



# Viewing TULP1\_sm\_291-536-FFX1FH\_reg-multi.table

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|                      |   |           |  |  |
|----------------------|---|-----------|--|--|
| All-Atom<br>Contacts | Clashscore, all atoms:  | 1.01      | 99 <sup>th</sup> percentile* (N=1784, all resolutions) |  |
|                      | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. |           |  |  |
| Protein<br>Geometry  | Poor rotamers   | 4         | 1.88%  | Goal: <1%  |
|                      | Ramachandran outliers   | 2         | 0.82%  | Goal: <0.05%                                     |
|                      | Ramachandran favored  | 229       | 93.85%   | Goal: >98%                                       |
|                      | MolProbity score^   | 1.41      |  | 97 <sup>th</sup> percentile* (N=27675, 0Å - 99Å) |
|                      | Cβ deviations >0.25Å  | 0         | 0.00%  | Goal: 0  |
|                      | Bad backbone bonds:   | 0 / 2017  | 0.00%  | Goal: 0%   |
|                      | Bad backbone angles:  | 11 / 2727 | 0.40%  | Goal: <0.1%                                      |

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

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

<sup>^</sup> 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: 1.01 | Outliers: 2 of 244                         | Poor rotamers: 4 of 213                               | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246 |
| A 291 | PRO | 50  | -          | -                | -  | 85% (Cg_exo)<br>chi angles: 331                       | 0.144Å             | -                  | -                   |
| A 292 | ARG | 50  | -          | -                | Favored (87.97%)<br>General / -59.9,-46.9  | 54.4% (ttm-85)<br>chi angles: 188.8,184.2,305.5,288.3 | 0.048Å             | -                  | -                   |
| A 293 | GLU | 50  | -          | -                | Favored (2.89%)<br>General / -59.5,-61.1   | 2.6% (tm-20)<br>chi angles: 156.4,279.5,330.8         | 0.134Å             | -                  | -                   |
| A 294 | PHE | 50  | -          | -                | Favored (55.31%)<br>General / -50.5,-49.5  | 73.7% (t80)<br>chi angles: 181.5,86.5                 | 0.09Å              | -                  | -                   |
| A 295 | VAL | 50  | -          | -                | Favored (43.36%)<br>Isoleucine or valine / | 26.7% (m)<br>chi angles: 301.8                        | 0.231Å             | -                  | -                   |

-63.2,-27.6

|          |     |    |   |   |   |        |   |   |
|----------|-----|----|---|---|---|--------|---|---|
| A<br>296 | LEU | 50 | - | Favored<br>(36.49%)<br>General /<br>-89.8,-13.5                 | 97.8% ( <i>mt</i> )<br>chi angles: 293.6,173.1                    | 0.082Å | - | - |
| A<br>297 | ARG | 50 | - | Favored<br>(41.8%)<br>Pre-proline /<br>-83.3,138.6              | 30.7% ( <i>mmm180</i> )<br>chi angles:<br>294,297.4,293.4,169.7   | 0.034Å | - | - |
| A<br>298 | PRO | 50 | - | Favored<br>(97.81%)<br>Trans-proline /<br>-59.7,145.6           | 98.4% ( <i>Cg_exo</i> )<br>chi angles: 329.4                      | 0.095Å | - | - |
| A<br>299 | ALA | 50 | - | Favored<br>(42.39%)<br>Pre-proline /<br>-55.8,147.4             | -   | 0.043Å | - | - |
| A<br>300 | PRO | 50 | - | Favored (91%)<br>Trans-proline /<br>-63.9,146.1                 | 49.4% ( <i>Cg_exo</i> )<br>chi angles: 326.6                      | 0.084Å | - | - |
| A<br>301 | GLN | 50 | - | Favored<br>(11.57%)<br>General /<br>-49.3,139.4                 | 6.1% ( <i>tp-100</i> )<br>chi angles:<br>184.1,61.6,272.9         | 0.062Å | - | - |
| A<br>302 | GLY | 50 | - | Favored<br>(29.18%)<br>Glycine / 65.7,6.4                       | -   | -      | - | - |
| A<br>303 | ARG | 50 | - | Favored<br>(10.9%)<br>General /<br>-108.9,166.3                 | 75.4% ( <i>mmt-85</i> )<br>chi angles:<br>295.2,293.6,168.8,279.7 | 0.041Å | - | - |
| A<br>304 | THR | 50 | - | Favored<br>(23.79%)<br>General /<br>-129.4,119.4                | 90.7% ( <i>m</i> )<br>chi angles: 302.3                           | 0.079Å | - | - |
| A<br>305 | VAL | 50 | - | Favored<br>(22.11%)<br>Isoleucine or<br>valine /<br>-91.4,110.1 | 59.5% ( <i>t</i> )<br>chi angles: 181                             | 0.043Å | - | - |
| A<br>306 | ARG | 50 | - | Favored<br>(44.45%)<br>General /<br>-97.0,129.7                 | 80% ( <i>mtt85</i> )<br>chi angles:<br>294.6,191.1,179.5,95.3     | 0.023Å | - | - |
| A<br>307 | CYS | 50 | - | Favored<br>(26.38%)<br>General /<br>-130.0,163.5                | 75.5% ( <i>m</i> )<br>chi angles: 298.7                           | 0.055Å | - | - |
| A        |     |    |   | Favored   | 20% ( <i>tpp85</i> )  |        |   |   |

| 308      | ARG     | 50         | -                                  | (46.31%)<br>General /<br>-120.9,125.0<br>Favored | chi angles:<br>186.9,64.1,71.4,84.6                           | 0.063Å             | -                  | -                                       |
|----------|---------|------------|------------------------------------|--|---|--------------------|--------------------|---|
| A<br>309 | LEU     | 50         | -                                  | (50.72%)<br>General /<br>-108.8,124.5<br>Favored | 7.7% ( <i>tt</i> )<br>chi angles: 193.4,157.2                 | 0.065Å             | -                  | -                                       |
| A<br>310 | THR     | 50         | -                                  | (25.79%)<br>General /<br>-121.9,160.0<br>Favored | 73.9% ( <i>p</i> )<br>chi angles: 60                          | 0.063Å             | -                  | -                                       |
| #        | Alt Res | High B     | Clash > 0.4Å                       | Ramachandran                                     | Rotamer   | Cβ deviation       | Bond lengths       | Bond angles                             |
|          |         | Avg: 54.27 | Clashscore: 1.01                   | Outliers: 2 of 244                               | Poor rotamers: 4 of 213                                       | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246                     |
| A<br>311 | ARG     | 50         | -                                  | (32.98%)<br>General /<br>-133.7,162.1<br>Favored | 40.4% ( <i>ptt180</i> )<br>chi angles: 61.9,183.1,180.9,186.1 | 0.043Å             | -                  | -                                       |
| A<br>312 | ASP     | 50         | -                                  | (41.67%)<br>General /<br>-61.4,129.5<br>Favored  | 33.7% ( <i>m-20</i> )<br>chi angles: 303.2,349.8              | 0.179Å             | -                  | OUTLIER(S)<br>worst is CA-CB-CG: 8.73 σ |
| A<br>313 | LYS     | 99.99      | -                                  | (25.89%)<br>General /<br>-54.8,143.3<br>Favored  | 64.7% ( <i>tttp</i> )<br>chi angles: 186,177.8,177.7,64.5     | 0.061Å             | -                  | -                                       |
| A<br>314 | LYS     | 99.99      | 0.455Å<br>HD2 with A<br>320 MET SD | (44.1%)<br>General /<br>-143.9,155.5<br>Favored  | 46.8% ( <i>mmtm</i> )<br>chi angles: 298.8,299.2,176.8,290.9  | 0.07Å              | -                  | -                                       |
| A<br>315 | GLY     | 99.99      | -                                  | (46.9%)<br>Glycine /<br>-84.7,-170.3<br>Favored  | -   | -                  | -                  | -                                       |
| A<br>316 | MET     | 99.99      | -                                  | (1.94%)<br>General /<br>-98.9,72.8<br>Allowed    | 18.5% ( <i>tpt</i> )<br>chi angles: 180.9,64.4,186.8          | 0.057Å             | -                  | -                                       |
| A<br>317 | ASP     | 99.99      | -                                  | (32.17%)<br>General /<br>-154.0,166.7<br>Favored | 28.7% ( <i>p-10</i> )<br>chi angles: 63.2,334.6               | 0.052Å             | -                  | -                                       |
| A<br>318 | ARG     | 99.99      | -                                  | (57.98%)<br>General /<br>-65.1,137.9<br>Favored  | 31.8% ( <i>ptt-85</i> )<br>chi angles: 57.5,184.4,176.2,267.5 | 0.043Å             | -                  | -                                       |
| A<br>319 | GLY     | 99.99      | -                                  | (2.96%)<br>Glycine /<br>Favored                  | -   | -                  | -                  | OUTLIER(S)<br>worst is C-N-CA: 5.292 σ  |

