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| | | | | |
|----------------------|---|-----------|--------|---|
| All-Atom Contacts | Clashscore, all atoms: | 65.92 | | 1 st percentile* (N=1784, all resolutions) |
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 12 | 1.78% | Goal: <1% |
| | Ramachandran outliers | 16 | 2.09% | Goal: <0.05% |
| | Ramachandran favored | 652 | 85.34% | Goal: >98% |
| | MolProbity score [^] | 3.13 | | 18 th percentile * (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 4 | 0.55% | Goal: 0 |
| | Bad backbone bonds: | 20 / 6252 | 0.32% | Goal: 0% |
| | Bad backbone angles: | 92 / 8404 | 1.09% | Goal: <0.1% |

In the two column results, the left column gives the raw count, right column gives the percentage.

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

[^] MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|-------|---------|------------|----------------------------------|---|--|--------------------|---------------------|---------------------|
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| A 407 | ASN | 50 | 0.539Å OD1 with A 410 ARG HB2 | - | 55.3% (t-20) chi angles: 182.4,339 | 0.064Å | - | - |
| A 408 | ALA | 50 | - | OUTLIER (0.02%) General / -169.4,-38.8 | - | 0.062Å | - | - |
| A 409 | SER | 50 | 0.678Å HB2 with A 449 LYS HD2 | Favored (58.86%) General / -81.2,-6.5 | 80% (p) chi angles: 60 | 0.123Å | - | - |
| A 410 | ARG | 50 | 0.54Å HH21 with A 447 ASN CG | Favored (64.1%) General / | 12.9% (mtp180) chi angles: 305.2,211.5,68.4,156.6 | 0.071Å | - | - |

| | | | | | | | | |
|----------|-----|----|--|---|--|--------|---|---|
| A 411 | ALA | 50 | - | -71.8,-29.1 Favored (63.75%) General / -73.4,-41.0 | - | 0.05Å | - | - |
| A 412 | GLU | 50 | - | Favored (81.94%) General / -60.6,-37.6 | 11.8% (<i>tm-20</i>) chi angles: 179.8,287.2,328.8 | 0.068Å | - | - |
| A 413 | PHE | 50 | 0.448Å CD1 with A 445 TRP HE3 | Favored (44.22%) General / -65.1,-53.5 | 88.9% (<i>t80</i>) chi angles: 178.5,82.1 | 0.035Å | - | - |
| A 414 | GLN | 50 | 0.561Å HA with A 417 ILE HG12 | Favored (81.56%) General / -59.5,-38.8 | 15.6% (<i>mt-30</i>) chi angles: 282.6,140.6,20.4 | 0.016Å | - | - |
| A 415 | ALA | 50 | - | Favored (80.73%) General / -68.5,-40.6 | - | 0.039Å | - | - |
| A 416 | LYS | 50 | - | Favored (8.88%) General / -69.9,-55.8 | 13.8% (<i>tppt?</i>) chi angles: 177.9,49.7,62.1,192.2 | 0.03Å | - | - |
| A 417 | ILE | 50 | 0.737Å O with A 420 ILE HG12 | Favored (33.54%) Isoleucine or valine / -58.1,-28.1 | 30% (<i>pt</i>) chi angles: 69.4,172.7 | 0.078Å | - | - |
| A 418 | ASP | 50 | - | Favored (92.98%) General / -65.4,-41.9 | 44.5% (<i>t0</i>) chi angles: 186.9,329.5 | 0.038Å | - | - |
| A 419 | SER | 50 | - | Favored (97.46%) General / -61.8,-44.1 | 40.1% (<i>t</i>) chi angles: 181.5 | 0.038Å | - | - |
| A 420 | ILE | 50 | 0.737Å HG12 with A 417 ILE O | Favored (65.2%) Isoleucine or valine / -58.7,-37.4 | 16.4% (<i>pt</i>) chi angles: 71.3,180.5 | 0.072Å | - | OUTLIER(S) worst is CB- CG1-CD1: 4.186 σ |
| A 421 | LYS | 50 | 0.648Å HG3 with A 417 ILE O | Favored (90.34%) General / -65.2,-38.4 Favored | 30.7% (<i>mtpp</i>) chi angles: 294,181,68,63.9 | 0.047Å | - | - |

| A 422 | GLN | 50 | - | (54.03%) General / -77.6,-33.0 | 19% (<i>mt-30</i>) chi angles: 298,166.1,183.6 | 0.087Å | - | - |
|----------|---------|------------|--|--|---|--------------------|---------------------|---|
| A 423 | TYR | 50 | 0.446Å CE1 with C 453 GLU HG3 | Favored (99.6%) General / -62.0,-42.9 | 71.9% (<i>t80</i>) chi angles: 172.6,84.8 | 0.05Å | - | - |
| A 424 | MET | 50 | 0.993Å SD with A 437 VAL HG11 | Favored (70.48%) General / -71.4,-40.7 | 69.9% (<i>mtm</i>) chi angles: 293.7,191.9,299.6 | 0.05Å | - | - |
| A 425 | GLN | 50 | - | Favored (79.46%) General / -67.7,-35.7 | 53.4% (<i>tt0</i>) chi angles: 185.3,179.2,57 | 0.012Å | - | - |
| A 426 | PHE | 50 | - | Favored (79.94%) General / -64.8,-35.1 | 11% (<i>t80</i>) chi angles: 182.8,38.1 | 0.025Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| A 427 | ARG | 99.99 | 0.989Å HB3 with C 473 HIS HE1 | Favored (57.36%) General / -92.0,-1.2 | 32.8% (<i>mmt180</i>) chi angles: 287.3,304.8,183.2,180 | 0.21Å | - | OUTLIER(S) worst is N-CA- CB: 4.945 σ |
| A 428 | LYS | 50 | - | Favored (28.26%) General / 54.1,38.0 | 88.4% (<i>mttt</i>) chi angles: 298.3,170.7,185,166.6 | 0.051Å | - | - |
| A 429 | VAL | 50 | 0.942Å HG21 with A 433 LEU HD22 | Favored (5.58%) Isoleucine or valine / -61.0,152.8 | 12.1% (<i>p</i>) chi angles: 62.1 | 0.168Å | - | - |
| A 430 | THR | 50 | 0.448Å HG22 with A 432 ASP H | Favored (7.51%) General / -57.2,156.3 | 98.9% (<i>m</i>) chi angles: 298.8 | 0.05Å | - | - |
| A 431 | LYS | 50 | 0.444Å O with A 435 THR HG23 | Favored (82.42%) General / -66.9,-36.5 | 32.8% (<i>mmmt</i>) chi angles: 296.3,295.3,295.3,181.1 | 0.032Å | - | - |
| A 432 | ASP | 50 | 0.448Å H with A 430 | Favored (80.59%) General / | 85.2% (<i>m-20</i>) chi angles: 293.9,349.1 | 0.053Å | - | - |

| | | | | | | | | |
|----------|-----|-------|--|---|---|--------|--|--|
| | | | THR HG22 | -65.3,-35.3 | | | | |
| A 433 | LEU | 50 | 0.942Å HD22 with A 429 VAL HG21 | Favored (63.85%) General / -73.5,-40.7 | 8.5% (<i>tt</i>) chi angles: 191.4,155.1 | 0.12Å | - | - |
| A 434 | GLU | 50 | 0.791Å O with A 437 VAL HG12 | Favored (93.67%) General / -63.9,-39.2 | 54.6% (<i>mt-10</i>) chi angles: 296.7,182.7,298.2 | 0.075Å | - | - |
| A 435 | THR | 50 | 0.444Å HG23 with A 431 LYS O | Favored (68.27%) General / -66.1,-49.3 | 77.9% (<i>p</i>) chi angles: 60.2 | 0.02Å | - | - |
| A 436 | ARG | 50 | - | Favored (72.82%) General / -58.2,-36.2 | 86.8% (<i>mtm-85</i>) chi angles: 285.7,187.7,294.2,260.3 | 0.068Å | - | - |
| A 437 | VAL | 50 | 0.993Å HG11 with A 424 MET SD | Favored (68.54%) Isoleucine or valine / -72.0,-41.3 | 4.9% (<i>p</i>) chi angles: 76.4 | 0.175Å | - | - |
| A 438 | ILE | 50 | 0.781Å HG12 with A 434 GLU O | Favored (28.75%) Isoleucine or valine / -58.1,-54.7 | 41.1% (<i>mm</i>) chi angles: 299.1,304.7 | 0.028Å | - | - |
| A 439 | ARG | 50 | 0.448Å O with A 443 TYR HD2 | Favored (77.74%) General / -60.0,-36.6 | 55.1% (<i>mmm-85</i>) chi angles: 293.6,298,293,278.7 | 0.033Å | - | - |
| A 440 | TRP | 99.99 | 0.829Å CH2 with A 444 LEU HD22 | Favored (42.13%) General / -62.5,-54.3 | 89.3% (<i>t90</i>) chi angles: 184.8,87.4 | 0.024Å | OUTLIER(S) worst is NE1-- CE2: 4.896 σ | OUTLIER(S) worst is CZ2- CH2-CZ3: 5.444 σ |
| A 441 | PHE | 50 | 0.791Å HE2 with A 437 VAL HG22 | Favored (61.53%) General / -51.0,-46.1 | 95.2% (<i>m-85</i>) chi angles: 292.2,275.1 | 0.075Å | - | - |
| A 442 | ASP | 50 | 0.4Å HB2 with A 439 ARG O | Favored (67.79%) General / -53.0,-45.5 | 51.3% (<i>m-20</i>) chi angles: 295.5,296.5 | 0.044Å | - | - |
| A 443 | TYR | 50 | 0.539Å CD2 with A 573 TYR CE1 | Favored (60.59%) General / -75.2,-30.6 | 95.2% (<i>m-85</i>) chi angles: 292.2,274.8 | 0.027Å | - | - |

| A 444 | LEU | 99.99 | 0.829Å HD22 with A 440 TRP CH2 | Favored (22.95%) General / -84.8,-33.5 | 21.3% (<i>tp</i>) chi angles: 187.1,74 | 0.098Å | - | - |
|----------|---------|------------|---|--|---|--------------------|--|--|
| A 445 | TRP | 50 | 0.453Å NE1 with A 444 LEU HD23 | Favored (8.95%) General / -119.4,-16.7 | 51.6% (<i>m0</i>) chi angles: 296.7,351.6 | 0.079Å | OUTLIER(S) worst is NE1-- CE2: 4.813 σ | OUTLIER(S) worst is CD2- CE3-CZ3: 4.178 σ |
| A 446 | ALA | 50 | - | Allowed (0.65%) General / 51.6,18.1 | - | 0.046Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| A 447 | ASN | 99.99 | 0.54Å CG with A 410 ARG HH21 | Favored (10.13%) General / 56.4,25.9 | 64.3% (<i>t-20</i>) chi angles: 184.8,348.6 | 0.098Å | - | OUTLIER(S) worst is OD1- CG-ND2: 5.744 σ |
| A 448 | LYS | 99.99 | - | Allowed (0.73%) General / -106.2,-72.1 | 29.5% (<i>tptp</i>) chi angles: 182.4,64.6,177.9,64.7 | 0.064Å | - | - |
| A 449 | LYS | 99.99 | 0.678Å HD2 with A 409 SER HB2 | Favored (49.15%) General / -125.2,147.2 | 27.9% (<i>tptp</i>) chi angles: 180.1,66.8,182.2,61.8 | 0.079Å | - | OUTLIER(S) worst is CG- CD-CE: 4.395 σ |
| A 450 | THR | 99.99 | 0.721Å HG22 with A 451 VAL H | Allowed (0.82%) General / -119.5,-160.6 | 48.8% (<i>m</i>) chi angles: 305 | 0.108Å | - | - |
| A 451 | VAL | 99.99 | 1.05Å HG22 with A 452 ASP HA | Allowed (0.43%) Isoleucine or valine / -48.1,151.1 | 6% (<i>p</i>) chi angles: 75 | 0.168Å | - | - |
| A 452 | ASP | 50 | 1.05Å HA with A 451 VAL HG22 | Allowed (1%) General / -104.9,44.8 | 2.2% (<i>m-20</i>) chi angles: 294.9,33.2 | 0.139Å | - | - |
| A 453 | GLU | 50 | 0.823Å HA with A 456 VAL HG22 | Allowed (0.61%) General / -40.4,-36.9 | 27.2% (<i>tt0</i>) chi angles: 193.5,193.3,40.1 | 0.049Å | - | - |
| A 454 | LYS | 50 | - | Favored (79.07%) General / 62.4,48.1 | 39% (<i>ttpt</i>) chi angles: 186.5,180,64.3,181.3 | 0.042Å | - | - |

| | | | | | | | | |
|----------|-----|----|---|---|---|--------|---|--|
| A 455 | GLU | 50 | 0.766Å HB3 with A 452 ASP HB3 | -63.4,-48.1 Favored (76.52%) General / -65.6,-47.2 | 10.8% (<i>tm-20</i>) chi angles: 181.5,289.9,325.1 | 0.055Å | - | - |
| A 456 | VAL | 50 | 0.823Å HG22 with A 453 GLU HA | Favored (84.79%) Isoleucine or valine / -58.1,-43.2 | 23.1% (<i>m</i>) chi angles: 302.6 | 0.057Å | - | - |
| A 457 | LEU | 50 | 0.485Å HB2 with A 453 GLU O | Favored (84.41%) General / -67.7,-40.6 | 0.6% chi angles: 254.3,39.5 | 0.031Å | - | - |
| A 458 | LYS | 50 | - | Favored (91.56%) General / -61.5,-39.6 | 28.6% (<i>tptp</i>) chi angles: 184.7,62.4,180.5,64.5 | 0.039Å | - | - |
| A 459 | SER | 50 | 0.646Å O with D 440 TRP CH2 | Favored (81.83%) General / -64.3,-35.7 | 68.7% (<i>m</i>) chi angles: 296.1 | 0.096Å | - | OUTLIER(S) worst is CA-C- O: 5.259 σ |
| A 460 | LEU | 50 | - | Favored (39.39%) Pre-proline / -70.6,166.1 | 80.5% (<i>mt</i>) chi angles: 298.8,182.5 | 0.042Å | - | - |
| A 461 | PRO | 50 | 0.782Å HD3 with D 440 TRP CE2 | Favored (6.38%) Trans-proline / -87.5,171.2 | 42.7% (<i>Cg_endo</i>) chi angles: 36 | 0.014Å | - | - |
| A 462 | ASP | 50 | - | Favored (96.91%) General / -63.9,-43.1 | 42.1% (<i>t0</i>) chi angles: 190.5,329.5 | 0.015Å | - | - |
| A 463 | LYS | 50 | 0.667Å HE2 with D 508 TYR H | Favored (73.89%) General / -57.9,-37.4 | 32.4% (<i>mmmt</i>) chi angles: 294.8,293.5,296.6,184.8 | 0.04Å | - | - |
| A 464 | LEU | 50 | 0.654Å HD12 with A 461 PRO HD2 | Favored (22.9%) General / -75.5,-48.4 | 59.3% (<i>mt</i>) chi angles: 286.4,177.4 | 0.038Å | - | - |
| A 465 | LYS | 50 | 0.581Å O with A 470 ILE HG12 | Favored (72.81%) General / -61.0,-33.1 | 54.9% (<i>mtmt</i>) chi angles: 294.7,178.6,295.9,178.8 | 0.136Å | - | - |
| A 466 | ALA | 50 | 0.722Å HA with A | Favored (83.81%) General / | | 0.110Å | - | - |

| 466 | ALA | 50 | HA with A 470 ILE CB | General / -66.6,-36.9 | - | 0.119Å | - | - |
|---|---------|--------|------------------------------------|---|--|--------------|---|--|
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: Clashscore: Outliers: 16 of Poor rotamers: 12 of Outliers: Outliers: 12 Outliers: 64 61.33 65.92 764 676 4 of 728 of 772 of 772 | | | | | | | | |
| A 467 | GLU | 50 | 0.589Å OE2 with D 433 LEU HD12 | Favored (79.53%) General / -68.8,-40.5 | 15.5% (<i>tt</i>) chi angles: 206.1,191.3,309.1 | 0.116Å | - | - |
| A 468 | ILE | 99.99 | 0.871Å HA with A 472 VAL HG12 | Favored (24.37%) Isoleucine or valine / -119.2,146.1 | 17.8% (<i>pt</i>) chi angles: 51.7,179.6 | 0.185Å | - | - |
| A 469 | ALA | 99.99 | 0.914Å H with A 473 HIS HD2 | Allowed (1.8%) General / 66.3,0.8 | - | 0.078Å | - | - |
| A 470 | ILE | 99.99 | 0.978Å HD12 with A 496 LEU HA | Allowed (0.75%) Isoleucine or valine / -132.4,-25.7 | 27.1% (<i>mm</i>) chi angles: 299,310.2 | 0.091Å | - | - |
| A 471 | ASN | 50 | 1.003Å HD21 with A 492 VAL HG12 | Allowed (0.47%) General / -140.4,-51.1 | 42.2% (<i>m-20</i>) chi angles: 278.7,302.3 | 0.195Å | - | OUTLIER(S) worst is CA-CB-CG: 4.049 σ |
| A 472 | VAL | 50 | 0.871Å HG12 with A 468 ILE HA | Favored (82.17%) Isoleucine or valine / -58.6,-41.5 | 15% (<i>p</i>) chi angles: 63.5 | 0.065Å | - | - |
| A 473 | HIS | 50 | 1.002Å HE1 with D 427 ARG HB3 | Favored (61.3%) General / -72.7,-25.5 | 84.1% (<i>m-70</i>) chi angles: 288,298.1 | 0.04Å | OUTLIER(S) worst is CD2--NE2: 7.05 σ | OUTLIER(S) worst is CD2-NE2-CE1: 12.768 σ |
| A 474 | LEU | 99.99 | 0.694Å C with A 474 LEU HD23 | Favored (38.13%) General / -53.1,132.5 | 7.2% (<i>tt</i>) chi angles: 184.9,162.9 | 0.126Å | - | - |
| A 475 | ASP | 99.99 | 0.527Å N with A 474 LEU HD23 | Favored (5.85%) General / -129.7,12.7 | 29.9% (<i>t70</i>) chi angles: 179.1,76.5 | 0.069Å | - | - |
| A 476 | THR | 99.99 | 0.473Å HB with A 522 ASN HA | Favored (2.21%) General / | 10.3% (<i>t</i>) chi angles: 184.2 | 0.074Å | - | - |

| 4/6 | | 523 ASX 11A | | General / | chi angles: 104.2 | | | | |
|-----|---------|-------------|--|--|---|-----------------|-----------------|----------------|---|
| | | | | -136.0,48.0 | | | | | |
| A | LEU | 99.99 | 1.1Å HG with A 483 PHE HB3 | Allowed (0.81%) General / -134.6,-52.3 | 10% (<i>tt</i>) chi angles: 185.3,154.6 | 0.239Å | - | - | |
| A | LYS | 50 | - | Favored (31.44%) General / -53.1,-29.6 | 27.1% (<i>tptp</i>) chi angles: 180.3,61.9,184.6,69.5 | 0.035Å | - | - | |
| A | LYS | 50 | - | Favored (49.45%) General / -89.1,-9.9 | 26.8% (<i>tptp</i>) chi angles: 188.6,61.2,182.7,67.3 | 0.051Å | - | - | |
| A | VAL | 50 | 1.093Å HG12 with A 477 LEU HA | Favored (23.98%) Isoleucine or valine / -117.0,108.1 | 11.5% (<i>p</i>) chi angles: 66.5 | 0.141Å | - | - | |
| A | ARG | 50 | 0.715Å HA with A 484 GLN HG2 | Favored (7.28%) General / -43.5,-47.1 | 57.9% (<i>mmm-85</i>) chi angles: 296.1,292.8,296.7,277.2 | 0.027Å | - | - | |
| A | ILE | 50 | 0.744Å HG12 with A 480 VAL HG22 | Favored (87.84%) Isoleucine or valine / -59.3,-42.6 | 42.2% (<i>pt</i>) chi angles: 65.5,172.5 | 0.067Å | - | - | |
| A | PHE | 50 | 1.1Å HB3 with A 477 LEU HG | Favored (28.76%) General / -79.7,-40.6 | 7.1% (<i>m-30</i>) chi angles: 278.5,9.7 | 0.047Å | - | | OUTLIER(S) worst is CA- CB-CG: 4.414 σ |
| A | GLN | 50 | 0.715Å HG2 with A 481 ARG HA | Favored (83.93%) General / -67.8,-38.8 | 19.8% (<i>pt20</i>) chi angles: 65.9,181.7,61.9 | 0.076Å | - | - | |
| A | ASP | 50 | - | Favored (4.67%) General / -97.0,26.4 | 48.7% (<i>t0</i>) chi angles: 190.7,338.3 | 0.039Å | - | - | |
| A | CYS | 99.99 | 0.624Å SG with A 490 LEU HD23 | Favored (27.27%) General / -115.1,155.3 | 52.7% (<i>t</i>) chi angles: 181.3 | 0.052Å | - | - | |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | |

Avg: Clashscore: Outliers: 16 of Poor rotamers: 12 of Outliers: Outliers: 12 Outliers: 64

61.22

65.02

76.4

676

4 of 729

6 of 772

6 of 772

| | 01.55 | | 05.92 | / 04 | 0/0 | 4 01 / 20 | 01 / / 2 | 01 / / 2 |
|----------|-----------|-------|--|---|--|-----------|----------|---|
| A 487 | GLU 99.99 | | - | Favored (8.68%) General / -57.2,120.8 | 87.8% (<i>mt-10</i>) chi angles: 301.3,182.2,337.1 | 0.064Å | - | - |
| A 488 | ALA | 50 | 0.728Å O with A 492 VAL HG13 | Favored (14.29%) General / -54.9,-22.3 | - | 0.016Å | - | - |
| A 489 | GLY | 50 | 0.497Å O with A 492 VAL HG22 | Favored (76.39%) Glycine / -67.5,-45.6 | - | - | - | - |
| A 490 | LEU | 99.99 | 0.748Å HD13 with A 591 TYR CD1 | Favored (93.9%) General / -65.5,-41.0 | 35.4% (<i>tp</i>) chi angles: 175.6,54.2 | 0.063Å | - | - |
| A 491 | LEU | 99.99 | 0.838Å HD13 with A 477 LEU HD11 | Favored (5.02%) General / -57.2,-59.5 | 94.3% (<i>mt</i>) chi angles: 298.4,175.6 | 0.075Å | - | - |
| A 492 | VAL | 50 | 1.003Å HG12 with A 471 ASN HD21 | Favored (14.91%) Isoleucine or valine / -48.6,-45.5 | 25.8% (<i>m</i>) chi angles: 302 | 0.023Å | - | - |
| A 493 | GLU | 50 | - | Favored (68.49%) General / -66.1,-28.0 | 14.3% (<i>tm-20</i>) chi angles: 183.8,285.3,333.8 | 0.107Å | - | - |
| A 494 | LEU | 50 | 0.701Å HD23 with A 483 PHE CE1 | Favored (12.94%) General / -80.0,-48.7 | 33.9% (<i>tp</i>) chi angles: 187.7,59.4 | 0.033Å | - | OUTLIER(S) worst is CD1- CG-CD2: 4.562 σ |
| A 495 | VAL | 50 | 0.758Å HG21 with A 470 ILE O | Favored (44.55%) Isoleucine or valine / -57.7,-33.2 | 20.8% (<i>m</i>) chi angles: 303.3 | 0.021Å | - | - |
| A 496 | LEU | 50 | 0.978Å HA with A 470 ILE HD12 | Favored (55.61%) General / -64.8,-13.4 | 8.9% (<i>tt</i>) chi angles: 190.5,154.5 | 0.155Å | - | - |
| A 497 | LYS | 50 | - | Favored (10.85%) General / -115.9,-18.0 | 64.5% (<i>mttp</i>) chi angles: 295.5,177.2,177.3,63.2 | 0.054Å | - | - |
| A | LEU | 50 | 0.640Å | Favored (44.40%) | 58.40% (<i>mt</i>) | 0.006Å | | |

