



Viewing TULP1_sm_291-536H-multi.table

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|----------------------|---|----------|--|--|
| All-Atom Contacts | Clashscore, all atoms: | 9.86 | 72 nd percentile* (N=1784, all resolutions) | |
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 0 | 0.00% | Goal: <1% |
| | Ramachandran outliers | 3 | 1.23% | Goal: <0.05% |
| | Ramachandran favored | 228 | 93.44% | Goal: >98% |
| | MolProbity score^ | 1.94 | | 79 th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 1 | 0.44% | Goal: 0 |
| | Bad backbone bonds: | 5 / 2017 | 0.25% | Goal: 0% |
| | Bad backbone angles: | 1 / 2727 | 0.04% | 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: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 291 | PRO | 50 | - | - | 55.4% (Cg _{exo}) chi angles: 326.9 | 0.047Å | - | - |
| A 292 | ARG | 50 | - | Favored (68.9%) General / -54.4,-41.2 | 50.3% (ttm-85) chi angles: 190.4,187.3,300.9,290.8 | 0.073Å | - | - |
| A 293 | GLU | 50 | - | Favored (3.72%) General / -63.1,-60.2 | 4.9% (tm-20) chi angles: 167.6,263.4,324 | 0.058Å | - | - |
| A 294 | PHE | 50 | - | Favored (43.73%) General / -52.8,-53.7 | 77.4% (t80) chi angles: 182.3,84.5 | 0.026Å | - | - |

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|----------|-----|----|---|---|---|--------|---|---|
| A 295 | VAL | 50 | - | Favored (21.57%) Isoleucine or valine / -59.3,-22.0 | 32.8% (<i>m</i>) chi angles: 300.3 | 0.124Å | - | - |
| A 296 | LEU | 50 | - | Favored (23.16%) General / -94.2,-16.9 | 87.8% (<i>mt</i>) chi angles: 290.9,175.2 | 0.046Å | - | - |
| A 297 | ARG | 50 | - | Favored (59.45%) Pre-proline / -78.8,135.4 | 90.8% (<i>mtt180</i>) chi angles: 285.3,195.7,181.5,175.3 | 0.092Å | - | - |
| A 298 | PRO | 50 | - | Favored (98.09%) Trans-proline / -59.9,142.2 | 82.2% (<i>Cg_exo</i>) chi angles: 330.8 | 0.085Å | - | - |
| A 299 | ALA | 50 | - | Favored (60.28%) Pre-proline / -55.8,143.4 | - | 0.014Å | - | - |
| A 300 | PRO | 50 | - | Favored (92.62%) Trans-proline / -60.0,147.5 | 89.8% (<i>Cg_exo</i>) chi angles: 329 | 0.067Å | - | - |
| A 301 | GLN | 50 | - | Favored (36.07%) General / -52.7,134.4 | 97.1% (<i>mm-40</i>) chi angles: 294.3,299.7,318.9 | 0.062Å | - | - |
| A 302 | GLY | 50 | - | Favored (56.78%) Glycine / 66.8,10.9 | - | - | - | - |
| A 303 | ARG | 50 | - | Favored (26.54%) General / -112.8,154.3 | 51.5% (<i>mtt180</i>) chi angles: 303.5,192.4,207.3,165.4 | 0.049Å | - | - |
| A 304 | THR | 50 | - | Favored (48.32%) General / -117.6,124.3 | 59% (<i>m</i>) chi angles: 304.1 | 0.068Å | - | - |
| A 305 | VAL | 50 | - | Favored (34.42%) Isoleucine or valine / -95.5,115.4 | 47.9% (<i>t</i>) chi angles: 182.9 | 0.046Å | - | - |
| A | ARG | 50 | - | Favored (51.33%) | 79.2% (<i>mtt85</i>) | 0.016Å | - | - |

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|---|-----|-------|----------------------------------|--|--|--------|---|---|
| 306 | | | | General / -103.9,126.9 | chi angles: 293.9,184.4,183.1,102.4 | | | |
| A 307 | CYS | 50 | - | Favored (38.69%) General / -128.1,158.2 | 64.6% (<i>m</i>) chi angles: 302.5 | 0.066Å | - | - |
| A 308 | ARG | 50 | - | Favored (45.13%) General / -117.9,123.1 | 59.2% (<i>ttt85</i>) chi angles: 182.3,178.6,178.1,90.8 | 0.073Å | - | - |
| A 309 | LEU | 50 | - | Favored (51.05%) General / -110.5,124.0 | 6.9% (<i>tt</i>) chi angles: 189.1,164.8 | 0.063Å | - | - |
| A 310 | THR | 50 | - | Favored (42.68%) General / -123.8,152.0 | 74.4% (<i>p</i>) chi angles: 60 | 0.052Å | - | - |
| <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: 54.27</div> <div>Clashscore: 9.86</div> <div>Outliers: 3 of 244</div> <div>Poor rotamers: 0 of 213</div> <div>Outliers: 1 of 229</div> <div>Outliers: 4 of 246</div> <div>Outliers: 1 of 246</div> </div> | | | | | | | | |
| A 311 | ARG | 50 | - | Favored (39.61%) General / -130.1,158.4 | 38.7% (<i>ptt180</i>) chi angles: 64.1,178.9,180.1,190.1 | 0.013Å | - | - |
| A 312 | ASP | 50 | - | Favored (42.76%) General / -53.9,135.0 | 79.7% (<i>m-20</i>) chi angles: 297.5,331.3 | 0.045Å | - | - |
| A 313 | LYS | 99.99 | - | Favored (48.14%) General / -63.5,131.4 | 22.6% (<i>pttp</i>) chi angles: 61.4,178.6,182.8,65.3 | 0.015Å | - | - |
| A 314 | LYS | 99.99 | - | Favored (50.77%) General / -130.3,151.5 | 22.6% (<i>pttp</i>) chi angles: 61.1,181,182.7,64.5 | 0.029Å | - | - |
| A 315 | GLY | 99.99 | - | Favored (43.58%) Glycine / -81.9,-169.8 | - | - | - | - |
| A 316 | MET | 99.99 | 0.43Å HG3 with A 316 MET O | Favored (2.55%) General / -99.8,82.2 Favored | 24.7% (<i>ptp</i>) chi angles: 58.9,178.4,71 | 0.045Å | - | - |

