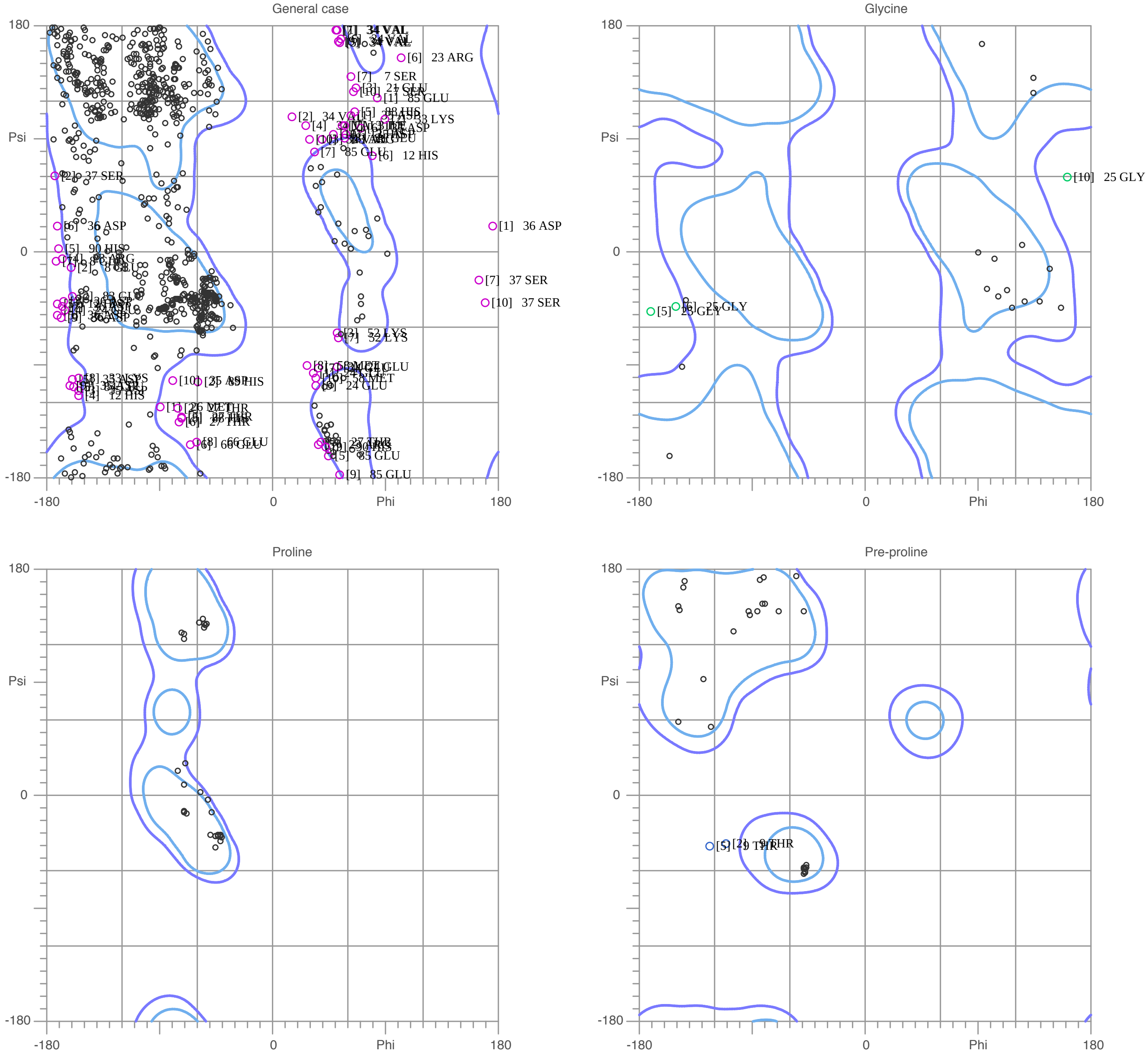
MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, all models



