET:CE | 2.29 | 0.60 |
| 1:B:1138:THR:HG23 | 1:B:1141:GLN:NE2 | 2.16 | 0.60 |
| 1:A:517:LYS:CD | 1:A:517:LYS:H | 2.05 | 0.60 |
| 1:A:288:GLN:CD | 1:A:302:ARG:HH21 | 2.05 | 0.60 |
| 1:B:1523:GLU:HG3 | 1:B:1524:GLN:N | 2.17 | 0.60 |
| 1:A:597:ILE:HD11 | 1:A:634:ILE:CD1 | 2.30 | 0.60 |
| 1:B:1605:THR:HA | 1:B:1672:TYR:O | 2.02 | 0.60 |
| 1:B:1565:LEU:HA | 1:B:1568:ILE:CG1 | 2.32 | 0.60 |
| 1:A:549:PHE:O | 1:A:561:PHE:HB3 | 2.02 | 0.60 |
| 1:B:1248:GLN:O | 1:B:1251:CYS:HB2 | 2.01 | 0.60 |
| 1:B:1571:LEU:O | 1:B:1575:TYR:O | 2.19 | 0.60 |
| 1:A:550:CYS:HB3 | 1:A:562:TRP:HB3 | 1.83 | 0.60 |
| 1:B:1598:LEU:HD23 | 1:B:1632:THR:HG22 | 1.84 | 0.59 |
| 1:A:137:VAL:CG2 | 1:A:262:ARG:HH22 | 2.13 | 0.59 |
| 1:B:1384:PHE:O | 1:B:1385:ASN:ND2 | 2.34 | 0.59 |
| 1:B:1270:LEU:O | 1:B:1274:GLN:HG3 | 2.02 | 0.59 |
| 1:A:672:TYR:HA | 1:A:677:ILE:O | 2.01 | 0.59 |
| 1:B:1155:VAL:O | 1:B:1159:GLU:HB2 | 2.01 | 0.59 |
| 1:A:512:PHE:CB | 1:A:519:GLY:HA2 | 2.31 | 0.59 |
| 1:A:171:ASP:HB2 | 1:A:206:MET:HE1 | 1.84 | 0.59 |
| 1:B:1550:CYS:HB3 | 1:B:1562:TRP:HB3 | 1.83 | 0.59 |
| 1:A:314:ARG:O | 1:A:318:LYS:HG3 | 2.02 | 0.59 |
| 1:B:1528:LEU:HA | 1:B:1531:LYS:HB2 | 1.84 | 0.59 |
| 1:B:1304:MET:HA | 1:B:1304:MET:CE | 2.31 | 0.59 |
| 1:B:1603:PRO:HB3 | 1:B:1632:THR:HG21 | 1.84 | 0.59 |
| 1:B:1668:SER:HB2 | 1:B:1669:PRO:HD2 | 1.84 | 0.59 |
| 1:B:1282:LYS:O | 1:B:1286:GLU:HG2 | 2.02 | 0.59 |
| 1:A:155:VAL:O | 1:A:159:GLU:HB2 | 2.03 | 0.59 |
| 1:B:1445:VAL:HB | 1:B:1452:ILE:HG22 | 1.84 | 0.59 |
| 1:A:597:ILE:C | 1:A:600:THR:HG22 | 2.22 | 0.59 |
| 1:A:172:PHE:HB2 | 1:A:206:MET:HE2 | 1.84 | 0.59 |
| 1:A:288:GLN:NE2 | 1:A:299:VAL:HA | 2.18 | 0.59 |
| 1:A:523:GLU:HG3 | 1:A:524:GLN:N | 2.18 | 0.59 |
| 1:B:1622:THR:HG22 | 1:B:1623:TRP:N | 2.18 | 0.59 |
| 1:B:1136:VAL:HG22 | 1:B:1137:VAL:H | 1.67 | 0.59 |
| 1:B:1412:THR:HG22 | 1:B:1413:LEU:N | 2.18 | 0.59 |
| 1:B:1179:LEU:HD22 | 1:B:1199:LYS:O | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:668:SER:HB2 | 1:A:669:PRO:HD2 | 1.84 | 0.58 |
| 1:A:412:THR:HG22 | 1:A:413:LEU:N | 2.17 | 0.58 |
| 1:B:1338:VAL:HG11 | 1:B:1470:MET:CE | 2.34 | 0.58 |
| 1:A:152:ARG:HH22 | 1:A:272:GLU:HB2 | 1.69 | 0.58 |
| 1:A:384:PHE:O | 1:A:385:ASN:ND2 | 2.37 | 0.58 |
| 1:B:1245:ARG:HE | 1:B:1249:ILE:HD11 | 1.69 | 0.58 |
| 1:A:576:ILE:O | 1:A:576:ILE:HG22 | 2.03 | 0.58 |
| 1:B:1314:ARG:O | 1:B:1318:LYS:HG3 | 2.04 | 0.58 |
| 1:B:1236:THR:O | 1:B:1240:LEU:HB3 | 2.02 | 0.58 |
| 1:A:528:LEU:HA | 1:A:531:LYS:HB2 | 1.84 | 0.58 |
| 1:A:283:LYS:O | 1:A:287:LEU:HD13 | 2.02 | 0.58 |
| 1:A:547:ALA:CA | 1:A:551:LYS:HB3 | 2.28 | 0.58 |
| 1:B:1441:PHE:O | 1:B:1442:GLU:HG3 | 2.04 | 0.58 |
| 1:A:565:LEU:HA | 1:A:568:ILE:CG1 | 2.33 | 0.58 |
| 1:A:686:TYR:N | 1:A:686:TYR:CD2 | 2.71 | 0.58 |
| 1:B:1654:ILE:HG21 | 1:B:1683:PHE:CD1 | 2.39 | 0.57 |
| 1:B:1637:VAL:HG22 | 1:B:1638:GLU:H | 1.69 | 0.57 |
| 1:B:1248:GLN:HE21 | 1:B:1481:ASN:HA | 1.69 | 0.57 |
| 1:A:591:LYS:O | 1:A:594:GLU:HB3 | 2.03 | 0.57 |
| 1:A:282:LYS:O | 1:A:286:GLU:HG2 | 2.05 | 0.57 |
| 1:B:1564:TRP:O | 1:B:1568:ILE:HG13 | 2.04 | 0.57 |
| 1:B:1549:PHE:O | 1:B:1561:PHE:HB3 | 2.03 | 0.57 |
| 1:B:1598:LEU:HD22 | 1:B:1623:TRP:O | 2.03 | 0.57 |
| 1:B:1258:ILE:HD12 | 1:B:1258:ILE:O | 2.04 | 0.57 |
| 1:B:1510:TRP:HA | 1:B:1513:SER:OG | 2.04 | 0.57 |
| 1:A:437:HIS:HD2 | 1:A:463:VAL:HG23 | 1.69 | 0.57 |
| 1:A:674:TYR:HB3 | 1:A:675:PRO:HD3 | 1.85 | 0.57 |
| 1:B:1633:GLN:C | 1:B:1634:ILE:HD12 | 2.25 | 0.57 |
| 1:B:1576:ILE:HG22 | 1:B:1576:ILE:O | 2.05 | 0.57 |
| 1:B:1288:GLN:NE2 | 1:B:1299:VAL:HA | 2.20 | 0.57 |
| 1:A:354:LYS:HG2 | 1:A:396:MET:CE | 2.33 | 0.57 |
| 1:A:248:GLN:HE21 | 1:A:481:ASN:HA | 1.69 | 0.57 |
| 1:B:1156:GLN:O | 1:B:1159:GLU:HB3 | 2.05 | 0.57 |
| 1:B:1559:PHE:CE2 | 1:B:1564:TRP:HB2 | 2.40 | 0.57 |
| 1:B:1498:ILE:HG22 | 1:B:1499:GLY:H | 1.70 | 0.57 |
| 1:B:1591:LYS:O | 1:B:1594:GLU:HB3 | 2.04 | 0.56 |
| 1:A:498:ILE:HG22 | 1:A:499:GLY:H | 1.70 | 0.56 |
| 1:A:248:GLN:O | 1:A:251:CYS:HB2 | 2.04 | 0.56 |
| 1:A:510:TRP:HA | 1:A:513:SER:OG | 2.04 | 0.56 |
| 1:A:658:LYS:NZ | 1:A:668:SER:HA | 2.20 | 0.56 |
| 1:B:1547:ALA:CA | 1:B:1551:LYS:HB3 | 2.26 | 0.56 |
| 1:A:623:TRP:CD1 | 1:A:623:TRP:N | 2.73 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1517:LYS:CD | 1:B:1517:LYS:H | 2.05 | 0.56 |
| 1:A:258:ILE:HD12 | 1:A:258:ILE:O | 2.04 | 0.56 |
| 1:B:1318:LYS:HA | 1:B:1454:LEU:CD2 | 2.35 | 0.56 |
| 1:B:1288:GLN:CD | 1:B:1302:ARG:HH21 | 2.08 | 0.56 |
| 1:A:653:ILE:N | 1:A:653:ILE:HD12 | 2.21 | 0.56 |
| 1:B:1284:LEU:HD22 | 1:B:1298:ILE:HD11 | 1.87 | 0.56 |
| 1:B:1284:LEU:HD22 | 1:B:1298:ILE:HD12 | 1.87 | 0.56 |
| 1:A:565:LEU:HA | 1:A:568:ILE:HG12 | 1.87 | 0.56 |
| 1:A:527:THR:HG21 | 1:A:589:ILE:HA | 1.88 | 0.56 |
| 1:B:1437:HIS:HD2 | 1:B:1463:VAL:HG23 | 1.69 | 0.56 |
| 1:B:1337:LEU:CA | 1:B:1461:VAL:HG22 | 2.35 | 0.56 |
| 1:A:664:ASN:O | 1:A:665:ILE:HD13 | 2.06 | 0.56 |
| 1:A:653:ILE:HD12 | 1:A:653:ILE:H | 1.71 | 0.56 |
| 1:B:1641:THR:CG2 | 1:B:1644:GLN:HE21 | 2.19 | 0.56 |
| 1:A:311:GLU:HA | 1:A:311:GLU:OE1 | 2.06 | 0.56 |
| 1:A:441:PHE:O | 1:A:442:GLU:HG3 | 2.05 | 0.56 |
| 1:B:1674:TYR:HB3 | 1:B:1675:PRO:HD3 | 1.87 | 0.56 |
| 1:B:1215:ARG:HH11 | 1:B:1215:ARG:HG2 | 1.70 | 0.56 |
