



Viewing TGFBI_sm_252-373H-multi.table

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| | | | | |
|-------------------|---|-----------|--------|---|
| All-Atom Contacts | Clashscore, all atoms: | 77.85 | | 0 th percentile* (N=1784, all resolutions) |
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 4 | 4.04% | Goal: <1% |
| | Ramachandran outliers | 5 | 4.17% | Goal: <0.05% |
| | Ramachandran favored | 97 | 80.83% | Goal: >98% |
| | MolProbity score^ | 3.54 | | 8 th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 3 | 2.68% | Goal: 0 |
| | Bad backbone bonds: | 4 / 914 | 0.44% | Goal: 0% |
| | Bad backbone angles: | 15 / 1243 | 1.21% | 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: 56.97 | Clashscore: 77.85 | Outliers: 5 of 120 | Poor rotamers: 4 of 99 | Outliers: 3 of 112 | Outliers: 2 of 122 | Outliers: 10 of 122 |
| A 252 | THR | 50 | - | - | 93.2% (m) chi angles: 300.2 | 0.071Å | - | - |
| A 253 | PHE | 50 | 0.843Å HB3 with A 257 ARG HB3 | Favored (2.97%) General / -133.8,42.1 | 45.3% (m-85) chi angles: 309.9,281.7 | 0.161Å | - | - |
| A 254 | GLU | 50 | - | Favored (65.46%) General / -67.5,-22.3 | 12.4% (pt-20) chi angles: 59.7,179.5,65.7 | 0.059Å | - | - |
| A 255 | THR | 50 | - | Favored (29.95%) General / -83.6,-26.4 | 13.8% (t) chi angles: 190.1 | 0.086Å | - | - |
| A 256 | LEU | 50 | 0.427Å HB2 with A 285 PHE CZ | Allowed (0.62%) General / -138.3,-53.6 | 3.3% (tm?) chi angles: 189.2,281.4 | 0.083Å | - | - |
| | | | 0.843Å | Favored | | | | |

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|----------|-----|----|--|--|---|--------|---|--|
| A 257 | ARG | 50 | HB3 with A 253 PHE HB3 | (64.2%) General / -73.7,-32.9 | 50.7% (<i>ttm-85</i>) chi angles: 174.3,190.6,298.7,279.3 | 0.112Å | - | - |
| A 258 | ALA | 50 | - | Favored (66.91%) General / -57.7,-31.9 | - | 0.059Å | - | - |
| A 259 | ALA | 50 | 0.454Å HA with A 262 ALA HB3 | Favored (61.26%) General / -72.8,-19.9 | - | 0.019Å | - | - |
| A 260 | VAL | 50 | 0.771Å HB with A 269 LEU HD12 | Allowed (0.81%) Isoleucine or valine / -52.0,-61.0 | 19.4% (<i>m</i>) chi angles: 303.9 | 0.151Å | - | OUTLIER(S) worst is CA- CB-CG2: 4.6 σ |
| A 261 | ALA | 50 | - | Favored (64.57%) General / -73.4,-32.8 | - | 0.048Å | - | - |
| A 262 | ALA | 50 | 0.454Å HB3 with A 259 ALA HA | Favored (40.85%) General / -76.8,-3.9 | - | 0.032Å | - | - |
| A 263 | SER | 50 | - | Favored (14.34%) General / -114.0,21.9 | 32.8% (<i>t</i>) chi angles: 183.9 | 0.018Å | - | - |
| A 264 | GLY | 50 | - | Favored (92.93%) Glycine / 64.2,36.2 | - | - | - | - |
| A 265 | LEU | 50 | 0.733Å HD12 with A 260 VAL HA | Favored (20.08%) General / -108.9,0.2 | 7% (<i>mt</i>) chi angles: 323.5,175.3 | 0.07Å | - | - |
| A 266 | ASN | 50 | - | Favored (16.24%) General / -50.8,-55.6 | 26.5% (<i>t-20</i>) chi angles: 184.8,300.2 | 0.054Å | - | - |
| A 267 | THR | 50 | - | Favored (62.23%) General / -71.7,-17.8 | 66.8% (<i>p</i>) chi angles: 59.5 | 0.031Å | - | - |
| A 268 | MET | 50 | 0.549Å HG2 with A 265 LEU HA | Favored (7.39%) General / -93.9,-46.0 | 20.4% (<i>ptp</i>) chi angles: 74.2,181.9,62.5 | 0.138Å | - | - |
| A | | | 0.771Å | Favored (30.02%) | 35.7% (<i>mt</i>) | | | |