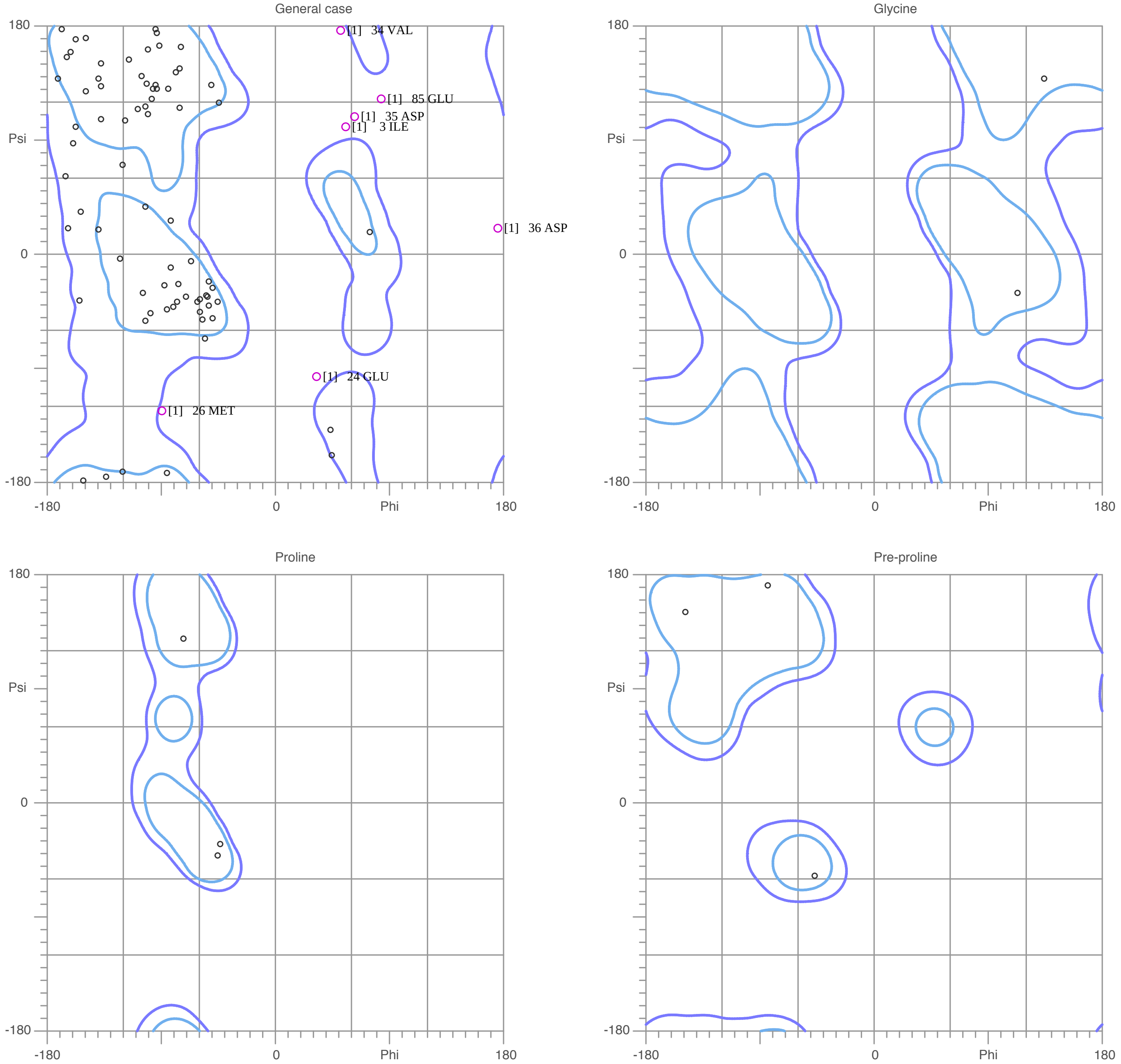
```
72.4% (644/890) of all residues were in favored (98%) regions.
91.7% (816/890) of all residues were in allowed (>99.8%) regions.

There were 74 outliers (phi, psi):
   [1]    3 ILE (55.1, 101.6)
   [1]   24 GLU (32.6, -96.9)
   [1]   26 MET (-90.5, -123.6)
   [1]   34 VAL (51.6, 177.9)
   [1]   35 ASP (62.5, 109.3)
   [1]   36 ASP (175.2, 21.1)
   [1]   85 GLU (83.3, 123.7)
   [2]    8 GLU (-161.2, -12.4)
   [2]    9 THR (-111.6, -38.8)
   [2]   27 THR (-76.7, -124.2)
   [2]   33 LYS (89.5, 106.6)
   [2]   34 VAL (15.6, 108.4)
   [2]   37 SER (-174.4, 61.0)
   [2]   83 GLU (-160.6, -35.1)
   [2]   89 HIS (-60.6, -103.5)
   [3]   21 GLU (66.1, 131.3)
   [3]   23 ARG (39.3, 90.3)
   [3]   24 GLU (51.3, -91.3)
   [3]   27 THR (38.8, -151.9)
   [3]   35 ASP (-155.6, -110.3)
   [3]   36 ASP (-167.9, -39.4)
   [3]   52 LYS (51.8, -64.2)
   [4]   12 HIS (-155.3, -114.4)
   [4]   23 ARG (-168.1, -5.4)
   [4]   24 GLU (-166.5, -46.6)
   [4]   34 VAL (26.6, 101.4)
   [5]    9 THR (-124.9, -40.4)
   [5]   12 HIS (-172.2, -41.8)
   [5]   23 ARG (36.4, -153.7)
   [5]   25 GLY (-171.7, -47.3)
   [5]   27 THR (-73.6, -131.5)
   [5]   34 VAL (53.7, 167.7)
   [5]   35 ASP (-160.1, -101.9)
   [5]   36 ASP (-172.5, -50.2)
   [5]   84 LEU (-159.7, -108.0)
   [5]   85 GLU (44.3, -162.5)
   [5]   88 HIS (65.3, 112.2)
   [5]   90 HIS (-171.8, 3.7)
   [6]   12 HIS (79.5, 77.3)
   [6]   23 ARG (102.3, 155.8)
   [6]   25 GLY (-151.2, -43.3)
   [6]   27 THR (-75.9, -135.9)
   [6]   34 VAL (54.9, 170.8)
   [6]   35 ASP (70.5, 99.1)
   [6]   36 ASP (-172.7, 21.1)
   [6]   66 GLU (-66.1, -153.6)
   [7]    3 ILE (57.4, 101.8)
   [7]    7 SER (62.2, 140.6)
   [7]    8 GLU (-173.7, -7.6)
   [7]   24 GLU (36.8, -92.5)
   [7]   34 VAL (50.2, 177.2)
   [7]   35 ASP (58.1, 94.9)
   [7]   36 ASP (-168.1, -43.5)
   [7]   37 SER (164.7, -22.3)
   [7]   52 LYS (52.3, -68.1)
   [7]   85 GLU (33.2, 80.3)
   [8]   21 GLU (57.8, 91.9)
   [8]   33 LYS (-155.5, -100.5)
   [8]   58 MET (28.0, -90.1)
   [8]   66 GLU (-61.6, -151.9)
   [8]   88 HIS (-73.9, -132.4)
   [9]   24 GLU (34.0, -106.9)
   [9]   34 VAL (52.7, 169.0)
   [9]   35 ASP (-162.6, -106.4)
   [9]   36 ASP (-169.1, -52.1)
   [9]   85 GLU (53.3, -177.2)
   [9]   90 HIS (42.0, -155.1)
   [10]   7 SER (65.0, 128.7)
   [10]  12 HIS (48.6, 94.0)
   [10]  25 GLY (161.8, 60.3)
   [10]  34 VAL (29.6, 91.0)
   [10]  35 ASP (-80.3, -102.8)
   [10]  37 SER (169.2, -40.6)
   [10]  58 MET (34.5, -100.3)
```

http://kinemage.biochem.duke.edu

Lovell, Davis, et al. Proteins 50:437 (2003)

MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 1



78.7% (70/89) of all residues were in favored (98%) regions.
92.1% (82/89) of all residues were in allowed (>99.8%) regions.

There were 7 outliers (phi, psi):

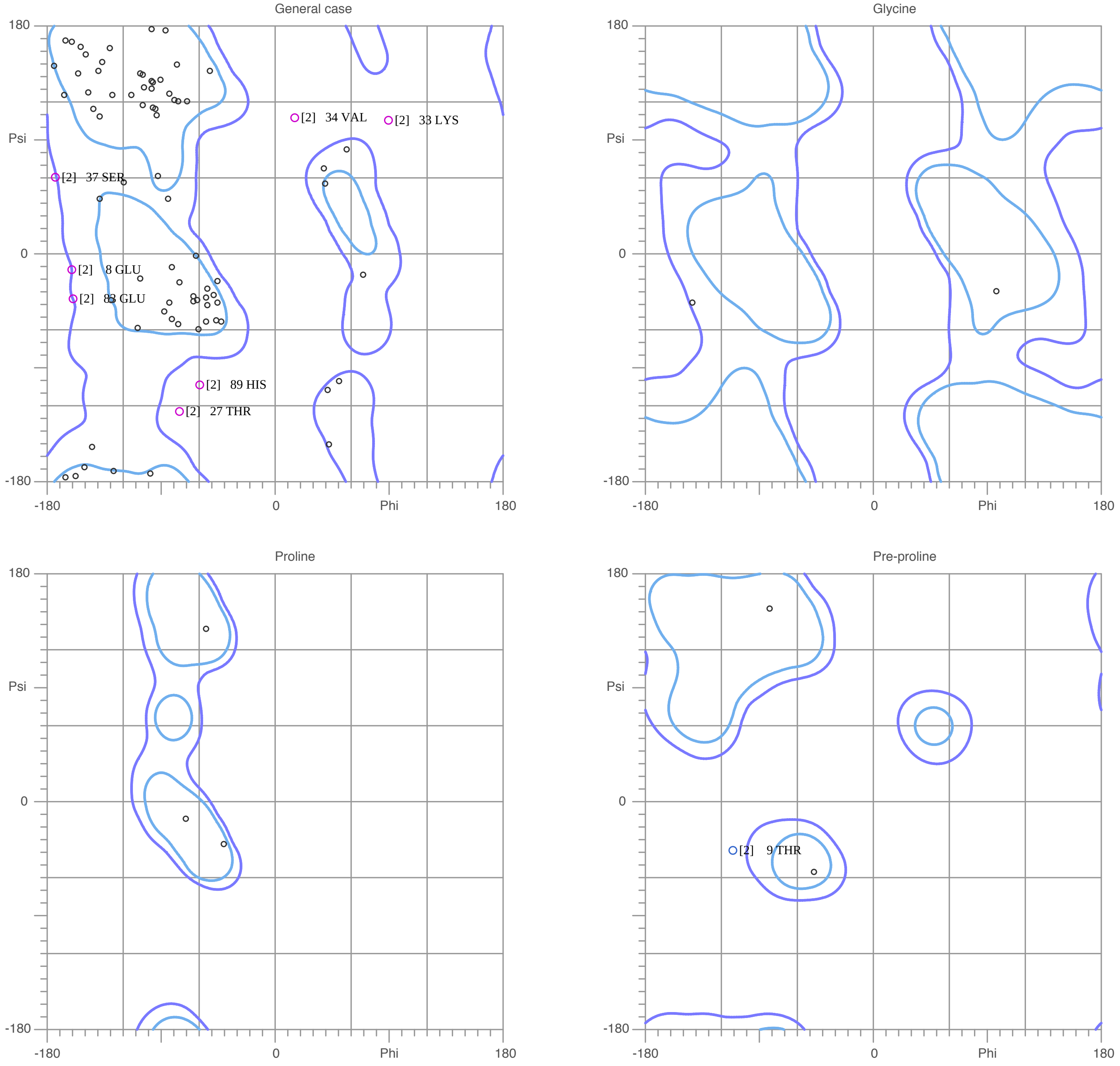
[1] 3 ILE (55.1, 101.6)
[1] 24 GLU (32.6, -96.9)
[1] 26 MET (-90.5, -123.6)
[1] 34 VAL (51.6, 177.9)
[1] 35 ASP (62.5, 109.3)
[1] 36 ASP (175.2, 21.1)
[1] 85 GLU (83.3, 123.7)