| 1:B:1575:TYR:O | 1:B:1576:ILE:HB | 2.06 | 0.56 |
| 1:A:575:TYR:C | 1:A:576:ILE:HD12 | 2.26 | 0.56 |
| 1:B:1252:ILE:HG23 | 1:B:1481:ASN:HD22 | 1.70 | 0.56 |
| 1:B:1498:ILE:CG2 | 1:B:1543:GLN:HB3 | 2.35 | 0.56 |
| 1:A:221:LEU:HD22 | 1:A:281:ILE:HD11 | 1.88 | 0.55 |
| 1:B:1215:ARG:NH1 | 1:B:1215:ARG:HG2 | 2.21 | 0.55 |
| 1:B:1584:TYR:O | 1:B:1608:LEU:HD12 | 2.06 | 0.55 |
| 1:A:575:TYR:O | 1:A:576:ILE:HB | 2.06 | 0.55 |
| 1:B:1512:PHE:CB | 1:B:1519:GLY:HA2 | 2.34 | 0.55 |
| 1:A:559:PHE:CE2 | 1:A:564:TRP:HB2 | 2.41 | 0.55 |
| 1:A:531:LYS:NZ | 1:A:612:GLU:HB3 | 2.21 | 0.55 |
| 1:B:1311:GLU:HA | 1:B:1311:GLU:OE1 | 2.06 | 0.55 |
| 1:A:594:GLU:HG3 | 1:A:607:LEU:CD2 | 2.36 | 0.55 |
| 1:A:368:ILE:HG21 | 1:A:385:ASN:HA | 1.89 | 0.55 |
| 1:A:349:VAL:O | 1:A:405:SER:HB2 | 2.06 | 0.55 |
| 1:B:1623:TRP:CD1 | 1:B:1623:TRP:N | 2.75 | 0.55 |
| 1:A:137:VAL:HG22 | 1:A:262:ARG:NH2 | 2.12 | 0.55 |
| 1:A:344:GLN:CG | 1:A:410:HIS:HA | 2.35 | 0.55 |
| 1:A:644:GLN:O | 1:A:646:ASN:N | 2.39 | 0.55 |
| 1:A:637:VAL:HG22 | 1:A:638:GLU:H | 1.71 | 0.55 |
| 1:A:215:ARG:HG2 | 1:A:215:ARG:NH1 | 2.22 | 0.55 |
| 1:B:1527:THR:HG21 | 1:B:1589:ILE:HA | 1.88 | 0.55 |
| 1:A:236:THR:O | 1:A:240:LEU:HB3 | 2.05 | 0.55 |
| 1:A:564:TRP:O | 1:A:568:ILE:HG12 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1567:ASN:O | 1:B:1571:LEU:HB2 | 2.07 | 0.55 |
| 1:A:279:GLN:NE2 | 1:A:282:LYS:HD2 | 2.22 | 0.55 |
| 1:A:365:LYS:HG3 | 1:A:391:THR:HG22 | 1.89 | 0.55 |
| 1:B:1669:PRO:HG2 | 1:B:1679:LYS:HE3 | 1.89 | 0.55 |
| 1:B:1279:GLN:NE2 | 1:B:1282:LYS:HD2 | 2.22 | 0.55 |
| 1:B:1686:TYR:N | 1:B:1686:TYR:HD1 | 2.04 | 0.55 |
| 1:A:522:ILE:N | 1:A:522:ILE:HD13 | 2.20 | 0.55 |
| 1:A:669:PRO:HG2 | 1:A:679:LYS:HE3 | 1.88 | 0.55 |
| 1:B:1195:VAL:HG12 | 1:B:1196:THR:N | 2.19 | 0.55 |
| 1:A:659:ILE:O | 1:A:660:MET:C | 2.46 | 0.55 |
| 1:B:1365:LYS:HG3 | 1:B:1391:THR:CG2 | 2.37 | 0.54 |
| 1:B:1368:ILE:HG21 | 1:B:1386:ILE:HG13 | 1.89 | 0.54 |
| 1:A:175:ASN:O | 1:A:178:THR:HG22 | 2.06 | 0.54 |
| 1:A:641:THR:CG2 | 1:A:644:GLN:HE21 | 2.19 | 0.54 |
| 1:B:1224:LEU:O | 1:B:1228:MET:HG3 | 2.07 | 0.54 |
| 1:B:1644:GLN:O | 1:B:1646:ASN:N | 2.40 | 0.54 |
| 1:A:215:ARG:HG2 | 1:A:215:ARG:HH11 | 1.72 | 0.54 |
| 1:B:1479:TRP:HD1 | 1:B:1492:PHE:CE1 | 2.25 | 0.54 |
| 1:A:179:LEU:HD21 | 1:A:200:MET:HA | 1.89 | 0.54 |
| 1:B:1314:ARG:HG3 | 1:B:1452:ILE:HD11 | 1.90 | 0.54 |
| 1:B:1610:PHE:HA | 1:B:1618:GLY:O | 2.06 | 0.54 |
| 1:A:414:ARG:HG2 | 1:A:415:GLU:H | 1.73 | 0.54 |
| 1:A:260:LEU:HB2 | 1:A:350:ARG:HH21 | 1.73 | 0.54 |
| 1:B:1195:VAL:HG11 | 1:B:1200:MET:HE1 | 1.90 | 0.54 |
| 1:B:1594:GLU:HG3 | 1:B:1607:LEU:HD22 | 1.89 | 0.54 |
| 1:B:1337:LEU:O | 1:B:1461:VAL:HG13 | 2.06 | 0.54 |
| 1:B:1325:ARG:NH1 | 1:B:1325:ARG:CB | 2.70 | 0.54 |
| 1:A:337:LEU:O | 1:A:461:VAL:HG13 | 2.07 | 0.54 |
| 1:A:337:LEU:CA | 1:A:461:VAL:HG22 | 2.37 | 0.54 |
| 1:B:1565:LEU:HA | 1:B:1568:ILE:HG13 | 1.89 | 0.54 |
| 1:A:559:PHE:HB3 | 1:A:615:LYS:HE3 | 1.90 | 0.54 |
| 1:A:567:ASN:O | 1:A:571:LEU:HB2 | 2.08 | 0.54 |
| 1:A:412:THR:CG2 | 1:A:413:LEU:N | 2.71 | 0.54 |
| 1:B:1632:THR:HG22 | 1:B:1632:THR:O | 2.08 | 0.54 |
| 1:B:1148:LEU:CD1 | 1:B:1231:VAL:HG11 | 2.37 | 0.54 |
| 1:A:621:PHE:O | 1:A:636:SER:HA | 2.08 | 0.54 |
| 1:A:398:GLU:O | 1:A:401:ASN:N | 2.41 | 0.54 |
| 1:B:1498:ILE:N | 1:B:1498:ILE:HD12 | 2.23 | 0.53 |
| 1:B:1504:VAL:HG12 | 1:B:1508:LEU:CD1 | 2.38 | 0.53 |
| 1:B:1414:ARG:HG2 | 1:B:1415:GLU:H | 1.74 | 0.53 |
| 1:A:488:LYS:HG3 | 1:A:488:LYS:O | 2.09 | 0.53 |
| 1:B:1597:ILE:CG1 | 1:B:1598:LEU:N | 2.68 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1564:TRP:CE2 | 1:B:1568:ILE:HD11 | 2.43 | 0.53 |
| 1:A:325:ARG:NH1 | 1:A:325:ARG:CB | 2.69 | 0.53 |
| 1:A:650:PHE:CD2 | 1:A:654:ILE:HD11 | 2.43 | 0.53 |
| 1:A:335:ARG:HG3 | 1:A:470:MET:SD | 2.49 | 0.53 |
| 1:A:156:GLN:O | 1:A:159:GLU:HB3 | 2.08 | 0.53 |
| 1:A:623:TRP:CE3 | 1:A:670:LEU:HD21 | 2.44 | 0.53 |
| 1:A:504:VAL:HG12 | 1:A:508:LEU:CD1 | 2.38 | 0.53 |
| 1:A:477:ILE:HG22 | 1:A:478:LEU:N | 2.24 | 0.53 |
| 1:B:1396:MET:HG3 | 1:B:1404:LEU:HD23 | 1.91 | 0.53 |
| 1:B:1175:ASN:O | 1:B:1178:THR:HG22 | 2.08 | 0.53 |
| 1:B:1619:VAL:O | 1:B:1619:VAL:HG23 | 2.09 | 0.53 |
| 1:A:158:LEU:HG | 1:A:220:GLU:OE1 | 2.09 | 0.53 |
| 1:A:287:LEU:N | 1:A:287:LEU:CD1 | 2.72 | 0.53 |
| 1:A:505:ALA:HB1 | 1:A:525:LEU:HD21 | 1.90 | 0.53 |
| 1:A:623:TRP:CD1 | 1:A:635:GLN:O | 2.62 | 0.53 |
| 1:A:660:MET:HB2 | 1:A:666:LEU:CG | 2.38 | 0.53 |
| 1:B:1557:LYS:H | 1:B:1557:LYS:HD2 | 1.74 | 0.53 |
| 1:A:685:LYS:HE3 | 1:A:686:TYR:HE2 | 1.74 | 0.53 |
| 1:B:1412:THR:CG2 | 1:B:1413:LEU:N | 2.71 | 0.53 |
| 1:B:1431:ILE:N | 1:B:1431:ILE:HD13 | 2.24 | 0.53 |
| 1:A:594:GLU:HG3 | 1:A:607:LEU:HD22 | 1.90 | 0.52 |
| 1:A:658:LYS:HZ3 | 1:A:668:SER:HA | 1.73 | 0.52 |
| 1:A:619:VAL:O | 1:A:619:VAL:HG23 | 2.08 | 0.52 |
| 1:B:1505:ALA:HB1 | 1:B:1525:LEU:HD21 | 1.91 | 0.52 |
| 1:B:1687:CYS:HA | 1:B:1688:ARG:HH21 | 1.74 | 0.52 |
| 1:A:248:GLN:NE2 | 1:A:485:ASN:HA | 2.23 | 0.52 |
| 1:B:1260:LEU:HB2 | 1:B:1350:ARG:HH21 | 1.74 | 0.52 |
| 1:A:621:PHE:CZ | 1:A:637:VAL:HG11 | 2.43 | 0.52 |
| 1:B:1678:PRO:O | 1:B:1680:GLU:N | 2.40 | 0.52 |
| 1:A:670:LEU:N | 1:A:670:LEU:CD2 | 2.68 | 0.52 |
