



Viewing RDH12_mb_33-610H-multi.table

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|----------------------|---|-----------|--------|---|
| All-Atom Contacts | Clashscore, all atoms: | 146.96 | | 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 | 11 | 4.70% | Goal: <1% |
| | Ramachandran outliers | 14 | 5.07% | Goal: <0.05% |
| | Ramachandran favored | 248 | 89.86% | Goal: >98% |
| | MolProbity score^ | 3.69 | | 6 th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 9 | 3.47% | Goal: 0 |
| | Bad backbone bonds: | 10 / 2208 | 0.45% | Goal: 0% |
| | Bad backbone angles: | 74 / 2985 | 2.48% | 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: Clashscore: 124.27 Outliers: 14 of 276 Poor rotamers: 11 of 234 Outliers: 9 of 259 Outliers: 8 of 278 Outliers: 60 of 278 | | | | | | | | |
| 33 | THR | 101.21 | 0.768Å HB with 258 ALA HB2 | - | 14.6% (t) chi angles: 187 | 0.072Å | - | - |
| 34 | ASN | 126.06 | - | Favored (70.82%) General / -65.1,-29.9 | 4.4% (p30) chi angles: 65.1,101.5 | 0.103Å | - | OUTLIER(S) worst is CA-CB-CG: 4.621 σ |
| 35 | VAL | 63.88 | 0.441Å H with 33 THR HG23 | Favored (47.69%) Isoleucine or valine / -57.8,-34.3 | 94.8% (t) chi angles: 175.9 | 0.06Å | - | - |
| 36 | GLN | 169.63 | 0.608Å HA with 36 GLN HE21 | Favored (70.91%) General / -63.9,-29.8 | 1% chi angles: 177.5,70.5,172.2 | 0.08Å | - | - |
| 37 | LEU | 112.63 | 0.589Å CD2 with 271 ALA HB2 | Favored (6.22%) Pre-proline / -47.5,142.6 | 90.4% (mt) chi angles: 297.3,180 | 0.106Å | - | - |

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|----|------------|--|--|--|--------|---|--|
| 38 | PRO 117.63 | 1.136Å HG2 with 119 LEU HD21 | Allowed (0.62%) Trans-proline / -93.0,-176.6 | 37.7% (<i>Cg_endo</i>) chi angles: 23.2 | 0.083Å | - | - |
| 39 | GLY 107.62 | 0.775Å O with 119 LEU HD13 | Favored (36.28%) Glycine / -94.7,178.2 | - | - | OUTLIER(S) worst is C--N: 5.744 σ | |
| 40 | LYS 241.57 | 1.135Å HD3 with 42 VAL HG23 | OUTLIER (0%) General / 153.0,177.1 | 0.1% chi angles: 41.6,55.4,181.4,63.7 | 0.097Å | - | - |
| 41 | VAL 174.29 | 1.1Å HG23 with 65 ARG HB2 | Favored (8%) Isoleucine or valine / -120.5,99.7 | 13.3% (<i>p</i>) chi angles: 62.8 | 0.156Å | - | - |
| 42 | VAL 86.48 | 1.135Å HG23 with 40 LYS HD3 | Favored (23.12%) Isoleucine or valine / -108.2,141.6 | 87.7% (<i>t</i>) chi angles: 175.1 | 0.069Å | - | - |
| 43 | VAL 127.51 | 0.751Å HG23 with 122 LEU HD12 | Favored (48.2%) Isoleucine or valine / -99.6,130.7 | 5.7% (<i>m</i>) chi angles: 285.4 | 0.094Å | - | - |
| 44 | ILE 72.86 | 0.522Å HG12 with 123 ILE HD12 | Favored (64.29%) Isoleucine or valine / -129.6,127.2 | 82% (<i>mt</i>) chi angles: 300.9,170.6 | 0.091Å | - | - |
| 45 | THR 49.61 | 0.435Å O with 125 ASN HB3 | Favored (31.09%) General / -82.5,143.5 | 67.6% (<i>p</i>) chi angles: 63.1 | 0.07Å | - | - |
| 46 | GLY 57.86 | - | Favored (20.32%) Glycine / -140.9,148.7 | - | - | - | OUTLIER(S) worst is C-N- CA: 6.545 σ |
| 47 | ALA 112.55 | 0.476Å O with 48 ASN HB2 | Favored (55.17%) General / -81.0,-15.8 | - | 0.063Å | - | - |
| 48 | ASN 89.79 | 0.476Å HB2 with 47 ALA O | Allowed (1.46%) General / 70.2,38.4 | 56.1% (<i>m-20</i>) chi angles: 275.4,330 | 0.112Å | - | - |
| 49 | THR 58.21 | 0.62Å HG22 with 50 GLY N | Favored (12.09%) General / -123.1,168.7 | 59.2% (<i>m</i>) chi angles: 304.1 | 0.055Å | - | - |
| | | 0.62Å | Favored (97.65%) | | | | |

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|----|-----|--------|--------------------------|---|---|--------------------------|--------------------|--------------------|---------------------|
| 50 | GLY | 55.63 | N with 49 THR HG22 | Glycine / -62.1,-39.4 | - | - | - | - | |
| 51 | ILE | 170.53 | O with 51 ILE HD13 | 0.686Å Favored (99.45%) Isoleucine or valine / -61.6,-44.9 | 0% chi angles: 193.7,294.1 | 0.044Å | - | - | |
| 52 | GLY | 48.34 | N with 51 ILE HG23 | 0.534Å Favored (97.06%) Glycine / -65.2,-40.9 | - | - | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 124.27 | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |
| 53 | LYS | 111.57 | HG3 with 88 LYS CE | 0.784Å Favored (90.34%) General / -63.4,-45.6 | 25% (<i>ttpt</i>) chi angles: 186.8,165.5,98.3,175 | 0.087Å | - | - | |
| 54 | GLU | 129.58 | HA with 57 ARG HG2 | 0.762Å Favored (92.34%) General / -65.7,-40.3 | 10% (<i>mm-40</i>) chi angles: 284.3,262.5,340.7 | 0.106Å | - | - | |
| 55 | THR | 165.86 | O with 59 LEU HG | 0.446Å Favored (99.22%) General / -61.0,-43.1 | 41.6% (<i>p</i>) chi angles: 54.4 | 0.101Å | - | - | |
| 56 | ALA | 60.53 | - | - Favored (97.95%) General / -63.7,-42.1 | - | 0.078Å | - | - | |
| 57 | ARG | 159.86 | HG2 with 54 GLU HA | 0.762Å Favored (92.61%) General / -64.0,-44.5 | 12.9% (<i>ptm180</i>) chi angles: 60.2,172.8,294.5,198.5 | 0.081Å | - | - | |
| 58 | GLU | 154.28 | HG2 with 266 LEU HD13 | 0.53Å Favored (90.29%) General / -66.2,-40.6 | 20.8% (<i>tp10</i>) chi angles: 171.5,53.5,42.8 | 0.078Å | - | - | |
| 59 | LEU | 93.02 | HD12 with 44 ILE HD11 | 0.493Å Favored (91.5%) General / -65.7,-42.1 | 86.6% (<i>mt</i>) chi angles: 299.3,180.3 | 0.042Å | - | - | |
| 60 | ALA | 57.5 | HB1 with 90 SER HB2 | 1.105Å Favored (91.38%) General / -60.4,-40.6 | - | 0.076Å | - | - | |
| 61 | SER | 52.86 | - | - Favored (67.83%) General / -59.7,-29.1 | 67.1% (<i>m</i>) chi angles: 296.3 | 0.084Å | - | - | |

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|----|-----|--------|----------------------------------|--|---|--------|---|---|
| 62 | ARG | 141.07 | - | Favored (64.03%) General / -69.1,-23.7 | 26.2% (<i>mmm180</i>) chi angles: 293,310.4,297.3,159.3 | 0.07Å | - | - |
| 63 | GLY | 49.05 | - | Favored (18.45%) Glycine / 110.6,11.8 | - | - | - | - |
| 64 | ALA | 67.18 | - | Favored (38.13%) General / -75.7,149.0 | - | 0.088Å | - | - |
| 65 | ARG | 127.01 | 1.1Å HB2 with 41 VAL HG23 | Favored (23.96%) General / -90.6,112.3 | 85.1% (<i>mtp180</i>) chi angles: 294,178.4,65.8,187.8 | 0.129Å | - | - |
| 66 | VAL | 63.89 | - | Favored (49.57%) Isoleucine or valine / -106.4,133.9 | 83.5% (<i>t</i>) chi angles: 174.8 | 0.077Å | - | - |
| 67 | TYR | 197.65 | 0.936Å HE2 with 69 ALA HB2 | Favored (26.96%) General / -111.9,114.2 | 26% (<i>t80</i>) chi angles: 161.6,72.2 | 0.143Å | - | OUTLIER(S) worst is CA- CB-CG: 6.959 σ |
| 68 | ILE | 59.25 | 0.451Å CD1 with 92 VAL CG1 | Favored (54.74%) Isoleucine or valine / -101.4,123.8 | 91% (<i>mt</i>) chi angles: 296.7,174.3 | 0.097Å | - | - |
| 69 | ALA | 63.09 | 0.936Å HB2 with 67 TYR HE2 | Favored (32.26%) General / -106.6,116.6 | - | 0.123Å | - | - |
| 70 | CYS | 85.61 | - | Favored (42.33%) General / -143.2,159.4 | 42.8% (<i>t</i>) chi angles: 184.5 | 0.085Å | - | - |
| 71 | ARG | 92.77 | - | Favored (70.41%) General / -69.2,-45.2 | 24.9% (<i>ttm-85</i>) chi angles: 180.1,194.6,288.8,251 | 0.096Å | - | - |
| 72 | ASP | 52.25 | - | Favored (7.21%) General / -103.4,97.1 | 39.5% (<i>t0</i>) chi angles: 192.2,328.5 | 0.08Å | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|------|-----|-----|--------|--------------------|---------------------|--------------------------|--------------------|--------------------|---------------------|
| Avg: | | | | Clashscore: 124.27 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |
| | | | | 146.96 | Favored | | | | |