http://kinemage.biochem.duke.edu

Lovell, Davis, et al. Proteins 50:437 (2003)

MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 2



74.2% (66/89) of all residues were in favored (98%) regions.
91.0% (81/89) of all residues were in allowed (>99.8%) regions.

There were 8 outliers (phi, psi):

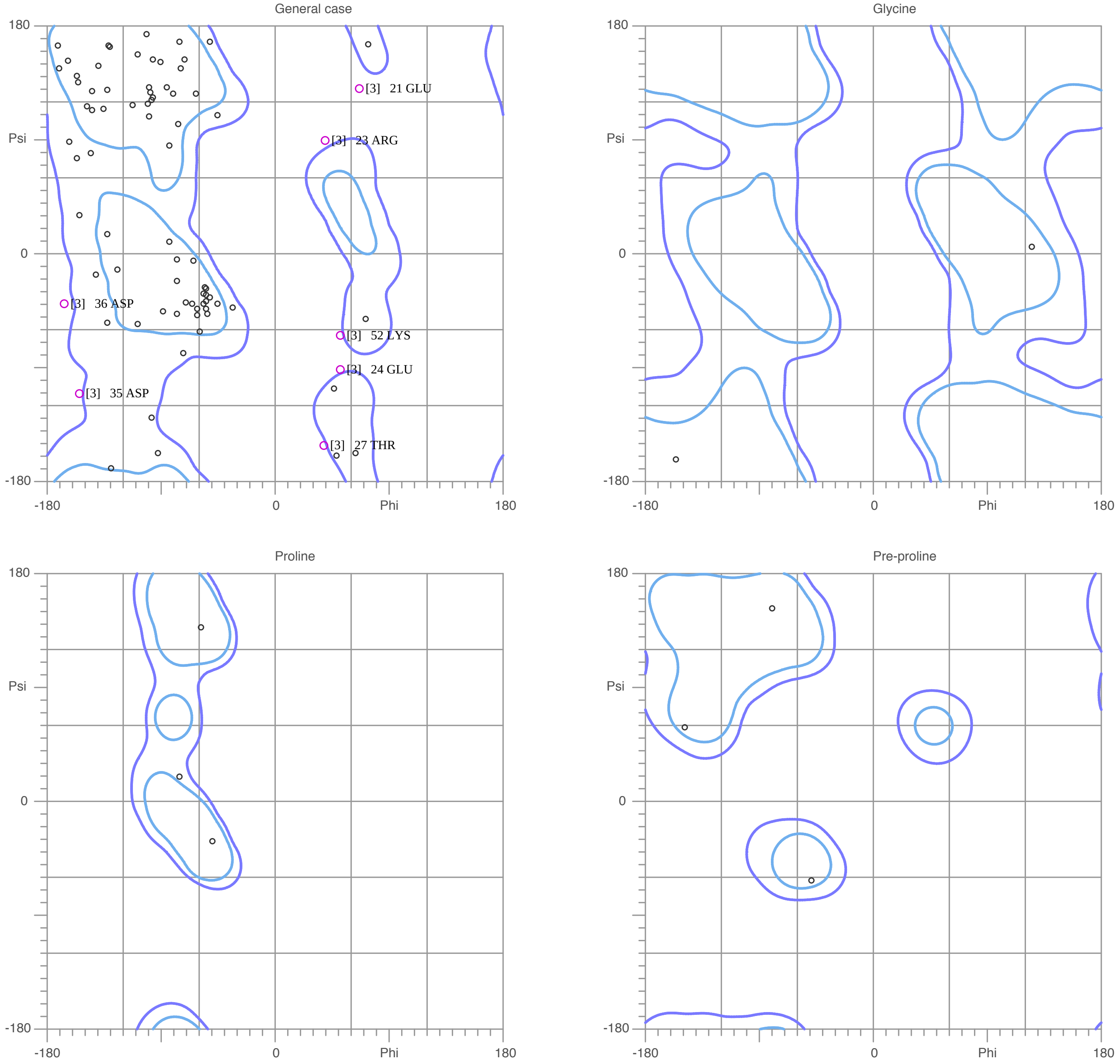
[2] 8 GLU (-161.2, -12.4)
[2] 9 THR (-111.6, -38.8)
[2] 27 THR (-76.7, -124.2)
[2] 33 LYS (89.5, 106.6)
[2] 34 VAL (15.6, 108.4)
[2] 37 SER (-174.4, 61.0)
[2] 83 GLU (-160.6, -35.1)
[2] 89 HIS (-60.6, -103.5)

http://kinemage.biochem.duke.edu

Lovell, Davis, et al. Proteins 50:437 (2003)

MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 3



70.8% (63/89) of all residues were in favored (98%) regions.
92.1% (82/89) of all residues were in allowed (>99.8%) regions.

There were 7 outliers (phi, psi):

