



Viewing TGFBI_sm_252-373-FFX1FH_reg-multi.table

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| | | | | |
|----------------------|---|-----------|--|--|
| All-Atom Contacts | Clashscore, all atoms: | 1.42 | 99 th percentile* (N=1784, all resolutions) | |
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 7 | 6.09% | Goal: <1% |
| | Ramachandran outliers | 1 | 0.74% | Goal: <0.05% |
| | Ramachandran favored | 111 | 82.22% | Goal: >98% |
| | MolProbity score^ | 2.18 | | 66 th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 2 | 1.56% | Goal: 0 |
| | Bad backbone bonds: | 0 / 1123 | 0.00% | Goal: 0% |
| | Bad backbone angles: | 11 / 1530 | 0.72% | 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: 81.34 | Clashscore: 1.42 | Outliers: 1 of 135 | Poor rotamers: 7 of 115 | Outliers: 2 of 128 | Outliers: 0 of 137 | Outliers: 11 of 137 |
| 621 | LEU | 38.1 | | 0.405Å N with 687 ASP OD2 | - | 23.3% (<i>mt</i>) chi angles: 301.4,192.2 | 0.269Å | - | OUTLIER(S) worst is C-CA-CB: 4.312 σ |
| 622 | HIS | 116.2 | | - | Favored (27.59%) General / -83.3,148.1 | 3.3% (<i>p80</i>) chi angles: 87.4,78.3 | 0.06Å | - | OUTLIER(S) worst is CA-CB-CG: 6.233 σ |
| 623 | GLN | 69.75 | | - | Favored (4.28%) General / -63.6,115.0 | 24.7% (<i>tp60</i>) chi angles: 175.2,48.7,78.4 | 0.031Å | - | - |
| 624 | GLY | 20.13 | | - | Favored (24.17%) Glycine / 132.7,-162.9 | - | - | - | OUTLIER(S) worst is C-N-CA: 4.234 σ |
| 625 | GLU | 93.64 | | - | Allowed (0.18%) General / | 0.9% chi angles: | 0.094Å | - | - |

-31.5,117.0 329.2,75.2,262

| | | | | | | | | |
|-----|-----|--------|---------------------------------|---|---|--------|---|---|
| 626 | ASN | 52.63 | - | Favored (4.19%) General / -142.7,103.3 | 54.7% (<i>m-20</i>) chi angles: 275.1,331.9 | 0.103Å | - | OUTLIER(S) worst is CA- CB-CG: 5.413 σ |
| 627 | LEU | 56.09 | - | Favored (34.84%) General / -85.2,129.3 | 25.5% (<i>tp</i>) chi angles: 180.4,74.1 | 0.057Å | - | - |
| 628 | PHE | 132.53 | - | Favored (8.42%) General / -108.2,98.9 | 11.2% (<i>t80</i>) chi angles: 180.6,218.3 | 0.03Å | - | - |
| 629 | GLU | 64.34 | - | Favored (46.02%) General / -73.1,146.0 | 86.4% (<i>mt-10</i>) chi angles: 299.2,178.1,12.6 | 0.081Å | - | - |
| 630 | LEU | 55.14 | - | Allowed (1.48%) General / -141.5,61.1 | 17.8% (<i>mt</i>) chi angles: 276.7,164.4 | 0.064Å | - | - |
| 631 | HIS | 80.09 | - | Favored (16.05%) General / -87.1,104.1 | 47.4% (<i>t-80</i>) chi angles: 178.4,276 | 0.029Å | - | - |
| 632 | ILE | 93.48 | - | Favored (29.77%) Isoleucine or valine / -85.7,117.0 | 34.1% (<i>mm</i>) chi angles: 306.9,307 | 0.051Å | - | - |
| 633 | HIS | 94.51 | - | Allowed (0.3%) General / -88.8,-80.0 | 24.9% (<i>t60</i>) chi angles: 177.6,44.5 | 0.131Å | - | - |
| 634 | GLN | 61.67 | - | Favored (14.35%) General / -135.6,171.5 | 50% (<i>mt-30</i>) chi angles: 286.5,191.9,71.8 | 0.051Å | - | - |
| 635 | ALA | 44.85 | - | Favored (9.96%) General / -130.4,108.4 | - | 0.056Å | - | - |
| 636 | PHE | 102.54 | 0.495Å O with 746 GLY HA2 | Favored (57.95%) General / -59.0,137.4 | 11.3% (<i>t80</i>) chi angles: 157.3,78 | 0.078Å | - | - |
| 637 | LEU | 92.95 | - | Favored (54.5%) General / -121.5,138.0 | 2.8% (<i>mp</i>) chi angles: 252.5,61.9 | 0.046Å | - | - |

