MolProbity Ramachandran analysis

2KHD_NMR.pdb, all models

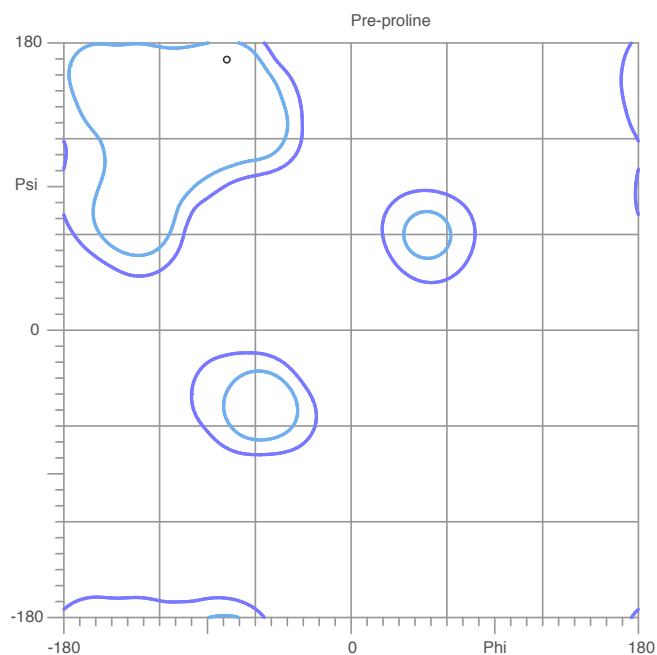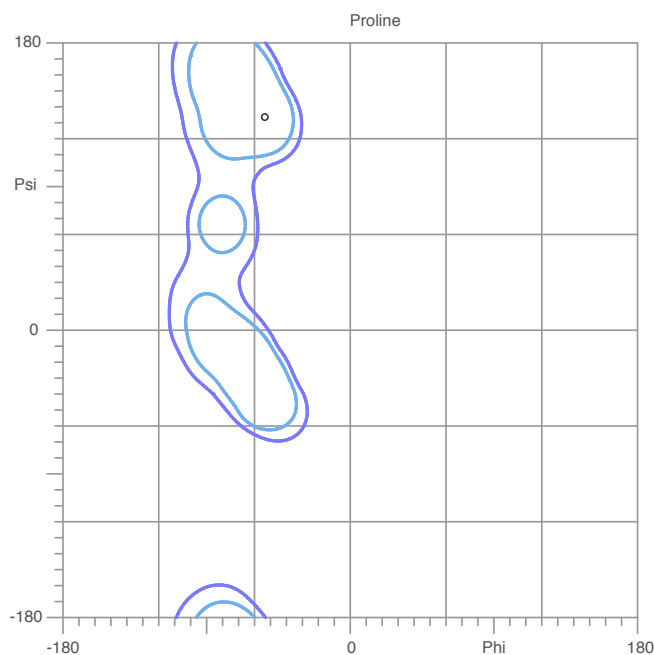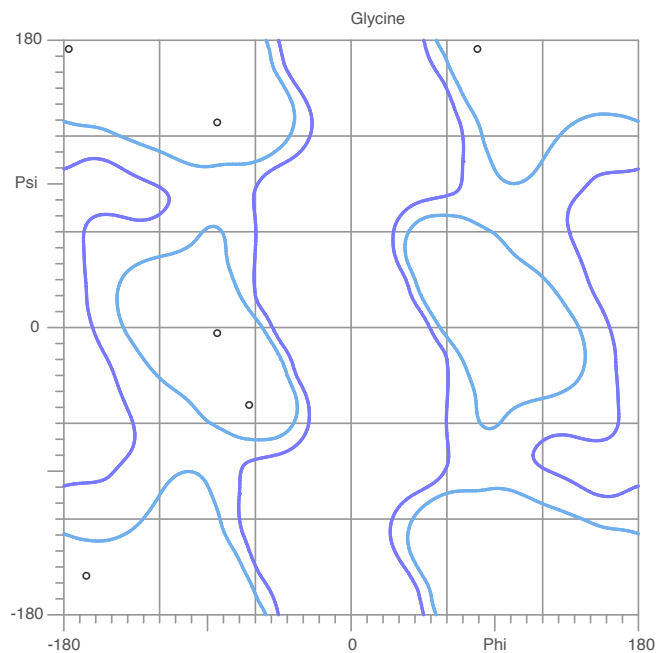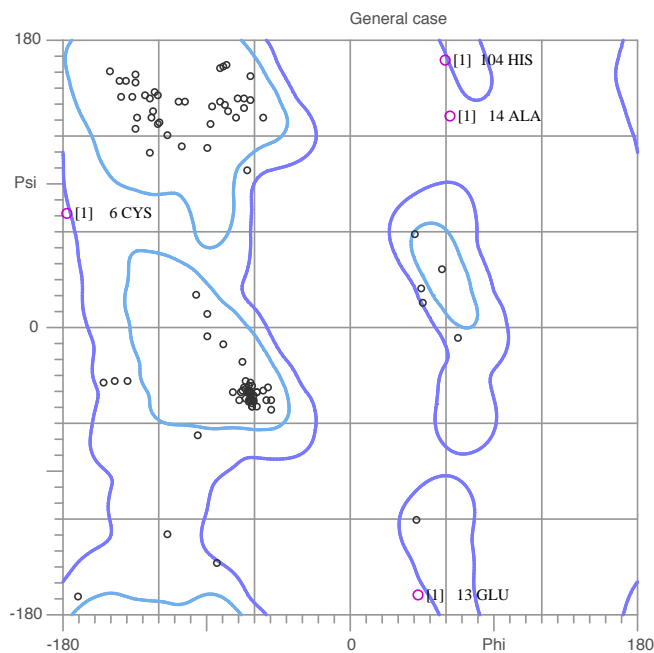Lovell, Davis, et al. Proteins 50:437 (2003)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 1

84.9% (90/106) of all residues were in favored (98%) regions.
96.2% (102/106) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
    [1]   6 CYS (-178.7, 72.1)
    [1]   13 GLU (42.4, -167.9)
    [1]   14 ALA (62.2, 133.3)
    [1] 104 HIS (59.7, 168.9)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 2
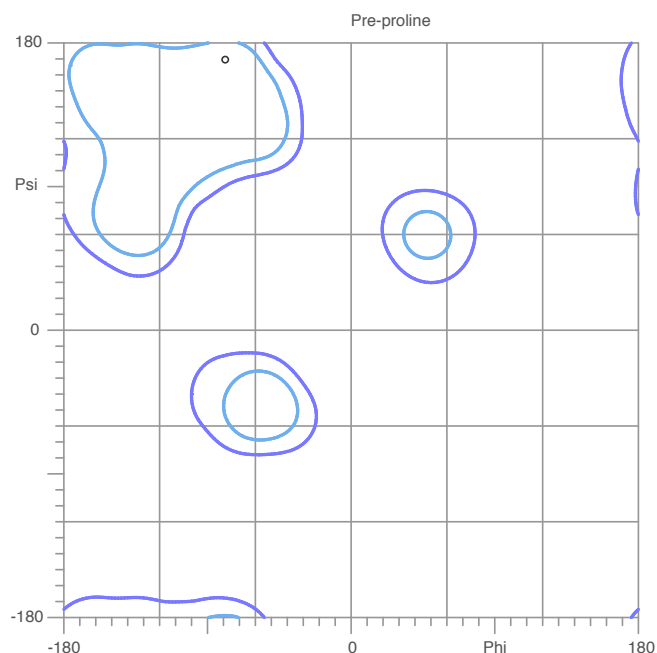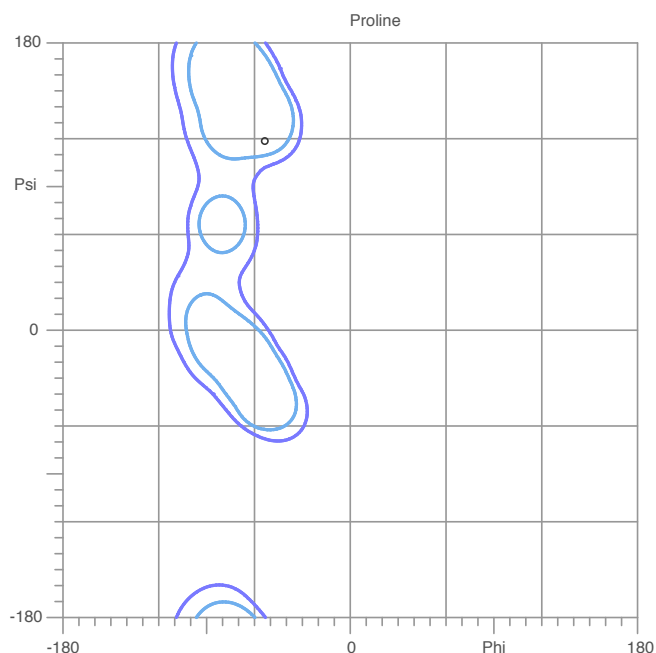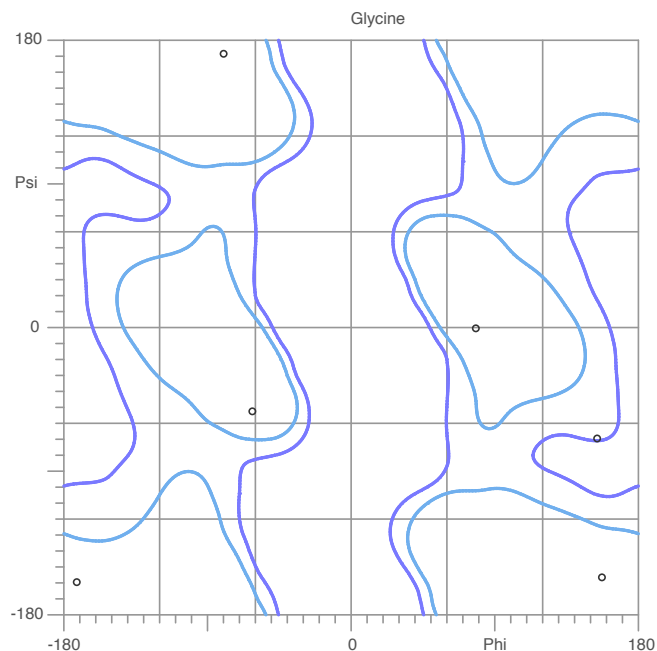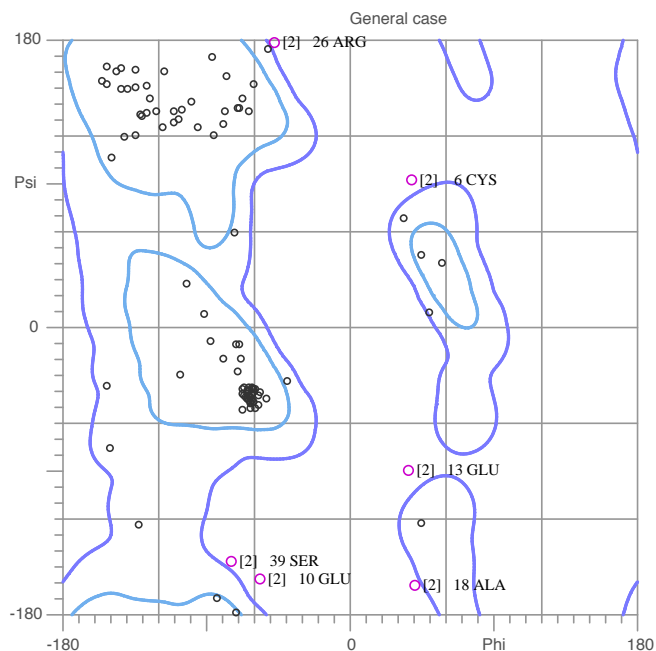
General case

Glycine

Proline

Pre-proline

84.9% (90/106) of all residues were in favored (98%) regions.
94.3% (100/106) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):
[2]   6 CYS (38.8, 93.9)

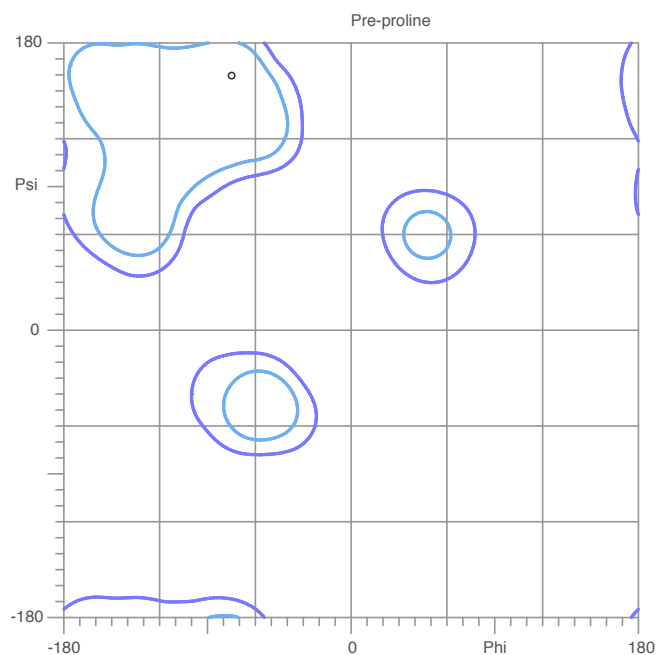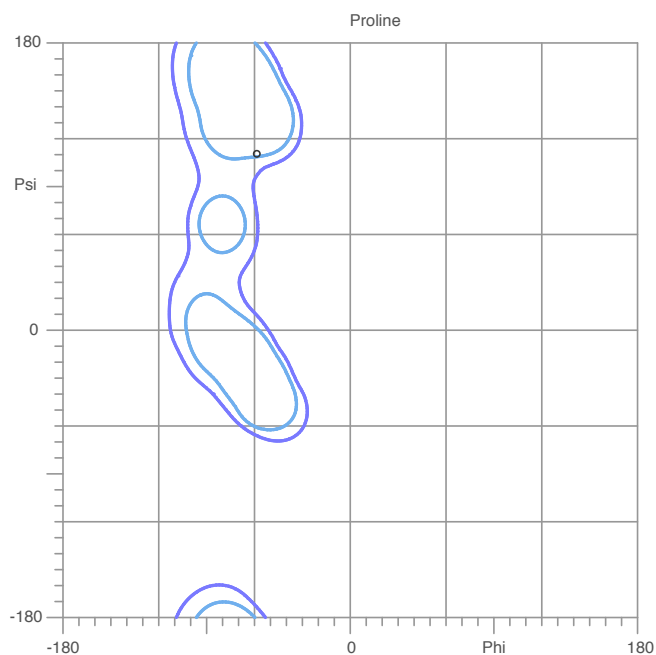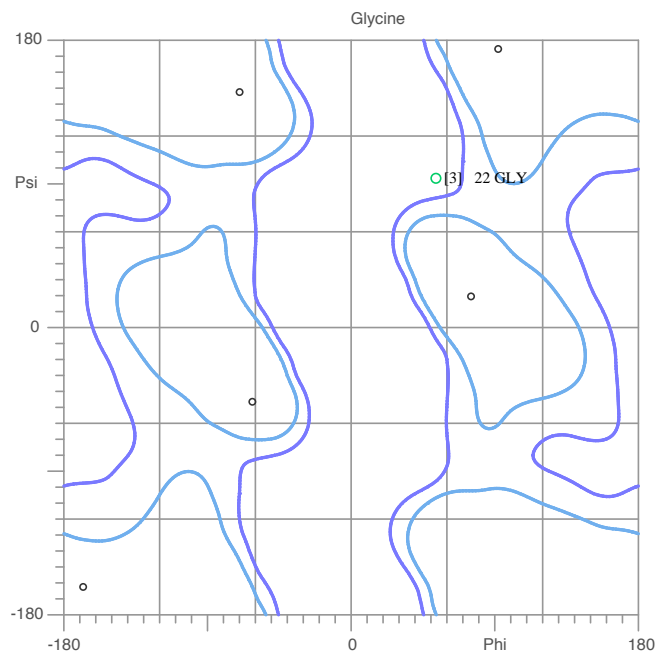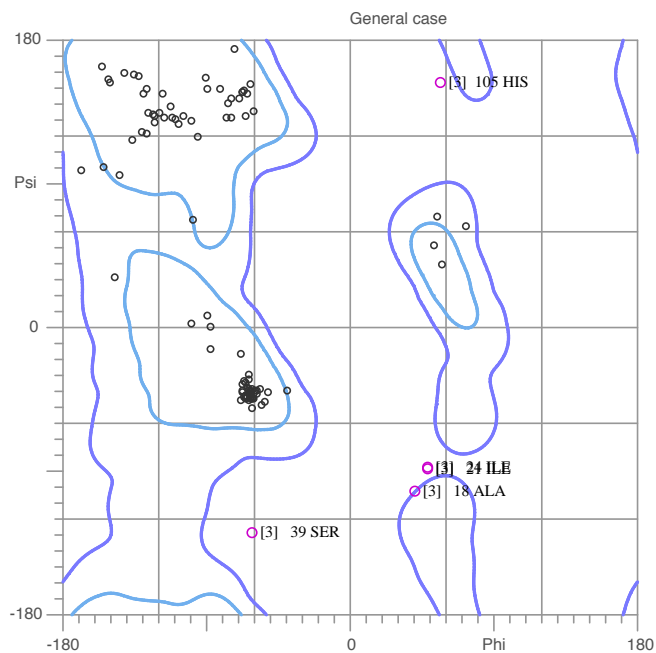[2]   10 GLU (-57.2, -157.6)
[2]   13 GLU (36.4, -89.0)
[2]   18 ALA (40.8, -161.5)
[2]   26 ARG (-48.6, 179.2)
[2]   39 SER (-75.8, -146.9)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 3

