



Viewing gucy2d_sm_871-1045-FFX1FH-multi.table

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|-------------------|---|-----------|--------|--|
| All-Atom Contacts | Clashscore, all atoms: | 0.74 | | 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 | 9 | 6.04% | Goal: <0.3% |
| | Favored rotamers | 127 | 85.23% | Goal: >98% |
| | Ramachandran outliers | 2 | 1.16% | Goal: <0.05% |
| | Ramachandran favored | 154 | 89.02% | Goal: >98% |
| | MolProbity score^ | 1.90 | | 81 st percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 1 | 0.62% | Goal: 0 |
| | Bad bonds: | 0 / 1380 | 0.00% | Goal: 0% |
| | Bad angles: | 19 / 1876 | 1.01% | Goal: <0.1% |
| Peptide Omegas | Cis Prolines: | 0 / 8 | 0.00% | Expected: ≤1 per chain, or ≤5% |
| | Cis nonProlines: | 3 / 166 | 1.81% | Goal: <0.05% |
| | Twisted Peptides: | 2 / 174 | 1.15% | Goal: 0 |

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 | Cis Peptides |
|-------|---------|------------|------------------|--|---|--------------------|--------------------|---------------------|---------------------------------|
| | | Avg: 56.86 | Clashscore: 0.74 | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 | Non-Trans: 5 of 174 |
| C 871 | VAL | 50 | - | - | Favored (19.3%) <i>m</i> chi angles: 302.7 | 0.22Å | - | - | - |
| C 872 | GLU | 50 | - | Favored (2.08%) Pre-Pro / -54.8,161.8 | OUTLIER (0%) chi angles: 74.5,319.6,305 | 0.09Å | - | - | Twisted nonPRO omega= 138.19 |
| C 873 | PRO | 50 | - | Allowed (0.2%) Trans-Pro / -103.6,150.0 | Favored (2.1%) <i>Cg_endo</i> chi angles: 41.1 | 0.12Å | - | - | Twisted PRO omega= 149.64 |
| C 874 | GLU | 50 | - | Favored (47.8%) General / -136.4,148.5 | Favored (68.4%) <i>tt0</i> chi angles: 180.4,165.2,359.9 | 0.03Å | - | - | - |
| C 875 | TYR | 50 | - | Allowed (0.89%) General / -113.6,74.9 | Favored (91%) <i>m-80</i> chi angles: 292.7,84.9 | 0.06Å | - | - | - |

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|-------|-----|---------|-------------------------------|---|---|-------|---|---|---|
| C 876 | PHE | 50 | - | Favored (42.89%) General / -54.2,136.4 | Favored (50%) <i>m-80</i> chi angles: 284.1,285 | 0.05Å | - | OUTLIER(S) worst is CA- CB-CG: 4.5 σ | - |
| C 877 | GLU | 50 | - | Allowed (0.75%) General / -111.5,-71.8 | Allowed (0.3%) <i>tp30</i> chi angles: 165,24.1,60.3 | 0.13Å | - | - | - |
| C 878 | GLN | 50 | - | Allowed (0.39%) General / -74.9,48.6 | Favored (6.5%) <i>mm-40</i> chi angles: 288.4,285,259.4 | 0.07Å | - | - | - |
| C 879 | VAL | 50 | - | Favored (15.87%) Ile or Val / -114.0,151.1 | OUTLIER (0.2%) chi angles: 149.6 | 0.13Å | - | - | - |
| C 880 | THR | 50 | - | Favored (29.91%) General / -122.9,119.2 | Favored (90.7%) <i>m</i> chi angles: 301.2 | 0.02Å | - | - | - |
| C 881 | LEU | 50 | - | Favored (27.9%) General / -80.5,153.8 | Favored (14.2%) <i>mt</i> chi angles: 314.6,176.6 | 0.06Å | - | - | - |
| C 882 | TYR | 99.99 O | 0.41Å with C 932 MET HA | Favored (14.38%) General / -138.1,119.1 | Favored (6.9%) <i>t80</i> chi angles: 168.9,280.1 | 0.10Å | - | - | - |
| C 883 | PHE | 50 | - | Favored (17.24%) General / -108.4,158.8 | Favored (5.9%) <i>m-80</i> chi angles: 267.6,88.6 | 0.07Å | - | - | - |
| C 884 | SER | 50 | - | Favored (4.74%) General / -167.2,145.0 | Favored (80.4%) <i>p</i> chi angles: 61.5 | 0.05Å | - | - | - |
| C 885 | ASP | 50 | - | Favored (33.11%) General / -142.8,163.3 | Allowed (0.8%) <i>p0</i> chi angles: 80.4,289.5 | 0.09Å | - | - | - |
| C 886 | ILE | 50 | - | Favored (35.04%) Ile or Val / -84.5,131.0 | Favored (48.5%) <i>mt</i> chi angles: 287.4,174.8 | 0.06Å | - | - | - |
| C 887 | VAL | 50 | - | Allowed (0.46%) Ile or Val / -75.4,75.3 | Favored (73.7%) <i>t</i> chi angles: 178.4 | 0.10Å | - | - | - |
| C 888 | GLY | 50 | - | Favored (3.54%) Glycine / 121.3,19.4 | - | - | - | - | - |
| C 889 | PHE | 50 | - | Favored (82.48%) General / -64.5,-35.9 | Favored (68.5%) <i>t80</i> chi angles: 181.5,67.9 | 0.14Å | - | - | - |