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|----------|-----|----|-------------------------------------|--|---|--------|---|---|
| A 498 | LEU | 50 | 0.047Å HB3 with A 577 PHE HB3 | (44.47%) General / -58.6,144.1 | 50.4% (ttt) chi angles: 305.2,173.5 | 0.096Å | - | - |
| A 499 | ARG | 50 | - | Favored (28.15%) Pre-proline / -118.9,124.7 | 40.1% (ptt180) chi angles: 62,179.4,181.4,181.7 | 0.069Å | - | - |
| A 500 | PRO | 50 | - | Favored (33.33%) Trans-proline / -68.0,134.9 | 92.8% (Cg_endo) chi angles: 30.9 | 0.035Å | - | - |
| A 501 | THR | 50 | - | Favored (30.25%) General / -144.9,142.9 | 63.4% (p) chi angles: 62.2 | 0.038Å | - | - |
| A 502 | VAL | 50 | - | Favored (36.42%) Isoleucine or valine / -115.5,140.6 | 74% (t) chi angles: 174 | 0.052Å | - | - |
| A 503 | PHE | 50 | - | Favored (50.81%) General / -127.0,145.2 | 63.9% (m-85) chi angles: 284.3,87.2 | 0.046Å | - | - |
| A 504 | SER | 50 | - | Favored (31.54%) Pre-proline / -101.6,158.6 | 70.2% (m) chi angles: 295.9 | 0.029Å | - | - |
| A 505 | PRO | 50 | - | Favored (52.29%) Trans-proline / -53.9,132.9 | 87.8% (Cg_exo) chi angles: 331.3 | 0.109Å | - | - |
| A 506 | GLY | 50 | - | Favored (9.88%) Glycine / 100.2,-30.6 | - | - | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|----------|-----|-----|------------------------------------|--|--|--------------------------|--------------------|---------------------|---------------------|
| Avg: | | | 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| A 507 | ASP | 50 | 0.454Å HA with C 463 LYS HE2 | Allowed (0.56%) General / -49.0,155.9 | 81.1% (<i>m</i> -20) chi angles: 283.3,337.3 | 0.05Å | - | - | |
| A 508 | TYR | 50 | 0.673Å H with C 463 LYS HE2 | Favored (5.14%) General / -108.5,94.6 | 11.4% (<i>m</i> -30) chi angles: 282.8,356.5 | 0.101Å | - | - | |

| | | | | | | | | |
|----------|-----|-------|---|---|---|--------|---|---|
| A 509 | ILE | 50 | 0.788Å HB with A 568 ILE HG23 | Favored (99.01%) Isoleucine or valine / -60.9,-45.0 | 69% (<i>mt</i>) chi angles: 303.1,168.1 | 0.091Å | - | - |
| A 510 | CYS | 99.99 | 1.027Å HB3 with A 568 ILE HG22 | Favored (28.07%) General / -144.3,138.6 | 4.8% (<i>t</i>) chi angles: 164.3 | 0.071Å | - | - |
| A 511 | LYS | 50 | 0.454Å NZ with A 508 TYR HD2 | Favored (37.7%) General / -108.1,142.8 | 68.4% (<i>mttm</i>) chi angles: 292.6,179.7,178.2,293.8 | 0.066Å | - | - |
| A 512 | LYS | 50 | - | Favored (31.24%) General / -61.9,152.7 | 38.6% (<i>ttpt</i>) chi angles: 184.7,182,62.4,181.3 | 0.071Å | - | - |
| A 513 | GLY | 50 | 0.447Å O with A 563 ARG HD2 | Favored (4.44%) Glycine / 78.9,-20.6 | - | - | - | - |
| A 514 | ASP | 50 | 0.477Å O with A 564 ARG HG2 | Favored (43.53%) General / -74.6,139.2 | 42.5% (<i>t0</i>) chi angles: 189,328.5 | 0.062Å | - | - |
| A 515 | ILE | 50 | - | Favored (12.76%) Isoleucine or valine / -63.5,121.6 | 27.2% (<i>mt</i>) chi angles: 311.5,178.4 | 0.032Å | - | - |
| A 516 | GLY | 50 | - | Favored (10.08%) Glycine / -98.5,130.0 | - | - | - | - |
| A 517 | LYS | 50 | 0.53Å HG2 with A 517 LYS O | Favored (9.22%) General / -124.0,19.7 | 61.9% (<i>tttm</i>) chi angles: 185.6,184.4,177.4,293.2 | 0.063Å | - | - |
| A 518 | GLU | 50 | - | Favored (7.59%) General / -169.3,157.6 | 12.6% (<i>pt-20</i>) chi angles: 61.5,180.2,62.4 | 0.013Å | - | - |
| A 519 | MET | 50 | - | Favored (8.78%) General / -124.8,173.1 | 27.1% (<i>ptm</i>) chi angles: 65.3,172.3,293.2 | 0.032Å | - | - |
| A | TYR | 50 | - | Favored (52.46%) General / -124.8,173.1 | 90.2% (<i>m-85</i>) chi angles: 184.7,182,62.4,181.3 | 0.071Å | - | - |

| A 520 | TYR | 50 | - | (32.48%) General / -130.9,149.6 | 30.2% (mt) chi angles: 299.1,87.1 | 0.071Å | - | - |
|----------|---------|------------|--|--|--|--------------------|---------------------|---|
| A 521 | ILE | 50 | 0.645Å HG12 with A 577 PHE HB2 | Favored (15.09%) Isoleucine or valine / -121.0,104.3 | 32% (pt) chi angles: 66.9,166.7 | 0.058Å | - | - |
| A 522 | ILE | 50 | - | Allowed (0.15%) Isoleucine or valine / -58.2,105.0 | 62.3% (mt) chi angles: 304.9,175.2 | 0.02Å | - | - |
| A 523 | ASN | 50 | 0.477Å HB3 with A 575 ASP O | Favored (20.01%) General / -76.9,-47.8 | 48.4% (t30) chi angles: 182.1,60.4 | 0.01Å | - | - |
| A 524 | GLU | 50 | - | Favored (6.4%) General / -157.0,127.2 | 11.3% (tm-20) chi angles: 179.9,288.4,328.6 | 0.08Å | - | - |
| A 525 | GLY | 50 | - | Favored (13.05%) Glycine / 132.8,172.6 | - | - | - | - |
| A 526 | LYS | 99.99 | 0.975Å HG3 with A 540 VAL HG13 | Favored (51.03%) General / -122.2,128.3 | 66.7% (tttt) chi angles: 165.7,169.7,180.8,162.5 | 0.107Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| A 527 | LEU | 50 | 0.877Å HB3 with A 568 ILE HD11 | Favored (29.48%) General / -119.4,156.8 | 9.5% (mp) chi angles: 281.9,69.5 | 0.069Å | - | OUTLIER(S) worst is CD1- CG-CD2: 4.488 σ |
| A 528 | ALA | 50 | 0.511Å O with A 568 ILE HD12 | Favored (54.91%) General / -118.4,128.8 | - | 0.07Å | - | - |
| A 529 | VAL | 50 | 0.682Å HG22 with A 568 ILE HD13 | Favored (70.26%) Isoleucine or valine / -113.0,127.5 | 22.5% (t) chi angles: 187.4 | 0.056Å | - | - |
| A 530 | VAL | 50 | - | Favored (3.12%) Isoleucine or | 7.3% (p) chi angles: 58.8 | 0.101Å | - | - |

| Chain | Res | Seq | Distance | Angle | Chi | Chi | Chi | Chi |
|-------|-----|-----|----------|--|---|---|--------|---|
| A | 531 | ALA | 99.99 | 0.872Å HB2 with A 566 ALA HB2 | valine / -130.1,97.0 Allowed (1.95%) General / -130.4,80.3 | - | 0.137Å | - |
| A | 532 | ASP | 99.99 | - | Favored (11.65%) General / 53.0,31.7 | 29.4% (<i>t70</i>) chi angles: 178.9,77 | 0.068Å | - |
| A | 533 | ASP | 99.99 | - | Favored (31.44%) General / -160.3,165.4 | 26.1% (<i>p30</i>) chi angles: 61.8,29.5 | 0.02Å | - |
| A | 534 | GLY | 99.99 | - | Allowed (0.82%) Glycine / -61.8,105.1 | - | - | - |
| A | 535 | VAL | 50 | 0.608Å HG22 with A 536 THR HG22 | OUTLIER (0%) Isoleucine or valine / -10.6,108.9 | 7.1% (<i>p</i>) chi angles: 58.4 | 0.01Å | - |
| A | 536 | THR | 99.99 | 0.608Å HG22 with A 535 VAL HG22 | Allowed (1.5%) General / 55.6,15.4 | 9.9% (<i>t</i>) chi angles: 184 | 0.055Å | - |
| A | 537 | GLN | 99.99 | 0.534Å HG2 with A 536 THR O | Favored (14.51%) General / 47.9,51.3 | 18.5% (<i>pt20</i>) chi angles: 64.8,180.9,57 | 0.097Å | - |
| A | 538 | PHE | 99.99 | 0.475Å CD2 with A 538 PHE O | Favored (14.34%) General / 63.5,32.4 | 85.3% (<i>t80</i>) chi angles: 180.7,81.9 | 0.055Å | - |
| A | 539 | VAL | 99.99 | 0.785Å HG12 with A 540 VAL H | Allowed (0.48%) Isoleucine or valine / -119.6,-168.6 | 63.1% (<i>t</i>) chi angles: 180 | 0.087Å | OUTLIER(S) worst is CA- CB-CG1: 4.474 σ |
| A | 540 | VAL | 99.99 | 0.975Å HG13 with A 526 LYS HG3 | OUTLIER (0.06%) Isoleucine or valine / -158.5,97.4 | 26.7% (<i>t</i>) chi angles: 164.6 | 0.381Å | OUTLIER(S) worst is N-CA- CB: 5.587 σ |
| A | 541 | LEU | 50 | - | Allowed (1.63%) General / -59.4,112.1 | 18.6% (<i>mt</i>) chi angles: 292,193.2 | 0.076Å | - |

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|----------|-----|-------|---|---|---|--------------------------|--------------------|---------------------|---------------------|
| A 542 | SER | 50 | - | Allowed (1.05%) General / -124.4,-162.1 | 20.8% (<i>t</i>) chi angles: 188.4 | 0.068Å | - | - | |
| A 543 | ASP | 50 | - | Favored (20.24%) General / -50.1,135.9 | 0.3% chi angles: 313.8,44.5 | 0.116Å | - | - | |
| A 544 | GLY | 50 | - | Favored (73.87%) Glycine / 79.3,18.6 | - | - | - | - | |
| A 545 | SER | 50 | - | Favored (28.28%) General / -124.4,160.4 | 72.6% (<i>m</i>) chi angles: 295.6 | 0.026Å | - | - | |
| A 546 | TYR | 50 | 0.615Å CE1 with A 482 ILE HD13 | Favored (7.79%) General / -134.8,177.4 | 45.9% (<i>p90</i>) chi angles: 59,275.2 | 0.048Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| A 547 | PHE | 50 | 0.519Å CE2 with A 527 LEU HD22 | Favored (4.1%) General / -173.7,162.6 | 43.6% (<i>p90</i>) chi angles: 60.5,83.6 | 0.022Å | - | - | |
| A 548 | GLY | 50 | - | Favored (62.81%) Glycine / 75.1,28.1 | - | - | - | - | |
| A 549 | GLU | 50 | - | Favored (29.19%) General / -86.9,-19.2 | 6.4% (<i>pm0</i>) chi angles: 70.4,293.3,339.2 | 0.053Å | - | - | |
| A 550 | ILE | 50 | - | Favored (97.65%) Isoleucine or valine / -62.3,-43.1 | 76.9% (<i>mt</i>) chi angles: 298.8,177 | 0.063Å | - | - | |
| A 551 | SER | 50 | - | Favored (66.23%) General / -68.4,-27.5 | 73.4% (<i>m</i>) chi angles: 295.3 | 0.038Å | - | - | |
| A | ILE | 99 99 | 0.812Å HG21 with A | Favored (58.47%) | 65.2% (<i>mt</i>) | 0.083Å | - | - | |

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|-------|-----------|------------------------------|---|--|--------|---|--|
| A 552 | LEU 99.99 | 584 LEU HD13 | Isoleucine or valine / -73.2,-42.2 | chi angles: 302.9,177.3 | 0.065Å | - | - |
| A 553 | LEU 99.99 | 0.479Å HD23 with A 554 ASN N | Favored (52.8%) General / -70.0,139.6 | 6.7% (tt) chi angles: 182.7,164 | 0.065Å | - | - |
| A 554 | ASN 99.99 | 0.479Å N with A 553 LEU HD23 | Favored (24.51%) General / -118.8,115.5 | 41% (p30) chi angles: 60.9,25.7 | 0.036Å | - | OUTLIER(S) worst is OD1-CG-ND2: 6.181 σ |
| A 555 | ILE 99.99 | 0.84Å H with A 560 SER HB3 | Favored (28.01%) Isoleucine or valine / -62.8,134.6 | 37.2% (pt) chi angles: 64,176.5 | 0.065Å | - | - |
| A 556 | LYS 99.99 | - | Favored (50.62%) General / -65.7,133.2 | 22.7% (pttp) chi angles: 61.9,180,182,64.6 | 0.024Å | - | - |
| A 557 | GLY 99.99 | - | Favored (33.75%) Glycine / 106.2,-21.2 | - | - | - | - |
| A 558 | SER 99.99 | - | Favored (2.7%) General / -151.6,-167.1 | 32.1% (t) chi angles: 184.5 | 0.087Å | - | - |
| A 559 | LYS 99.99 | - | Favored (30.42%) General / -115.6,117.5 | 22.6% (pttp) chi angles: 59.8,180.7,181.7,66.3 | 0.056Å | - | - |
| A 560 | SER 99.99 | 0.84Å HB3 with A 555 ILE H | Favored (5.02%) General / -130.5,27.4 | 45.1% (t) chi angles: 178.7 | 0.049Å | - | OUTLIER(S) worst is O-C-N: 4.559 σ |
| A 561 | GLY 50 | - | Allowed (0.74%) Glycine / 48.5,17.4 | - | - | - | - |
| A 562 | ASN 50 | 0.644Å ND2 with A 563 ARG H | Allowed (0.31%) General / -125.8,-144.1 | 59% (t30) chi angles: 188.9,50.1 | 0.12Å | - | - |
| A 563 | ARG 50 | 0.644Å H with A 562 ASN ND2 | Favored (22.72%) General / -101.8,150.9 | 12.2% (mmt180) chi angles: 305,301.9,193.1,133.1 | 0.097Å | - | - |
| A | | 0.477Å | Favored (2.5%) | 28.1% (mmt180) | | | |

| A 564 | ARG | 50 | 0.177Å HG2 with A 514 ASP O | Favored (2.17%) General / -59.0,114.3 | 28.1% (m-100) chi angles: 296.1,296.9,204.3,186.3 | 0.057Å | - | - |
|---|---------|-----------|--------------------------------------|---|---|-----------------|-----------------|----------------|
| A 565 | THR | 50 | - | Allowed (0.75%) General / -71.9,10.2 | 63.3% (p) chi angles: 64.8 | 0.021Å | - | - |
| A 566 | ALA | 50 | 0.872Å HB2 with A 531 ALA HB2 | Allowed (0.63%) General / -173.3,-170.6 | - | 0.204Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: Clashscore: Outliers: 16 of Poor rotamers: 12 of Outliers: Outliers: 12 Outliers: 64 61.33 65.92 764 676 4 of 728 of 772 of 772 | | | | | | | | |
| A 567 | ASN | 50 | - | Favored (54.23%) General / -121.7,138.7 | 28.5% (t-20) chi angles: 187.7,301.4 | 0.124Å | - | - |
| A 568 | ILE | 50 | 1.027Å HG22 with A 510 CYS HB3 | Favored (74.3%) Isoleucine or valine / -117.4,125.9 | 8.6% (tp) chi angles: 183.2,64.9 | 0.129Å | - | - |
| A 569 | ARG | 50 | - | Favored (46.23%) General / -124.8,126.9 | 50.3% (ttp180) chi angles: 184.2,189.1,74.3,213.1 | 0.114Å | - | - |
| A 570 | SER | 50 | - | Favored (53%) General / -69.3,137.4 | 34.4% (t) chi angles: 183.1 | 0.109Å | - | - |
| A 571 | ILE | 50 | 0.939Å HG12 with A 526 LYS HG2 | Favored (3.98%) Isoleucine or valine / -101.1,-34.6 | 0.8% chi angles: 77.1,123.2 | 0.071Å | - | - |
| A 572 | GLY | 50 | 0.612Å N with A 571 ILE HG13 | Favored (14.71%) Glycine / -118.7,172.9 | - | - | - | - |
| A 573 | TYR | 50 | 0.539Å CE1 with A 443 TYR CD2 | OUTLIER (0.02%) General / -60.4,90.5 | 22.6% (m-85) chi angles: 274.5,272.2 | 0.028Å | - | - |
| A 574 | SER | 50 | - | Favored (40.49%) General / -76.0,145.1 | 53.7% (m) chi angles: 299.9 | 0.062Å | - | - |
| ~ ~ ~ ~ ~ | | | | Favored | | | | |

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|----------|-----|-------|--|--|--|--------|---|---|
| A 575 | ASP | 50 | 0.477Å O with A 523 ASN HB3 | Favored (6.37%) General / -125.7,100.3 | 90% (<i>m-20</i>) chi angles: 294.2,344 | 0.005Å | - | - |
| A 576 | LEU | 50 | - | Favored (9.84%) General / -109.0,167.8 | 37.2% (<i>mt</i>) chi angles: 310.5,176.1 | 0.111Å | - | - |
| A 577 | PHE | 50 | 0.649Å HB3 with A 498 LEU HB3 | Favored (51.56%) General / -126.1,133.8 | 88.9% (<i>m-85</i>) chi angles: 300.1,90 | 0.044Å | - | - |
| A 578 | CYS | 99.99 | - | Favored (31.6%) General / -104.5,144.5 | 52.3% (<i>t</i>) chi angles: 180 | 0.035Å | - | - |
| A 579 | LEU | 50 | 0.556Å HD22 with A 494 LEU HD11 | Favored (44.24%) General / -129.0,128.7 | 30.8% (<i>tp</i>) chi angles: 188.6,66.7 | 0.096Å | - | - |
| A 580 | SER | 50 | - | Favored (21.27%) General / -83.9,159.8 | 84% (<i>p</i>) chi angles: 68.6 | 0.017Å | - | - |
| A 581 | LYS | 50 | 0.727Å HG3 with A 552 ILE HG23 | Favored (79.78%) General / -60.1,-37.4 | 39.2% (<i>ttpt</i>) chi angles: 187,179.1,66.9,179.8 | 0.066Å | - | - |
| A 582 | ASP | 50 | - | Allowed (0.83%) General / -52.3,-64.4 | 5.6% (<i>m-20</i>) chi angles: 306.4,84.2 | 0.075Å | - | - |
| A 583 | ASP | 50 | - | Favored (78.54%) General / -63.6,-34.8 | 61.9% (<i>m-20</i>) chi angles: 294.3,302.7 | 0.03Å | - | - |
| A 584 | LEU | 99.99 | 0.812Å HD13 with A 552 ILE HG21 | Favored (73.82%) General / -61.0,-50.3 | 10.3% (<i>tt</i>) chi angles: 183.9,150 | 0.045Å | - | - |
| A 585 | MET | 50 | 0.629Å O with A 589 THR HG23 | Favored (69.05%) General / -69.1,-30.7 | 60.7% (<i>mtt</i>) chi angles: 292.3,183.8,173.7 | 0.026Å | - | - |
| A 586 | GLU | 50 | - | Favored (45.07%) General / -66.7,-52.4 | 62.4% (<i>tt0</i>) chi angles: 185.1,189.7,338.7 | 0.069Å | - | - |

High Clash > Cβ Bond Bond

| # | Alt | Res | B | 0.4Å | kamachandran | rotamer | deviation | lengths | angles |
|--|-----|-----|----------------------------------|------|---|---|-----------|---------|--------|
| Avg: Clashscore: 61.33 Outliers: 16 of 764 Poor rotamers: 12 of 676 Outliers: 4 of 728 Outliers: 12 of 772 Outliers: 64 of 772 | | | | | | | | | |
| A587 | ALA | 50 | - | - | Favored (70.58%) General / -61.5,-30.4 | - | 0.091Å | - | - |
| A588 | LEU | 50 | - | - | Favored (26.72%) General / -86.3,-22.5 | 48.9% (<i>mt</i>) chi angles: 293.2,185.6 | 0.112Å | - | - |
| A589 | THR | 50 | 0.629Å HG23 with A585 MET O | - | Favored (65.07%) General / -72.8,-31.9 | 77.8% (<i>p</i>) chi angles: 60.2 | 0.017Å | - | - |
| A590 | GLU | 50 | - | - | Favored (57.13%) General / -77.0,-32.5 | 80.4% (<i>tt0</i>) chi angles: 180.2,177.5,15.6 | 0.094Å | - | - |
| A591 | TYR | 50 | 0.748Å CD1 with A490 LEU HD13 | - | Favored (65.41%) Pre-proline / -133.8,76.7 | 90.7% (<i>m-85</i>) chi angles: 301.5,99.4 | 0.05Å | - | - |
| A592 | PRO | 50 | - | - | Favored (32.53%) Trans-proline / -60.1,-43.9 | 82.1% (<i>Cg_exo</i>) chi angles: 331.9 | 0.085Å | - | - |
| A593 | GLU | 50 | - | - | Allowed (0.79%) General / -42.2,-34.6 | 52.3% (<i>mm-40</i>) chi angles: 290.9,289.4,0.6 | 0.08Å | - | - |
| A594 | ALA | 50 | - | - | Favored (60.22%) General / -74.2,-20.4 | - | 0.035Å | - | - |
| A595 | LYS | 50 | 0.412Å O with A599 GLU HG3 | - | Favored (83.92%) General / -59.5,-39.5 | 63.6% (<i>tttp</i>) chi angles: 183.3,182.1,179.2,63.2 | 0.022Å | - | - |
| A596 | LYS | 50 | - | - | Favored (80.88%) General / -64.0,-35.5 | 64% (<i>tttp</i>) chi angles: 184.1,180.4,179.1,62.3 | 0.017Å | - | - |
| A597 | ALA | 50 | - | - | Favored (64.25%) General / -56.5,-52.6 | - | 0.031Å | - | - |