General case

Glycine

Proline

Pre-proline

88.7% (94/106) of all residues were in favored (98%) regions.

94.3% (100/106) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):

  [3]   18 ALA (41.0, -102.0)

  [3]   21 ILE (48.8, -88.3)
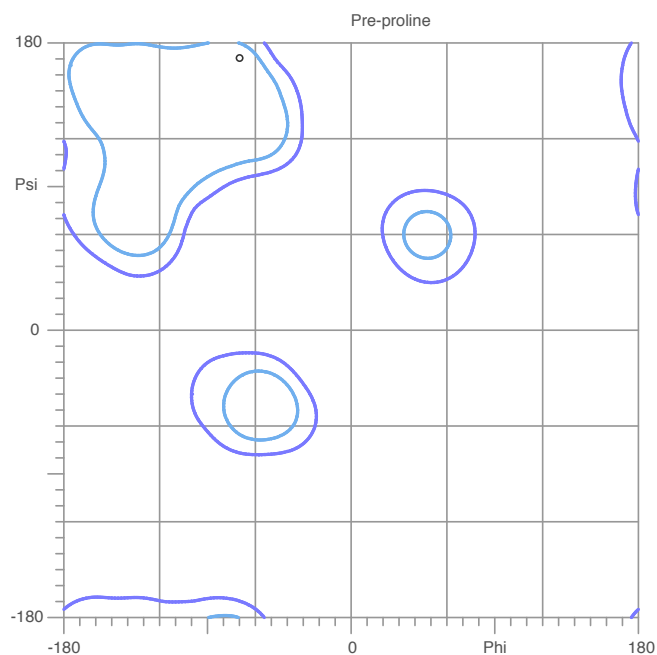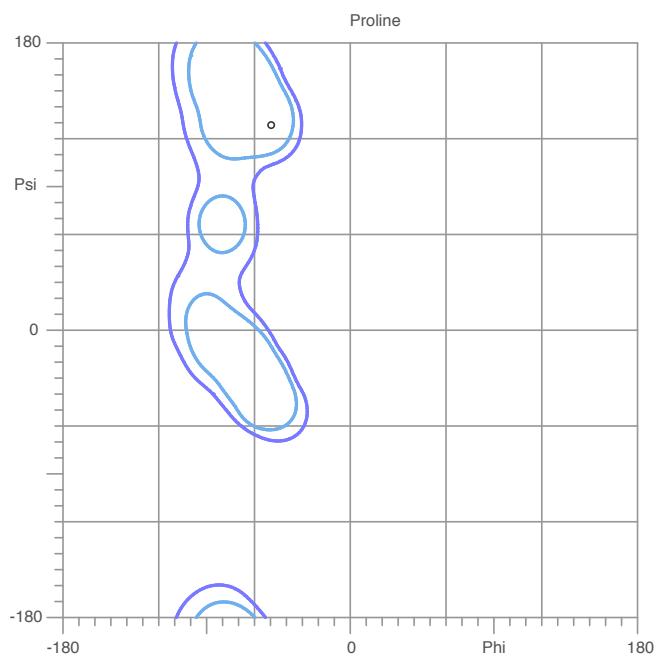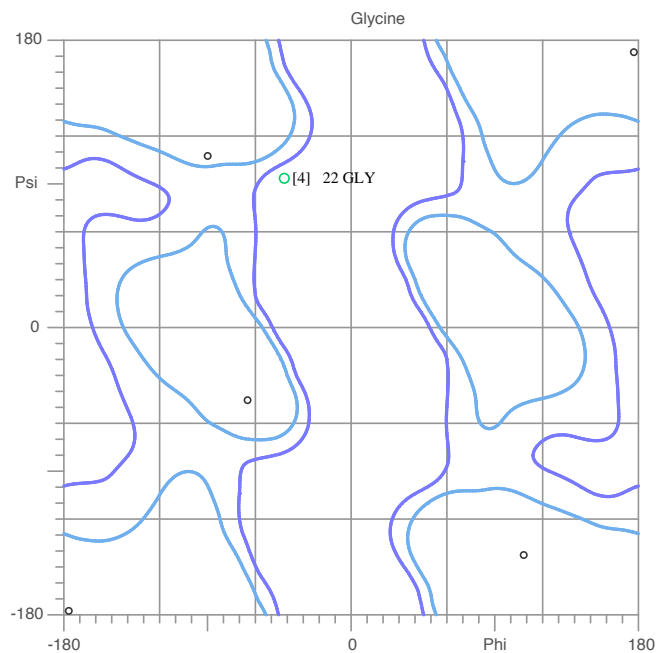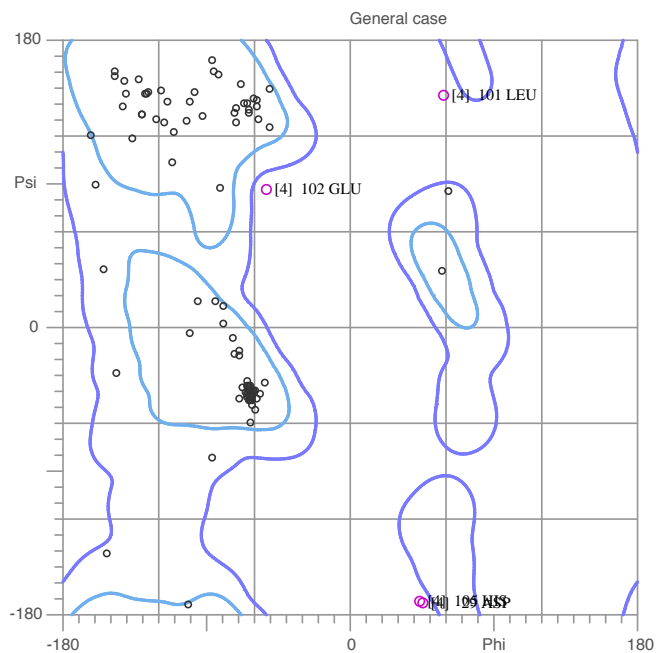 [3]   22 GLY (53.1, 94.3)
  [3]   24 ILE (48.9, -87.6)
  [3]   39 SER (-62.6, -128.3)
  [3]   105 HIS (56.6, 155.0)

MolProbity Ramachandran analysis
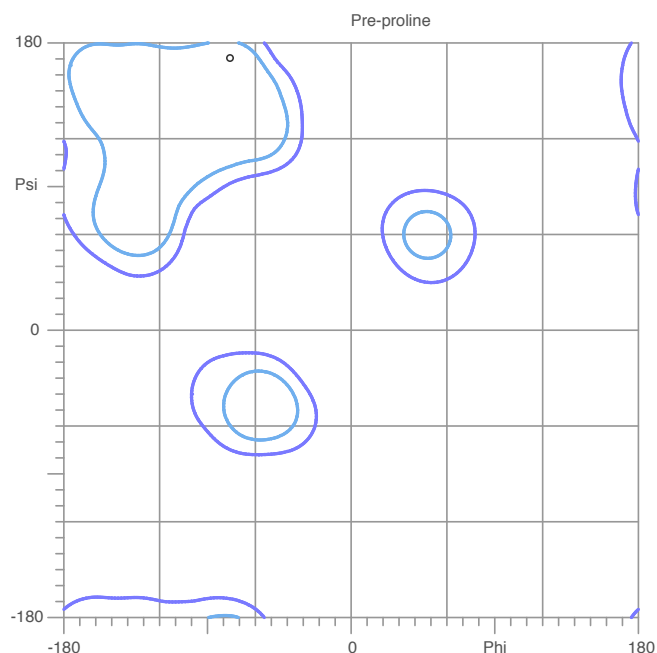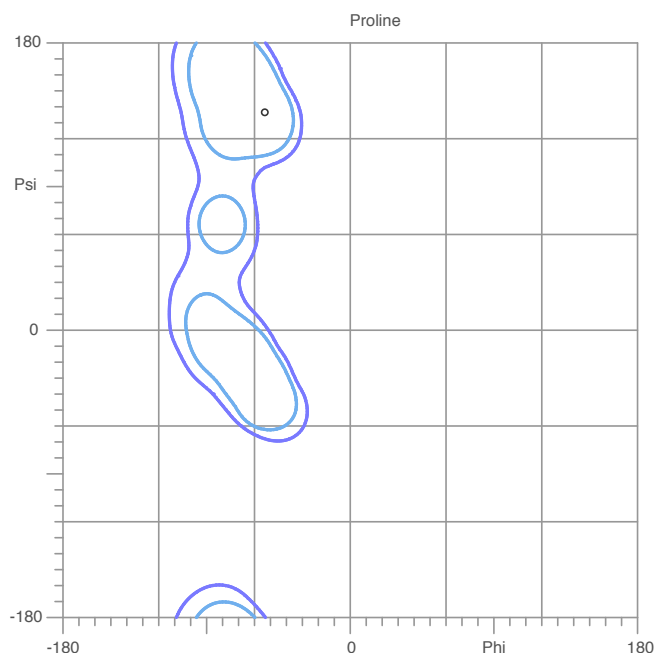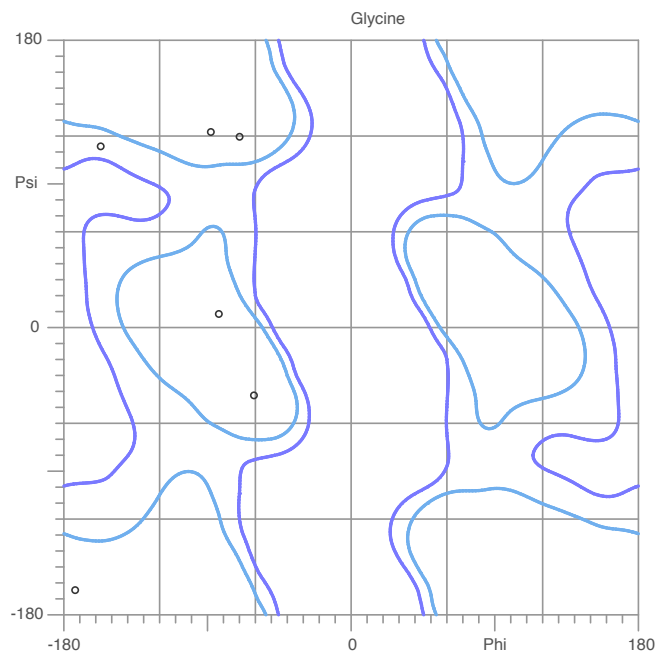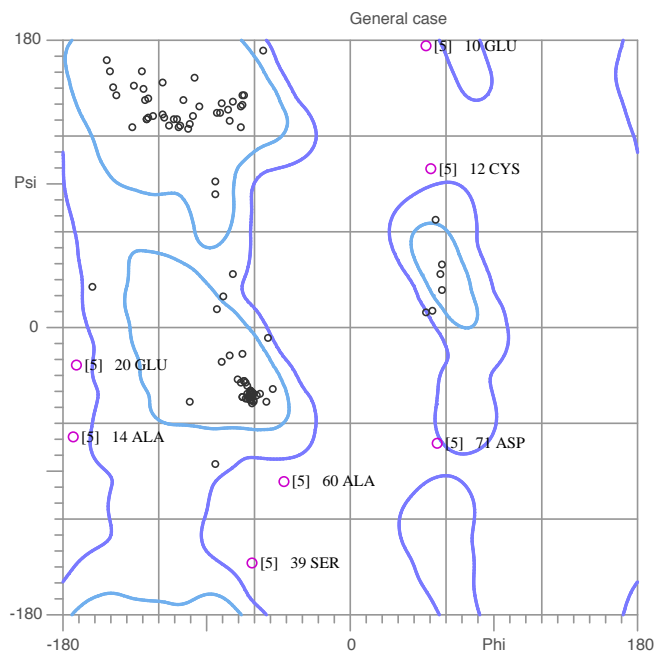
2KHD_NMR.pdb, model 4

88.7% (94/106) of all residues were in favored (98%) regions.
95.3% (101/106) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[4]   22 GLY (-42.2, 94.5)
[4]   29 ASP (45.0, -172.4)
[4] 101 LEU (58.8, 146.6)
[4] 102 GLU (-53.1, 87.3)
[4] 105 HIS (43.9, -171.2)