| 638 | THR | 114.84 | - | Favored (6.68%) General / -78.4,179.9 | 4.4% (<i>t</i>) chi angles: 198.8 | 0.16Å | - | - | |
|-----|-----|--------|---------------|---|--|----------------------------|--------------------|--|------------------------|
| 639 | SER | 70.56 | - | Favored (80.28%) General / -68.5,-37.7 | 85.2% (<i>p</i>) chi angles: 61.1 | 0.13Å | - | - | |
| 640 | ALA | 44.87 | - | Favored (76.39%) General / -65.2,-33.6 | - | 0.082Å | - | - | |
| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | | Avg: 81.34 | Clashscore: 1.42 | Outliers: 1 of 135 | Poor rotamers: 7 of 115 | Outliers: 2 of 128 | Outliers: 0 of 137 | Outliers: 11 of 137 |
| 641 | ALA | 58.54 | - | Favored (89.89%) General / -64.9,-38.1 | - | 0.079Å | - | - | |
| 642 | LEU | 141.39 | - | Favored (84.74%) General / -61.0,-38.0 | 59.1% (<i>tp</i>) chi angles: 181.2,63.9 | 0.071Å | - | - | |
| 643 | ALA | 43.44 | - | Favored (83.63%) General / -63.0,-36.5 | - | 0.097Å | - | - | |
| 644 | GLN | 75.48 | - | Favored (55.4%) General / -79.1,-17.2 | 16.9% (<i>mt-30</i>) chi angles: 289,157.5,114.7 | 0.106Å | - | - | |
| 645 | ALA | 55.96 | - | Favored (49.7%) General / -77.6,-24.2 | - | 0.044Å | - | - | |
| 646 | GLY | 45.12 | - | Favored (72.45%) Glycine / 73.0,25.9 | - | - | - | - | |
| 647 | ASP | 64.91 | - | Favored (4.15%) General / 51.2,28.4 | 12.7% (<i>m-20</i>) chi angles: 301.3,5.9 | 0.158Å | - | OUTLIER(S) worst is C-N- CA: 4.017 σ | |
| 648 | THR | 108.4 | - | Favored (4.41%) General / -115.7,178.1 | 96.4% (<i>m</i>) chi angles: 299.5 | 0.133Å | - | - | |
| | | | | Favored (2.01%) | 37.8% (<i>mt-30</i>) | | | | |

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|-----|-----|--------|--------------------------------|---|--|--------|---|---|
| 649 | GLN | 73.46 | - | Pre-proline / -96.0,95.6 | chi angles: 296.6,186.1,251 | 0.031Å | - | - |
| 650 | PRO | 83.32 | - | Favored (24.14%) Trans-proline / -79.0,151.7 | 82.9% (<i>Cg_endo</i>) chi angles: 29.9 | 0.07Å | - | - |
| 651 | THR | 110.27 | 0.437Å HA with 669 SER O | Favored (35.58%) General / -93.2,122.5 | 88.9% (<i>m</i>) chi angles: 302.1 | 0.058Å | - | - |
| 652 | THR | 44.26 | - | Favored (44.94%) General / -133.4,157.7 | 62% (<i>p</i>) chi angles: 62.8 | 0.029Å | - | - |
| 653 | PHE | 67.73 | - | Favored (30.62%) General / -155.9,167.4 | 15.3% (<i>p90</i>) chi angles: 76.9,284.1 | 0.024Å | - | - |
| 654 | CYS | 51.54 | - | Favored (44.98%) General / -131.9,157.1 | 2.3% (<i>p</i>) chi angles: 42.9 | 0.122Å | - | - |
| 655 | THR | 124.52 | - | Favored (50.47%) General / -133.5,145.8 | 2.9% (<i>t</i>) chi angles: 200.9 | 0.103Å | - | - |
| 656 | TYR | 67.33 | - | Favored (14.38%) General / -164.0,172.1 | 23.1% (<i>p90</i>) chi angles: 74,101.8 | 0.062Å | - | - |
| 657 | SER | 73.86 | - | Favored (5.96%) General / -155.4,-176.5 | 23% (<i>t</i>) chi angles: 187.6 | 0.101Å | - | - |
| 658 | PHE | 60.88 | - | Allowed (0.07%) General / 178.2,133.5 | 74.1% (<i>t80</i>) chi angles: 185.3,72.9 | 0.075Å | - | - |
| 659 | TYR | 78.28 | - | Favored (8.06%) General / 65.2,35.1 | 12% (<i>t80</i>) chi angles: 201.5,97.8 | 0.168Å | - | - |
| 660 | ASP | 47.8 | - | Favored (23.44%) General / 57.7,33.6 | 22.9% (<i>m-20</i>) chi angles: 310.8,320.8 | 0.134Å | - | - |