| C 890 | THR | 50 | - | Favored (80.49%) General / -56.3,-45.1 | Favored (5.1%) <i>p</i> chi angles: 44.7 | 0.11Å | - | - | - |
|------------|---------|--------|--------------|--|---|-------------------------|--------------------|---------------------|---------------------|
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
| Avg: 56.86 | | | | Clashscore: 0.74 | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 |
| | | | | | | Outliers: 0 of 175 | Outliers: 0 of 175 | Outliers: 16 of 175 | Non-Trans: 5 of 174 |
| C 891 | THR | 50 | - | Favored (77.46%) General / -67.3,-34.5 | OUTLIER (0.2%) chi angles: 34.5 | 0.21Å | - | - | - |
| C 892 | ILE | 50 | - | Favored (79.89%) Ile or Val / -59.4,-39.8 | Favored (83.8%) <i>mt</i> chi angles: 290.3,166.9 | 0.13Å | - | - | - |
| C 893 | SER | 50 | - | Favored (2.42%) General / -69.7,3.5 | Favored (7.2%) <i>t</i> chi angles: 193.5 | 0.10Å | - | - | - |
| C 894 | ALA | 50 | - | Favored (2.74%) General / -138.4,10.4 | - | 0.02Å | - | - | - |
| C 895 | MET | 50 | - | Favored (2.09%) General / -141.8,23.3 | Favored (68.1%) <i>mtt</i> chi angles: 295.1,178.1,176.6 | 0.04Å | - | - | - |
| C 896 | SER | 99.99 | - | Favored (13.97%) General / -151.4,173.9 | Favored (5.4%) <i>m</i> chi angles: 310.8 | 0.09Å | - | - | - |
| C 897 | GLU | 50 | - | Favored (62.35%) Pre-Pro / -83.3,159.3 | Favored (4.2%) <i>pt0</i> chi angles: 83.3,197.4,2.8 | 0.07Å | - | - | - |
| C 898 | PRO | 50 | - | Favored (94.16%) Trans-Pro / -59.3,-30.9 | Favored (89.5%) <i>Cg_exo</i> chi angles: 329.8 | 0.08Å | - | - | - |
| C 899 | ILE | 50 | - | Favored (64.39%) Ile or Val / -67.8,-50.0 | Favored (45.9%) <i>mm</i> chi angles: 304.1,303.7 | 0.08Å | - | - | - |
| C 900 | GLU | 99.99 | - | Favored (60.32%) General / -75.7,-14.0 | Favored (3.4%) <i>pt0</i> chi angles: 81.2,195.7,132.9 | 0.20Å | - | - | - |
| C 901 | VAL | 50 | - | Favored (69.25%) Ile or Val / -60.1,-36.7 | Favored (94.8%) <i>t</i> chi angles: 174.8 | 0.10Å | - | - | - |
| C 902 | VAL | 50 | - | Favored (3.82%) Ile or Val / | Favored (28.4%) <i>m</i> chi angles: 300.8 | 0.24Å | - | - | - |

-96.7,-28.6

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|-------|-----|-------|---|---|---|-------|---|--|---|
| C 903 | ASP | 50 | - | Favored (12.74%) General / -47.3,-53.8 | Favored (43.6%) <i>m</i> - 30 chi angles: 300.1,347.9 | 0.12Å | - | - | - |
| C 904 | LEU | 50 | - | Favored (53.06%) General / -54.0,-32.1 | Favored (47.2%) <i>tp</i> chi angles: 176.1,55.9 | 0.08Å | - | - | - |
| C 905 | LEU | 50 | - | Favored (63.57%) General / -71.4,-27.8 | Favored (39.3%) <i>mt</i> chi angles: 308.1,180.4 | 0.14Å | - | - | - |
| C 906 | ASN | 50 | - | Favored (80.4%) General / -68.4,-41.6 | Favored (16.1%) <i>m</i> - 40 chi angles: 307.4,274.9 | 0.13Å | - | - | - |
| C 907 | ASP | 99.99 | - | Favored (6.84%) General / -52.7,-58.4 | Allowed (0.5%) <i>m</i> - 30 chi angles: 308.2,36.8 | 0.11Å | - | OUTLIER(S) worst is CA- CB-CG: 5.7 σ | - |
| C 908 | LEU | 50 | - | Favored (4.7%) General / -74.4,-56.6 | Favored (5.2%) <i>mt</i> chi angles: 308.2,196.7 | 0.13Å | - | - | - |
| C 909 | TYR | 50 | - | Favored (68.9%) General / -70.8,-32.0 | Favored (8.7%) <i>m</i> - 10 chi angles: 297.6,354.5 | 0.18Å | - | - | - |
| C 910 | THR | 50 | - | Favored (93.59%) General / -65.2,-42.3 | Favored (4.2%) <i>m</i> chi angles: 315 | 0.15Å | - | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|---|-----|-----|------------|------------------|--------------------|-------------------------|--------------------|--------------------|---------------------|---------------------|
| | | | Avg: 56.86 | Clashscore: 0.74 | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 | Non-Trans: 5 of 174 |