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|----------|-----|-------|--------------------------------------|---|--|--------|--|---|
| A 317 | ASP | 99.99 | - | (10.91%) General / -169.3,164.9 | 29.7% (<i>p-10</i>) chi angles: 64.6,336.7 | 0.032Å | - | - |
| A 318 | ARG | 99.99 | O with A 320 MET HE2 | Favored (50.72%) General / -61.2,145.6 | 30.2% (<i>ptt-85</i>) chi angles: 56.6,191.4,181.8,263.7 | 0.016Å | - | - |
| A 319 | GLY | 99.99 | 0.402Å HA3 with A 320 MET CB | Favored (20.01%) Glycine / -179.9,-157.4 | - | - | - | OUTLIER(S) worst is C-N- CA: 5.483 σ |
| A 320 | MET | 50 | 0.455Å HE2 with A 318 ARG O | Allowed (0.07%) General / 170.9,175.4 | 2% (<i>mtm</i>) chi angles: 244.1,163.2,290.4 | 0.111Å | - | - |
| A 321 | TYR | 50 | - | Favored (62.99%) Pre-proline / -136.1,67.8 | 53% (<i>m-85</i>) chi angles: 308,274.5 | 0.042Å | - | - |
| A 322 | PRO | 50 | - | Favored (26.25%) Trans-proline / -77.5,148.3 | 68% (<i>Cg_endo</i>) chi angles: 33.7 | 0.037Å | - | - |
| A 323 | SER | 50 | - | Favored (31.21%) General / -80.5,146.6 | 48.7% (<i>m</i>) chi angles: 300.5 | 0.051Å | - | - |
| A 324 | TYR | 50 | - | Favored (48.66%) General / -119.7,142.2 | 88.9% (<i>m-85</i>) chi angles: 299.1,86.4 | 0.081Å | - | - |
| A 325 | PHE | 50 | - | Favored (51.84%) General / -130.6,145.2 | 57.8% (<i>m-85</i>) chi angles: 307,273.8 | 0.045Å | - | - |
| A 326 | LEU | 50 | - | Favored (30.18%) General / -128.7,122.2 | 25% (<i>tp</i>) chi angles: 190.2,68.8 | 0.053Å | - | - |
| A 327 | HIS | 50 | - | Favored (39.5%) General / -122.8,153.5 | 77.5% (<i>m80</i>) chi angles: 295.9,80.8 | 0.088Å | OUTLIER(S) worst is CG-- ND1: 4.479 σ | - |
| A 328 | LEU | 50 | 0.403Å HD12 with A 334 VAL CG1 | Favored (58.4%) General / -62.7,138.0 | 44% (<i>mt</i>) chi angles: 291,185.2 | 0.04Å | - | - |

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|----------|----------------|-------------------|---|---|--|-------------------------|-------------------------|------------------------|
| A 329 | ASP | 50 | - | Allowed (1.28%) General / -88.1,45.4 | 29.9% (<i>t0</i>) chi angles: 193.8,32 | 0.089Å | - | - |
| A 330 | THR | 50 | 0.494Å HG23 with A 332 LYS O | Favored (9.94%) General / -103.5,167.2 | 6.4% (<i>t</i>) chi angles: 177.8 | 0.057Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 331 | GLU | 50 | - | Favored (71.48%) General / -62.5,-30.7 | 2.4% (<i>mm-40</i>) chi angles: 320.2,319.6,278.4 | 0.052Å | - | - |
| A 332 | LYS | 50 | 0.494Å O with A 330 THR HG23 | Favored (4.1%) General / -94.1,81.3 | 50.7% (<i>tttt</i>) chi angles: 182.7,209.6,177.5,187.4 | 0.077Å | - | - |
| A 333 | LYS | 50 | - | Allowed (0.08%) General / -66.0,80.1 | 54.8% (<i>mttp</i>) chi angles: 304,171.7,182.2,61.4 | 0.048Å | - | - |
| A 334 | VAL | 50 | 0.403Å CG1 with A 328 LEU HD12 | Favored (26.05%) Isoleucine or valine / -72.9,136.2 | 8.6% (<i>p</i>) chi angles: 68.5 | 0.118Å | - | - |
| A 335 | PHE | 50 | 0.447Å CE1 with A 356 PRO HB3 | Favored (52.34%) General / -70.3,141.5 | 84.6% (<i>t80</i>) chi angles: 173.6,78.3 | 0.077Å | - | - |
| A 336 | LEU | 50 | - | Allowed (1.77%) General / -118.0,-60.7 | 90.1% (<i>mt</i>) chi angles: 298.8,179.4 | 0.025Å | - | - |
| A 337 | LEU | 50 | - | Favored (33.12%) General / -148.3,150.2 | 86.1% (<i>mt</i>) chi angles: 293.3,168.6 | 0.074Å | - | - |
| A 338 | ALA | 50 | - | Favored (52.21%) General / -132.5,150.1 | - | 0.045Å | - | - |
| A 339 | GLY | 50 | - | Favored (23.19%) Glycine / -146.5,150.9 | - | - | - | - |

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|----------|-----|----|---|--|--|--------|---|---|
| A 340 | ARG | 50 | 0.673Å HH11 with A 359 LEU CD1 | Favored (16.75%) General / -154.6,139.0 | 34.9% (<i>ttt180</i>) chi angles: 185.4,173.1,178,230.6 | 0.02Å | - | - |
| A 341 | LYS | 50 | - | Favored (42.88%) General / -73.3,132.2 | 87.1% (<i>tttt</i>) chi angles: 188.2,175.1,180.7,176.2 | 0.095Å | - | - |
| A 342 | ARG | 50 | 0.773Å HH22 with A 344 ARG NH2 | Favored (32.35%) General / -80.6,127.3 | 61.3% (<i>mtp85</i>) chi angles: 295.5,174.3,64.3,67.5 | 0.104Å | - | - |
| A 343 | LYS | 50 | - | Favored (60.57%) General / -74.4,-27.4 | 12.3% (<i>ptmt</i>) chi angles: 53.9,209.8,301,182.7 | 0.134Å | - | - |
| A 344 | ARG | 50 | 0.773Å NH2 with A 342 ARG HH22 | Allowed (1.27%) General / -94.4,34.7 | 27.5% (<i>ptt-85</i>) chi angles: 65.6,171.2,177.8,283.4 | 0.098Å | - | - |
| A 345 | SER | 50 | - | Favored (46.41%) General / -115.9,142.7 | 61.4% (<i>m</i>) chi angles: 292 | 0.017Å | - | - |
| A 346 | LYS | 50 | - | Favored (81.37%) General / -63.5,-35.7 | 83.8% (<i>mttt</i>) chi angles: 308.3,174.9,190.5,181.3 | 0.049Å | - | - |
| A 347 | THR | 50 | - | Favored (17.55%) General / -119.2,163.2 | 81.4% (<i>p</i>) chi angles: 61.1 | 0.051Å | - | - |
| A 348 | ALA | 50 | - | Favored (14.89%) General / -55.4,123.7 | - | 0.021Å | - | - |
| A 349 | ASN | 50 | - | Favored (4.54%) General / -144.1,107.3 | 57.7% (<i>t-20</i>) chi angles: 184.1,339.9 | 0.068Å | - | - |
| A 350 | TYR | 50 | 0.534Å HB2 with A 370 LEU HB3 | Favored (48.77%) General / -102.2,131.5 | 62.4% (<i>m-85</i>) chi angles: 291.3,78.2 | 0.077Å | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|------|-----|-----|-------------|-----------------|---------------------|-----------|-----------------|-----------------|----------------|
| Avg: | | | Clashscore: | Outliers: 3 of | Poor rotamers: 0 of | Outliers: | Outliers: 4 | Outliers: 1 | |
| 54 | 27 | | | 0.00 | 0.11 | 0.10 | 1.6000 | 0.016 | 0.016 |