MolProbity Ramachandran analysis
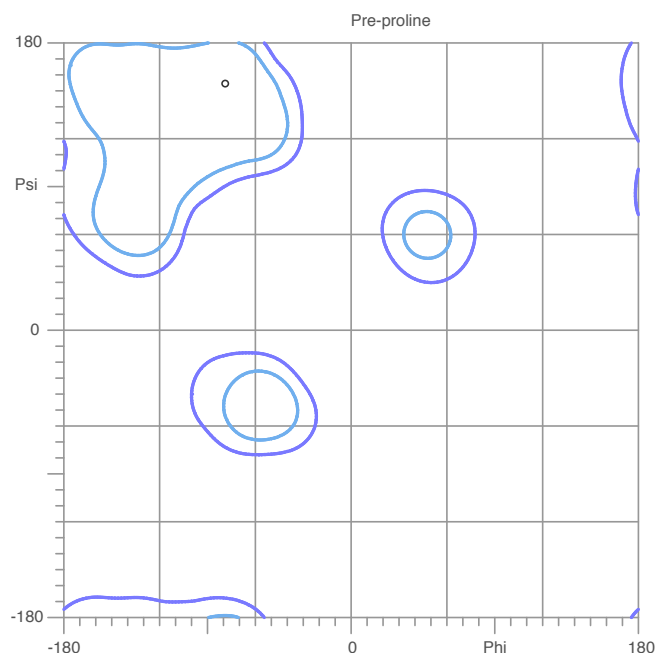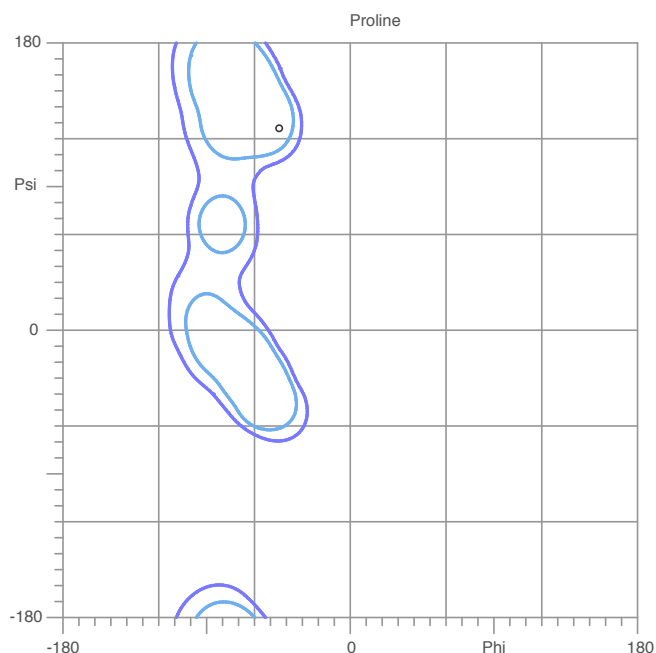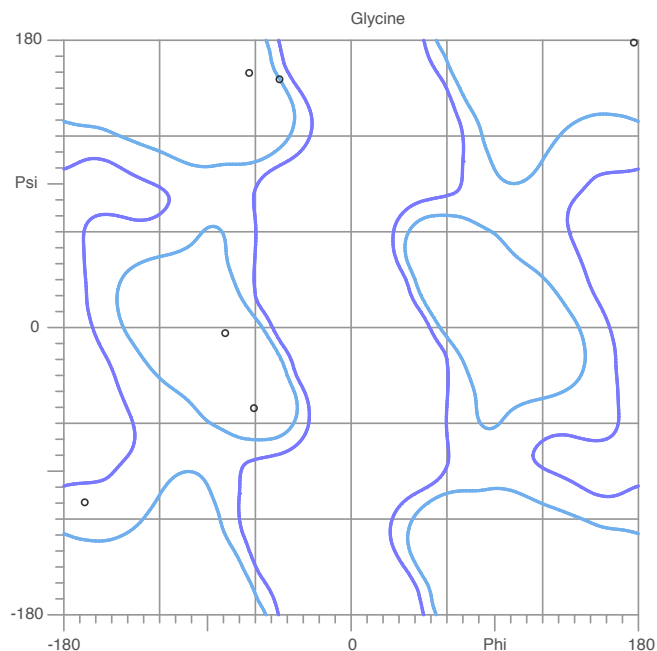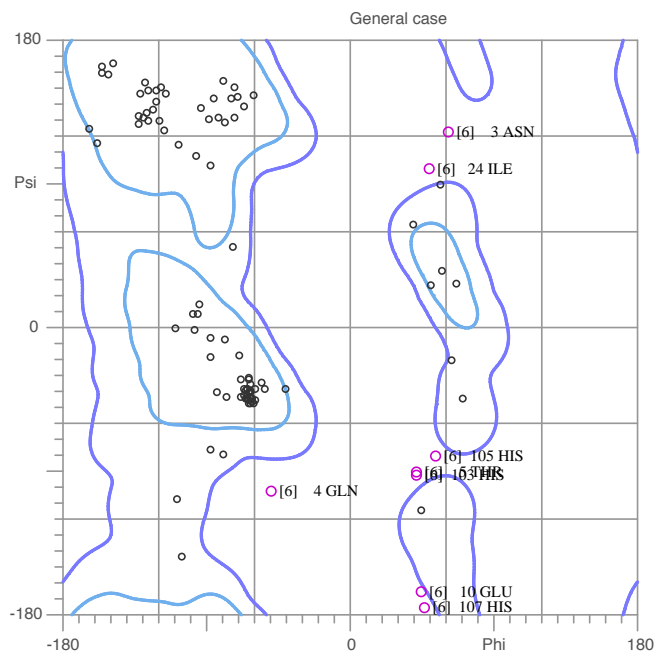
2KHD_NMR.pdb, model 5

84.0% (89/106) of all residues were in favored (98%) regions.
93.4% (99/106) of all residues were in allowed (>99.8%) regions.

There were 7 outliers (phi, psi):
   [5]   10 GLU (47.7, 177.9)

[5]   12 CYS (50.4, 100.8)
[5]   14 ALA (-174.3, -68.2)
[5]   20 GLU (-172.0, -23.7)
[5]   39 SER (-62.6, -147.6)
[5]   60 ALA (-42.3, -97.0)
[5]   71 ASP (54.8, -72.5)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 6

81.1% (86/106) of all residues were in favored (98%) regions.

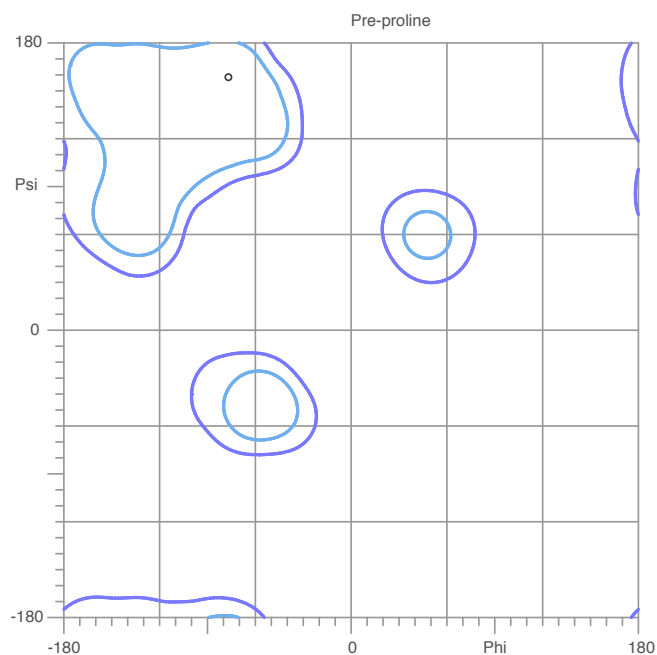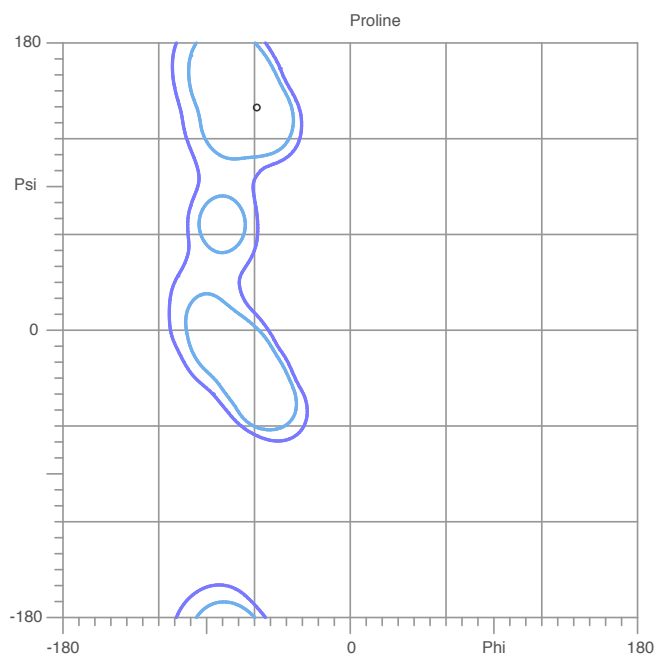92.5% (98/106) of all residues were in allowed (>99.8%) regions.

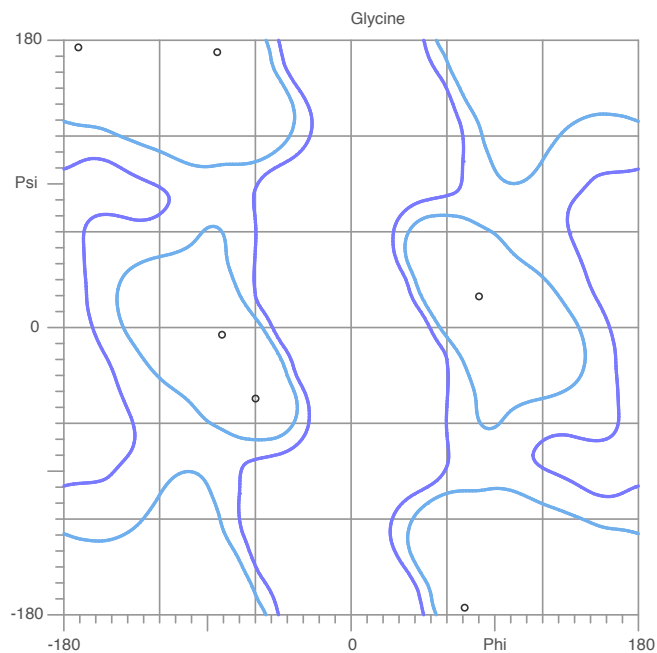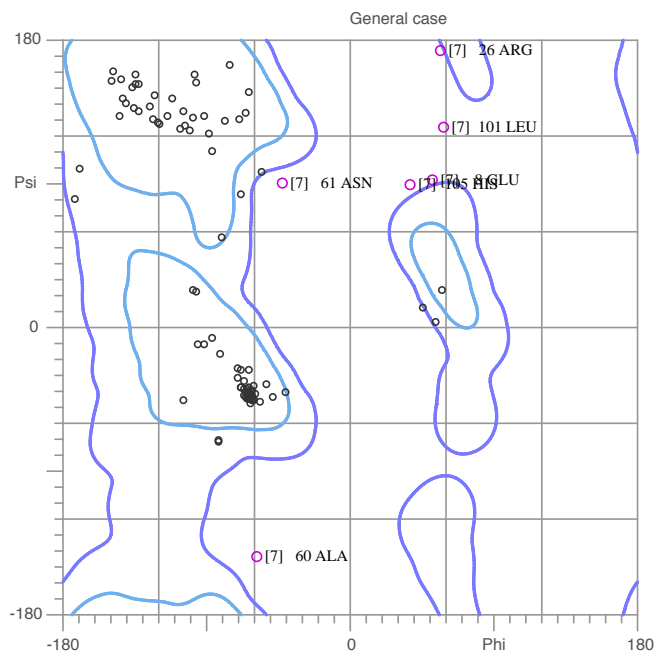There were 8 outliers (phi, psi):

   [6]   3 ASN (61.8, 124.0)

   [6]   4 GLN (-50.9, -102.1)

   [6]   5 THR (41.4, -90.2)

   [6] 10 GLU (44.6, -166.0)

   [6] 24 ILE (49.4, 100.4)

   [6] 103 HIS (41.4, -92.6)

   [6] 105 HIS (53.7, -80.6)

   [6] 107 HIS (46.3, -175.7)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 7

General case

Glycine

[7]   26 ARG
[7] 101 LEU
[7]   61 ASN
[7] 105 HIS
[7]   8 GLU
[7]   60 ALA

Proline

Pre-proline

86.8% (92/106) of all residues were in favored (98%) regions.
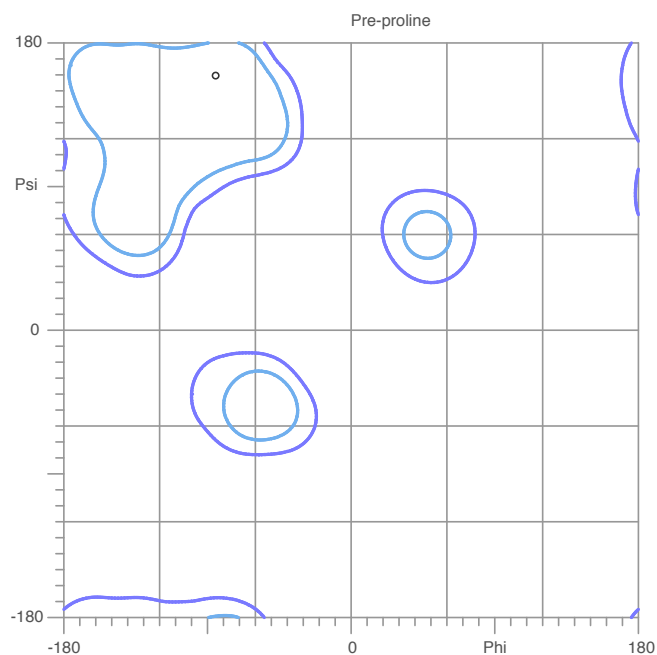94.3% (100/106) of all residues were in allowed (>99.8%) regions.
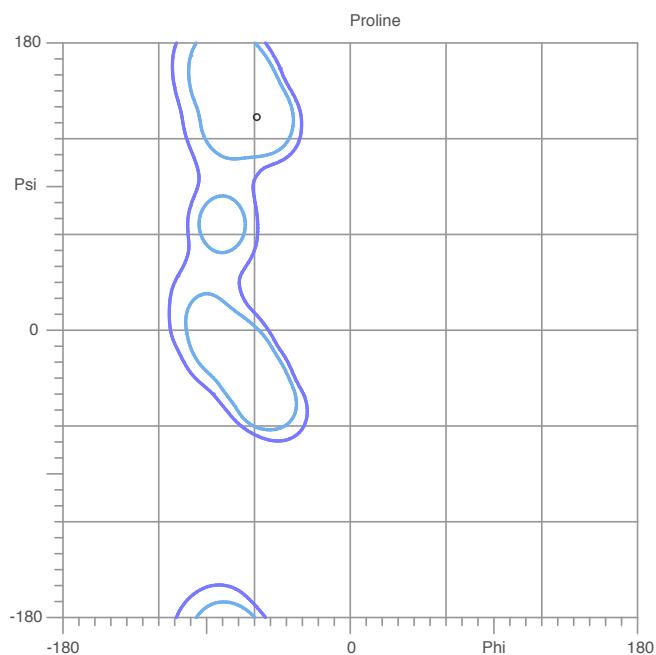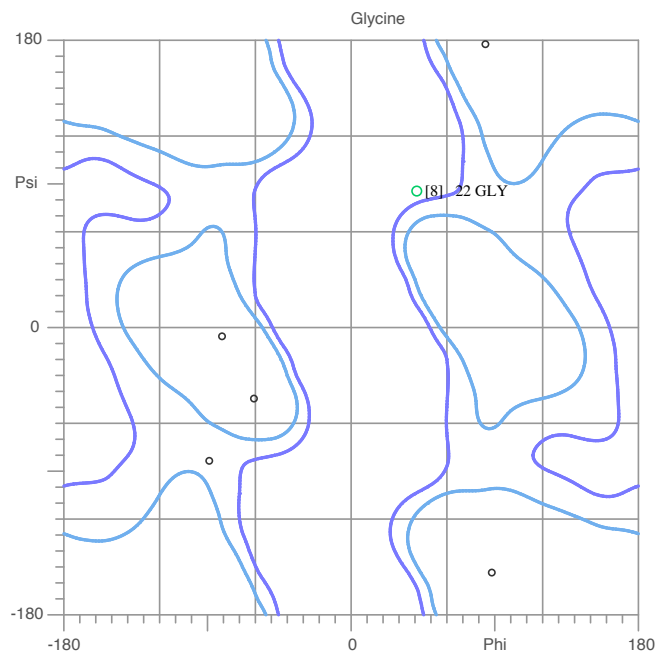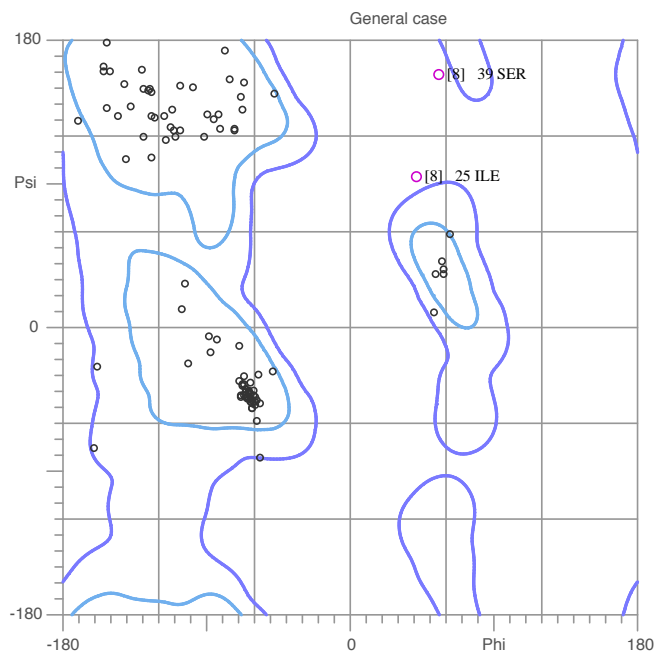
There were 6 outliers (phi, psi):
[7]   8 GLU (51.4, 93.3)