| 1:A:610:PHE:HA | 1:A:618:GLY:O | 2.10 | 0.52 |
| 1:B:1379:ARG:NH1 | 1:B:1380:GLY:H | 2.02 | 0.52 |
| 1:B:1559:PHE:CD2 | 1:B:1564:TRP:HB2 | 2.44 | 0.52 |
| 1:A:659:ILE:O | 1:A:667:VAL:CG2 | 2.57 | 0.52 |
| 1:A:441:PHE:C | 1:A:442:GLU:HG3 | 2.30 | 0.52 |
| 1:A:633:GLN:CG | 1:A:634:ILE:N | 2.72 | 0.52 |
| 1:B:1201:GLN:C | 1:B:1203:LEU:H | 2.12 | 0.52 |
| 1:A:364:ILE:HD13 | 1:A:443:THR:HG21 | 1.92 | 0.52 |
| 1:B:1195:VAL:HB | 1:B:1200:MET:HE2 | 1.92 | 0.52 |
| 1:B:1477:ILE:HG22 | 1:B:1478:LEU:N | 2.24 | 0.52 |
| 1:A:559:PHE:CD2 | 1:A:564:TRP:HB2 | 2.45 | 0.52 |
| 1:A:557:LYS:HD2 | 1:A:557:LYS:H | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:340:LYS:HB3 | 1:A:343:VAL:HG21 | 1.91 | 0.52 |
| 1:A:633:GLN:HG3 | 1:A:634:ILE:H | 1.74 | 0.52 |
| 1:A:386:ILE:CG2 | 1:A:411:LEU:HD22 | 2.38 | 0.52 |
| 1:A:366:VAL:HA | 1:A:440:THR:O | 2.09 | 0.52 |
| 1:A:600:THR:HG23 | 1:A:601:LYS:HG2 | 1.92 | 0.51 |
| 1:B:1594:GLU:HG3 | 1:B:1607:LEU:CD2 | 2.39 | 0.51 |
| 1:B:1571:LEU:HD11 | 1:B:1576:ILE:HD12 | 1.91 | 0.51 |
| 1:A:438:LEU:HD21 | 1:A:460:PRO:HG3 | 1.91 | 0.51 |
| 1:A:658:LYS:CE | 1:A:669:PRO:HD3 | 2.40 | 0.51 |
| 1:B:1609:ARG:NH1 | 1:B:1620:THR:HG21 | 2.25 | 0.51 |
| 1:B:1521:SER:O | 1:B:1525:LEU:HB2 | 2.10 | 0.51 |
| 1:A:362:LEU:HD11 | 1:A:445:VAL:HG22 | 1.92 | 0.51 |
| 1:A:475:ALA:HB2 | 1:A:562:TRP:HE1 | 1.76 | 0.51 |
| 1:A:479:TRP:HD1 | 1:A:492:PHE:CE1 | 2.25 | 0.51 |
| 1:B:1438:LEU:HD21 | 1:B:1460:PRO:HG3 | 1.93 | 0.51 |
| 1:A:654:ILE:HG22 | 1:A:654:ILE:O | 2.10 | 0.51 |
| 1:A:476:SER:HB3 | 1:A:493:PHE:CE2 | 2.46 | 0.51 |
| 1:B:1493:PHE:CD1 | 1:B:1496:PRO:HG3 | 2.45 | 0.51 |
| 1:A:671:VAL:HG12 | 1:A:679:LYS:HZ3 | 1.75 | 0.51 |
| 1:B:1379:ARG:C | 1:B:1381:SER:H | 2.14 | 0.51 |
| 1:A:498:ILE:CG2 | 1:A:543:GLN:HB3 | 2.36 | 0.51 |
| 1:B:1550:CYS:HB3 | 1:B:1562:TRP:CB | 2.40 | 0.51 |
| 1:B:1340:LYS:HB3 | 1:B:1343:VAL:HG21 | 1.92 | 0.51 |
| 1:A:609:ARG:NH1 | 1:A:620:THR:HG21 | 2.26 | 0.51 |
| 1:A:605:THR:HA | 1:A:671:VAL:O | 2.11 | 0.51 |
| 1:A:517:LYS:CD | 1:A:517:LYS:N | 2.71 | 0.51 |
| 1:A:512:PHE:CZ | 1:A:569:ILE:HD13 | 2.45 | 0.51 |
| 1:A:172:PHE:HD1 | 1:A:206:MET:HB3 | 1.75 | 0.51 |
| 1:A:302:ARG:N | 1:A:303:PRO:CD | 2.74 | 0.51 |
| 1:B:1475:ALA:HB2 | 1:B:1562:TRP:HE1 | 1.75 | 0.51 |
| 1:A:144:LEU:C | 1:A:146:GLN:N | 2.63 | 0.51 |
| 1:A:288:GLN:CG | 1:A:299:VAL:HG12 | 2.41 | 0.51 |
| 1:A:493:PHE:O | 1:A:496:PRO:HD3 | 2.11 | 0.51 |
| 1:B:1332:HIS:HB3 | 1:B:1335:ARG:HB2 | 1.92 | 0.51 |
| 1:B:1276:GLN:O | 1:B:1280:GLN:HG2 | 2.11 | 0.51 |
| 1:B:1287:LEU:CD1 | 1:B:1287:LEU:N | 2.73 | 0.51 |
| 1:B:1604:GLY:O | 1:B:1670:LEU:HB3 | 2.11 | 0.50 |
| 1:A:176:TYR:HA | 1:A:203:LEU:HD21 | 1.93 | 0.50 |
| 1:A:332:HIS:HB3 | 1:A:335:ARG:HB2 | 1.92 | 0.50 |
| 1:A:521:SER:O | 1:A:525:LEU:HB2 | 2.12 | 0.50 |
| 1:B:1520:LEU:HB2 | 1:B:1525:LEU:HD13 | 1.93 | 0.50 |
| 1:B:1252:ILE:HG21 | 1:B:1481:ASN:HD22 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:634:ILE:C | 1:A:635:GLN:HG3 | 2.32 | 0.50 |
| 1:B:1600:THR:HG23 | 1:B:1601:LYS:HG2 | 1.93 | 0.50 |
| 1:A:332:HIS:CE1 | 1:A:467:ILE:HD11 | 2.47 | 0.50 |
| 1:B:1144:LEU:C | 1:B:1146:GLN:N | 2.62 | 0.50 |
| 1:B:1654:ILE:HG22 | 1:B:1654:ILE:O | 2.11 | 0.50 |
| 1:A:473:ALA:O | 1:A:476:SER:N | 2.45 | 0.50 |
| 1:A:584:TYR:O | 1:A:608:LEU:HD12 | 2.12 | 0.50 |
| 1:B:1670:LEU:N | 1:B:1670:LEU:CD2 | 2.69 | 0.50 |
| 1:A:473:ALA:C | 1:A:475:ALA:N | 2.65 | 0.50 |
| 1:B:1594:GLU:O | 1:B:1597:ILE:HG12 | 2.12 | 0.50 |
| 1:A:280:GLN:NE2 | 1:A:280:GLN:HA | 2.16 | 0.50 |
| 1:B:1302:ARG:N | 1:B:1303:PRO:CD | 2.74 | 0.50 |
| 1:A:148:LEU:CD1 | 1:A:231:VAL:HG11 | 2.42 | 0.50 |
| 1:A:288:GLN:NE2 | 1:A:302:ARG:HH21 | 2.09 | 0.50 |
| 1:A:550:CYS:HB3 | 1:A:562:TRP:CB | 2.41 | 0.50 |
| 1:B:1586:MET:O | 1:B:1588:PHE:N | 2.45 | 0.50 |
| 1:A:585:ILE:HG22 | 1:A:587:GLY:N | 2.27 | 0.49 |
| 1:A:573:LYS:CA | 1:A:577:LEU:HD13 | 2.41 | 0.49 |
| 1:B:1285:GLU:O | 1:B:1289:GLN:HG3 | 2.12 | 0.49 |
| 1:B:1476:SER:HB3 | 1:B:1493:PHE:CE2 | 2.47 | 0.49 |
| 1:B:1441:PHE:C | 1:B:1442:GLU:HG3 | 2.30 | 0.49 |
| 1:A:530:GLU:C | 1:A:532:LEU:H | 2.15 | 0.49 |
| 1:A:605:THR:HG22 | 1:A:672:TYR:CB | 2.35 | 0.49 |
| 1:A:201:GLN:C | 1:A:203:LEU:H | 2.14 | 0.49 |
| 1:A:493:PHE:CD1 | 1:A:496:PRO:HG3 | 2.47 | 0.49 |
| 1:B:1488:LYS:O | 1:B:1488:LYS:HG3 | 2.12 | 0.49 |
| 1:B:1576:ILE:HA | 1:B:1579:LEU:CD1 | 2.31 | 0.49 |
| 1:A:209:ALA:O | 1:A:213:MET:HG2 | 2.13 | 0.49 |
| 1:B:1622:THR:C | 1:B:1623:TRP:HD1 | 2.16 | 0.49 |
| 1:B:1606:PHE:HZ | 1:B:1679:LYS:HB3 | 1.78 | 0.49 |
| 1:B:1573:LYS:CA | 1:B:1577:LEU:HD13 | 2.40 | 0.49 |
| 1:B:1550:CYS:CB | 1:B:1562:TRP:HB3 | 2.42 | 0.49 |
| 1:B:1554:MET:O | 1:B:1555:ALA:C | 2.51 | 0.49 |
| 1:A:591:LYS:HE2 | 1:A:609:ARG:HH22 | 1.72 | 0.49 |
| 1:A:657:TYR:CZ | 1:A:659:ILE:HG12 | 2.48 | 0.49 |
| 1:B:1288:GLN:CG | 1:B:1299:VAL:HG12 | 2.43 | 0.49 |
| 1:A:285:GLU:O | 1:A:289:GLN:HG3 | 2.12 | 0.49 |
| 1:A:482:MET:HE3 | 1:A:483:LEU:CD2 | 2.43 | 0.49 |
| 1:B:1344:GLN:CG | 1:B:1410:HIS:HA | 2.43 | 0.49 |
| 1:B:1601:LYS:HE3 | 1:B:1674:TYR:CE2 | 2.48 | 0.49 |
| 1:A:678:PRO:O | 1:A:680:GLU:N | 2.41 | 0.49 |
| 1:B:1604:GLY:HA2 | 1:B:1670:LEU:HB3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:576:ILE:HA | 1:A:579:LEU:CD1 | 2.32 | 0.49 |