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|----------|----------------|-------------------|--|---|--|-------------------------|-------------------------|------------------------|
| A 598 | LEU | 50 | - | Favored (92.89%) General / -64.8,-39.0 | 10.5% (<i>mp</i>) chi angles: 280.6,63.7 | 0.026Å | - | - |
| A 599 | GLU | 99.99 | 0.412Å HG3 with A 595 LYS O | - | 74.9% (<i>mt-10</i>) chi angles: 293.7,191.7,332 | 0.049Å | - | - |
| B 407 | ASN | 99.99 | - | - | 85% (<i>m-20</i>) chi angles: 296.7,336.5 | 0.058Å | - | - |
| B 408 | ALA | 50 | - | OUTLIER (0.02%) General / -171.2,-39.6 | - | 0.063Å | - | - |
| B 409 | SER | 50 | 0.688Å HB2 with B 449 LYS HD2 | Favored (58.86%) General / -81.7,-6.2 | 80.2% (<i>p</i>) chi angles: 60 | 0.123Å | - | - |
| B 410 | ARG | 50 | 0.541Å HH21 with B 447 ASN CG | Favored (66.01%) General / -71.2,-30.2 | 10.9% (<i>mtp180</i>) chi angles: 302.7,214.3,69.6,156.8 | 0.073Å | - | - |
| B 411 | ALA | 50 | - | Favored (63.85%) General / -73.4,-40.9 | - | 0.052Å | - | - |
| B 412 | GLU | 50 | - | Favored (81.99%) General / -60.7,-37.5 | 11.8% (<i>tm-20</i>) chi angles: 179.8,287.3,328.8 | 0.069Å | - | - |
| B 413 | PHE | 50 | 0.45Å CD1 with B 445 TRP HE3 | Favored (45.25%) General / -65.1,-53.5 | 88.8% (<i>t80</i>) chi angles: 178.5,82.1 | 0.037Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| B 414 | GLN | 50 | 0.544Å HA with B 417 ILE HG12 | Favored (81.81%) General / -59.5,-38.7 | 15.8% (<i>mt-30</i>) chi angles: 282.5,140.6,20.1 | 0.015Å | - | - |
| B 415 | ALA | 50 | - | Favored (80.73%) General / -68.5,-40.6 | - | 0.039Å | - | - |
| B | LYS | 50 | - | Favored (8.88%) | 13.8% (<i>tppt?</i>) | 0.03Å | - | - |

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| 416 | | | | General / -69.9,-55.8 | chi angles: 177.9,49.7,62.1,192.2 | | | |
| B 417 | ILE | 50 | 0.736Å O with B 420 ILE HG12 | Favored (33.54%) Isoleucine or valine / -58.1,-28.1 | 30% (<i>pt</i>) chi angles: 69.4,172.7 | 0.078Å | - | - |
| B 418 | ASP | 50 | - | Favored (92.98%) General / -65.4,-41.9 | 44.5% (<i>t0</i>) chi angles: 186.9,329.5 | 0.038Å | - | - |
| B 419 | SER | 50 | - | Favored (97.46%) General / -61.8,-44.1 | 40.1% (<i>t</i>) chi angles: 181.5 | 0.038Å | - | - |
| B 420 | ILE | 50 | 0.736Å HG12 with B 417 ILE O | Favored (65.2%) Isoleucine or valine / -58.7,-37.4 | 16.4% (<i>pt</i>) chi angles: 71.3,180.5 | 0.072Å | - | OUTLIER(S) worst is CB- CG1-CD1: 4.186 σ |
| B 421 | LYS | 50 | 0.672Å HG3 with B 417 ILE O | Favored (90.34%) General / -65.2,-38.4 | 30.7% (<i>mtpp</i>) chi angles: 294,181,68,63.9 | 0.047Å | - | - |
| B 422 | GLN | 50 | - | Favored (54.03%) General / -77.6,-33.0 | 19% (<i>mt-30</i>) chi angles: 298,166.1,183.6 | 0.087Å | - | - |
| B 423 | TYR | 50 | 0.445Å CE1 with D 453 GLU HG3 | Favored (99.6%) General / -62.0,-42.9 | 71.9% (<i>t80</i>) chi angles: 172.6,84.8 | 0.05Å | - | - |
| B 424 | MET | 50 | 1.002Å SD with B 437 VAL HG11 | Favored (70.48%) General / -71.4,-40.7 | 69.9% (<i>mtm</i>) chi angles: 293.7,191.9,299.6 | 0.05Å | - | - |
| B 425 | GLN | 50 | - | Favored (79.46%) General / -67.7,-35.7 | 53.4% (<i>tt0</i>) chi angles: 185.3,179.2,57 | 0.012Å | - | - |
| B 426 | PHE | 50 | - | Favored (79.94%) General / -64.8,-35.1 | 11% (<i>t80</i>) chi angles: 182.8,38.1 | 0.025Å | - | - |
| B 427 | ARG | 99.99 | 1.003Å HB3 with D 473 HIS HE1 | Favored (57.36%) General / -92.0,-1.2 | 32.8% (<i>mmt180</i>) chi angles: 287.3,304.8,183.2,180 | 0.21Å | - | OUTLIER(S) worst is N-CA- CB: 4.945 σ |

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| B 428 | LYS | 50 | - | Favored (28.26%) General / 54.1,38.0 | 88.4% (<i>mttt</i>) chi angles: 298.3,170.7,185,166.6 | 0.051Å | - | - |
| B 429 | VAL | 50 | 0.914Å HG21 with B 433 LEU HD22 | Favored (5.58%) Isoleucine or valine / -61.0,152.8 | 12.1% (<i>p</i>) chi angles: 62.1 | 0.168Å | - | - |
| B 430 | THR | 50 | 0.455Å HG22 with B 432 ASP H | Favored (7.51%) General / -57.2,156.3 | 98.9% (<i>m</i>) chi angles: 298.8 | 0.05Å | - | - |
| B 431 | LYS | 50 | 0.441Å O with B 435 THR HG23 | Favored (82.42%) General / -66.9,-36.5 | 32.8% (<i>mmmt</i>) chi angles: 296.3,295.3,295.3,181.1 | 0.032Å | - | - |
| B 432 | ASP | 50 | 0.455Å H with B 430 THR HG22 | Favored (80.59%) General / -65.3,-35.3 | 85.2% (<i>m-20</i>) chi angles: 293.9,349.1 | 0.053Å | - | - |
| B 433 | LEU | 50 | 0.914Å HD22 with B 429 VAL HG21 | Favored (63.84%) General / -73.5,-40.7 | 8.5% (<i>tt</i>) chi angles: 191.4,155.1 | 0.12Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: | Clashscore: | Outliers: 16 of | Poor rotamers: 12 of | Outliers: | Outliers: 12 | Outliers: 64 |
| | | 61.33 | 65.92 | 764 | 676 | 4 of 728 | of 772 | of 772 |
| B 434 | GLU | 50 | 0.786Å O with B 438 ILE HG12 | Favored (93.61%) General / -63.9,-39.2 | 54.6% (<i>mt-10</i>) chi angles: 296.7,182.7,298.1 | 0.075Å | - | - |
| B 435 | THR | 50 | 0.441Å HG23 with B 431 LYS O | Favored (68.27%) General / -66.1,-49.3 | 77.9% (<i>p</i>) chi angles: 60.2 | 0.02Å | - | - |
| B 436 | ARG | 50 | - | Favored (72.82%) General / -58.2,-36.2 | 86.8% (<i>mtm-85</i>) chi angles: 285.7,187.7,294.2,260.3 | 0.068Å | - | - |
| B 437 | VAL | 50 | 1.002Å HG11 with B 424 MET SD | Favored (68.54%) Isoleucine or valine / -72.0,-41.3 | 4.9% (<i>p</i>) chi angles: 76.4 | 0.175Å | - | - |
| - | | | 0.706 Å | Favored | | | | |

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| B 438 | ILE | 50 | U. / OOA HG12 with B 434 GLU O | (28.75%) Isoleucine or valine / -58.1,-54.7 | 41.1% (<i>mm</i>) chi angles: 299.1,304.7 | 0.028Å | - | - |
| B 439 | ARG | 50 | 0.437Å O with B 443 TYR HD2 | Favored (77.74%) General / -60.0,-36.6 | 55.1% (<i>mmm-85</i>) chi angles: 293.6,298,293,278.7 | 0.033Å | - | - |
| B 440 | TRP | 99.99 | 0.842Å CH2 with B 444 LEU HD22 | Favored (42.13%) General / -62.5,-54.3 | 89.3% (<i>t90</i>) chi angles: 184.8,87.4 | 0.024Å | OUTLIER(S) worst is NE1-- CE2: 4.896 σ | OUTLIER(S) worst is CZ2- CH2-CZ3: 5.444 σ |
| B 441 | PHE | 50 | 0.775Å HE2 with B 437 VAL HG22 | Favored (61.2%) General / -51.0,-46.2 | 95.4% (<i>m-85</i>) chi angles: 292.2,275.1 | 0.073Å | - | - |
| B 442 | ASP | 50 | 0.404Å HB2 with B 439 ARG O | Favored (67.79%) General / -53.0,-45.5 | 51.3% (<i>m-20</i>) chi angles: 295.4,296.5 | 0.044Å | - | - |
| B 443 | TYR | 50 | 0.552Å CE2 with B 573 TYR CZ | Favored (60.59%) General / -75.2,-30.6 | 95.2% (<i>m-85</i>) chi angles: 292.2,274.8 | 0.027Å | - | - |
| B 444 | LEU | 99.99 | 0.842Å HD22 with B 440 TRP CH2 | Favored (22.95%) General / -84.8,-33.5 | 21.3% (<i>tp</i>) chi angles: 187.1,74 | 0.098Å | - | - |
| B 445 | TRP | 50 | 0.458Å NE1 with B 444 LEU HD23 | Favored (8.95%) General / -119.4,-16.7 | 51.6% (<i>m0</i>) chi angles: 296.7,351.6 | 0.079Å | OUTLIER(S) worst is NE1-- CE2: 4.813 σ | OUTLIER(S) worst is CD2- CE3-CZ3: 4.178 σ |
| B 446 | ALA | 50 | - | Allowed (0.65%) General / 51.6,18.1 | - | 0.046Å | - | - |
| B 447 | ASN | 99.99 | 0.541Å CG with B 410 ARG HH21 | Favored (10.17%) General / 56.4,26.0 | 64.3% (<i>t-20</i>) chi angles: 184.8,348.8 | 0.097Å | - | OUTLIER(S) worst is OD1- CG-ND2: 5.666 σ |
| B 448 | LYS | 99.99 | - | Allowed (0.73%) General / -106.2,-72.0 | 29.5% (<i>tptp</i>) chi angles: 182.4,64.6,177.9,64.7 | 0.065Å | - | - |
| B 449 | LYS | 99.99 | 0.688Å HD2 with B 409 SER HB2 | Favored (49.19%) General / -125.3,147.2 | 27.9% (<i>tptp</i>) chi angles: 180.1,66.8,182.2,61.9 | 0.079Å | - | OUTLIER(S) worst is CG- CD-CE: 4.38 σ |

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| B 450 | THR | 99.99 | 0.721Å HG22 with B 451 VAL H | Allowed (0.82%) General / -119.5,-160.6 | 48.5% (<i>m</i>) chi angles: 305 | 0.108Å | - | - | |
| B 451 | VAL | 99.99 | 1.088Å HG22 with B 452 ASP HA | Allowed (0.43%) Isoleucine or valine / -48.1,151.1 | 6% (<i>p</i>) chi angles: 75 | 0.168Å | - | - | |
| B 452 | ASP | 50 | 1.088Å HA with B 451 VAL HG22 | Allowed (1%) General / -104.9,44.8 | 2.2% (<i>m-20</i>) chi angles: 294.9,33.2 | 0.139Å | - | - | |
| B 453 | GLU | 50 | 0.835Å HA with B 456 VAL HG22 | Allowed (0.61%) General / -40.4,-36.9 | 27.2% (<i>tt0</i>) chi angles: 193.5,193.3,40.1 | 0.049Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: | | | 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| B 454 | LYS | 50 | - | - | Favored (79.07%) General / -63.4,-48.1 | 39% (<i>ttpt</i>) chi angles: 186.5,180,64.3,181.3 | 0.042Å | - | - |
| B 455 | GLU | 50 | 0.752Å HB3 with B 452 ASP HB3 | Favored (76.52%) General / -65.6,-47.2 | 10.8% (<i>tm-20</i>) chi angles: 181.5,289.9,325.1 | 0.055Å | - | - | |
| B 456 | VAL | 50 | 0.835Å HG22 with B 453 GLU HA | Favored (84.79%) Isoleucine or valine / -58.1,-43.2 | 23.1% (<i>m</i>) chi angles: 302.6 | 0.057Å | - | - | |
| B 457 | LEU | 50 | 0.476Å HB2 with B 453 GLU O | Favored (84.41%) General / -67.7,-40.6 | 0.6% chi angles: 254.3,39.5 | 0.031Å | - | - | |
| B 458 | LYS | 50 | - | - | Favored (91.56%) General / -61.5,-39.6 | 28.6% (<i>tptp</i>) chi angles: 184.7,62.4,180.5,64.5 | 0.039Å | - | - |
| B 459 | SER | 50 | 0.641Å O with C 440 TRP CH2 | Favored (81.95%) General / -64.2,-35.8 | 68.2% (<i>m</i>) chi angles: 296.2 | 0.096Å | - | OUTLIER(S) worst is CA-C- O: 5.239 σ | |
| B | LEU | 50 | - | - | Favored (80.5%) | 80.5% (<i>mt</i>) | 0.042 Å | - | - |

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| B 460 | LEU | 50 | - | (39.39%) Pre-proline / -70.6,166.1 | chi angles: 298.8,182.5 | 0.042Å | - | - |
| B 461 | PRO | 50 | 0.778Å HD3 with C 440 TRP CE2 | Favored (6.38%) Trans-proline / -87.5,171.2 | 42.7% (<i>Cg_endo</i>) chi angles: 36 | 0.014Å | - | - |
| B 462 | ASP | 50 | - | Favored (96.91%) General / -63.9,-43.1 | 42.1% (<i>t0</i>) chi angles: 190.5,329.5 | 0.015Å | - | - |
| B 463 | LYS | 50 | 0.686Å HE2 with C 508 TYR H | Favored (73.89%) General / -57.9,-37.4 | 32.4% (<i>mmmt</i>) chi angles: 294.8,293.5,296.6,184.8 | 0.04Å | - | - |
| B 464 | LEU | 50 | 0.669Å HD12 with B 461 PRO HD2 | Favored (22.9%) General / -75.5,-48.4 | 59.3% (<i>mt</i>) chi angles: 286.4,177.4 | 0.038Å | - | - |
| B 465 | LYS | 50 | 0.593Å O with B 470 ILE HG12 | Favored (72.81%) General / -61.0,-33.1 | 54.9% (<i>mtmt</i>) chi angles: 294.7,178.6,295.9,178.8 | 0.136Å | - | - |
| B 466 | ALA | 50 | 0.72Å HA with B 470 ILE CB | Favored (83.81%) General / -66.6,-36.9 | - | 0.119Å | - | - |
| B 467 | GLU | 50 | 0.599Å OE2 with C 433 LEU HD12 | Favored (79.53%) General / -68.8,-40.5 | 15.5% (<i>tt0</i>) chi angles: 206.1,191.3,309.1 | 0.116Å | - | - |
| B 468 | ILE | 99.99 | 0.867Å HA with B 472 VAL HG12 | Favored (24.37%) Isoleucine or valine / -119.2,146.1 | 17.8% (<i>pt</i>) chi angles: 51.7,179.6 | 0.185Å | - | - |
| B 469 | ALA | 99.99 | 0.977Å H with B 473 HIS HD2 | Allowed (1.8%) General / 66.3,0.8 | - | 0.078Å | - | - |
| B 470 | ILE | 99.99 | 0.966Å HD12 with B 496 LEU HA | Allowed (0.75%) Isoleucine or valine / -132.4,-25.7 | 27.1% (<i>mm</i>) chi angles: 299,310.2 | 0.091Å | - | - |
| B 471 | ASN | 50 | 1.034Å HD21 with B 492 VAL HG12 | Allowed (0.47%) General / -140.4,-51.1 | 42.2% (<i>m-20</i>) chi angles: 278.7,302.3 | 0.195Å | - | OUTLIER(S) worst is CA- CB-CG: 4.049 σ |

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| B 472 | VAL | 50 | 0.867Å HG12 with B 468 ILE HA | Favored (82.17%) Isoleucine or valine / -58.6,-41.5 | 15% (<i>p</i>) chi angles: 63.5 | 0.065Å | - | - | |
| B 473 | HIS | 50 | 1.019Å HE1 with C 427 ARG HB3 | Favored (61.3%) General / -72.7,-25.5 | 84.1% (<i>m-70</i>) chi angles: 288,298.1 | 0.04Å | OUTLIER(S) worst is CD2-- NE2: 7.05 σ | OUTLIER(S) worst is CD2- NE2-CE1: 12.768 σ | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| B 474 | LEU | 99.99 | 0.696Å C with B 474 LEU HD23 | Favored (38.13%) General / -53.1,132.5 | 7.2% (<i>tt</i>) chi angles: 184.9,162.9 | 0.126Å | - | - | |
| B 475 | ASP | 99.99 | 0.542Å N with B 474 LEU HD23 | Favored (5.85%) General / -129.7,12.7 | 29.9% (<i>t70</i>) chi angles: 179.1,76.4 | 0.069Å | - | - | |
| B 476 | THR | 99.99 | 0.49Å HB with B 523 ASN HA | Favored (2.21%) General / -136.0,48.0 | 10.3% (<i>t</i>) chi angles: 184.2 | 0.074Å | - | - | |
| B 477 | LEU | 99.99 | 1.093Å HG with B 483 PHE HB3 | Allowed (0.81%) General / -134.6,-52.3 | 10% (<i>tt</i>) chi angles: 185.3,154.6 | 0.239Å | - | - | |
| B 478 | LYS | 50 | - | Favored (31.44%) General / -53.1,-29.6 | 27.1% (<i>tptp</i>) chi angles: 180.3,61.9,184.6,69.5 | 0.035Å | - | - | |
| B 479 | LYS | 50 | - | Favored (49.45%) General / -89.1,-9.9 | 26.8% (<i>tptp</i>) chi angles: 188.6,61.2,182.7,67.3 | 0.051Å | - | - | |
| B 480 | VAL | 50 | 1.051Å HG12 with B 477 LEU HA | Favored (23.98%) Isoleucine or valine / -117.0,108.1 | 11.5% (<i>p</i>) chi angles: 66.5 | 0.141Å | - | - | |
| B 481 | ARG | 50 | 0.724Å HA with B 484 GLN HG2 | Favored (7.28%) General / -43.5,-47.1 | 57.9% (<i>mmm-85</i>) chi angles: 296.1,292.8,296.7,277.2 | 0.027Å | - | - | |
| B | ILE | 50 | 0.741Å HG12 with B | Favored (87.84%) | 42.2% (<i>pt</i>) | 0.067Å | - | - | |

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| B 482 | ILE | 50 | HG12 with B 480 VAL HG22 | (8/.84%) Isoleucine or valine / -59.3,-42.6 | chi angles: 65.5,172.5 | 0.007Å | - | - |
| B 483 | PHE | 50 | 1.093Å HB3 with B 477 LEU HG | Favored (28.76%) General / -79.7,-40.6 | 7.1% (<i>m-30</i>) chi angles: 278.5,9.7 | 0.047Å | - | OUTLIER(S) worst is CA-CB-CG: 4.414 σ |
| B 484 | GLN | 50 | 0.724Å HG2 with B 481 ARG HA | Favored (83.93%) General / -67.8,-38.8 | 19.8% (<i>pt20</i>) chi angles: 65.9,181.7,61.9 | 0.076Å | - | - |
| B 485 | ASP | 50 | - | Favored (4.67%) General / -97.0,26.4 | 48.7% (<i>t0</i>) chi angles: 190.7,338.3 | 0.039Å | - | - |
| B 486 | CYS | 99.99 | 0.636Å SG with B 490 LEU HD23 | Favored (27.27%) General / -115.1,155.3 | 52.7% (<i>t</i>) chi angles: 181.3 | 0.052Å | - | - |
| B 487 | GLU | 99.99 | - | Favored (8.68%) General / -57.2,120.8 | 87.8% (<i>mt-10</i>) chi angles: 301.3,182.2,337.1 | 0.064Å | - | - |
| B 488 | ALA | 50 | 0.722Å O with B 492 VAL HG13 | Favored (14.29%) General / -54.9,-22.3 | - | 0.016Å | - | - |
| B 489 | GLY | 50 | 0.492Å O with B 492 VAL HG22 | Favored (76.39%) Glycine / -67.5,-45.6 | - | - | - | - |
| B 490 | LEU | 99.99 | 0.748Å HD13 with B 591 TYR CD1 | Favored (93.9%) General / -65.5,-41.0 | 35.4% (<i>tp</i>) chi angles: 175.6,54.2 | 0.063Å | - | - |
| B 491 | LEU | 99.99 | 0.829Å HD13 with B 477 LEU HD11 | Favored (5.02%) General / -57.2,-59.5 | 94.3% (<i>mt</i>) chi angles: 298.4,175.6 | 0.075Å | - | - |
| B 492 | VAL | 50 | 1.034Å HG12 with B 471 ASN HD21 | Favored (14.91%) Isoleucine or valine / -48.6,-45.5 | 25.8% (<i>m</i>) chi angles: 302 | 0.023Å | - | - |
| B 493 | GLU | 50 | - | Favored (68.49%) General / -66.1,-28.0 | 14.3% (<i>tm-20</i>) chi angles: 183.8,285.3,333.8 | 0.107Å | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | C β deviation | Bond lengths | Bond angles |
|----------|-----|-----|------------|--|--|--|------------------------|---------------------|--|
| | | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| B 494 | LEU | 50 | | 0.689Å HD23 with B 483 PHE CE1 | Favored (12.94%) General / -80.0,-48.7 | 33.9% (<i>tp</i>) chi angles: 187.7,59.4 | 0.033Å | - | OUTLIER(S) worst is CD1- CG-CD2: 4.562 σ |
| B 495 | VAL | 50 | | 0.749Å HG21 with B 470 ILE O | Favored (44.55%) Isoleucine or valine / -57.7,-33.2 | 20.8% (<i>m</i>) chi angles: 303.3 | 0.021Å | - | - |
| B 496 | LEU | 50 | | 0.966Å HA with B 470 ILE HD12 | Favored (55.61%) General / -64.8,-13.4 | 8.9% (<i>tt</i>) chi angles: 190.5,154.5 | 0.155Å | - | - |
| B 497 | LYS | 50 | | - | Favored (10.85%) General / -115.9,-18.0 | 64.5% (<i>mttp</i>) chi angles: 295.5,177.2,177.3,63.2 | 0.054Å | - | - |
| B 498 | LEU | 50 | | 0.639Å HB3 with B 577 PHE HB3 | Favored (44.49%) General / -58.6,144.1 | 58.4% (<i>mt</i>) chi angles: 305.2,173.5 | 0.096Å | - | - |
| B 499 | ARG | 50 | | - | Favored (28.15%) Pre-proline / -118.9,124.7 | 40.1% (<i>ptt180</i>) chi angles: 62,179.4,181.4,181.7 | 0.069Å | - | - |
| B 500 | PRO | 50 | | - | Favored (33.33%) Trans-proline / -68.0,134.9 | 92.8% (<i>Cg_endo</i>) chi angles: 30.9 | 0.035Å | - | - |
| B 501 | THR | 50 | | - | Favored (30.25%) General / -144.9,142.9 | 63.4% (<i>p</i>) chi angles: 62.2 | 0.038Å | - | - |
| B 502 | VAL | 50 | | - | Favored (36.42%) Isoleucine or valine / -115.5,140.6 | 74% (<i>t</i>) chi angles: 174 | 0.052Å | - | - |
| B 503 | PHE | 50 | | - | Favored (50.81%) General / -127.0,145.2 | 63.9% (<i>m-85</i>) chi angles: 284.3,87.2 | 0.046Å | - | - |