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

Avg: 81.34 Clashscore: 1.42 Outliers: 1 of 135 Poor rotamers: 7 of 115 Outliers: 2 of 128 Outliers: 0 of 137 Outliers: 11 of 137

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|-----|-----|--------|--------------------------------|--|---|--------|---|---|
| 661 | PHE | 71.15 | - | Favored (11.63%) General / -79.3,174.4 | 17.1% (<i>m-85</i>) chi angles: 273.5,255.8 | 0.095Å | - | - |
| 662 | GLU | 77.3 | - | Allowed (0.05%) General / -39.6,149.8 | 21.7% (<i>pt-20</i>) chi angles: 66.4,189.7,351.6 | 0.072Å | - | - |
| 663 | THR | 100.09 | - | Favored (5.83%) General / -74.8,105.4 | 30.8% (<i>p</i>) chi angles: 51.4 | 0.029Å | - | - |
| 664 | HIS | 37.23 | - | Favored (35.12%) General / -81.7,139.0 | 78.5% (<i>m80</i>) chi angles: 297.6,83.7 | 0.081Å | - | - |
| 665 | CYS | 78.71 | - | Favored (36.25%) General / -138.2,136.1 | 1.9% (<i>p</i>) chi angles: 41.6 | 0.038Å | - | - |
| 666 | THR | 45.77 | - | Favored (3.89%) Pre-proline / -69.5,173.5 | 74.8% (<i>p</i>) chi angles: 61.7 | 0.046Å | - | - |
| 667 | PRO | 82.06 | - | Favored (53.61%) Trans-proline / -69.0,159.5 | 46.8% (<i>Cg_endo</i>) chi angles: 24.7 | 0.033Å | - | - |
| 668 | LEU | 99.99 | - | Favored (26.82%) General / -86.3,119.7 | 11.1% (<i>mp</i>) chi angles: 275.3,63.7 | 0.038Å | - | - |
| 669 | SER | 34.99 | 0.437Å O with 651 THR HA | Favored (16.74%) General / -95.6,155.4 | 23.2% (<i>t</i>) chi angles: 187.3 | 0.075Å | - | - |
| 670 | VAL | 36.25 | - | Favored (13.25%) Isoleucine or valine / -129.2,105.9 | 77.3% (<i>t</i>) chi angles: 172.3 | 0.095Å | - | - |
| 671 | GLY | 40.97 | - | Favored (7.57%) Glycine / 149.4,157.2 | - | - | - | - |
| 672 | PRO | 169.99 | - | Favored (57.6%) Trans-proline / -63.6,-35.7 | 81.7% (<i>Cg_exo</i>) chi angles: 330.7 | 0.074Å | - | - |