| 269 | LEU | 50 | HD12 with A 260 VAL HB | General / -70.5,-51.3 | chi angles: 287.8,184.2 | 0.08Å | - | - |
|----------|---------|-----------|---|---|--|------------------------|--------------------|--|
| A 270 | GLU | 50 | 0.485Å CD with A 270 GLU O | Allowed (1.57%) General / -98.2,36.5 | 14.7% (<i>tm</i> -20) chi angles: 185.6,283,325.1 | 0.129Å | - | - |
| A 271 | GLY | 50 | - | Allowed (0.27%) Glycine / -53.4,-74.8 | - | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 56.97 | Clashscore: 77.85 | Outliers: 5 of 120 | Poor rotamers: 4 of 99 | Outliers: 3 of 112 | Outliers: 2 of 122 |
| | | | OUTLIER | | | | | |
| A 272 | ASN | 50 | - | (0.01%) General / -178.8,81.7 | 28.7% (<i>t</i> -20) chi angles: 187.3,301.5 | 0.066Å | - | - |
| A 273 | GLY | 50 | - | Favored (7.56%) Glycine / 150.5,157.0 | - | - | - | - |
| A 274 | GLN | 50 | - | Favored (2.3%) General / -59.5,113.6 | 18.3% (<i>pt</i> 20) chi angles: 64,176.3,61.8 | 0.046Å | - | - |
| A 275 | TYR | 99.99 | 0.4Å CD1 with A 269 LEU O | Favored (53.78%) General / -116.5,126.8 | 55.8% (<i>p</i> 90) chi angles: 62.6,271 | 0.022Å | - | - |
| A 276 | THR | 50 | 0.513Å CG2 with A 312 LEU HB2 | Favored (35.53%) General / -93.8,121.7 | 4.7% (<i>t</i>) chi angles: 175.2 | 0.033Å | - | - |
| A 277 | LEU | 50 | - | Favored (12.97%) General / -134.2,114.4 | 8.9% (<i>tt</i>) chi angles: 188.4,157.9 | 0.075Å | - | - |
| A 278 | LEU | 50 | 0.629Å HA with A 365 HIS O | Allowed (1.28%) General / -73.0,84.8 | 71.3% (<i>mt</i>) chi angles: 298.5,169 | 0.069Å | - | - |
| A 279 | ALA | 50 | 0.646Å HB3 with A 257 ARG HH21 | Favored (61.6%) Pre-proline / -99.0,111.8 | - | 0.158Å | - | OUTLIER(S) worst is N- CA-CB: 4.005 σ |
| A 280 | PRO | 50 | 0.69Å HB3 with A 367 ILE HG13 | Favored (27.22%) Trans-proline / -58.7,157.7 | 55.4% (<i>Cg_endo</i>) chi angles: 25.6 | 0.043Å | - | - |
| A | | | 0.553Å HB with A | Favored | 0.1% | | | |

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|----------|-----|----|--|---|---|--------|---|---|
| 281 | THR | 50 | 283 GLU HG2 | (43.06%) General / -69.1,153.8 Favored | chi angles: 18.6 | 0.047Å | - | - |
| A 282 | ASN | 50 | - | (50.73%) General / -54.9,-28.4 Favored | 52.2% (<i>t30</i>) chi angles: 184.7,58 | 0.028Å | - | - |
| A 283 | GLU | 50 | 0.553Å HG2 with A 281 THR HB | (73.04%) General / -69.9,-34.1 Favored | 12.3% (<i>pt-20</i>) chi angles: 65.3,177.9,64.1 | 0.058Å | - | - |
| A 284 | ALA | 50 | - | (97.15%) General / -64.0,-42.1 Favored | - | 0.057Å | - | - |
| A 285 | PHE | 50 | 0.929Å CD2 with A 296 ILE HD12 | (97.98%) General / -62.6,-43.8 Favored | 2.6% (<i>m-85</i>) chi angles: 260.8,68.5 | 0.036Å | - | - |
| A 286 | GLU | 50 | 0.809Å HA with A 293 LEU HD12 | (61.71%) General / -71.8,-24.3 Favored | 12.7% (<i>pt-20</i>) chi angles: 63.7,181.3,65.4 | 0.192Å | - | - |
| A 287 | LYS | 50 | - | (88.13%) General / -66.8,-41.1 Favored | 27.9% (<i>tptp</i>) chi angles: 185.1,61.5,183.2,64.8 | 0.028Å | - | - |
| A 288 | ILE | 50 | 1.034Å HD11 with A 296 ILE HD13 | (67.21%) Pre-proline / -57.9,124.1 Favored | 20.6% (<i>pt</i>) chi angles: 66.8,181.9 | 0.093Å | - | - |
| A 289 | PRO | 50 | - | (0.34%) Trans-proline / -73.1,-167.3 Allowed | 68.5% (<i>Cg_endo</i>) chi angles: 33.6 | 0.019Å | - | - |
| A 290 | SER | 50 | - | (0.18%) General / 53.5,-156.9 Allowed | 70.4% (<i>m</i>) chi angles: 297.3 | 0.049Å | - | - |
| A 291 | GLU | 50 | 0.461Å O with A 295 ARG HG3 | (3.68%) General / -91.4,22.8 Favored | 11.9% (<i>pt-20</i>) chi angles: 62.2,176.8,64 | 0.034Å | - | - |