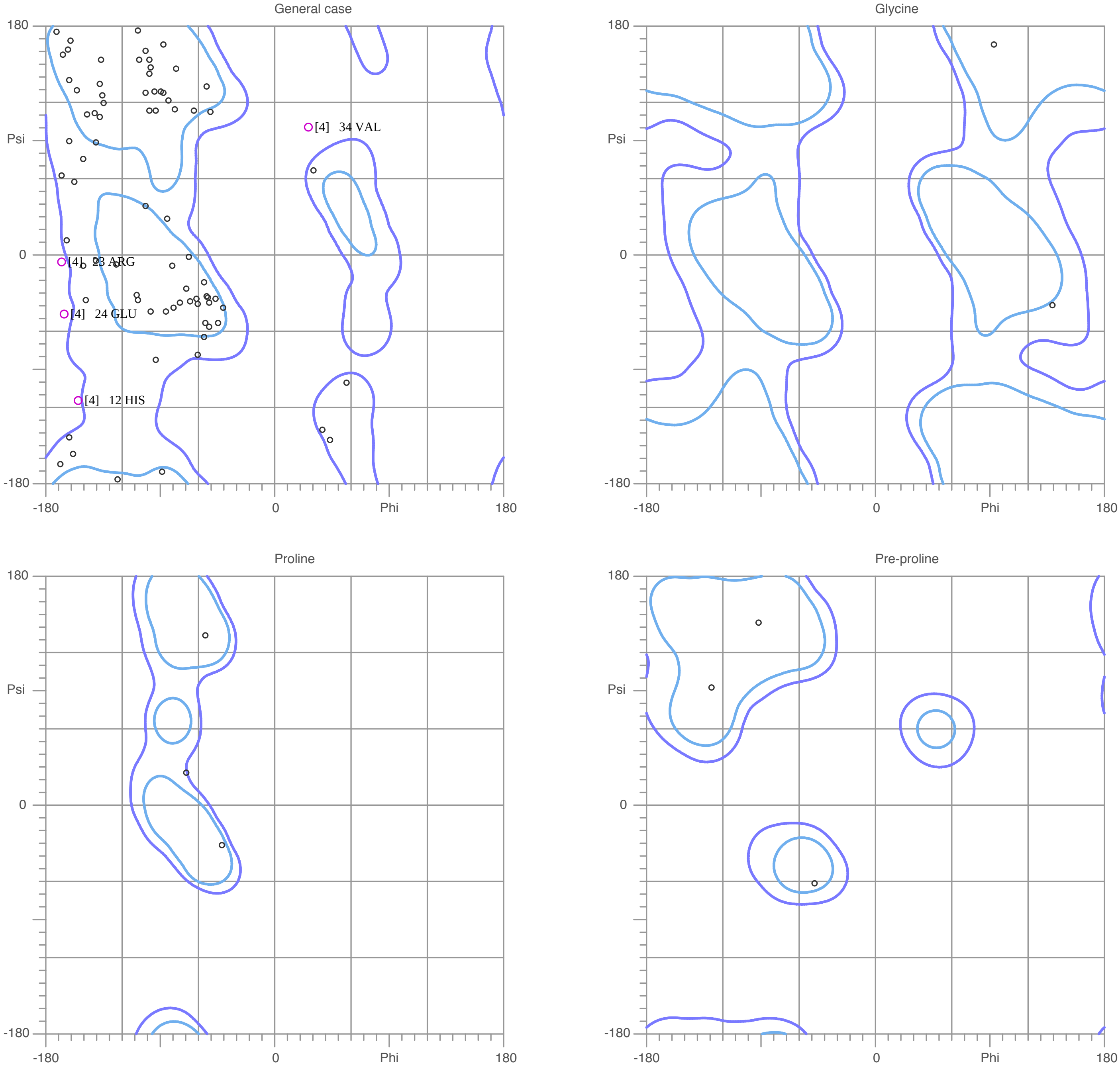
[3] 21 GLU (66.1, 131.3)
[3] 23 ARG (39.3, 90.3)
[3] 24 GLU (51.3, -91.3)
[3] 27 THR (38.8, -151.9)
[3] 35 ASP (-155.6, -110.3)
[3] 36 ASP (-167.9, -39.4)
[3] 52 LYS (51.8, -64.2)

http://kinemage.biochem.duke.edu

Lovell, Davis, et al. Proteins 50:437 (2003)

MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 4



69.7% (62/89) of all residues were in favored (98%) regions.
95.5% (85/89) of all residues were in allowed (>99.8%) regions.

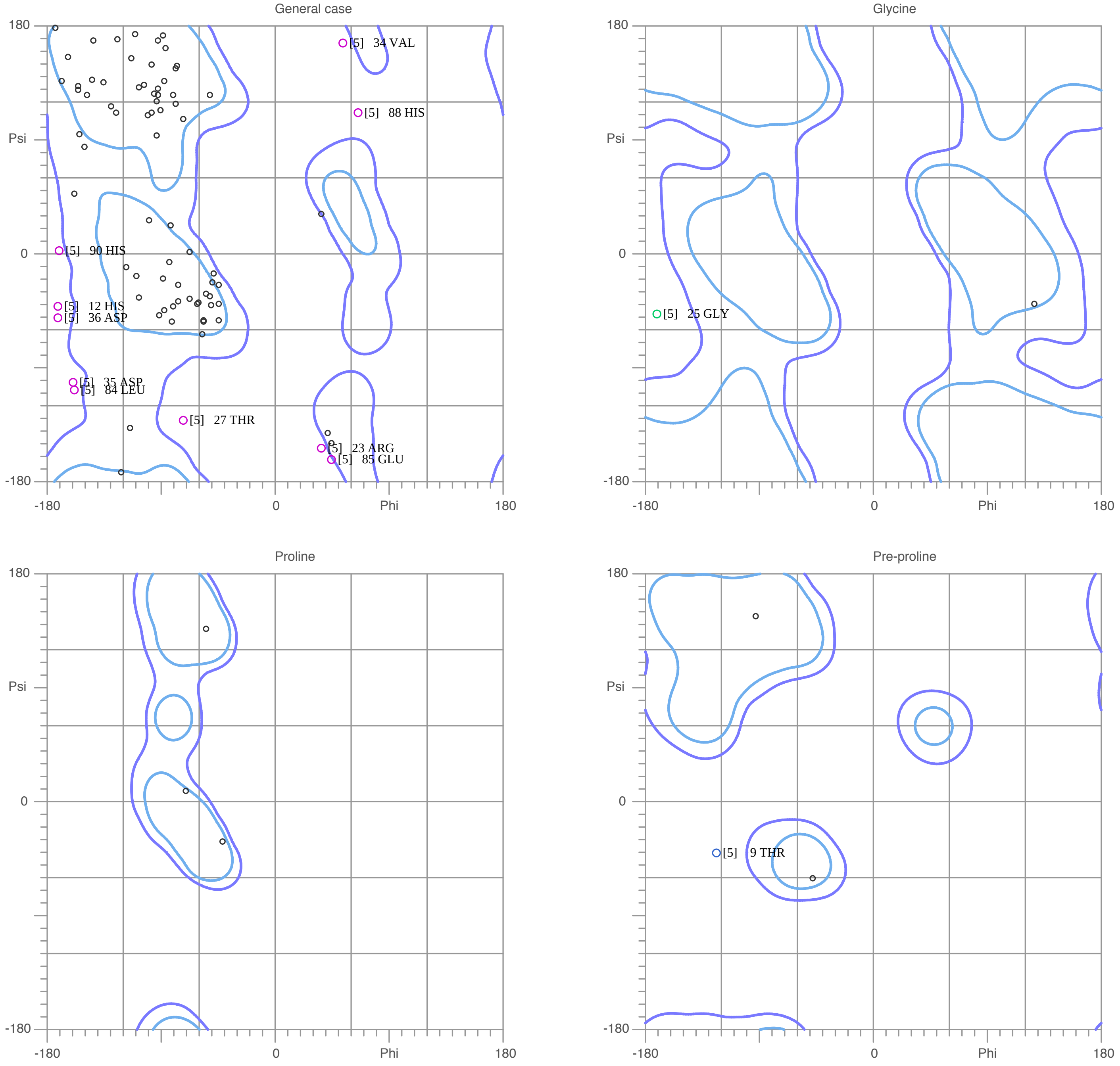
There were 4 outliers (phi, psi):

[4] 12 HIS (-155.3, -114.4)
[4] 23 ARG (-168.1, -5.4)
[4] 24 GLU (-166.5, -46.6)
[4] 34 VAL (26.6, 101.4)

Lovell, Davis, et al. Proteins 50:437 (2003)

MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 5



75.3% (67/89) of all residues were in favored (98%) regions.
86.5% (77/89) of all residues were in allowed (>99.8%) regions.