[7]   26 ARG (56.1, 174.5)
[7]   60 ALA (-59.8, -143.3)
[7]   61 ASN (-43.7, 91.6)
[7] 101 LEU (58.4, 126.1)
[7] 105 HIS (37.8, 90.3)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 8

90.6% (96/106) of all residues were in favored (98%) regions.
97.2% (103/106) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
  [8]   22 GLY (41.6, 86.4)
  [8]   25 ILE (41.6, 95.0)
  [8]   39 SER (55.7, 159.8)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 9

General case

Glycine

Proline

Pre-proline

85.8% (91/106) of all residues were in favored (98%) regions.
96.2% (102/106) of all residues were in allowed (>99.8%) regions.
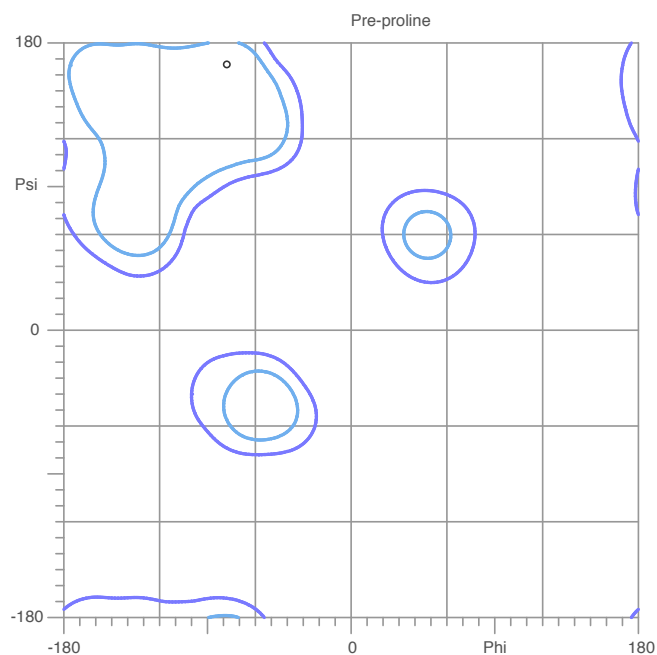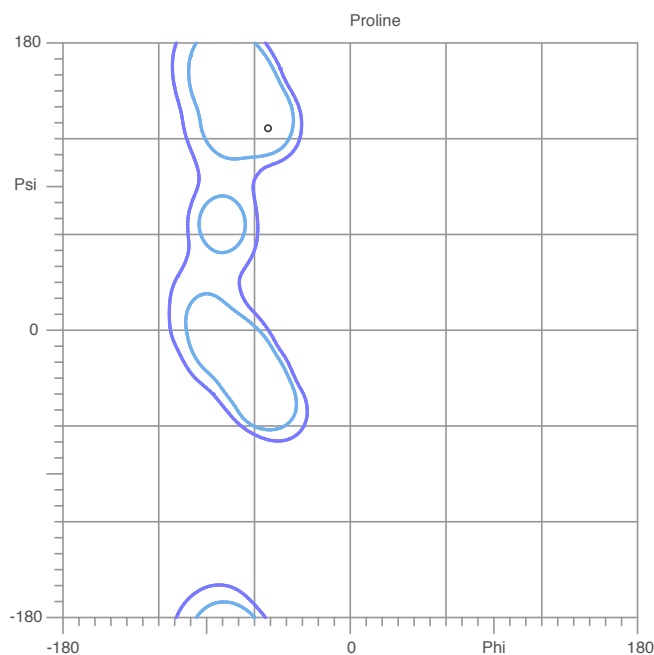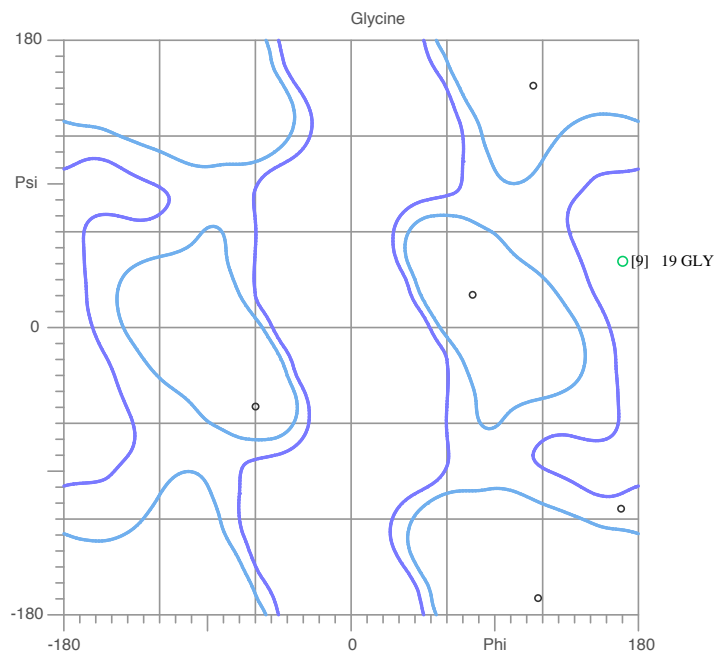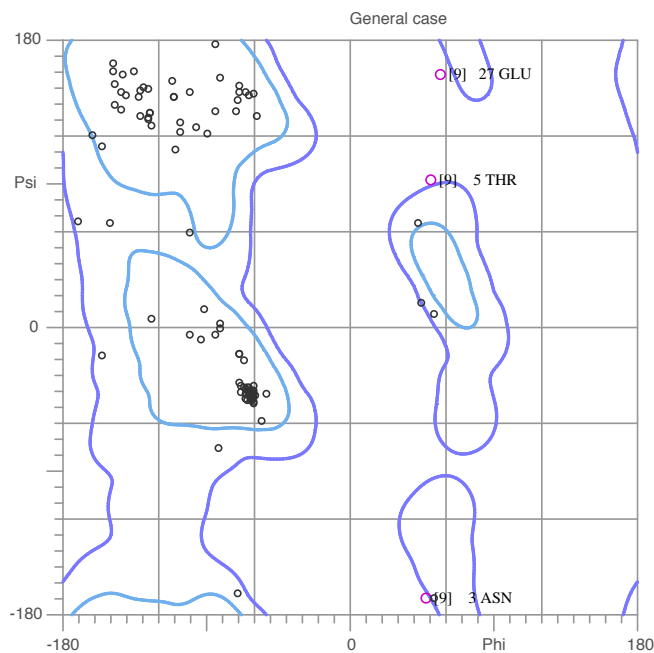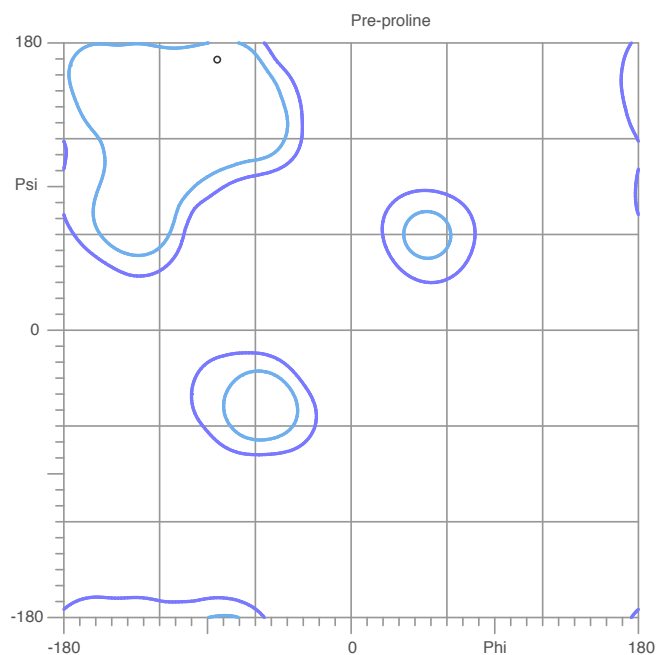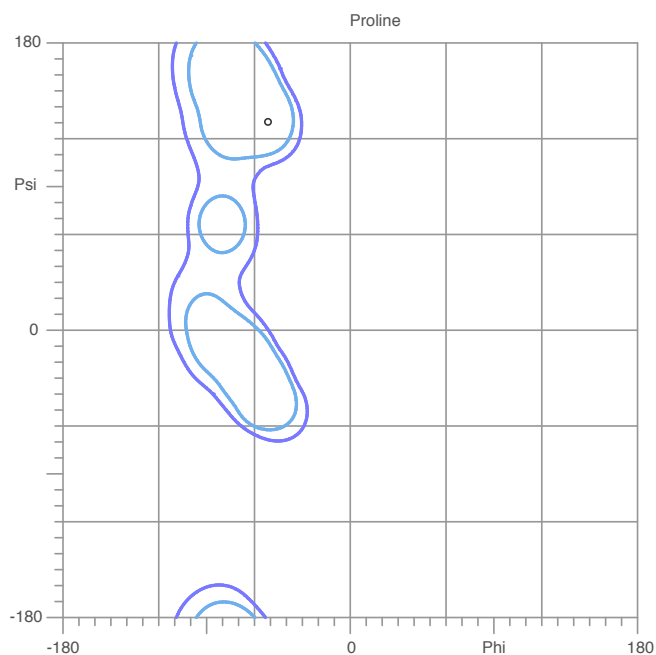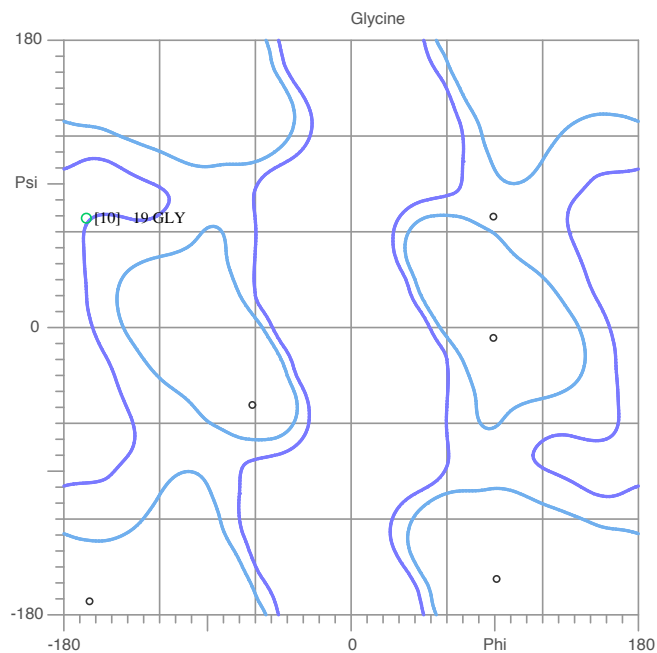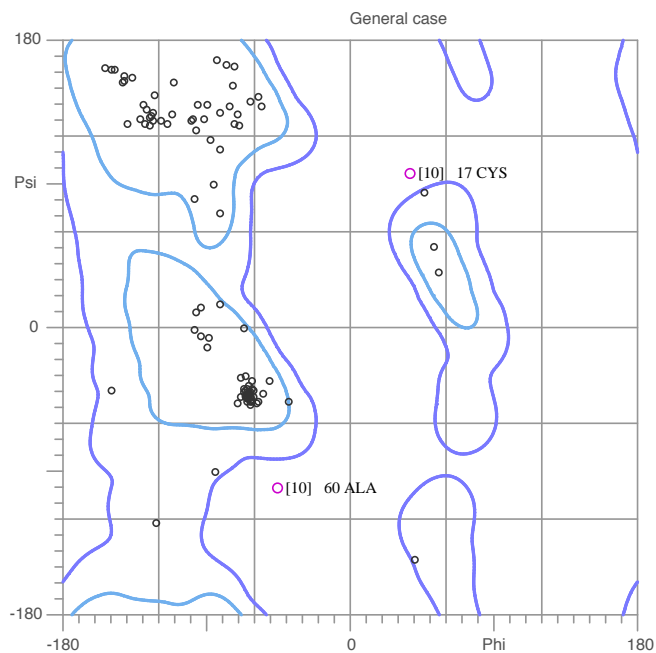
There were 4 outliers (phi, psi):
    [9]   3 ASN (47.9, -169.7)
    [9]   5 THR (50.1, 93.0)
    [9] 19 GLY (170.9, 43.0)
    [9] 27 GLU (56.1, 159.5)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 10