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| B 504 | SER | 50 | - | Favored (31.54%) Pre-proline / -101.6,158.6 | 70.2% (<i>m</i>) chi angles: 295.9 | 0.029Å | - | - |
| B 505 | PRO | 50 | - | Favored (52.29%) Trans-proline / -53.9,132.9 | 87.8% (<i>Cg_exo</i>) chi angles: 331.3 | 0.109Å | - | - |
| B 506 | GLY | 50 | - | Favored (9.88%) Glycine / 100.2,-30.6 | - | - | - | - |
| B 507 | ASP | 50 | 0.443Å HA with D 463 LYS HE2 | Allowed (0.56%) General / -49.0,155.9 | 81.1% (<i>m-20</i>) chi angles: 283.3,337.3 | 0.05Å | - | - |
| B 508 | TYR | 50 | 0.684Å H with D 463 LYS HE2 | Favored (5.14%) General / -108.5,94.6 | 11.4% (<i>m-30</i>) chi angles: 282.8,356.5 | 0.101Å | - | - |
| B 509 | ILE | 50 | 0.806Å HB with B 568 ILE HG23 | Favored (99.01%) Isoleucine or valine / -60.9,-45.0 | 69% (<i>mt</i>) chi angles: 303.1,168.1 | 0.091Å | - | - |
| B 510 | CYS | 99.99 | 1.038Å HB3 with B 568 ILE HG22 | Favored (28.07%) General / -144.3,138.6 | 4.8% (<i>t</i>) chi angles: 164.3 | 0.071Å | - | - |
| B 511 | LYS | 50 | 0.449Å NZ with B 508 TYR HD2 | Favored (37.7%) General / -108.1,142.8 | 68.4% (<i>mttm</i>) chi angles: 292.6,179.7,178.2,293.8 | 0.066Å | - | - |
| B 512 | LYS | 50 | - | Favored (31.24%) General / -61.9,152.7 | 38.6% (<i>ttpt</i>) chi angles: 184.7,182,62.4,181.3 | 0.071Å | - | - |
| B 513 | GLY | 50 | 0.446Å O with B 563 ARG HD2 | Favored (4.44%) Glycine / 78.9,-20.6 | - | - | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|---|-----|-----|-----------|-----------------|--------------|---------|-----------------|-----------------|----------------|
|---|-----|-----|-----------|-----------------|--------------|---------|-----------------|-----------------|----------------|

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|-------|-------------|-----------------|----------------------|-----------|--------------|--------------|
| Avg: | Clashscore: | Outliers: 16 of | Poor rotamers: 12 of | Outliers: | Outliers: 12 | Outliers: 64 |
| 61.33 | 65.92 | 764 | 676 | 4 of 728 | of 772 | of 772 |

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|----------|-----|----|------------------------|----------------------------------|---|--------|---|---|
| B 514 | ASP | 50 | 0.477Å O with B 564 | Favored (43.53%) General / | 42.5% (<i>t0</i>) chi angles: 189.3,28.5 | 0.062Å | - | - |
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| B 514 | | | | General / -74.6,139.2 | chi angles: 189,328.3 | | | |
| B 515 | ILE | 50 | - | Favored (12.76%) Isoleucine or valine / -63.5,121.6 | 27.2% (<i>mt</i>) chi angles: 311.5,178.4 | 0.032Å | - | - |
| B 516 | GLY | 50 | - | Favored (10.08%) Glycine / -98.5,130.0 | - | - | - | - |
| B 517 | LYS | 50 | 0.528Å HG2 with B 517 LYS O | Favored (9.22%) General / -124.0,19.7 | 61.9% (<i>tttm</i>) chi angles: 185.6,184.4,177.4,293.2 | 0.063Å | - | - |
| B 518 | GLU | 50 | - | Favored (7.59%) General / -169.3,157.6 | 12.6% (<i>pt-20</i>) chi angles: 61.5,180.2,62.4 | 0.013Å | - | - |
| B 519 | MET | 50 | - | Favored (8.78%) General / -124.8,173.1 | 27.1% (<i>ptm</i>) chi angles: 65.3,172.3,293.2 | 0.032Å | - | - |
| B 520 | TYR | 50 | - | Favored (52.46%) General / -130.9,149.6 | 90.2% (<i>m-85</i>) chi angles: 299.1,87.1 | 0.071Å | - | - |
| B 521 | ILE | 50 | 0.646Å HG12 with B 577 PHE HB2 | Favored (15.09%) Isoleucine or valine / -121.0,104.3 | 32% (<i>pt</i>) chi angles: 66.9,166.7 | 0.058Å | - | - |
| B 522 | ILE | 50 | - | Allowed (0.15%) Isoleucine or valine / -58.2,105.0 | 62.3% (<i>mt</i>) chi angles: 304.9,175.2 | 0.02Å | - | - |
| B 523 | ASN | 50 | 0.49Å HA with B 476 THR HB | Favored (20.01%) General / -76.9,-47.8 | 48.4% (<i>t30</i>) chi angles: 182.1,60.4 | 0.01Å | - | - |
| B 524 | GLU | 50 | - | Favored (6.4%) General / -157.0,127.2 | 11.3% (<i>tm-20</i>) chi angles: 179.9,288.5,328.5 | 0.08Å | - | - |
| B 525 | GLY | 50 | - | Favored (13.05%) Glycine / 132.8,172.6 | - | - | - | - |

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| B 526 | LYS | 99.99 | 0.955Å HG3 with B 540 VAL HG13 | Favored (51.03%) General / -122.2,128.3 | 66.7% (tttt) chi angles: 165.7,169.7,180.8,162.5 | 0.107Å | - | - |
| B 527 | LEU | 50 | 0.871Å HB3 with B 568 ILE HD11 | Favored (29.48%) General / -119.4,156.8 | 9.5% (mp) chi angles: 281.9,69.5 | 0.069Å | - | OUTLIER(S) worst is CD1- CG-CD2: 4.488 σ |
| B 528 | ALA | 50 | 0.499Å O with B 568 ILE HD12 | Favored (54.91%) General / -118.4,128.8 | - | 0.07Å | - | - |
| B 529 | VAL | 50 | 0.683Å HG22 with B 568 ILE HD13 | Favored (70.26%) Isoleucine or valine / -113.0,127.5 | 22.5% (t) chi angles: 187.4 | 0.056Å | - | - |
| B 530 | VAL | 50 | - | Favored (3.12%) Isoleucine or valine / -130.1,97.0 | 7.3% (p) chi angles: 58.8 | 0.101Å | - | - |
| B 531 | ALA | 99.99 | 0.856Å HB2 with B 566 ALA HB2 | Allowed (1.95%) General / -130.4,80.3 | - | 0.137Å | - | - |
| B 532 | ASP | 99.99 | - | Favored (11.65%) General / 53.0,31.7 | 29.4% (t70) chi angles: 178.9,77 | 0.068Å | - | - |
| B 533 | ASP | 99.99 | - | Favored (31.44%) General / -160.3,165.4 | 26.1% (p30) chi angles: 61.8,29.5 | 0.02Å | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|------|-----|-----|-----------|-----------------|--------------|---------------------|--------------------------|---------------------|---------------------|
| Avg: | | | 61.33 | Clashscore: | 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 |
| | | | | | | | | Outliers: 64 of 772 | |

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|----------|-----|-------|--------------------------------|--|------------------------------|-------|---|---|
| B 534 | GLY | 99.99 | - | Allowed (0.82%) Glycine / -61.8,105.1 | - | - | - | - |
| B 535 | VAL | 50 | 0.6Å HG22 with B 536 THR | OUTLIER (0%) Isoleucine or valine / -10.6,108.9 | 7.1% (p) chi angles: 58.4 | 0.01Å | - | - |
| | | | HG22 0.6Å | Allowed | | | | |

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| B 536 | THR | 99.99 | 0.07Å HG22 with B 535 VAL HG22 | (1.5%) General / 55.6,15.4 | 9.9% (<i>t</i>) chi angles: 184 | 0.055Å | - | - |
| B 537 | GLN | 99.99 | 0.517Å HG2 with B 536 THR O | Favored (14.51%) General / 47.9,51.3 | 18.5% (<i>pt20</i>) chi angles: 64.8,180.9,57 | 0.097Å | - | - |
| B 538 | PHE | 99.99 | 0.475Å CD2 with B 538 PHE O | Favored (14.34%) General / 63.5,32.4 | 85.3% (<i>t80</i>) chi angles: 180.7,81.9 | 0.055Å | - | - |
| B 539 | VAL | 99.99 | 0.806Å HG12 with B 540 VAL H | Allowed (0.48%) Isoleucine or valine / -119.6,-168.6 | 63.1% (<i>t</i>) chi angles: 180 | 0.087Å | - | OUTLIER(S) worst is CA- CB-CG1: 4.474 σ |
| B 540 | VAL | 99.99 | 0.955Å HG13 with B 526 LYS HG3 | OUTLIER (0.06%) Isoleucine or valine / -158.5,97.4 | 26.7% (<i>t</i>) chi angles: 164.6 | 0.381Å | - | OUTLIER(S) worst is N-CA- CB: 5.587 σ |
| B 541 | LEU | 50 | - | Allowed (1.63%) General / -59.4,112.1 | 18.6% (<i>mt</i>) chi angles: 292,193.2 | 0.076Å | - | - |
| B 542 | SER | 50 | - | Allowed (1.05%) General / -124.4,-162.1 | 20.8% (<i>t</i>) chi angles: 188.4 | 0.068Å | - | - |
| B 543 | ASP | 50 | - | Favored (20.24%) General / -50.1,135.9 | 0.3% chi angles: 313.8,44.5 | 0.116Å | - | - |
| B 544 | GLY | 50 | - | Favored (73.87%) Glycine / 79.3,18.6 | - | - | - | - |
| B 545 | SER | 50 | - | Favored (28.28%) General / -124.4,160.4 | 72.6% (<i>m</i>) chi angles: 295.6 | 0.026Å | - | - |
| B 546 | TYR | 50 | 0.619Å CE1 with B 482 ILE HD13 | Favored (7.79%) General / -134.8,177.4 | 45.9% (<i>p90</i>) chi angles: 59,275.2 | 0.048Å | - | - |
| B 547 | PHE | 50 | 0.512Å CE2 with B 527 LEU | Favored (4.1%) General / | 43.6% (<i>p90</i>) chi angles: 60.5,83.6 | 0.022Å | - | - |

| | | HD22 | | -173.7,162.6 | | | | | |
|----------|---------|-----------|---|---|---|--------------------|---------------------|---|---|
| B 548 | GLY | 50 | - | Favored (62.81%) Glycine / 75.1,28.1 | - | - | - | - | - |
| B 549 | GLU | 50 | - | Favored (29.19%) General / -86.9,-19.2 | 6.4% (<i>pm0</i>) chi angles: 70.4,293.3,339.2 | 0.053Å | - | - | - |
| B 550 | ILE | 50 | - | Favored (97.65%) Isoleucine or valine / -62.3,-43.1 | 76.9% (<i>mt</i>) chi angles: 298.8,177 | 0.063Å | - | - | - |
| B 551 | SER | 50 | - | Favored (66.23%) General / -68.4,-27.5 | 73.4% (<i>m</i>) chi angles: 295.3 | 0.038Å | - | - | - |
| B 552 | ILE | 99.99 | 0.79Å HG21 with B 584 LEU HD13 | Favored (58.47%) Isoleucine or valine / -73.2,-42.2 | 65.2% (<i>mt</i>) chi angles: 302.9,177.3 | 0.083Å | - | - | - |
| B 553 | LEU | 99.99 | 0.485Å HD23 with B 554 ASN N | Favored (52.8%) General / -70.0,139.6 | 6.7% (<i>tt</i>) chi angles: 182.7,164 | 0.065Å | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | |
| Avg: | | 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 | |
| B 554 | ASN | 99.99 | 0.485Å N with B 553 LEU HD23 | Favored (24.51%) General / -118.8,115.5 | 41% (<i>p30</i>) chi angles: 60.9,25.7 | 0.036Å | - | OUTLIER(S) worst is OD1- CG-ND2: 6.181 σ | |
| B 555 | ILE | 99.99 | 0.861Å H with B 560 SER HB3 | Favored (28.01%) Isoleucine or valine / -62.8,134.6 | 37.2% (<i>pt</i>) chi angles: 64,176.5 | 0.065Å | - | - | - |
| B 556 | LYS | 99.99 | - | Favored (50.62%) General / -65.7,133.2 | 22.7% (<i>pttp</i>) chi angles: 61.9,180,182,64.6 | 0.024Å | - | - | - |
| B 557 | GLY | 99.99 | - | Favored (33.75%) Glycine / | - | - | - | - | - |

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| | | | | 106.2,-21.2 | | | | |
| B 558 | SER | 99.99 | - | Favored (2.7%) General / -151.6,-167.1 | 32.1% (t) chi angles: 184.5 | 0.087Å | - | - |
| B 559 | LYS | 99.99 | - | Favored (30.42%) General / -115.6,117.5 | 22.6% (pttp) chi angles: 59.8,180.7,181.7,66.3 | 0.056Å | - | - |
| B 560 | SER | 99.99 | 0.861Å HB3 with B 555 ILE H | Favored (5.02%) General / -130.5,27.4 | 45.1% (t) chi angles: 178.7 | 0.049Å | - | OUTLIER(S) worst is O-C- N: 4.559 σ |
| B 561 | GLY | 50 | - | Allowed (0.74%) Glycine / 48.5,17.4 | - | - | - | - |
| B 562 | ASN | 50 | 0.654Å ND2 with B 563 ARG H | Allowed (0.31%) General / -125.8,-144.1 | 59% (t30) chi angles: 188.9,50.1 | 0.12Å | - | - |
| B 563 | ARG | 50 | 0.654Å H with B 562 ASN ND2 | Favored (22.72%) General / -101.8,150.9 | 12.2% (mmt180) chi angles: 305,301.9,193.1,133.1 | 0.097Å | - | - |
| B 564 | ARG | 50 | 0.477Å HG2 with B 514 ASP O | Favored (2.5%) General / -59.0,114.3 | 28.1% (mmt180) chi angles: 296.1,296.9,204.3,186.3 | 0.057Å | - | - |
| B 565 | THR | 50 | - | Allowed (0.75%) General / -71.9,10.2 | 63.3% (p) chi angles: 64.8 | 0.021Å | - | - |
| B 566 | ALA | 50 | 0.856Å HB2 with B 531 ALA HB2 | Allowed (0.63%) General / -173.3,-170.6 | - | 0.204Å | - | - |
| B 567 | ASN | 50 | - | Favored (54.23%) General / -121.7,138.7 | 28.5% (t-20) chi angles: 187.7,301.4 | 0.124Å | - | - |
| B 568 | ILE | 50 | 1.038Å HG22 with B 510 CYS HB3 | Favored (74.3%) Isoleucine or valine / -117.4,125.9 | 8.6% (tp) chi angles: 183.2,64.9 | 0.129Å | - | - |
| B 569 | ARG | 50 | - | Favored (46.23%) General / -124.8,126.9 | 50.3% (ttp180) chi angles: 184.2,189.1,74.3,213.1 | 0.114Å | - | - |

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|-------|---------|------------|------------------------------------|---|---|--------------------|---------------------|---------------------|
| B 570 | SER | 50 | - | Favored (53%) General / -69.3,137.4 | 34.4% (t) chi angles: 183.1 | 0.109Å | - | - |
| B 571 | ILE | 50 | 0.945Å HG12 with B 526 LYS HG2 | Favored (3.98%) Isoleucine or valine / -101.1,-34.6 | 0.8% chi angles: 77.1,123.2 | 0.071Å | - | - |
| B 572 | GLY | 50 | 0.62Å N with B 571 ILE HG13 | Favored (14.71%) Glycine / -118.7,172.9 | - | - | - | - |
| B 573 | TYR | 50 | 0.552Å CZ with B 443 TYR CE2 | OUTLIER (0.02%) General / -60.4,90.5 | 22.6% (m-85) chi angles: 274.5,272.2 | 0.028Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| B 574 | SER | 50 | - | Favored (40.49%) General / -76.0,145.1 | 53.7% (m) chi angles: 299.9 | 0.062Å | - | - |
| B 575 | ASP | 50 | 0.488Å O with B 523 ASN HB3 | Favored (6.37%) General / -125.7,100.3 | 90% (m-20) chi angles: 294.2,344 | 0.005Å | - | - |
| B 576 | LEU | 50 | - | Favored (9.84%) General / -109.0,167.8 | 37.2% (mt) chi angles: 310.5,176.1 | 0.111Å | - | - |
| B 577 | PHE | 50 | 0.646Å HB2 with B 521 ILE HG12 | Favored (51.56%) General / -126.1,133.8 | 88.9% (m-85) chi angles: 300.1,90 | 0.044Å | - | - |
| B 578 | CYS | 99.99 | - | Favored (31.6%) General / -104.5,144.5 | 52.3% (t) chi angles: 180 | 0.035Å | - | - |
| B 579 | LEU | 50 | 0.541Å HD22 with B 494 LEU HD11 | Favored (44.24%) General / -129.0,128.7 | 30.8% (tp) chi angles: 188.6,66.7 | 0.096Å | - | - |
| B 580 | SER | 50 | - | Favored (21.27%) General / | 84% (p) chi angles: 68.6 | 0.017Å | - | - |

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| | | | | -83.9,159.8 | | | | |
| B 581 | LYS | 50 | 0.721Å HG3 with B 552 ILE HG23 | Favored (79.78%) General / -60.1,-37.4 | 39.2% (<i>ttpt</i>) chi angles: 187,179.1,66.9,179.8 | 0.066Å | - | - |
| B 582 | ASP | 50 | - | Allowed (0.83%) General / -52.3,-64.4 | 5.6% (<i>m-20</i>) chi angles: 306.4,84.2 | 0.075Å | - | - |
| B 583 | ASP | 50 | - | Favored (78.54%) General / -63.6,-34.8 | 61.9% (<i>m-20</i>) chi angles: 294.3,302.7 | 0.03Å | - | - |
| B 584 | LEU | 99.99 | 0.79Å HD13 with B 552 ILE HG21 | Favored (73.82%) General / -61.0,-50.3 | 10.3% (<i>tt</i>) chi angles: 183.9,150 | 0.045Å | - | - |
| B 585 | MET | 50 | 0.624Å O with B 589 THR HG23 | Favored (69.05%) General / -69.1,-30.7 | 60.7% (<i>mtt</i>) chi angles: 292.3,183.8,173.7 | 0.026Å | - | - |
| B 586 | GLU | 50 | - | Favored (45.07%) General / -66.7,-52.4 | 62.4% (<i>tt0</i>) chi angles: 185.1,189.7,338.7 | 0.069Å | - | - |
| B 587 | ALA | 50 | - | Favored (70.58%) General / -61.5,-30.4 | - | 0.091Å | - | - |
| B 588 | LEU | 50 | - | Favored (26.72%) General / -86.3,-22.5 | 48.9% (<i>mt</i>) chi angles: 293.2,185.6 | 0.112Å | - | - |
| B 589 | THR | 50 | 0.624Å HG23 with B 585 MET O | Favored (65.07%) General / -72.8,-31.9 | 77.8% (<i>p</i>) chi angles: 60.2 | 0.017Å | - | - |
| B 590 | GLU | 50 | - | Favored (57.13%) General / -77.0,-32.5 | 80.4% (<i>tt0</i>) chi angles: 180.2,177.5,15.6 | 0.094Å | - | - |
| B 591 | TYR | 50 | 0.748Å CD1 with B 490 LEU HD13 | Favored (65.41%) Pre-proline / -133.8,76.7 | 90.7% (<i>m-85</i>) chi angles: 301.5,99.4 | 0.05Å | - | - |
| B 592 | PRO | 50 | - | Favored (32.53%) | 82.1% (<i>Cg_exo</i>) chi angles: 331.9 | 0.085Å | - | - |

| B 593 | GLU | 50 | - | Trans-proline / -60.1,-43.9 Allowed (0.79%) General / -42.2,-34.6 | 52.3% (<i>mm-40</i>) chi angles: 290.9,289.4,0.6 | 0.08Å | - | - |
|----------------------------------|---------|-----------|-------------------------------------|--|--|-----------------|---------------------|---------------------|
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: Clashscore: Outliers: 16 of | | | | 764 | Poor rotamers: 12 of | 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| B 594 | ALA | 50 | - | Favored (60.22%) General / -74.2,-20.4 | - | 0.035Å | - | - |
| B 595 | LYS | 50 | 0.405Å O with B 599 GLU HG3 | Favored (83.92%) General / -59.5,-39.5 | 63.6% (<i>tttp</i>) chi angles: 183.3,182.1,179.2,63.2 | 0.022Å | - | - |
| B 596 | LYS | 50 | - | Favored (80.88%) General / -64.0,-35.5 | 64% (<i>tttp</i>) chi angles: 184.1,180.4,179.1,62.3 | 0.017Å | - | - |
| B 597 | ALA | 50 | - | Favored (64.25%) General / -56.5,-52.6 | - | 0.031Å | - | - |
| B 598 | LEU | 50 | - | Favored (92.89%) General / -64.8,-39.0 | 10.5% (<i>mp</i>) chi angles: 280.6,63.7 | 0.026Å | - | - |
| B 599 | GLU | 99.99 | 0.405Å HG3 with B 595 LYS O | - | 74.9% (<i>mt-10</i>) chi angles: 293.7,191.7,332 | 0.049Å | - | - |
| C 407 | ASN | 99.99 | - | - | 85% (<i>m-20</i>) chi angles: 296.7,336.5 | 0.058Å | - | - |
| C 408 | ALA | 50 | - | OUTLIER (0.02%) General / -171.2,-39.6 | - | 0.063Å | - | - |
| C 409 | SER | 50 | 0.675Å HB2 with C 449 LYS HD2 | Favored (58.86%) General / -81.7,-6.2 | 80.2% (<i>p</i>) chi angles: 60 | 0.123Å | - | - |
| C 410 | ARG | 50 | 0.545Å HH21 with C 447 ASN CG | Favored (66.01%) General / -71.2,-30.2 | 10.9% (<i>mtp180</i>) chi angles: 302.7,214.3,69.6,156.8 | 0.073Å | - | - |