| | | 54.2% | 9.86 | 244 | 213 | 1 of 229 | of 246 | of 246 |
|----------|-----|-------|---|--|--|----------|--------|--------|
| A 351 | LEU | 50 | 0.724Å HD22 with A 361 ARG HD3 | Favored (40.45%) General / -95.9,133.1 | 74.9% (<i>mt</i>) chi angles: 300.5,183.1 | 0.04Å | - | - |
| A 352 | ILE | 50 | - | Favored (53.95%) Isoleucine or valine / -115.8,136.0 | 61.9% (<i>mt</i>) chi angles: 305.6,171.6 | 0.073Å | - | - |
| A 353 | SER | 50 | - | Favored (50.94%) General / -135.0,155.3 | 46% (<i>t</i>) chi angles: 178.9 | 0.07Å | - | - |
| A 354 | ILE | 50 | - | Favored (6.54%) Isoleucine or valine / -101.3,12.7 | 48.1% (<i>pt</i>) chi angles: 59.5,172.5 | 0.064Å | - | - |
| A 355 | ASP | 50 | - | Favored (29.47%) Pre-proline / -124.4,107.8 | 46.9% (<i>t0</i>) chi angles: 187.4,331.1 | 0.021Å | - | - |
| A 356 | PRO | 50 | 0.447Å HB3 with A 335 PHE CE1 | Favored (63.69%) Trans-proline / -64.9,-22.0 | 94.7% (<i>Cg_endo</i>) chi angles: 32.2 | 0.058Å | - | - |
| A 357 | THR | 50 | - | Favored (56.88%) General / -93.0,-1.2 | 30.8% (<i>p</i>) chi angles: 69.8 | 0.006Å | - | - |
| A 358 | ASN | 99.99 | - | Favored (56.82%) General / -116.5,131.9 | 53.5% (<i>t30</i>) chi angles: 184.4,26.4 | 0.056Å | - | - |
| A 359 | LEU | 99.99 | 0.673Å CD1 with A 340 ARG HH11 | Favored (11.74%) General / -105.6,-26.7 | 7.3% (<i>tt</i>) chi angles: 184.6,162.3 | 0.045Å | - | - |
| A 360 | SER | 99.99 | - | Favored (29.51%) General / -57.9,147.2 | 46.3% (<i>t</i>) chi angles: 180.5 | 0.061Å | - | - |
| A 361 | ARG | 99.99 | 0.883Å HA with A 366 PHE HB2 | Allowed (1.39%) General / -117.5,79.7 | 16.7% (<i>ptt180</i>) chi angles: 68.3,156.6,170.9,198 | 0.122Å | - | - |

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|----------|---------|------------|--|---|--|--------------------|--------------------|--------------------|
| A 362 | GLY | 99.99 | - | Favored (23.9%) Glycine / 173.4,161.6 | - | - | - | - |
| A 363 | GLY | 99.99 | - | Allowed (0.64%) Glycine / 64.7,-102.5 | - | - | - | - |
| A 364 | GLU | 99.99 | 0.566Å HG2 with A 365 ASN ND2 | Favored (34.08%) General / -81.9,-26.5 | 5.1% (<i>pm0</i>) chi angles: 59.8,291.7,338.6 | 0.295Å | - | - |
| A 365 | ASN | 50 | 0.566Å ND2 with A 364 GLU HG2 | Allowed (0.46%) General / -149.2,-1.8 | 70.7% (<i>m-80</i>) chi angles: 299.2,293.6 | 0.176Å | - | - |
| A 366 | PHE | 50 | 0.883Å HB2 with A 361 ARG HA | Favored (26.76%) General / -64.3,126.1 | 16.2% (<i>t80</i>) chi angles: 175.2,45.6 | 0.2Å | - | - |
| A 367 | ILE | 50 | - | Allowed (1.97%) Isoleucine or valine / -119.0,-28.7 | 9.8% (<i>tp</i>) chi angles: 199,65.4 | 0.158Å | - | - |
| A 368 | GLY | 50 | - | Favored (43.04%) Glycine / -168.8,176.3 | - | - | - | - |
| A 369 | LYS | 50 | - | Favored (24.69%) General / -148.5,141.4 | 36% (<i>ttpt</i>) chi angles: 173.5,164.3,60.2,180.2 | 0.053Å | - | - |
| A 370 | LEU | 50 | 0.534Å HB3 with A 350 TYR HB2 | Favored (19.52%) General / -114.2,110.2 | 50.7% (<i>tp</i>) chi angles: 177,68.4 | 0.044Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 371 | ARG | 50 | - | Favored (56.98%) General / -114.9,130.8 | 42.7% (<i>ttp180</i>) chi angles: 182.1,199.5,63.1,178.4 | 0.097Å | - | - |
| A 372 | SER | 50 | - | Favored (17.19%) General / | 59.5% (<i>p</i>) chi angles: 71.5 | 0.052Å | - | - |