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|-------|-----|-------|---|---|---|-------|---|--|---|
| C 911 | LEU | 99.99 | - | Favored (61.04%) General / -75.2,-37.5 | Favored (17.7%) <i>tp</i> chi angles: 184.7,50.2 | 0.13Å | - | - | - |
| C 912 | PHE | 50 | - | Favored (96.59%) General / -63.0,-44.2 | Favored (8.4%) <i>m</i> - 10 chi angles: 298.3,354 | 0.13Å | - | OUTLIER(S) worst is CA- CB-CG: 6.8 σ | - |
| C 913 | ASP | 50 | - | Favored (62.87%) General / -71.9,-27.5 | Favored (34.5%) <i>m</i> - 30 chi angles: 295.6,0.3 | 0.15Å | - | - | - |
| C 914 | ALA | 50 | - | Favored (86.21%) General / -63.3,-37.2 | - | 0.08Å | - | - | - |
| C 915 | ILE | 50 | - | Favored (9.85%) Ile or Val / | Favored (9.2%) <i>pt</i> chi angles: 59.6,155.3 | 0.25Å | - | - | - |

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|-------|-----|----|-------------------------------------|---|---|-------|---|---|---|
| | | | | -92.0,-10.2 | | | | | |
| C 916 | ILE | 50 | - | Favored (73.44%) Ile or Val / -57.9,-39.8 | Favored (11.9%) <i>pt</i> chi angles: 62.2,184.7 | 0.24Å | - | - | - |
| C 917 | GLY | 50 | - | Favored (68.63%) Glycine / -63.4,-25.6 | - | - | - | - | - |
| C 918 | SER | 50 | - | Favored (16.52%) General / -80.5,5.0 | Favored (9%) <i>t</i> chi angles: 191.9 | 0.08Å | - | - | - |
| C 919 | HIS | 50 | - | Allowed (1.87%) General / -142.0,8.2 | Favored (6.2%) <i>m90</i> chi angles: 317.5,86.4 | 0.06Å | - | - | - |
| C 920 | ASP | 50 | - | Favored (16.48%) General / 52.9,51.1 | Favored (31.6%) <i>t0</i> chi angles: 196.3,27.6 | 0.13Å | - | - | - |
| C 921 | VAL | 50 | 0.43Å HG12 with C 935 SER HB2 | Favored (58.36%) Ile or Val / -115.3,134.5 | Favored (28.1%) <i>m</i> chi angles: 298.5 | 0.09Å | - | - | - |
| C 922 | TYR | 50 | - | Favored (55.07%) General / -108.1,130.8 | Favored (29.6%) <i>m-80</i> chi angles: 301.2,255.7 | 0.06Å | - | - | - |
| C 923 | LYS | 50 | - | Favored (39.6%) General / -77.2,138.7 | Favored (29.8%) <i>ttpt</i> chi angles: 195,169.7,71.2,177.6 | 0.05Å | - | - | - |
| C 924 | VAL | 50 | - | Favored (6.91%) Ile or Val / -104.0,150.9 | Favored (72.6%) <i>t</i> chi angles: 178.5 | 0.10Å | - | - | - |
| C 925 | GLU | 50 | - | Favored (4.78%) General / -73.3,105.5 | Favored (16.1%) <i>mm-30</i> chi angles: 302.6,319.2,298.6 | 0.03Å | - | - | - |
| C 926 | THR | 50 | - | Favored (3.66%) General / -109.3,-178.8 | Favored (16.7%) <i>p</i> chi angles: 48.9 | 0.09Å | - | - | - |
| C 927 | ILE | 50 | - | Favored (39.51%) Ile or Val / -132.2,143.6 | Favored (75.1%) <i>mt</i> chi angles: 295.8,175.8 | 0.10Å | - | - | - |
| C 928 | GLY | 50 | - | Favored (41.73%) Glycine / 63.6,-135.9 | - | - | - | - | - |
| C 929 | ASP | 50 | - | Favored (59.02%) General / -81.6,-11.7 | Favored (15.8%) <i>p0</i> chi angles: 58.5,309.6 | 0.07Å | - | - | - |