| 1:B:1280:GLN:NE2 | 1:B:1280:GLN:HA | 2.16 | 0.49 |
| 1:A:276:GLN:O | 1:A:280:GLN:HG2 | 2.13 | 0.49 |
| 1:B:1386:ILE:C | 1:B:1387:LEU:HD23 | 2.34 | 0.49 |
| 1:A:179:LEU:CD2 | 1:A:200:MET:HA | 2.43 | 0.49 |
| 1:A:504:VAL:O | 1:A:508:LEU:HD12 | 2.12 | 0.49 |
| 1:B:1504:VAL:O | 1:B:1508:LEU:HD12 | 2.13 | 0.49 |
| 1:A:328:CYS:SG | 1:A:336:PRO:HA | 2.52 | 0.49 |
| 1:B:1600:THR:HG23 | 1:B:1601:LYS:N | 2.28 | 0.48 |
| 1:B:1328:CYS:SG | 1:B:1336:PRO:HA | 2.53 | 0.48 |
| 1:B:1346:THR:CG2 | 1:B:1409:LYS:HA | 2.38 | 0.48 |
| 1:A:325:ARG:CZ | 1:A:325:ARG:CB | 2.91 | 0.48 |
| 1:A:357:GLU:CD | 1:A:357:GLU:H | 2.17 | 0.48 |
| 1:A:224:LEU:O | 1:A:228:MET:HG3 | 2.12 | 0.48 |
| 1:A:600:THR:HG23 | 1:A:601:LYS:H | 1.78 | 0.48 |
| 1:A:520:LEU:HB2 | 1:A:525:LEU:HD13 | 1.94 | 0.48 |
| 1:A:674:TYR:O | 1:A:675:PRO:C | 2.51 | 0.48 |
| 1:B:1178:THR:O | 1:B:1182:GLN:HG2 | 2.13 | 0.48 |
| 1:B:1293:TYR:CE1 | 1:B:1296:ASP:HA | 2.48 | 0.48 |
| 1:A:550:CYS:CB | 1:A:562:TRP:HB3 | 2.43 | 0.48 |
| 1:B:1439:ILE:N | 1:B:1439:ILE:HD12 | 2.28 | 0.48 |
| 1:A:654:ILE:HD13 | 1:A:683:PHE:HE1 | 1.78 | 0.48 |
| 1:A:498:ILE:HG22 | 1:A:499:GLY:N | 2.28 | 0.48 |
| 1:B:1473:ALA:O | 1:B:1476:SER:N | 2.47 | 0.48 |
| 1:B:1665:ILE:O | 1:B:1667:VAL:N | 2.46 | 0.48 |
| 1:A:634:ILE:HG22 | 1:A:635:GLN:N | 2.28 | 0.48 |
| 1:A:658:LYS:C | 1:A:659:ILE:HG13 | 2.34 | 0.48 |
| 1:A:673:LEU:O | 1:A:674:TYR:C | 2.52 | 0.48 |
| 1:B:1136:VAL:HG22 | 1:B:1137:VAL:N | 2.28 | 0.48 |
| 1:A:586:MET:O | 1:A:588:PHE:N | 2.47 | 0.48 |
| 1:A:364:ILE:HD13 | 1:A:443:THR:CG2 | 2.44 | 0.48 |
| 1:A:665:ILE:O | 1:A:667:VAL:N | 2.47 | 0.48 |
| 1:B:1498:ILE:HG22 | 1:B:1499:GLY:N | 2.28 | 0.48 |
| 1:B:1616:GLU:O | 1:B:1642:LYS:HE3 | 2.14 | 0.48 |
| 1:B:1585:ILE:HG22 | 1:B:1587:GLY:N | 2.28 | 0.48 |
| 1:B:1622:THR:HG23 | 1:B:1634:ILE:HG23 | 1.95 | 0.48 |
| 1:B:1622:THR:CG2 | 1:B:1623:TRP:N | 2.77 | 0.48 |
| 1:A:600:THR:HG23 | 1:A:601:LYS:N | 2.29 | 0.48 |
| 1:B:1517:LYS:N | 1:B:1517:LYS:CD | 2.73 | 0.48 |
| 1:A:139:GLU:HA | 1:A:142:GLN:CG | 2.37 | 0.48 |
| 1:B:1179:LEU:HD11 | 1:B:1195:VAL:HG12 | 1.96 | 0.48 |
| 1:A:659:ILE:O | 1:A:667:VAL:HG22 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1195:VAL:CB | 1:B:1200:MET:HE2 | 2.44 | 0.48 |
| 1:B:1582:GLU:OE2 | 1:B:1582:GLU:N | 2.38 | 0.48 |
| 1:A:634:ILE:CG2 | 1:A:635:GLN:N | 2.76 | 0.47 |
| 1:B:1493:PHE:O | 1:B:1496:PRO:HD3 | 2.13 | 0.47 |
| 1:B:1530:GLU:C | 1:B:1532:LEU:H | 2.16 | 0.47 |
| 1:A:379:ARG:HH11 | 1:A:380:GLY:N | 2.12 | 0.47 |
| 1:A:688:ARG:H | 1:A:688:ARG:HE | 1.62 | 0.47 |
| 1:B:1600:THR:HG23 | 1:B:1601:LYS:H | 1.78 | 0.47 |
| 1:B:1201:GLN:O | 1:B:1203:LEU:N | 2.39 | 0.47 |
| 1:B:1532:LEU:HD12 | 1:B:1561:PHE:HE2 | 1.79 | 0.47 |
| 1:A:554:MET:O | 1:A:555:ALA:C | 2.52 | 0.47 |
| 1:A:326:GLN:OE1 | 1:A:458:SER:HB2 | 2.14 | 0.47 |
| 1:B:1623:TRP:NE1 | 1:B:1635:GLN:O | 2.48 | 0.47 |
| 1:B:1673:LEU:O | 1:B:1674:TYR:C | 2.53 | 0.47 |
| 1:B:1671:VAL:HG12 | 1:B:1679:LYS:HZ3 | 1.80 | 0.47 |
| 1:A:204:GLU:HG3 | 1:A:204:GLU:H | 1.40 | 0.47 |
| 1:A:318:LYS:HA | 1:A:454:LEU:CD2 | 2.44 | 0.47 |
| 1:B:1565:LEU:CD1 | 1:B:1568:ILE:HD12 | 2.45 | 0.47 |
| 1:B:1674:TYR:O | 1:B:1675:PRO:C | 2.52 | 0.47 |
| 1:A:243:TRP:NE1 | 1:A:258:ILE:HB | 2.29 | 0.47 |
| 1:B:1243:TRP:NE1 | 1:B:1258:ILE:HB | 2.30 | 0.47 |
| 1:B:1288:GLN:HG3 | 1:B:1299:VAL:HG12 | 1.97 | 0.47 |
| 1:B:1288:GLN:NE2 | 1:B:1302:ARG:HH21 | 2.13 | 0.47 |
| 1:A:278:ARG:HD3 | 1:A:448:GLN:OE1 | 2.15 | 0.47 |
| 1:B:1172:PHE:HD1 | 1:B:1206:MET:HB3 | 1.80 | 0.47 |
| 1:A:585:ILE:HD13 | 1:A:608:LEU:HD13 | 1.96 | 0.47 |
| 1:A:146:GLN:O | 1:A:147:HIS:C | 2.52 | 0.47 |
| 1:B:1357:GLU:H | 1:B:1357:GLU:CD | 2.17 | 0.47 |
| 1:A:136:VAL:HG22 | 1:A:137:VAL:H | 1.80 | 0.47 |
| 1:A:288:GLN:HG3 | 1:A:299:VAL:HG12 | 1.97 | 0.47 |
| 1:A:252:ILE:HG21 | 1:A:481:ASN:HD22 | 1.77 | 0.47 |
| 1:A:386:ILE:C | 1:A:387:LEU:HD23 | 2.34 | 0.47 |
| 1:B:1580:TRP:C | 1:B:1580:TRP:CD1 | 2.88 | 0.47 |
| 1:A:595:ARG:O | 1:A:597:ILE:N | 2.42 | 0.47 |
| 1:B:1447:HIS:C | 1:B:1449:GLY:N | 2.66 | 0.47 |
| 1:A:252:ILE:HG23 | 1:A:481:ASN:ND2 | 2.27 | 0.47 |
| 1:A:656:GLY:O | 1:A:657:TYR:C | 2.53 | 0.46 |
| 1:B:1622:THR:CG2 | 1:B:1634:ILE:HG23 | 2.44 | 0.46 |
| 1:B:1246:ARG:HD2 | 1:B:1257:ASN:O | 2.16 | 0.46 |
| 1:B:1296:ASP:HB3 | 1:B:1299:VAL:HG22 | 1.97 | 0.46 |
| 1:A:414:ARG:HG2 | 1:A:415:GLU:N | 2.30 | 0.46 |
| 1:B:1566:ASP:HA | 1:B:1569:ILE:HD12 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:592:GLU:OE1 | 1:A:592:GLU:C | 2.54 | 0.46 |
| 1:B:1325:ARG:CZ | 1:B:1325:ARG:CB | 2.93 | 0.46 |
| 1:A:662:ALA:C | 1:A:664:ASN:H | 2.18 | 0.46 |
| 1:B:1583:GLY:C | 1:B:1585:ILE:N | 2.68 | 0.46 |
| 1:A:152:ARG:O | 1:A:156:GLN:HG2 | 2.15 | 0.46 |
| 1:B:1201:GLN:HA | 1:B:1204:GLU:CG | 2.45 | 0.46 |
| 1:B:1443:THR:O | 1:B:1454:LEU:HB2 | 2.15 | 0.46 |
| 1:B:1656:GLY:O | 1:B:1658:LYS:HE3 | 2.15 | 0.46 |
| 1:A:447:HIS:C | 1:A:449:GLY:N | 2.66 | 0.46 |
| 1:B:1482:MET:HE3 | 1:B:1483:LEU:CD2 | 2.45 | 0.46 |
| 1:B:1644:GLN:C | 1:B:1646:ASN:N | 2.67 | 0.46 |
| 1:B:1152:ARG:O | 1:B:1156:GLN:HG2 | 2.15 | 0.46 |
| 1:A:201:GLN:HA | 1:A:204:GLU:CG | 2.46 | 0.46 |