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|----------|-----|----|--|--|---|--------|---|---|
| A 373 | ASN | 50 | - | General / -92.8,156.1 Favored (7.38%) General / -70.2,172.9 | 41.9% (<i>p-10</i>) chi angles: 65.5,340.6 | 0.046Å | - | - |
| A 374 | LEU | 50 | - | Favored (80.45%) General / -58.4,-39.7 | 3% (<i>tt</i>) chi angles: 200.2,141.4 | 0.069Å | - | - |
| A 375 | LEU | 50 | - | Favored (93.36%) General / -65.4,-40.3 | 86.5% (<i>mt</i>) chi angles: 294.6,179.3 | 0.079Å | - | - |
| A 376 | GLY | 50 | - | Favored (42.09%) Glycine / 97.9,13.8 | - | - | - | - |
| A 377 | ASN | 50 | - | Favored (16.29%) General / -108.0,-7.1 | 34.1% (<i>p-10</i>) chi angles: 64.9,334.6 | 0.033Å | - | - |
| A 378 | ARG | 50 | - | Favored (51.92%) General / -127.5,140.8 | 83.6% (<i>mtt180</i>) chi angles: 297.5,187.1,180.2,204.8 | 0.012Å | - | - |
| A 379 | PHE | 50 | - | Favored (49.35%) General / -133.8,145.0 | 88.5% (<i>m-85</i>) chi angles: 295.8,83.2 | 0.082Å | - | - |
| A 380 | THR | 50 | - | Favored (50.59%) General / -121.8,142.1 | 55.4% (<i>m</i>) chi angles: 304.5 | 0.038Å | - | - |
| A 381 | VAL | 50 | - | Favored (67.69%) Isoleucine or valine / -110.4,126.2 | 46.2% (<i>t</i>) chi angles: 183.5 | 0.063Å | - | - |
| A 382 | PHE | 50 | - | Favored (35.61%) General / -116.5,151.7 | 90.6% (<i>m-85</i>) chi angles: 302.2,276.8 | 0.098Å | - | - |
| A 383 | ASP | 50 | 0.424Å OD2 with A 401 GLN HG2 | OUTLIER (0.03%) General / -71.2,-156.2 Favored (12.22%) | 50.3% (<i>p-10</i>) chi angles: 67.5,355.7 | 0.097Å | - | - |
| A | ASN | 50 | | (12.22%) | 50.3% (<i>p-10</i>) | 0.097Å | | |

| A 384 | ASN | 50 | - | (15.32%) General / -97.4,19.4 | 52.4% (<i>pt0</i>) chi angles: 62.5,359.4 | 0.002Å | - | - |
|----------|---------|------------|-------------------------------------|---|---|--------------------|--------------------|--------------------|
| A 385 | GLY | 50 | 0.427Å HA3 with A 400 ARG HA | Favored (54.85%) Glycine / -75.0,168.1 | - | - | - | - |
| A 386 | GLN | 50 | 0.421Å HG2 with A 387 ASN N | Favored (42.9%) General / -74.9,145.2 | 10.2% (<i>tt0</i>) chi angles: 187.1,202.1,108.6 | 0.06Å | - | - |
| A 387 | ASN | 50 | 0.421Å N with A 386 GLN HG2 | Favored (90.28%) Pre-proline / -71.9,127.8 | 55.2% (<i>t-20</i>) chi angles: 183.1,338 | 0.049Å | - | - |
| A 388 | PRO | 50 | - | Favored (40.88%) Trans-proline / -66.0,-33.5 | 78.1% (<i>Cg_exo</i>) chi angles: 332.1 | 0.075Å | - | - |
| A 389 | GLN | 50 | 0.455Å HE22 with A 441 ASN HA | Favored (65.04%) General / -62.5,-20.9 | 2.9% (<i>mp0</i>) chi angles: 270.1,49.4,256.2 | 0.022Å | - | - |
| A 390 | ARG | 50 | - | Favored (56.94%) General / -84.5,-11.0 | 6% (<i>mmp_?</i>) chi angles: 299.3,276.8,109.4,113.8 | 0.038Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 391 | GLY | 50 | - | Allowed (0.12%) Glycine / 178.9,98.7 | - | - | - | - |
| A 392 | TYR | 50 | - | Favored (64.78%) General / -68.3,-21.3 | 13.8% (<i>t80</i>) chi angles: 195.7,54.6 | 0.049Å | - | - |
| A 393 | SER | 50 | - | Favored (58.85%) General / -87.8,-4.6 | 61.1% (<i>m</i>) chi angles: 299 | 0.034Å | - | - |
| A 394 | THR | 50 | - | Favored (58.82%) General / -64.8,140.0 | 98.8% (<i>m</i>) chi angles: 298.9 | 0.09Å | - | - |

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|----------|-----|----|-------------------------------------|---|--|--------|---|---|
| A 395 | ASN | 50 | - | Favored (44.46%) General / -54.5,136.5 | 45.8% (<i>t30</i>) chi angles: 182.2,22.6 | 0.073Å | - | - |
| A 396 | VAL | 50 | - | Favored (60.25%) Isoleucine or valine / -56.2,-39.6 | 62% (<i>t</i>) chi angles: 181.5 | 0.021Å | - | - |
| A 397 | ALA | 50 | - | Favored (68.36%) General / -60.2,-28.9 | - | 0.02Å | - | - |
| A 398 | SER | 50 | - | Favored (57.11%) General / -86.4,-9.1 | 60.9% (<i>m</i>) chi angles: 299.1 | 0.04Å | - | - |
| A 399 | LEU | 50 | - | Favored (49.41%) General / -71.8,140.4 | 89.1% (<i>mt</i>) chi angles: 298.1,180.2 | 0.016Å | - | - |
| A 400 | ARG | 50 | 0.427Å HA with A 385 GLY HA3 | Favored (57.29%) General / -61.8,142.4 | 40.1% (<i>ptt180</i>) chi angles: 65.5,184.2,188.6,185.4 | 0.014Å | - | - |
| A 401 | GLN | 50 | 0.424Å HG2 with A 383 ASP OD2 | Favored (20.71%) General / -105.9,154.3 | 15.9% (<i>pt20</i>) chi angles: 69.8,184.3,285.6 | 0.043Å | - | - |
| A 402 | GLU | 50 | - | Favored (38.95%) General / -96.1,122.4 | 71.9% (<i>mt-10</i>) chi angles: 295.5,188.6,18.1 | 0.034Å | - | - |
| A 403 | LEU | 50 | - | Favored (15.18%) General / -96.3,-26.9 | 95.9% (<i>mt</i>) chi angles: 295.9,174.2 | 0.018Å | - | - |
| A 404 | ALA | 50 | - | Favored (2.72%) General / -172.4,152.6 | - | 0.045Å | - | - |
| A 405 | ALA | 50 | - | Favored (49.17%) General / -132.7,142.7 | - | 0.079Å | - | - |
| A 406 | VAL | 50 | - | Favored (69.77%) Isoleucine or | 40.4% (<i>t</i>) chi angles: 184.8 | 0.037Å | - | - |