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| C 411 | ALA | 50 | - | Favored (63.85%) General / -73.4,-40.9 | - | 0.052Å | - | - |
| C 412 | GLU | 50 | - | Favored (81.99%) General / -60.7,-37.5 | 11.8% (<i>tm</i> -20) chi angles: 179.8,287.3,328.8 | 0.069Å | - | - |
| C 413 | PHE | 50 | 0.454Å CD1 with C 445 TRP HE3 | Favored (45.25%) General / -65.1,-53.5 | 88.8% (<i>t80</i>) chi angles: 178.5,82.1 | 0.037Å | - | - |
| C 414 | GLN | 50 | 0.553Å HA with C 417 ILE HG12 | Favored (81.81%) General / -59.5,-38.7 | 15.8% (<i>mt</i> -30) chi angles: 282.5,140.6,20.1 | 0.015Å | - | - |
| C 415 | ALA | 50 | - | Favored (80.73%) General / -68.5,-40.6 | - | 0.039Å | - | - |
| C 416 | LYS | 50 | - | Favored (9%) General / -69.9,-55.7 | 13.8% (<i>tppt</i> ?) chi angles: 177.9,49.7,62.1,192.2 | 0.03Å | - | - |
| C 417 | ILE | 50 | 0.74Å O with C 420 ILE HG12 | Favored (33.85%) Isoleucine or valine / -58.2,-28.1 | 30.1% (<i>pt</i>) chi angles: 69.3,172.7 | 0.077Å | - | - |
| C 418 | ASP | 50 | - | Favored (92.98%) General / -65.4,-41.9 | 44.5% (<i>t0</i>) chi angles: 186.9,329.5 | 0.038Å | - | - |
| C 419 | SER | 50 | - | Favored (97.46%) General / -61.8,-44.1 | 40.1% (<i>t</i>) chi angles: 181.5 | 0.038Å | - | - |
| C 420 | ILE | 50 | 0.74Å HG12 with C 417 ILE O | Favored (65.2%) Isoleucine or valine / -58.7,-37.4 | 16.4% (<i>pt</i>) chi angles: 71.3,180.5 | 0.072Å | - | OUTLIER(S) worst is CB- CG1-CD1: 4.186 σ |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|------|---------|-------------|-----------------|----------------------|--------------------|---------------------|---------------------|-------------|
| Avg: | | Clashscore: | Outliers: 16 of | Poor rotamers: 12 of | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 | |
| | | 61.33 | 65.92 | 764 | 676 | | | |

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|---|-----|--------|---------------------|-----------------------|---|--|--|--|
| C | ... | 0.661Å | Favored (60.24%) | 30.7% (<i>mtpp</i>) | 0 | | | |
|---|-----|--------|---------------------|-----------------------|---|--|--|--|

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|-----|-----|-------|--|--|---|--------|---|--|
| 421 | LYS | 50 | HG3 with C 417 ILE O | (90.34%) General / -65.2,-38.4 | chi angles: 294,181,68,63.9 | 0.047Å | - | - |
| 422 | GLN | 50 | - | Favored (54.03%) General / -77.6,-33.0 | 19% (<i>mt-30</i>) chi angles: 298,166.1,183.5 | 0.087Å | - | - |
| 423 | TYR | 50 | 0.445Å CE1 with B 453 GLU HG3 | Favored (99.6%) General / -62.0,-42.9 | 71.9% (<i>t80</i>) chi angles: 172.6,84.8 | 0.05Å | - | - |
| 424 | MET | 50 | 1.002Å SD with C 437 VAL HG11 | Favored (70.48%) General / -71.4,-40.7 | 69.9% (<i>mtm</i>) chi angles: 293.7,191.9,299.6 | 0.05Å | - | - |
| 425 | GLN | 50 | - | Favored (79.46%) General / -67.7,-35.7 | 53.4% (<i>tt0</i>) chi angles: 185.3,179.2,57 | 0.012Å | - | - |
| 426 | PHE | 50 | - | Favored (79.94%) General / -64.8,-35.1 | 11% (<i>t80</i>) chi angles: 182.8,38.1 | 0.025Å | - | - |
| 427 | ARG | 99.99 | 1.019Å HB3 with B 473 HIS HE1 | Favored (57.36%) General / -92.0,-1.2 | 32.8% (<i>mmt180</i>) chi angles: 287.3,304.8,183.2,180 | 0.21Å | - | OUTLIER(S) worst is N-CA- CB: 4.945 σ |
| 428 | LYS | 50 | - | Favored (28.26%) General / 54.1,38.0 | 88.4% (<i>mttt</i>) chi angles: 298.3,170.7,185,166.6 | 0.051Å | - | - |
| 429 | VAL | 50 | 0.926Å HG21 with C 433 LEU HD22 | Favored (5.58%) Isoleucine or valine / -61.0,152.8 | 12.1% (<i>p</i>) chi angles: 62.1 | 0.168Å | - | - |
| 430 | THR | 50 | 0.449Å HG22 with C 432 ASP H | Favored (7.51%) General / -57.2,156.3 | 98.9% (<i>m</i>) chi angles: 298.8 | 0.05Å | - | - |
| 431 | LYS | 50 | 0.437Å O with C 435 THR HG23 | Favored (82.42%) General / -66.9,-36.5 | 32.8% (<i>mmmt</i>) chi angles: 296.3,295.3,295.3,181.1 | 0.032Å | - | - |
| 432 | ASP | 50 | 0.449Å H with C 430 THR HG22 | Favored (80.59%) General / -65.3,-35.3 | 85.2% (<i>m-20</i>) chi angles: 293.9,349.1 | 0.053Å | - | - |

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| C 433 | LEU | 50 | 0.926Å HD22 with C 429 VAL HG21 | Favored (63.82%) General / -73.5,-40.7 | 8.5% (<i>tt</i>) chi angles: 191.4,155.1 | 0.12Å | - | - |
| C 434 | GLU | 50 | 0.784Å O with C 438 ILE HG12 | Favored (93.68%) General / -63.9,-39.2 | 54.6% (<i>mt-10</i>) chi angles: 296.7,182.7,298.1 | 0.075Å | - | - |
| C 435 | THR | 50 | 0.437Å HG23 with C 431 LYS O | Favored (68.27%) General / -66.1,-49.3 | 77.9% (<i>p</i>) chi angles: 60.2 | 0.02Å | - | - |
| C 436 | ARG | 50 | - | Favored (72.82%) General / -58.2,-36.2 | 86.8% (<i>mtm-85</i>) chi angles: 285.7,187.7,294.2,260.3 | 0.068Å | - | - |
| C 437 | VAL | 50 | 1.002Å HG11 with C 424 MET SD | Favored (68.54%) Isoleucine or valine / -72.0,-41.3 | 4.9% (<i>p</i>) chi angles: 76.4 | 0.175Å | - | - |
| C 438 | ILE | 50 | 0.784Å HG12 with C 434 GLU O | Favored (28.75%) Isoleucine or valine / -58.1,-54.7 | 41.3% (<i>mm</i>) chi angles: 299.1,304.7 | 0.028Å | - | - |
| C 439 | ARG | 50 | 0.445Å O with C 443 TYR HD2 | Favored (77.74%) General / -60.0,-36.6 | 55.1% (<i>mmm-85</i>) chi angles: 293.6,298,293,278.7 | 0.033Å | - | - |
| C 440 | TRP | 99.99 | 0.834Å CH2 with C 444 LEU HD22 | Favored (42.13%) General / -62.5,-54.3 | 89.3% (<i>t90</i>) chi angles: 184.8,87.3 | 0.024Å | OUTLIER(S) worst is NE1-- CE2: 4.769 σ | OUTLIER(S) worst is CZ2- CH2-CZ3: 5.295 σ |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| C 441 | PHE | 50 | 0.787Å HE2 with C 437 VAL HG22 | Favored (61.2%) General / -51.0,-46.2 | 95.6% (<i>m-85</i>) chi angles: 292.3,275.1 | 0.072Å | - | - |
| C 442 | ASP | 50 | 0.407Å HB2 with C 439 ARG O | Favored (67.79%) General / -53.0,-45.5 | 51.3% (<i>m-20</i>) chi angles: 295.4,296.5 | 0.044Å | - | - |
| C | TYR | 50 | 0.543Å CE2 with C | Favored (60.59%) | 95.2% (<i>m-85</i>) | 0.027Å | - | - |

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| C 443 | TRP | 50 | CE2 with C 573 TYR CZ | General / -75.2,-30.6 | chi angles: 292.2,274.8 | 0.027 Å | - | - |
| C 444 | LEU | 99.99 | 0.834 Å HD22 with C 440 TRP CH2 | Favored (22.95%) General / -84.8,-33.5 | 21.3% (<i>tp</i>) chi angles: 187.1,74 | 0.098 Å | - | - |
| C 445 | TRP | 50 | 0.454 Å HE3 with C 413 PHE CD1 | Favored (8.96%) General / -119.3,-16.7 | 51.6% (<i>m0</i>) chi angles: 296.7,351.6 | 0.079 Å | OUTLIER(S) worst is NE1-- CE2: 4.757 σ | OUTLIER(S) worst is CD2- CE3-CZ3: 4.172 σ |
| C 446 | ALA | 50 | - | Allowed (0.66%) General / 51.6,18.1 | - | 0.046 Å | - | - |
| C 447 | ASN | 99.99 | 0.545 Å CG with C 410 ARG HH21 | Favored (10.17%) General / 56.4,26.0 | 64.3% (<i>t-20</i>) chi angles: 184.8,348.8 | 0.097 Å | - | OUTLIER(S) worst is OD1- CG-ND2: 5.666 σ |
| C 448 | LYS | 99.99 | - | Allowed (0.73%) General / -106.2,-72.0 | 29.5% (<i>tptp</i>) chi angles: 182.4,64.6,177.9,64.7 | 0.065 Å | - | - |
| C 449 | LYS | 99.99 | 0.675 Å HD2 with C 409 SER HB2 | Favored (49.27%) General / -125.4,147.2 | 27.9% (<i>tptp</i>) chi angles: 180.1,66.8,182.2,61.9 | 0.078 Å | - | OUTLIER(S) worst is CG- CD-CE: 4.38 σ |
| C 450 | THR | 99.99 | 0.709 Å HG22 with C 451 VAL H | Allowed (0.82%) General / -119.5,-160.6 | 48.8% (<i>m</i>) chi angles: 305 | 0.108 Å | - | - |
| C 451 | VAL | 99.99 | 1.053 Å HG22 with C 452 ASP HA | Allowed (0.44%) Isoleucine or valine / -48.1,151.2 | 6% (<i>p</i>) chi angles: 75 | 0.168 Å | - | - |
| C 452 | ASP | 50 | 1.053 Å HA with C 451 VAL HG22 | Allowed (1.01%) General / -104.8,44.7 | 2.2% (<i>m-20</i>) chi angles: 294.9,33.2 | 0.14 Å | - | - |
| C 453 | GLU | 50 | 0.825 Å HA with C 456 VAL HG22 | Allowed (0.6%) General / -40.4,-36.9 | 27.1% (<i>tt0</i>) chi angles: 193.5,193.3,40.1 | 0.048 Å | - | - |
| C 454 | LYS | 50 | - | Favored (79.14%) General / -63.5,-48.0 | 39% (<i>ttpt</i>) chi angles: 186.5,179.9,64.3,181.3 | 0.041 Å | - | - |

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|--|------|-------|---|---|---|--------|---|--|
| C 455 | GLU | 50 | 0.762Å HB3 with C 452 ASP HB3 | Favored (75.69%) General / -65.6,-47.4 | 10.8% (<i>tm-20</i>) chi angles: 181.5,289.8,325.2 | 0.055Å | - | - |
| C 456 | VAL | 50 | 0.825Å HG22 with C 453 GLU HA | Favored (85.34%) Isoleucine or valine / -58.9,-42.3 | 22.1% (<i>m</i>) chi angles: 302.9 | 0.037Å | - | - |
| C 457 | LEU | 50 | 0.469Å HB2 with C 453 GLU O | Favored (82.27%) General / -68.2,-40.5 | 0.5% chi angles: 254.3,39.3 | 0.042Å | - | - |
| C 458 | LYS | 50 | - | Favored (93.83%) General / -61.1,-40.4 | 28.6% (<i>tptp</i>) chi angles: 184.5,62.4,180.5,64.5 | 0.04Å | - | - |
| C 459 | SER | 99.99 | 0.653Å O with A 440 TRP CH2 | Favored (77.29%) General / -64.6,-34.0 | 95.4% (<i>p</i>) chi angles: 66.7 | 0.102Å | - | OUTLIER(S) worst is CA-C- O: 5.595 σ |
| C 460 | LEU | 50 | - | Favored (38.7%) Pre-proline / -71.6,166.5 | 81% (<i>mt</i>) chi angles: 298.2,182.5 | 0.042Å | - | - |
| <div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash > 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div> <div> <div>Avg: 61.33</div> <div>Clashscore: 65.92</div> <div>Outliers: 16 of 764</div> <div>Poor rotamers: 12 of 676</div> <div>Outliers: 4 of 728</div> <div>Outliers: 12 of 772</div> <div>Outliers: 64 of 772</div> </div> | | | | | | | | |
| C 461 | PRO | 50 | 0.778Å HD3 with A 440 TRP CE2 | Favored (6.07%) Trans-proline / -87.7,171.3 | 42.9% (<i>Cg_endo</i>) chi angles: 35.9 | 0.014Å | - | - |
| C 462 | ASP | 50 | - | Favored (96.45%) General / -64.0,-43.1 | 42.1% (<i>t0</i>) chi angles: 190.5,329.5 | 0.016Å | - | - |
| C 463 | LYS | 50 | 0.673Å HE2 with A 508 TYR H | Favored (73.75%) General / -57.8,-37.4 | 32.4% (<i>mmmt</i>) chi angles: 294.8,293.5,296.6,184.8 | 0.04Å | - | - |
| C 464 | LEU | 50 | 0.666Å HD12 with C 461 PRO HD2 | Favored (22.9%) General / -75.5,-48.4 | 59.3% (<i>mt</i>) chi angles: 286.4,177.4 | 0.038Å | - | - |
| C | ---- | ---- | 0.585Å | Favored (72.01%) | 54.9% (<i>mtmt</i>) | 0 | - | - |

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| ~ 465 | LYS | 50 | O with C 470 ILE HG12 | (χ^2 of 2.01 / 0) General / -61.0,-33.1 | chi angles: 294.7,178.6,295.9,178.8 | 0.135Å | - | - |
| C 466 | ALA | 50 | 0.723Å HA with C 470 ILE CB | Favored (83.8%) General / -66.6,-36.9 | - | 0.118Å | - | - |
| C 467 | GLU | 50 | 0.601Å OE2 with A 433 LEU HD12 | Favored (79.54%) General / -68.8,-40.5 | 15.5% (<i>tt0</i>) chi angles: 206.1,191.3,309.1 | 0.116Å | - | - |
| C 468 | ILE | 99.99 | 0.892Å HA with C 472 VAL HG12 | Favored (24.44%) Isoleucine or valine / -119.2,146.0 | 17.8% (<i>pt</i>) chi angles: 51.7,179.6 | 0.186Å | - | - |
| C 469 | ALA | 99.99 | 0.922Å H with C 473 HIS HD2 | Allowed (1.81%) General / 66.3,0.8 | - | 0.078Å | - | - |
| C 470 | ILE | 99.99 | 0.986Å HD12 with C 496 LEU HA | Allowed (0.75%) Isoleucine or valine / -132.4,-25.7 | 26.9% (<i>mm</i>) chi angles: 299,310.2 | 0.091Å | - | - |
| C 471 | ASN | 50 | 1.066Å HD21 with C 492 VAL HG12 | Allowed (0.47%) General / -140.4,-51.1 | 42.2% (<i>m-20</i>) chi angles: 278.7,302.3 | 0.195Å | - | OUTLIER(S) worst is CA- CB-CG: 4.049 σ |
| C 472 | VAL | 50 | 0.892Å HG12 with C 468 ILE HA | Favored (82.17%) Isoleucine or valine / -58.6,-41.5 | 15% (<i>p</i>) chi angles: 63.5 | 0.065Å | - | - |
| C 473 | HIS | 99.99 | 0.989Å HE1 with A 427 ARG HB3 | Favored (61.3%) General / -72.7,-25.5 | 84.1% (<i>m-70</i>) chi angles: 288,298.1 | 0.04Å | OUTLIER(S) worst is CD2-- NE2: 7.083 σ | OUTLIER(S) worst is CD2- NE2-CE1: 12.71 σ |
| C 474 | LEU | 99.99 | 0.684Å C with C 474 LEU HD23 | Favored (38.13%) General / -53.1,132.5 | 7.2% (<i>tt</i>) chi angles: 184.9,162.9 | 0.126Å | - | - |
| C 475 | ASP | 99.99 | 0.542Å N with C 474 LEU HD23 | Favored (5.85%) General / -129.7,12.7 | 29.9% (<i>t70</i>) chi angles: 179.1,76.4 | 0.069Å | - | - |
| C 476 | THR | 99.99 | 0.483Å HB with C 523 ASN HA | Favored (2.21%) General / -136.0,18.0 | 10.3% (<i>t</i>) chi angles: 184.2 | 0.074Å | - | - |

| C 477 | LEU | 99.99 | 1.097Å HG with C 483 PHE HB3 | Allowed (0.81%) General / -134.6,-52.3 | 10% (<i>tt</i>) chi angles: 185.3,154.6 | 0.239Å | - | - |
|----------|---------|------------|--|--|---|--------------------|---------------------|---|
| C 478 | LYS | 50 | - | Favored (31.44%) General / -53.1,-29.6 | 27.1% (<i>tptp</i>) chi angles: 180.3,61.9,184.6,69.5 | 0.035Å | - | - |
| C 479 | LYS | 50 | - | Favored (49.45%) General / -89.1,-9.9 | 26.8% (<i>tptp</i>) chi angles: 188.6,61.2,182.7,67.3 | 0.051Å | - | - |
| C 480 | VAL | 50 | 1.043Å HG12 with C 477 LEU HA | Favored (23.98%) Isoleucine or valine / -117.0,108.1 | 11.5% (<i>p</i>) chi angles: 66.6 | 0.141Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| C 481 | ARG | 50 | 0.713Å HA with C 484 GLN HG2 | Favored (7.28%) General / -43.5,-47.1 | 57.9% (<i>mmm-85</i>) chi angles: 296.1,292.8,296.7,277.2 | 0.027Å | - | - |
| C 482 | ILE | 50 | 0.745Å HG12 with C 480 VAL HG22 | Favored (87.84%) Isoleucine or valine / -59.3,-42.6 | 42.2% (<i>pt</i>) chi angles: 65.5,172.5 | 0.067Å | - | - |
| C 483 | PHE | 50 | 1.097Å HB3 with C 477 LEU HG | Favored (28.76%) General / -79.7,-40.6 | 7.1% (<i>m-30</i>) chi angles: 278.5,9.7 | 0.047Å | - | OUTLIER(S) worst is CA- CB-CG: 4.414 σ |
| C 484 | GLN | 50 | 0.713Å HG2 with C 481 ARG HA | Favored (83.93%) General / -67.8,-38.8 | 19.8% (<i>pt20</i>) chi angles: 65.9,181.7,61.9 | 0.076Å | - | - |
| C 485 | ASP | 50 | - | Favored (4.67%) General / -97.0,26.4 | 48.7% (<i>t0</i>) chi angles: 190.7,338.3 | 0.039Å | - | - |
| C 486 | CYS | 99.99 | 0.639Å SG with C 490 LEU HD23 | Favored (27.27%) General / -115.1,155.3 | 52.7% (<i>t</i>) chi angles: 181.3 | 0.052Å | - | - |

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|----------|-----|-------|--|---|--|--------|---|---|
| C 487 | GLU | 99.99 | - | Favored (8.68%) General / -57.2,120.8 | 87.8% (<i>mt-10</i>) chi angles: 301.3,182.2,337.1 | 0.064Å | - | - |
| C 488 | ALA | 50 | 0.723Å O with C 492 VAL HG13 | Favored (14.29%) General / -54.9,-22.3 | - | 0.016Å | - | - |
| C 489 | GLY | 50 | 0.483Å O with C 492 VAL HG22 | Favored (76.39%) Glycine / -67.5,-45.6 | - | - | - | - |
| C 490 | LEU | 99.99 | 0.749Å HD13 with C 591 TYR CD1 | Favored (93.9%) General / -65.5,-41.0 | 35.4% (<i>tp</i>) chi angles: 175.6,54.2 | 0.063Å | - | - |
| C 491 | LEU | 99.99 | 0.835Å HD13 with C 477 LEU HD11 | Favored (5.02%) General / -57.2,-59.5 | 94.3% (<i>mt</i>) chi angles: 298.4,175.6 | 0.075Å | - | - |
| C 492 | VAL | 50 | 1.066Å HG12 with C 471 ASN HD21 | Favored (14.9%) Isoleucine or valine / -48.6,-45.5 | 25.8% (<i>m</i>) chi angles: 302 | 0.023Å | - | - |
| C 493 | GLU | 50 | - | Favored (68.45%) General / -66.2,-28.0 | 14.3% (<i>tm-20</i>) chi angles: 183.8,285.4,333.7 | 0.107Å | - | - |
| C 494 | LEU | 50 | 0.699Å HD23 with C 483 PHE CE1 | Favored (12.94%) General / -80.0,-48.7 | 33.9% (<i>tp</i>) chi angles: 187.7,59.4 | 0.033Å | - | OUTLIER(S) worst is CD1- CG-CD2: 4.562 σ |
| C 495 | VAL | 50 | 0.756Å HG21 with C 470 ILE O | Favored (44.55%) Isoleucine or valine / -57.7,-33.2 | 20.8% (<i>m</i>) chi angles: 303.3 | 0.021Å | - | - |
| C 496 | LEU | 50 | 0.986Å HA with C 470 ILE HD12 | Favored (55.61%) General / -64.8,-13.4 | 8.9% (<i>tt</i>) chi angles: 190.5,154.5 | 0.155Å | - | - |
| C 497 | LYS | 50 | - | Favored (10.85%) General / -115.9,-18.0 | 64.5% (<i>mttp</i>) chi angles: 295.5,177.2,177.3,63.2 | 0.054Å | - | - |
| - | - | - | 0.651 Å | Favored | | | | |

| C 498 | LEU | 50 | 0.851 Å HB3 with C 577 PHE HB3 | (44.49%) General / -58.6,144.1 | 58.4% (<i>mt</i>) chi angles: 305.2,173.5 | 0.096 Å | - | - |
|----------|---------|------------|--------------------------------------|--|--|--------------------|---------------------|---------------------|
| C 499 | ARG | 50 | - | Favored (28.15%) Pre-proline / -118.9,124.7 | 40.1% (<i>ptt180</i>) chi angles: 62,179.4,181.4,181.7 | 0.069 Å | - | - |
| C 500 | PRO | 50 | - | Favored (33.36%) Trans-proline / -68.0,135.0 | 92.8% (<i>Cg_endo</i>) chi angles: 30.9 | 0.035 Å | - | - |
| # | Alt Res | High B | Clash > 0.4 Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| C 501 | THR | 50 | - | Favored (30.24%) General / -144.9,142.9 | 63.1% (<i>p</i>) chi angles: 62.3 | 0.038 Å | - | - |
| C 502 | VAL | 50 | - | Favored (36.42%) Isoleucine or valine / -115.5,140.6 | 74% (<i>t</i>) chi angles: 174 | 0.052 Å | - | - |
| C 503 | PHE | 50 | - | Favored (50.81%) General / -127.0,145.2 | 63.9% (<i>m-85</i>) chi angles: 284.3,87.2 | 0.046 Å | - | - |
| C 504 | SER | 50 | - | Favored (31.54%) Pre-proline / -101.6,158.6 | 70.2% (<i>m</i>) chi angles: 295.9 | 0.029 Å | - | - |
| C 505 | PRO | 50 | - | Favored (52.06%) Trans-proline / -53.9,132.9 | 88.3% (<i>Cg_exo</i>) chi angles: 331.4 | 0.107 Å | - | - |
| C 506 | GLY | 50 | - | Favored (9.88%) Glycine / 100.2,-30.6 | - | - | - | - |
| C 507 | ASP | 50 | 0.441 Å HA with B 463 LYS HE2 | Allowed (0.56%) General / -49.0,155.9 | 81.1% (<i>m-20</i>) chi angles: 283.3,337.3 | 0.05 Å | - | - |
| C 508 | TYR | 50 | 0.686 Å H with B 463 LYS HF2 | Favored (5.14%) General / -108.5,94.6 | 11.4% (<i>m-30</i>) chi angles: 282.8,356.5 | 0.101 Å | - | - |