| 1:A:144:LEU:C | 1:A:146:GLN:H | 2.18 | 0.46 |
| 1:A:669:PRO:O | 1:A:670:LEU:C | 2.54 | 0.46 |
| 1:A:671:VAL:HG12 | 1:A:679:LYS:NZ | 2.31 | 0.46 |
| 1:B:1493:PHE:C | 1:B:1496:PRO:HD3 | 2.36 | 0.46 |
| 1:A:161:LYS:NZ | 1:A:216:SER:OG | 2.48 | 0.46 |
| 1:B:1669:PRO:O | 1:B:1670:LEU:C | 2.54 | 0.46 |
| 1:A:246:ARG:HD2 | 1:A:257:ASN:O | 2.16 | 0.46 |
| 1:A:293:TYR:CE1 | 1:A:296:ASP:HA | 2.50 | 0.46 |
| 1:A:296:ASP:HB3 | 1:A:299:VAL:HG22 | 1.97 | 0.46 |
| 1:B:1144:LEU:C | 1:B:1146:GLN:H | 2.17 | 0.46 |
| 1:B:1607:LEU:HB3 | 1:B:1608:LEU:H | 1.56 | 0.46 |
| 1:A:530:GLU:OE2 | 1:B:1593:ARG:NH1 | 2.41 | 0.46 |
| 1:B:1473:ALA:C | 1:B:1475:ALA:N | 2.66 | 0.46 |
| 1:A:441:PHE:CD1 | 1:A:441:PHE:N | 2.84 | 0.46 |
| 1:A:433:THR:CG2 | 1:A:469:GLN:HB3 | 2.46 | 0.46 |
| 1:A:653:ILE:CD1 | 1:A:653:ILE:H | 2.28 | 0.46 |
| 1:A:205:GLN:C | 1:A:207:LEU:N | 2.68 | 0.46 |
| 1:A:252:ILE:HG21 | 1:A:478:LEU:HA | 1.98 | 0.46 |
| 1:A:582:GLU:CD | 1:A:582:GLU:N | 2.68 | 0.46 |
| 1:B:1158:LEU:HG | 1:B:1220:GLU:OE1 | 2.16 | 0.46 |
| 1:B:1589:ILE:HD13 | 1:B:1607:LEU:HD21 | 1.98 | 0.46 |
| 1:A:417:ARG:HG2 | 1:A:418:CYS:N | 2.27 | 0.46 |
| 1:B:1414:ARG:HG2 | 1:B:1415:GLU:N | 2.30 | 0.46 |
| 1:A:607:LEU:HB3 | 1:A:608:LEU:H | 1.58 | 0.46 |
| 1:B:1592:GLU:OE1 | 1:B:1592:GLU:C | 2.54 | 0.46 |
| 1:A:214:ARG:CZ | 1:A:298:ILE:HD12 | 2.46 | 0.46 |
| 1:B:1366:VAL:HA | 1:B:1440:THR:O | 2.15 | 0.46 |
| 1:B:1656:GLY:O | 1:B:1657:TYR:C | 2.55 | 0.45 |
| 1:A:288:GLN:NE2 | 1:A:298:ILE:HG22 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1330:PRO:HD2 | 1:B:1344:GLN:O | 2.16 | 0.45 |
| 1:B:1209:ALA:O | 1:B:1213:MET:HG2 | 2.16 | 0.45 |
| 1:B:1318:LYS:HA | 1:B:1454:LEU:HD22 | 1.98 | 0.45 |
| 1:B:1162:MET:O | 1:B:1165:VAL:HG12 | 2.16 | 0.45 |
| 1:B:1686:TYR:O | 1:B:1688:ARG:NH2 | 2.50 | 0.45 |
| 1:A:358:LEU:O | 1:A:361:GLN:HB3 | 2.17 | 0.45 |
| 1:B:1605:THR:HA | 1:B:1671:VAL:O | 2.17 | 0.45 |
| 1:A:329:MET:HE1 | 1:A:338:VAL:O | 2.16 | 0.45 |
| 1:A:201:GLN:O | 1:A:204:GLU:HG3 | 2.16 | 0.45 |
| 1:B:1288:GLN:NE2 | 1:B:1298:ILE:HG22 | 2.29 | 0.45 |
| 1:B:1611:SER:N | 1:B:1618:GLY:O | 2.43 | 0.45 |
| 1:A:287:LEU:N | 1:A:287:LEU:HD12 | 2.31 | 0.45 |
| 1:A:493:PHE:C | 1:A:496:PRO:HD3 | 2.37 | 0.45 |
| 1:B:1326:GLN:OE1 | 1:B:1458:SER:HB2 | 2.17 | 0.45 |
| 1:B:1433:THR:CG2 | 1:B:1469:GLN:HB3 | 2.46 | 0.45 |
| 1:B:1585:ILE:HD13 | 1:B:1608:LEU:HD13 | 1.98 | 0.45 |
| 1:B:1279:GLN:OE1 | 1:B:1448:GLN:NE2 | 2.49 | 0.45 |
| 1:A:447:HIS:O | 1:A:449:GLY:N | 2.50 | 0.45 |
| 1:B:1358:LEU:O | 1:B:1361:GLN:HB3 | 2.15 | 0.45 |
| 1:A:531:LYS:HZ1 | 1:A:557:LYS:HE2 | 1.82 | 0.45 |
| 1:A:610:PHE:CD1 | 1:A:619:VAL:HG12 | 2.52 | 0.45 |
| 1:B:1201:GLN:O | 1:B:1204:GLU:HG3 | 2.16 | 0.45 |
| 1:B:1652:GLU:OE1 | 1:B:1652:GLU:HA | 2.16 | 0.45 |
| 1:A:443:THR:O | 1:A:454:LEU:HB2 | 2.16 | 0.45 |
| 1:B:1362:LEU:HD11 | 1:B:1445:VAL:HG22 | 1.98 | 0.45 |
| 1:B:1139:GLU:HA | 1:B:1142:GLN:CG | 2.43 | 0.45 |
| 1:A:532:LEU:HD12 | 1:A:561:PHE:HE2 | 1.79 | 0.45 |
| 1:A:596:ALA:HB1 | 1:B:1535:PRO:HB3 | 1.97 | 0.45 |
| 1:A:459:LEU:HD23 | 1:A:459:LEU:HA | 1.84 | 0.45 |
| 1:B:1521:SER:OG | 1:B:1524:GLN:HG2 | 2.16 | 0.45 |
| 1:A:283:LYS:HA | 1:A:286:GLU:CG | 2.47 | 0.45 |
| 1:A:330:PRO:HD2 | 1:A:344:GLN:O | 2.16 | 0.45 |
| 1:B:1336:PRO:O | 1:B:1337:LEU:HB2 | 2.16 | 0.45 |
| 1:B:1470:MET:CB | 1:B:1471:PRO:CD | 2.94 | 0.45 |
| 1:A:243:TRP:HE1 | 1:A:258:ILE:HB | 1.82 | 0.45 |
| 1:A:201:GLN:O | 1:A:203:LEU:N | 2.41 | 0.45 |
| 1:A:382:ARG:HB2 | 1:A:384:PHE:HE1 | 1.82 | 0.45 |
| 1:A:384:PHE:CD1 | 1:A:384:PHE:N | 2.85 | 0.45 |
| 1:B:1287:LEU:HD12 | 1:B:1287:LEU:N | 2.32 | 0.45 |
| 1:B:1503:GLN:HG3 | 1:B:1503:GLN:H | 1.49 | 0.45 |
| 1:B:1146:GLN:O | 1:B:1147:HIS:C | 2.54 | 0.45 |
| 1:B:1172:PHE:HB2 | 1:B:1206:MET:HE2 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:660:MET:CG | 1:A:666:LEU:HD12 | 2.47 | 0.45 |
| 1:B:1597:ILE:HD11 | 1:B:1622:THR:HG22 | 1.97 | 0.45 |
| 1:A:442:GLU:HG2 | 1:A:455:GLU:HB2 | 1.99 | 0.45 |
| 1:B:1622:THR:C | 1:B:1623:TRP:CD1 | 2.90 | 0.44 |
| 1:A:470:MET:HB3 | 1:A:471:PRO:CD | 2.33 | 0.44 |
| 1:A:277:THR:O | 1:A:281:ILE:HG12 | 2.16 | 0.44 |
| 1:B:1182:GLN:C | 1:B:1184:ASP:H | 2.21 | 0.44 |
| 1:A:521:SER:OG | 1:A:524:GLN:HG2 | 2.16 | 0.44 |
| 1:A:611:SER:N | 1:A:618:GLY:O | 2.43 | 0.44 |
| 1:B:1578:ALA:O | 1:B:1581:ASN:HB2 | 2.17 | 0.44 |
| 1:B:1523:GLU:CG | 1:B:1524:GLN:N | 2.80 | 0.44 |
| 1:B:1447:HIS:O | 1:B:1449:GLY:N | 2.50 | 0.44 |
| 1:B:1582:GLU:CD | 1:B:1582:GLU:N | 2.68 | 0.44 |
| 1:A:272:GLU:O | 1:A:276:GLN:HG3 | 2.17 | 0.44 |
| 1:A:409:LYS:HB2 | 1:A:409:LYS:HZ2 | 1.82 | 0.44 |
| 1:B:1442:GLU:HG2 | 1:B:1455:GLU:HB2 | 1.99 | 0.44 |
| 1:A:340:LYS:HE3 | 1:A:343:VAL:CG2 | 2.48 | 0.44 |
| 1:A:680:GLU:O | 1:A:684:GLY:HA3 | 2.17 | 0.44 |
| 1:A:652:GLU:OE1 | 1:A:652:GLU:HA | 2.17 | 0.44 |
| 1:A:431:ILE:O | 1:A:435:GLU:HB2 | 2.16 | 0.44 |
| 1:A:658:LYS:HE2 | 1:A:668:SER:HA | 2.00 | 0.44 |
| 1:A:656:GLY:O | 1:A:658:LYS:HE3 | 2.18 | 0.44 |
| 1:A:660:MET:HG3 | 1:A:666:LEU:HD12 | 1.99 | 0.44 |
| 1:B:1650:PHE:O | 1:B:1654:ILE:HG12 | 2.18 | 0.44 |
| 1:B:1643:GLN:O | 1:B:1646:ASN:HB2 | 2.18 | 0.44 |
| 1:A:482:MET:HE3 | 1:A:483:LEU:HD21 | 1.98 | 0.44 |