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|--|-----|-------|---|--|--|------------|---|---|
| 673 | GLN | 139.8 | - | Favored (28.67%) Pre-proline / -97.7,105.8 | 13.7% (<i>tp60</i>) chi angles: 174.9,57.4,94 | 0.043Å | - | - |
| 674 | PRO | 77.1 | - | Favored (9.3%) Trans-proline / -86.4,154.3 | 88.1% (<i>Cg_endo</i>) chi angles: 31.8 | 0.029Å | - | - |
| 675 | LEU | 70.84 | - | Favored (49.66%) General / -123.3,144.1 | 3.1% (<i>mt</i>) chi angles: 267.9,152 | 0.071Å | - | - |
| 676 | TYR | 55.87 | - | Allowed (0.72%) General / -132.8,-65.3 | 30.9% (<i>m-85</i>) chi angles: 299.7,307.5 | 0.1Å | - | - |
| 677 | ASP | 46.2 | - | Favored (24.68%) General / 50.9,47.4 | 3.4% (<i>m-20</i>) chi angles: 286.1,261.5 | 0.188Å | - | - |
| 678 | PHE | 55.18 | - | Favored (4.1%) General / -77.9,87.1 | 84.7% (<i>t80</i>) chi angles: 182.6,74.4 | 0.045Å | - | - |
| 679 | THR | 46.88 | - | Favored (8.14%) General / -81.6,69.0 | 49.3% (<i>m</i>) chi angles: 305 | 0.057Å | - | - |
| 680 | SER | 87.33 | - | Favored (19.21%) General / -83.7,165.1 | 16.5% (<i>t</i>) chi angles: 189.6 | 0.037Å | - | - |
| <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: 81.34</div> <div>Clashscore: 1.42</div> <div>Outliers: 1 of 135</div> <div>Poor rotamers: 7 of 115</div> <div>Outliers: 2 of 128</div> <div>Outliers: 0 of 137</div> <div>Outliers: 11 of 137</div> </div> | | | | | | | | |
| 681 | GLN | 55.82 | - | Allowed (1.04%) General / -177.4,154.9 | 21.3% (<i>pt20</i>) chi angles: 58.6,184.4,358.2 | 0.063Å | - | - |
| 682 | TYR | 89.63 | - | Favored (4.95%) General / -146.5,-175.9 | 11.9% (<i>p90</i>) chi angles: 56.5,71.9 | 0.141Å | - | - |
| 683 | VAL | 40.3 | - | Favored (26.44%) Isoleucine or valine / -121.3,146.4 | 84.9% (<i>t</i>) chi angles: 174.9 | 0.082Å | - | - |
| | | | | Allowed | 31.8% (<i>tpp</i>) | OUTLIER(S) | | |

| | | | | | | | | |
|-----|-----|--------|---------------------------------|--|--|--------|---|--|
| 684 | MET | 86.14 | - | (0.88%) General / -160.0,89.8 | chi angles: 188.2,48.4,56.7 | 0.032Å | - | worst is C-N- CA: 5.227 σ |
| 685 | GLU | 130.39 | - | OUTLIER (0.04%) General / -66.8,49.9 | 4.4% (<i>mp0</i>) chi angles: 305.2,94.8,306.4 | 0.051Å | - | - |
| 686 | THR | 91.25 | - | Favored (42.68%) General / -150.4,161.3 | 17.3% (<i>m</i>) chi angles: 311.3 | 0.051Å | - | - |
| 687 | ASP | 108.83 | 0.405Å OD2 with 621 LEU N | Allowed (0.74%) General / -108.6,-72.1 | 42.2% (<i>m-20</i>) chi angles: 293.4,4.2 | 0.06Å | - | OUTLIER(S) worst is CA- CB-CG: 4.218 σ |
| 688 | SER | 47.82 | - | Favored (28.17%) General / -47.6,-48.6 | 70.7% (<i>p</i>) chi angles: 57.7 | 0.119Å | - | - |
| 689 | LEU | 51.68 | - | Favored (84.31%) General / -67.7,-39.4 | 66% (<i>mt</i>) chi angles: 305.2,180.7 | 0.127Å | - | - |
| 690 | PHE | 116.92 | - | Favored (89.54%) General / -66.5,-41.0 | 70.4% (<i>t80</i>) chi angles: 175.3,267.2 | 0.083Å | - | - |
| 691 | LEU | 48.45 | - | Favored (60.59%) General / -74.2,-27.0 | 53.7% (<i>mt</i>) chi angles: 302.7,169.8 | 0.11Å | - | - |
| 692 | HIS | 69.78 | - | Favored (91.19%) General / -64.7,-44.1 | 66.3% (<i>t-80</i>) chi angles: 192.8,283.4 | 0.074Å | - | - |
| 693 | TYR | 46.82 | - | Favored (84.39%) General / -63.5,-36.6 | 11.2% (<i>t80</i>) chi angles: 193.4,288.2 | 0.083Å | - | - |
| 694 | LEU | 143.63 | - | Favored (69.77%) General / -54.7,-41.0 | 53% (<i>tp</i>) chi angles: 180.3,57.9 | 0.051Å | - | - |
| 695 | GLN | 67.23 | - | Favored (33.61%) General / -82.6,-25.0 | 17.7% (<i>mm100</i>) chi angles: 307.9,316.7,129.4 | 0.153Å | - | - |
| 696 | GLU | 86.47 | - | Favored (11.75%) General / | 5.3% (<i>pt-20</i>) chi angles: 75.6,210.6,327.9 | 0.092Å | - | - |