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|----------|-----|-------|---|---|---|--------|---|---|
| C 509 | ILE | 50 | 0.801Å HB with C 568 ILE HG23 | Favored (99.01%) Isoleucine or valine / -60.9,-45.0 | 69% (<i>mt</i>) chi angles: 303.1,168.1 | 0.091Å | - | - |
| C 510 | CYS | 99.99 | 1.016Å HB3 with C 568 ILE HG22 | Favored (28.07%) General / -144.3,138.6 | 4.8% (<i>t</i>) chi angles: 164.3 | 0.071Å | - | - |
| C 511 | LYS | 50 | 0.457Å NZ with C 508 TYR HD2 | Favored (37.7%) General / -108.1,142.8 | 68.4% (<i>mttm</i>) chi angles: 292.6,179.7,178.2,293.8 | 0.066Å | - | - |
| C 512 | LYS | 50 | - | Favored (31.24%) General / -61.9,152.7 | 38.6% (<i>ttpt</i>) chi angles: 184.7,182,62.4,181.3 | 0.071Å | - | - |
| C 513 | GLY | 50 | 0.441Å O with C 563 ARG HD2 | Favored (4.44%) Glycine / 78.9,-20.6 | - | - | - | - |
| C 514 | ASP | 50 | 0.479Å O with C 564 ARG HG2 | Favored (43.53%) General / -74.6,139.2 | 42.5% (<i>t0</i>) chi angles: 189,328.5 | 0.062Å | - | - |
| C 515 | ILE | 50 | - | Favored (12.76%) Isoleucine or valine / -63.5,121.6 | 27.2% (<i>mt</i>) chi angles: 311.5,178.4 | 0.032Å | - | - |
| C 516 | GLY | 50 | - | Favored (10.08%) Glycine / -98.5,130.0 | - | - | - | - |
| C 517 | LYS | 50 | 0.524Å HG2 with C 517 LYS O | Favored (9.22%) General / -124.0,19.7 | 61.9% (<i>tttm</i>) chi angles: 185.6,184.4,177.4,293.2 | 0.063Å | - | - |
| C 518 | GLU | 50 | - | Favored (7.59%) General / -169.3,157.6 | 12.6% (<i>pt-20</i>) chi angles: 61.5,180.2,62.4 | 0.013Å | - | - |
| C 519 | MET | 50 | - | Favored (8.78%) General / -124.8,173.1 | 27.1% (<i>ptm</i>) chi angles: 65.3,172.3,293.2 | 0.032Å | - | - |
| C 520 | GLY | 50 | - | Favored (52.46%) Glycine / -98.5,130.0 | 90.0% (<i>mt-85</i>) chi angles: 311.5,178.4 | 0.032Å | - | - |

| 520 | TYR | 50 | - | (52.46%) General / -130.9,149.6 | 50.2% (mt 65) chi angles: 299.1,87.1 | 0.071Å | - | - |
|-------|---------|------------|------------------------------------|--|---|--------------------|---------------------|---|
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| C 521 | ILE | 50 | 0.644Å CG1 with C 577 PHE HB2 | Favored (15.09%) Isoleucine or valine / -121.0,104.3 | 32% (pt) chi angles: 66.9,166.7 | 0.058Å | - | - |
| C 522 | ILE | 50 | - | Allowed (0.15%) Isoleucine or valine / -58.2,105.0 | 62.3% (mt) chi angles: 304.9,175.2 | 0.02Å | - | - |
| C 523 | ASN | 50 | 0.483Å HA with C 476 THR HB | Favored (20.01%) General / -76.9,-47.8 | 48.4% (t30) chi angles: 182.1,60.4 | 0.01Å | - | - |
| C 524 | GLU | 50 | - | Favored (6.4%) General / -157.0,127.2 | 11.3% (tm-20) chi angles: 179.9,288.5,328.5 | 0.08Å | - | - |
| C 525 | GLY | 50 | - | Favored (13.05%) Glycine / 132.8,172.6 | - | - | - | - |
| C 526 | LYS | 99.99 | 0.972Å HG2 with C 571 ILE HG12 | Favored (51.03%) General / -122.2,128.3 | 66.7% (tttt) chi angles: 165.7,169.7,180.8,162.5 | 0.107Å | - | - |
| C 527 | LEU | 50 | 0.885Å HB3 with C 568 ILE HD11 | Favored (29.48%) General / -119.4,156.8 | 9.5% (mp) chi angles: 281.9,69.5 | 0.069Å | - | OUTLIER(S) worst is CD1- CG-CD2: 4.488 σ |
| C 528 | ALA | 50 | 0.51Å O with C 568 ILE HD12 | Favored (54.91%) General / -118.4,128.8 | - | 0.07Å | - | - |
| C 529 | VAL | 50 | 0.695Å HG22 with C 568 ILE HD13 | Favored (70.26%) Isoleucine or valine / -113.0,127.5 | 22.5% (t) chi angles: 187.4 | 0.056Å | - | - |
| C 530 | VAL | 50 | - | Favored (3.12%) Isoleucine or | 7.3% (p) chi angles: 58.8 | 0.101Å | - | - |

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|----------|-----|-------|--|--|---|--------|---|---|
| C 531 | ALA | 99.99 | 0.87Å HB2 with C 566 ALA HB2 | Isoleucine or valine / -130.1,97.0 Allowed (1.95%) General / -130.4,80.3 | - | 0.137Å | - | - |
| C 532 | ASP | 99.99 | - | Favored (11.65%) General / 53.0,31.7 | 29.4% (<i>t</i> 70) chi angles: 178.9,77 | 0.068Å | - | - |
| C 533 | ASP | 99.99 | - | Favored (31.44%) General / -160.3,165.4 | 26.1% (<i>p</i> 30) chi angles: 61.8,29.5 | 0.02Å | - | - |
| C 534 | GLY | 99.99 | - | Allowed (0.82%) Glycine / -61.8,105.1 | - | - | - | - |
| C 535 | VAL | 50 | 0.596Å HG22 with C 536 THR HG22 | OUTLIER (0%) Isoleucine or valine / -10.6,108.9 | 7.1% (<i>p</i>) chi angles: 58.4 | 0.01Å | - | - |
| C 536 | THR | 99.99 | 0.596Å HG22 with C 535 VAL HG22 | Allowed (1.5%) General / 55.6,15.4 | 9.9% (<i>t</i>) chi angles: 184 | 0.055Å | - | - |
| C 537 | GLN | 99.99 | 0.526Å HG2 with C 536 THR O | Favored (14.51%) General / 47.9,51.3 | 18.5% (<i>pt</i> 20) chi angles: 64.8,180.9,57 | 0.097Å | - | - |
| C 538 | PHE | 99.99 | 0.484Å CD2 with C 538 PHE O | Favored (14.34%) General / 63.5,32.4 | 85.3% (<i>t</i> 80) chi angles: 180.7,81.9 | 0.055Å | - | - |
| C 539 | VAL | 99.99 | 0.791Å HG12 with C 540 VAL H | Allowed (0.48%) Isoleucine or valine / -119.6,-168.6 | 63.1% (<i>t</i>) chi angles: 180 | 0.087Å | - | OUTLIER(S) worst is CA- CB-CG1: 4.474 σ |
| C 540 | VAL | 99.99 | 0.956Å HG13 with C 526 LYS HG3 | OUTLIER (0.06%) Isoleucine or valine / -158.5,97.4 | 26.7% (<i>t</i>) chi angles: 164.6 | 0.381Å | - | OUTLIER(S) worst is N-CA- CB: 5.587 σ |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | C β deviation | Bond lengths | Bond angles |
|---|---------|-----------|-----------------|--------------|---------|------------------------|-----------------|----------------|
| Avg: Clashscore: Outliers: 16 of Poor rotamers: 12 of Outliers: Outliers: 12 Outliers: 64 | | | | | | | | |
| 61.22 | | 65.02 | 76.4 | 676 | 4.66722 | 66772 | 66772 | 66772 |

| | | 01.55 | 05.92 | / 04 | 0/0 | 4 01 / 20 | 01 / / 2 | 01 / / 2 |
|----------|-----|-------|---|---|--|-----------|----------|----------|
| C 541 | LEU | 50 | - | Allowed (1.63%) General / -59.4,112.1 | 18.6% (<i>mt</i>) chi angles: 292,193.2 | 0.076Å | - | - |
| C 542 | SER | 50 | - | Allowed (1.05%) General / -124.4,-162.1 | 20.8% (<i>t</i>) chi angles: 188.4 | 0.068Å | - | - |
| C 543 | ASP | 50 | - | Favored (20.24%) General / -50.1,135.9 | 0.3% chi angles: 313.8,44.5 | 0.116Å | - | - |
| C 544 | GLY | 50 | - | Favored (73.87%) Glycine / 79.3,18.6 | - | - | - | - |
| C 545 | SER | 50 | - | Favored (28.28%) General / -124.4,160.4 | 72.6% (<i>m</i>) chi angles: 295.6 | 0.026Å | - | - |
| C 546 | TYR | 50 | 0.622Å CE1 with C 482 ILE HD13 | Favored (7.79%) General / -134.8,177.4 | 45.9% (<i>p90</i>) chi angles: 59,275.2 | 0.048Å | - | - |
| C 547 | PHE | 50 | 0.52Å CE2 with C 527 LEU HD22 | Favored (4.1%) General / -173.7,162.6 | 43.6% (<i>p90</i>) chi angles: 60.5,83.6 | 0.022Å | - | - |
| C 548 | GLY | 50 | - | Favored (62.81%) Glycine / 75.1,28.1 | - | - | - | - |
| C 549 | GLU | 50 | - | Favored (29.19%) General / -86.9,-19.2 | 6.4% (<i>pm0</i>) chi angles: 70.4,293.3,339.2 | 0.053Å | - | - |
| C 550 | ILE | 50 | - | Favored (97.65%) Isoleucine or valine / -62.3,-43.1 | 76.9% (<i>mt</i>) chi angles: 298.8,177 | 0.063Å | - | - |
| C 551 | SER | 50 | - | Favored (66.23%) General / -68.4,-27.5 | 73.4% (<i>m</i>) chi angles: 295.3 | 0.038Å | - | - |
| C | ... | ... | 0.785Å HG21 with C | Favored (58.47%) | 65.2% (<i>mt</i>) | ... | - | - |

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|-------|-----|-------|------------------------------|---|--|--------|---|---|
| 552 | ILE | 99.99 | HD23 with C 584 LEU HD13 | Isoleucine or valine / -73.2,-42.2 | chi angles: 302.9,177.3 | 0.083Å | - | - |
| C 553 | LEU | 99.99 | 0.483Å HD23 with C 554 ASN N | Favored (52.8%) General / -70.0,139.6 | 6.7% (tt) chi angles: 182.7,164 | 0.065Å | - | - |
| C 554 | ASN | 99.99 | 0.483Å N with C 553 LEU HD23 | Favored (24.51%) General / -118.8,115.5 | 41% (p30) chi angles: 60.9,25.7 | 0.036Å | - | OUTLIER(S) worst is OD1-CG-ND2: 6.181 σ |
| C 555 | ILE | 99.99 | 0.843Å H with C 560 SER HB3 | Favored (28.01%) Isoleucine or valine / -62.8,134.6 | 37.2% (pt) chi angles: 64,176.5 | 0.065Å | - | - |
| C 556 | LYS | 99.99 | - | Favored (50.62%) General / -65.7,133.2 | 22.7% (pttp) chi angles: 61.9,180,182,64.6 | 0.024Å | - | - |
| C 557 | GLY | 99.99 | - | Favored (33.75%) Glycine / 106.2,-21.2 | - | - | - | - |
| C 558 | SER | 99.99 | - | Favored (2.7%) General / -151.6,-167.1 | 32.1% (t) chi angles: 184.5 | 0.087Å | - | - |
| C 559 | LYS | 99.99 | - | Favored (30.42%) General / -115.6,117.5 | 22.6% (pttp) chi angles: 59.8,180.7,181.7,66.3 | 0.056Å | - | - |
| C 560 | SER | 99.99 | 0.843Å HB3 with C 555 ILE H | Favored (5.02%) General / -130.5,27.4 | 45.1% (t) chi angles: 178.7 | 0.049Å | - | OUTLIER(S) worst is O-C-N: 4.559 σ |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|------|-----|-----|--------|-------------------|---------------------|--------------------------|--------------------|---------------------|---------------------|
| Avg: | | | 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |

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|-------|-----|----|-----------------------------|---|----------------------------------|-------|---|---|
| C 561 | GLY | 50 | - | Allowed (0.75%) Glycine / 48.6,17.4 | - | - | - | - |
| C 562 | ASN | 50 | 0.645Å ND2 with C 563 ARG H | Allowed (0.31%) General / -125.8,-144.1 | 59% (t30) chi angles: 188.9,50.1 | 0.12Å | - | - |

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|----------|-----|----|--------------------------------------|---|---|--------|---|---|
| C 563 | ARG | 50 | 0.645Å H with C 562 ASN ND2 | Favored (22.72%) General / -101.8,150.9 | 12.2% (<i>mmt180</i>) chi angles: 305,301.9,193.1,133.1 | 0.097Å | - | - |
| C 564 | ARG | 50 | 0.479Å HG2 with C 514 ASP O | Favored (2.5%) General / -59.0,114.3 | 28.1% (<i>mmt180</i>) chi angles: 296.1,296.9,204.3,186.3 | 0.057Å | - | - |
| C 565 | THR | 50 | - | Allowed (0.75%) General / -71.9,10.2 | 63.3% (<i>p</i>) chi angles: 64.8 | 0.021Å | - | - |
| C 566 | ALA | 50 | 0.87Å HB2 with C 531 ALA HB2 | Allowed (0.63%) General / -173.3,-170.6 | - | 0.204Å | - | - |
| C 567 | ASN | 50 | - | Favored (54.23%) General / -121.7,138.7 | 28.5% (<i>t-20</i>) chi angles: 187.7,301.4 | 0.124Å | - | - |
| C 568 | ILE | 50 | 1.016Å HG22 with C 510 CYS HB3 | Favored (74.3%) Isoleucine or valine / -117.4,125.9 | 8.6% (<i>tp</i>) chi angles: 183.2,64.9 | 0.129Å | - | - |
| C 569 | ARG | 50 | - | Favored (46.23%) General / -124.8,126.9 | 50.3% (<i>ttp180</i>) chi angles: 184.2,189.1,74.3,213.1 | 0.114Å | - | - |
| C 570 | SER | 50 | - | Favored (53%) General / -69.3,137.4 | 34.4% (<i>t</i>) chi angles: 183.1 | 0.109Å | - | - |
| C 571 | ILE | 50 | 0.972Å HG12 with C 526 LYS HG2 | Favored (3.98%) Isoleucine or valine / -101.1,-34.6 | 0.8% chi angles: 77.1,123.2 | 0.071Å | - | - |
| C 572 | GLY | 50 | 0.628Å N with C 571 ILE HG13 | Favored (14.71%) Glycine / -118.7,172.9 | - | - | - | - |
| C 573 | TYR | 50 | 0.543Å CZ with C 443 TYR CE2 | OUTLIER (0.02%) General / -60.4,90.5 | 22.6% (<i>m-85</i>) chi angles: 274.5,272.2 | 0.028Å | - | - |
| C 574 | SER | 50 | - | Favored (40.49%) General / -76.0,145.1 | 53.7% (<i>m</i>) chi angles: 299.9 | 0.062Å | - | - |

| C 575 | ASP | 50 | 0.474Å O with C 523 ASN HB3 | Favored (6.37%) General / -125.7,100.3 | 90% (<i>m-20</i>) chi angles: 294.2,344 | 0.005Å | - | - |
|----------|---------|------------|--|--|--|--------------------|---------------------|---------------------|
| C 576 | LEU | 50 | - | Favored (9.84%) General / -109.0,167.8 | 37.2% (<i>mt</i>) chi angles: 310.5,176.1 | 0.111Å | - | - |
| C 577 | PHE | 50 | 0.651Å HB3 with C 498 LEU HB3 | Favored (51.56%) General / -126.1,133.8 | 88.9% (<i>m-85</i>) chi angles: 300.1,90 | 0.044Å | - | - |
| C 578 | CYS | 99.99 | - | Favored (31.6%) General / -104.5,144.5 | 52.3% (<i>t</i>) chi angles: 180 | 0.035Å | - | - |
| C 579 | LEU | 50 | 0.551Å HD22 with C 494 LEU HD11 | Favored (44.24%) General / -129.0,128.7 | 30.8% (<i>tp</i>) chi angles: 188.6,66.7 | 0.096Å | - | - |
| C 580 | SER | 50 | - | Favored (21.27%) General / -83.9,159.8 | 84% (<i>p</i>) chi angles: 68.6 | 0.017Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| C 581 | LYS | 50 | 0.728Å HG3 with C 552 ILE HG23 | Favored (79.78%) General / -60.1,-37.4 | 39.2% (<i>ttpt</i>) chi angles: 187,179.1,66.9,179.8 | 0.066Å | - | - |
| C 582 | ASP | 50 | - | Allowed (0.83%) General / -52.3,-64.4 | 5.6% (<i>m-20</i>) chi angles: 306.4,84.2 | 0.075Å | - | - |
| C 583 | ASP | 50 | - | Favored (78.54%) General / -63.6,-34.8 | 62% (<i>m-20</i>) chi angles: 294.3,302.8 | 0.03Å | - | - |
| C 584 | LEU | 99.99 | 0.785Å HD13 with C 552 ILE HG21 | Favored (73.82%) General / -61.0,-50.3 | 10.3% (<i>tt</i>) chi angles: 183.9,150 | 0.045Å | - | - |
| C 585 | MET | 50 | 0.625Å O with C 589 THR HG23 | Favored (69.05%) General / | 60.7% (<i>mtt</i>) chi angles: 292.3,183.8,173.7 | 0.026Å | - | - |

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|----------|-----|----|---|--|--|--------|---|---|
| C 586 | GLU | 50 | - | -69.1,-30.7 Favored (45.07%) General / -66.7,-52.4 | 62.4% (<i>tt0</i>) chi angles: 185.1,189.7,338.7 | 0.069Å | - | - |
| C 587 | ALA | 50 | - | Favored (70.58%) General / -61.5,-30.4 | - | 0.091Å | - | - |
| C 588 | LEU | 50 | - | Favored (26.72%) General / -86.3,-22.5 | 48.9% (<i>mt</i>) chi angles: 293.2,185.6 | 0.112Å | - | - |
| C 589 | THR | 50 | 0.625Å HG23 with C 585 MET O | Favored (65.07%) General / -72.8,-31.9 | 77.8% (<i>p</i>) chi angles: 60.2 | 0.017Å | - | - |
| C 590 | GLU | 50 | - | Favored (57.13%) General / -77.0,-32.5 | 80.4% (<i>tt0</i>) chi angles: 180.2,177.5,15.6 | 0.094Å | - | - |
| C 591 | TYR | 50 | 0.749Å CD1 with C 490 LEU HD13 | Favored (65.41%) Pre-proline / -133.8,76.7 | 90.7% (<i>m-85</i>) chi angles: 301.5,99.4 | 0.05Å | - | - |
| C 592 | PRO | 50 | - | Favored (32.53%) Trans-proline / -60.1,-43.9 | 82.1% (<i>Cg_exo</i>) chi angles: 331.9 | 0.085Å | - | - |
| C 593 | GLU | 50 | - | Allowed (0.79%) General / -42.2,-34.6 | 52.3% (<i>mm-40</i>) chi angles: 290.9,289.4,0.6 | 0.08Å | - | - |
| C 594 | ALA | 50 | - | Favored (60.22%) General / -74.2,-20.4 | - | 0.035Å | - | - |
| C 595 | LYS | 50 | 0.412Å O with C 599 GLU HG3 | Favored (83.92%) General / -59.5,-39.5 | 63.6% (<i>tttp</i>) chi angles: 183.3,182.1,179.2,63.2 | 0.022Å | - | - |
| C 596 | LYS | 50 | - | Favored (80.88%) General / -64.0,-35.5 | 64% (<i>tttp</i>) chi angles: 184.1,180.4,179.1,62.3 | 0.017Å | - | - |
| C 597 | ALA | 50 | - | Favored (64.25%) General / | - | 0.031Å | - | - |

| | | | | General / -56.5,-52.6 | | | | |
|----------------------------------|---------|-----------|--|---|--|------------------------|-----------------|----------------|
| C 598 | LEU | 50 | - | Favored (92.89%) General / -64.8,-39.0 | 10.5% (<i>mp</i>) chi angles: 280.6,63.7 | 0.026Å | - | - |
| C 599 | GLU | 99.99 | 0.412Å HG3 with C 595 LYS O | - | 74.9% (<i>mt-10</i>) chi angles: 293.7,191.7,332 | 0.049Å | - | - |
| D 407 | ASN | 99.99 | - | - | 85% (<i>m-20</i>) chi angles: 296.7,336.5 | 0.058Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | C β deviation | Bond lengths | Bond angles |
| Avg: Clashscore: Outliers: 16 of | | | | Poor rotamers: 12 of | Outliers: 12 Outliers: 64 | | | |
| 61.33 | | | | 65.92 | 764 | 676 | 4 of 728 | of 772 |
| D 408 | ALA | 50 | - | OUTLIER (0.02%) General / -171.2,-39.6 | - | 0.063Å | - | - |
| D 409 | SER | 50 | 0.671Å HB2 with D 449 LYS HD2 | Favored (58.86%) General / -81.7,-6.2 | 80.2% (<i>p</i>) chi angles: 60 | 0.123Å | - | - |
| D 410 | ARG | 50 | 0.546Å HH21 with D 447 ASN CG | Favored (66.01%) General / -71.2,-30.2 | 10.9% (<i>mtp180</i>) chi angles: 302.7,214.3,69.6,156.8 | 0.073Å | - | - |
| D 411 | ALA | 50 | - | Favored (63.85%) General / -73.4,-40.9 | - | 0.052Å | - | - |
| D 412 | GLU | 50 | - | Favored (81.99%) General / -60.7,-37.5 | 11.8% (<i>tm-20</i>) chi angles: 179.8,287.3,328.8 | 0.069Å | - | - |
| D 413 | PHE | 50 | 0.445Å CD1 with D 445 TRP HE3 | Favored (45.25%) General / -65.1,-53.5 | 88.8% (<i>t80</i>) chi angles: 178.5,82.1 | 0.037Å | - | - |
| D 414 | GLN | 50 | 0.558Å HA with D 417 ILE HG12 | Favored (81.81%) General / -59.5,-38.7 | 15.8% (<i>mt-30</i>) chi angles: 282.5,140.6,20.1 | 0.015Å | - | - |
| D 415 | ALA | 50 | - | Favored (80.73%) General / -68.5,-40.6 | - | 0.039Å | - | - |