| 1:A:526:THR:C | 1:A:528:LEU:N | 2.71 | 0.44 |
| 1:A:285:GLU:HA | 1:A:288:GLN:HB2 | 2.00 | 0.44 |
| 1:A:503:GLN:H | 1:A:503:GLN:HG3 | 1.47 | 0.44 |
| 1:A:162:MET:O | 1:A:165:VAL:HG12 | 2.17 | 0.44 |
| 1:B:1652:GLU:OE2 | 1:B:1688:ARG:NE | 2.50 | 0.44 |
| 1:B:1610:PHE:CD1 | 1:B:1619:VAL:HG12 | 2.53 | 0.44 |
| 1:B:1685:LYS:HB2 | 1:B:1686:TYR:CD1 | 2.52 | 0.44 |
| 1:B:1531:LYS:NZ | 1:B:1557:LYS:HE2 | 2.33 | 0.44 |
| 1:A:336:PRO:O | 1:A:337:LEU:HB2 | 2.18 | 0.44 |
| 1:B:1205:GLN:C | 1:B:1207:LEU:N | 2.70 | 0.44 |
| 1:B:1589:ILE:HG23 | 1:B:1589:ILE:O | 2.17 | 0.44 |
| 1:B:1671:VAL:HG12 | 1:B:1679:LYS:HG2 | 2.00 | 0.44 |
| 1:B:1335:ARG:HB3 | 1:B:1470:MET:HE1 | 2.00 | 0.44 |
| 1:B:1162:MET:CE | 1:B:1283:LYS:HB3 | 2.47 | 0.44 |
| 1:A:214:ARG:NH2 | 1:A:287:LEU:HB3 | 2.33 | 0.44 |
| 1:A:589:ILE:HG23 | 1:A:589:ILE:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:671:VAL:HG12 | 1:A:679:LYS:HG2 | 2.00 | 0.44 |
| 1:B:1592:GLU:O | 1:B:1594:GLU:N | 2.51 | 0.44 |
| 1:B:1272:GLU:O | 1:B:1276:GLN:HG3 | 2.18 | 0.44 |
| 1:B:1382:ARG:HB2 | 1:B:1384:PHE:HE1 | 1.82 | 0.44 |
| 1:A:583:GLY:C | 1:A:585:ILE:N | 2.70 | 0.43 |
| 1:B:1243:TRP:HE1 | 1:B:1258:ILE:HB | 1.83 | 0.43 |
| 1:A:225:LEU:CD2 | 1:A:308:ARG:HB3 | 2.48 | 0.43 |
| 1:B:1663:THR:O | 1:B:1665:ILE:HG13 | 2.17 | 0.43 |
| 1:A:256:PRO:HB2 | 1:A:257:ASN:H | 1.66 | 0.43 |
| 1:B:1284:LEU:HD23 | 1:B:1284:LEU:HA | 1.83 | 0.43 |
| 1:B:1441:PHE:N | 1:B:1441:PHE:CD1 | 2.85 | 0.43 |
| 1:A:340:LYS:O | 1:A:343:VAL:HG23 | 2.18 | 0.43 |
| 1:B:1533:LEU:HD21 | 1:B:1544:ILE:HG12 | 1.99 | 0.43 |
| 1:B:1576:ILE:HA | 1:B:1579:LEU:HB2 | 1.99 | 0.43 |
| 1:B:1255:PRO:HA | 1:B:1256:PRO:HD2 | 1.82 | 0.43 |
| 1:A:447:HIS:O | 1:A:448:GLN:C | 2.56 | 0.43 |
| 1:B:1340:LYS:O | 1:B:1343:VAL:HG23 | 2.19 | 0.43 |
| 1:B:1214:ARG:NH2 | 1:B:1287:LEU:HB3 | 2.33 | 0.43 |
| 1:B:1651:ALA:HB3 | 1:B:1688:ARG:NH2 | 2.31 | 0.43 |
| 1:A:279:GLN:HE21 | 1:A:282:LYS:HD2 | 1.82 | 0.43 |
| 1:B:1531:LYS:HZ1 | 1:B:1557:LYS:HE2 | 1.84 | 0.43 |
| 1:A:578:ALA:O | 1:A:581:ASN:HB2 | 2.18 | 0.43 |
| 1:B:1592:GLU:C | 1:B:1594:GLU:N | 2.72 | 0.43 |
| 1:B:1651:ALA:O | 1:B:1655:MET:HG2 | 2.18 | 0.43 |
| 1:B:1681:GLU:O | 1:B:1685:LYS:CE | 2.66 | 0.43 |
| 1:A:361:GLN:HG2 | 1:A:361:GLN:O | 2.19 | 0.43 |
| 1:A:650:PHE:CE2 | 1:A:654:ILE:HD11 | 2.52 | 0.43 |
| 1:A:364:ILE:CD1 | 1:A:443:THR:HG21 | 2.49 | 0.43 |
| 1:B:1384:PHE:N | 1:B:1384:PHE:CD1 | 2.86 | 0.43 |
| 1:A:523:GLU:CG | 1:A:524:GLN:N | 2.81 | 0.43 |
| 1:A:685:LYS:HE3 | 1:A:686:TYR:CE2 | 2.52 | 0.43 |
| 1:B:1225:LEU:CD2 | 1:B:1308:ARG:HB3 | 2.48 | 0.43 |
| 1:A:592:GLU:O | 1:A:594:GLU:N | 2.51 | 0.43 |
| 1:A:619:VAL:HG23 | 1:A:650:PHE:CE1 | 2.53 | 0.43 |
| 1:A:205:GLN:O | 1:A:207:LEU:N | 2.51 | 0.43 |
| 1:A:308:ARG:O | 1:A:311:GLU:HB3 | 2.18 | 0.43 |
| 1:A:136:VAL:HG22 | 1:A:137:VAL:N | 2.34 | 0.43 |
| 1:A:470:MET:CB | 1:A:471:PRO:CD | 2.95 | 0.43 |
| 1:A:432:VAL:C | 1:A:434:GLU:H | 2.22 | 0.43 |
| 1:B:1623:TRP:CB | 1:B:1670:LEU:HG | 2.49 | 0.42 |
| 1:B:1201:GLN:HA | 1:B:1204:GLU:OE1 | 2.19 | 0.42 |
| 1:A:205:GLN:O | 1:A:208:THR:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:288:GLN:HE22 | 1:A:302:ARG:HH21 | 1.67 | 0.42 |
| 1:A:253:GLY:O | 1:A:510:TRP:HB3 | 2.19 | 0.42 |
| 1:B:1671:VAL:HG12 | 1:B:1679:LYS:NZ | 2.33 | 0.42 |
| 1:A:512:PHE:O | 1:A:516:THR:OG1 | 2.29 | 0.42 |
| 1:A:621:PHE:CZ | 1:A:637:VAL:CG1 | 3.03 | 0.42 |
| 1:B:1340:LYS:HE3 | 1:B:1343:VAL:CG2 | 2.48 | 0.42 |
| 1:B:1205:GLN:O | 1:B:1208:THR:N | 2.52 | 0.42 |
| 1:A:623:TRP:NE1 | 1:A:635:GLN:O | 2.53 | 0.42 |
| 1:B:1466:ASN:ND2 | 1:B:1467:ILE:H | 2.18 | 0.42 |
| 1:A:575:TYR:CB | 1:A:576:ILE:HD12 | 2.49 | 0.42 |
| 1:A:283:LYS:HA | 1:A:283:LYS:HD2 | 1.83 | 0.42 |
| 1:B:1359:ASN:O | 1:B:1360:TYR:HB2 | 2.19 | 0.42 |
| 1:A:655:MET:HG3 | 1:A:687:CYS:SG | 2.59 | 0.42 |
| 1:A:576:ILE:HA | 1:A:579:LEU:HB2 | 2.00 | 0.42 |
| 1:A:285:GLU:HB2 | 1:A:302:ARG:HD3 | 2.01 | 0.42 |
| 1:A:515:THR:HG21 | 1:A:573:LYS:CG | 2.49 | 0.42 |
| 1:B:1515:THR:HG21 | 1:B:1573:LYS:CG | 2.48 | 0.42 |
| 1:B:1482:MET:HE3 | 1:B:1483:LEU:HD21 | 2.01 | 0.42 |
| 1:A:643:GLN:O | 1:A:646:ASN:HB2 | 2.19 | 0.42 |
| 1:A:580:TRP:CD1 | 1:A:580:TRP:C | 2.91 | 0.42 |
| 1:A:221:LEU:CD1 | 1:A:281:ILE:HD13 | 2.33 | 0.42 |
| 1:A:592:GLU:C | 1:A:594:GLU:N | 2.73 | 0.42 |
| 1:B:1609:ARG:HH11 | 1:B:1620:THR:CG2 | 2.32 | 0.42 |
| 1:B:1606:PHE:CZ | 1:B:1679:LYS:HB3 | 2.55 | 0.42 |
| 1:A:263:LEU:O | 1:A:267:ILE:CG1 | 2.68 | 0.42 |
| 1:B:1447:HIS:O | 1:B:1448:GLN:C | 2.58 | 0.42 |
| 1:A:206:MET:O | 1:A:210:LEU:HG | 2.19 | 0.42 |
| 1:A:531:LYS:NZ | 1:A:557:LYS:HE2 | 2.33 | 0.42 |
| 1:A:254:GLY:HA2 | 1:A:510:TRP:CD2 | 2.55 | 0.42 |
| 1:A:388:GLY:O | 1:A:390:ASN:N | 2.53 | 0.42 |
| 1:A:654:ILE:HD13 | 1:A:683:PHE:CE1 | 2.54 | 0.42 |
| 1:A:445:VAL:HB | 1:A:452:ILE:CG2 | 2.50 | 0.42 |
| 1:B:1256:PRO:HB2 | 1:B:1257:ASN:H | 1.67 | 0.42 |
| 1:B:1196:THR:HG22 | 1:B:1197:ARG:N | 2.34 | 0.42 |
| 1:A:382:ARG:HB2 | 1:A:384:PHE:CE1 | 2.55 | 0.42 |
| 1:B:1172:PHE:N | 1:B:1206:MET:HE1 | 2.35 | 0.42 |
| 1:A:591:LYS:CE | 1:A:609:ARG:NH2 | 2.77 | 0.42 |
| 1:A:658:LYS:CE | 1:A:668:SER:HA | 2.50 | 0.42 |
| 1:A:623:TRP:HB2 | 1:A:670:LEU:HG | 2.01 | 0.42 |
| 1:B:1279:GLN:HE21 | 1:B:1282:LYS:HD2 | 1.83 | 0.42 |