-176.9,-138.5

|          |     |    |                                    |   |   |        |   |   |
|----------|-----|----|------------------------------------|---|---|--------|---|---|
| A<br>320 | MET | 50 | 0.455Å<br>SD with A<br>314 LYS HD2 | Favored<br>(3.31%)<br>General /<br>-156.7,-170.4      | 2.4% ( <i>t</i> <sub>tm</sub> )<br>chi angles:<br>236.3,164.3,289 | 0.075Å | - | - |
| A<br>321 | TYR | 50 | -                                  | Favored<br>(19.65%)<br>Pre-proline /<br>-142.8,69.8   | 55% ( <i>m</i> -85)<br>chi angles: 307.6,274.6                    | 0.048Å | - | - |
| A<br>322 | PRO | 50 | -                                  | Favored<br>(23.32%)<br>Trans-proline /<br>-79.7,154.1 | 40% ( <i>Cg_endo</i> )<br>chi angles: 36.5                        | 0.06Å  | - | - |
| A<br>323 | SER | 50 | -                                  | Favored<br>(26.48%)<br>General /<br>-82.2,152.3       | 58.5% ( <i>m</i> )<br>chi angles: 290.9                           | 0.038Å | - | - |
| A<br>324 | TYR | 50 | -                                  | Favored<br>(51.87%)<br>General /<br>-126.1,141.6      | 86.5% ( <i>m</i> -85)<br>chi angles: 299,84.7                     | 0.092Å | - | - |
| A<br>325 | PHE | 50 | -                                  | Favored<br>(51.63%)<br>General /<br>-131.2,144.9      | 55.2% ( <i>m</i> -85)<br>chi angles: 307.6,274.6                  | 0.066Å | - | - |
| A<br>326 | LEU | 50 | -                                  | Favored<br>(44.86%)<br>General /<br>-127.2,127.7      | 20.9% ( <i>tp</i> )<br>chi angles: 191.3,70.6                     | 0.1Å   | - | - |
| A<br>327 | HIS | 50 | -                                  | Favored<br>(27.02%)<br>General /<br>-123.3,160.2      | 37.6% ( <i>m</i> -70)<br>chi angles: 300.3,250.4                  | 0.072Å | - | - |
| A<br>328 | LEU | 50 | -                                  | Favored<br>(55.81%)<br>General /<br>-68.4,140.4       | 70% ( <i>mt</i> )<br>chi angles: 290.7,179.8                      | 0.07Å  | - | - |
| A<br>329 | ASP | 50 | -                                  | Favored<br>(2.84%)<br>General /<br>-90.1,54.6         | 10.9% ( <i>t</i> <sub>0</sub> )<br>chi angles: 208.3,24.1         | 0.075Å | - | - |
| A<br>330 | THR | 50 | -                                  | Favored<br>(19.75%)<br>General /<br>-114.4,159.9      | 52% ( <i>p</i> )<br>chi angles: 55.9                              | 0.037Å | - | - |

| #     | Alt | Res | High<br>B   | Clash ><br>0.4Å | Ramachandran        | Rotamer   | Cβ<br>deviation | Bond<br>lengths | Bond<br>angles |
|-------|-----|-----|-------------|-----------------|---------------------|-----------|-----------------|-----------------|----------------|
| Avg:  |     |     | Clashscore: | Outliers: 2 of  | Poor rotamers: 4 of | Outliers: | Outliers:       | Outliers: 11    |                |
| 54.27 |     |     | 1.01        | 244             | 213                 | 0 of 229  | 0 of 246        | of 246          |                |

|          |     |    |                                   |   |   |        |   |   |
|----------|-----|----|-----------------------------------|---|---|--------|---|---|
| A<br>331 | GLU | 50 | -                                 | Favored<br>(47.27%)<br>General /<br>-49.4,-46.2                 | 14% ( <i>tm-20</i> )<br>chi angles:<br>179.7,281.2,332.3          | 0.114Å | - | - |
| A<br>332 | LYS | 50 | -                                 | Favored<br>(5.83%)<br>General /<br>-80.3,85.2                   | 46.7% ( <i>mmtm</i> )<br>chi angles:<br>299.2,293.2,175.4,292     | 0.053Å | - | - |
| A<br>333 | LYS | 50 | -                                 | Allowed<br>(1.92%)<br>General /<br>-74.7,70.9                   | 45.2% ( <i>mttp</i> )<br>chi angles:<br>298.9,163.9,190.3,63.7    | 0.036Å | - | - |
| A<br>334 | VAL | 50 | -                                 | Favored<br>(27.14%)<br>Isoleucine or<br>valine /<br>-61.7,134.3 | 8.1% ( <i>p</i> )<br>chi angles: 70.2                             | 0.12Å  | - | - |
| A<br>335 | PHE | 50 | -                                 | Favored<br>(50.02%)<br>General /<br>-70.9,145.8                 | 81.2% ( <i>t80</i> )<br>chi angles: 172.3,77.9                    | 0.053Å | - | - |
| A<br>336 | LEU | 50 | -                                 | Allowed<br>(1.04%)<br>General /<br>-120.8,-66.6                 | 86.1% ( <i>mt</i> )<br>chi angles: 300.1,179.9                    | 0.049Å | - | - |
| A<br>337 | LEU | 50 | -                                 | Favored<br>(42.62%)<br>General /<br>-142.9,153.0                | 88.2% ( <i>mt</i> )<br>chi angles: 292.8,168.9                    | 0.098Å | - | - |
| A<br>338 | ALA | 50 | -                                 | Favored<br>(52.53%)<br>General /<br>-132.0,149.0                | -   | 0.041Å | - | - |
| A<br>339 | GLY | 50 | 0.407Å<br>HA2 with A<br>351 LEU O | Favored<br>(21.93%)<br>Glycine /<br>-139.4,151.5                | -   | -      | - | - |
| A<br>340 | ARG | 50 | -                                 | Favored<br>(15.46%)<br>General /<br>-156.1,139.2                | 34.3% ( <i>ttt180</i> )<br>chi angles:<br>187.1,171.9,175.8,225.8 | 0.03Å  | - | - |
| A<br>341 | LYS | 50 | -                                 | Favored<br>(39.34%)<br>General /<br>-72.7,129.9                 | 86.4% ( <i>tttt</i> )<br>chi angles:<br>189.2,175.2,180.9,175.9   | 0.048Å | - | - |
| A<br>342 | ARG | 50 | -                                 | Favored<br>(29.35%)<br>General /<br>-78.5,125.4                 | 72.4% ( <i>mtp85</i> )<br>chi angles:<br>297.4,176.1,57.6,77.8    | 0.1Å   | - | - |

| A<br>343 | LYS     | 50         | -                                      | Favored<br>(71.14%)<br>General /<br>-70.6,-33.6                  | 87.2% ( <i>tttt</i> )<br>chi angles:<br>180.8,174.3,182.4,182.4  | 0.086Å             | -                  | -                   |
|----------|---------|------------|--|--|--|--------------------|--------------------|---------------------|
| A<br>344 | ARG     | 50         | -                                      | Allowed<br>(1.09%)<br>General /<br>-95.0,44.3                    | 83.8% ( <i>mtp180</i> )<br>chi angles:<br>291.4,181.1,65.1,185.3 | 0.058Å             | -                  | -                   |
| A<br>345 | SER     | 50         | -                                      | Favored (46%)<br>General /<br>-122.9,148.0                       | 34.1% ( <i>t</i> )<br>chi angles: 183.2                          | 0.073Å             | -                  | -                   |
| A<br>346 | LYS     | 50         | -                                      | Favored<br>(70.64%)<br>General /<br>-71.5,-35.1                  | 26.9% ( <i>tptp</i> )<br>chi angles:<br>183.8,65.6,187.4,65.6    | 0.037Å             | -                  | -                   |
| A<br>347 | THR     | 50         | -                                      | Favored<br>(11.73%)<br>General /<br>-115.9,166.7                 | 80.5% ( <i>p</i> )<br>chi angles: 61.4                           | 0.049Å             | -                  | -                   |
| A<br>348 | ALA     | 50         | -                                      | Favored<br>(49.75%)<br>General /<br>-60.4,131.1                  | -  | 0.014Å             | -                  | -                   |
| A<br>349 | ASN     | 50         | -                                      | Favored<br>(2.84%)<br>General /<br>-150.4,100.1                  | 58.4% ( <i>t-20</i> )<br>chi angles: 185.3,339.7                 | 0.111Å             | -                  | -                   |
| A<br>350 | TYR     | 50         | -                                      | Favored<br>(33.9%)<br>General /<br>-95.1,137.7                   | 22.2% ( <i>m-85</i> )<br>chi angles: 294.7,69.9                  | 0.081Å             | -                  | -                   |
| #        | Alt Res | High<br>B  | Clash ><br>0.4Å                        | Ramachandran   | Rotamer  | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles      |
|          |         | Avg: 54.27 | Clashscore: 1.01                       | Outliers: 2 of 244   | Poor rotamers: 4 of 213  | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246 |
| A<br>351 | LEU     | 50         | 0.423Å<br>CD2 with A<br>361 ARG<br>HD2 | Favored<br>(43.49%)<br>General /<br>-101.0,134.8                 | 66.3% ( <i>mt</i> )<br>chi angles: 303.2,183.6                   | 0.052Å             | -                  | -                   |
| A<br>352 | ILE     | 50         | -                                      | Favored<br>(72.93%)<br>Isoleucine or<br>valine /<br>-117.5,130.1 | 64.7% ( <i>mt</i> )<br>chi angles: 305,171.4                     | 0.077Å             | -                  | -                   |
| A<br>353 | SER     | 50         | -                                      | Favored<br>(46.55%)<br>General /<br>-128.5,154.0                 | 41% ( <i>t</i> )<br>chi angles: 177.2                            | 0.128Å             | -                  | -                   |