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|----|-----|--------|-----------------------------------|---|---|--------|---|---|
| 73 | VAL | 43.52 | 0.555Å HG13 with 94 VAL CG1 | Favored (72.59%) Isoleucine or valine / -68.4,-35.9 | 92% (<i>t</i>) chi angles: 177 | 0.059Å | - | - |
| 74 | LEU | 120.77 | 0.528Å C with 74 LEU HD13 | Favored (89.81%) General / -61.2,-46.6 | 3.1% (<i>tm?</i>) chi angles: 184.8,290.2 | 0.06Å | - | - |
| 75 | LYS | 92.14 | - | Favored (93.44%) General / -63.8,-44.4 | 1.9% (<i>ttmp?</i>) chi angles: 178.7,169.7,273.1,55 | 0.12Å | - | - |
| 76 | GLY | 28.71 | - | Favored (99.77%) Glycine / -62.9,-42.0 | - | - | - | - |
| 77 | GLU | 73.29 | - | Favored (96.89%) General / -64.2,-41.8 | 3.6% (<i>tp10</i>) chi angles: 189.9,79.2,298.3 | 0.08Å | - | - |
| 78 | SER | 28.67 | - | Favored (81.94%) General / -59.7,-48.4 | 95.5% (<i>p</i>) chi angles: 63.6 | 0.085Å | - | - |
| 79 | ALA | 36.58 | - | Favored (90.66%) General / -65.4,-43.5 | - | 0.085Å | - | - |
| 80 | ALA | 66.25 | 0.487Å HA with 88 LYS HD2 | Favored (75.08%) General / -70.2,-39.5 | - | 0.072Å | - | - |
| 81 | SER | 195.76 | - | Favored (7.97%) General / -95.9,172.5 | 96.4% (<i>p</i>) chi angles: 64.8 | 0.097Å | - | - |
| 82 | GLU | 265.7 | 1.015Å HB3 with 86 ASP HA | Favored (50.72%) General / -107.2,134.2 | 1.9% (<i>pp20?</i>) chi angles: 64.9,87.7,48.1 | 0.106Å | - | - |
| 83 | ILE | 88.92 | 0.447Å O with 83 ILE HG22 | Allowed (0.75%) Isoleucine or valine / -109.2,84.9 | 96.1% (<i>mt</i>) chi angles: 295.5,168.4 | 0.128Å | - | - |
| 84 | ARG | 198.75 | - | Favored (2.46%) General / 65.0,4.3 | 60.9% (<i>mtt180</i>) chi angles: 291.7,190.6,180,217.8 | 0.075Å | - | - |
| 85 | VAL | 77.25 | 0.596Å C with 82 GLU HB2 | Favored (2.67%) Isoleucine or valine / | 73.5% (<i>t</i>) chi angles: 173.9 | 0.106Å | - | - |

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|---|-----|--------|-----------------------------------|--|---|--------|---|---|
| | | | | -155.4,133.4 | | | | |
| 86 | ASP | 128.54 | 1.015Å HA with 82 GLU HB3 | Favored (10.61%) General / -77.4,108.6 | 52.6% (<i>m-20</i>) chi angles: 293.1,1.8 | 0.105Å | - | OUTLIER(S) worst is CA- CB-CG: 4.792 σ |
| 87 | THR | 87.12 | - | Favored (82.61%) General / -64.9,-46.2 | 74.1% (<i>p</i>) chi angles: 58.1 | 0.066Å | - | - |
| 88 | LYS | 69.92 | 0.784Å CE with 53 LYS HG3 | Favored (36.27%) General / -109.5,118.3 | 96.9% (<i>mttt</i>) chi angles: 285.6,176.7,176.2,180.6 | 0.12Å | - | - |
| 89 | ASN | 57.49 | - | Favored (46.14%) General / -73.3,145.3 | 89.3% (<i>m-20</i>) chi angles: 286.7,328.1 | 0.072Å | - | OUTLIER(S) worst is CA- CB-CG: 5.24 σ |
| 90 | SER | 164.78 | 1.105Å HB2 with 60 ALA HB1 | OUTLIER (0%) General / 95.0,-165.2 | 16.2% (<i>m</i>) chi angles: 307.8 | 0.096Å | - | - |
| 91 | GLN | 82.79 | - | Favored (21.34%) General / -106.9,109.4 | 71.5% (<i>mt-30</i>) chi angles: 292.6,188.7,57.1 | 0.13Å | - | - |
| 92 | VAL | 61.77 | 0.451Å CG1 with 68 ILE CD1 | Favored (39.91%) Isoleucine or valine / -121.7,113.6 | 79.7% (<i>t</i>) chi angles: 174.5 | 0.103Å | - | - |
| <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: 124.27</div> <div>Clashscore: 146.96</div> <div>Outliers: 14 of 276</div> <div>Poor rotamers: 11 of 234</div> <div>Outliers: 9 of 259</div> <div>Outliers: 8 of 278</div> <div>Outliers: 60 of 278</div> </div> | | | | | | | | |
| 93 | LEU | 148.87 | 0.572Å N with 93 LEU HD22 | Favored (24.2%) General / -104.9,151.2 | 1.9% (<i>mm?</i>) chi angles: 295.6,296.3 | 0.086Å | - | - |
| 94 | VAL | 116.56 | 0.555Å CG1 with 73 VAL HG13 | Favored (62.69%) Isoleucine or valine / -121.5,135.1 | 1% chi angles: 86.8 | 0.037Å | - | - |
| 95 | ARG | 134.86 | 0.68Å HB2 with 67 TYR CE1 | Favored (33.29%) General / -134.7,162.1 | 44.3% (<i>mtm180</i>) chi angles: 301.6,202.1,301.3,185.6 | 0.185Å | - | OUTLIER(S) worst is N- CA-CB: 4.407 σ |
| 96 | LYS | 110.69 | 0.721Å NZ with 98 ASP HB2 | Favored (34.37%) General / -84.7,134.0 | 5.7% (<i>tmtt?</i>) chi angles: 197.2,290.9,182.5,158 | 0.034Å | - | - |
| | | | | Favored | | | | |

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|-----|-----|--------|-----------------------------------|---|---|--------|---|---|
| 97 | LEU | 74.49 | 0.65Å N with 96 LYS HD3 | (11.91%) General / -151.2,129.4 | 62.2% (<i>tp</i>) chi angles: 175.3,61.6 | 0.094Å | - | - |
| 98 | ASP | 63.07 | 0.721Å HB2 with 96 LYS NZ | Favored (11.04%) General / -117.7,104.5 | 66.2% (<i>t0</i>) chi angles: 186,356.3 | 0.113Å | - | - |
| 99 | LEU | 81.38 | - | Favored (68.16%) General / -64.1,-25.6 | 68.6% (<i>mt</i>) chi angles: 290.5,179.9 | 0.061Å | - | - |
| 100 | SER | 66.61 | - | Favored (36.54%) General / -76.8,-3.1 | 71.2% (<i>m</i>) chi angles: 295.8 | 0.079Å | - | - |
| 101 | ASP | 64.01 | - | Favored (13.85%) General / -132.2,113.9 | 60.4% (<i>t0</i>) chi angles: 187.9,344.2 | 0.084Å | - | - |
| 102 | THR | 107.33 | 0.825Å O with 105 ILE HG22 | Favored (78.85%) General / -62.5,-35.2 | 15% (<i>t</i>) chi angles: 188.3 | 0.073Å | - | - |
| 103 | LYS | 66.57 | 0.496Å N with 102 THR HG23 | Favored (97.36%) General / -63.0,-40.3 | 74.1% (<i>tttt</i>) chi angles: 191.6,162.8,181,169.4 | 0.078Å | - | - |
| 104 | SER | 88.71 | - | Favored (74.45%) General / -68.4,-33.6 | 78.4% (<i>p</i>) chi angles: 59.2 | 0.098Å | - | - |
| 105 | ILE | 131.35 | 0.856Å HD11 with 154 LEU HA | Favored (90.59%) Isoleucine or valine / -62.8,-41.0 | 0.1% chi angles: 198.4,292.5 | 0.061Å | - | - |
| 106 | ARG | 134.57 | 0.425Å N with 105 ILE CG2 | Favored (93.73%) General / -63.0,-45.2 | 13.4% (<i>mmm180</i>) chi angles: 288.4,271.4,304.4,139.5 | 0.1Å | - | - |
| 107 | ALA | 23.77 | - | Favored (99.75%) General / -63.1,-42.9 | - | 0.089Å | - | - |
| 108 | PHE | 63.38 | 0.553Å CZ with 112 PHE CD1 | Favored (91.25%) General / -63.9,-45.0 | 37% (<i>t80</i>) chi angles: 164.2,72.5 | 0.084Å | - | OUTLIER(S) worst is CA- CB-CG: 8.957 σ |
| 109 | ALA | 42.58 | - | Favored (90.45%) General / | - | 0.084Å | - | - |