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

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|-------|-------------|----------------|---------------------|-----------|-------------|--------------|
| Avg: | Clashscore: | Outliers: 5 of | Poor rotamers: 4 of | Outliers: | Outliers: 2 | Outliers: 10 |
| 56.97 | 77.85 | 120 | 99 | 3 of 112 | of 122 | of 122 |

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|----------|-----|----|--|----------------------------------|---|--------|---|---|
| A 292 | THR | 50 | 0.768Å HG22 with A 288 ILE HD12 | (71.85%) General / Favored | 47.3% (<i>m</i>) chi angles: 305.1 | 0.029Å | - | - |
|----------|-----|----|--|----------------------------------|---|--------|---|---|

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|----------|-----|-------|--|---|---|--------|---|--|
| A 293 | LEU | 50 | 0.809Å HD12 with A 286 GLU HA | -70.3,-33.7 Favored (88.32%) General / -66.3,-38.7 | 6.3% (<i>tt</i>) chi angles: 189.7,167.7 | 0.149Å | - | - |
| A 294 | ASN | 50 | - | Favored (76.21%) General / -69.9,-38.6 | 54% (<i>t30</i>) chi angles: 185.8,55.9 | 0.078Å | - | - |
| A 295 | ARG | 50 | 0.461Å HG3 with A 291 GLU O | Favored (79.59%) General / -68.9,-38.6 | 77.2% (<i>mtp85</i>) chi angles: 293.3,178.2,68.4,82.6 | 0.025Å | - | - |
| A 296 | ILE | 50 | 1.034Å HD13 with A 288 ILE HD11 | Favored (17.62%) Isoleucine or valine / -74.0,-20.2 | 37.5% (<i>pt</i>) chi angles: 65.2,175.1 | 0.046Å | - | OUTLIER(S) worst is CB- CG1-CD1: 4.517 σ |
| A 297 | LEU | 50 | - | Favored (59.32%) General / -75.9,-31.5 | 8.4% (<i>tp</i>) chi angles: 197.9,81.9 | 0.051Å | - | - |
| A 298 | GLY | 50 | 0.492Å C with A 300 PRO HD2 | Favored (38.63%) Glycine / -68.5,142.3 | - | - | - | - |
| A 299 | ASP | 99.99 | 0.515Å OD1 with A 300 PRO HD3 | Favored (73.8%) Pre-proline / -60.5,-40.2 | 15.3% (<i>p-10</i>) chi angles: 66.9,312.7 | 0.078Å | - | - |
| A 300 | PRO | 99.99 | 0.515Å HD3 with A 299 ASP OD1 | Favored (13.19%) Trans-proline / -61.5,123.7 | 85.6% (<i>Cg_endo</i>) chi angles: 33 | 0.041Å | - | - |
| A 301 | GLU | 99.99 | - | Allowed (0.36%) General / -118.8,-141.3 | 21.1% (<i>pm0</i>) chi angles: 66.4,283.6,4.6 | 0.219Å | - | - |
| A 302 | ALA | 50 | - | OUTLIER (0%) General / 163.6,-35.0 | - | 0.111Å | - | - |
| A 303 | LEU | 50 | 0.424Å CD1 with A 256 LEU HD21 | Favored (67.73%) General / -58.0,-32.2 | 14.4% (<i>mt</i>) chi angles: 274.7,162.4 | 0.043Å | - | - |
| A 304 | ARG | 50 | 0.561Å O with A 307 LEU HD22 | Favored (92.24%) General / -64.0,-44.6 | 78.2% (<i>ttt-85</i>) chi angles: 183.7,178.1,178,277.8 | 0.032Å | - | - |
| A | ASP | 50 | - | Favored (81.24%) | 38.4% (<i>t70</i>) | 0.014Å | - | - |