|          |     |       |  |   |   |        |   |   |
|----------|-----|-------|--|---|---|--------|---|---|
| A<br>354 | ILE | 50    | -                                      | Favored<br>(9.04%)<br>Isoleucine or<br>valine / -97.0,5.2 | 43.5% ( <i>pt</i> )<br>chi angles: 57.1,171.6               | 0.179Å | - | -   |
| A<br>355 | ASP | 50    | -                                      | Favored<br>(29.67%)<br>Pre-proline /<br>-118.3,123.0      | 58.6% ( <i>t0</i> )<br>chi angles: 177.6,352.6              | 0.109Å | - | OUTLIER(S)<br>worst is CA-<br>CB-CG: 4.188<br>σ |
| A<br>356 | PRO | 50    | -                                      | Favored<br>(17.48%)<br>Trans-proline /<br>-76.3,-16.3     | 41.2% ( <i>Cg_endo</i> )<br>chi angles: 36.3                | 0.053Å | - | -   |
| A<br>357 | THR | 50    | -                                      | Favored<br>(25.5%)<br>General /<br>-90.4,-18.4            | 91.8% ( <i>m</i> )<br>chi angles: 302.5                     | 0.123Å | - | -   |
| A<br>358 | ASN | 99.99 | -                                      | Favored<br>(48.33%)<br>General /<br>-101.5,127.2          | 50.9% ( <i>t30</i> )<br>chi angles: 187.3,15.1              | 0.043Å | - | -   |
| A<br>359 | LEU | 99.99 | -                                      | Favored<br>(15.53%)<br>General /<br>-98.8,-23.1           | 91.7% ( <i>mt</i> )<br>chi angles: 297.4,172.1              | 0.058Å | - | -   |
| A<br>360 | SER | 99.99 | -                                      | Favored<br>(48.01%)<br>General /<br>-63.7,148.8           | 27.5% ( <i>t</i> )<br>chi angles: 185.4                     | 0.017Å | - | -   |
| A<br>361 | ARG | 99.99 | 0.423Å<br>HD2 with A<br>351 LEU<br>CD2 | Allowed<br>(0.86%)<br>General /<br>-119.7,70.4            | 9% ( <i>ptm-85</i> )<br>chi angles:<br>60.7,173,293.1,281.3 | 0.125Å | - | -   |
| A<br>362 | GLY | 99.99 | -                                      | Favored<br>(42.45%)<br>Glycine /<br>-172.7,-178.0         | -   | -      | - | -   |
| A<br>363 | GLY | 99.99 | -                                      | Favored<br>(29.09%)<br>Glycine /<br>55.4,-123.2           | -   | -      | - | OUTLIER(S)<br>worst is C-N-<br>CA: 5.955 σ      |
| A<br>364 | GLU | 99.99 | -                                      | Favored<br>(87.96%)<br>General /<br>-60.6,-39.4           | 2.1% ( <i>pm0</i> )<br>chi angles:<br>60.1,305.2,330.3      | 0.139Å | - | OUTLIER(S)<br>worst is CB-<br>CG-CD:<br>5.637 σ |
| A<br>365 | ASN | 50    | -                                      | Favored<br>(2.39%)<br>General /<br>-139.0,6.5             | 72.7% ( <i>m-80</i> )<br>chi angles: 291.2,298.6            | 0.159Å | - | -   |

Favored

|          |     |    |   |   |  |        |   |   |
|----------|-----|----|---|---|--|--------|---|---|
| A<br>366 | PHE | 50 | - | (49.58%)<br>General /<br>-64.2,132.2                            | 12% ( <i>t80</i> )<br>chi angles: 181.6,39.1                   | 0.096Å | - | - |
| A<br>367 | ILE | 50 | - | Allowed<br>(1.23%)<br>Isoleucine or<br>valine /<br>-128.1,-26.0 | 7.1% ( <i>tp</i> )<br>chi angles: 204.1,69.7                   | 0.164Å | - | - |
| A<br>368 | GLY | 50 | - | Favored<br>(45.99%)<br>Glycine /<br>-173.0,175.2                | -  | -      | - | - |
| A<br>369 | LYS | 50 | - | Favored<br>(29.57%)<br>General /<br>-145.4,142.7                | 34.2% ( <i>ttpt</i> )<br>chi angles:<br>171.2,165.8,56.9,183.6 | 0.084Å | - | - |
| A<br>370 | LEU | 50 | - | Favored<br>(36.06%)<br>General /<br>-111.7,118.6                | 28.8% ( <i>tp</i> )<br>chi angles: 175.6,72.6                  | 0.094Å | - | - |

| #        | Alt | Res | High<br>B  | Clash ><br>0.4Å  | Ramachandran                                     | Rotamer  | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles      |
|----------|-----|-----|------------|------------------|--|--|--------------------|--------------------|---------------------|
|          |     |     | Avg: 54.27 | Clashscore: 1.01 | Outliers: 2 of 244                               | Poor rotamers: 4 of 213  | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246 |
| A<br>371 | ARG | 50  | -          |                  | Favored<br>(36.46%)<br>General /<br>-124.6,122.0 | 30.1% ( <i>ttp180</i> )<br>chi angles:<br>175.8,208.9,62,182.3 | 0.115Å             | -                  | -                   |
| A<br>372 | SER | 50  | -          |                  | Favored<br>(25.22%)<br>General /<br>-79.8,162.3  | 59.9% ( <i>p</i> )<br>chi angles: 72.6                         | 0.084Å             | -                  | -                   |
| A<br>373 | ASN | 50  | -          |                  | Favored<br>(2.99%)<br>General /<br>-72.2,-179.7  | 35.5% ( <i>p-10</i> )<br>chi angles: 65.6,335.5                | 0.073Å             | -                  | -                   |
| A<br>374 | LEU | 50  | -          |                  | Favored<br>(86.78%)<br>General /<br>-65.0,-37.2  | 48% ( <i>tp</i> )<br>chi angles: 184.8,63.3                    | 0.141Å             | -                  | -                   |
| A<br>375 | LEU | 50  | -          |                  | Favored<br>(62.8%)<br>General /<br>-72.4,-28.2   | 74.5% ( <i>mt</i> )<br>chi angles: 301.4,172.4                 | 0.086Å             | -                  | -                   |
| A<br>376 | GLY | 50  | -          |                  | Favored<br>(67.95%)<br>Glycine / 91.9,3.6        | -  | -                  | -                  | -                   |