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|-------|---------|------------|----------------------------------|--------------------|---|---|--------------------|--------------------|---|
| A 407 | ILE | 50 | - | - | Favored (69.59%) Isoleucine or valine / -127.3,128.1 -117.3,122.3 | 4.2% (<i>mp</i>) chi angles: 305.6,81.2 | 0.015Å | - | - |
| A 408 | TYR | 50 | - | - | Favored (45.92%) General / -104.7,135.5 | 91.2% (<i>m-85</i>) chi angles: 291.1,273.5 | 0.083Å | - | - |
| A 409 | GLU | 50 | - | - | Favored (40.22%) General / -75.7,146.3 | 67.8% (<i>mt-10</i>) chi angles: 286.2,184.6,23 | 0.042Å | - | - |
| A 410 | THR | 50 | - | - | Favored (43.99%) General / -97.0,131.2 | 89.8% (<i>m</i>) chi angles: 297.8 | 0.08Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | |
| | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 | |
| A 411 | ASN | 50 | 0.812Å ND2 with A 417 GLY HA3 | - | Favored (23.4%) General / -83.3,155.8 | 87.1% (<i>m-20</i>) chi angles: 296.2,332.7 | 0.032Å | - | - |
| A 412 | VAL | 99.99 | - | - | Favored (43.07%) Isoleucine or valine / -132.2,157.3 | 14.7% (<i>p</i>) chi angles: 64 | 0.099Å | - | - |
| A 413 | LEU | 99.99 | 0.408Å C with A 413 LEU HD23 | - | Favored (42.83%) General / -55.6,130.4 | 7.1% (<i>tt</i>) chi angles: 184.5,163.3 | 0.052Å | - | - |
| A 414 | GLY | 99.99 | - | - | Favored (33.07%) Glycine / 105.7,-22.0 | - | - | - | - |
| A 415 | PHE | 99.99 | - | - | Favored (43.48%) General / -116.8,145.5 | 72.7% (<i>t80</i>) chi angles: 185.5,80.8 | 0.078Å | - | - |
| A 416 | ARG | 99.99 | - | - | Favored (21.54%) General / -90.3,151.3 | 32.8% (<i>ptt-85</i>) chi angles: 62.3,176.9,178.274.6 | 0.051Å | - | - |

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|----------|-----|-------|--|--|---|--------|--|---|
| A 417 | GLY | 99.99 | 0.812Å HA3 with A 411 ASN ND2 | OUTLIER (0.09%) Glycine / -176.1,93.3 | - | - | - | - |
| A 418 | PRO | 50 | 0.692Å O with A 417 GLY HA2 | OUTLIER (0.07%) Trans-proline / -30.6,127.8 | 61% (<i>Cg_endo</i>) chi angles: 27.3 | 0.037Å | OUTLIER(S) worst is C--N: 6.839 σ | - |
| A 419 | ARG | 50 | - | Favored (26.48%) General / -88.4,144.3 | 89.6% (<i>mtm180</i>) chi angles: 291.9,177.2,296.2,168.8 | 0.04Å | - | - |
| A 420 | ARG | 50 | - | Favored (54.7%) General / -68.3,137.4 | 98.9% (<i>mtt180</i>) chi angles: 295.4,184,186.9,170.5 | 0.032Å | - | - |
| A 421 | MET | 50 | - | Favored (48.9%) General / -119.9,142.2 | 78.7% (<i>mtp</i>) chi angles: 299.2,177.5,57.1 | 0.132Å | - | - |
| A 422 | THR | 50 | - | Favored (53.69%) General / -121.4,130.6 | 68.8% (<i>m</i>) chi angles: 303.3 | 0.04Å | - | - |
| A 423 | VAL | 50 | - | Favored (75.97%) Isoleucine or valine / -120.3,128.3 | 64.5% (<i>t</i>) chi angles: 179.8 | 0.05Å | - | - |
| A 424 | ILE | 50 | - | Favored (73.73%) Isoleucine or valine / -118.5,130.2 | 40.9% (<i>mm</i>) chi angles: 307.2,299.2 | 0.044Å | - | - |
| A 425 | ILE | 50 | - | Favored (66.6%) Pre-proline / -131.1,160.5 | 49.9% (<i>pt</i>) chi angles: 61.5,172.1 | 0.089Å | - | - |
| A 426 | PRO | 50 | - | Favored (94.48%) Trans-proline / -62.6,144.6 | 90.4% (<i>Cg_exo</i>) chi angles: 330 | 0.07Å | - | - |
| A 427 | GLY | 50 | - | Favored (34.97%) Glycine / -63.6,161.8 | - | - | - | - |
| A | | | | Favored | 86% (<i>mmm</i>) | | | |

| 428 | MET | 50 | - | Favored (39.57%) General / -114.8,147.6 | chi angles: 308.2,299.1,286.6 | 0.089Å | - | - |
|----------|---------|------------|---------------------------------------|--|---|------------------------|--------------------|--------------------|
| A 429 | SER | 50 | 0.515Å OG with A 431 GLU HB3 | Favored (11.79%) General / -77.3,173.6 | 78.9% (<i>p</i>) chi angles: 59.5 | 0.05Å | - | - |
| A 430 | ALA | 50 | - | Favored (66.67%) General / -65.5,-21.8 | - | 0.021Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | C β deviation | Bond lengths | Bond angles |
| | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 431 | GLU | 50 | 0.515Å HB3 with A 429 SER OG | Favored (66.44%) General / -66.0,-22.1 | 14.1% (<i>tp10</i>) chi angles: 178.9,89.7,22.9 | 0.098Å | - | - |
| A 432 | ASN | 50 | - | Allowed (1.44%) General / 72.9,32.1 | 9.2% (<i>m120</i>) chi angles: 301.2,158.9 | 0.097Å | - | - |
| A 433 | GLU | 50 | - | Favored (31.94%) General / -118.3,154.6 | 69.3% (<i>mt-10</i>) chi angles: 282.7,183.2,325 | 0.031Å | - | - |
| A 434 | ARG | 50 | - | Favored (48.22%) General / -60.6,145.7 | 68.4% (<i>mtm-85</i>) chi angles: 276.7,192.5,299.7,291.6 | 0.082Å | - | - |
| A 435 | VAL | 50 | - | Favored (20.64%) Pre-proline / -102.6,101.5 | 58.4% (<i>t</i>) chi angles: 180.7 | 0.04Å | - | - |
| A 436 | PRO | 50 | - | Favored (61.49%) Trans-proline / -69.9,147.1 | 81% (<i>Cg_exo</i>) chi angles: 330.6 | 0.073Å | - | - |
| A 437 | ILE | 50 | - | Favored (30.23%) Isoleucine or valine / -115.2,110.0 | 94.9% (<i>mt</i>) chi angles: 297.7,169.1 | 0.044Å | - | - |
| A 438 | ARG | 50 | - | Favored (62.01%) Pre-proline / | 40.4% (<i>ttm-85</i>) chi angles: 198.1,181.5,302.1,259.9 | 0.127Å | - | - |