-105.4,-26.9

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|-----|-----|--------|---|--|---|--------|---|---|
| 697 | ALA | 33.03 | - | Allowed (1.73%) General / -140.1,50.1 | - | 0.062Å | - | - |
| 698 | SER | 80.78 | - | Favored (2.18%) General / -45.3,142.2 | 18.2% (<i>t</i>) chi angles: 169.4 | 0.063Å | - | - |
| 699 | ALA | 41.79 | - | Favored (33.47%) General / -62.5,152.8 | - | 0.014Å | - | OUTLIER(S) worst is C-N- CA: 4.33 σ |
| 700 | ARG | 111.88 | - | Favored (51.14%) General / -134.2,151.1 | 52.2% (<i>ttt85</i>) chi angles: 182.1,188.6,170.3,90 | 0.144Å | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
|-----|-----|--------|---------------|---|--|----------------------------|--------------------|---|------------------------|
| | | | Avg: 81.34 | Clashscore: 1.42 | Outliers: 1 of 135 | Poor rotamers: 7 of 115 | Outliers: 2 of 128 | Outliers: 0 of 137 | Outliers: 11 of 137 |
| 701 | LEU | 74.18 | - | Favored (4.71%) General / -148.0,110.6 | 13.7% (<i>tp</i>) chi angles: 172.6,79.9 | 0.081Å | - | - | |
| 702 | ASP | 51.95 | - | Favored (39.69%) General / -104.4,139.2 | 87.8% (<i>m-20</i>) chi angles: 288.5,353.4 | 0.039Å | - | - | |
| 703 | ILE | 100.62 | - | Favored (15.2%) Isoleucine or valine / -103.2,143.5 | 15.8% (<i>tt</i>) chi angles: 197.1,169.3 | 0.111Å | - | - | |
| 704 | HIS | 61.86 | - | Favored (51.63%) General / -130.6,144.8 | 23.9% (<i>m-70</i>) chi angles: 320.3,284.5 | 0.144Å | - | - | |
| 705 | GLN | 55.38 | - | Favored (9.99%) General / -96.3,98.1 | 18.9% (<i>tt0</i>) chi angles: 187.7,183.4,115.7 | 0.04Å | - | - | |
| 706 | ALA | 46.22 | - | Favored (9.91%) General / -84.4,67.6 | - | 0.033Å | - | - | |
| 707 | MET | 100.62 | - | Allowed (0.13%) General / | 3.9% (<i>ppp?</i>) chi angles: 60.9,94.7,81.2 | 0.32Å | - | OUTLIER(S) worst is C- CA-CB: 4.678 | |

| | | | | -85.1,-150.8 | | | | σ |
|-----|-----|--------|---|--|--|--------|---|--|
| 708 | ALA | 30.22 | - | Favored (7.27%) General / -78.3,-53.5 | - | 0.068Å | - | - |
| 709 | SER | 48.93 | - | Allowed (1.78%) General / -98.5,-59.3 | 56.2% (<i>p</i>) chi angles: 55.4 | 0.098Å | - | - |
| 710 | GLU | 61.29 | - | Favored (38.74%) General / -76.5,145.9 | 0.3% chi angles: 225.7,305.6,278.7 | 0.051Å | - | - |
| 711 | HIS | 82.81 | - | Allowed (0.96%) General / -146.2,5.0 | 76.7% (<i>m80</i>) chi angles: 297.9,81.9 | 0.059Å | - | - |
| 712 | SER | 45.61 | - | Favored (6.86%) General / -88.1,177.6 | 19.2% (<i>m</i>) chi angles: 306.5 | 0.033Å | - | - |
| 713 | THR | 77.82 | - | Favored (20.98%) General / -62.5,124.5 | 99.9% (<i>m</i>) chi angles: 298.5 | 0.025Å | - | - |
| 714 | LEU | 180.94 | - | Favored (14.72%) General / -102.8,-19.4 | 19.1% (<i>tp</i>) chi angles: 189.5,51.4 | 0.082Å | - | - |
| 715 | ALA | 62.75 | - | Favored (15.37%) General / -156.1,139.0 | - | 0.032Å | - | - |
| 716 | ALA | 49.31 | - | Favored (36.08%) General / -93.2,122.9 | - | 0.091Å | - | - |
| 717 | GLY | 22.06 | - | Favored (11.95%) Glycine / -112.1,134.3 | - | - | - | - |
| 718 | TRP | 158.33 | - | Favored (55.45%) General / -109.0,129.4 | 9.6% (<i>t-105</i>) chi angles: 204.6,276.9 | 0.045Å | - | OUTLIER(S) worst is CE3- CD2-CG: 4.848 σ |
| 719 | ILE | 106.65 | - | Allowed (0.29%) Isoleucine or valine / -137.9,72.2 | 9.5% (<i>tt</i>) chi angles: 186.9,182 | 0.157Å | - | - |