Favored



|          |     |    |   |  |   |        |   |   |
|----------|-----|----|---|--|---|--------|---|---|
| A<br>377 | ASN | 50 | - | (19.71%)<br>General /<br>-98.9,-14.1                             | 31.7% ( <i>p</i> -10)<br>chi angles: 66,331.9                   | 0.093Å | - | - |
| A<br>378 | ARG | 50 | - | Favored<br>(49.16%)<br>General /<br>-123.5,145.0                 | 90.4% ( <i>mtt</i> 180)<br>chi angles:<br>297.9,187,177.2,198.3 | 0.03Å  | - | - |
| A<br>379 | PHE | 50 | - | Favored<br>(52.39%)<br>General /<br>-132.5,148.8                 | 77.7% ( <i>m</i> -85)<br>chi angles: 296.9,80.7                 | 0.089Å | - | - |
| A<br>380 | THR | 50 | - | Favored<br>(49.67%)<br>General /<br>-117.7,140.4                 | 7.2% ( <i>m</i> )<br>chi angles: 314.8                          | 0.079Å | - | - |
| A<br>381 | VAL | 50 | - | Favored<br>(62.88%)<br>Isoleucine or<br>valine /<br>-106.9,126.1 | 38.8% ( <i>t</i> )<br>chi angles: 185.3                         | 0.07Å  | - | - |
| A<br>382 | PHE | 50 | - | Favored<br>(20.45%)<br>General /<br>-114.0,159.0                 | 86.5% ( <i>m</i> -85)<br>chi angles: 302.5,281.7                | 0.103Å | - | - |
| A<br>383 | ASP | 50 | - | OUTLIER<br>(0.04%)<br>General /<br>-74.4,-154.1                  | 49.8% ( <i>p</i> -10)<br>chi angles: 66.3,353.3                 | 0.187Å | - | - |
| A<br>384 | ASN | 50 | - | Favored<br>(51.04%)<br>General /<br>-95.6,-1.1                   | 43.3% ( <i>p</i> -10)<br>chi angles: 57.9,354.3                 | 0.125Å | - | - |
| A<br>385 | GLY | 50 | - | Favored<br>(21.77%)<br>Glycine /<br>-66.3,174.7                  | -   | -      | - | - |
| A<br>386 | GLN | 50 | - | Favored<br>(34.49%)<br>General /<br>-79.3,144.2                  | 14.5% ( <i>tt</i> 0)<br>chi angles:<br>192.8,191.7,113.2        | 0.037Å | - | - |
| A<br>387 | ASN | 50 | - | Favored<br>(89.21%)<br>Pre-proline /<br>-74.2,123.5              | 35.1% ( <i>t</i> 30)<br>chi angles: 177.9,36.9                  | 0.085Å | - | - |
| A<br>388 | PRO | 50 | - | Favored<br>(93.52%)<br>Trans-proline /<br>-59.0,-30.5            | 53.1% ( <i>Cg</i> _exo)<br>chi angles: 334.8                    | 0.08Å  | - | - |
|          |     |    |   | Favored  | 98.1% ( <i>mt</i> -30)  |        |   |   |

| A<br>389 | GLN     | 50         | -                | (25.56%)<br>General /<br>-69.0,-6.0                             | chi angles:<br>295.6,179.2,329                                 | 0.059Å             | -                  | -                   |
|----------|---------|------------|------------------|---|--|--------------------|--------------------|---------------------|
| A<br>390 | ARG     | 50         | -                | Favored<br>(23.9%)<br>General /<br>-91.6,-18.5                  | 42.4% ( <i>tpt85</i> )<br>chi angles:<br>187.2,61.3,195.3,82.2 | 0.127Å             | -                  | -                   |
| #        | Alt Res | High<br>B  | Clash ><br>0.4Å  | Ramachandran  | Rotamer  | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles      |
|          |         | Avg: 54.27 | Clashscore: 1.01 | Outliers: 2 of 244  | Poor rotamers: 4 of 213  | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246 |
| A<br>391 | GLY     | 50         | -                | Allowed<br>(0.11%)<br>Glycine /<br>-176.2,96.7                  | -  | -                  | -                  | -                   |
| A<br>392 | TYR     | 50         | -                | Favored<br>(69.55%)<br>General /<br>-66.1,-29.3                 | 31.9% ( <i>t80</i> )<br>chi angles: 191.6,61.3                 | 0.133Å             | -                  | -                   |
| A<br>393 | SER     | 50         | -                | Favored<br>(55.34%)<br>General /<br>-74.1,-8.2                  | 6.4% ( <i>m</i> )<br>chi angles: 313.3                         | 0.053Å             | -                  | -                   |
| A<br>394 | THR     | 50         | -                | Favored<br>(57.78%)<br>General /<br>-61.5,135.7                 | 90.9% ( <i>m</i> )<br>chi angles: 300.6                        | 0.049Å             | -                  | -                   |
| A<br>395 | ASN     | 50         | -                | Favored<br>(5.28%)<br>General /<br>-46.8,139.6                  | 45.8% ( <i>t30</i> )<br>chi angles: 182,10.7                   | 0.049Å             | -                  | -                   |
| A<br>396 | VAL     | 50         | -                | Favored<br>(87.25%)<br>Isoleucine or<br>valine /<br>-59.8,-41.9 | 53% ( <i>t</i> )<br>chi angles: 182.2                          | 0.09Å              | -                  | -                   |
| A<br>397 | ALA     | 50         | -                | Favored<br>(67.71%)<br>General /<br>-58.6,-31.0                 | -  | 0.073Å             | -                  | -                   |
| A<br>398 | SER     | 50         | -                | Favored<br>(52.56%)<br>General /<br>-83.6,-14.2                 | 22.4% ( <i>m</i> )<br>chi angles: 305.1                        | 0.059Å             | -                  | -                   |
| A<br>399 | LEU     | 50         | -                | Favored<br>(47.87%)<br>General /<br>-71.6,137.3                 | 85.9% ( <i>mt</i> )<br>chi angles: 300.8,179.5                 | 0.058Å             | -                  | -                   |

|          |     |    |   |  |  |        |   |   |
|----------|-----|----|---|--|--|--------|---|---|
| A<br>400 | ARG | 50 | - | Favored<br>(41.95%)<br>General /<br>-57.3,142.8                  | 36.5% ( <i>ptt180</i> )<br>chi angles:<br>64.9,190.4,190.5,178.9 | 0.063Å | - | - |
| A<br>401 | GLN | 50 | - | Favored<br>(16.44%)<br>General /<br>-102.7,158.2                 | 5.7% ( <i>pt20</i> )<br>chi angles:<br>77.5,193.2,260.3          | 0.063Å | - | - |
| A<br>402 | GLU | 50 | - | Favored<br>(31.75%)<br>General /<br>-102.3,116.0                 | 52.2% ( <i>mt-10</i> )<br>chi angles:<br>292.5,202.6,357.9       | 0.035Å | - | - |
| A<br>403 | LEU | 50 | - | Favored<br>(16.71%)<br>General /<br>-94.3,-26.1                  | 70.8% ( <i>mt</i> )<br>chi angles: 301.1,171.4                   | 0.054Å | - | - |
| A<br>404 | ALA | 50 | - | Favored<br>(9.68%)<br>General /<br>-167.9,157.1                  | -  | 0.043Å | - | - |
| A<br>405 | ALA | 50 | - | Favored<br>(46.87%)<br>General /<br>-134.6,142.3                 | -  | 0.057Å | - | - |
| A<br>406 | VAL | 50 | - | Favored<br>(72.59%)<br>Isoleucine or<br>valine /<br>-125.6,130.9 | 34.1% ( <i>t</i> )<br>chi angles: 185.8                          | 0.047Å | - | - |
| A<br>407 | ILE | 50 | - | Favored (63%)<br>Isoleucine or<br>valine /<br>-119.7,120.3       | 5.4% ( <i>mp</i> )<br>chi angles: 302.4,90.3                     | 0.038Å | - | - |
| A<br>408 | TYR | 50 | - | Favored<br>(42.95%)<br>General /<br>-102.1,135.8                 | 85.5% ( <i>m-85</i> )<br>chi angles: 289.7,274.8                 | 0.095Å | - | - |
| A<br>409 | GLU | 50 | - | Favored<br>(41.13%)<br>General /<br>-75.2,146.4                  | 67.4% ( <i>mt-10</i> )<br>chi angles:<br>287.3,177.6,26.7        | 0.065Å | - | - |
| A<br>410 | THR | 50 | - | Favored<br>(43.66%)<br>General /<br>-97.7,132.1                  | 69.6% ( <i>p</i> )<br>chi angles: 59.2                           | 0.038Å | - | - |