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| --- | | | | -128.1,84.9 | | | | |
| A 439 | PRO | 50 | - | Favored (79.24%) Trans-proline / -66.6,146.3 | 78.2% (<i>Cg_exo</i>) chi angles: 328.4 | 0.064Å | - | - |
| A 440 | ARG | 50 | - | Favored (33.05%) General / -91.6,-12.9 | 7.4% (<i>mmm-85</i>) chi angles: 315.4,300.5,265.4,261 | 0.019Å | - | - |
| A 441 | ASN | 50 | 0.455Å HA with A 389 GLN HE22 | Favored (17.71%) General / -166.2,164.9 | 37.5% (<i>p30</i>) chi angles: 59.3,27.1 | 0.025Å | - | - |
| A 442 | ALA | 50 | - | Allowed (0.09%) General / -72.4,18.3 | - | 0.063Å | - | - |
| A 443 | SER | 50 | - | Favored (47.74%) General / -97.2,6.8 | 24.8% (<i>p</i>) chi angles: 78.8 | 0.029Å | - | - |
| A 444 | ASP | 50 | - | Favored (43%) General / -146.7,156.2 | 30.7% (<i>t0</i>) chi angles: 186.7,32.9 | 0.048Å | - | - |
| A 445 | GLY | 50 | - | Favored (28.43%) Glycine / 150.8,-178.1 | - | - | - | - |
| A 446 | LEU | 50 | - | Favored (57.51%) General / -63.8,-53.0 | 85.5% (<i>mt</i>) chi angles: 291.4,177.3 | 0.043Å | - | - |
| A 447 | LEU | 50 | - | Favored (86.48%) General / -61.0,-38.5 | 95.1% (<i>mt</i>) chi angles: 294.3,175.8 | 0.026Å | - | - |
| A 448 | VAL | 50 | - | Favored (63.22%) Isoleucine or valine / -61.1,-52.3 | 95% (<i>t</i>) chi angles: 175.9 | 0.057Å | - | - |
| A 449 | ARG | 50 | - | Favored (84.9%) General / -65.0,-36.6 | 98.3% (<i>mtt180</i>) chi angles: 297.4,183.6,187.4,183.1 | 0.036Å | - | - |
| A 450 | TRP | 50 | - | Favored (64.39%) General / | 57.4% (<i>t-105</i>) chi angles: 168.9,249.9 | 0.026Å | - | - |

-57.4,-52.7

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|----------|-----|-----|-----------------------------------|------------------|--|---|--------------------|--------------------|--------------------|
| | | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 451 | GLN | 50 | - | - | Favored (65.34%) General / -69.7,-27.8 | 12.8% (<i>pt20</i>) chi angles: 53.9,186.7,23.1 | 0.152Å | - | - |
| A 452 | ASN | 50 | - | - | Favored (53.06%) General / -80.0,-17.3 | 90.7% (<i>m-20</i>) chi angles: 291.3,348 | 0.039Å | - | - |
| A 453 | LYS | 50 | - | - | Favored (7.74%) General / 62.0,45.0 | 75.4% (<i>mmtt</i>) chi angles: 300.6,297.7,177.1,184.4 | 0.093Å | - | - |
| A 454 | THR | 50 | - | - | Allowed (1.66%) General / -111.0,82.8 | 54.4% (<i>p</i>) chi angles: 56.1 | 0.05Å | - | - |
| A 455 | LEU | 50 | - | - | Favored (18.32%) General / -106.1,20.8 | 62.2% (<i>mt</i>) chi angles: 306.6,177 | 0.057Å | - | - |
| A 456 | GLU | 50 | - | - | Favored (83.79%) General / -61.4,-47.9 | 29.4% (<i>tt0</i>) chi angles: 188.7,168.6,281.9 | 0.041Å | - | - |
| A 457 | SER | 50 | - | - | Favored (12.26%) General / -90.0,14.4 | 78.6% (<i>p</i>) chi angles: 59.3 | 0.056Å | - | - |
| A 458 | LEU | 50 | - | - | Favored (23.94%) General / -124.4,162.4 | 36.6% (<i>mt</i>) chi angles: 307.4,185.9 | 0.027Å | - | - |
| A 459 | ILE | 50 | - | - | Favored (69.25%) Isoleucine or valine / -119.5,132.4 | 86.7% (<i>mt</i>) chi angles: 300.1,173 | 0.053Å | - | - |
| A 460 | GLU | 50 | 0.5Å OE2 with A 462 HIS HE1 | - | Favored (52.98%) General / -107.3,132.5 | 65% (<i>tt0</i>) chi angles: 183.2,183.2,333.9 | 0.109Å | - | - |

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| A 461 | LEU | 50 | - | Favored (51.02%) General / -134.5,155.1 | 66.7% (<i>mt</i>) chi angles: 304.3,174.6 | 0.093Å | - | - |
| A 462 | HIS | 50 | 0.5Å HE1 with A 460 GLU OE2 | Favored (46.25%) General / -140.9,155.7 | 71.7% (<i>m80</i>) chi angles: 298.9,96.2 | 0.053Å | OUTLIER(S) worst is CG-- ND1: 4.921 σ | - |
| A 463 | ASN | 50 | - | Favored (58.79%) General / -63.8,139.7 | 8.1% (<i>p-10</i>) chi angles: 73.4,291.6 | 0.019Å | - | - |
| A 464 | LYS | 50 | - | Favored (75.95%) Pre-proline / -75.5,132.2 | 86.9% (<i>tttt</i>) chi angles: 184.5,173.2,178.3,173.3 | 0.055Å | - | - |
| A 465 | PRO | 50 | - | Favored (42.74%) Trans-proline / -68.0,138.0 | 90.2% (<i>Cg_exo</i>) chi angles: 329 | 0.058Å | - | - |
| A 466 | PRO | 50 | - | Favored (75.37%) Trans-proline / -68.3,152.8 | 99.6% (<i>Cg_exo</i>) chi angles: 329.5 | 0.056Å | - | - |
| A 467 | VAL | 50 | - | Favored (27.63%) Isoleucine or valine / -122.5,156.8 | 33.4% (<i>m</i>) chi angles: 299.7 | 0.068Å | - | - |
| A 468 | TRP | 50 | - | Favored (26.99%) General / -66.8,125.8 | 68% (<i>t-105</i>) chi angles: 186.3,245.4 | 0.007Å | - | - |
| A 469 | ASN | 50 | 0.49Å HD22 with A 472 SER H | Favored (9.11%) General / -106.5,99.5 | 1.6% (<i>t30</i>) chi angles: 194.3,101 | 0.051Å | - | - |
| A 470 | ASP | 50 | - | Favored (64.46%) General / -62.2,-20.7 | 4% (<i>t0</i>) chi angles: 212.8,321.9 | 0.036Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 471 | ASP | 50 | - | Favored (30.88%) | 31% (<i>t70</i>) chi angles: 181.6,76.8 | 0.063Å | - | - |