91.5% (97/106) of all residues were in favored (98%) regions.
97.2% (103/106) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
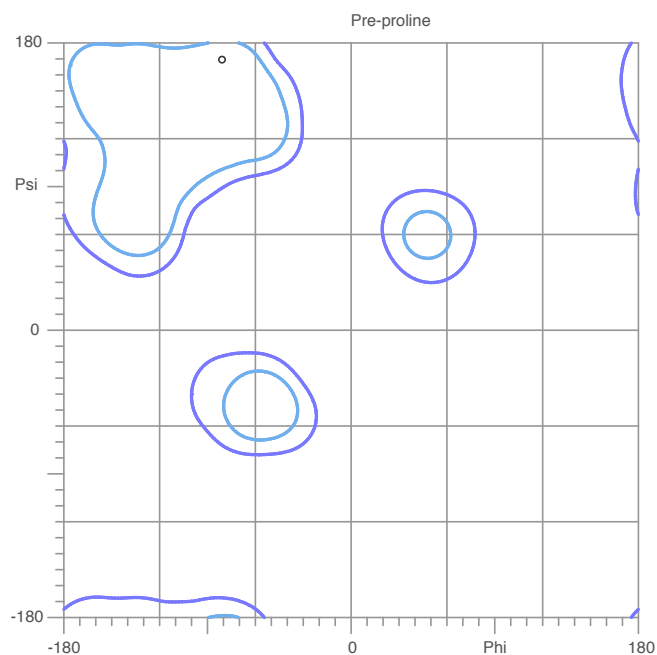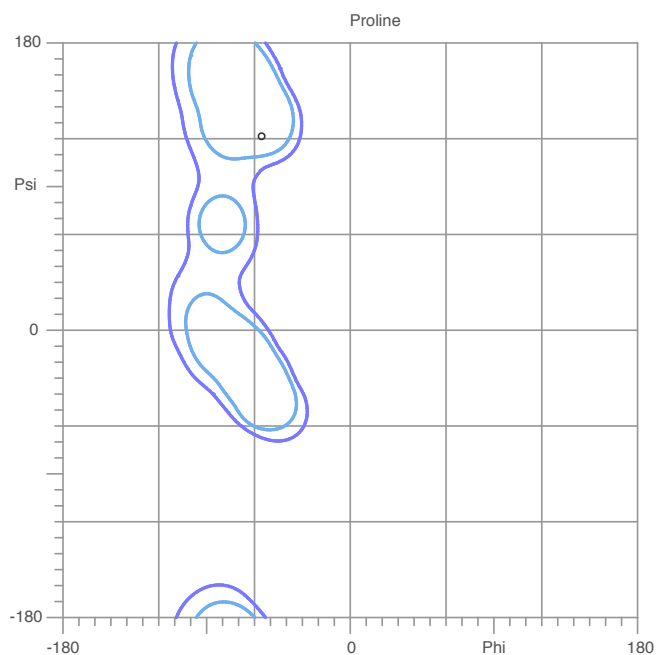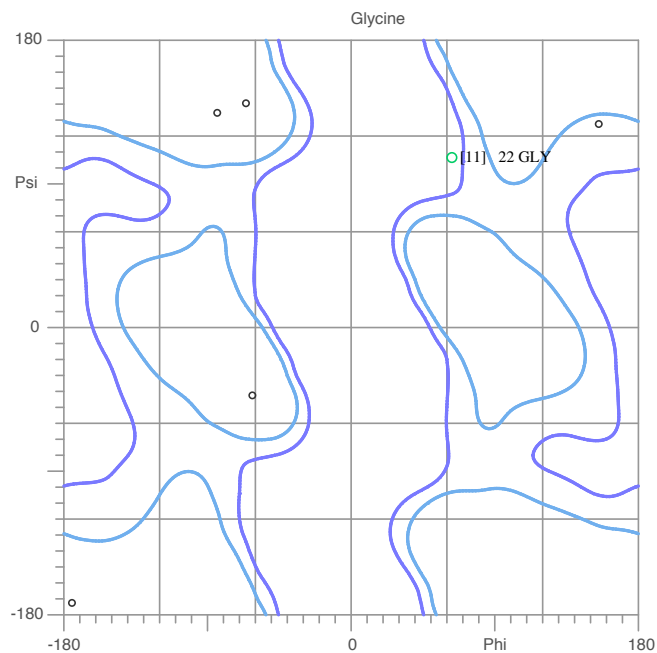   [10]   17 CYS (37.5, 97.0)
    [10]   19 GLY (-166.3, 69.9)
    [10]   60 ALA (-46.5, -100.0)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 11

91.5% (97/106) of all residues were in favored (98%) regions.
98.1% (104/106) of all residues were in allowed (>99.8%) regions.

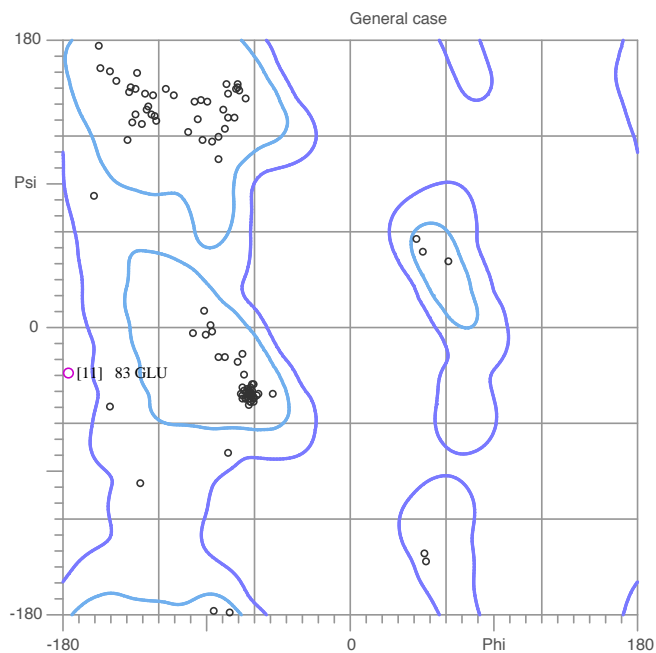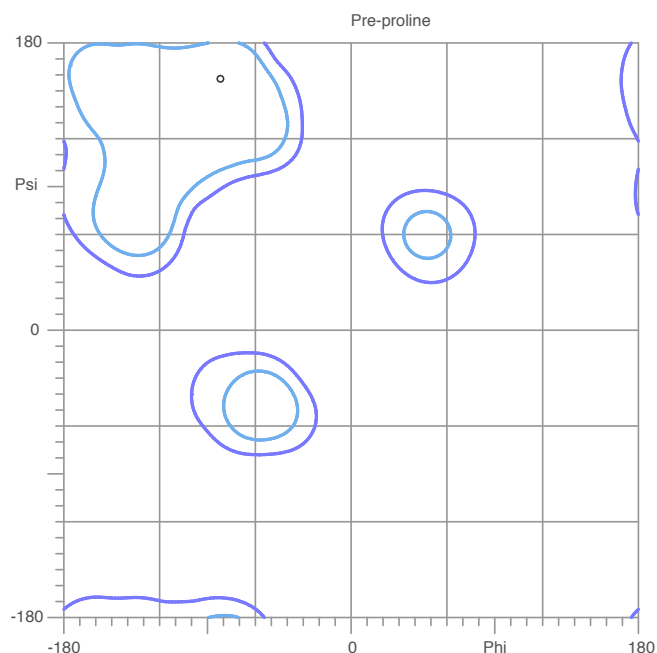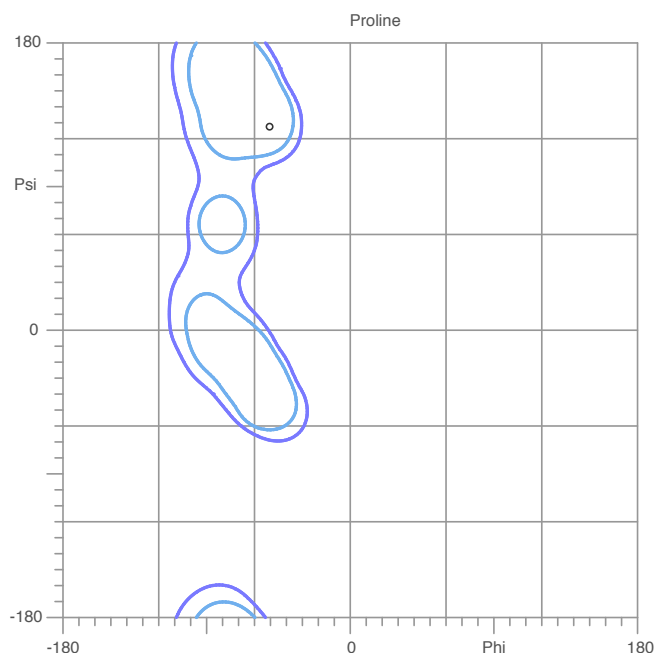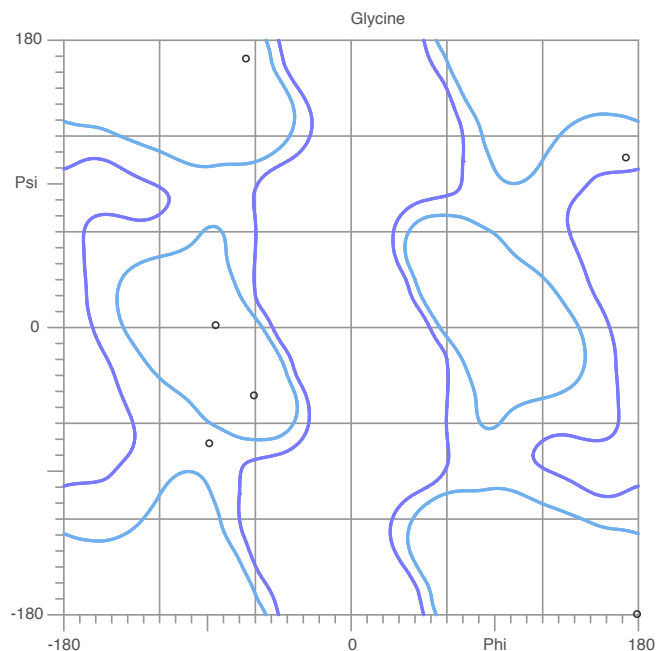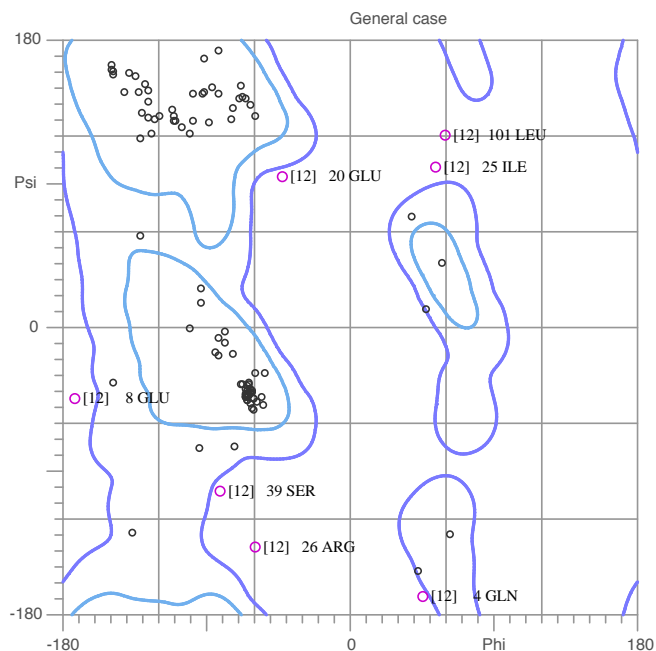There were 2 outliers (phi, psi):
    [11]   22 GLY (63.7, 107.3)
    [11]   83 GLU (-177.3, -28.9)

MolProbity Ramachandran analysis
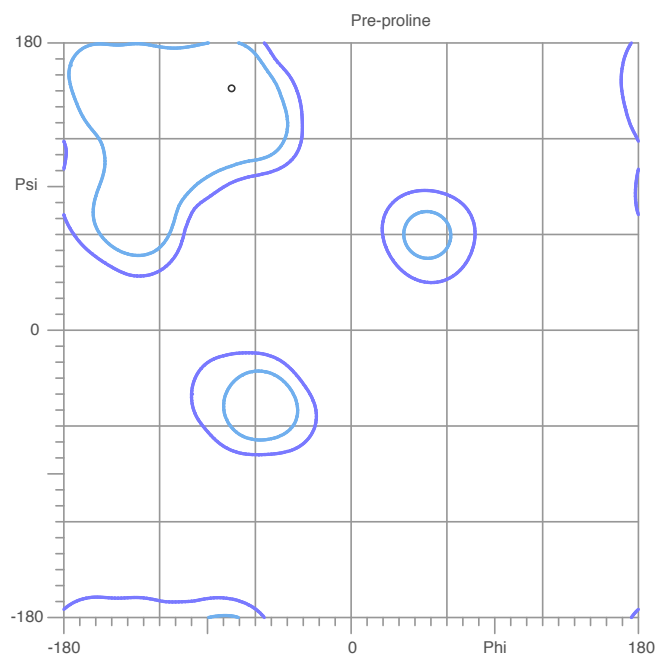
2KHD_NMR.pdb, model 12

83.0% (88/106) of all residues were in favored (98%) regions.
93.4% (99/106) of all residues were in allowed (>99.8%) regions.

There were 7 outliers (phi, psi):
   [12]   4 GLN (45.6, -168.4)

[12]   8 GLU (-173.3, -44.7)
[12] 20 GLU (-43.6, 95.1)
[12] 25 ILE (53.4, 101.7)
[12] 26 ARG (-60.2, -137.1)
[12] 39 SER (-82.7, -102.9)
[12] 101 LEU (59.5, 121.4)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 13

General case

Glycine

Proline

Pre-proline

84.0% (89/106) of all residues were in favored (98%) regions.
94.3% (100/106) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):
  [13]   9 ASN (-73.1, -119.6)

[13]   13 GLU (53.9, -90.4)
[13]   21 ILE (58.3, 139.8)
[13]   26 ARG (59.8, 121.2)
[13] 103 HIS (57.5, 118.2)
[13] 105 HIS (38.6, 84.4)