| 1:A:409:LYS:CB | 1:A:409:LYS:NZ | 2.83 | 0.42 |
| 1:A:368:ILE:CD1 | 1:A:413:LEU:HD21 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1331:MET:HE2 | 1:B:1331:MET:HA | 2.02 | 0.42 |
| 1:A:281:ILE:HD12 | 1:A:305:LEU:HB3 | 2.02 | 0.42 |
| 1:B:1283:LYS:HA | 1:B:1286:GLU:CG | 2.45 | 0.42 |
| 1:A:530:GLU:C | 1:A:532:LEU:N | 2.73 | 0.42 |
| 1:B:1517:LYS:HE2 | 1:B:1581:ASN:OD1 | 2.20 | 0.42 |
| 1:B:1518:ARG:HG2 | 1:B:1519:GLY:O | 2.19 | 0.42 |
| 1:B:1526:THR:C | 1:B:1528:LEU:N | 2.72 | 0.42 |
| 1:B:1205:GLN:O | 1:B:1207:LEU:N | 2.53 | 0.42 |
| 1:B:1598:LEU:HD13 | 1:B:1623:TRP:HA | 2.02 | 0.41 |
| 1:B:1540:SER:C | 1:B:1542:CYS:H | 2.23 | 0.41 |
| 1:A:621:PHE:CE1 | 1:A:637:VAL:HB | 2.54 | 0.41 |
| 1:B:1368:ILE:O | 1:B:1369:ASP:HB2 | 2.20 | 0.41 |
| 1:B:1169:GLN:O | 1:B:1169:GLN:HG2 | 2.20 | 0.41 |
| 1:A:180:LYS:O | 1:A:180:LYS:HG2 | 2.20 | 0.41 |
| 1:B:1379:ARG:C | 1:B:1379:ARG:HD3 | 2.41 | 0.41 |
| 1:A:246:ARG:NH1 | 1:A:258:ILE:HA | 2.35 | 0.41 |
| 1:A:362:LEU:HD23 | 1:A:362:LEU:HA | 1.77 | 0.41 |
| 1:A:205:GLN:O | 1:A:206:MET:C | 2.59 | 0.41 |
| 1:B:1180:LYS:O | 1:B:1180:LYS:HG2 | 2.19 | 0.41 |
| 1:A:506:GLU:O | 1:A:509:SER:HB3 | 2.20 | 0.41 |
| 1:B:1181:SER:O | 1:B:1182:GLN:HB3 | 2.20 | 0.41 |
| 1:B:1283:LYS:HA | 1:B:1283:LYS:HD2 | 1.85 | 0.41 |
| 1:A:245:ARG:HD3 | 1:A:485:ASN:HB3 | 2.02 | 0.41 |
| 1:B:1368:ILE:HG21 | 1:B:1385:ASN:HA | 2.02 | 0.41 |
| 1:A:154:ARG:HB2 | 1:A:224:LEU:HD13 | 2.02 | 0.41 |
| 1:B:1601:LYS:HB3 | 1:B:1602:PRO:CD | 2.43 | 0.41 |
| 1:A:335:ARG:HA | 1:A:335:ARG:HD3 | 1.90 | 0.41 |
| 1:A:332:HIS:HE1 | 1:A:467:ILE:HD11 | 1.84 | 0.41 |
| 1:A:260:LEU:HB2 | 1:A:350:ARG:NH2 | 2.35 | 0.41 |
| 1:A:172:PHE:C | 1:A:172:PHE:CD2 | 2.94 | 0.41 |
| 1:B:1530:GLU:C | 1:B:1532:LEU:N | 2.74 | 0.41 |
| 1:A:304:MET:HA | 1:A:304:MET:HE1 | 2.02 | 0.41 |
| 1:A:602:PRO:O | 1:A:603:PRO:C | 2.59 | 0.41 |
| 1:A:146:GLN:O | 1:A:149:GLN:N | 2.52 | 0.41 |
| 1:A:340:LYS:HA | 1:A:464:ILE:HG13 | 2.03 | 0.41 |
| 1:B:1409:LYS:NZ | 1:B:1409:LYS:CB | 2.84 | 0.41 |
| 1:A:245:ARG:HH11 | 1:A:485:ASN:HB3 | 1.85 | 0.41 |
| 1:B:1382:ARG:HB2 | 1:B:1384:PHE:CE1 | 2.55 | 0.41 |
| 1:B:1433:THR:HG21 | 1:B:1472:ASN:HB2 | 2.03 | 0.41 |
| 1:A:535:PRO:CG | 1:B:1600:THR:HB | 2.47 | 0.41 |
| 1:B:1670:LEU:N | 1:B:1670:LEU:HD22 | 2.11 | 0.41 |
| 1:A:279:GLN:OE1 | 1:A:448:GLN:OE1 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1252:ILE:HG23 | 1:B:1481:ASN:ND2 | 2.34 | 0.41 |
| 1:A:623:TRP:HH2 | 1:A:659:ILE:HG21 | 1.86 | 0.41 |
| 1:A:466:ASN:ND2 | 1:A:467:ILE:H | 2.19 | 0.41 |
| 1:A:309:ILE:C | 1:A:309:ILE:HD13 | 2.40 | 0.41 |
| 1:A:604:GLY:HA2 | 1:A:670:LEU:HB3 | 2.01 | 0.41 |
| 1:B:1677:ILE:HG13 | 1:B:1677:ILE:H | 1.67 | 0.41 |
| 1:B:1470:MET:HB3 | 1:B:1471:PRO:CD | 2.33 | 0.41 |
| 1:A:280:GLN:CA | 1:A:280:GLN:HE21 | 2.13 | 0.41 |
| 1:B:1524:GLN:HE21 | 1:B:1524:GLN:HB3 | 1.59 | 0.41 |
| 1:B:1246:ARG:NH1 | 1:B:1258:ILE:HA | 2.36 | 0.41 |
| 1:B:1285:GLU:HA | 1:B:1288:GLN:HB2 | 2.02 | 0.41 |
| 1:A:284:LEU:C | 1:A:286:GLU:H | 2.24 | 0.41 |
| 1:A:522:ILE:CD1 | 1:A:522:ILE:H | 2.13 | 0.41 |
| 1:B:1172:PHE:C | 1:B:1172:PHE:CD2 | 2.95 | 0.41 |
| 1:B:1195:VAL:HG11 | 1:B:1200:MET:CE | 2.51 | 0.41 |
| 1:B:1308:ARG:O | 1:B:1311:GLU:HB3 | 2.21 | 0.41 |
| 1:B:1234:THR:O | 1:B:1238:GLU:HB2 | 2.21 | 0.41 |
| 1:A:240:LEU:HD13 | 1:A:263:LEU:HD13 | 2.02 | 0.40 |
| 1:B:1243:TRP:CZ2 | 1:B:1260:LEU:HD21 | 2.56 | 0.40 |
| 1:B:1196:THR:CB | 1:B:1199:LYS:HB2 | 2.49 | 0.40 |
| 1:B:1361:GLN:HG2 | 1:B:1361:GLN:O | 2.20 | 0.40 |
| 1:A:337:LEU:HD22 | 1:A:461:VAL:HG23 | 2.03 | 0.40 |
| 1:B:1314:ARG:CA | 1:B:1452:ILE:HD11 | 2.44 | 0.40 |
| 1:A:288:GLN:NE2 | 1:A:302:ARG:HE | 2.20 | 0.40 |
| 1:B:1365:LYS:HA | 1:B:1391:THR:HG22 | 2.01 | 0.40 |
| 1:B:1277:THR:O | 1:B:1281:ILE:HG13 | 2.21 | 0.40 |
| 1:B:1388:GLY:O | 1:B:1390:ASN:N | 2.54 | 0.40 |
| 1:B:1459:LEU:HD23 | 1:B:1459:LEU:HA | 1.84 | 0.40 |
| 1:A:359:ASN:O | 1:A:360:TYR:HB2 | 2.21 | 0.40 |
| 1:B:1335:ARG:N | 1:B:1336:PRO:CD | 2.84 | 0.40 |
| 1:B:1576:ILE:HG23 | 1:B:1579:LEU:HB2 | 2.03 | 0.40 |
| 1:A:526:THR:C | 1:A:528:LEU:H | 2.23 | 0.40 |
| 1:B:1228:MET:HE1 | 1:B:1274:GLN:N | 2.36 | 0.40 |
| 1:A:651:ALA:O | 1:A:655:MET:HG2 | 2.21 | 0.40 |
| 1:B:1496:PRO:HA | 1:B:1497:PRO:HD3 | 1.86 | 0.40 |
| 1:A:144:LEU:HA | 1:A:144:LEU:HD12 | 1.94 | 0.40 |
| 1:A:592:GLU:O | 1:A:595:ARG:N | 2.53 | 0.40 |
| 1:A:671:VAL:CG1 | 1:A:679:LYS:NZ | 2.84 | 0.40 |
| 1:B:1592:GLU:O | 1:B:1595:ARG:N | 2.53 | 0.40 |
| 1:B:1335:ARG:HA | 1:B:1335:ARG:HD3 | 1.91 | 0.40 |
| 1:A:243:TRP:CZ2 | 1:A:260:LEU:HD21 | 2.56 | 0.40 |
| 1:A:533:LEU:HD13 | 1:A:542:CYS:HB3 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:B:1683:PHE:O | 1:B:1687:CYS:SG | 2.80 | 0.40 |
| 1:A:337:LEU:HD13 | 1:A:460:PRO:O | 2.21 | 0.40 |
| 1:A:570:ASP:O | 1:A:574:LYS:HB2 | 2.21 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-------------------------|-------------|----------|
| 1:B:1575:TYR:OH | 1:B:1643:GLN:OE1[5_554] | 2.14 | 0.06 |

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|-----------|----------|-------------|----|
| 1 | A | 485/562 (86%) | 362 (75%) | 91 (19%) | 32 (7%) | 2 | 12 |