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|-------|-----|-------|---|--|---|---------------------------|---|---|------------------------|
| A 305 | | | | | General / -62.1,-36.3 | chi angles: 183.4,59.2 | | | |
| A 306 | LEU | 99.99 | 0.658Å O with A 372 ILE HD11 | Favored (6.91%) General / -109.9,30.2 | 80.6% (<i>mt</i>) chi angles: 296.9,169.6 | 0.037Å | - | - | |
| A 307 | LEU | 50 | 0.561Å HD22 with A 304 ARG O | Favored (70.35%) General / -62.3,-29.4 | 2.4% (<i>pt?</i>) chi angles: 78.3,170.7 | 0.035Å | - | - | |
| A 308 | ASN | 50 | 0.886Å HA with A 311 ILE HG22 | Favored (74.07%) General / -56.4,-40.1 | 31.8% (<i>m120</i>) chi angles: 292.1,118.5 | 0.079Å | - | - | |
| A 309 | ASN | 50 | 0.424Å ND2 with A 333 THR HG21 | Favored (70.25%) General / -65.5,-29.6 | 27.5% (<i>t-20</i>) chi angles: 188,300.7 | 0.054Å | - | - | |
| A 310 | HIS | 50 | 0.813Å HB2 with A 372 ILE HD12 | Favored (24.62%) General / -87.3,-23.4 | 0.3% chi angles: 218.7,351.9 | 0.082Å | OUTLIER(S) worst is CG-- ND1: 4.608 σ | OUTLIER(S) worst is CB- CG-CD2: 4.284 σ | |
| A 311 | ILE | 50 | 0.886Å HG22 with A 308 ASN HA | Favored (56.41%) Isoleucine or valine / -102.3,126.7 | 9% (<i>tp</i>) chi angles: 184.2,63.9 | 0.055Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 56.97 | Clashscore: 77.85 | Outliers: 5 of 120 | Poor rotamers: 4 of 99 | Outliers: 3 of 112 | Outliers: 2 of 122 | Outliers: 10 of 122 |
| A 312 | LEU | 99.99 | 0.819Å HG with A 329 THR HA | Favored (5.8%) General / -144.7,111.5 | 4.6% (<i>mp</i>) chi angles: 295.9,63.6 | 0.055Å | - | OUTLIER(S) worst is CD1- CG-CD2: 4.994 σ | |
| A 313 | LYS | 99.99 | - | Favored (43.15%) General / -74.0,135.6 | 99.3% (<i>mttt</i>) chi angles: 293.8,181.9,179.1,180.2 | 0.038Å | - | - | |
| A 314 | SER | 50 | - | Allowed (0.49%) General / 57.7,72.9 | 43.3% (<i>t</i>) chi angles: 181 | 0.036Å | - | - | |
| A 315 | ALA | 50 | - | Favored (4.98%) General / -128.2,98.1 | - | 0.024Å | - | - | |
| A 316 | MET | 50 | - | Favored (26.33%) General / | 25.7% (<i>ptp</i>) chi angles: | 0.016Å | - | - | |