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

|       |             |                |                     |           |           |              |
|-------|-------------|----------------|---------------------|-----------|-----------|--------------|
| Avg:  | Clashscore: | Outliers: 2 of | Poor rotamers: 4 of | Outliers: | Outliers: | Outliers: 11 |
| 54.27 | 1.01        | 244            | 213                 | 0 of 229  | 0 of 246  | of 246       |

|          |           |   |  |   |        |   |   |
|----------|-----------|---|--|---|--------|---|---|
| A<br>411 | ASN 50    | - | Favored<br>(18.23%)<br>General /<br>-86.5,162.1                  | 60.4% ( <i>m-20</i> )<br>chi angles: 305.7,324.3                  | 0.038Å | - | - |
| A<br>412 | VAL 99.99 | - | Favored<br>(37.26%)<br>Isoleucine or<br>valine /<br>-136.0,156.5 | 12.9% ( <i>p</i> )<br>chi angles: 65.4                            | 0.097Å | - | - |
| A<br>413 | LEU 99.99 | - | Favored<br>(32.58%)<br>General /<br>-52.5,136.3                  | 9.9% ( <i>tt</i> )<br>chi angles: 186.8,155                       | 0.058Å | - | - |
| A<br>414 | GLY 99.99 | - | Favored<br>(52.57%)<br>Glycine /<br>93.4,-19.4                   | -   | -      | - | - |
| A<br>415 | PHE 99.99 | - | Favored<br>(43.1%)<br>General /<br>-110.9,142.3                  | 80.5% ( <i>t80</i> )<br>chi angles: 184.2,76.7                    | 0.088Å | - | - |
| A<br>416 | ARG 99.99 | - | Favored<br>(21.94%)<br>General /<br>-85.9,153.9                  | 99.8% ( <i>mtt180</i> )<br>chi angles:<br>295.1,180,179.3,180     | 0.085Å | - | - |
| A<br>417 | GLY 99.99 | - | Allowed<br>(0.21%)<br>Glycine /<br>-176.6,106.1                  | -   | -      | - | - |
| A<br>418 | PRO 50    | - | Allowed<br>(0.17%)<br>Trans-proline /<br>-39.3,113.3             | 56.9% ( <i>Cg_endo</i> )<br>chi angles: 26.1                      | 0.045Å | - | - |
| A<br>419 | ARG 50    | - | Favored<br>(53.38%)<br>General /<br>-69.5,143.5                  | 90.3% ( <i>mtm180</i> )<br>chi angles:<br>291.1,177.6,296.4,173.4 | 0.067Å | - | - |
| A<br>420 | ARG 50    | - | Favored<br>(53.56%)<br>General /<br>-69.7,140.3                  | 98.2% ( <i>mtt180</i> )<br>chi angles:<br>296,183.3,187.8,169     | 0.045Å | - | - |
| A<br>421 | MET 50    | - | Favored<br>(54.62%)<br>General /<br>-121.9,137.9                 | 87.6% ( <i>mtp</i> )<br>chi angles:<br>300.1,176.6,62.9           | 0.11Å  | - | - |
| A<br>422 | THR 50    | - | Favored<br>(55.18%)<br>General /<br>-113.4,133.4                 | 70.9% ( <i>m</i> )<br>chi angles: 296.7                           | 0.04Å  | - | - |

|          |     |     |               |  |  |                            |                    |                    |                        |
|----------|-----|-----|---------------|--|--|----------------------------|--------------------|--------------------|------------------------|
| A<br>423 | VAL | 50  | -             | Favored<br>(75.19%)<br>Isoleucine or<br>valine /<br>-122.2,127.2 | 95.9% ( <i>t</i> )<br>chi angles: 176.7                  | 0.062Å                     | -                  | -                  |                        |
| A<br>424 | ILE | 50  | -             | Favored<br>(72.52%)<br>Isoleucine or<br>valine /<br>-117.6,130.4 | 45% ( <i>mm</i> )<br>chi angles: 305.2,303.5             | 0.075Å                     | -                  | -                  |                        |
| A<br>425 | ILE | 50  | -             | Favored<br>(27.11%)<br>Pre-proline /<br>-128.7,166.1             | 35.5% ( <i>pt</i> )<br>chi angles: 58.1,176.9            | 0.084Å                     | -                  | -                  |                        |
| A<br>426 | PRO | 50  | -             | Favored<br>(89.13%)<br>Trans-proline /<br>-64.2,145.5            | 72.8% ( <i>Cg_exo</i> )<br>chi angles: 328               | 0.102Å                     | -                  | -                  |                        |
| A<br>427 | GLY | 50  | -             | Favored<br>(16.56%)<br>Glycine /<br>-61.3,165.5                  | -  | -                          | -                  | -                  |                        |
| A<br>428 | MET | 50  | -             | Favored<br>(41.38%)<br>General /<br>-117.5,148.9                 | 84.2% ( <i>mmm</i> )<br>chi angles:<br>307.9,303.7,285.8 | 0.097Å                     | -                  | -                  |                        |
| A<br>429 | SER | 50  | -             | Favored<br>(9.36%)<br>General /<br>-79.5,176.8                   | 27.4% ( <i>p</i> )<br>chi angles: 51.7                   | 0.057Å                     | -                  | -                  |                        |
| A<br>430 | ALA | 50  | -             | Favored<br>(67.3%)<br>General /<br>-67.5,-27.8                   | -  | 0.09Å                      | -                  | -                  |                        |
| #        | Alt | Res | High<br>B     | Clash ><br>0.4Å  | Ramachandran   | Rotamer                    | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles         |
|          |     |     | Avg:<br>54.27 | Clashscore:<br>1.01  | Outliers: 2 of<br>244                                    | Poor rotamers: 4 of<br>213 | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11<br>of 246 |
| A<br>431 | GLU | 50  | -             | Favored<br>(70.27%)<br>General /<br>-57.2,-36.0                  | 84.6% ( <i>tt0</i> )<br>chi angles:<br>182.1,184.9,2.4   | 0.05Å                      | -                  | -                  |                        |
| A<br>432 | ASN | 50  | -             | OUTLIER<br>(0.01%)<br>General /<br>93.2,25.5                     | 70.3% ( <i>m-80</i> )<br>chi angles: 296.2,287.6         | 0.204Å                     | -                  | -                  |                        |
| A<br>433 | GLU | 50  | -             | Favored<br>(15.74%)<br>General /                                 | 30.4% ( <i>tp10</i> )<br>chi angles:<br>188.9,51.4,29.6  | 0.058Å                     | -                  | -                  |                        |

-109.5,161.0

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|----------|-----|----|---|--|---|--------|---|---|
| A<br>434 | ARG | 50 | - | Favored<br>(57.15%)<br>General /<br>-66.2,143.6                  | 74% ( <i>mtm-85</i> )<br>chi angles:<br>278.8,187.2,299.7,289.8   | 0.094Å | - | - |
| A<br>435 | VAL | 50 | - | Allowed<br>(0.84%)<br>Pre-proline /<br>-91.7,95.1                | 61.4% ( <i>t</i> )<br>chi angles: 181.3                           | 0.105Å | - | - |
| A<br>436 | PRO | 50 | - | Favored<br>(71.83%)<br>Trans-proline /<br>-59.4,136.4            | 78.5% ( <i>Cg_exo</i> )<br>chi angles: 333.5                      | 0.079Å | - | - |
| A<br>437 | ILE | 50 | - | Favored<br>(31.94%)<br>Isoleucine or<br>valine /<br>-106.8,110.5 | 97.4% ( <i>mt</i> )<br>chi angles: 293.4,167.9                    | 0.072Å | - | - |
| A<br>438 | ARG | 50 | - | Favored<br>(75.29%)<br>Pre-proline /<br>-127.8,78.3              | 33.9% ( <i>ttm-85</i> )<br>chi angles:<br>199.4,177.7,302.9,256.3 | 0.135Å | - | - |
| A<br>439 | PRO | 50 | - | Favored<br>(94.75%)<br>Trans-proline /<br>-57.3,141.8            | 95.7% ( <i>Cg_exo</i> )<br>chi angles: 329.7                      | 0.09Å  | - | - |
| A<br>440 | ARG | 50 | - | Favored<br>(27.77%)<br>General /<br>-86.0,-21.4                  | 85.3% ( <i>mtp180</i> )<br>chi angles:<br>293.6,177.4,64.8,187    | 0.084Å | - | - |
| A<br>441 | ASN | 50 | - | Favored<br>(5.17%)<br>General /<br>-147.7,-176.2                 | 55.1% ( <i>t30</i> )<br>chi angles: 184.1,33                      | 0.124Å | - | - |
| A<br>442 | ALA | 50 | - | Favored<br>(4.12%)<br>General /<br>-86.6,17.1                    | -   | 0.024Å | - | - |
| A<br>443 | SER | 50 | - | Favored<br>(57.41%)<br>General /<br>-91.6,-1.6                   | 72.8% ( <i>p</i> )<br>chi angles: 57.9                            | 0.152Å | - | - |
| A<br>444 | ASP | 50 | - | Favored<br>(20.68%)<br>General /<br>-134.5,167.5                 | 41.3% ( <i>t0</i> )<br>chi angles: 187.6,26                       | 0.082Å | - | - |
| A<br>445 | GLY | 50 | - | Favored<br>(12.01%)<br>Glycine /                                 | -   | -      | - | - |