| 1 | B | 491/562 (87%) | 362 (74%) | 95 (19%) | 34 (7%) | 2 | 11 |
| All | All | 976/1124 (87%) | 724 (74%) | 186 (19%) | 66 (7%) | 2 | 11 |

All (66) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 256 | PRO |
| 1 | A | 368 | ILE |
| 1 | A | 555 | ALA |
| 1 | A | 557 | LYS |
| 1 | A | 667 | VAL |
| 1 | A | 676 | ASP |
| 1 | A | 679 | LYS |
| 1 | B | 1256 | PRO |
| 1 | B | 1555 | ALA |
| 1 | B | 1557 | LYS |
| 1 | B | 1584 | TYR |
| 1 | B | 1633 | GLN |
| 1 | B | 1664 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1667 | VAL |
| 1 | B | 1676 | ASP |
| 1 | B | 1679 | LYS |
| 1 | A | 542 | CYS |
| 1 | A | 584 | TYR |
| 1 | A | 587 | GLY |
| 1 | A | 600 | THR |
| 1 | A | 632 | THR |
| 1 | A | 645 | LEU |
| 1 | A | 657 | TYR |
| 1 | A | 666 | LEU |
| 1 | B | 1182 | GLN |
| 1 | B | 1542 | CYS |
| 1 | B | 1587 | GLY |
| 1 | B | 1600 | THR |
| 1 | B | 1645 | LEU |
| 1 | B | 1657 | TYR |
| 1 | B | 1666 | LEU |
| 1 | A | 202 | GLN |
| 1 | A | 369 | ASP |
| 1 | A | 593 | ARG |
| 1 | A | 670 | LEU |
| 1 | B | 1202 | GLN |
| 1 | B | 1593 | ARG |
| 1 | B | 1670 | LEU |
| 1 | A | 147 | HIS |
| 1 | A | 596 | ALA |
| 1 | A | 608 | LEU |
| 1 | A | 637 | VAL |
| 1 | B | 1147 | HIS |
| 1 | B | 1369 | ASP |
| 1 | B | 1608 | LEU |
| 1 | B | 1632 | THR |
| 1 | B | 1637 | VAL |
| 1 | A | 354 | LYS |
| 1 | A | 538 | ASN |
| 1 | A | 675 | PRO |
| 1 | B | 1354 | LYS |
| 1 | B | 1368 | ILE |
| 1 | B | 1538 | ASN |
| 1 | B | 1665 | ILE |
| 1 | B | 1675 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 206 | MET |
| 1 | A | 252 | ILE |
| 1 | A | 255 | PRO |
| 1 | B | 1252 | ILE |
| 1 | B | 1255 | PRO |
| 1 | B | 1495 | LYS |
| 1 | A | 495 | LYS |
| 1 | A | 576 | ILE |
| 1 | B | 1576 | ILE |
| 1 | A | 477 | ILE |
| 1 | B | 1477 | ILE |

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 | 458/505 (91%) | 416 (91%) | 42 (9%) | 13 | 45 |
| 1 | B | 464/505 (92%) | 422 (91%) | 42 (9%) | 14 | 46 |
| All | All | 922/1010 (91%) | 838 (91%) | 84 (9%) | 14 | 46 |

All (84) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 152 | ARG |
| 1 | A | 158 | LEU |
| 1 | A | 168 | LEU |
| 1 | A | 178 | THR |
| 1 | A | 201 | GLN |
| 1 | A | 203 | LEU |
| 1 | A | 204 | GLU |
| 1 | A | 218 | VAL |
| 1 | A | 229 | GLU |
| 1 | A | 235 | LEU |
| 1 | A | 242 | ASP |
| 1 | A | 280 | GLN |
| 1 | A | 287 | LEU |
| 1 | A | 304 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 309 | ILE |
| 1 | A | 350 | ARG |
| 1 | A | 379 | ARG |
| 1 | A | 397 | GLU |
| 1 | A | 453 | ASP |
| 1 | A | 503 | GLN |
| 1 | A | 515 | THR |
| 1 | A | 517 | LYS |
| 1 | A | 522 | ILE |
| 1 | A | 523 | GLU |
| 1 | A | 524 | GLN |
| 1 | A | 532 | LEU |
| 1 | A | 552 | GLU |
| 1 | A | 553 | ASN |
| 1 | A | 575 | TYR |
| 1 | A | 580 | TRP |
| 1 | A | 582 | GLU |
| 1 | A | 586 | MET |
| 1 | A | 592 | GLU |
| 1 | A | 623 | TRP |
| 1 | A | 632 | THR |
| 1 | A | 637 | VAL |
| 1 | A | 652 | GLU |
| 1 | A | 659 | ILE |
| 1 | A | 670 | LEU |
| 1 | A | 676 | ASP |
| 1 | A | 686 | TYR |
| 1 | A | 688 | ARG |
| 1 | B | 1152 | ARG |
| 1 | B | 1168 | LEU |
| 1 | B | 1178 | THR |
| 1 | B | 1182 | GLN |
| 1 | B | 1201 | GLN |
| 1 | B | 1203 | LEU |
| 1 | B | 1204 | GLU |
| 1 | B | 1218 | VAL |
| 1 | B | 1229 | GLU |
| 1 | B | 1235 | LEU |
| 1 | B | 1242 | ASP |
| 1 | B | 1280 | GLN |
| 1 | B | 1287 | LEU |
| 1 | B | 1304 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1350 | ARG |
| 1 | B | 1379 | ARG |
| 1 | B | 1397 | GLU |
| 1 | B | 1431 | ILE |
| 1 | B | 1453 | ASP |
| 1 | B | 1503 | GLN |
| 1 | B | 1515 | THR |
| 1 | B | 1517 | LYS |
| 1 | B | 1522 | ILE |
| 1 | B | 1523 | GLU |
| 1 | B | 1524 | GLN |
| 1 | B | 1532 | LEU |
| 1 | B | 1552 | GLU |
| 1 | B | 1553 | ASN |
| 1 | B | 1575 | TYR |
| 1 | B | 1580 | TRP |
| 1 | B | 1582 | GLU |
| 1 | B | 1586 | MET |
| 1 | B | 1592 | GLU |
| 1 | B | 1597 | ILE |
| 1 | B | 1621 | PHE |
| 1 | B | 1623 | TRP |
| 1 | B | 1637 | VAL |
| 1 | B | 1652 | GLU |
| 1 | B | 1670 | LEU |
| 1 | B | 1676 | ASP |
| 1 | B | 1686 | TYR |
| 1 | B | 1688 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 167 | ASN |
| 1 | A | 201 | GLN |
| 1 | A | 205 | GLN |
| 1 | A | 248 | GLN |
| 1 | A | 279 | GLN |
| 1 | A | 280 | GLN |
| 1 | A | 332 | HIS |
| 1 | A | 385 | ASN |
| 1 | A | 401 | ASN |
| 1 | A | 437 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 466 | ASN |
| 1 | A | 481 | ASN |
| 1 | A | 503 | GLN |
| 1 | A | 644 | GLN |
| 1 | B | 1167 | ASN |
| 1 | B | 1248 | GLN |
| 1 | B | 1279 | GLN |
| 1 | B | 1280 | GLN |
| 1 | B | 1332 | HIS |
| 1 | B | 1385 | ASN |
| 1 | B | 1390 | ASN |
| 1 | B | 1437 | HIS |
| 1 | B | 1466 | ASN |
| 1 | B | 1472 | ASN |
| 1 | B | 1481 | ASN |
| 1 | B | 1503 | GLN |
| 1 | B | 1644 | GLN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 | 501/562 (89%) | 0.06 | 0 | 100 | 100 | 43, 92, 127, 139 | 0 |
| 1 | B | 507/562 (90%) | 0.09 | 2 (0%) | 90 | 42 | 36, 101, 131, 143 | 0 |
| All | All | 1008/1124 (89%) | 0.07 | 2 (0%) | 93 | 56 | 36, 97, 130, 143 | 0 |

All (2) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1199 | LYS | 2.5 |
| 1 | B | 1198 | GLN | 2.3 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.