| C 930 | ALA | 50 | - | | Favored (42.07%) General / -69.3,130.2 | - | 0.03Å | - | - | - |
|-------|---------|------------|--|--|--|---|--------------------|--|-----------------------------------|---|
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides | |
| | | Avg: 56.86 | Clashscore: 0.74 | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 | Non-Trans: 5 of 174 | |
| C 931 | TYR | 50 | - | | Favored (17.76%) General / -134.9,119.2 | Favored (51.2%) <i>t80</i> chi angles: 180,274.5 | 0.08Å | - | - | - |
| C 932 | MET | 50 | 0.41Å HA with C 882 TYR O | Favored (50.71%) General / -125.0,143.8 | Favored (19.4%) <i>ttt</i> chi angles: 183.7,191.5,173.7 | 0.08Å | - | - | - | |
| C 933 | VAL | 50 | - | Favored (4.85%) lle or Val / -135.0,178.8 | Favored (16.9%) <i>m</i> chi angles: 303.7 | 0.14Å | - | - | - | |
| C 934 | ALA | 50 | - | Favored (8.75%) General / -160.1,136.3 | - | 0.12Å | - | - | - | |
| C 935 | SER | 50 | 0.43Å HB2 with C 921 VAL HG12 | Favored (19.61%) General / -111.2,157.9 | Favored (16.4%) <i>t</i> chi angles: 187.3 | 0.10Å | - | - | - | |
| C 936 | GLY | 99.99 | - | Favored (52.79%) Glycine / 94.6,13.7 | - | - | - | - | - | |
| C 937 | LEU | 99.99 | - | Favored (7.45%) Pre-Pro / -66.5,-34.1 | Favored (6.5%) <i>tt</i> chi angles: 182,143.4 | 0.10Å | - | - | - | |
| C 938 | PRO | 99.99 | - | Favored (4.19%) Trans-Pro / -48.4,-22.6 | Favored (4.5%) <i>Cg_exo</i> chi angles: 351.7 | 0.15Å | - | OUTLIER(S) worst is N- CA-C: 5.4 σ | - | |
| C 939 | GLN | 50 | - | Favored (19.71%) General / -79.4,116.6 | Favored (76.9%) <i>mt0</i> chi angles: 298.1,185.9,44.8 | 0.06Å | - | - | Cis nonPRO omega= -25.43 | |
| C 940 | ARG | 99.99 | - | Allowed (0.08%) General / 75.4,50.0 | Favored (62.9%) <i>mtp180</i> chi angles: 293.7,192.3,64.5,175.1 | 0.16Å | - | - | - | |
| C 941 | ASN | 99.99 | - | Favored (4.69%) General / -92.5,67.5 | Favored (72.9%) <i>m-40</i> chi angles: 296.6,346.1 | 0.07Å | - | - | - | |
| | | | | Favored (16.69%) | | | | | | |

| C 942 | GLY | 99.99 | - | Glycine / 118.1,-2.7 | - | - | - | - | - |
|------------------------|---------|-----------|-----------------|--|--|--------------------|--------------------|--|-----------------------------------|
| C 943 | GLN | 99.99 | - | Favored (10.49%) General / -109.5,166.9 | Favored (13.3%) <i>mp10</i> chi angles: 302,89,19.6 | 0.05Å | - | OUTLIER(S) worst is C-N- CA: 7.1 σ | - |
| C 944 | ARG | 50 | - | Allowed (0.07%) General / 83.8,31.1 | Favored (10.1%) <i>mtm110</i> chi angles: 317.8,174,303.9,103.7 | 0.22Å | - | - | Cis nonPRO omega= -11.43 |
| C 945 | HIS | 50 | - | Favored (70.56%) General / -63.1,-29.1 | Favored (36.4%) <i>p90</i> chi angles: 70.2,85.7 | 0.23Å | - | OUTLIER(S) worst is CA- CB-CG: 4.1 σ | - |
| C 946 | ALA | 50 | - | Favored (35.43%) General / -80.5,-34.4 | - | 0.14Å | - | - | - |
| C 947 | ALA | 50 | - | Favored (86.52%) General / -63.1,-46.6 | - | 0.04Å | - | - | - |
| C 948 | GLU | 50 | - | Favored (76.98%) General / -66.3,-34.0 | Favored (19.4%) <i>mm-30</i> chi angles: 281.9,306.8,338.3 | 0.13Å | - | - | - |
| C 949 | ILE | 50 | - | Favored (80.58%) Ile or Val / -66.4,-37.9 | Allowed (0.4%) <i>mm</i> chi angles: 279,273.8 | 0.18Å | - | - | - |
| C 950 | ALA | 50 | - | Favored (88.88%) General / -65.1,-37.9 | - | 0.11Å | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
| Avg: Clashscore: 56.86 | | | | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 | Non-Trans: 5 of 174 |
| C 951 | ASN | 50 | - | Favored (73.44%) General / -61.8,-50.2 | Favored (28.9%) <i>m-40</i> chi angles: 302.2,346.2 | 0.10Å | - | - | - |
| C 952 | MET | 50 | - | Favored (66.82%) General / -54.0,-40.4 | Favored (9.6%) <i>tpt</i> chi angles: 180.9,79.5,187.9 | 0.05Å | - | - | - |
| C 953 | SER | 50 | - | Favored (70.11%) General / -64.4,-29.0 | Favored (5%) <i>t</i> chi angles: 195.8 | 0.14Å | - | - | - |
| C 954 | LEU | 50 | - | Favored (43.66%) General / -75.6,-44.3 | Favored (29.9%) <i>mt</i> chi angles: 301.4,165.8 | 0.07Å | - | - | - |