138.4,171.0

|          |     |    |   |   |   |        |   |  |
|----------|-----|----|---|---|---|--------|---|--|
| A<br>446 | LEU | 50 | - | Favored<br>(88.46%)<br>General /<br>-58.3,-44.3                 | 95.1% ( <i>mt</i> )<br>chi angles: 293.3,171.4                    | 0.074Å | - | -  |
| A<br>447 | LEU | 50 | - | Favored<br>(69.31%)<br>General /<br>-69.2,-31.0                 | 90.7% ( <i>mt</i> )<br>chi angles: 294.2,170.6                    | 0.127Å | - | -  |
| A<br>448 | VAL | 50 | - | Favored<br>(50.21%)<br>Isoleucine or<br>valine /<br>-68.7,-51.0 | 77.7% ( <i>t</i> )<br>chi angles: 172.7                           | 0.075Å | - | -  |
| A<br>449 | ARG | 50 | - | Favored<br>(73.71%)<br>General /<br>-66.1,-32.3                 | 96.3% ( <i>mtt180</i> )<br>chi angles:<br>298.4,178.6,192.3,183.1 | 0.052Å | - | -  |
| A<br>450 | TRP | 50 | - | Favored<br>(99.15%)<br>General /<br>-63.3,-42.7                 | 52.4% ( <i>t-105</i> )<br>chi angles: 167.6,255.7                 | 0.128Å | - | OUTLIER(S)<br>worst is CE3-<br>CD2-CG:<br>5.015 $\sigma$ |

| #        | Alt | Res | High<br>B  | Clash ><br>0.4Å  | Ramachandran                                    | Rotamer   | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles                             |
|----------|-----|-----|------------|------------------|---|---|--------------------|--------------------|--|
|          |     |     | Avg: 54.27 | Clashscore: 1.01 | Outliers: 2 of 244                              | Poor rotamers: 4 of 213                                       | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246                        |
| A<br>451 |     | GLN | 50         | -                | Favored<br>(38.07%)<br>General /<br>-80.6,-26.1 | 46.8% ( <i>tp60</i> )<br>chi angles:<br>185.8,58,73.4         | 0.117Å             | -                  | -  |
| A<br>452 |     | ASN | 50         | -                | Favored<br>(52.28%)<br>General /<br>-82.0,-15.8 | 48% ( <i>m-20</i> )<br>chi angles: 300.9,351.3                | 0.092Å             | -                  | -  |
| A<br>453 |     | LYS | 50         | -                | Favored<br>(5.95%)<br>General /<br>67.1,32.9    | 32.4% ( <i>mmmt</i> )<br>chi angles:<br>294.1,295.6,291.9,178 | 0.16Å              | -                  | -  |
| A<br>454 |     | THR | 50         | -                | Allowed<br>(1.81%)<br>General /<br>-102.5,79.3  | 80.3% ( <i>p</i> )<br>chi angles: 61.5                        | 0.094Å             | -                  | -  |
| A<br>455 |     | LEU | 50         | -                | Favored<br>(47.25%)<br>General /<br>-99.0,5.0   | 59.1% ( <i>mt</i> )<br>chi angles: 306.6,180.5                | 0.061Å             | -                  | OUTLIER(S)<br>worst is C-N-<br>CA: 4.132 σ |
| A<br>456 |     | GLU | 50         | -                | Favored<br>(77.92%)<br>General /                | 55.2% ( <i>mp0</i> )<br>chi angles:<br>300.3,78.2,2.5         | 0.038Å             | -                  | OUTLIER(S)<br>worst is CB-<br>CG-CD:       |

|          |     |    |                                      |  |   |        |   |   |
|----------|-----|----|--------------------------------------|--|---|--------|---|---|
|          |     |    |                                      | -56.9,-48.5  |   |        |   |   |
| A<br>457 | SER | 50 | -                                    | Favored<br>(3.63%)<br>General /<br>-86.6,17.9                    | 74.9% ( <i>p</i> )<br>chi angles: 58.2                          | 0.092Å | - | - |
| A<br>458 | LEU | 50 | -                                    | Favored<br>(21.51%)<br>General /<br>-128.6,165.1                 | 30% ( <i>mt</i> )<br>chi angles: 307.2,187.7                    | 0.076Å | - | - |
| A<br>459 | ILE | 50 | -                                    | Favored<br>(75.38%)<br>Isoleucine or<br>valine /<br>-122.9,129.0 | 96.7% ( <i>mt</i> )<br>chi angles: 297.3,169.7                  | 0.057Å | - | - |
| A<br>460 | GLU | 50 | -                                    | Favored<br>(48.99%)<br>General /<br>-102.7,132.2                 | 65.2% ( <i>tt0</i> )<br>chi angles:<br>181.8,175.5,333.4        | 0.068Å | - | - |
| A<br>461 | LEU | 50 | -                                    | Favored<br>(47.04%)<br>General /<br>-135.8,157.4                 | 55.5% ( <i>mt</i> )<br>chi angles: 305.4,173.1                  | 0.09Å  | - | - |
| A<br>462 | HIS | 50 | -                                    | Favored<br>(21.78%)<br>General /<br>-136.7,167.2                 | 96% ( <i>m-70</i> )<br>chi angles: 298.2,276.9                  | 0.013Å | - | - |
| A<br>463 | ASN | 50 | -                                    | Favored<br>(51.88%)<br>General /<br>-70.4,143.2                  | 5.7% ( <i>p-10</i> )<br>chi angles: 72.1,281.9                  | 0.083Å | - | - |
| A<br>464 | LYS | 50 | 0.42Å<br>NZ with A<br>500 ASP<br>OD1 | Favored<br>(83.48%)<br>Pre-proline /<br>-72.0,134.2              | 79.8% ( <i>tttt</i> )<br>chi angles:<br>190.1,166.3,177.8,173.5 | 0.038Å | - | - |
| A<br>465 | PRO | 50 | -                                    | Favored<br>(37.58%)<br>Trans-proline /<br>-67.4,135.8            | 34.7% ( <i>Cg_exo</i> )<br>chi angles: 325.5                    | 0.101Å | - | - |
| A<br>466 | PRO | 50 | -                                    | Favored<br>(89.87%)<br>Trans-proline /<br>-62.9,149.9            | 33.1% ( <i>Cg_exo</i> )<br>chi angles: 325.4                    | 0.061Å | - | - |
| A<br>467 | VAL | 50 | -                                    | Favored<br>(15.91%)<br>Isoleucine or<br>valine /<br>-117.9,162.4 | 34.9% ( <i>m</i> )<br>chi angles: 298.4                         | 0.069Å | - | - |



|          |     |    |   |   |   |        |   |  |
|----------|-----|----|---|---|---|--------|---|--|
| A<br>468 | TRP | 50 | - | Favored<br>(35.71%)<br>General /<br>-72.8,128.5 | 71% ( <i>t</i> -105)<br>chi angles: 183.5,245.7 | 0.028Å | - | OUTLIER(S)<br>worst is CE3-<br>CD2-CG:<br>4.295 $\sigma$ |
| A<br>469 | ASN | 50 | - | Favored<br>(7.62%)<br>General /<br>-112.3,98.9  | 1%<br>chi angles: 199,105.2                     | 0.031Å | - | -  |
| A<br>470 | ASP | 50 | - | Favored<br>(95.41%)<br>General /<br>-62.4,-40.1 | 0.5%<br>chi angles: 232.6,338.1                 | 0.128Å | - | -  |