| | | | | | -61.9,-39.0 | | | | |
|-----|---------|-------------|-----------------------------------|--|---|--|--------------------|--|---|
| 110 | GLU | 80.26 | - | | Favored (72.86%) General / -60.7,-33.5 | 40.6% (<i>tt0</i>) chi angles: 180.6,178.4,304.3 | 0.066Å | - | - |
| 111 | GLY | 36.4 | 0.493Å C with 95 ARG HH22 | | Favored (93.48%) Glycine / -64.0,-36.6 | - | - | - | - |
| 112 | PHE | 80.44 | 0.648Å O with 161 ARG HD3 | | Favored (20.78%) General / -80.8,116.3 | 8.8% (<i>m-85</i>) chi angles: 267.9,89.6 | 0.175Å | - | OUTLIER(S) worst is CA- CB-CG: 8.593 σ |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | |
| | | Avg: 124.27 | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 | |
| 113 | LEU | 134.77 | 0.848Å HD22 with 114 ALA N | Favored (85.29%) General / -67.5,-40.5 | 0% chi angles: 52.4,301.6 | 0.073Å | - | - | |
| 114 | ALA | 51.84 | 0.848Å N with 113 LEU HD22 | Favored (2.09%) General / -175.7,157.9 | - | 0.098Å | - | - | |
| 115 | GLU | 119.5 | 0.91Å HB2 with 121 ILE CG1 | Favored (54.03%) General / -121.6,131.3 | 0.3% chi angles: 25.7,265,11.6 | 0.066Å | - | OUTLIER(S) worst is CB- CG-CD: 4.01 σ | |
| 116 | GLU | 175.54 | 0.833Å CG with 41 VAL HG12 | Favored (70.34%) General / -57.1,-51.2 | 8.5% (<i>mm-40</i>) chi angles: 278.7,268.3,20 | 0.139Å | - | - | |
| 117 | LYS | 262.06 | 1.052Å HB3 with 167 PRO HA | Favored (12.25%) General / 61.5,41.8 | 23.8% (<i>tttt</i>) chi angles: 215.1,161.7,170.4,197.8 | 0.089Å | - | - | |
| 118 | GLN | 130.36 | - | Favored (90.52%) General / -63.3,-38.3 | 7.9% (<i>tt0</i>) chi angles: 179.9,182.2,180.6 | 0.159Å | - | - | |
| 119 | LEU | 232.59 | 1.136Å HD21 with 38 PRO HG2 | Allowed (1.7%) General / -107.3,-170.4 | 8% (<i>mp</i>) chi angles: 280.7,53.1 | 0.079Å | - | - | |
| 120 | HIS | 212.87 | 0.679Å CG with 171 VAL HG23 | Favored (49.02%) General / -57.6,131.1 | 22.8% (<i>m-70</i>) chi angles: 287.7,242.5 | 0.191Å | - | OUTLIER(S) worst is C-N- CA: 4.467 σ | |
| | | | | | Favored | | | | |

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|-----|-----|--------|--|--|--|--------|---|---|
| 121 | ILE | 246.39 | 1.089Å HD12 with 42 VAL HG22 | (11.18%) Isoleucine or valine / -108.7,-9.1 | 4.8% (<i>tp</i>) chi angles: 206,54.1 | 0.136Å | - | - |
| 122 | LEU | 69.93 | 0.751Å HD12 with 43 VAL HG23 | Favored (44.57%) General / -119.8,123.8 | 65.6% (<i>tp</i>) chi angles: 175.9,62.8 | 0.111Å | - | - |
| 123 | ILE | 63.03 | 0.522Å HD12 with 44 ILE HG12 | Favored (44.82%) Isoleucine or valine / -116.1,114.0 | 99.2% (<i>mt</i>) chi angles: 297.5,171.8 | 0.086Å | - | - |
| 124 | ASN | 77.78 | 0.55Å HD22 with 172 ASN ND2 | Favored (5.85%) General / -91.1,78.9 | 86.8% (<i>m-20</i>) chi angles: 292.6,315.9 | 0.098Å | - | OUTLIER(S) worst is CA- CB-CG: 4.505 σ |
| 125 | ASN | 107.01 | 0.435Å HB3 with 45 THR O | Favored (17.51%) General / -87.2,-37.1 | 31.4% (<i>t30</i>) chi angles: 179.9,71.4 | 0.073Å | - | OUTLIER(S) worst is CA- CB-CG: 4.449 σ |
| 126 | ALA | 52.42 | - | Favored (55.36%) General / -62.4,144.8 | - | 0.081Å | - | - |
| 127 | GLY | 42.59 | 0.497Å HA2 with 147 ASN OD1 | Favored (24.09%) Glycine / -163.8,153.6 | - | - | - | - |
| 128 | VAL | 123.43 | 0.806Å HG12 with 146 VAL HG21 | Favored (19.15%) Isoleucine or valine / -117.3,152.3 | 9% (<i>p</i>) chi angles: 60.3 | 0.095Å | - | - |
| 129 | MET | 125.09 | 0.453Å HE2 with 200 TYR CZ | Favored (22.78%) General / -142.7,131.5 | 40.7% (<i>ttm</i>) chi angles: 192.3,179.9,304 | 0.094Å | - | - |
| 130 | MET | 139.48 | 0.506Å HG2 with 130 MET O | Favored (20.07%) General / 51.9,49.8 | 55.3% (<i>ttm</i>) chi angles: 188.6,181.4,294.7 | 0.071Å | - | - |
| 131 | CYS | 40.41 | 0.647Å H with 143 HIS CE1 | Allowed (1.59%) Pre-proline / -100.2,177.2 | 87.9% (<i>m</i>) chi angles: 293 | 0.096Å | - | - |
| 132 | PRO | 63.86 | 0.438Å HD2 with 131 CYS HB3 | Favored (37.31%) Trans-proline / -71.4,164.0 | 71.9% (<i>Cg_exo</i>) chi angles: 332.6 | 0.092Å | - | - |

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| # | Alt | Res | High B | 0.4Å | Ramachandran | Rotamer | deviation | lengths | angles |
|-----|-----|--------|----------------------------------|------|--|--|--------------------|--------------------|---|
| | | | Avg: Clashscore: Outliers: 14 of | | Poor rotamers: 11 of | | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |
| | | | 124.27 146.96 | | 276 | | 234 | | |
| 133 | TYR | 139.16 | - | | Favored (26.89%) General / -71.5,125.4 | 74.7% (<i>t80</i>) chi angles: 177.3,87.3 | 0.049Å | - | - |
| 134 | SER | 54.02 | 0.757Å O with 142 THR HG23 | | Favored (37.16%) General / -158.5,160.9 | 44.9% (<i>p</i>) chi angles: 54.1 | 0.062Å | - | - |
| 135 | LYS | 72.92 | - | | Favored (28.21%) General / -116.1,155.4 | 53.8% (<i>mtmt</i>) chi angles: 290.5,177.3,291.4,178.9 | 0.115Å | - | - |
| 136 | THR | 33.03 | - | | Favored (6.19%) General / -86.7,-177.7 | 59.2% (<i>p</i>) chi angles: 62.4 | 0.089Å | - | - |
| 137 | ALA | 34.67 | - | | Favored (88.57%) General / -61.2,-39.0 | - | 0.098Å | - | - |
| 138 | ASP | 77.41 | 0.454Å CB with 140 PHE CE2 | | Favored (62.47%) General / -70.9,-21.0 | 62.2% (<i>m-20</i>) chi angles: 291.4,0.6 | 0.065Å | - | OUTLIER(S) worst is CA-CB-CG: 5.106 σ |
| 139 | GLY | 39.01 | - | | Favored (35.41%) Glycine / 99.7,14.2 | - | - | - | - |
| 140 | PHE | 102.17 | 0.578Å HD1 with 189 GLN OE1 | | Favored (20.24%) General / -89.9,154.0 | 28.6% (<i>m-85</i>) chi angles: 308.8,302.2 | 0.18Å | - | - |
| 141 | GLU | 147.02 | 0.513Å OE2 with 143 HIS HB2 | | Favored (55.59%) General / -66.2,145.6 | 1.1% (<i>pp20?</i>) chi angles: 80.1,92.9,351.3 | 0.086Å | - | - |
| 142 | THR | 128.56 | 0.757Å HG23 with 134 SER O | | Favored (99.58%) General / -62.1,-42.8 | 66.9% (<i>p</i>) chi angles: 59.5 | 0.081Å | - | - |
| 143 | HIS | 88.83 | 0.647Å CE1 with 131 CYS H | | Favored (65.21%) General / -68.1,-48.5 | 75.3% (<i>m80</i>) chi angles: 295.1,78.2 | 0.048Å | - | OUTLIER(S) worst is CD2-NE2-CE1: 4.418 σ |
| 144 | LEU | 96.48 | 0.963Å HD22 with 188 LEU HG | | Favored (96.82%) General / | 21.3% (<i>tp</i>) chi angles: 175.4,75.6 | 0.165Å | - | - |