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|-------|-----|-------|---|--|--|-------|---|---|---|
| C 955 | ASP | 50 | - | Favored (81.79%) General / -62.0,-36.5 | OUTLIER (0.3%) chi angles: 309.9,16.6 | 0.13Å | - | OUTLIER(S) worst is CA- CB-CG: 4.3 σ | - |
| C 956 | ILE | 50 | - | Favored (95.53%) Ile or Val / -60.5,-43.9 | Allowed (1.4%) <i>mm</i> chi angles: 290.3,272.7 | 0.09Å | - | - | - |
| C 957 | LEU | 50 | - | Favored (93.76%) General / -61.1,-40.4 | Favored (95.1%) <i>mt</i> chi angles: 296.9,175.3 | 0.12Å | - | - | - |
| C 958 | SER | 50 | - | Favored (97.47%) General / -63.5,-43.3 | Favored (36%) <i>m</i> chi angles: 302.3 | 0.07Å | - | - | - |
| C 959 | ALA | 50 | - | Favored (73.37%) General / -67.2,-32.4 | - | 0.10Å | - | - | - |
| C 960 | VAL | 50 | - | Favored (69.55%) Ile or Val / -71.9,-41.9 | Favored (13.1%) <i>m</i> chi angles: 305.2 | 0.24Å | - | - | - |
| C 961 | GLY | 50 | - | Favored (70.9%) Glycine / -69.0,-16.8 | - | - | - | - | - |
| C 962 | THR | 50 | - | Favored (59.45%) General / -74.7,-21.4 | Allowed (1.1%) <i>p</i> chi angles: 39.9 | 0.12Å | - | - | - |
| C 963 | PHE | 99.99 | - | Favored (4.29%) General / -115.9,178.5 | Favored (47.9%) <i>m-80</i> chi angles: 306.6,293.5 | 0.04Å | - | - | - |
| C 964 | ARG | 50 | - | Favored (3.45%) General / -153.3,110.4 | Favored (32.3%) <i>mmt-90</i> chi angles: 283.2,310.6,185.4,277.5 | 0.07Å | - | - | - |
| C 965 | MET | 50 | - | Allowed (1.76%) General / -47.6,147.6 | Favored (3.1%) <i>ppp</i> chi angles: 65.8,93.4,70 | 0.04Å | - | OUTLIER(S) worst is C-N- CA: 4.2 σ | - |
| C 966 | ARG | 99.99 | - | Allowed (0.1%) General / -46.0,-20.8 | Favored (2.8%) <i>ttt90</i> chi angles: 186.6,156.2,144,62.5 | 0.17Å | - | - | - |
| C 967 | HIS | 50 | - | Favored (59.93%) General / -77.0,-13.8 | Favored (7.5%) <i>m-70</i> chi angles: 300.9,336.8 | 0.15Å | - | OUTLIER(S) worst is CA- CB-CG: 6.0 σ | - |
| C 968 | MET | 99.99 | - | Allowed (0.72%) Pre-Pro / 63.3,46.3 | Favored (12.1%) <i>mmt</i> chi angles: 297.2,295.2,131.8 | 0.17Å | - | - | - |

| C 969 | PRO | 99.99 | - | Favored (6.19%) Trans-Pro / -87.3,172.0 | OUTLIER (0.1%) chi angles: 44.3 | 0.10Å | - | - | - |
|------------|---------|--------|--------------|---|--|-------------------------|--------------------|---|------------------------------|
| C 970 | GLU | 99.99 | - | Favored (66.52%) General / -60.3,-52.1 | OUTLIER (0%) chi angles: 202,326.9,93.9 | 0.08Å | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | C β deviation | Bond lengths | Bond angles | Cis Peptides |
| Avg: 56.86 | | | | Clashscore: 0.74 | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 |
| | | | | | | | | | |
| C 971 | VAL | 99.99 | - | Favored (26.14%) Pre-Pro / -52.1,123.1 | Favored (17.6%) <i>m</i> chi angles: 293.2 | 0.10Å | - | - | - |
| C 972 | PRO | 99.99 | - | Favored (77.51%) Trans-Pro / -62.4,-27.4 | Allowed (1.9%) <i>Cg_exo</i> chi angles: 357.4 | 0.24Å | - | OUTLIER(S) worst is C-N- CA: 7.6 σ | - |
| C 973 | VAL | 50 | - | Allowed (0.45%) Ile or Val / -53.5,159.9 | Favored (16.9%) <i>m</i> chi angles: 293 | 0.04Å | - | - | Cis nonPRO omega= 1.61 |
| C 974 | ARG | 50 | - | Favored (18.7%) General / -87.4,159.5 | Favored (11.2%) <i>mtt-85</i> chi angles: 300.5,189.8,211.8,296.2 | 0.06Å | - | - | - |
| C 975 | ILE | 50 | - | Favored (32.38%) Ile or Val / -126.7,150.2 | Allowed (0.9%) <i>tp</i> chi angles: 198.4,88.9 | 0.17Å | - | - | - |
| C 976 | ARG | 50 | - | Favored (18.42%) General / -95.5,152.4 | Favored (35%) <i>mtm-85</i> chi angles: 274.9,174.5,282.5,261 | 0.09Å | - | - | - |
| C 977 | ILE | 50 | - | Favored (23.94%) Ile or Val / -144.4,139.4 | Favored (40.9%) <i>mt</i> chi angles: 288.6,177.9 | 0.13Å | - | - | - |
| C 978 | GLY | 50 | - | Allowed (0.88%) Glycine / -141.8,114.1 | - | - | - | - | - |
| C 979 | LEU | 50 | - | Favored (45.75%) General / -100.6,132.8 | Favored (4.4%) <i>mp</i> chi angles: 285.4,57.1 | 0.09Å | - | - | - |
| C 980 | HIS | 50 | - | Favored (3.31%) General / -142.2,98.4 | Favored (7.4%) <i>t-90</i> chi angles: 179.4,296.9 | 0.11Å | - | OUTLIER(S) worst is CA- CB-CG: 5.1 σ | - |
| C 981 | SER | 50 | - | Favored (47.42%) General / | Favored (70.3%) <i>m</i> chi angles: 295 | 0.03Å | - | - | - |