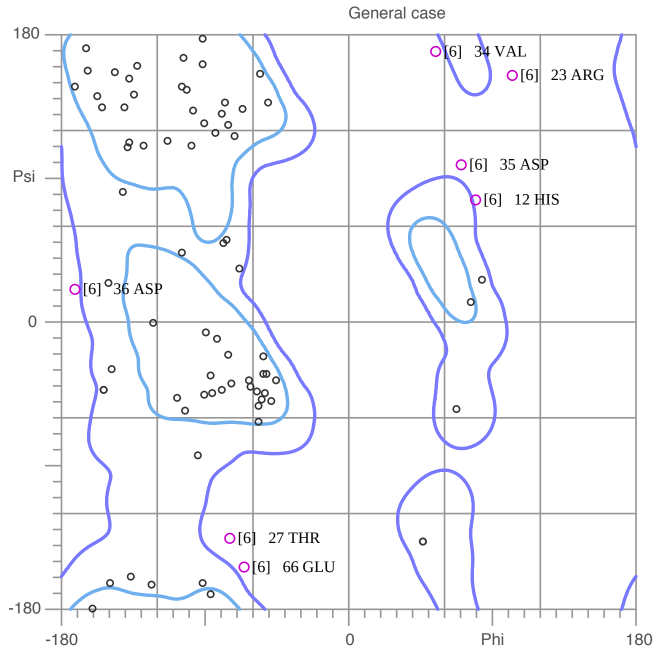
There were 12 outliers (phi, psi):
[5] 9 THR (-124.9, -40.4)
[5] 12 HIS (-172.2, -41.8)
[5] 23 ARG (36.4, -153.7)
[5] 25 GLY (-171.7, -47.3)
[5] 27 THR (-73.6, -131.5)
[5] 34 VAL (53.7, 167.7)
[5] 35 ASP (-160.1, -101.9)
[5] 36 ASP (-172.5, -50.2)
[5] 84 LEU (-159.7, -108.0)
[5] 85 GLU (44.3, -162.5)
[5] 88 HIS (65.3, 112.2)
[5] 90 HIS (-171.8, 3.7)

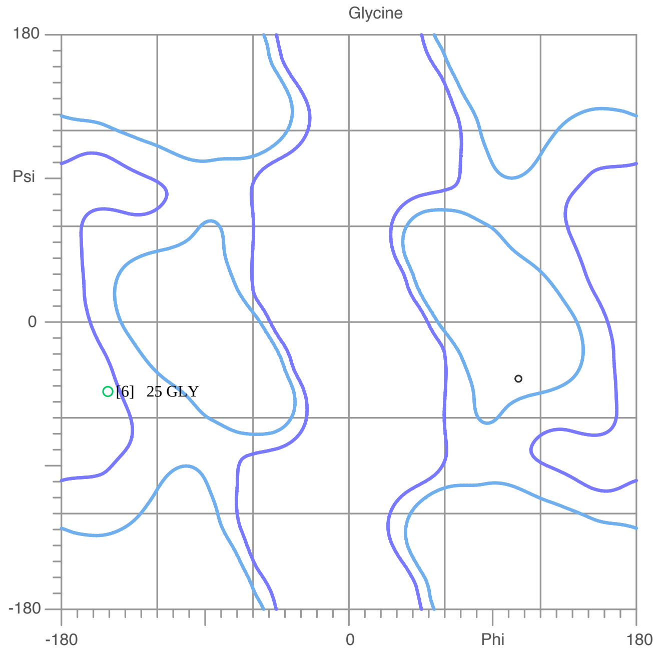
http://kinemage.biochem.duke.edu

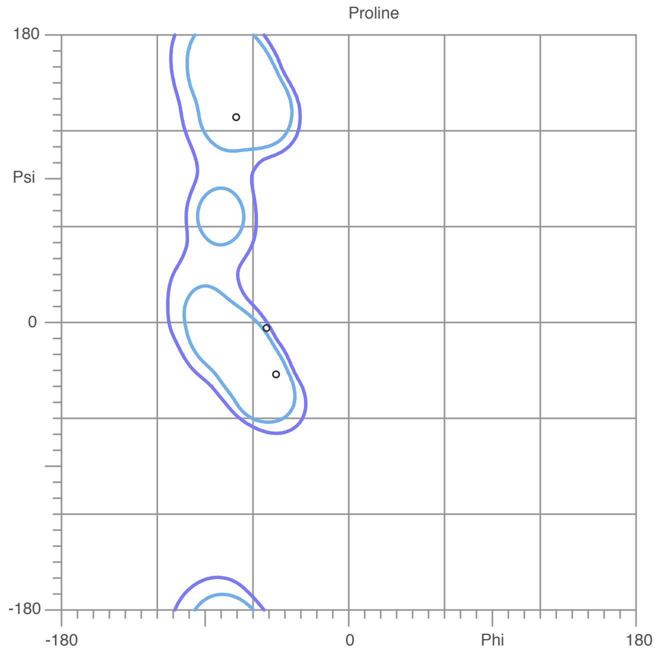
Lovell, Davis, et al. Proteins 50:437 (2003)

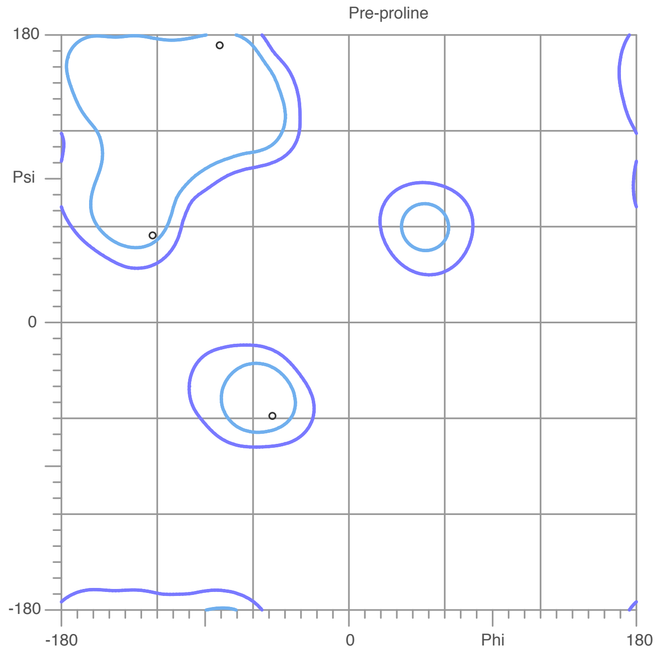
MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 6









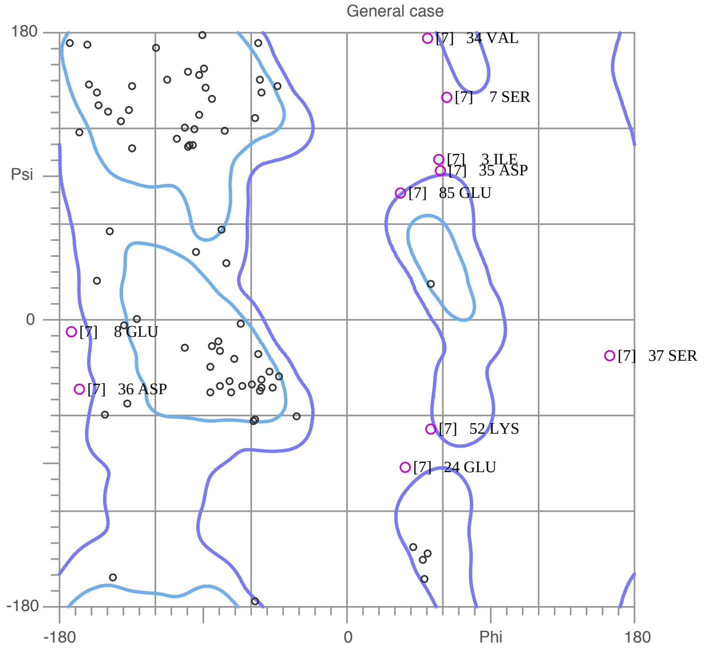
69.7% (62/89) of all residues were in favored (98%) regions.
91.0% (81/89) of all residues were in allowed (>99.8%) regions.