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|-----|-----|--------|--|--|--|--------|---|---|
| 145 | GLY | 44.64 | - | -64.0,-40.6 Favored (90.89%) Glycine / -64.0,-46.6 | - | - | - | - |
| 146 | VAL | 115.9 | 0.806Å HG21 with 128 VAL HG12 | Favored (22%) Isoleucine or valine / -74.3,-51.8 | 30.4% (<i>m</i>) chi angles: 294.3 | 0.052Å | - | - |
| 147 | ASN | 82.24 | 0.606Å N with 146 VAL HG23 | Favored (38.02%) General / -70.4,-50.5 | 91.6% (<i>m-20</i>) chi angles: 294.3,331.1 | 0.075Å | - | OUTLIER(S) worst is CA- CB-CG: 4.899 σ |
| 148 | HIS | 107.98 | 0.531Å HD2 with 149 LEU HD22 | Favored (2.18%) General / -91.0,-59.4 | 86.3% (<i>t60</i>) chi angles: 180.7,69 | 0.075Å | - | OUTLIER(S) worst is CD2- NE2-CE1: 4.464 σ |
| 149 | LEU | 124.52 | 0.857Å HD23 with 144 LEU HG | Favored (90.17%) General / -63.8,-45.3 | 2.1% (<i>mm?</i>) chi angles: 283.5,283.4 | 0.079Å | - | - |
| 150 | GLY | 29.97 | - | Favored (98.4%) Glycine / -63.8,-40.4 | - | - | - | - |
| 151 | HIS | 65.7 | - | Favored (80.49%) General / -67.6,-36.3 | 29.3% (<i>m170</i>) chi angles: 284.2,146.9 | 0.055Å | - | OUTLIER(S) worst is CD2- NE2-CE1: 4.458 σ |
| 152 | PHE | 59.27 | - | Favored (81.4%) General / -60.1,-48.5 | 79.8% (<i>t80</i>) chi angles: 180.1,84.7 | 0.094Å | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | C β deviation | Bond lengths | Bond angles |
|-------------|-----|-----|--------|--------------------|---------------------|--------------------------|------------------------|--------------------|---------------------|
| Avg: 124.27 | | | | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |

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|-----|-----|--------|-----------------------------------|---|--|--------|---|---|
| 153 | LEU | 98.03 | - | Favored (92.18%) General / -65.3,-43.1 | 81.8% (<i>mt</i>) chi angles: 297.8,182.4 | 0.09Å | - | - |
| 154 | LEU | 52.29 | 0.856Å HA with 105 ILE HD11 | Favored (98.36%) General / -61.9,-43.7 | 63.1% (<i>tp</i>) chi angles: 179.7,63.5 | 0.096Å | - | - |
| 155 | THR | 47.6 | 0.601Å O with 159 LEU HG | Favored (91.19%) General / -65.2,-43.6 | 86.6% (<i>m</i>) chi angles: 301.2 | 0.046Å | - | - |
| 156 | TYR | 104.02 | - | Favored (96.35%) | 24.8% (<i>t80</i>) | 0.123Å | - | OUTLIER(S) worst is CA- CB-CG: 4.68 |

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| | | | | General / -60.2,-43.2 | chi angles: 161,76.4 | | | σ |
| 157 | LEU | 59.98 | - | Favored (94.6%) General / -65.0,-42.3 | 83.8% (<i>mt</i>) chi angles: 294.7,180 | 0.076Å | - | - |
| 158 | LEU | 83.5 | 0.624Å O with 162 LEU HD13 | Favored (62.63%) General / -73.9,-30.5 | 81.5% (<i>mt</i>) chi angles: 294.4,180.3 | 0.081Å | - | - |
| 159 | LEU | 77.13 | 0.601Å HG with 155 THR O | Favored (67.83%) General / -53.7,-42.2 | 55.6% (<i>mt</i>) chi angles: 288.2,180.1 | 0.1Å | - | - |
| 160 | GLU | 71.75 | - | Favored (98.92%) General / -62.3,-41.9 | 62.6% (<i>mm-40</i>) chi angles: 291.1,289,303.7 | 0.073Å | - | - |
| 161 | ARG | 90.56 | 0.648Å HD3 with 112 PHE O | Favored (98.56%) General / -62.1,-41.8 | 82.5% (<i>mtt-85</i>) chi angles: 308,179.3,194.3,275.1 | 0.154Å | - | - |
| 162 | LEU | 151.09 | 0.925Å HD23 with 117 LYS HD2 | Favored (5.79%) General / -79.3,77.2 | 5% (<i>mp</i>) chi angles: 291.5,56.3 | 0.112Å | - | - |
| 163 | LYS | 231.57 | 0.595Å N with 167 PRO HG2 | Favored (5.98%) General / -54.0,152.2 | 0.1% chi angles: 179.7,160.6,254.4,52.9 | 0.081Å | - | - |
| 164 | VAL | 160.06 | 0.601Å HG13 with 165 SER N | Favored (90.19%) Isoleucine or valine / -58.7,-46.9 | 6.3% (<i>p</i>) chi angles: 55.3 | 0.049Å | - | - |
| 165 | SER | 51.06 | 0.601Å N with 164 VAL HG13 | OUTLIER (0.04%) General / -60.9,-78.1 | 79.9% (<i>p</i>) chi angles: 59.9 | 0.079Å | - | - |
| 166 | ALA | 54.33 | 0.903Å HB3 with 167 PRO HD3 | Favored (41%) Pre-proline / -67.7,-48.9 | - | 0.092Å | - | - |
| 167 | PRO | 228.32 | 1.052Å HA with 117 LYS HB3 | Favored (6.49%) Trans-proline / -72.3,120.0 | 84.3% (<i>Cg_exo</i>) chi angles: 331 | 0.288Å | - | - |
| 168 | ALA | 103.41 | 0.867Å HB1 with 169 ARG HD2 | Favored (6.89%) General / -72.0,-55.7 | - | 0.089Å | - | - |

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|--------|-----|--------|--------------------------------------|--|--|-----------|-----------------|--|----------------|
| 169 | ARG | 235.77 | 0.867Å HD2 with 168 ALA HB1 | Favored (11.99%) General / -166.3,171.6 | 8.5% (<i>mpt_?</i>) chi angles: 292,85.7,171.5,159.8 | 0.14Å | - | - | |
| 170 | VAL | 75.62 | - | Favored (69.94%) Isoleucine or valine / -121.7,132.8 | 79.8% (<i>t</i>) chi angles: 174.5 | 0.125Å | - | - | |
| 171 | VAL | 90.06 | 0.679Å HG23 with 120 HIS CG | Favored (73.91%) Isoleucine or valine / -116.8,125.8 | 77.7% (<i>t</i>) chi angles: 172.3 | 0.208Å | - | - | |
| 172 | ASN | 74.14 | 0.55Å ND2 with 124 ASN HD22 | Favored (55.8%) General / -113.8,132.6 | 8.8% (<i>m120</i>) chi angles: 286.1,75.9 | 0.127Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: | | | Clashscore: | Outliers: 14 of | Poor rotamers: 11 of | Outliers: | Outliers: 8 | Outliers: 60 | |
| 124.27 | | | 146.96 | 276 | 234 | 9 of 259 | of 278 | of 278 | |
| 173 | VAL | 77.62 | - | Favored (46.1%) Isoleucine or valine / -94.6,128.1 | 78.1% (<i>t</i>) chi angles: 179.2 | 0.058Å | - | - | |
| 174 | SER | 143.26 | 0.633Å O with 229 HIS HB2 | Allowed (0.5%) General / -115.7,-152.4 | 60.3% (<i>p</i>) chi angles: 72.2 | 0.104Å | - | - | |
| 175 | SER | 107.93 | 0.512Å OG with 234 ARG HB3 | Favored (25.23%) General / -162.2,166.6 | 41.6% (<i>t</i>) chi angles: 177.5 | 0.114Å | - | - | |
| 176 | VAL | 169.83 | 0.429Å HG13 with 177 ALA N | Favored (40.89%) Isoleucine or valine / -63.2,-26.4 | 14.5% (<i>p</i>) chi angles: 63.3 | 0.109Å | - | - | |
| 177 | ALA | 104.75 | 0.429Å N with 176 VAL HG13 | Favored (62.14%) General / -58.4,-25.4 | - | 0.079Å | - | - | |
| 178 | HIS | 136.37 | 0.714Å NE2 with 291 SER HB3 | Favored (67.33%) General / -64.5,-23.6 | 4% (<i>p-80</i>) chi angles: 69.4,240.8 | 0.17Å | - | OUTLIER(S) worst is CD2- NE2-CE1: 4.372 σ | |
| 179 | HIS | 105.73 | - | Favored (71.76%) General / | 58.3% (<i>t-80</i>) chi angles: 197.3,286.1 | 0.067Å | - | OUTLIER(S) worst is CD2- NE2-CE1: | |