-70.8,134.5

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|-------|-----|----|---|---|---|-------|---|---|---|
| C 982 | GLY | 50 | - | Favored (16.45%) Glycine / 150.3,169.5 | - | - | - | - | - |
| C 983 | PRO | 50 | - | Favored (18.65%) Trans-Pro / -81.6,156.4 | Favored (42.9%) <i>Cg_endo</i> chi angles: 33.7 | 0.08Å | - | - | - |
| C 984 | CYS | 50 | - | Favored (4.63%) General / -150.2,-174.1 | Favored (15.9%) <i>p</i> chi angles: 56.5 | 0.07Å | - | - | - |
| C 985 | VAL | 50 | - | Favored (21.75%) Ile or Val / -119.4,150.9 | Favored (4.4%) <i>p</i> chi angles: 72.2 | 0.11Å | - | - | - |
| C 986 | ALA | 50 | - | Favored (36.79%) General / -128.9,159.1 | - | 0.12Å | - | - | - |
| C 987 | GLY | 50 | - | Allowed (0.23%) Glycine / -157.3,103.5 | - | - | - | - | - |
| C 988 | VAL | 50 | - | Favored (26.72%) Ile or Val / -63.0,129.6 | Favored (80.3%) <i>t</i> chi angles: 173.1 | 0.08Å | - | - | - |
| C 989 | VAL | 50 | - | Allowed (0.17%) Ile or Val / -109.4,63.6 | Favored (98%) <i>t</i> chi angles: 175.2 | 0.15Å | - | - | - |
| C 990 | GLY | 50 | - | Favored (48.61%) Glycine / 179.0,-179.5 | - | - | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|---|---------|------------|------------------|--------------------|-------------------------|--------------------|--------------------|---------------------|---------------------|
| | | Avg: 56.86 | Clashscore: 0.74 | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 | Non-Trans: 5 of 174 |

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|-------|-----|----|---|--|---|-------|---|---|---|
| C 991 | LEU | 50 | - | OUTLIER (0.05%) General / -161.4,-53.3 | Favored (5.8%) <i>tt</i> chi angles: 186.8,143.4 | 0.08Å | - | - | - |
| C 992 | THR | 50 | - | Favored (61.56%) General / -71.5,-45.8 | Favored (5.7%) <i>p</i> chi angles: 45 | 0.10Å | - | - | - |
| C 993 | MET | 50 | - | Favored (30.68%) Pre-Pro / -118.7,141.9 | Favored (78.3%) <i>mmm</i> chi angles: 283.8,295.8,285.2 | 0.08Å | - | - | - |
| | | | | Favored | Favored (21.5%) | | | | |