-87.0,146.0 62.3,181.3,69.1

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|----------|-----|----|-------------------------------------|--|--|--------|---|---|
| A 317 | CYS | 50 | 0.746Å HB2 with A 357 ILE CD1 | Favored (29.88%) General / -58.4,147.9 | 9.6% (<i>t</i>) chi angles: 196.2 | 0.195Å | - | - |
| A 318 | ALA | 50 | - | Favored (78.5%) General / -58.6,-38.7 | - | 0.026Å | - | - |
| A 319 | GLU | 50 | 0.647Å HG2 with A 317 CYS SG | Favored (64.94%) General / -58.2,-28.5 | 12.5% (<i>pt</i> -20) chi angles: 67,181.3,58.8 | 0.04Å | - | - |
| A 320 | ALA | 50 | - | Favored (71.88%) General / -61.1,-32.2 | - | 0.019Å | - | - |
| A 321 | ILE | 50 | 0.889Å HG13 with A 322 VAL H | Allowed (0.18%) Isoleucine or valine / -113.3,-86.8 | 23.8% (<i>pt</i>) chi angles: 57.2,162.1 | 0.154Å | - | - |
| A 322 | VAL | 50 | 0.889Å H with A 321 ILE HG13 | Favored (41.05%) Isoleucine or valine / -130.6,154.7 | 14.7% (<i>p</i>) chi angles: 64 | 0.101Å | - | - |
| A 323 | ALA | 50 | - | Favored (21.83%) General / -88.9,111.2 | - | 0.047Å | - | - |
| A 324 | GLY | 50 | - | Allowed (0.63%) Glycine / 113.9,74.4 | - | - | - | - |
| A 325 | LEU | 50 | 0.846Å HG with A 326 SER H | Favored (2.3%) General / -130.5,-170.2 | 38% (<i>tp</i>) chi angles: 186.8,60.6 | 0.085Å | - | - |
| A 326 | SER | 50 | 0.846Å H with A 325 LEU HG | Favored (21.03%) General / -122.1,162.5 | 87.8% (<i>p</i>) chi angles: 65.5 | 0.058Å | - | - |
| A 327 | VAL | 50 | 0.58Å CG1 with A 335 LEU HB2 | Favored (3.74%) Isoleucine or valine / -126.0,96.6 | 12.1% (<i>p</i>) chi angles: 66.1 | 0.138Å | - | - |
| A 328 | GLU | 50 | 0.453Å HA with A 333 THR O | Favored (37.68%) General / | 57.6% (<i>tt0</i>) chi angles: 188.2,189.6,334.4 | 0.098Å | - | - |

| A 329 | THR | 50 | 0.819Å HA with A 312 LEU HG | -78.8,141.5 Favored (23.23%) General / -105.7,152.4 | 6.3% (<i>p</i>) chi angles: 79.7 | 0.021Å | - | - | |
|----------|-----|-----|--|---|--|------------------------|--------------------|--------------------|---------------------|
| A 330 | LEU | 50 | 0.592Å HD22 with A 308 ASN ND2 | Favored (75.45%) General / -56.0,-41.9 | 7.4% (<i>tt</i>) chi angles: 187.4,162.8 | 0.028Å | - | - | |
| A 331 | GLU | 50 | - | Favored (67.03%) General / -54.3,-39.4 | 14.9% (<i>tt0</i>) chi angles: 193,199.3,281.7 | 0.085Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 56.97 | Clashscore: 77.85 | Outliers: 5 of 120 | Poor rotamers: 4 of 99 | Outliers: 3 of 112 | Outliers: 2 of 122 | Outliers: 10 of 122 |
| A 332 | GLY | 50 | - | Allowed (0.34%) Glycine / 120.2,72.1 | - | - | - | - | - |
| A 333 | THR | 50 | 0.453Å O with A 328 GLU HA | Favored (8.14%) General / -149.5,121.3 | 72.4% (<i>p</i>) chi angles: 63.7 | 0.07Å | - | - | |
| A 334 | THR | 50 | - | Favored (11.92%) General / -101.5,101.4 | 66.8% (<i>p</i>) chi angles: 57.3 | 0.021Å | - | - | |
| A 335 | LEU | 50 | 0.58Å HB2 with A 327 VAL CG1 | Favored (9.99%) General / -88.4,171.6 | 7.1% (<i>mp</i>) chi angles: 287.2,58.6 | 0.032Å | - | - | |
| A 336 | GLU | 50 | 0.414Å O with A 346 ILE HA | Favored (25.92%) General / -106.3,112.8 | 10.5% (<i>pt-20</i>) chi angles: 57,175.3,70.9 | 0.014Å | - | - | |
| A 337 | VAL | 50 | 0.454Å HG22 with A 346 ILE HD13 | Favored (15.32%) Isoleucine or valine / -95.3,104.0 | 16% (<i>t</i>) chi angles: 190.2 | 0.04Å | - | - | |
| A 338 | GLY | 50 | - | Favored (16.49%) Glycine / -112.6,140.8 | - | - | - | - | |
| A 339 | CYS | 50 | - | Allowed (1.03%) General / -121.5,-66.6 | 81.6% (<i>m</i>) chi angles: 299.8 | 0.025Å | - | - | |