| #        | Alt | Res | High<br>B  | Clash ><br>0.4Å                                  | Ramachandran                                     | Rotamer                 | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles      |
|----------|-----|-----|------------|--|--|-------------------------|--------------------|--------------------|---------------------|
|          |     |     | Avg: 54.27 | Clashscore: 1.01                                 | Outliers: 2 of 244                               | Poor rotamers: 4 of 213 | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246 |
| A<br>471 | ASP | 50  | -          | Favored<br>(63.16%)<br>General /<br>-55.4,-33.1  | 33% ( <i>t</i> 70)<br>chi angles: 178.6,70.1     | 0.062Å                  | -                  | -                  |                     |
| A<br>472 | SER | 50  | -          | Favored<br>(15.25%)<br>General /<br>-111.4,-3.4  | 92.7% ( <i>p</i> )<br>chi angles: 65.1           | 0.107Å                  | -                  | -                  |                     |
| A<br>473 | GLY | 50  | -          | Favored<br>(91.67%)<br>Glycine /<br>59.7,37.0    | -  | -                       | -                  | -                  |                     |
| A<br>474 | SER | 50  | -          | Favored<br>(30.52%)<br>General /<br>-148.9,149.0 | 29% ( <i>t</i> )<br>chi angles: 185.1            | 0.078Å                  | -                  | -                  |                     |
| A<br>475 | TYR | 50  | -          | Favored<br>(14.38%)<br>General /<br>-83.0,105.9  | 21.4% ( <i>m</i> -85)<br>chi angles: 274.4,276   | 0.049Å                  | -                  | -                  |                     |
| A<br>476 | THR | 50  | -          | Allowed<br>(1.79%)<br>General /<br>-142.3,-164.3 | 13.9% ( <i>t</i> )<br>chi angles: 190            | 0.202Å                  | -                  | -                  |                     |
| A<br>477 | LEU | 50  | -          | Favored<br>(47.65%)<br>General /<br>-139.4,153.7 | 94.5% ( <i>mt</i> )<br>chi angles: 293.3,171.1   | 0.055Å                  | -                  | -                  |                     |
| A<br>478 | ASN | 50  | -          | Favored<br>(6.42%)<br>General /<br>-79.9,96.6    | 60.4% ( <i>t</i> -20)<br>chi angles: 187.9,341.5 | 0.052Å                  | -                  | -                  |                     |

Favored

|          |     |    |   |  |   |        |   |   |
|----------|-----|----|---|--|---|--------|---|---|
| A<br>479 | PHE | 50 | - | (58.06%)<br>General /<br>-82.5,-4.8                              | 98.2% ( <i>m-85</i> )<br>chi angles: 296.9,279.1                  | 0.106Å | - | - |
| A<br>480 | GLN | 50 | - | Favored<br>(5.63%)<br>General /<br>65.3,38.7                     | 96.3% ( <i>mt-30</i> )<br>chi angles:<br>293.9,180.3,341.2        | 0.097Å | - | - |
| A<br>481 | GLY | 50 | - | Favored<br>(50.7%)<br>Glycine / 66.7,9.2                         | -   | -      | - | - |
| A<br>482 | ARG | 50 | - | Favored<br>(41.84%)<br>General /<br>-79.8,-23.8                  | 28.5% ( <i>mmm180</i> )<br>chi angles:<br>299.6,292.5,295.6,150.2 | 0.056Å | - | - |
| A<br>483 | VAL | 50 | - | Favored<br>(61.13%)<br>Isoleucine or<br>valine /<br>-128.0,123.7 | 96.1% ( <i>t</i> )<br>chi angles: 178.6                           | 0.106Å | - | - |
| A<br>484 | THR | 50 | - | Favored<br>(9.91%)<br>General /<br>-118.3,-12.6                  | 38.5% ( <i>p</i> )<br>chi angles: 53.2                            | 0.075Å | - | - |
| A<br>485 | GLN | 50 | - | Favored<br>(47.72%)<br>General /<br>-131.4,136.1                 | 70.2% ( <i>mt-30</i> )<br>chi angles:<br>302.4,191.6,330.3        | 0.085Å | - | - |
| A<br>486 | ALA | 50 | - | Favored<br>(40.88%)<br>General /<br>-55.2,139.8                  | -   | 0.044Å | - | - |
| A<br>487 | SER | 50 | - | Favored<br>(2.53%)<br>General /<br>-170.8,145.9                  | 32.7% ( <i>t</i> )<br>chi angles: 184                             | 0.092Å | - | - |
| A<br>488 | VAL | 50 | - | Favored<br>(26.43%)<br>Isoleucine or<br>valine /<br>-67.5,-20.4  | 32.9% ( <i>m</i> )<br>chi angles: 300.2                           | 0.126Å | - | - |
| A<br>489 | LYS | 50 | - | Favored<br>(59.25%)<br>General /<br>-83.1,-9.4                   | 29.7% ( <i>mtmm</i> )<br>chi angles:<br>290.5,172.7,277,295.8     | 0.051Å | - | - |
| A<br>490 | ASN | 50 | - | Favored<br>(26.49%)<br>General /<br>-71.7,125.2                  | 79.7% ( <i>m-20</i> )<br>chi angles: 296,347.5                    | 0.093Å | - | - |

| #        | Alt | Res | High<br>B  | Clash ><br>0.4Å                   | Ramachandran   | Rotamer   | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles                                  |
|----------|-----|-----|------------|-----------------------------------|--|---|--------------------|--------------------|---|
|          |     |     | Avg: 54.27 | Clashscore: 1.01                  | Outliers: 2 of 244   | Poor rotamers: 4 of 213                                 | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246                             |
| A<br>491 |     | PHE | 50         | -                                 | Favored<br>(39.65%)<br>General /<br>-156.9,162.2                 | 18.3% ( <i>p90</i> )<br>chi angles: 61.4,74.7           | 0.038Å             | -                  | -   |
| A<br>492 |     | GLN | 50         | -                                 | Favored<br>(54.76%)<br>General /<br>-122.4,137.7                 | 98.6% ( <i>mt-30</i> )<br>chi angles: 291.2,178.8,334.7 | 0.104Å             | -                  | -   |
| A<br>493 |     | ILE | 50         | -                                 | Favored<br>(66.75%)<br>Isoleucine or<br>valine /<br>-109.6,125.1 | 44% ( <i>mm</i> )<br>chi angles: 301.8,305.1            | 0.068Å             | -                  | -   |
| A<br>494 |     | VAL | 50         | -                                 | Favored<br>(25.47%)<br>Isoleucine or<br>valine /<br>-130.1,167.4 | 28% ( <i>m</i> )<br>chi angles: 296.6                   | 0.062Å             | -                  | -   |
| A<br>495 |     | HIS | 50         | -                                 | Favored<br>(18.47%)<br>General /<br>-98.1,153.4                  | 45.8% ( <i>t-80</i> )<br>chi angles: 192,263.2          | 0.059Å             | -                  | -   |
| A<br>496 |     | ALA | 50         | -                                 | Favored<br>(73.53%)<br>General /<br>-58.0,-37.0                  | -   | 0.083Å             | -                  | -   |
| A<br>497 |     | ASP | 50         | -                                 | Favored<br>(64.16%)<br>General /<br>-69.0,-24.0                  | 0.1%<br>chi angles: 321.7,1.4                           | 0.114Å             | -                  | OUTLIER(S)<br>worst is CA-<br>CB-CG: 5.948<br>σ |
| A<br>498 |     | ASP | 50         | -                                 | Favored<br>(3.93%)<br>Pre-proline /<br>-146.8,101.8              | 63.2% ( <i>t0</i> )<br>chi angles: 186.8,346.5          | 0.025Å             | -                  | -   |
| A<br>499 |     | PRO | 50         | -                                 | Favored<br>(11.06%)<br>Trans-proline /<br>-79.6,-0.9             | 69.4% ( <i>Cg_endo</i> )<br>chi angles: 33.5            | 0.055Å             | -                  | -   |
| A<br>500 |     | ASP | 50         | 0.42Å<br>OD1 with A<br>464 LYS NZ | Favored<br>(14.42%)<br>General /<br>-111.1,-8.4                  | 75.4% ( <i>m-20</i> )<br>chi angles: 298.8,330.8        | 0.169Å             | -                  | -   |
| A<br>501 |     | TYR | 50         | -                                 | Favored<br>(6.01%)<br>General /<br>-81.0,90.6                    | 36.7% ( <i>t80</i> )<br>chi angles: 192,274.1           | 0.051Å             | -                  | -   |