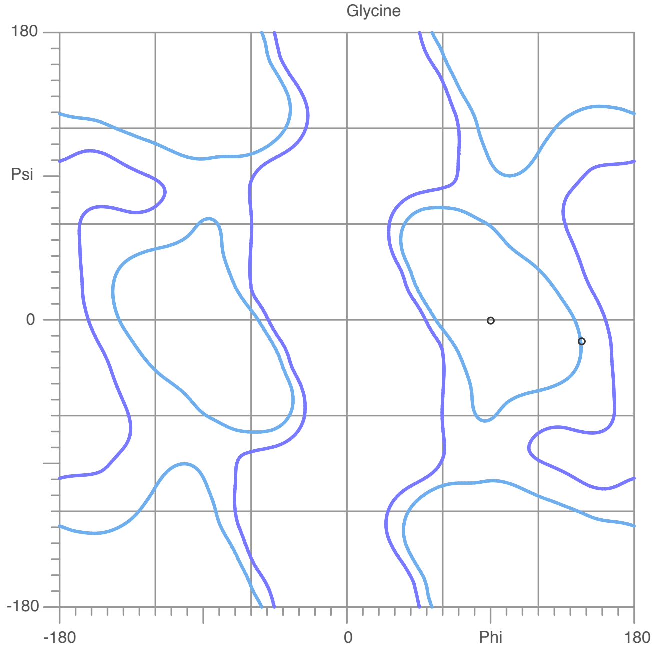
There were 8 outliers (phi, psi):
[6] 12 HIS (79.5, 77.3)
[6] 23 ARG (102.3, 155.8)
[6] 25 GLY (-151.2, -43.3)
[6] 27 THR (-75.9, -135.9)
[6] 34 VAL (54.9, 170.8)
[6] 35 ASP (70.5, 99.1)
[6] 36 ASP (-172.7, 21.1)
[6] 66 GLU (-66.1, -153.6)

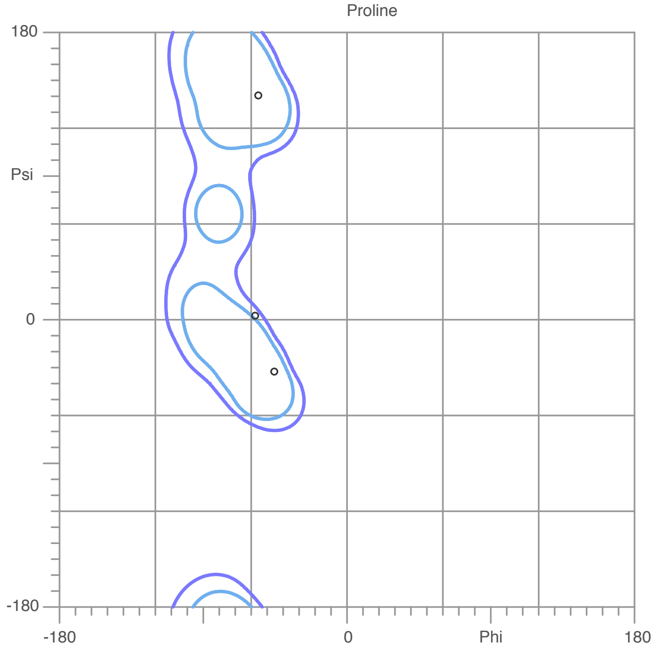
http://kinemage.biochem.duke.edu
Lovell, Davis, et al. Proteins 50:437 (2003)

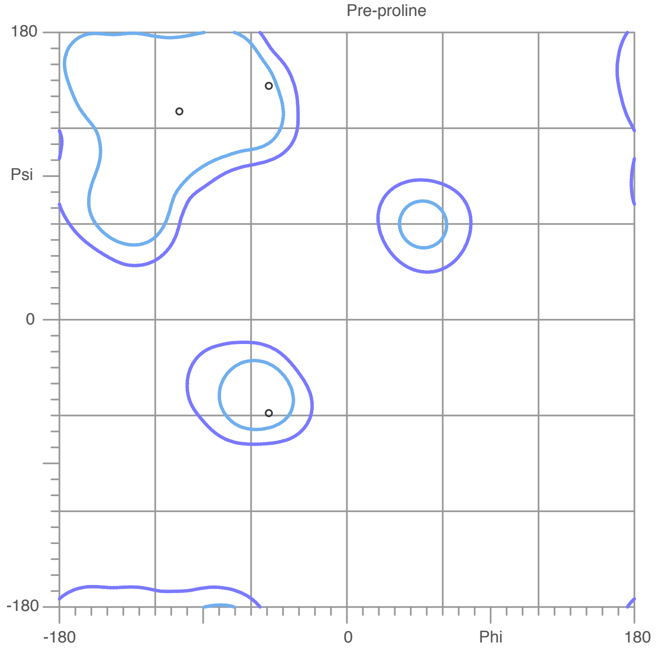
MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 7









67.4% (60/89) of all residues were in favored (98%) regions.
88.8% (79/89) of all residues were in allowed (>99.8%) regions.

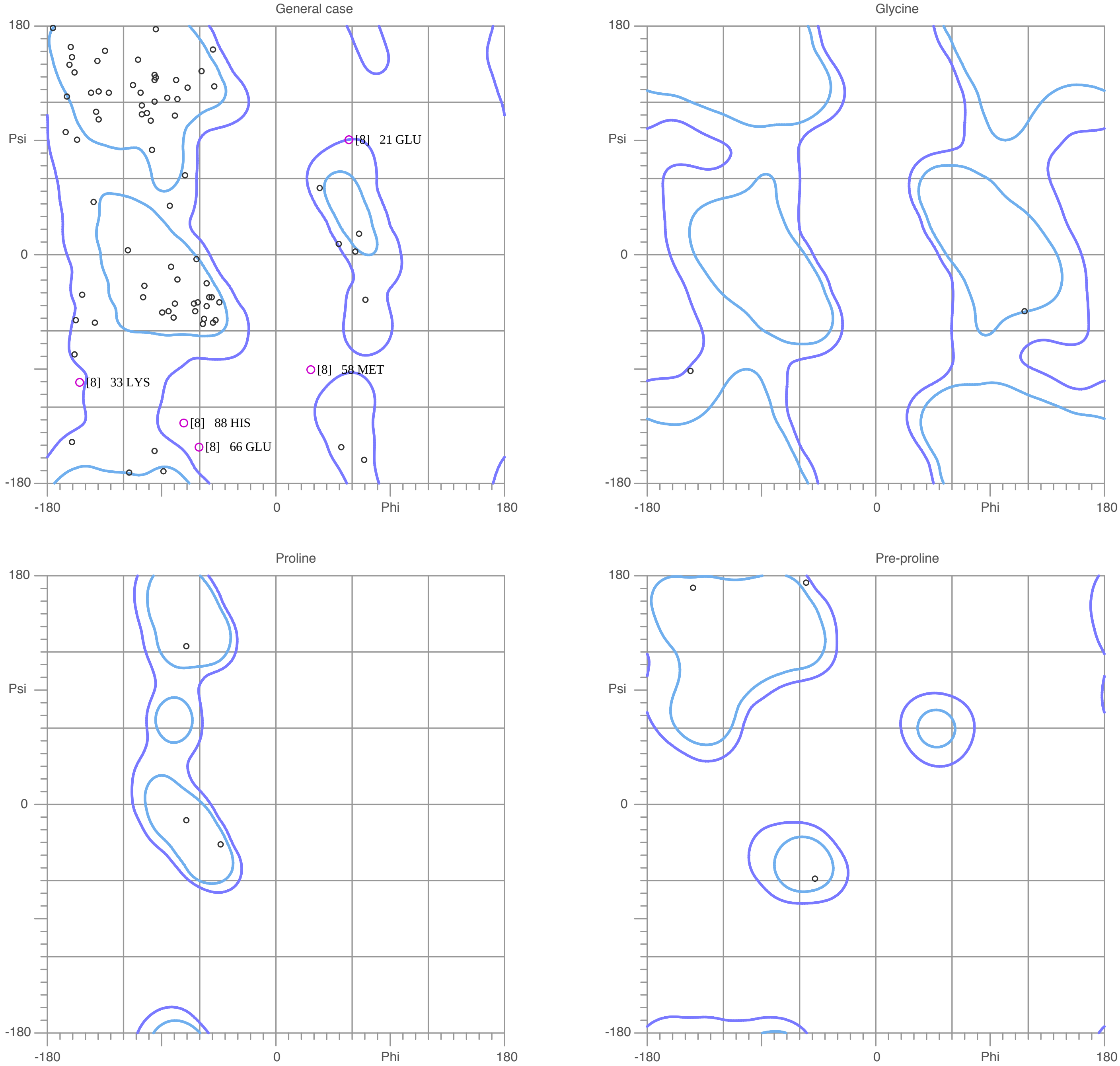
There were 10 outliers (phi, psi):
[7] 3 ILE (57.4, 101.8)
[7] 7 SER (62.2, 140.6)
[7] 8 GLU (-173.7, -7.6)
[7] 24 GLU (36.8, -92.5)
[7] 34 VAL (50.2, 177.2)
[7] 35 ASP (58.1, 94.9)
[7] 36 ASP (-168.1, -43.5)
[7] 37 SER (164.7, -22.3)
[7] 52 LYS (52.3, -68.1)
[7] 85 GLU (33.2, 80.3)