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|----------|-----|-------|---|--|---|--------|---|---|
| A 340 | SER | 50 | - | Favored (39.15%) General / -61.9,149.9 | 32.6% (<i>t</i>) chi angles: 184.1 | 0.041Å | - | - |
| A 341 | GLY | 50 | - | Favored (67.71%) Glycine / 58.4,32.1 | - | - | - | - |
| A 342 | ASP | 99.99 | 0.491Å OD2 with A 345 THR HG23 | Favored (13.74%) General / -165.7,156.8 | 38.3% (<i>t70</i>) chi angles: 184.7,63.7 | 0.083Å | - | - |
| A 343 | MET | 99.99 | 0.462Å C with A 344 LEU HG | Favored (52.73%) General / -77.7,-34.7 | 23.8% (<i>ptp</i>) chi angles: 58.6,185.5,67 | 0.111Å | - | - |
| A 344 | LEU | 99.99 | 0.559Å HB3 with A 352 ILE HG13 | OUTLIER (0.01%) General / 177.9,69.9 | 0% chi angles: 335,133.7 | 0.241Å | - | OUTLIER(S) worst is O-C- N: 4.582 σ |
| A 345 | THR | 50 | 0.663Å HB with A 348 GLY O | Favored (57.03%) General / -116.1,131.1 | 26.5% (<i>p</i>) chi angles: 71.5 | 0.564Å | - | - |
| A 346 | ILE | 50 | 0.542Å HD11 with A 327 VAL CG1 | Favored (2.07%) Isoleucine or valine / -137.6,101.4 | 8.8% (<i>tp</i>) chi angles: 184.7,60.6 | 0.108Å | - | - |
| A 347 | ASN | 50 | - | Favored (13.93%) General / 56.8,28.2 | 65.3% (<i>t30</i>) chi angles: 191.3,28.2 | 0.057Å | - | - |
| A 348 | GLY | 99.99 | 0.663Å O with A 345 THR HB | Favored (36.76%) Glycine / 163.1,-166.0 | - | - | - | - |
| A 349 | LYS | 99.99 | - | Favored (47.25%) General / -123.1,147.0 | 22.8% (<i>pttp</i>) chi angles: 61.3,179.4,181.6,65.2 | 0.031Å | - | - |
| A 350 | ALA | 99.99 | - | Favored (29.11%) General / 51.3,44.0 | - | 0.05Å | - | - |
| A 351 | ILE | 99.99 | 0.895Å HD11 with A 371 LEU HG | Favored (11.62%) Isoleucine or valine / -101.0,-47.3 | 18.3% (<i>tt</i>) chi angles: 182.5,166.1 | 0.112Å | - | OUTLIER(S) worst is CA- C-O: 4.33 σ |

Alt Res High Clash > Ramachandran Rotamer Cβ Bond Bond

| | | B | | 0.4Å | | deviation | lengths | angles |
|-------|-----|------------|--------------------------------------|---|---|--------------------|--------------------|--|
| | | Avg: 56.97 | Clashscore: 77.85 | Outliers: 5 of 120 | Poor rotamers: 4 of 99 | Outliers: 3 of 112 | Outliers: 2 of 122 | Outliers: 10 of 122 |
| A 352 | ILE | 99.99 | 0.988Å HA with A 367 ILE HA | Allowed (0.12%) Isoleucine or valine / -94.7,-164.4 | 21.8% (<i>pt</i>) chi angles: 56.4,181.5 | 0.228Å | - | - |
| A 353 | SER | 50 | - | OUTLIER (0.01%) General / -178.2,-55.5 | 0.3% chi angles: 240.5 | 0.06Å | - | - |
| A 354 | ASN | 50 | - | Favored (2.19%) General / -123.1,83.9 | 50.9% (<i>t30</i>) chi angles: 183.8,58.8 | 0.056Å | - | - |
| A 355 | LYS | 50 | 0.846Å HD3 with A 352 ILE HD12 | Allowed (1.81%) General / -69.7,102.1 | 28.9% (<i>mmmt</i>) chi angles: 296,294.8,275.3,178.1 | 0.019Å | - | - |
| A 356 | ASP | 50 | 0.604Å O with A 357 ILE HG22 | Favored (51.18%) General / -76.8,-39.5 | 40.3% (<i>t0</i>) chi angles: 185,327.8 | 0.079Å | - | - |
| A 357 | ILE | 50 | 0.746Å CD1 with A 317 CYS HB2 | Allowed (0.27%) Isoleucine or valine / 74.4,-60.0 | 8% (<i>tp</i>) chi angles: 185.7,56.7 | 0.261Å | - | OUTLIER(S) worst is CA- CB-CG2: 5.865 σ |
| A 358 | LEU | 50 | - | Favored (18.32%) General / -104.8,107.4 | 55.4% (<i>tp</i>) chi angles: 182.3,64.4 | 0.052Å | - | - |
| A 359 | ALA | 50 | 0.476Å HB2 with A 364 ILE HG23 | Favored (10.89%) General / -80.1,175.2 | - | 0.016Å | - | - |
| A 360 | THR | 50 | - | Favored (66.81%) General / -68.5,-28.2 | 80.5% (<i>p</i>) chi angles: 60.4 | 0.03Å | - | - |
| A 361 | ASN | 50 | - | Favored (3.12%) General / -136.8,14.9 | 52.7% (<i>t30</i>) chi angles: 184.2,47.3 | 0.064Å | - | - |
| A 362 | GLY | 50 | 0.438Å C with A 359 ALA HB3 | Allowed (0.71%) Glycine / 178.6,-120.5 Favored | - | - | - | - |