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|-------|-----|----|---|--|---|-------|---|---|---|
| C 994 | PRO | 50 | - | (3.05%) Trans-Pro / -89.9,138.8 | <i>Cg_endo</i> chi angles: 36.7 | 0.07Å | - | - | - |
| C 995 | ARG | 50 | - | Favored (41.43%) General / -109.8,120.1 | Favored (50%) <i>mtp180</i> chi angles: 293.1,198.7,68.3,198.6 | 0.04Å | - | OUTLIER(S) worst is CD- NE-CZ: 4.1 σ | - |
| C 996 | TYR | 50 | - | Favored (3.7%) General / -95.2,81.8 | Favored (86.4%) <i>m-80</i> chi angles: 295.2,104.3 | 0.06Å | - | - | - |
| C 997 | CYS | 50 | - | Favored (22.53%) General / -81.3,118.3 | Favored (84.2%) <i>m</i> chi angles: 295.3 | 0.04Å | - | - | - |
| C 998 | LEU | 50 | - | Favored (30.41%) General / -110.3,149.3 | Favored (25.6%) <i>mt</i> chi angles: 304.9,187.8 | 0.04Å | - | - | - |
| C 999 | PHE | 50 | - | Favored (13.49%) General / -145.0,172.1 | Favored (56.9%) <i>t80</i> chi angles: 184.5,66.1 | 0.10Å | - | - | - |
| C1000 | GLY | 50 | - | Favored (16.54%) Glycine / 113.1,166.3 | - | - | - | - | - |
| C1001 | ASP | 50 | - | Favored (59.99%) General / -77.1,-12.8 | Favored (7.3%) <i>t70</i> chi angles: 205,47.4 | 0.18Å | - | - | - |
| C1002 | THR | 50 | - | Favored (81.65%) General / -63.5,-35.8 | Allowed (1.3%) <i>p</i> chi angles: 40.2 | 0.13Å | - | - | - |
| C1003 | VAL | 50 | - | Favored (40.14%) Ile or Val / -71.6,-50.4 | Favored (59.3%) <i>t</i> chi angles: 170.7 | 0.12Å | - | - | - |
| C1004 | ASN | 50 | - | Favored (54.98%) General / -76.1,-24.4 | Favored (4.4%) <i>t0</i> chi angles: 198.5,255.7 | 0.24Å | - | - | - |
| C1005 | THR | 50 | - | Favored (76.01%) General / -58.1,-38.1 | Favored (7.3%) <i>p</i> chi angles: 45.7 | 0.21Å | - | OUTLIER(S) worst is N- CA-CB: 4.2 σ | - |
| C1006 | ALA | 50 | - | Favored (85.31%) General / -61.7,-37.8 | - | 0.11Å | - | - | - |
| C1007 | SER | 50 | - | Favored (69.7%) General / -69.3,-31.3 | Favored (35.7%) <i>t</i> chi angles: 181.3 | 0.12Å | - | - | - |
| | | | | Favored (74%) General / | Allowed (1.5%) <i>mpp-170</i> | | | | |

| C1008 | ARG | 50 | - | -64.2,-32.4 | chi angles: 279.9,95.5,76.7,179 | 0.21Å | - | - | - |
|------------|---------|--------|--------------|---|--|-------------------------|--------------------|--------------------|---------------------|
| C1009 | MET | 50 | - | Favored (73.14%) General / -70.0,-34.3 | Allowed (1.9%) <i>mtt</i> chi angles: 294,143.6,200.8 | 0.15Å | - | - | - |
| C1010 | GLU | 50 | - | Favored (61.71%) General / -60.6,-53.1 | Favored (32.1%) <i>tt0</i> chi angles: 182.4,189.7,44.8 | 0.10Å | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
| Avg: 56.86 | | | | Clashscore: 0.74 | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 |
| C1011 | SER | 50 | - | Favored (69.63%) General / -62.6,-28.1 | Favored (8.7%) <i>t</i> chi angles: 192.2 | 0.12Å | - | - | - |
| C1012 | THR | 50 | - | Favored (55.01%) General / -95.1,1.9 | Favored (27.7%) <i>p</i> chi angles: 52.4 | 0.14Å | - | - | - |
| C1013 | GLY | 50 | - | Favored (29.45%) Glycine / -73.7,141.4 | - | - | - | - | - |
| C1014 | LEU | 50 | - | Favored (56.22%) Pre-Pro / -79.3,137.6 | Allowed (1.4%) <i>tt</i> chi angles: 201.9,150.2 | 0.05Å | - | - | - |
| C1015 | PRO | 50 | - | Favored (20.22%) Trans-Pro / -49.1,128.7 | OUTLIER (0%) chi angles: 317.3 | 0.07Å | - | - | - |
| C1016 | TYR | 50 | - | Favored (6.34%) General / 65.3,37.6 | Favored (7.3%) <i>t80</i> chi angles: 204.2,87.4 | 0.16Å | - | - | - |
| C1017 | ARG | 50 | - | Favored (47.07%) General / -139.2,156.4 | Favored (50.8%) <i>mtt180</i> chi angles: 297.2,203,190.5,179.8 | 0.06Å | - | - | - |
| C1018 | ILE | 50 | - | Favored (7.37%) Ile or Val / -99.3,98.7 | Favored (55%) <i>mt</i> chi angles: 302,179 | 0.09Å | - | - | - |
| C1019 | HIS | 50 | - | Favored (3.67%) General / -77.2,89.7 | Favored (17.4%) <i>t-170</i> chi angles: 181.8,183.9 | 0.12Å | - | - | - |
| C1020 | VAL | 50 | - | Favored (4.9%) Ile or Val / -70.6,111.9 | Favored (70.2%) <i>t</i> chi angles: 178.7 | 0.07Å | - | - | - |
| | | | | Favored | | | | | |