http://kinemage.biochem.duke.edu

Lovell, Davis, et al. Proteins 50:437 (2003)

MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 8



68.5% (61/89) of all residues were in favored (98%) regions.
94.4% (84/89) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

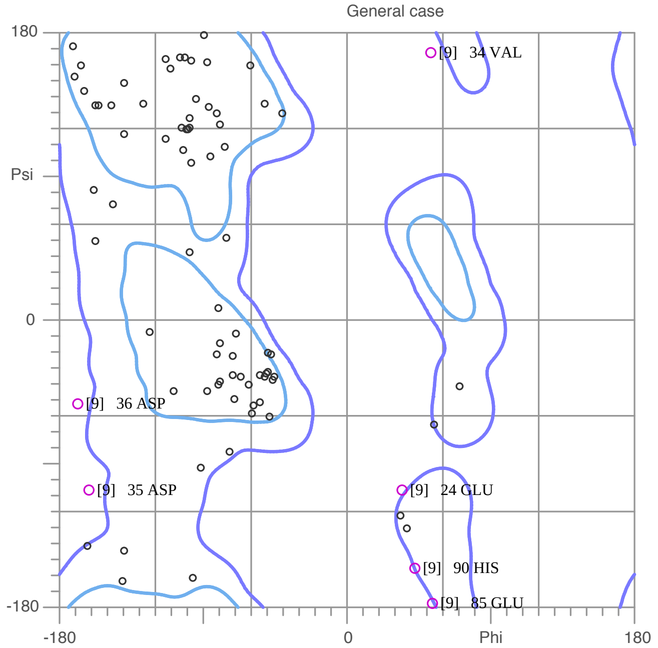
[8] 21 GLU (57.8, 91.9)
[8] 33 LYS (-155.5, -100.5)
[8] 58 MET (28.0, -90.1)
[8] 66 GLU (-61.6, -151.9)
[8] 88 HIS (-73.9, -132.4)

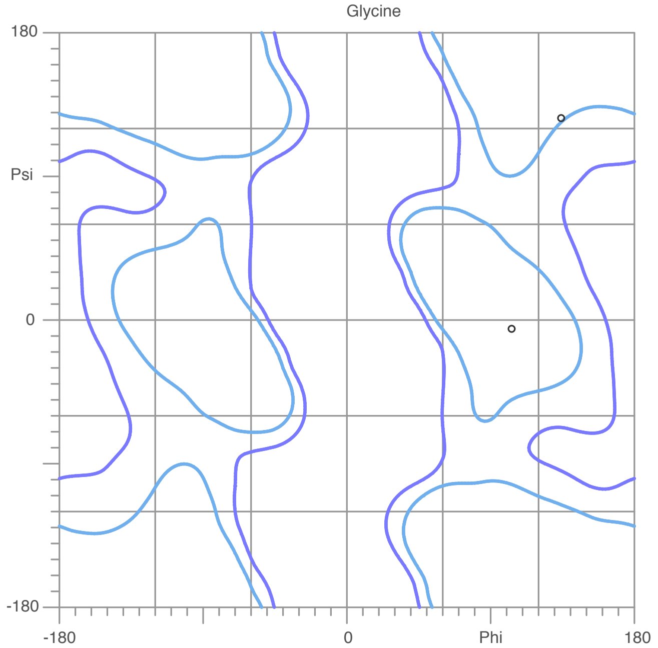
http://kinemage.biochem.duke.edu

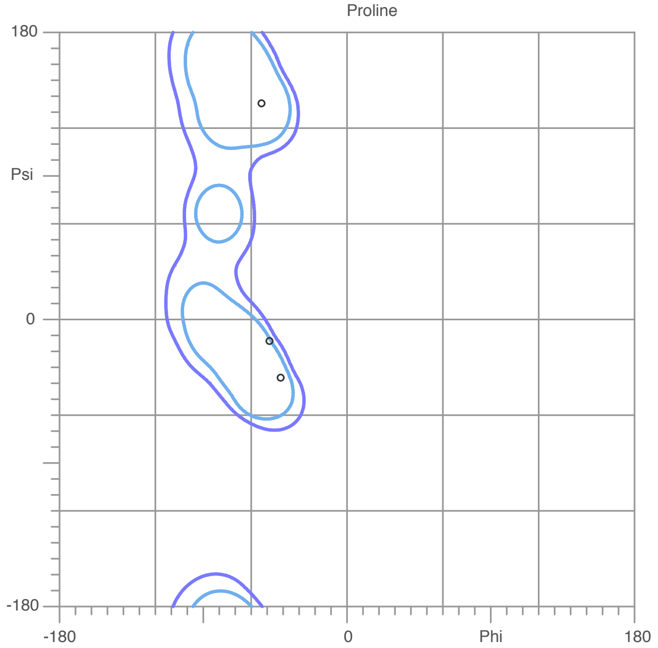
Lovell, Davis, et al. Proteins 50:437 (2003)

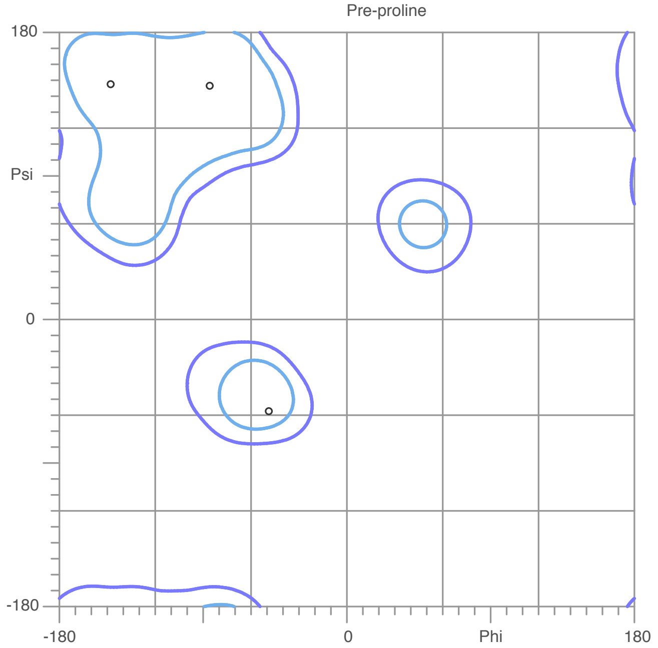
MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 9