MolProbity Ramachandran analysis
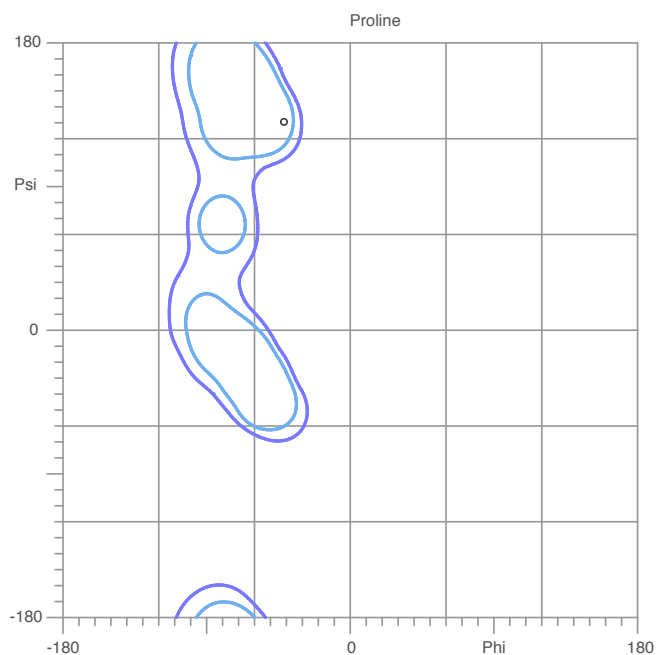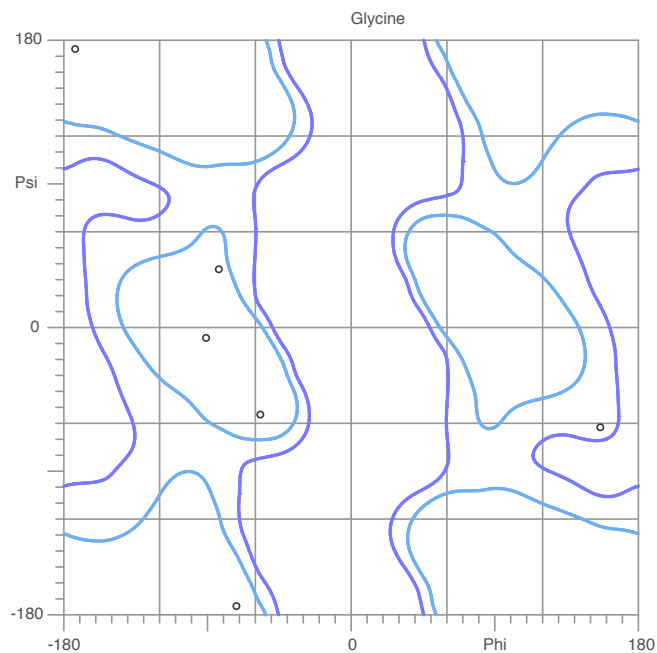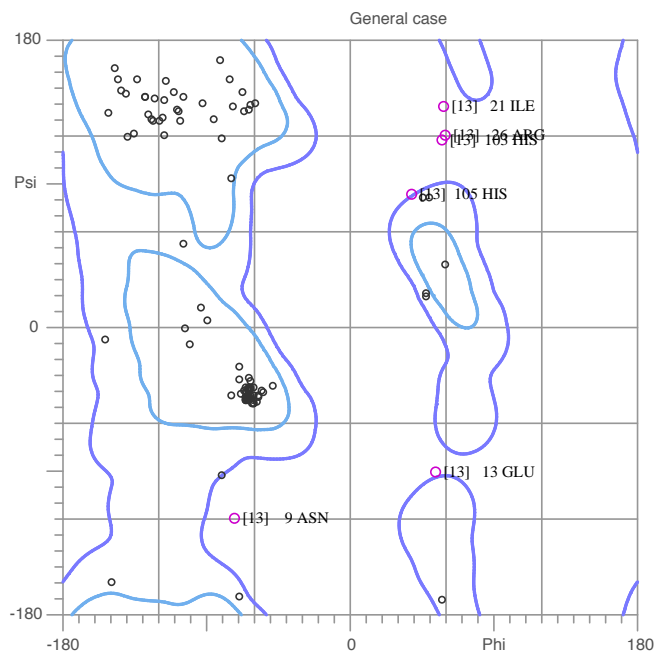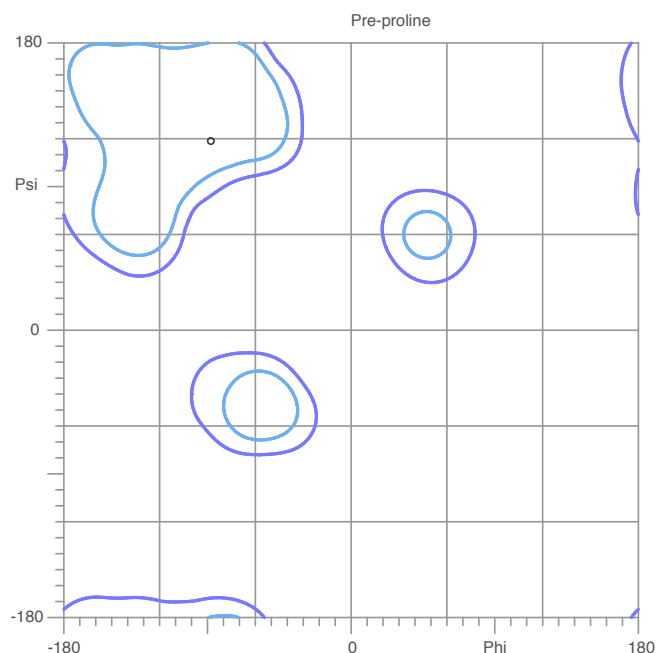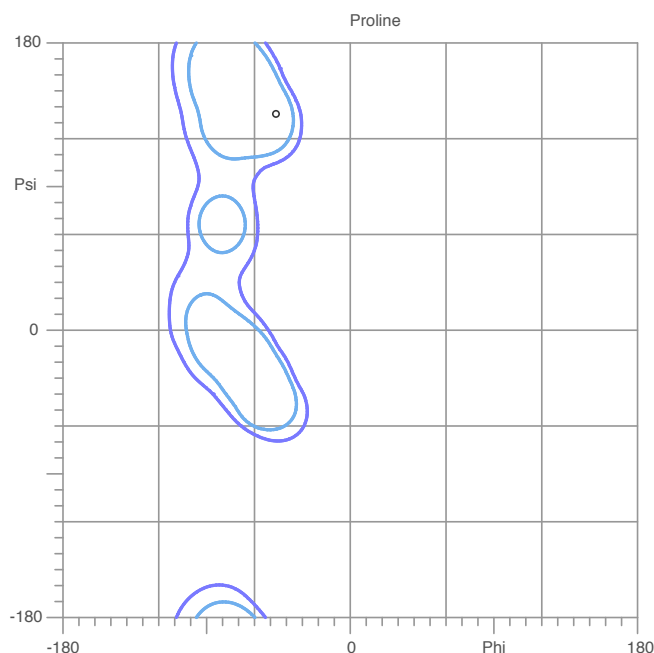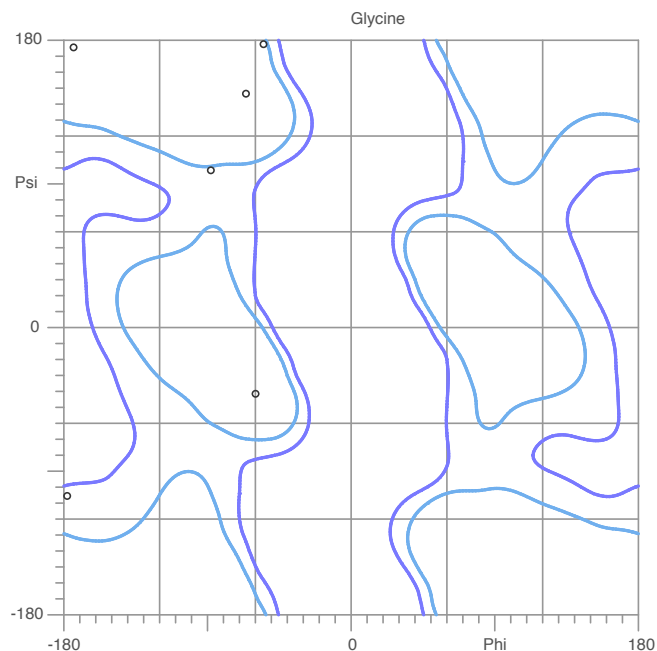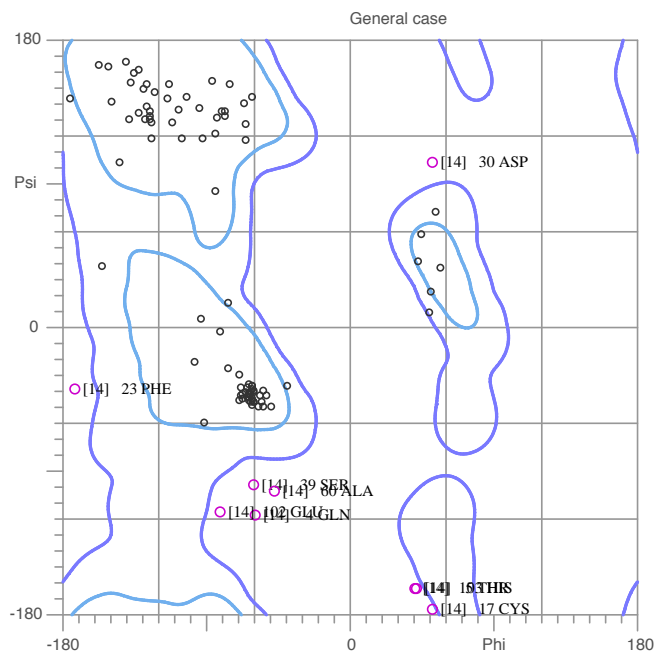
2KHD_NMR.pdb, model 14

84.0% (89/106) of all residues were in favored (98%) regions.
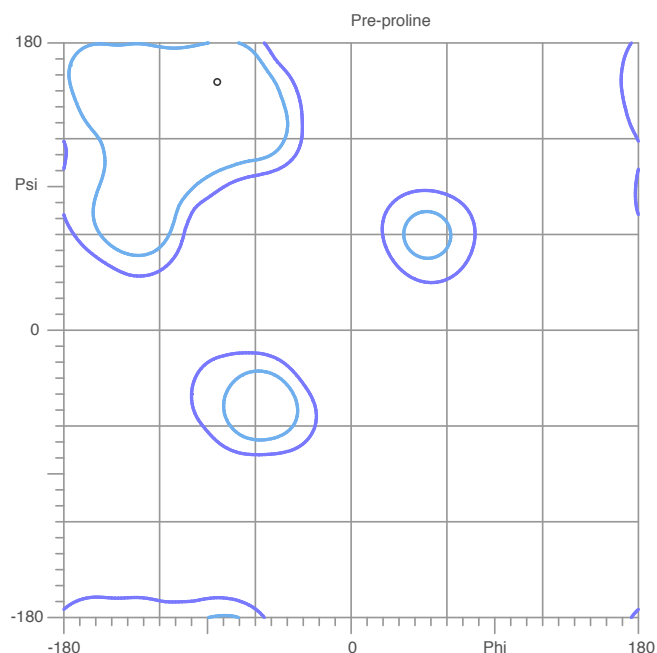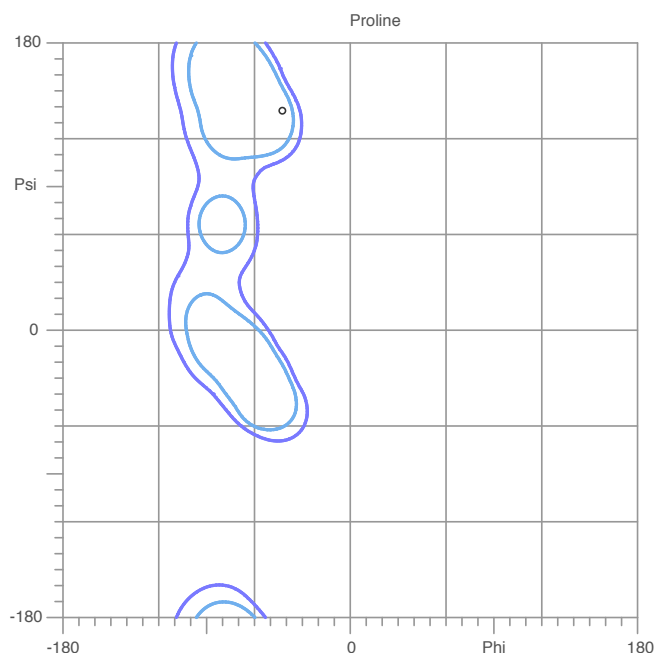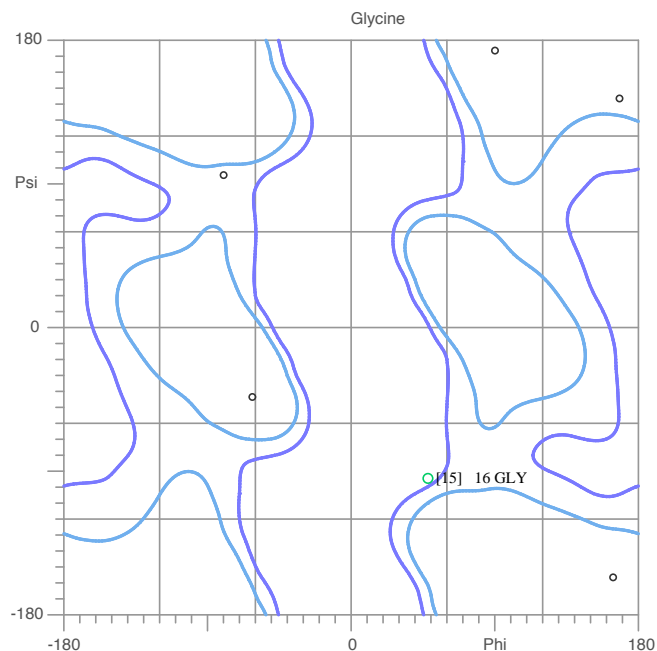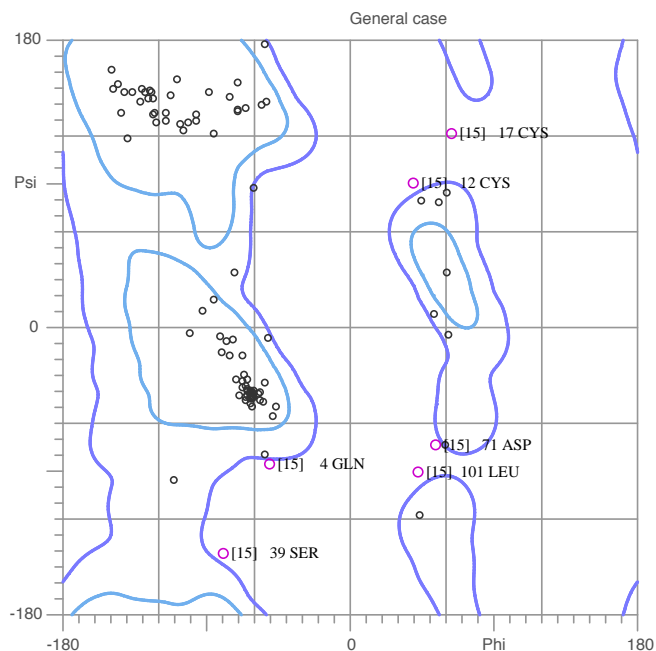91.5% (97/106) of all residues were in allowed (>99.8%) regions.