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|-------|-----|-------|---|--|---|-------|---|---|---|
| C1021 | ASN | 50 | - | (17.62%) General / -59.4,154.0 | Favored (46.4%) <i>tO</i> chi angles: 183.4,37.1 | 0.06Å | - | - | - |
| C1022 | LEU | 50 | - | Favored (67.98%) General / -57.6,-33.3 | Favored (50.4%) <i>mt</i> chi angles: 305.9,182 | 0.17Å | - | - | - |
| C1023 | SER | 50 | - | Favored (94.4%) General / -63.6,-44.4 | Favored (86.5%) <i>p</i> chi angles: 67.2 | 0.13Å | - | - | - |
| C1024 | THR | 50 | - | Favored (91.44%) General / -63.9,-38.5 | Allowed (2%) <i>m</i> chi angles: 318.5 | 0.10Å | - | - | - |
| C1025 | VAL | 50 | - | Favored (81.36%) Ile or Val / -65.2,-37.9 | OUTLIER (0.3%) chi angles: 86.5 | 0.23Å | - | - | - |
| C1026 | GLY | 50 | - | Favored (72.76%) Glycine / -68.2,-45.1 | - | - | - | - | - |
| C1027 | ILE | 50 | - | Favored (50.72%) Ile or Val / -69.7,-32.0 | Favored (7.1%) <i>tp</i> chi angles: 185.3,57.4 | 0.28Å | - | - | - |
| C1028 | LEU | 50 | - | Favored (87%) General / -61.3,-38.5 | Favored (73.6%) <i>mt</i> chi angles: 287,167.8 | 0.10Å | - | - | - |
| C1029 | ARG | 50 | - | Favored (59.94%) General / -76.1,-11.5 | Favored (5.6%) <i>tpp-160</i> chi angles: 199.6,57.7,57.2,213.5 | 0.11Å | - | - | - |
| C1030 | ALA | 99.99 | - | Favored (23.67%) General / -107.8,16.4 | - | 0.04Å | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|---|---------|------------|------------------|--------------------|-------------------------|--------------------|--------------------|---------------------|---------------------|
| | | Avg: 56.86 | Clashscore: 0.74 | Outliers: 2 of 173 | Poor rotamers: 9 of 149 | Outliers: 1 of 160 | Outliers: 0 of 175 | Outliers: 16 of 175 | Non-Trans: 5 of 174 |

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|-------|-----|-------|---|--|--|-------|---|--|---|
| C1031 | LEU | 99.99 | - | Allowed (0.26%) General / -127.0,-140.2 | Favored (75.9%) <i>mt</i> chi angles: 299.9,172.2 | 0.15Å | - | OUTLIER(S) worst is C-N-CA: 4.8 σ | - |
| C1032 | ASP | 99.99 | - | Allowed (0.08%) General / -67.7,63.4 | OUTLIER (0.1%) chi angles: 319,37.7 | 0.04Å | - | OUTLIER(S) worst is CA-CB-CG: 6.7 σ | - |
| C1033 | SER | 99.99 | - | OUTLIER (0.02%) General / -64.8,52.5 | Favored (36.3%) <i>t</i> chi angles: 181.3 | 0.11Å | - | - | - |
| | | | | Favored | | | | | |

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|-------|-----|-------|---|---|---|-------|---|--|---|
| C1034 | GLY | 50 | - | (17.75%) Glycine / -100.0,-19.9 | - | - | - | - | - |
| C1035 | TYR | 50 | - | Favored (44.08%) General / -58.5,143.9 | Favored (44.6%) <i>m-80</i> chi angles: 308.8,288.7 | 0.06Å | - | - | - |
| C1036 | GLN | 50 | - | Favored (39.93%) General / -118.8,150.4 | Favored (13.3%) <i>tp-100</i> chi angles: 184.5,56.7,273.8 | 0.09Å | - | - | - |
| C1037 | VAL | 50 | - | Favored (18.82%) Ile or Val / -142.7,158.8 | Favored (3.2%) <i>p</i> chi angles: 74.3 | 0.11Å | - | - | - |
| C1038 | GLU | 50 | - | Favored (25.18%) General / -90.8,144.9 | Favored (11.2%) <i>pt0</i> chi angles: 65.6,177.6,316.2 | 0.07Å | - | - | - |
| C1039 | LEU | 50 | - | Favored (7.75%) General / -88.8,77.6 | Favored (30.8%) <i>mt</i> chi angles: 309,183.3 | 0.08Å | - | - | - |
| C1040 | ARG | 50 | - | Favored (44.63%) General / -68.8,153.0 | Favored (66.9%) <i>mtp180</i> chi angles: 299.1,192.9,69.5,185.3 | 0.05Å | - | - | - |
| C1041 | GLY | 50 | - | Favored (48.4%) Glycine / -74.6,176.4 | - | - | - | - | - |
| C1042 | ARG | 50 | - | Favored (61.96%) General / -71.7,-20.3 | Favored (20.2%) <i>tpt90</i> chi angles: 192.2,67,200.7,85.8 | 0.12Å | - | - | - |
| C1043 | THR | 50 | - | Favored (60.32%) General / -75.5,-16.4 | Favored (6.2%) <i>p</i> chi angles: 45.3 | 0.03Å | - | - | - |
| C1044 | GLU | 50 | - | Favored (29.61%) General / -105.7,13.6 | Favored (28.8%) <i>mt-10</i> chi angles: 301.6,186.3,269.7 | 0.05Å | - | OUTLIER(S) worst is C-N- CA: 5.4 σ | - |
| C1045 | LEU | 99.99 | - | - | Favored (6.7%) <i>tp</i> chi angles: 177.9,44.7 | 0.07Å | - | - | - |

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