| | | | | | | | | |
|----------|---------|------------|--|--|--|--------------------|---|---|
| A 363 | VAL | 50 | 0.532Å HG13 with A 357 ILE O | (41.77%) Isoleucine or valine / -129.2,143.2 | 85.6% (<i>t</i>) chi angles: 175 | 0.063Å | - | - |
| A 364 | ILE | 50 | 0.84Å HB with A 366 TYR CE1 | Favored (17.55%) Isoleucine or valine / -143.7,130.8 | 20.9% (<i>pt</i>) chi angles: 52.7,178.9 | 0.09Å | - | - |
| A 365 | HIS | 50 | 0.821Å HB3 with A 355 LYS HZ2 | Favored (11.54%) General / -146.7,123.9 | 32.6% (<i>m170</i>) chi angles: 294.9,139.4 | 0.317Å | OUTLIER(S) worst is CG-- ND1: 5.648 σ | OUTLIER(S) worst is C- CA-CB: 4.998 σ |
| A 366 | TYR | 50 | 0.84Å CE1 with A 364 ILE HB | Favored (56.37%) General / -114.4,128.5 | 3.1% (<i>m-30</i>) chi angles: 290,23.2 | 0.17Å | - | OUTLIER(S) worst is CG- CD1-CE1: 5.266 σ |
| A 367 | ILE | 50 | 0.988Å HA with A 352 ILE HA | Favored (28.72%) Isoleucine or valine / -87.2,134.0 | 38.1% (<i>pt</i>) chi angles: 56.7,168.2 | 0.145Å | - | - |
| A 368 | ASP | 50 | 0.636Å HB2 with A 352 ILE O | Favored (65.61%) General / -64.0,-20.1 | 9.7% (<i>t0</i>) chi angles: 209,26.1 | 0.055Å | - | - |
| A 369 | GLU | 50 | 0.853Å HG2 with A 351 ILE HA | Allowed (0.3%) General / -123.5,-138.1 | 12% (<i>pt-20</i>) chi angles: 66.4,177,61.8 | 0.137Å | - | - |
| A 370 | LEU | 50 | 0.416Å N with A 369 GLU HG3 | Favored (49.02%) General / -121.1,143.6 | 9.9% (<i>tt</i>) chi angles: 185.3,154.8 | 0.112Å | - | - |
| A 371 | LEU | 50 | 0.895Å HG with A 351 ILE HD11 | Favored (5.46%) General / -123.7,177.9 | 1.2% (<i>mt</i>) chi angles: 245.5,170.5 | 0.055Å | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 56.97 | Clashscore: 77.85 | Outliers: 5 of 120 | Poor rotamers: 4 of 99 | Outliers: 3 of 112 | Outliers: 2 of 122 | Outliers: 10 of 122 |
| A 372 | ILE | 99.99 | 0.813Å HD12 with A 310 HIS HB2 | OUTLIER (0.08%) Pre-proline / 59.5,149.3 | 3.1% (<i>tt</i>) chi angles: 187.3,192 | 0.184Å | - | - |
| A 373 | PRO | 99.99 | 0.484Å HD2 with A 372 ILE CG1 | - | 61% (<i>Cg_endo</i>) chi angles: 27.3 | 0.035Å | - | - |