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| | | | | -56.1,-50.2 | | | | 4.44 σ |
| 180 | ILE | 157.37 | 0.432Å CG2 with 201 CYS SG | Favored (36.62%) Isoleucine or valine / -69.2,-27.9 | 11.2% (<i>tp</i>) chi angles: 192.1,66.6 | 0.075Å | - | - |
| 181 | GLY | 63.94 | - | Favored (33.76%) Glycine / -60.3,154.3 | - | - | - | - |
| 182 | LYS | 87.5 | - | Favored (36.11%) General / -142.2,147.2 | 53.6% (<i>mttm</i>) chi angles: 290.5,167.8,168.5,291.3 | 0.138Å | - | - |
| 183 | ILE | 138.76 | 0.602Å HD13 with 202 HIS CD2 | Favored (65.37%) Pre-proline / -98.4,114.5 | 43.9% (<i>mm</i>) chi angles: 303.1,296 | 0.097Å | - | - |
| 184 | PRO | 120.69 | 0.632Å HD2 with 202 HIS CE1 | Allowed (1.94%) Trans-proline / -84.3,115.3 | 12.5% (<i>Cg_endo</i>) chi angles: 15.5 | 0.121Å | - | - |
| 185 | PHE | 115.05 | - | Favored (66.6%) General / -70.7,-44.5 | 46.3% (<i>m-85</i>) chi angles: 308.8,273 | 0.14Å | - | OUTLIER(S) worst is CA- CB-CG: 5.928 σ |
| 186 | HIS | 90.21 | - | Favored (64.62%) General / -64.0,-51.4 | 71.8% (<i>m80</i>) chi angles: 298.1,77.6 | 0.075Å | - | OUTLIER(S) worst is CD2- NE2-CE1: 4.457 σ |
| 187 | ASP | 180.94 | 0.78Å HB3 with 190 SER HB3 | Allowed (1.21%) General / -123.7,73.6 | 75.5% (<i>m-20</i>) chi angles: 290.5,323.4 | 0.15Å | - | - |
| 188 | LEU | 97.32 | 0.963Å HG with 144 LEU HD22 | Favored (72.35%) General / -63.4,-49.8 | 27.4% (<i>tp</i>) chi angles: 190.5,65 | 0.121Å | - | OUTLIER(S) worst is C-N- CA: 4.289 σ |
| 189 | GLN | 140.17 | 0.578Å OE1 with 140 PHE HD1 | Favored (17.86%) General / -90.2,-30.0 | 22.5% (<i>mt-30</i>) chi angles: 300.8,172.8,188.9 | 0.136Å | - | OUTLIER(S) worst is C-N- CA: 6.985 σ |
| 190 | SER | 196.77 | 0.78Å HB3 with 187 ASP HB3 | OUTLIER (0.03%) General / -66.0,-165.3 | 2.1% (<i>t</i>) chi angles: 205.1 | 0.14Å | - | OUTLIER(S) worst is C-N- CA: 7.645 σ |
| 191 | GLU | 141.52 | - | Favored (67.06%) General / -56.1,-35.5 | 13.3% (<i>pt-20</i>) chi angles: 64.1,180.1,54 | 0.109Å | - | - |
| | | | | Favored | | | | |

| 192 | LYS | 115.39 | 0.421Å NZ with 184 PRO HG3 | (3.74%) General / -56.3,159.1 | 19% (<i>pttm</i>) chi angles: 61.6,164.9,174.3,283.6 | 0.086Å | - | - | |
|-----|-----|--------|------------------------------------|-------------------------------------|--|---|--------------------|--------------------|---|
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 124.27 | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |
| 193 | ARG | 112.01 | - | - | Favored (9.18%) General / -53.9,149.1 | 17.4% (<i>ptm180</i>) chi angles: 62.6,186,293.3,171.5 | 0.107Å | - | - |
| 194 | TYR | 91.21 | - | - | Favored (44.79%) General / -102.6,135.2 | 79.5% (<i>t80</i>) chi angles: 184.4,78.2 | 0.07Å | - | - |
| 195 | SER | 100.86 | 0.773Å OG with 198 PHE HB2 | - | Favored (46.81%) General / -127.6,129.2 | 93.6% (<i>p</i>) chi angles: 66.9 | 0.107Å | - | - |
| 196 | ARG | 107.71 | 0.628Å HG2 with 131 CYS O | - | Favored (92.61%) General / -61.6,-45.8 | 77.2% (<i>mtm180</i>) chi angles: 293.4,173.3,290,153.4 | 0.075Å | - | - |
| 197 | GLY | 51.63 | - | - | Favored (77.77%) Glycine / -67.9,-44.9 | - | - | - | - |
| 198 | PHE | 72.95 | 0.773Å HB2 with 195 SER OG | - | Favored (75.89%) General / -67.8,-34.0 | 34.7% (<i>m-85</i>) chi angles: 278.5,80.8 | 0.159Å | - | - |
| 199 | ALA | 42.08 | - | - | Favored (95.4%) General / -62.5,-40.0 | - | 0.086Å | - | - |
| 200 | TYR | 78.18 | 0.552Å OH with 204 LYS HE3 | - | Favored (93.75%) General / -64.0,-44.1 | 66.5% (<i>t80</i>) chi angles: 183.2,66.6 | 0.036Å | - | - |
| 201 | CYS | 60.18 | 0.432Å SG with 180 ILE CG2 | - | Favored (91.47%) General / -63.2,-38.5 | 68.8% (<i>m</i>) chi angles: 301.8 | 0.036Å | - | - |
| 202 | HIS | 75.92 | 0.828Å CE1 with 188 LEU HD12 | - | Favored (98.19%) General / -61.4,-42.1 | 5.1% (<i>t-160</i>) chi angles: 180,163.1 | 0.102Å | - | OUTLIER(S) worst is CD2- NE2-CE1: 4.56 σ |
| 203 | SER | 101.46 | - | - | Favored (92.16%) General / | 17.8% (<i>m</i>) chi angles: 307.1 | 0.173Å | - | - |

-65.7,-41.5

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|-------------|-----|--------|---------------------------------------|---|--|--------------------------|--------------------|--------------------|---------------------|
| 204 | LYS | 143.54 | 0.552Å HE3 with 200 TYR OH | Favored (77.38%) General / -69.0,-36.0 | 37.3% (<i>mm</i> tt) chi angles: 287.1,303.7,151,185.3 | 0.109Å | - | - | |
| 205 | LEU | 132.3 | 0.772Å O with 208 VAL HG22 | Favored (92.78%) General / -65.4,-40.0 | 1% chi angles: 192.5,304.9 | 0.142Å | - | - | |
| 206 | ALA | 49.87 | - | Favored (82.9%) General / -61.2,-37.4 | - | 0.086Å | - | - | |
| 207 | ASN | 81.16 | - | Favored (85.55%) General / -59.3,-40.3 | 25.6% (<i>m</i> 120) chi angles: 292,132.1 | 0.142Å | - | - | |
| 208 | VAL | 152.71 | 0.782Å HG11 with 248 TRP CZ3 | Favored (61.22%) Isoleucine or valine / -72.8,-41.7 | 20.8% (<i>m</i>) chi angles: 303.3 | 0.113Å | - | - | |
| 209 | LEU | 71.19 | 0.569Å HG with 205 LEU CD1 | Favored (82.63%) General / -62.1,-36.7 | 79.3% (<i>mt</i>) chi angles: 292.8,179.9 | 0.09Å | - | - | |
| 210 | PHE | 78.7 | - | Favored (88.79%) General / -59.5,-46.5 | 61.1% (<i>t</i> 80) chi angles: 168.6,79.9 | 0.094Å | - | - | |
| 211 | THR | 69.96 | 0.51Å HG23 with 225 THR HG23 | Favored (95.3%) General / -64.7,-40.4 | 92.2% (<i>m</i>) chi angles: 300.4 | 0.051Å | - | - | |
| 212 | ARG | 182.06 | 0.613Å HB2 with 212 ARG NH1 | Favored (78.47%) General / -65.1,-47.1 | 12.7% (<i>ttm</i> 105) chi angles: 168.4,172,277.8,84.9 | 0.083Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: 124.27 | | | | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |
| 213 | GLU | 102.08 | 0.525Å HG3 with 217 ARG HE | Favored (85.1%) General / -67.5,-40.3 | 19.1% (<i>tp</i> 10) chi angles: 178.1,65.9,345.5 | 0.066Å | - | - | |
| 214 | LEU | 144.29 | 0.99Å HD13 with 218 LEU HD13 | Favored (91.76%) General / -59.0,-44.9 | 1.8% (<i>tm</i> ?) chi angles: 186.1,299.8 | 0.135Å | - | - | |
| | | | | Favored | | | | | |