There were 9 outliers (phi, psi):
  [14]   4 GLN (-60.1, -117.1)
  [14]   5 THR (40.5, -163.6)

[14]   17 CYS (51.0, -176.2)
[14]   23 PHE (-173.6, -38.3)
[14]   30 ASP (51.2, 104.3)
[14]   39 SER (-61.4, -99.0)
[14]   60 ALA (-48.2, -103.0)
[14] 102 GLU (-82.5, -115.5)
[14] 103 HIS (41.2, -163.5)

MolProbity Ramachandran analysis
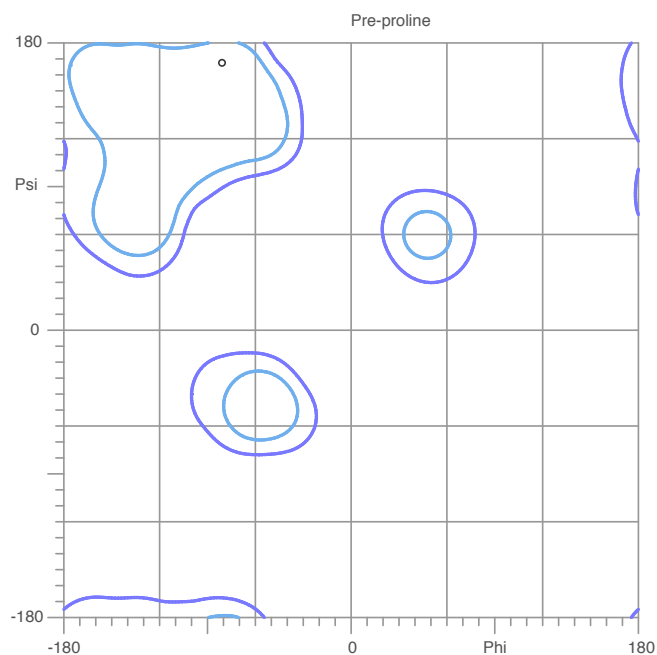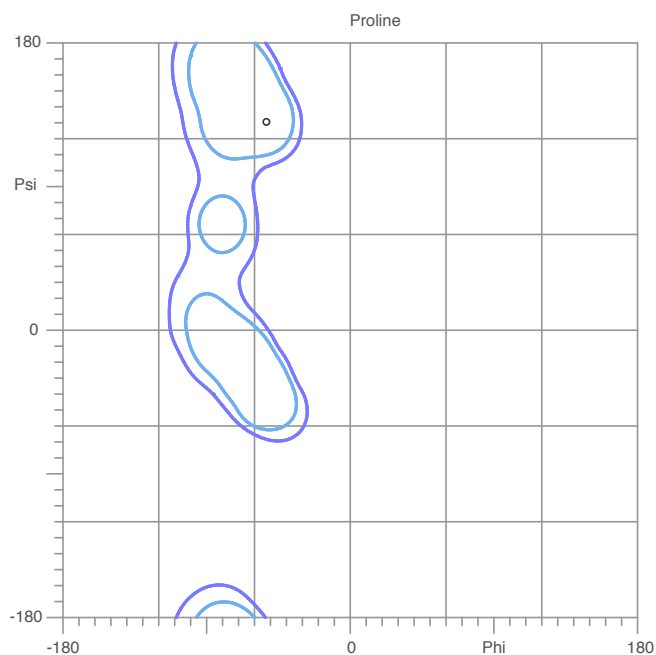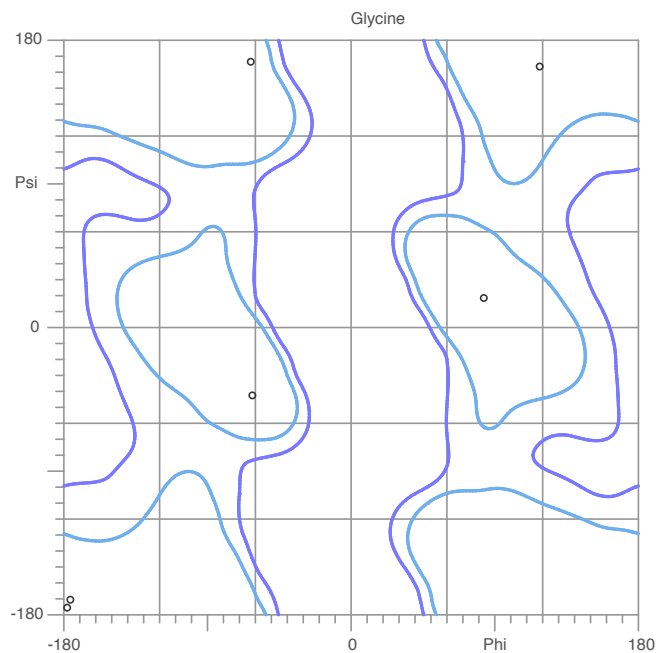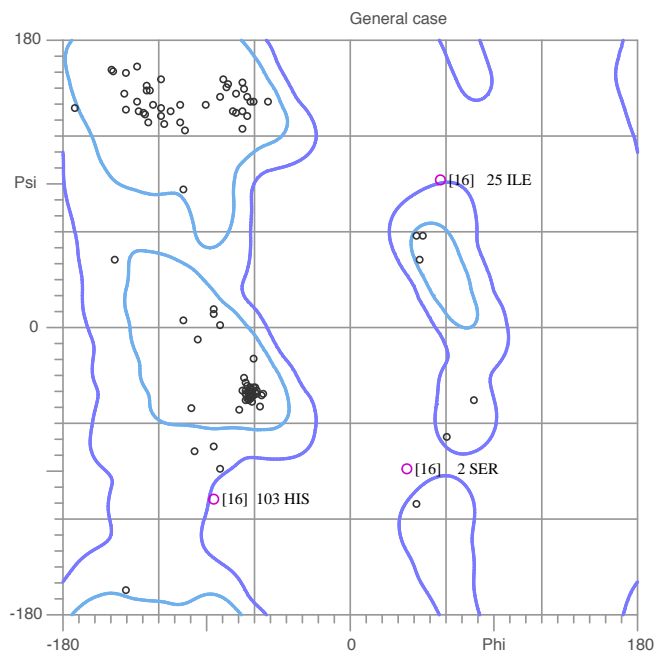
2KHD_NMR.pdb, model 15

80.2% (85/106) of all residues were in favored (98%) regions.
93.4% (99/106) of all residues were in allowed (>99.8%) regions.

There were 7 outliers (phi, psi):
   [15]   4 GLN (-51.3, -85.1)

[15]   12 CYS (39.3, 91.5)
[15]   16 GLY (48.2, -94.3)
[15]   17 CYS (63.9, 122.2)
[15]   39 SER (-80.4, -141.5)
[15]   71 ASP (53.4, -73.4)
[15] 101 LEU (42.6, -90.1)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 16

88.7% (94/106) of all residues were in favored (98%) regions.
97.2% (103/106) of all residues were in allowed (>99.8%) regions.

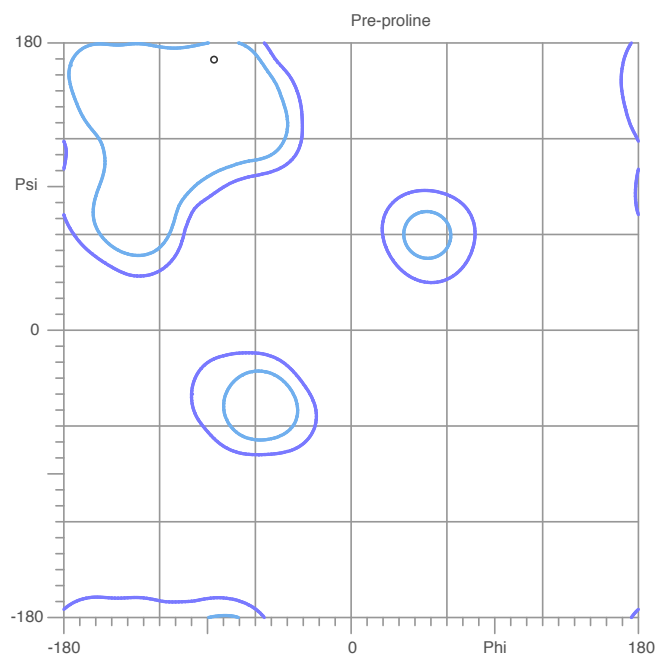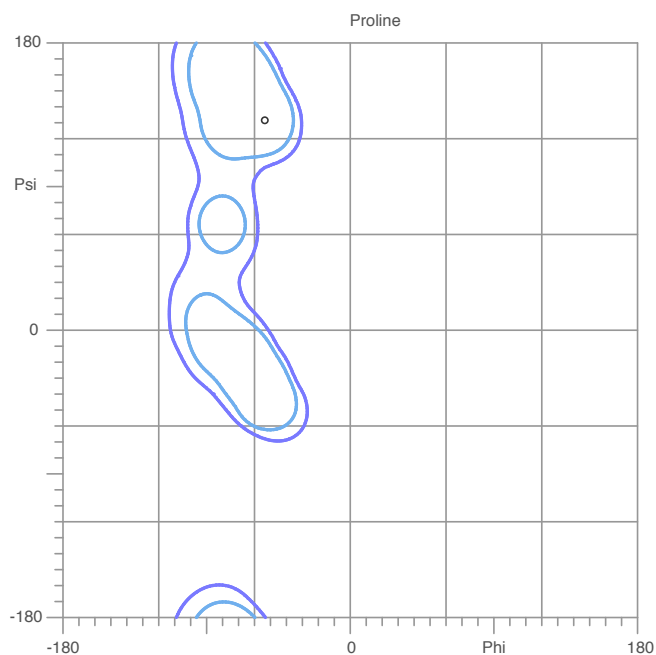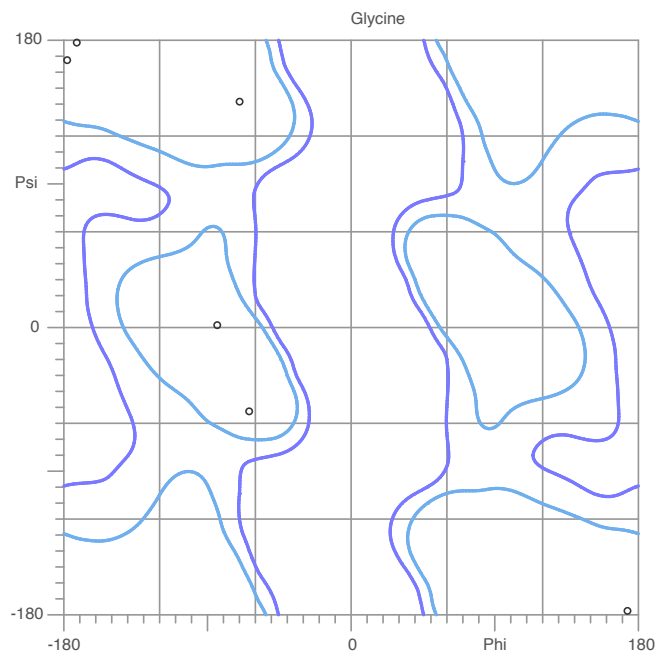There were 3 outliers (phi, psi):
    [16]   2 SER (35.2, -88.8)
    [16]   25 ILE (56.9, 93.8)
    [16] 103 HIS (-86.0, -107.5)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 17

General case

Glycine

Proline

Pre-proline

90.6% (96/106) of all residues were in favored (98%) regions.
95.3% (101/106) of all residues were in allowed (>99.8%) regions.
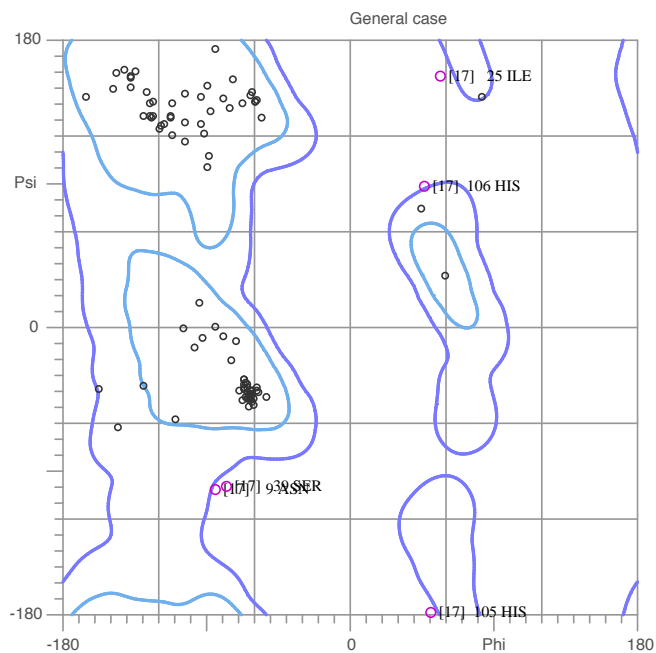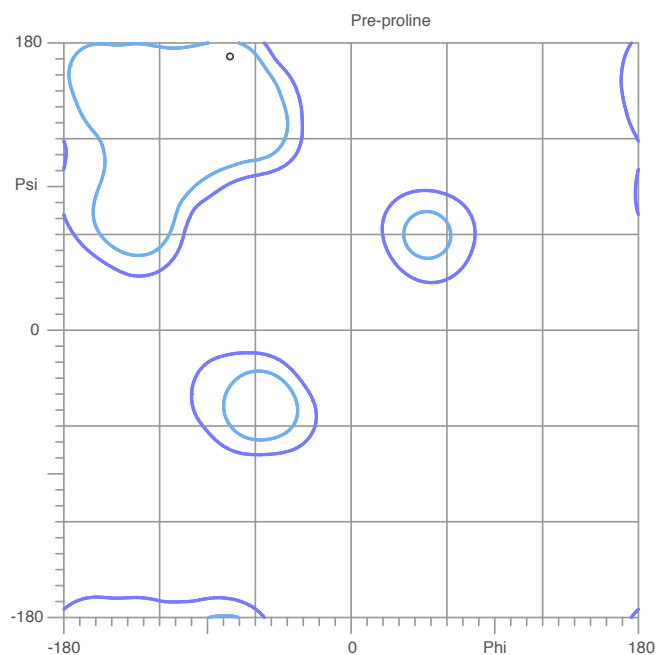
There were 5 outliers (phi, psi):

[17]   9 ASN (-85.5, -101.3)
[17]   25 ILE (56.4, 158.1)
[17]   39 SER (-78.5, -99.3)
[17] 105 HIS (50.5, -178.9)
[17] 106 HIS (46.6, 89.9)