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|----------|-----|-------|--|---|--|--------|---|---|
| D 416 | LYS | 50 | - | Favored (8.88%) General / -69.9,-55.8 | 13.8% (<i>tppt?</i>) chi angles: 177.9,49.7,62.1,192.2 | 0.03Å | - | - |
| D 417 | ILE | 50 | 0.733Å O with D 420 ILE HG12 | Favored (33.54%) Isoleucine or valine / -58.1,-28.1 | 30% (<i>pt</i>) chi angles: 69.4,172.7 | 0.078Å | - | - |
| D 418 | ASP | 50 | - | Favored (93.02%) General / -65.4,-41.9 | 44.6% (<i>t0</i>) chi angles: 186.9,329.6 | 0.038Å | - | - |
| D 419 | SER | 50 | - | Favored (97.44%) General / -61.8,-44.1 | 40.5% (<i>t</i>) chi angles: 181.4 | 0.038Å | - | - |
| D 420 | ILE | 50 | 0.733Å HG12 with D 417 ILE O | Favored (65.2%) Isoleucine or valine / -58.7,-37.4 | 16.4% (<i>pt</i>) chi angles: 71.3,180.5 | 0.072Å | - | OUTLIER(S) worst is CB- CG1-CD1: 4.186 σ |
| D 421 | LYS | 50 | 0.659Å HG3 with D 417 ILE O | Favored (90.34%) General / -65.2,-38.4 | 30.7% (<i>mtpp</i>) chi angles: 294,181,68,63.9 | 0.047Å | - | - |
| D 422 | GLN | 50 | - | Favored (54.03%) General / -77.6,-33.0 | 19% (<i>mt-30</i>) chi angles: 298,166.1,183.5 | 0.087Å | - | - |
| D 423 | TYR | 50 | 0.446Å CE1 with A 453 GLU HG3 | Favored (99.6%) General / -62.0,-42.9 | 71.9% (<i>t80</i>) chi angles: 172.6,84.8 | 0.05Å | - | - |
| D 424 | MET | 50 | 0.987Å SD with D 437 VAL HG11 | Favored (70.48%) General / -71.4,-40.5 | 69.9% (<i>mtm</i>) chi angles: 293.7,191.9,299.6 | 0.051Å | - | - |
| D 425 | GLN | 50 | - | Favored (79.45%) General / -67.7,-35.8 | 53.4% (<i>tt0</i>) chi angles: 185.3,179.2,57.1 | 0.012Å | - | - |
| D 426 | PHE | 50 | - | Favored (79.9%) General / -64.7,-35.1 | 11% (<i>t80</i>) chi angles: 182.8,38.1 | 0.025Å | - | - |
| D | ARG | 99 99 | 1.002Å HR3 with A | Favored (57.36%) | 32.8% (<i>mmt180</i>) chi angles: | 0.21Å | - | OUTLIER(S) worst is NL-CA- |

| 427 | ARG | 50 | HD3 with D 473 HIS HE1 | General / -92.0,-1.2 | Chi angles: 287.3,304.8,183.2,180 | 0.21 Å | - | - | Worst case CB: 4.945 σ |
|-------|-----|-----|------------------------------------|---|--|--|--------------------|---------------------|------------------------|
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| D 428 | LYS | 50 | - | - | Favored (28.26%) General / 54.1,38.0 | 88.4% (<i>mttt</i>) chi angles: 298.3,170.7,185,166.5 | 0.051Å | - | - |
| D 429 | VAL | 50 | 0.935Å HG21 with D 433 LEU HD22 | Favored (5.58%) Isoleucine or valine / -61.0,152.8 | 12.1% (<i>p</i>) chi angles: 62.1 | 0.168Å | - | - | |
| D 430 | THR | 50 | 0.449Å HG22 with D 432 ASP H | Favored (7.51%) General / -57.2,156.3 | 98.9% (<i>m</i>) chi angles: 298.8 | 0.05Å | - | - | |
| D 431 | LYS | 50 | 0.445Å O with D 435 THR HG23 | Favored (82.42%) General / -66.9,-36.5 | 32.8% (<i>mmmt</i>) chi angles: 296.3,295.3,295.3,181.1 | 0.032Å | - | - | |
| D 432 | ASP | 50 | 0.449Å H with D 430 THR HG22 | Favored (80.59%) General / -65.3,-35.3 | 85.2% (<i>m-20</i>) chi angles: 293.9,349.1 | 0.053Å | - | - | |
| D 433 | LEU | 50 | 0.935Å HD22 with D 429 VAL HG21 | Favored (63.81%) General / -73.5,-40.7 | 8.5% (<i>tt</i>) chi angles: 191.4,155.1 | 0.12Å | - | - | |
| D 434 | GLU | 50 | 0.783Å O with D 438 ILE HG12 | Favored (93.62%) General / -63.9,-39.2 | 54.6% (<i>mt-10</i>) chi angles: 296.7,182.7,298.1 | 0.075Å | - | - | |
| D 435 | THR | 50 | 0.445Å HG23 with D 431 LYS O | Favored (68.27%) General / -66.1,-49.3 | 77.9% (<i>p</i>) chi angles: 60.2 | 0.02Å | - | - | |
| D 436 | ARG | 50 | - | Favored (72.82%) General / -58.2,-36.2 | 86.8% (<i>mtm-85</i>) chi angles: 285.7,187.7,294.2,260.3 | 0.068Å | - | - | |
| D 437 | VAL | 50 | 0.987Å HG11 with D 424 MET SD | Favored (68.54%) Isoleucine or | 4.9% (<i>p</i>) chi angles: 76.4 | 0.175Å | - | - | |

| D 438 | ILE | 50 | 0.783Å HG12 with D 434 GLU O | valine / -72.0,-41.3 Favored (28.75%) Isoleucine or valine / -58.1,-54.7 | 41.3% (<i>mm</i>) chi angles: 299.1,304.7 | 0.028Å | - | - |
|----------|---------|-----------|---|--|---|-----------------|--|--|
| D 439 | ARG | 50 | 0.456Å O with D 443 TYR HD2 | Favored (77.74%) General / -60.0,-36.6 | 55.1% (<i>mmm-85</i>) chi angles: 293.6,298,293,278.7 | 0.033Å | - | - |
| D 440 | TRP | 99.99 | 0.837Å CH2 with D 444 LEU HD22 | Favored (42.13%) General / -62.5,-54.3 | 89.3% (<i>t90</i>) chi angles: 184.8,87.3 | 0.024Å | OUTLIER(S) worst is NE1-- CE2: 4.769 σ | OUTLIER(S) worst is CZ2- CH2-CZ3: 5.295 σ |
| D 441 | PHE | 50 | 0.791Å HE2 with D 437 VAL HG22 | Favored (61.2%) General / -51.0,-46.2 | 95.6% (<i>m-85</i>) chi angles: 292.3,275.1 | 0.072Å | - | - |
| D 442 | ASP | 50 | 0.403Å HB2 with D 439 ARG O | Favored (67.79%) General / -53.0,-45.5 | 51.3% (<i>m-20</i>) chi angles: 295.4,296.5 | 0.044Å | - | - |
| D 443 | TYR | 50 | 0.55Å CE2 with D 573 TYR CZ | Favored (60.59%) General / -75.2,-30.6 | 95.2% (<i>m-85</i>) chi angles: 292.2,274.8 | 0.027Å | - | - |
| D 444 | LEU | 99.99 | 0.837Å HD22 with D 440 TRP CH2 | Favored (22.95%) General / -84.8,-33.5 | 21.3% (<i>tp</i>) chi angles: 187.1,74 | 0.098Å | - | - |
| D 445 | TRP | 50 | 0.445Å HE3 with D 413 PHE CD1 | Favored (8.96%) General / -119.3,-16.7 | 51.6% (<i>m0</i>) chi angles: 296.7,351.6 | 0.079Å | OUTLIER(S) worst is NE1-- CE2: 4.757 σ | OUTLIER(S) worst is CD2- CE3-CZ3: 4.172 σ |
| D 446 | ALA | 50 | - | Allowed (0.66%) General / 51.6,18.1 | - | 0.046Å | - | - |
| D 447 | ASN | 99.99 | 0.546Å CG with D 410 ARG HH21 | Favored (10.17%) General / 56.4,26.0 | 64.3% (<i>t-20</i>) chi angles: 184.8,348.8 | 0.097Å | - | OUTLIER(S) worst is OD1- CG-ND2: 5.666 σ |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |

Avg: Clashscore: 61.33 Outliers: 65.92 of 764 Poor rotamers: 676 of 728 Outliers: 4 of 728 Outliers: 12 of 772 Outliers: 64 of 772

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|----------|-----|-------|--|---|---|--------|---|--|
| D 448 | LYS | 99.99 | - | (0.73%) General / -106.2,-72.0 | 29.5% (<i>tpip</i>) chi angles: 182.4,64.6,177.9,64.7 | 0.065Å | - | - |
| D 449 | LYS | 99.99 | 0.671Å HD2 with D 409 SER HB2 | Favored (49.27%) General / -125.4,147.2 | 27.9% (<i>tptp</i>) chi angles: 180.1,66.8,182.2,61.9 | 0.078Å | - | OUTLIER(S) worst is CG- CD-CE: 4.38 σ |
| D 450 | THR | 99.99 | 0.72Å HG22 with D 451 VAL H | Allowed (0.82%) General / -119.5,-160.6 | 48.8% (<i>m</i>) chi angles: 305 | 0.108Å | - | - |
| D 451 | VAL | 99.99 | 1.03Å HG22 with D 452 ASP HA | Allowed (0.44%) Isoleucine or valine / -48.1,151.2 | 6% (<i>p</i>) chi angles: 75 | 0.168Å | - | - |
| D 452 | ASP | 50 | 1.03Å HA with D 451 VAL HG22 | Allowed (1.01%) General / -104.8,44.7 | 2.2% (<i>m-20</i>) chi angles: 294.9,33.2 | 0.14Å | - | - |
| D 453 | GLU | 50 | 0.836Å HA with D 456 VAL HG22 | Allowed (0.6%) General / -40.4,-36.9 | 27.1% (<i>tt0</i>) chi angles: 193.5,193.3,40.1 | 0.048Å | - | - |
| D 454 | LYS | 50 | - | Favored (79.14%) General / -63.5,-48.0 | 39% (<i>ttpt</i>) chi angles: 186.5,179.9,64.3,181.3 | 0.041Å | - | - |
| D 455 | GLU | 50 | 0.762Å HB3 with D 452 ASP HB3 | Favored (75.69%) General / -65.6,-47.4 | 10.8% (<i>tm-20</i>) chi angles: 181.5,289.8,325.2 | 0.055Å | - | - |
| D 456 | VAL | 50 | 0.836Å HG22 with D 453 GLU HA | Favored (85.34%) Isoleucine or valine / -58.9,-42.3 | 22.1% (<i>m</i>) chi angles: 302.9 | 0.037Å | - | - |
| D 457 | LEU | 50 | 0.477Å HB2 with D 453 GLU O | Favored (82.27%) General / -68.2,-40.5 | 0.5% chi angles: 254.3,39.3 | 0.042Å | - | - |
| D 458 | LYS | 50 | - | Favored (93.83%) General / -61.1,-40.4 | 28.6% (<i>tptp</i>) chi angles: 184.5,62.4,180.5,64.5 | 0.04Å | - | - |
| D 459 | SER | 99.99 | 0.652Å O with B 440 TRP CH2 | Favored (77.29%) General / | 95.9% (<i>p</i>) chi angles: 66.7 | 0.102Å | - | OUTLIER(S) worst is CA-C- O: 5.505 Å |

| | | | Clash | | Ramachandran | | Rotamer | | C β deviation | | Bond lengths | | Bond angles | |
|-------|-----|-------|-----------------------------------|--------------|---|--|--|--|---------------------|--|---------------------|--|---------------------|--|
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | | Rotamer | | C β deviation | | Bond lengths | | Bond angles | |
| Avg: | | | 61.33 | 65.92 | Outliers: 16 of 764 | | Poor rotamers: 12 of 676 | | Outliers: 4 of 728 | | Outliers: 12 of 772 | | Outliers: 64 of 772 | |
| D 460 | LEU | 50 | - | - | Favored (38.7%) Pre-proline / -71.6,166.5 | | 81% (<i>mt</i>) chi angles: 298.2,182.5 | | 0.042Å | | - | | - | |
| D 461 | PRO | 50 | 0.774Å HD3 with B 440 TRP CE2 | - | Favored (6.07%) Trans-proline / -87.7,171.3 | | 42.9% (<i>Cg_endo</i>) chi angles: 35.9 | | 0.014Å | | - | | - | |
| D 462 | ASP | 50 | - | - | Favored (96.45%) General / -64.0,-43.1 | | 42.1% (<i>t0</i>) chi angles: 190.5,329.5 | | 0.016Å | | - | | - | |
| D 463 | LYS | 50 | 0.684Å HE2 with B 508 TYR H | - | Favored (73.75%) General / -57.8,-37.4 | | 32.4% (<i>mmmt</i>) chi angles: 294.8,293.5,296.6,184.8 | | 0.04Å | | - | | - | |
| D 464 | LEU | 50 | 0.657Å HD12 with D 461 PRO HD2 | - | Favored (22.9%) General / -75.5,-48.4 | | 59.3% (<i>mt</i>) chi angles: 286.4,177.4 | | 0.038Å | | - | | - | |
| D 465 | LYS | 50 | 0.591Å O with D 470 ILE HG12 | - | Favored (72.81%) General / -61.0,-33.1 | | 54.9% (<i>mtmt</i>) chi angles: 294.7,178.6,295.9,178.8 | | 0.135Å | | - | | - | |
| D 466 | ALA | 50 | 0.727Å HA with D 470 ILE CB | - | Favored (83.8%) General / -66.6,-36.9 | | - | | 0.118Å | | - | | - | |
| D 467 | GLU | 50 | 0.6Å OE2 with B 433 LEU HD12 | - | Favored (79.54%) General / -68.8,-40.5 | | 15.5% (<i>tt0</i>) chi angles: 206.1,191.3,309.1 | | 0.116Å | | - | | - | |
| D 468 | ILE | 99.99 | 0.887Å HA with D 472 VAL HG12 | - | Favored (24.44%) Isoleucine or valine / -119.2,146.0 | | 17.8% (<i>pt</i>) chi angles: 51.7,179.6 | | 0.186Å | | - | | - | |
| D 469 | ALA | 99.99 | 0.947Å H with D 473 HIS HD2 | - | Allowed (1.81%) General / 66.3,0.8 | | - | | 0.078Å | | - | | - | |

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|----------|-----|-------|--|--|---|--------|--|--|
| D 470 | ILE | 99.99 | 0.973Å HD12 with D 496 LEU HA | (0.75%) Isoleucine or valine / -132.4,-25.7 | 26.9% (<i>mm</i>) chi angles: 299,310.2 | 0.091Å | - | - |
| D 471 | ASN | 50 | 1.036Å HD21 with D 492 VAL HG12 | Allowed (0.47%) General / -140.4,-51.1 | 42.2% (<i>m-20</i>) chi angles: 278.7,302.3 | 0.195Å | - | OUTLIER(S) worst is CA- CB-CG: 4.049 σ |
| D 472 | VAL | 50 | 0.887Å HG12 with D 468 ILE HA | Favored (82.17%) Isoleucine or valine / -58.6,-41.5 | 15% (<i>p</i>) chi angles: 63.5 | 0.065Å | - | - |
| D 473 | HIS | 99.99 | 1.003Å HE1 with B 427 ARG HB3 | Favored (61.3%) General / -72.7,-25.5 | 84.1% (<i>m-70</i>) chi angles: 288,298.1 | 0.04Å | OUTLIER(S) worst is CD2-- NE2: 7.083 σ | OUTLIER(S) worst is CD2- NE2-CE1: 12.71 σ |
| D 474 | LEU | 99.99 | 0.699Å C with D 474 LEU HD23 | Favored (38.13%) General / -53.1,132.5 | 7.2% (<i>tt</i>) chi angles: 184.9,162.9 | 0.126Å | - | - |
| D 475 | ASP | 99.99 | 0.538Å N with D 474 LEU HD23 | Favored (5.85%) General / -129.7,12.7 | 29.9% (<i>t70</i>) chi angles: 179.1,76.4 | 0.069Å | - | - |
| D 476 | THR | 99.99 | 0.485Å HB with D 523 ASN HA | Favored (2.21%) General / -136.0,48.0 | 10.3% (<i>t</i>) chi angles: 184.2 | 0.074Å | - | - |
| D 477 | LEU | 99.99 | 1.099Å HG with D 483 PHE HB3 | Allowed (0.81%) General / -134.6,-52.3 | 10% (<i>tt</i>) chi angles: 185.3,154.6 | 0.239Å | - | - |
| D 478 | LYS | 50 | - | Favored (31.44%) General / -53.1,-29.6 | 27.1% (<i>tptp</i>) chi angles: 180.3,61.9,184.6,69.5 | 0.035Å | - | - |
| D 479 | LYS | 50 | - | Favored (49.45%) General / -89.1,-9.9 | 26.8% (<i>tptp</i>) chi angles: 188.6,61.2,182.7,67.3 | 0.051Å | - | - |
| D 480 | VAL | 50 | 1.033Å HG12 with D 477 LEU HA | Favored (23.98%) Isoleucine or valine / -117.0,108.1 | 11.5% (<i>p</i>) chi angles: 66.6 | 0.141Å | - | - |
| D 481 | ARG | 50 | 0.722Å HA with D 484 C1N1 | Favored (7.28%) General / -117.0,108.1 | 57.9% (<i>mmm-85</i>) chi angles: | 0.027Å | - | - |

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|----------|-----|-------|--|---|--|--------|---|---|
| 401 | | | 404 GLN HG2 | General / -43.5,-47.1 | 296.1,292.8,296.7,277.2 | | | |
| D 482 | ILE | 50 | 0.739Å HG12 with D 480 VAL HG22 | Favored (87.84%) Isoleucine or valine / -59.3,-42.6 | 42.2% (<i>pt</i>) chi angles: 65.5,172.5 | 0.067Å | - | - |
| D 483 | PHE | 50 | 1.099Å HB3 with D 477 LEU HG | Favored (28.76%) General / -79.7,-40.6 | 7.1% (<i>m-30</i>) chi angles: 278.5,9.7 | 0.047Å | - | OUTLIER(S) worst is CA- CB-CG: 4.414 σ |
| D 484 | GLN | 50 | 0.722Å HG2 with D 481 ARG HA | Favored (83.93%) General / -67.8,-38.8 | 19.8% (<i>pt20</i>) chi angles: 65.9,181.7,61.9 | 0.076Å | - | - |
| D 485 | ASP | 50 | - | Favored (4.67%) General / -97.0,26.4 | 48.7% (<i>t0</i>) chi angles: 190.7,338.3 | 0.039Å | - | - |
| D 486 | CYS | 99.99 | 0.633Å SG with D 490 LEU HD23 | Favored (27.27%) General / -115.1,155.3 | 52.7% (<i>t</i>) chi angles: 181.3 | 0.052Å | - | - |
| D 487 | GLU | 99.99 | - | Favored (8.68%) General / -57.2,120.8 | 87.8% (<i>mt-10</i>) chi angles: 301.3,182.2,337.1 | 0.064Å | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | | |
|------|---------|-----------|-----------------|--------------|---------|-----------------|----------------------|--------------------|---------------------|---------------------|
| Avg: | | | 61.33 | Clashscore: | 65.92 | Outliers: 16 of | Poor rotamers: 12 of | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |

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|----------|-----|-------|--|---|--|--------|---|---|
| D 488 | ALA | 50 | 0.732Å O with D 492 VAL HG13 | Favored (14.29%) General / -54.9,-22.3 | - | 0.016Å | - | - |
| D 489 | GLY | 50 | 0.49Å O with D 492 VAL HG22 | Favored (76.39%) Glycine / -67.5,-45.6 | - | - | - | - |
| D 490 | LEU | 99.99 | 0.748Å HD13 with D 591 TYR CD1 | Favored (93.9%) General / -65.5,-41.0 | 35.4% (<i>tp</i>) chi angles: 175.6,54.2 | 0.063Å | - | - |
| D 491 | LEU | 99.99 | 0.837Å HD13 with D 477 LEU HD11 | Favored (5.02%) General / -57.2,-59.5 | 94.3% (<i>mt</i>) chi angles: 298.4,175.6 | 0.075Å | - | - |

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|----------|-----|----|--|--|--|--------|---|--|
| D 492 | VAL | 50 | 1.036Å HG12 with D 471 ASN HD21 | Favored (14.9%) Isoleucine or valine / -48.6,-45.5 | 25.8% (<i>m</i>) chi angles: 302 | 0.023Å | - | - |
| D 493 | GLU | 50 | - | Favored (68.45%) General / -66.2,-28.0 | 14.3% (<i>tm-20</i>) chi angles: 183.8,285.4,333.7 | 0.107Å | - | - |
| D 494 | LEU | 50 | 0.694Å HD23 with D 483 PHE CE1 | Favored (12.94%) General / -80.0,-48.7 | 33.9% (<i>tp</i>) chi angles: 187.7,59.4 | 0.033Å | - | OUTLIER(S) worst is CD1- CG-CD2: 4.562 σ |
| D 495 | VAL | 50 | 0.752Å HG21 with D 470 ILE O | Favored (44.55%) Isoleucine or valine / -57.7,-33.2 | 20.8% (<i>m</i>) chi angles: 303.3 | 0.021Å | - | - |
| D 496 | LEU | 50 | 0.973Å HA with D 470 ILE HD12 | Favored (55.61%) General / -64.8,-13.4 | 8.9% (<i>tt</i>) chi angles: 190.5,154.5 | 0.155Å | - | - |
| D 497 | LYS | 50 | - | Favored (10.85%) General / -115.9,-18.0 | 64.5% (<i>mttp</i>) chi angles: 295.5,177.2,177.3,63.2 | 0.054Å | - | - |
| D 498 | LEU | 50 | 0.636Å HB3 with D 577 PHE HB3 | Favored (44.49%) General / -58.6,144.1 | 58.4% (<i>mt</i>) chi angles: 305.2,173.5 | 0.096Å | - | - |
| D 499 | ARG | 50 | - | Favored (28.15%) Pre-proline / -118.9,124.7 | 40.1% (<i>ptt180</i>) chi angles: 62,179.4,181.4,181.7 | 0.069Å | - | - |
| D 500 | PRO | 50 | - | Favored (33.36%) Trans-proline / -68.0,135.0 | 92.8% (<i>Cg_endo</i>) chi angles: 30.9 | 0.035Å | - | - |
| D 501 | THR | 50 | - | Favored (30.24%) General / -144.9,142.9 | 63.1% (<i>p</i>) chi angles: 62.3 | 0.038Å | - | - |
| D 502 | VAL | 50 | - | Favored (36.42%) Isoleucine or valine / -115.5,140.6 | 74% (<i>t</i>) chi angles: 174 | 0.052Å | - | - |