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|-----|-----|--------|---------------------------------------|--|---|--------|---|--|
| 215 | ALA | 61.08 | - | (91.1%) General / -64.3,-38.5 | - | 0.074Å | - | - |
| 216 | LYS | 146.29 | 0.62Å C with 216 LYS HD2 | Favored (97.12%) General / -61.8,-44.3 | 3.6% (<i>tmmm?</i>) chi angles: 179.7,286.7,286.6,294.8 | 0.014Å | - | - |
| 217 | ARG | 70.09 | 0.525Å HE with 213 GLU HG3 | Favored (94.7%) General / -65.2,-41.2 | 86.3% (<i>mtt-85</i>) chi angles: 298.2,171.5,185.7,261.7 | 0.019Å | - | - |
| 218 | LEU | 139 | 1.07Å HD23 with 223 VAL HG23 | Favored (64.71%) General / -68.3,-22.1 | 10.1% (<i>mp</i>) chi angles: 278,56.2 | 0.104Å | - | - |
| 219 | GLN | 89.88 | - | Favored (68.41%) General / -56.3,-36.2 | 64.6% (<i>tt0</i>) chi angles: 179.9,181.4,359.2 | 0.133Å | - | - |
| 220 | GLY | 45.97 | - | Favored (71.64%) Glycine / -64.8,-48.5 | - | - | - | - |
| 221 | THR | 130.17 | 0.903Å HG22 with 218 LEU HA | Favored (49.24%) General / -69.6,-49.9 | 7.1% (<i>t</i>) chi angles: 194.1 | 0.108Å | - | - |
| 222 | GLY | 54.18 | 0.582Å N with 221 THR HG23 | Favored (4.08%) Glycine / 121.6,-34.0 | - | - | - | - |
| 223 | VAL | 132.42 | 1.07Å HG23 with 218 LEU HD23 | Favored (5.29%) Isoleucine or valine / -77.3,157.4 | 27.8% (<i>m</i>) chi angles: 295.5 | 0.07Å | - | - |
| 224 | THR | 155.12 | 0.646Å HG23 with 169 ARG HG2 | Favored (30.6%) General / -128.5,161.0 | 10.1% (<i>t</i>) chi angles: 181.3 | 0.172Å | - | - |
| 225 | THR | 133.18 | 0.602Å HB with 214 LEU HD12 | Favored (55.21%) General / -121.2,133.9 | 14.8% (<i>t</i>) chi angles: 188.7 | 0.057Å | - | - |
| 226 | TYR | 124.84 | 0.893Å CG with 274 LEU HB2 | Favored (10.91%) General / -133.0,173.9 | 0.9% chi angles: 314.7,352.2 | 0.265Å | - | OUTLIER(S) worst is N- CA-CB: 4.747 σ |
| | | | 1.021Å | Favored | | | | |

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|-----|-----|--------|---------------------------------------|--|--|--------|---|--|
| 227 | ALA | 85.56 | HB3 with 277 LEU HG | (22.82%) General / -142.2,167.1 Favored (3.54%) | - | 0.088Å | - | - |
| 228 | VAL | 158.02 | 0.779Å HG21 with 264 THR C | Isoleucine or valine / -154.4,158.7 Favored (29.58%) | 13.4% (<i>p</i>) chi angles: 62.8 | 0.155Å | - | - |
| 229 | HIS | 152.9 | 0.877Å NE2 with 247 LEU HB3 | Pre-proline / -149.7,149.9 Favored (26.59%) | 0.9% chi angles: 90.4,69.1 | 0.324Å | - | OUTLIER(S) worst is CA- CB-CG: 6.445 σ |
| 230 | PRO | 164.25 | 0.967Å HB2 with 244 LEU HD22 | Trans-proline / -72.9,-13.3 Favored (19.11%) | 23.5% (<i>Cg_endo</i>) chi angles: 19.9 | 0.172Å | - | OUTLIER(S) worst is C-N- CA: 4.702 σ |
| 231 | GLY | 98.78 | 0.748Å HA3 with 245 CYS C | Glycine / 100.0,-151.0 Favored (32.85%) | - | - | - | - |
| 232 | VAL | 157.39 | 0.759Å HG13 with 284 ASP O | Isoleucine or valine / -56.0,-32.3 Favored (28.86%) | 34.5% (<i>m</i>) chi angles: 298.7 | 0.085Å | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | C β deviation | Bond lengths | Bond angles |
|-------------|-----|-----|--------|--------------------|---------------------|--------------------------|------------------------|--------------------|---------------------|
| Avg: 124.27 | | | | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |

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|-----|-----|--------|--------------------------------------|---|---|--------|--|---|
| 233 | VAL | 181.19 | 1.194Å HG21 with 240 HIS HB3 | Favored (28.86%) Isoleucine or valine / -69.9,-25.8 | 86.7% (<i>t</i>) chi angles: 177.7 | 0.339Å | - | OUTLIER(S) worst is CA- CB-CG2: 5.339 σ |
| 234 | ARG | 269.11 | 0.803Å HG2 with 230 PRO HG2 | Favored (21.11%) General / -77.8,1.2 | 15.8% (<i>mmt85</i>) chi angles: 275.9,304.5,178.4,91.2 | 0.145Å | - | - |
| 235 | SER | 136.67 | - | Allowed (0.16%) General / -88.2,-148.8 | 96.4% (<i>p</i>) chi angles: 66.4 | 0.161Å | - | OUTLIER(S) worst is N- CA-C: 4.003 σ |
| 236 | GLU | 224.8 | 0.548Å HG2 with 236 GLU O | Favored (62.37%) General / -59.1,-23.7 | 38.1% (<i>tt0</i>) chi angles: 180.1,191.9,43.9 | 0.085Å | OUTLIER(S) worst is C--N: 4.235 σ | OUTLIER(S) worst is C-N- CA: 5.005 σ |
| 237 | LEU | 328.28 | 0.636Å N with 237 LEU HD12 | Allowed (0.11%) General / -83.9,-150.4 | 4% (<i>mp</i>) chi angles: 299.3,69 | 0.135Å | OUTLIER(S) worst is C--N: 7.431 σ | OUTLIER(S) worst is C-N- CA: 6.299 σ |
| | | | 0.664Å | OUTLIER (0%) Isoleucine or | 39.6% (<i>t</i>) | | | OUTLIER(S) |