75.3% (67/89) of all residues were in favored (98%) regions.
93.3% (83/89) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):

[9] 24 GLU (34.0, -106.9)
[9] 34 VAL (52.7, 169.0)
[9] 35 ASP (-162.6, -106.4)
[9] 36 ASP (-169.1, -52.1)
[9] 85 GLU (53.3, -177.2)
[9] 90 HIS (42.0, -155.1)

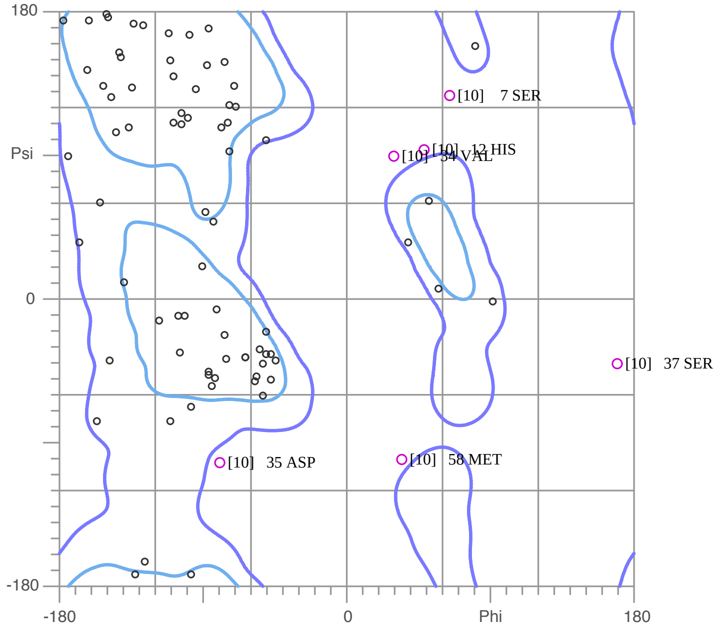
http://kinemage.biochem.duke.edu

Lovell, Davis, et al. Proteins 50:437 (2003)

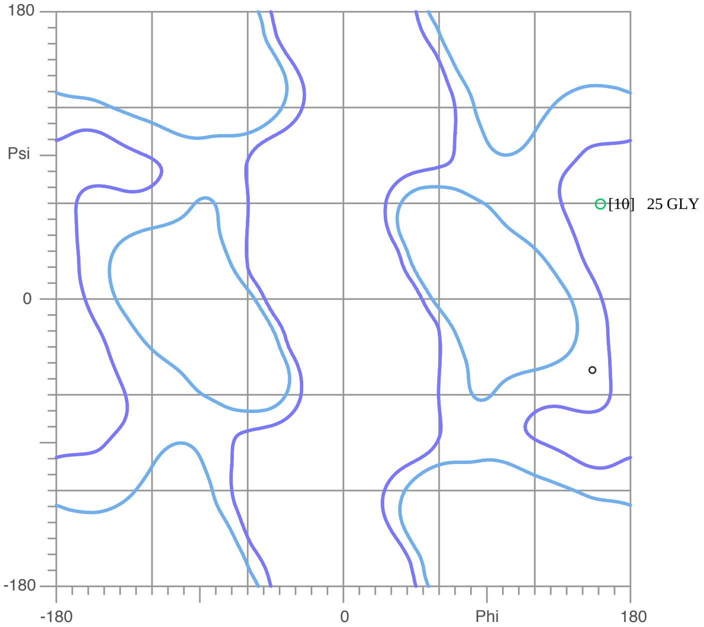
MolProbity Ramachandran analysis

ZR18_NMR_em_bcr3.pdb, model 10

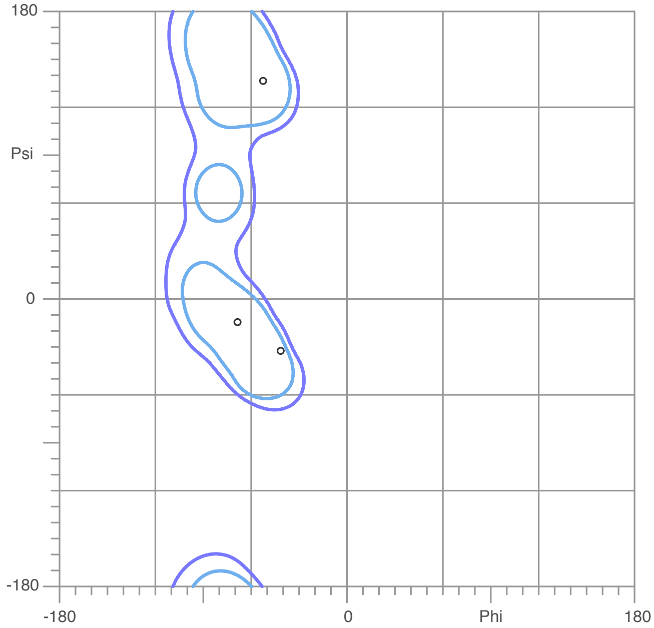
General case



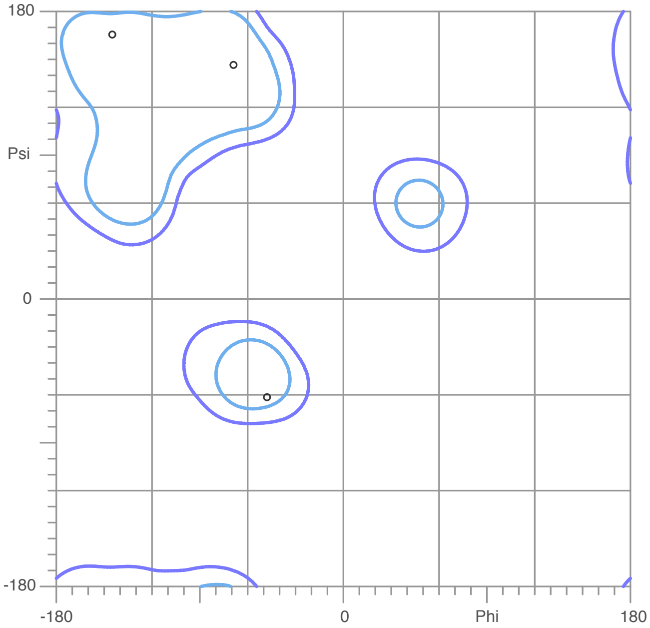
Glycine



Proline



Pre-proline



74.2% (66/89) of all residues were in favored (98%) regions.
92.1% (82/89) of all residues were in allowed (>99.8%) regions.

There were 7 outliers (phi, psi):

[10] 7 SER (65.0, 128.7)
[10] 12 HIS (48.6, 94.0)
[10] 25 GLY (161.8, 60.3)
[10] 34 VAL (29.6, 91.0)
[10] 35 ASP (-80.3, -102.8)
[10] 37 SER (169.2, -40.6)
[10] 58 MET (34.5, -100.3)

http://kinemage.biochem.duke.edu

Lovell, Davis, et al. Proteins 50:437 (2003)