Favored

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|-------|-----|-------|---|---|---|--------------------------|--------------------|---------------------|---------------------|
| D 503 | PHE | 50 | - | (50.81%) General / -127.0,145.2 | 63.9% (<i>m-85</i>) chi angles: 284.3,87.2 | 0.046Å | - | - | |
| D 504 | SER | 50 | - | Favored (31.54%) Pre-proline / -101.6,158.6 | 70.2% (<i>m</i>) chi angles: 295.9 | 0.029Å | - | - | |
| D 505 | PRO | 50 | - | Favored (52.06%) Trans-proline / -53.9,132.9 | 88.3% (<i>Cg_exo</i>) chi angles: 331.4 | 0.107Å | - | - | |
| D 506 | GLY | 50 | - | Favored (9.88%) Glycine / 100.2,-30.6 | - | - | - | - | |
| D 507 | ASP | 50 | 0.458Å HA with A 463 LYS HE2 | Allowed (0.56%) General / -49.0,155.9 | 81.1% (<i>m-20</i>) chi angles: 283.3,337.3 | 0.05Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 61.33 | Clashscore: 65.92 | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| D 508 | TYR | 50 | 0.667Å H with A 463 LYS HE2 | Favored (5.14%) General / -108.5,94.6 | 11.4% (<i>m-30</i>) chi angles: 282.8,356.5 | 0.101Å | - | - | |
| D 509 | ILE | 50 | 0.814Å HB with D 568 ILE HG23 | Favored (99.01%) Isoleucine or valine / -60.9,-45.0 | 69% (<i>mt</i>) chi angles: 303.1,168.1 | 0.091Å | - | - | |
| D 510 | CYS | 99.99 | 1.035Å HB3 with D 568 ILE HG22 | Favored (28.07%) General / -144.3,138.6 | 4.8% (<i>t</i>) chi angles: 164.3 | 0.071Å | - | - | |
| D 511 | LYS | 50 | 0.455Å NZ with D 508 TYR HD2 | Favored (37.7%) General / -108.1,142.8 | 68.4% (<i>mttm</i>) chi angles: 292.6,179.7,178.2,293.8 | 0.066Å | - | - | |
| D 512 | LYS | 50 | - | Favored (31.24%) General / -61.9,152.7 | 38.6% (<i>ttpt</i>) chi angles: 184.7,182,62.4,181.3 | 0.071Å | - | - | |
| D 513 | GLY | 50 | 0.45Å O with D 563 ASP HD2 | Favored (4.44%) Glycine / | - | - | - | - | |

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|----------|-----|----|-------------------------------------|--|---|--------|---|---|
| | | | ARG HD2 | System / 78.9,-20.6 | | | | |
| D 514 | ASP | 50 | 0.475Å O with D 564 ARG HG2 | Favored (43.53%) General / -74.6,139.2 | 42.6% (<i>t0</i>) chi angles: 189,328.5 | 0.062Å | - | - |
| D 515 | ILE | 50 | - | Favored (12.76%) Isoleucine or valine / -63.5,121.6 | 27.2% (<i>mt</i>) chi angles: 311.5,178.4 | 0.032Å | - | - |
| D 516 | GLY | 50 | - | Favored (10.08%) Glycine / -98.5,130.0 | - | - | - | - |
| D 517 | LYS | 50 | 0.533Å HG2 with D 517 LYS O | Favored (9.22%) General / -124.0,19.7 | 61.9% (<i>tttm</i>) chi angles: 185.6,184.4,177.4,293.2 | 0.063Å | - | - |
| D 518 | GLU | 50 | - | Favored (7.59%) General / -169.3,157.6 | 12.6% (<i>pt-20</i>) chi angles: 61.5,180.2,62.4 | 0.013Å | - | - |
| D 519 | MET | 50 | - | Favored (8.78%) General / -124.8,173.1 | 27.1% (<i>ptm</i>) chi angles: 65.3,172.3,293.2 | 0.032Å | - | - |
| D 520 | TYR | 50 | - | Favored (52.46%) General / -130.9,149.6 | 90.2% (<i>m-85</i>) chi angles: 299.1,87.1 | 0.071Å | - | - |
| D 521 | ILE | 50 | 0.645Å CG1 with D 577 PHE HB2 | Favored (15.09%) Isoleucine or valine / -121.0,104.3 | 32% (<i>pt</i>) chi angles: 66.9,166.7 | 0.058Å | - | - |
| D 522 | ILE | 50 | - | Allowed (0.15%) Isoleucine or valine / -58.2,105.0 | 62.3% (<i>mt</i>) chi angles: 304.9,175.2 | 0.02Å | - | - |
| D 523 | ASN | 50 | 0.485Å HA with D 476 THR HB | Favored (20.01%) General / -76.9,-47.8 | 48.4% (<i>t30</i>) chi angles: 182.1,60.4 | 0.01Å | - | - |
| D 524 | GLU | 50 | - | Favored (6.4%) General / -157.0,127.2 | 11.3% (<i>tm-20</i>) chi angles: 179.9,288.5,328.5 | 0.08Å | - | - |
| | | | | Favored | | | | |

| D 525 | GLY | 50 | - | 0.979Å HG3 with D 540 VAL HG13 | Favored (13.05%) Glycine / 132.8,172.6 | - | - | - | - |
|---|-----|-------|--|--|--|---------|-----------------|-----------------|---|
| D 526 | LYS | 99.99 | 0.979Å HG3 with D 540 VAL HG13 | Favored (51.03%) General / -122.2,128.3 | 66.7% (tttt) chi angles: 165.7,169.7,180.8,162.5 | 0.107Å | - | - | - |
| D 527 | LEU | 50 | 0.906Å HB3 with D 568 ILE HD11 | Favored (29.48%) General / -119.4,156.8 | 9.5% (mp) chi angles: 281.9,69.5 | 0.069Å | - | - | OUTLIER(S) worst is CD1- CG-CD2: 4.488 σ |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: Clashscore: Outliers: 16 of Poor rotamers: 12 of Outliers: Outliers: 12 Outliers: 64 61.33 65.92 764 676 4 of 728 of 772 of 772 | | | | | | | | | |
| D 528 | ALA | 50 | 0.492Å O with D 568 ILE HD12 | Favored (54.91%) General / -118.4,128.8 | - | 0.07Å | - | - | - |
| D 529 | VAL | 50 | 0.696Å HG22 with D 568 ILE HD13 | Favored (70.26%) Isoleucine or valine / -113.0,127.5 | 22.5% (t) chi angles: 187.4 | 0.056Å | - | - | - |
| D 530 | VAL | 50 | - | Favored (3.12%) Isoleucine or valine / -130.1,97.0 | 7.3% (p) chi angles: 58.8 | 0.101Å | - | - | - |
| D 531 | ALA | 99.99 | 0.85Å HB2 with D 566 ALA HB2 | Allowed (1.95%) General / -130.4,80.3 | - | 0.137Å | - | - | - |
| D 532 | ASP | 99.99 | - | Favored (11.65%) General / 53.0,31.7 | 29.4% (t70) chi angles: 178.9,77 | 0.068Å | - | - | - |
| D 533 | ASP | 99.99 | - | Favored (31.44%) General / -160.3,165.4 | 26.1% (p30) chi angles: 61.8,29.5 | 0.02Å | - | - | - |
| D 534 | GLY | 99.99 | - | Allowed (0.82%) Glycine / -61.8,105.1 | - | - | - | - | - |
| D | | | 0.6Å | OUTLIER (0%) | 7.1% (p) | - | - | - | - |

| | | | | | | | | |
|-------|-----|-------|--------------------------------|--|--|--------|---|---|
| D 535 | VAL | 50 | HG22 with D 536 THR HG22 | isoleucine or valine / -10.6,108.9 | chi angles: 58.4 | 0.01Å | - | - |
| D 536 | THR | 99.99 | HG22 with D 535 VAL HG22 | Allowed (1.5%) General / 55.6,15.4 | 9.9% (t) chi angles: 184 | 0.055Å | - | - |
| D 537 | GLN | 99.99 | 0.524Å HG2 with D 536 THR O | Favored (14.51%) General / 47.9,51.3 | 18.5% (pt20) chi angles: 64.8,180.9,57 | 0.097Å | - | - |
| D 538 | PHE | 99.99 | 0.489Å CD2 with D 538 PHE O | Favored (14.34%) General / 63.5,32.4 | 85.3% (t80) chi angles: 180.7,81.9 | 0.055Å | - | - |
| D 539 | VAL | 99.99 | 0.8Å HG12 with D 540 VAL H | Allowed (0.48%) Isoleucine or valine / -119.6,-168.6 | 63.1% (t) chi angles: 180 | 0.087Å | - | OUTLIER(S) worst is CA-CB-CG1: 4.474 σ |
| D 540 | VAL | 99.99 | 0.979Å HG13 with D 526 LYS HG3 | OUTLIER (0.06%) Isoleucine or valine / -158.5,97.4 | 26.7% (t) chi angles: 164.6 | 0.381Å | - | OUTLIER(S) worst is N-CA-CB: 5.587 σ |
| D 541 | LEU | 50 | - | Allowed (1.63%) General / -59.4,112.1 | 18.6% (mt) chi angles: 292,193.2 | 0.076Å | - | - |
| D 542 | SER | 50 | - | Allowed (1.05%) General / -124.4,-162.1 | 20.8% (t) chi angles: 188.4 | 0.068Å | - | - |
| D 543 | ASP | 50 | - | Favored (20.24%) General / -50.1,135.9 | 0.3% chi angles: 313.8,44.5 | 0.116Å | - | - |
| D 544 | GLY | 50 | - | Favored (73.87%) Glycine / 79.3,18.6 | - | - | - | - |
| D 545 | SER | 50 | - | Favored (28.28%) General / -124.4,160.4 | 72.6% (m) chi angles: 295.6 | 0.026Å | - | - |
| D 546 | TYR | 50 | 0.621Å CE1 with D 482 ILE HD13 | Favored (7.79%) General / -134.8,177.4 | 45.9% (p90) chi angles: 59,275.2 | 0.048Å | - | - |

| D 547 | PHE | 50 | 0.514Å CE2 with D 527 LEU HD22 | Favored (4.1%) General / -173.7,162.6 | 43.6% (<i>p90</i>) chi angles: 60.5,83.6 | 0.022Å | - | - |
|------------------------|---------|-----------|--|---|---|--------------------|---------------------|---|
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: Clashscore: 61.33 | | | | Outliers: 16 of 764 | Poor rotamers: 12 of 676 | Outliers: 4 of 728 | Outliers: 12 of 772 | Outliers: 64 of 772 |
| D 548 | GLY | 50 | - | Favored (62.81%) Glycine / 75.1,28.1 | - | - | - | - |
| D 549 | GLU | 50 | - | Favored (29.19%) General / -86.9,-19.2 | 6.4% (<i>pm0</i>) chi angles: 70.4,293.3,339.2 | 0.053Å | - | - |
| D 550 | ILE | 50 | - | Favored (97.65%) Isoleucine or valine / -62.3,-43.1 | 76.9% (<i>mt</i>) chi angles: 298.8,177 | 0.063Å | - | - |
| D 551 | SER | 50 | - | Favored (66.23%) General / -68.4,-27.5 | 73.4% (<i>m</i>) chi angles: 295.3 | 0.038Å | - | - |
| D 552 | ILE | 99.99 | 0.808Å HG21 with D 584 LEU HD13 | Favored (58.47%) Isoleucine or valine / -73.2,-42.2 | 65.2% (<i>mt</i>) chi angles: 302.9,177.3 | 0.083Å | - | - |
| D 553 | LEU | 99.99 | 0.479Å HD23 with D 554 ASN N | Favored (52.8%) General / -70.0,139.6 | 6.7% (<i>tt</i>) chi angles: 182.7,164 | 0.065Å | - | - |
| D 554 | ASN | 99.99 | 0.479Å N with D 553 LEU HD23 | Favored (24.51%) General / -118.8,115.5 | 41% (<i>p30</i>) chi angles: 60.9,25.7 | 0.036Å | - | OUTLIER(S) worst is OD1- CG-ND2: 6.181 σ |
| D 555 | ILE | 99.99 | 0.855Å H with D 560 SER HB3 | Favored (28.01%) Isoleucine or valine / -62.8,134.6 | 37.2% (<i>pt</i>) chi angles: 64,176.5 | 0.065Å | - | - |
| D 556 | LYS | 99.99 | - | Favored (50.62%) General / -65.7,133.2 | 22.7% (<i>pttp</i>) chi angles: 61.9,180,182,64.6 | 0.024Å | - | - |

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|-------|-----|-------|------------------------------------|--|--|--------|---|---|
| D 557 | GLY | 99.99 | - | Favored (33.75%) Glycine / 106.2,-21.2 | - | - | - | - |
| D 558 | SER | 99.99 | - | Favored (2.7%) General / -151.6,-167.1 | 32.1% (t) chi angles: 184.5 | 0.087Å | - | - |
| D 559 | LYS | 99.99 | - | Favored (30.42%) General / -115.6,117.5 | 22.6% (pttp) chi angles: 59.8,180.7,181.7,66.3 | 0.056Å | - | - |
| D 560 | SER | 99.99 | 0.855Å HB3 with D 555 ILE H | Favored (5.02%) General / -130.5,27.4 | 45.1% (t) chi angles: 178.7 | 0.049Å | - | OUTLIER(S) worst is O-C- N: 4.559 σ |
| D 561 | GLY | 50 | - | Allowed (0.75%) Glycine / 48.6,17.4 | - | - | - | - |
| D 562 | ASN | 50 | 0.645Å ND2 with D 563 ARG H | Allowed (0.31%) General / -125.8,-144.1 | 59% (t30) chi angles: 188.9,50.1 | 0.12Å | - | - |
| D 563 | ARG | 50 | 0.645Å H with D 562 ASN ND2 | Favored (22.72%) General / -101.8,150.9 | 12.2% (mmt180) chi angles: 305,301.9,193.1,133.1 | 0.097Å | - | - |
| D 564 | ARG | 50 | 0.475Å HG2 with D 514 ASP O | Favored (2.5%) General / -59.0,114.3 | 28.1% (mmt180) chi angles: 296.1,296.9,204.3,186.3 | 0.057Å | - | - |
| D 565 | THR | 50 | - | Allowed (0.75%) General / -71.9,10.2 | 63.3% (p) chi angles: 64.8 | 0.021Å | - | - |
| D 566 | ALA | 50 | 0.85Å HB2 with D 531 ALA HB2 | Allowed (0.63%) General / -173.3,-170.6 | - | 0.204Å | - | - |
| D 567 | ASN | 50 | - | Favored (54.23%) General / -121.7,138.7 | 28.5% (t-20) chi angles: 187.7,301.4 | 0.124Å | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|---|---------|--------|--------------|--------------|---------|--------------|--------------|-------------|
|---|---------|--------|--------------|--------------|---------|--------------|--------------|-------------|

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|-------|-------------|-----------------|----------------------|----------------|-----------------|-----------------|
| Avg: | Clashscore: | Outliers: 16 of | Poor rotamers: 12 of | Outliers: 4 of | Outliers: 12 of | Outliers: 64 of |
| 61.33 | 65.92 | 764 | 676 | 728 | 772 | 772 |

| | | |
|---|---------|---------------------|
| - | 1.035 Å | Favored (74.20%) |
|---|---------|---------------------|

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|----------|-----|-------|--|---|--|--------|---|---|
| D 568 | ILE | 50 | 1.055Å HG22 with D 510 CYS HB3 | (/ 4.5%) Isoleucine or valine / -117.4,125.9 | 8.6% (<i>tp</i>) chi angles: 183.2,64.9 | 0.129Å | - | - |
| D 569 | ARG | 50 | - | Favored (46.23%) General / -124.8,126.9 | 50.3% (<i>ttp180</i>) chi angles: 184.2,189.1,74.3,213.1 | 0.114Å | - | - |
| D 570 | SER | 50 | - | Favored (53%) General / -69.3,137.4 | 34.4% (<i>t</i>) chi angles: 183.1 | 0.109Å | - | - |
| D 571 | ILE | 50 | 0.956Å HG12 with D 526 LYS HG2 | Favored (3.98%) Isoleucine or valine / -101.1,-34.6 | 0.8% chi angles: 77.1,123.2 | 0.071Å | - | - |
| D 572 | GLY | 50 | 0.619Å N with D 571 ILE HG13 | Favored (14.7%) Glycine / -118.8,172.9 | - | - | - | - |
| D 573 | TYR | 50 | 0.55Å CZ with D 443 TYR CE2 | OUTLIER (0.02%) General / -60.3,90.5 | 22.6% (<i>m-85</i>) chi angles: 274.5,272.2 | 0.028Å | - | - |
| D 574 | SER | 50 | - | Favored (40.49%) General / -76.0,145.1 | 53.7% (<i>m</i>) chi angles: 299.9 | 0.062Å | - | - |
| D 575 | ASP | 50 | 0.484Å O with D 523 ASN HB3 | Favored (6.37%) General / -125.7,100.3 | 90% (<i>m-20</i>) chi angles: 294.2,344 | 0.005Å | - | - |
| D 576 | LEU | 50 | - | Favored (9.84%) General / -109.0,167.8 | 37.2% (<i>mt</i>) chi angles: 310.5,176.1 | 0.111Å | - | - |
| D 577 | PHE | 50 | 0.645Å HB2 with D 521 ILE CG1 | Favored (51.56%) General / -126.1,133.8 | 88.9% (<i>m-85</i>) chi angles: 300.1,90 | 0.044Å | - | - |
| D 578 | CYS | 99.99 | - | Favored (31.6%) General / -104.5,144.5 | 52.3% (<i>t</i>) chi angles: 180 | 0.035Å | - | - |
| D 579 | LEU | 50 | 0.549Å HD22 with D 494 LEU HD11 | Favored (44.24%) General / -129.0,128.7 | 30.8% (<i>tp</i>) chi angles: 188.6,66.7 | 0.096Å | - | - |

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|--|-----|-------|--|---|--|--------|---|---|
| D 580 | SER | 50 | - | Favored (21.27%) General / -83.9,159.8 | 84% (<i>p</i>) chi angles: 68.6 | 0.017Å | - | - |
| D 581 | LYS | 50 | 0.714Å HG3 with D 552 ILE HG23 | Favored (79.78%) General / -60.1,-37.4 | 39.2% (<i>ttpt</i>) chi angles: 187,179.1,66.9,179.8 | 0.066Å | - | - |
| D 582 | ASP | 50 | - | Allowed (0.83%) General / -52.3,-64.4 | 5.6% (<i>m-20</i>) chi angles: 306.4,84.2 | 0.075Å | - | - |
| D 583 | ASP | 50 | - | Favored (78.54%) General / -63.6,-34.8 | 62% (<i>m-20</i>) chi angles: 294.3,302.8 | 0.03Å | - | - |
| D 584 | LEU | 99.99 | 0.808Å HD13 with D 552 ILE HG21 | Favored (73.82%) General / -61.0,-50.3 | 10.3% (<i>tt</i>) chi angles: 183.9,150 | 0.045Å | - | - |
| D 585 | MET | 50 | 0.625Å O with D 589 THR HG23 | Favored (69.05%) General / -69.1,-30.7 | 60.7% (<i>mtt</i>) chi angles: 292.3,183.8,173.7 | 0.026Å | - | - |
| D 586 | GLU | 50 | - | Favored (45.07%) General / -66.7,-52.4 | 62.4% (<i>tt0</i>) chi angles: 185.1,189.7,338.7 | 0.069Å | - | - |
| D 587 | ALA | 50 | - | Favored (70.58%) General / -61.5,-30.4 | - | 0.091Å | - | - |
| <div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash > 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div> <div> <div>Avg: 61.33</div> <div>Clashscore: 65.92</div> <div>Outliers: 16 of 764</div> <div>Poor rotamers: 12 of 676</div> <div>Outliers: 4 of 728</div> <div>Outliers: 12 of 772</div> <div>Outliers: 64 of 772</div> </div> | | | | | | | | |
| D 588 | LEU | 50 | - | Favored (26.72%) General / -86.3,-22.5 | 48.9% (<i>mt</i>) chi angles: 293.2,185.6 | 0.112Å | - | - |
| D 589 | THR | 50 | 0.625Å HG23 with D 585 MET O | Favored (65.07%) General / -72.8,-31.9 | 77.8% (<i>p</i>) chi angles: 60.2 | 0.017Å | - | - |
| D 590 | GLU | 50 | - | Favored (57.13%) General / | 80.4% (<i>tt0</i>) chi angles: | 0.094Å | - | - |

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|----------|-----------|----|---|---|--|--------|---|---|
| | | | | General / -77.0,-32.5 | 180.2,177.5,15.6 | | | |
| D 591 | TYR | 50 | 0.748Å CD1 with D 490 LEU HD13 | Favored (65.41%) Pre-proline / -133.8,76.7 | 90.7% (<i>m-85</i>) chi angles: 301.5,99.4 | 0.05Å | - | - |
| D 592 | PRO | 50 | - | Favored (32.53%) Trans-proline / -60.1,-43.9 | 82.1% (<i>Cg_exo</i>) chi angles: 331.9 | 0.085Å | - | - |
| D 593 | GLU | 50 | - | Allowed (0.79%) General / -42.2,-34.6 | 52.3% (<i>mm-40</i>) chi angles: 290.9,289.4,0.6 | 0.08Å | - | - |
| D 594 | ALA | 50 | - | Favored (60.22%) General / -74.2,-20.4 | - | 0.035Å | - | - |
| D 595 | LYS | 50 | 0.411Å O with D 599 GLU HG3 | Favored (83.92%) General / -59.5,-39.5 | 63.6% (<i>tttp</i>) chi angles: 183.3,182.1,179.2,63.2 | 0.022Å | - | - |
| D 596 | LYS | 50 | - | Favored (80.88%) General / -64.0,-35.5 | 64% (<i>tttp</i>) chi angles: 184.1,180.4,179.1,62.3 | 0.017Å | - | - |
| D 597 | ALA | 50 | - | Favored (64.25%) General / -56.5,-52.6 | - | 0.031Å | - | - |
| D 598 | LEU | 50 | - | Favored (92.89%) General / -64.8,-39.0 | 10.5% (<i>mp</i>) chi angles: 280.6,63.7 | 0.026Å | - | - |
| D 599 | GLU 99.99 | | 0.411Å HG3 with D 595 LYS O | - | 74.9% (<i>mt-10</i>) chi angles: 293.7,191.7,332 | 0.049Å | - | - |

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