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|-----|------------|---------------------------------------|---|---|--------|--|---|
| 238 | VAL 361.18 | HG12 with 239 ARG N | valine / -161.2,-125.8 | chi angles: 185.1 | 0.04Å | - | worst is C-N- CA: 5.731 σ |
| 239 | ARG 374.78 | 0.664Å N with 238 VAL HG12 | OUTLIER (0%) General / -0.7,63.3 | 50.3% (<i>mtm180</i>) chi angles: 293.8,196.5,298.1,148.7 | 0.093Å | - | - |
| 240 | HIS 277.74 | 1.194Å HB3 with 233 VAL HG21 | Allowed (1.95%) General / -138.7,-0.2 | 15% (<i>p-80</i>) chi angles: 45.1,273.9 | 0.604Å | OUTLIER(S) worst is CA-- C: 5.154 σ | OUTLIER(S) worst is CB- CA-C: 9.31 σ |
| 241 | SER 148.65 | 0.64Å HA with 240 HIS CD2 | Favored (9.62%) General / -49.9,-56.7 | 5.5% (<i>t</i>) chi angles: 198.9 | 0.081Å | - | - |
| 242 | SER 133.54 | 0.603Å O with 260 GLU HB3 | Favored (4.99%) General / -70.5,-57.2 | 47.3% (<i>t</i>) chi angles: 180.1 | 0.09Å | - | - |
| 243 | LEU 201.95 | 0.49Å HA with 260 GLU HA | Favored (59.3%) General / -69.4,-49.0 | 62.7% (<i>tp</i>) chi angles: 179.9,63.5 | 0.119Å | - | OUTLIER(S) worst is C-N- CA: 4.324 σ |
| 244 | LEU 277.91 | 1.105Å HD23 with 233 VAL HB | OUTLIER (0.01%) General / -2.5,115.6 | 2.3% (<i>mp</i>) chi angles: 313.1,93.4 | 0.212Å | - | OUTLIER(S) worst is N- CA-CB: 4.214 σ |
| 245 | CYS 110.49 | 1.1Å HB3 with 285 CYS HA | Favored (8.14%) General / -92.9,93.0 | 96.3% (<i>m</i>) chi angles: 294.8 | 0.126Å | - | OUTLIER(S) worst is C-N- CA: 9.838 σ |
| 246 | LEU 264.8 | 1.048Å HD11 with 261 GLY HA2 | OUTLIER (0%) General / -28.3,176.4 | 0.1% chi angles: 319.5,311.4 | 0.155Å | - | - |
| 247 | LEU 344.54 | 0.877Å HB3 with 229 HIS NE2 | Favored (2.35%) General / -161.2,119.0 | 61.7% (<i>tp</i>) chi angles: 174.9,61.8 | 0.122Å | - | - |
| 248 | TRP 450.74 | 1.028Å CG with 277 LEU HB2 | OUTLIER (0%) General / 152.2,145.8 | 1.9% (<i>t-105</i>) chi angles: 201.7,299 | 0.272Å | - | OUTLIER(S) worst is N- CA-CB: 4.192 σ |
| 249 | ARG 426.24 | 0.779Å HB3 with 288 THR C | OUTLIER (0%) General / 146.7,173.1 | 2.3% (<i>tpm_?</i>) chi angles: 189.1,67.5,264.7,265.7 | 0.14Å | - | - |
| 250 | LEU 311.48 | 0.619Å N with 249 ARG HG3 | Favored (8.99%) General / -96.2,170.8 | 59.9% (<i>tp</i>) chi angles: 180,60.4 | 0.101Å | - | - |
| | | 0.568Å | Favored (36.45%) | 87.4% (<i>m-85</i>) | | | OUTLIER(S) worst is CA- |

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|-------------|-----|--------|---------------------------------------|--|---|--------------------|-----------------------|---|----------------|
| 251 | PHE | 250.74 | N with 250 LEU HG | General / -77.0,129.7 | chi angles: 291.5,280.3 | 0.116Å | - | CB-CG: 6.175 σ | |
| 252 | SER | 163.36 | - | Favored (31.17%) Pre-proline / -116.5,122.9 | 66.8% (<i>m</i>) chi angles: 292.7 | 0.101Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| Avg: 124.27 | | | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 | |
| 253 | PRO | 153.91 | - | Favored (54.64%) Trans-proline / -57.4,-23.3 | 91.3% (<i>Cg_endo</i>) chi angles: 30.2 | 0.054Å | - | - | |
| 254 | PHE | 183.36 | - | Favored (51.82%) General / -66.1,148.4 | 82.2% (<i>m-85</i>) chi angles: 301.6,88.3 | 0.054Å | - | OUTLIER(S) worst is CA- CB-CG: 8.788 σ | |
| 255 | VAL | 139.98 | 0.774Å HG12 with 287 ARG NH2 | Allowed (0.87%) Isoleucine or valine / -127.8,-172.6 | 35.1% (<i>m</i>) chi angles: 298.3 | 0.087Å | - | - | |
| 256 | LYS | 305.67 | 0.524Å HG3 with 256 LYS O | Favored (12.94%) General / 58.1,48.5 | 13.1% (<i>tppt?</i>) chi angles: 187.3,62.6,48.9,181.9 | 0.089Å | - | - | |
| 257 | THR | 276.04 | - | Favored (33.11%) General / -79.4,145.9 | 59.8% (<i>p</i>) chi angles: 62.4 | 0.068Å | - | - | |
| 258 | ALA | 210.82 | 0.768Å HB2 with 33 THR HB | Favored (16.98%) General / -80.4,170.0 | - | 0.104Å | - | - | |
| 259 | ARG | 213.72 | 0.919Å HG2 with 280 LYS HZ1 | Favored (23.26%) General / -118.5,114.7 | 73.8% (<i>mtt-85</i>) chi angles: 305.8,186.9,201.3,275.2 | 0.189Å | - | - | |
| 260 | GLU | 247.55 | 1.112Å HB2 with 263 GLN HB2 | Favored (15.85%) General / -154.8,138.2 | 6% (<i>mp0</i>) chi angles: 292.9,94.2,49 | 0.159Å | - | - | |
| 261 | GLY | 105.41 | 1.048Å HA2 with 246 LEU HD11 | Favored (86.94%) Glycine / -65.9,-45.6 | - | - | - | - | |
| 262 | ALA | 78.65 | 0.577Å O with 266 LEU HG | Favored (72.21%) General / -63.8,-31.1 | - | 0.105Å | - | - | |

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|-----|------------|---------------------------------------|--|--|--------|---|---|
| 263 | GLN 161.92 | 1.112Å HB2 with 260 GLU HB2 | Favored (98.29%) General / -60.9,-43.5 | 53.8% (<i>tt0</i>) chi angles: 179.9,176.8,329.4 | 0.302Å | - | OUTLIER(S) worst is C-N- CA: 6.135 σ |
| 264 | THR 202.67 | 0.983Å HG21 with 279 GLY HA2 | Favored (80.91%) General / -65.8,-35.5 | 23.1% (<i>p</i>) chi angles: 49.6 | 0.352Å | - | OUTLIER(S) worst is N- CA-CB: 6.274 σ |
| 265 | SER 84.86 | 0.617Å HA with 228 VAL HG11 | Favored (93.97%) General / -61.5,-40.2 | 69.4% (<i>m</i>) chi angles: 296 | 0.11Å | - | - |
| 266 | LEU 87.95 | 0.577Å HG with 262 ALA O | Favored (96.14%) General / -63.9,-40.3 | 82.6% (<i>mt</i>) chi angles: 294.2,179.9 | 0.057Å | - | - |
| 267 | HIS 94.4 | 0.661Å O with 272 GLU HG2 | Favored (94.8%) General / -64.6,-43.1 | 9.5% (<i>t-160</i>) chi angles: 198.9,174.6 | 0.085Å | - | OUTLIER(S) worst is CD2- NE2-CE1: 4.401 σ |
| 268 | CYS 116.65 | 0.795Å SG with 226 TYR HB2 | Favored (65.81%) General / -68.6,-27.2 | 42.8% (<i>t</i>) chi angles: 178.3 | 0.09Å | - | - |
| 269 | ALA 131.85 | 0.5Å O with 120 HIS HB2 | Favored (27.38%) General / -51.4,-32.8 | - | 0.083Å | - | - |
| 270 | LEU 308.31 | 0.948Å CD2 with 119 LEU HA | OUTLIER (0%) General / 143.4,18.3 | 47.9% (<i>tp</i>) chi angles: 183.5,65.8 | 0.203Å | - | OUTLIER(S) worst is N- CA-CB: 5.959 σ |
| 271 | ALA 133.76 | 0.589Å HB2 with 37 LEU CD2 | Favored (75.74%) General / -59.7,-36.0 | - | 0.149Å | - | OUTLIER(S) worst is N- CA-C: 4.054 σ |
| 272 | GLU 143.4 | 0.756Å HG3 with 274 LEU HD11 | Favored (2.12%) General / -130.8,-169.2 | 22.3% (<i>pt-20</i>) chi angles: 61.1,180,351.7 | 0.089Å | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | C β deviation | Bond lengths | Bond angles |
|-------------|------------|----------------------------------|---|---------------------|--------------------------|------------------------------|-----------------------------|---------------------|
| Avg: 124.27 | | | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |
| 273 | GLY 71.24 | 0.766Å C with 274 LEU HD12 | Favored (18.9%) Glycine / -116.8,147.6 | - | - | - | - | - |
| 274 | LEU 210.77 | 0.893Å HB2 with | Allowed (0.15%) | 5.7% (<i>mp</i>) | 0.17Å | OUTLIER(S) worst is C--N: | OUTLIER(S) worst is C-N- | |