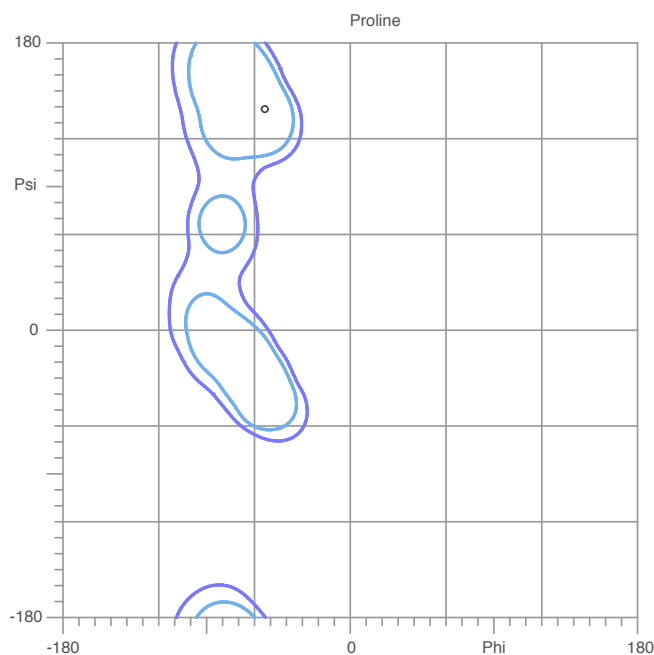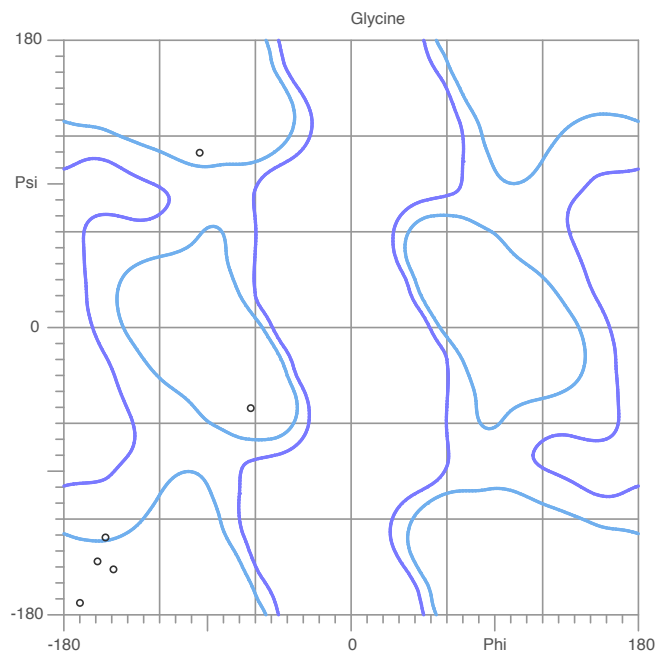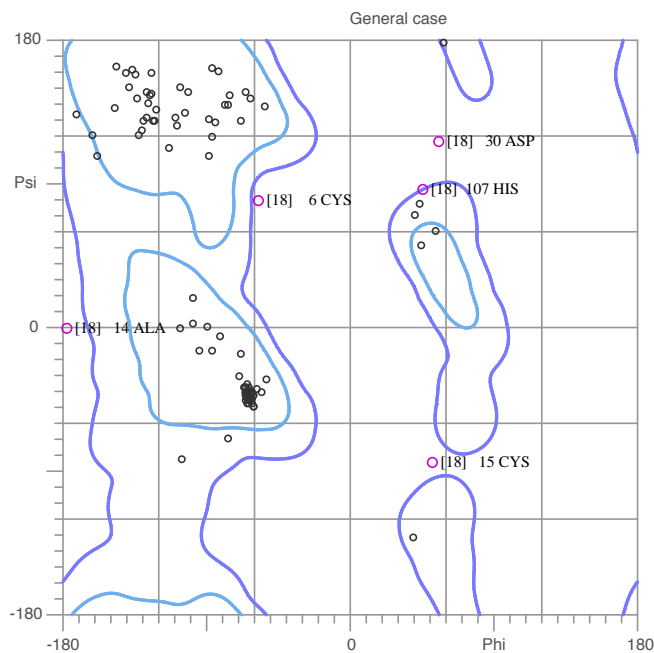# MolProbity Ramachandran analysis
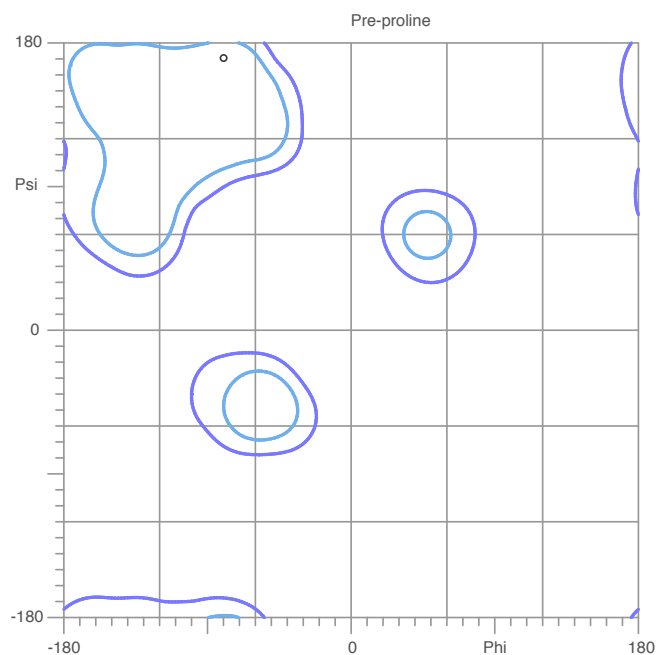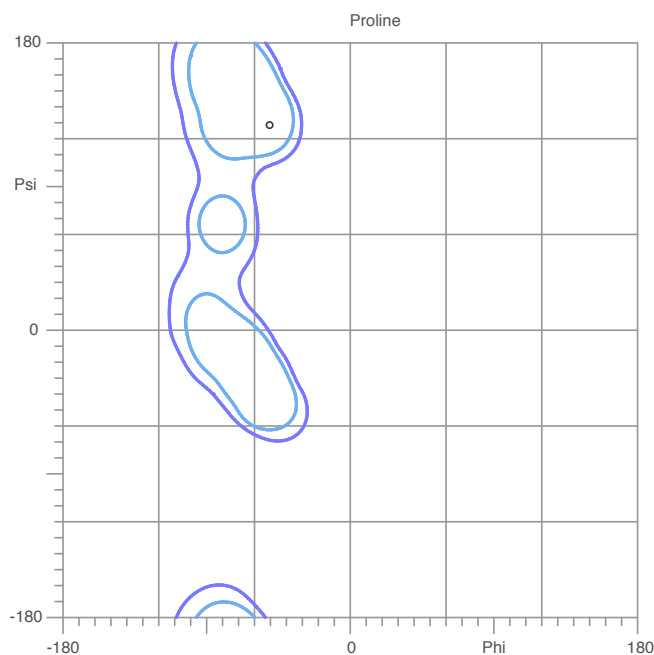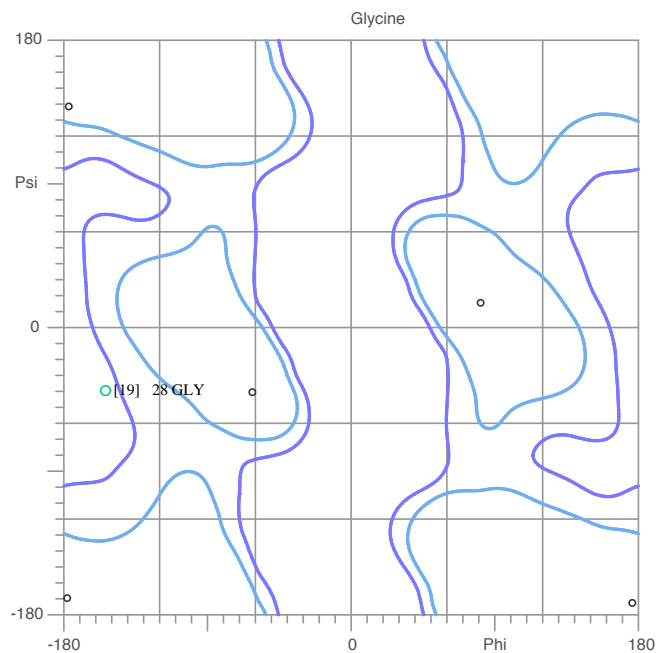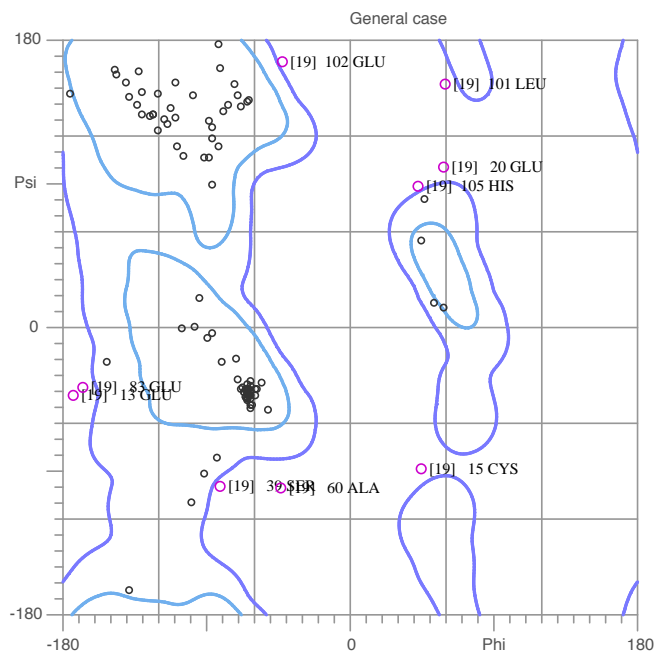
2KHD_NMR.pdb, model 18

85.8% (91/106) of all residues were in favored (98%) regions.
95.3% (101/106) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[18]   6 CYS (-58.9, 80.8)
[18]   14 ALA (-178.4, 0.0)
[18]   15 CYS (51.1, -84.7)
[18]   30 ASP (55.8, 117.9)
[18] 107 HIS (45.1, 87.5)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 19

83.0% (88/106) of all residues were in favored (98%) regions.
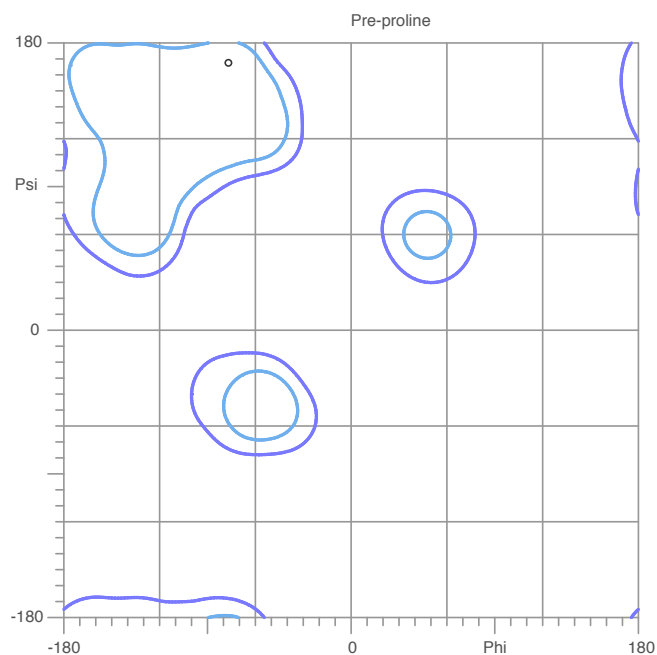90.6% (96/106) of all residues were in allowed (>99.8%) regions.
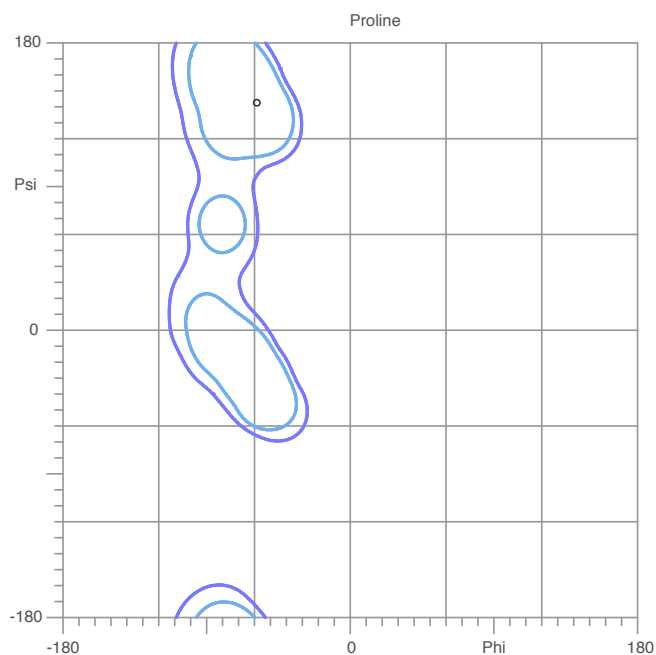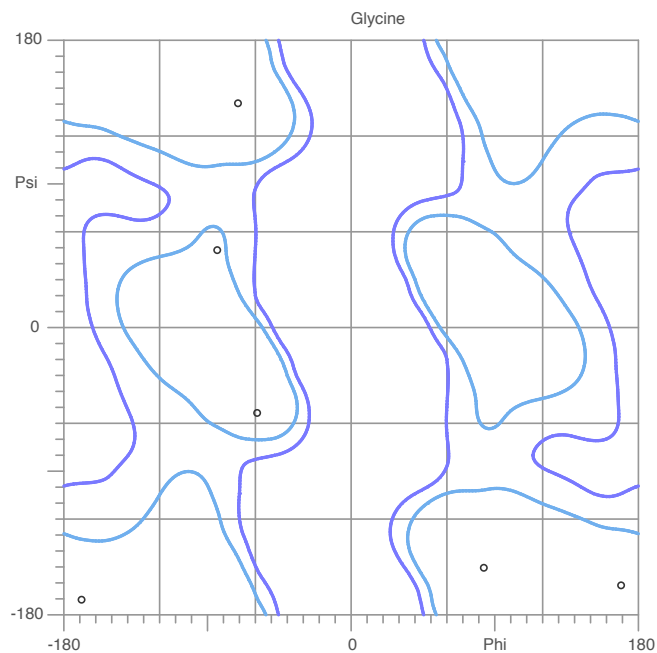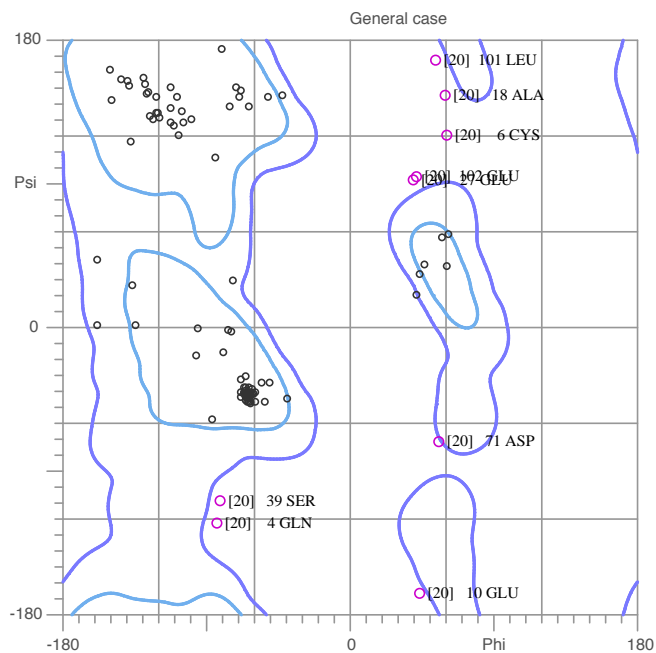
There were 10 outliers (phi, psi):
   [19] 13 GLU (-174.1, -42.2)
   [19] 15 CYS (44.6, -88.1)
   [19] 20 GLU (58.3, 101.5)

   [19] 28 GLY (-154.6, -39.7)
   [19] 39 SER (-82.2, -99.4)
   [19] 60 ALA (-44.4, -100.0)
   [19] 83 GLU (-168.8, -38.0)
   [19] 101 LEU (59.3, 153.7)
   [19] 102 GLU (-43.2, 168.0)
   [19] 105 HIS (42.2, 89.7)

MolProbity Ramachandran analysis

2KHD_NMR.pdb, model 20

85.8% (91/106) of all residues were in favored (98%) regions.
91.5% (97/106) of all residues were in allowed (>99.8%) regions.

There were 9 outliers (phi, psi):
   [20]   4 GLN (-84.0, -122.5)
   [20]   6 CYS (60.9, 121.5)

[20]   10 GLU (43.1, -166.5)
[20]   18 ALA (59.6, 147.0)
[20]   27 GLU (40.0, 93.5)
[20]   39 SER (-82.4, -108.9)
[20]   71 ASP (55.6, -71.7)
[20]   101 LEU (53.7, 168.3)
[20]   102 GLU (41.5, 95.1)