| 720 | CYS | 84.05 | - | Favored (41.23%) General / -75.1,146.8 | 18.2% (t) chi angles: 192.2 | 0.026Å | - | - |
|-----|---------|---------------|---------------------|---|--|--------------------|--------------------|---------------------|
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles |
| | | Avg: 81.34 | Clashscore: 1.42 | Outliers: 1 of 135 | Poor rotamers: 7 of 115 | Outliers: 2 of 128 | Outliers: 0 of 137 | Outliers: 11 of 137 |
| 721 | PHE | 72.36 | - | Allowed (0.78%) General / -104.6,50.8 | 16.2% (m-85) chi angles: 310,309.6 | 0.057Å | - | - |
| 722 | ASP | 109.07 | - | Favored (69.44%) General / -55.4,-38.8 | 18.2% (p-10) chi angles: 64,315.4 | 0.049Å | - | - |
| 723 | ARG | 79.32 | - | Favored (60.37%) General / -75.6,-13.9 | 25.7% (mmm180) chi angles: 304.1,306.9,303.3,149.2 | 0.116Å | - | - |
| 724 | VAL | 49.38 | - | Favored (9.86%) Isoleucine or valine / -80.8,-6.6 | 24% (t) chi angles: 187.1 | 0.136Å | - | - |
| 725 | LEU | 156.87 | - | Favored (58.66%) General / -79.3,-15.0 | 30.9% (tp) chi angles: 188.4,67.1 | 0.039Å | - | - |
| 726 | GLU | 103.33 | - | Allowed (0.4%) General / -134.7,-85.9 | 15.2% (tt0) chi angles: 186.1,206.6,312.1 | 0.129Å | - | - |
| 727 | THR | 60.75 | - | Favored (4.86%) General / -78.7,82.8 | 31.8% (p) chi angles: 51.5 | 0.064Å | - | - |
| 728 | VAL | 120.12 | - | Allowed (0.71%) Isoleucine or valine / -77.0,80.5 | 27.9% (m) chi angles: 295.5 | 0.173Å | - | - |
| 729 | GLU | 78.6 | - | Allowed (1.05%) General / -156.0,-160.8 | 0.8% chi angles: 227.4,303.8,292 | 0.178Å | - | - |
| 730 | LYS | 122.19 | - | Allowed (1.25%) General / -75.8,59.8 | 43.5% (mttm) chi angles: 293.7,156.9,185,286.3 | 0.06Å | - | - |

| | | | | | | | | |
|---|-----|--------|---|---|--|--------|---|---|
| 731 | VAL | 111.58 | - | Allowed (1.87%) Isoleucine or valine / -83.8,83.8 | 11.8% (<i>p</i>) chi angles: 61.9 | 0.202Å | - | - |
| 732 | HIS | 75.19 | - | Allowed (1.02%) General / -39.3,135.4 | 22.5% (<i>t60</i>) chi angles: 156.5,81.4 | 0.121Å | - | - |
| 733 | GLY | 20.13 | - | Favored (16.62%) Glycine / -123.1,177.1 | - | - | - | - |
| 734 | LEU | 49.75 | - | Favored (45.9%) General / -127.1,153.5 | 95% (<i>mt</i>) chi angles: 297.9,174.8 | 0.037Å | - | - |
| 735 | ALA | 37.22 | - | Favored (14.32%) General / -147.2,128.0 | - | 0.048Å | - | - |
| 736 | THR | 90.01 | - | Favored (31.66%) General / -82.1,126.1 | 19.5% (<i>p</i>) chi angles: 48.1 | 0.065Å | - | - |
| 737 | LEU | 73.55 | - | Favored (14.29%) General / -103.8,104.3 | 2.6% (<i>mt</i>) chi angles: 328.4,179 | 0.049Å | - | - |
| 738 | ILE | 87.79 | - | Favored (41.72%) Isoleucine or valine / -88.4,125.0 | 4.8% (<i>mp</i>) chi angles: 296,91.5 | 0.044Å | - | - |
| 739 | GLY | 39.66 | - | Favored (34.67%) Glycine / -97.0,-178.4 | - | - | - | - |
| 740 | ALA | 33.6 | - | Favored (69.41%) General / -60.5,-29.9 | - | 0.105Å | - | - |
| <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: 81.34</div> <div>Clashscore: 1.42</div> <div>Outliers: 1 of 135</div> <div>Poor rotamers: 7 of 115</div> <div>Outliers: 2 of 128</div> <div>Outliers: 0 of 137</div> <div>Outliers: 11 of 137</div> </div> | | | | | | | | |
| 741 | GLY | 72.45 | - | Favored (73.63%) Glycine / -83.3,6.1 | - | - | - | - |