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|-----|------------|---------------------------------------|--|---|--------|----------------|--|
| | | 226 TYR CG | General / -166.5,-153.1 | chi angles: 295.7,78.3 | | 4.372 σ | CA: 10.582 σ |
| 275 | GLU 359.39 | 0.744Å HB3 with 276 PRO HD3 | OUTLIER (0%) Pre-proline / 146.8,-33.6 | 65.7% (<i>tt0</i>) chi angles: 180,179.9,28.6 | 0.185Å | - | OUTLIER(S) worst is N- CA-C: 5.65 σ |
| 276 | PRO 211.07 | 0.744Å HD3 with 275 GLU HB3 | Favored (8.5%) Trans-proline / -66.3,172.7 | 32.9% (<i>Cg_exo</i>) chi angles: 325.4 | 0.167Å | - | - |
| 277 | LEU 186.18 | 1.028Å HB2 with 248 TRP CG | Favored (5.31%) General / -115.3,175.9 | 0.6% chi angles: 304.4,54.3 | 0.114Å | - | - |
| 278 | SER 125.06 | 0.474Å HA with 248 TRP O | Favored (40.31%) General / -122.8,152.9 | 47.4% (<i>t</i>) chi angles: 180 | 0.107Å | - | - |
| 279 | GLY 95.24 | 0.983Å HA2 with 264 THR HG21 | Favored (5.11%) Glycine / 150.0,149.8 | - | - | - | OUTLIER(S) worst is C-N- CA: 4.273 σ |
| 280 | LYS 167.75 | 0.936Å HD2 with 245 CYS HB3 | Favored (27.83%) General / -54.4,142.2 | 42.2% (<i>mttm</i>) chi angles: 304,193.7,162.2,298.3 | 0.117Å | - | OUTLIER(S) worst is C-N- CA: 4.381 σ |
| 281 | TYR 159.78 | 0.739Å HB3 with 286 LYS HB3 | Favored (86.39%) General / -65.7,-44.3 | 82.5% (<i>t80</i>) chi angles: 178.9,84.3 | 0.072Å | - | - |
| 282 | PHE 226.87 | 0.745Å H with 286 LYS HB2 | Favored (63.34%) General / -69.9,-20.6 | 34.3% (<i>t80</i>) chi angles: 195.2,87.1 | 0.085Å | - | OUTLIER(S) worst is CA- CB-CG: 9.749 σ |
| 283 | SER 265 | 0.708Å OG with 247 LEU HD22 | OUTLIER (0.02%) General / 90.7,-43.2 | 47.9% (<i>t</i>) chi angles: 179.8 | 0.088Å | - | - |
| 284 | ASP 112.42 | 0.759Å O with 232 VAL HG13 | Favored (61.54%) General / -75.2,-34.6 | 70.2% (<i>m-20</i>) chi angles: 293.9,355.5 | 0.107Å | - | OUTLIER(S) worst is CA- CB-CG: 4.465 σ |
| 285 | CYS 124.36 | 1.1Å HA with 245 CYS HB3 | Favored (30.21%) General / -158.2,167.3 | 25.6% (<i>p</i>) chi angles: 57.8 | 0.09Å | - | - |
| 286 | LYS 198.14 | 0.803Å H with 280 LYS HD3 | OUTLIER (0%) General / 125.9,-161.4 | 29.6% (<i>mmmt</i>) chi angles: 283.7,297.5,296.8,180.9 | 0.218Å | - | OUTLIER(S) worst is N- CA-CB: 4.087 σ |
| 287 | ARG 169.79 | 0.774Å NH2 with 255 VAL | Favored (17.23%) General / | 7.2% (<i>ptp180</i>) chi angles: | 0.144Å | - | - |

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|-----|-----|--------|--|--|---|-----------------------------|---|---|------------------------|
| | | | HG12 | -94.4,154.9 | 62.3,161.3,78.1,171.5 | | | | |
| 288 | THR | 258.81 | 0.831Å HA with 279 GLY O | Favored (47.82%) General / -59.5,130.6 | 70% (<i>p</i>) chi angles: 63.3 | 0.086Å | OUTLIER(S) worst is C--N: 5.808 σ | OUTLIER(S) worst is C-N- CA: 4.42 σ | |
| 289 | TRP | 288.47 | 0.687Å HA with 249 ARG O | Favored (2.7%) General / -170.2,145.2 | 16.4% (<i>t-105</i>) chi angles: 163.3,268.1 | 0.105Å | OUTLIER(S) worst is C--N: 5.71 σ | OUTLIER(S) worst is C-N- CA: 10.755 σ | |
| 290 | VAL | 243.63 | 1.033Å HG11 with 295 ARG HH21 | Allowed (1.64%) Isoleucine or valine / -72.4,169.2 | 9.2% (<i>p</i>) chi angles: 71 | 0.053Å | OUTLIER(S) worst is C--N: 8.205 σ | OUTLIER(S) worst is C-N- CA: 5.873 σ | |
| 291 | SER | 177.14 | 0.714Å HB3 with 178 HIS NE2 | Favored (31.47%) Pre-proline / -118.9,142.2 | 60% (<i>p</i>) chi angles: 71.9 | 0.178Å | - | - | |
| 292 | PRO | 130.67 | 0.605Å O with 295 ARG HB2 | Favored (3.86%) Trans-proline / -66.9,-45.8 | 12.4% (<i>Cg_endo</i>) chi angles: 15.5 | 0.292Å | - | OUTLIER(S) worst is N- CA-C: 5.189 σ | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 124.27 | Clashscore: 146.96 | Outliers: 14 of 276 | Poor rotamers: 11 of 234 | Outliers: 9 of 259 | Outliers: 8 of 278 | Outliers: 60 of 278 |
| 293 | ARG | 189.56 | - | Favored (69.29%) General / -65.5,-28.6 | 61.1% (<i>ttt85</i>) chi angles: 185.6,181.2,184.8,84.7 | 0.111Å | - | - | |
| 294 | ALA | 74.64 | 0.612Å CB with 208 VAL HG21 | Favored (69.4%) General / -62.2,-28.0 | - | 0.065Å | - | - | |
| 295 | ARG | 114.88 | 1.033Å HH21 with 290 VAL HG11 | Favored (64.26%) General / -68.8,-22.8 | 52% (<i>mtt180</i>) chi angles: 292.3,191.4,179.3,224.7 | 0.09Å | - | - | |
| 296 | ASN | 64.72 | 0.758Å O with 299 THR HG22 | Favored (3.84%) General / -66.2,112.2 | 21.4% (<i>t-20</i>) chi angles: 194.3,302.1 | 0.061Å | - | OUTLIER(S) worst is CA- CB-CG: 4.39 σ | |
| 297 | ASN | 84.45 | - | Favored (80.64%) General / -68.7,-39.6 | 20.5% (<i>p-10</i>) chi angles: 63.9,313.5 | 0.09Å | - | OUTLIER(S) worst is CA- CB-CG: 4.372 σ | |
| 298 | LYS | 89.34 | 0.652Å O with 301 GLU HG2 | Favored (99.7%) General / -62.8,-42.4 | 35.6% (<i>ttmt</i>) chi angles: 183,167,288.2,179.7 | 0.085Å | - | - | |

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|-----|-----|--------|--|---|---|--------|---|---|
| 299 | THR | 103.53 | 0.758Å HG22 with 296 ASN O | Favored (89.59%) General / -65.3,-38.2 | 12.2% (<i>t</i>) chi angles: 191.4 | 0.061Å | - | - |
| 300 | ALA | 40.25 | 0.473Å N with 299 THR HG23 | Favored (99.6%) General / -61.6,-43.0 | - | 0.08Å | - | - |
| 301 | GLU | 86.77 | 0.652Å HG2 with 298 LYS O | Favored (85.32%) General / -67.5,-40.5 | 22.4% (<i>pt</i> -20) chi angles: 59,187.9,354.5 | 0.057Å | - | - |
| 302 | ARG | 72.72 | - | Favored (91.51%) General / -65.9,-40.5 | 15.7% (<i>mtp</i> -105) chi angles: 298.5,193.7,94.2,247.5 | 0.067Å | - | - |
| 303 | LEU | 56.07 | 0.711Å O with 306 VAL HG12 | Favored (83.88%) General / -64.2,-36.4 | 62% (<i>tp</i>) chi angles: 179.3,60.8 | 0.072Å | - | - |
| 304 | TRP | 70.38 | - | Favored (99.72%) General / -62.4,-42.8 | 40.5% (<i>t</i> -105) chi angles: 186.5,275.5 | 0.096Å | - | - |
| 305 | ASN | 69.55 | - | Favored (97.75%) General / -61.8,-44.0 | 26.4% (<i>t</i> -20) chi angles: 180.6,254.3 | 0.074Å | - | OUTLIER(S) worst is CA- CB-CG: 4.157 σ |
| 306 | VAL | 85.59 | 0.711Å HG12 with 303 LEU O | Favored (84.54%) Isoleucine or valine / -65.2,-39.1 | 7.5% (<i>p</i>) chi angles: 69.2 | 0.068Å | - | - |
| 307 | SER | 48.37 | 0.49Å N with 306 VAL HG13 | Favored (95.27%) General / -64.8,-40.5 | 74.2% (<i>m</i>) chi angles: 294.1 | 0.078Å | - | - |
| 308 | CYS | 77.9 | - | Favored (84.31%) General / -66.4,-37.0 | 7.2% (<i>p</i>) chi angles: 49.4 | 0.09Å | - | - |
| 309 | GLU | 23.43 | - | Favored (97.12%) General / -64.1,-42.1 | 98% (<i>mt</i> -10) chi angles: 292.9,177.6,359.4 | 0.059Å | - | - |
| 310 | LEU | 34.93 | 0.797Å HD12 with 149 LEU HD11 | - | 79.5% (<i>mt</i>) chi angles: 293.5,180.3 | 0.065Å | - | - |