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|----------|-----|----|-----------------------------------|--|---|--------|---|---|
| A 472 | SER | 50 | 0.49Å H with A 469 ASN HD22 | General / -82.0,-32.0 Favored (18.4%) General / -109.1,-2.0 | 89.2% (<i>p</i>) chi angles: 62.2 | 0.024Å | - | - |
| A 473 | GLY | 50 | - | Favored (33.06%) Glycine / 54.3,54.3 | - | - | - | - |
| A 474 | SER | 50 | - | Favored (18.08%) General / -159.1,147.6 | 35% (<i>t</i>) chi angles: 182.9 | 0.068Å | - | - |
| A 475 | TYR | 50 | - | Favored (13.7%) General / -82.0,106.1 | 27.1% (<i>m-85</i>) chi angles: 276.2,275.3 | 0.023Å | - | - |
| A 476 | THR | 50 | - | Favored (3.64%) General / -143.7,-172.0 | 13% (<i>t</i>) chi angles: 190.8 | 0.098Å | - | - |
| A 477 | LEU | 50 | - | Favored (35.54%) General / -125.9,158.3 | 95% (<i>mt</i>) chi angles: 296.5,173 | 0.047Å | - | - |
| A 478 | ASN | 50 | - | Favored (9.99%) General / -84.3,98.4 | 61.2% (<i>t-20</i>) chi angles: 184.1,344.1 | 0.015Å | - | - |
| A 479 | PHE | 50 | - | Favored (53.26%) General / -87.9,1.8 | 98.3% (<i>m-85</i>) chi angles: 295.4,276.2 | 0.029Å | - | - |
| A 480 | GLN | 50 | - | Favored (13.25%) General / 63.2,34.7 | 46.3% (<i>mm-40</i>) chi angles: 302.4,293.6,355.3 | 0.035Å | - | - |
| A 481 | GLY | 50 | - | Favored (65.76%) Glycine / 64.0,21.6 | - | - | - | - |
| A 482 | ARG | 50 | - | Favored (30.55%) General / -84.3,-22.8 | 31.4% (<i>mmm180</i>) chi angles: 295.8,293.8,293.4,159.1 | 0.015Å | - | - |
| A | VAL | 50 | - | Favored (60.27%) | 64.7% (<i>t</i>) | 0.079Å | - | - |

| 483 | VAL | 50 | - | Isoleucine or valine / -128.7,123.9 | chi angles: 179.8 | 0.073Å | - | - |
|-------|---------|------------|------------------|--|--|--------------------|--------------------|--------------------|
| A 484 | THR | 50 | - | Favored (10.24%) General / -117.6,-14.1 | 82.1% (<i>p</i>) chi angles: 60.5 | 0.063Å | - | - |
| A 485 | GLN | 50 | - | Favored (52.79%) General / -125.7,140.3 | 51.4% (<i>mt-30</i>) chi angles: 308.5,192.3,341.2 | 0.003Å | - | - |
| A 486 | ALA | 50 | - | Favored (58.45%) General / -62.3,138.5 | - | 0.052Å | - | - |
| A 487 | SER | 50 | - | Favored (5.09%) General / -166.4,143.6 | 40.3% (<i>t</i>) chi angles: 176.7 | 0.084Å | - | - |
| A 488 | VAL | 50 | - | Favored (26.75%) Isoleucine or valine / -65.4,-20.0 | 32% (<i>m</i>) chi angles: 300.6 | 0.068Å | - | - |
| A 489 | LYS | 50 | - | Favored (52.15%) General / -79.8,-17.9 | 32.1% (<i>mtmm</i>) chi angles: 284.4,179.7,281.5,290.6 | 0.055Å | - | - |
| A 490 | ASN | 50 | - | Favored (27.04%) General / -66.3,125.9 | 65% (<i>m-20</i>) chi angles: 298.9,348.6 | 0.046Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 491 | PHE | 50 | - | Favored (29%) General / -159.7,157.1 | 21% (<i>p90</i>) chi angles: 63.8,76.3 | 0.039Å | - | - |
| A 492 | GLN | 50 | - | Favored (54.68%) General / -122.7,135.7 | 97.9% (<i>mt-30</i>) chi angles: 295.9,177.8,328.7 | 0.09Å | - | - |
| A 493 | ILE | 50 | - | Favored (63.58%) Isoleucine or valine / -107.9,123.8 | 51.3% (<i>mm</i>) chi angles: 302.6,300.7 | 0.042Å | - | - |

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|----------|-----|----|--|--|--|--------|--|---|
| A 494 | VAL | 50 | - | Favored (42.82%) Isoleucine or valine / -131.4,156.6 | 34.4% (<i>m</i>) chi angles: 298.8 | 0.06Å | - | - |
| A 495 | HIS | 50 | - | Favored (25.28%) General / -86.0,149.3 | 59.9% (<i>t-80</i>) chi angles: 190.7,274.8 | 0.072Å | OUTLIER(S) worst is CG-- ND1: 4.705 σ | - |
| A 496 | ALA | 50 | - | Favored (61.64%) General / -56.4,-29.6 | - | 0.016Å | - | - |
| A 497 | ASP | 50 | - | Favored (61.58%) General / -72.5,-25.8 | 83.6% (<i>m-20</i>) chi angles: 293.7,350.4 | 0.126Å | - | - |
| A 498 | ASP | 50 | - | Favored (3.87%) Pre-proline / -147.8,98.4 | 50% (<i>t0</i>) chi angles: 192.2,346.5 | 0.058Å | - | - |
| A 499 | PRO | 50 | - | Favored (9.86%) Trans-proline / -72.3,-1.3 | 96.8% (<i>Cg_endo</i>) chi angles: 30.6 | 0.095Å | - | - |
| A 500 | ASP | 50 | - | Favored (17.73%) General / -106.7,-6.6 | 70.7% (<i>m-20</i>) chi angles: 287.9,322.5 | 0.063Å | - | - |
| A 501 | TYR | 50 | - | Favored (15.8%) General / -94.3,103.8 | 55.6% (<i>t80</i>) chi angles: 186.3,270.8 | 0.065Å | - | - |
| A 502 | ILE | 50 | - | Favored (5.8%) Isoleucine or valine / -89.2,96.0 | 25.4% (<i>mm</i>) chi angles: 312.2,304 | 0.057Å | - | - |
| A 503 | VAL | 50 | - | Favored (80.17%) Isoleucine or valine / -62.3,-38.1 | 46% (<i>t</i>) chi angles: 183.5 | 0.055Å | - | - |
| A 504 | LEU | 50 | 0.458Å HD11 with A 516 LEU HD11 | Favored (9.07%) General / -154.1,128.4 | 39.6% (<i>tp</i>) chi angles: 186.8,63 | 0.055Å | - | - |
| A 505 | GLN | 50 | - | Favored (53.28%) General / -134.1,124.0 | 29.5% (<i>tt0</i>) chi angles: 125.7,175.0,271.1 | 0.069Å | - | - |