| | | | | | | | | |
|-----|-----|--------|---------------------------------|--|---|--------|---|--|
| 742 | GLY | 302.96 | - | Favored (58.51%) Glycine / 72.4,38.3 | - | - | - | - |
| 743 | GLU | 336.37 | - | Favored (18.46%) General / -117.1,162.0 | 16.3% (<i>pt-20</i>) chi angles: 64.3,185.4,297.6 | 0.106Å | - | - |
| 744 | GLU | 170.94 | - | Favored (7.25%) General / -88.1,63.4 | 1.7% (<i>pp20?</i>) chi angles: 68,103.5,199.3 | 0.109Å | - | - |
| 745 | PHE | 115.64 | - | Favored (63.41%) General / -51.7,-48.8 | 57.4% (<i>t80</i>) chi angles: 181.9,92.7 | 0.095Å | - | - |
| 746 | GLY | 39.67 | 0.495Å HA2 with 636 PHE O | Favored (22.73%) Glycine / -135.4,156.6 | - | - | - | - |
| 747 | VAL | 30.27 | - | Favored (13.82%) Isoleucine or valine / -130.7,107.2 | 90.6% (<i>t</i>) chi angles: 177.9 | 0.049Å | - | - |
| 748 | LEU | 47.29 | - | Favored (44.99%) General / -74.0,144.6 | 7.7% (<i>tp</i>) chi angles: 205.1,76.7 | 0.071Å | - | - |
| 749 | GLU | 76.92 | - | Favored (33.16%) General / -115.5,118.4 | 0.1% chi angles: 191.1,300.1,276.1 | 0.062Å | - | - |
| 750 | TYR | 64.12 | - | Favored (28.88%) General / -150.3,166.8 | 33.1% (<i>p90</i>) chi angles: 61.5,101.1 | 0.073Å | - | - |
| 751 | TRP | 66.7 | - | Favored (13.86%) General / -152.2,132.8 | 0.6% chi angles: 29,275.9 | 0.063Å | - | OUTLIER(S) worst is CE3- CD2-CG: 4.135 σ |
| 752 | MET | 126.29 | - | Favored (29.16%) General / -137.1,164.1 | 0% chi angles: 71,288.8,155.6 | 0.079Å | - | - |
| 753 | ARG | 135.06 | - | Allowed (0.09%) General / -176.9,112.4 | 0.3% chi angles: 41.8,131.2,283.4,185.8 | 0.08Å | - | - |

| | | | | | | | | |
|-----|-----|--------|---|--|---|--------|---|---|
| 754 | LEU | 193.6 | - | Favored (31.72%) General / -90.3,120.7 | 1.2% (<i>tt</i>) chi angles: 174.9,128.1 | 0.045Å | - | - |
| 755 | ARG | 144.16 | - | Allowed (0.33%) General / 179.7,150.1 | 8.6% (<i>ptm-85</i>) chi angles: 53.4,184.8,294.2,281.2 | 0.074Å | - | - |
| 756 | PHE | 109.12 | - | Favored (7.96%) Pre-proline / -46.5,127.9 | 53.4% (<i>t80</i>) chi angles: 174.6,91.3 | 0.096Å | - | - |
| 757 | PRO | 61.62 | - | - | 33.7% (<i>Cg_endo</i>) chi angles: 37 | 0.014Å | - | - |

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