|          |     |     |            |   |   |                         |                    |                    |                     |
|----------|-----|-----|------------|---|---|-------------------------|--------------------|--------------------|---------------------|
| A<br>502 | ILE | 50  | -          | Allowed<br>(1.12%)<br>Isoleucine or<br>valine /<br>-73.9,98.6   | 15.8% ( <i>mm</i> )<br>chi angles: 311.6,311.6                    | 0.077Å                  | -                  | -                  |                     |
| A<br>503 | VAL | 50  | -          | Favored<br>(87.03%)<br>Isoleucine or<br>valine /<br>-67.5,-42.4 | 53.6% ( <i>t</i> )<br>chi angles: 182.2                           | 0.058Å                  | -                  | -                  |                     |
| A<br>504 | LEU | 50  | -          | Favored<br>(22.21%)<br>General /<br>-146.2,134.8                | 32.2% ( <i>tp</i> )<br>chi angles: 188.7,60.5                     | 0.077Å                  | -                  | -                  |                     |
| A<br>505 | GLN | 50  | -          | Favored<br>(54.13%)<br>General /<br>-123.2,134.9                | 23.9% ( <i>tt0</i> )<br>chi angles:<br>189.6,171.7,257.5          | 0.095Å                  | -                  | -                  |                     |
| A<br>506 | PHE | 50  | -          | Favored<br>(37.38%)<br>General /<br>-139.5,142.1                | 33.1% ( <i>t80</i> )<br>chi angles: 185.7,55.7                    | 0.077Å                  | -                  | -                  |                     |
| A<br>507 | GLY | 50  | -          | Favored<br>(26.27%)<br>Glycine /<br>179.3,161.1                 | -   | -                       | -                  | -                  |                     |
| A<br>508 | ARG | 50  | -          | Favored<br>(45.2%)<br>General /<br>-74.2,140.5                  | 78.4% ( <i>ttt180</i> )<br>chi angles:<br>186.4,177.1,178.2,188.5 | 0.087Å                  | -                  | -                  |                     |
| A<br>509 | VAL | 50  | -          | Favored<br>(2.33%)<br>Isoleucine or<br>valine /<br>-122.3,-25.1 | 28.9% ( <i>m</i> )<br>chi angles: 295.2                           | 0.18Å                   | -                  | -                  |                     |
| A<br>510 | ALA | 50  | -          | Favored<br>(4.43%)<br>General /<br>-149.3,-173.6                | -   | 0.038Å                  | -                  | -                  |                     |
| #        | Alt | Res | High<br>B  | Clash ><br>0.4Å   | Ramachandran  | Rotamer                 | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles      |
|          |     |     | Avg: 54.27 | Clashscore: 1.01  | Outliers: 2 of 244  | Poor rotamers: 4 of 213 | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246 |
| A<br>511 | GLU | 50  | -          | Favored<br>(75.71%)<br>General /<br>-56.9,-40.1                 | 18.2% ( <i>pt-20</i> )<br>chi angles:<br>60.1,180.3,335.6         | 0.105Å                  | -                  | -                  |                     |

Favored

|          |     |    |   |   |  |        |   |   |
|----------|-----|----|---|---|--|--------|---|---|
| A<br>512 | ASP | 50 | - | (3.61%)<br>General /<br>-134.8,23.5                 | 65.2% ( <i>m-20</i> )<br>chi angles: 301.5,308.8                 | 0.071Å | - | - |
| A<br>513 | ALA | 50 | - | Favored<br>(51.16%)<br>General /<br>-129.7,140.2    | -  | 0.04Å  | - | - |
| A<br>514 | PHE | 50 | - | Favored<br>(45.63%)<br>General /<br>-141.2,154.0    | 45.7% ( <i>m-85</i> )<br>chi angles: 306.1,81.7                  | 0.176Å | - | - |
| A<br>515 | THR | 50 | - | Favored<br>(18.02%)<br>General /<br>-97.8,153.8     | 33% ( <i>p</i> )<br>chi angles: 51.8                             | 0.036Å | - | - |
| A<br>516 | LEU | 50 | - | Favored<br>(3.68%)<br>General /<br>-147.8,105.3     | 50.3% ( <i>tp</i> )<br>chi angles: 181.5,67                      | 0.058Å | - | - |
| A<br>517 | ASP | 50 | - | Favored<br>(36.93%)<br>General /<br>-118.6,120.3    | 47.3% ( <i>m-20</i> )<br>chi angles: 303.4,341.9                 | 0.071Å | - | - |
| A<br>518 | TYR | 50 | - | Favored<br>(36.37%)<br>General /<br>-120.8,153.9    | 47.9% ( <i>p90</i> )<br>chi angles: 68.4,272.1                   | 0.043Å | - | - |
| A<br>519 | ARG | 50 | - | Favored<br>(13.05%)<br>General /<br>-127.1,169.8    | 70.9% ( <i>mtp180</i> )<br>chi angles:<br>300.5,194.8,68.3,193.3 | 0.061Å | - | - |
| A<br>520 | TYR | 50 | - | Favored<br>(73.37%)<br>Pre-proline /<br>-56.0,136.0 | 80.9% ( <i>t80</i> )<br>chi angles: 179,84.8                     | 0.075Å | - | - |
| A<br>521 | PRO | 50 | - | Favored<br>(58.18%)<br>Cis-proline /<br>-93.3,7.0   | 6.2% ( <i>Cg_endo</i> )<br>chi angles: 41                        | 0.044Å | - | - |
| A<br>522 | LEU | 50 | - | Favored<br>(41.78%)<br>General /<br>-74.7,147.0     | 83% ( <i>mt</i> )<br>chi angles: 296.9,181.7                     | 0.058Å | - | - |
| A<br>523 | CYS | 50 | - | Favored<br>(8.38%)<br>General /<br>-98.3,171.2      | 29.5% ( <i>p</i> )<br>chi angles: 66.1                           | 0.044Å | - | - |
| A        |     |    |   | Favored<br>(83.97%)                                 |  |        |   |   |

|          |     |    |   |   |  |        |   |   |
|----------|-----|----|---|---|--|--------|---|---|
| 524      | ALA | 50 | - | General /<br>-62.1,-37.1  | -  | 0.12Å  | - | - |
| A<br>525 | LEU | 50 | - | Favored<br>(91.52%)<br>General /<br>-65.6,-42.5                 | 44.6% ( <i>tp</i> )<br>chi angles: 180.6,56              | 0.115Å | - | - |
| A<br>526 | GLN | 50 | - | Favored<br>(64.89%)<br>General /<br>-62.4,-52.1                 | 78.7% ( <i>mt-30</i> )<br>chi angles:<br>291.4,165.7,305 | 0.083Å | - | - |
| A<br>527 | ALA | 50 | - | Favored<br>(68.23%)<br>General /<br>-54.0,-49.7                 | -  | 0.023Å | - | - |
| A<br>528 | PHE | 50 | - | Favored<br>(94.68%)<br>General /<br>-62.6,-45.0                 | 37.9% ( <i>t80</i> )<br>chi angles: 184.5,57.3           | 0.039Å | - | - |
| A<br>529 | ALA | 50 | - | Favored<br>(77.59%)<br>General /<br>-68.3,-35.3                 | -  | 0.071Å | - | - |
| A<br>530 | ILE | 50 | - | Favored<br>(93.19%)<br>Isoleucine or<br>valine /<br>-65.2,-45.7 | 66.1% ( <i>mt</i> )<br>chi angles: 295.9,160.9           | 0.113Å | - | - |

| #        | Alt | Res | High<br>B  | Clash ><br>0.4Å  | Ramachandran                                    | Rotamer  | Cβ<br>deviation    | Bond<br>lengths    | Bond<br>angles      |
|----------|-----|-----|------------|------------------|---|--|--------------------|--------------------|---------------------|
|          |     |     | Avg: 54.27 | Clashscore: 1.01 | Outliers: 2 of 244                              | Poor rotamers: 4 of 213                        | Outliers: 0 of 229 | Outliers: 0 of 246 | Outliers: 11 of 246 |
| A<br>531 | ALA | 50  | -          | -                | Favored<br>(85.7%)<br>General /<br>-60.1,-39.3  | -  | 0.07Å              | -                  | -                   |
| A<br>532 | LEU | 50  | -          | -                | Favored<br>(71.73%)<br>General /<br>-63.5,-30.6 | 73.7% ( <i>mt</i> )<br>chi angles: 290.2,178.6 | 0.135Å             | -                  | -                   |
| A<br>533 | SER | 50  | -          | -                | Favored<br>(61.63%)<br>General /<br>-72.6,-17.9 | 51.8% ( <i>p</i> )<br>chi angles: 75.3         | 0.17Å              | -                  | -                   |
| A<br>534 | SER | 50  | -          | -                | Favored<br>(41.33%)<br>General /<br>-83.5,-17.6 | 18.1% ( <i>p</i> )<br>chi angles: 81           | 0.143Å             | -                  | -                   |

|          |     |       |   |   |  |        |   |   |
|----------|-----|-------|---|---|--|--------|---|---|
| A<br>535 | PHE | 50    | - | Favored<br>(27.27%)<br>General /<br>-80.6,154.7 | 94.3% ( <i>m</i> -85)<br>chi angles: 297.9,266.9 | 0.107Å | - | -   |
| A<br>536 | ASP | 99.99 | - | -   | 0%<br>chi angles: 15.8,43.4                      | 0.169Å | - | OUTLIER(S)<br>worst is CA-<br>CB-CG: 7.951<br>σ |

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