-124.1,134.8 185.7,175.9,271.1

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|----------|-----|-----|--|---|---|----------------------------|-----------------------|-----------------------|-----------------------|
| A 506 | PHE | 50 | - | Favored (32%) General / -141.1,136.5 | 37.7% (<i>t80</i>) chi angles: 187.6,59.2 | 0.085Å | - | - | |
| A 507 | GLY | 50 | - | Favored (31.92%) Glycine / -170.5,159.6 | - | - | - | - | |
| A 508 | ARG | 50 | - | Favored (35.53%) General / -81.6,136.4 | 55.6% (<i>ttm-85</i>) chi angles: 182.8,187.6,288.8,279.9 | 0.083Å | - | - | |
| A 509 | VAL | 50 | - | Favored (5.6%) Isoleucine or valine / -118.0,-20.0 | 24.2% (<i>m</i>) chi angles: 293.4 | 0.112Å | - | - | |
| A 510 | ALA | 50 | 0.433Å HB3 with A 513 ALA HB3 | Favored (4.49%) General / -155.5,-173.3 | - | 0.06Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 511 | GLU | 50 | - | Favored (97.86%) General / -61.2,-42.0 | 26.2% (<i>tp10</i>) chi angles: 187.6,55.4,42.4 | 0.018Å | - | - | |
| A 512 | ASP | 50 | - | Favored (5.37%) General / -129.8,24.3 | 47% (<i>m-20</i>) chi angles: 299.6,294.9 | 0.067Å | - | - | |
| A 513 | ALA | 50 | 0.433Å HB3 with A 510 ALA HB3 | Favored (50.65%) General / -130.4,143.3 | - | 0.023Å | - | - | |
| A 514 | PHE | 50 | - | Favored (43.67%) General / -144.2,155.0 | 54.9% (<i>m-85</i>) chi angles: 304.8,82.2 | 0.112Å | - | - | |
| A 515 | THR | 50 | - | Favored (37.3%) General / -104.6,140.9 | 67.7% (<i>p</i>) chi angles: 59.6 | 0.019Å | - | - | |
| A 516 | LEU | 50 | 0.458Å HD11 with A 504 LEU HD11 | Favored (5.15%) | 48.7% (<i>tp</i>) chi angles: 183.1,66.1 | 0.026Å | - | - | |

| RDT | | | | General / -136.5,103.2 | | | | |
|----------|-----|----|---|---|--|--------|---|---|
| A 517 | ASP | 50 | - | Favored (38.45%) General / -115.8,120.2 | 21.4% (<i>m-20</i>) chi angles: 309.5,332.2 | 0.046Å | - | - |
| A 518 | TYR | 50 | - | Favored (38.18%) General / -119.5,151.7 | 49% (<i>p90</i>) chi angles: 67.7,273.2 | 0.038Å | - | - |
| A 519 | ARG | 50 | - | Favored (15.78%) General / -126.2,167.2 | 73.5% (<i>mtp180</i>) chi angles: 299.4,192.4,65.5,183.4 | 0.074Å | - | - |
| A 520 | TYR | 50 | - | Favored (48.21%) Pre-proline / -53.1,128.5 | 73.4% (<i>t80</i>) chi angles: 182,86.4 | 0.076Å | - | - |
| A 521 | PRO | 50 | - | Favored (8.21%) Cis-proline / -106.5,8.3 | 44.7% (<i>Cg_endo</i>) chi angles: 35.6 | 0.03Å | - | - |
| A 522 | LEU | 50 | - | Favored (38.26%) General / -76.1,147.8 | 77.5% (<i>mt</i>) chi angles: 295.7,182.1 | 0.025Å | - | - |
| A 523 | CYS | 50 | - | Favored (6.84%) General / -104.8,172.3 | 26.9% (<i>p</i>) chi angles: 66.9 | 0.043Å | - | - |
| A 524 | ALA | 50 | - | Favored (88.86%) General / -61.8,-38.6 | - | 0.011Å | - | - |
| A 525 | LEU | 50 | - | Favored (98.96%) General / -63.1,-43.2 | 42.8% (<i>tp</i>) chi angles: 182.5,56.1 | 0.074Å | - | - |
| A 526 | GLN | 50 | - | Favored (92.22%) General / -63.6,-45.0 | 89.1% (<i>mt-30</i>) chi angles: 290,173.4,305.5 | 0.052Å | - | - |
| A 527 | ALA | 50 | - | Favored (88.48%) General / -64.5,-45.1 | - | 0.048Å | - | - |
| A | PHE | 50 | - | Favored (90.37%) | 35.2% (<i>t80</i>) | 0.039Å | - | - |

| 528 | | | | General / -64.6,-44.5 | chi angles: 184.7,56.1 | | | | |
|----------|-----|-------|------------|--|--|-------------------------|--------------------|--------------------|--------------------|
| A 529 | ALA | 50 | - | Favored (81.59%) General / -68.3,-38.5 | - | 0.05Å | - | - | |
| A 530 | ILE | 50 | - | Favored (93.9%) Isoleucine or valine / -63.7,-41.8 | 95.2% (<i>mt</i>) chi angles: 297.7,169.1 | 0.036Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 54.27 | Clashscore: 9.86 | Outliers: 3 of 244 | Poor rotamers: 0 of 213 | Outliers: 1 of 229 | Outliers: 4 of 246 | Outliers: 1 of 246 |
| A 531 | ALA | 50 | - | Favored (92.44%) General / -65.2,-39.2 | - | 0.026Å | - | - | |
| A 532 | LEU | 50 | - | Favored (78.97%) General / -62.6,-35.3 | 60.9% (<i>mt</i>) chi angles: 287.8,178.8 | 0.054Å | - | - | |
| A 533 | SER | 50 | - | Favored (66.7%) General / -63.9,-21.9 | 52.4% (<i>p</i>) chi angles: 74.9 | 0.071Å | - | - | |
| A 534 | SER | 50 | - | Favored (45.77%) General / -78.5,-24.8 | 61.7% (<i>p</i>) chi angles: 71.4 | 0.104Å | - | - | |
| A 535 | PHE | 50 | - | Favored (33.91%) General / -71.2,159.8 | 97.6% (<i>m-85</i>) chi angles: 296.2,270.7 | 0.051Å | - | - | |
| A 536 | ASP | 99.99 | - | - | 24.3% (<i>p30</i>) chi angles: 54.4,24.9 | 0.085Å | - | - | |

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