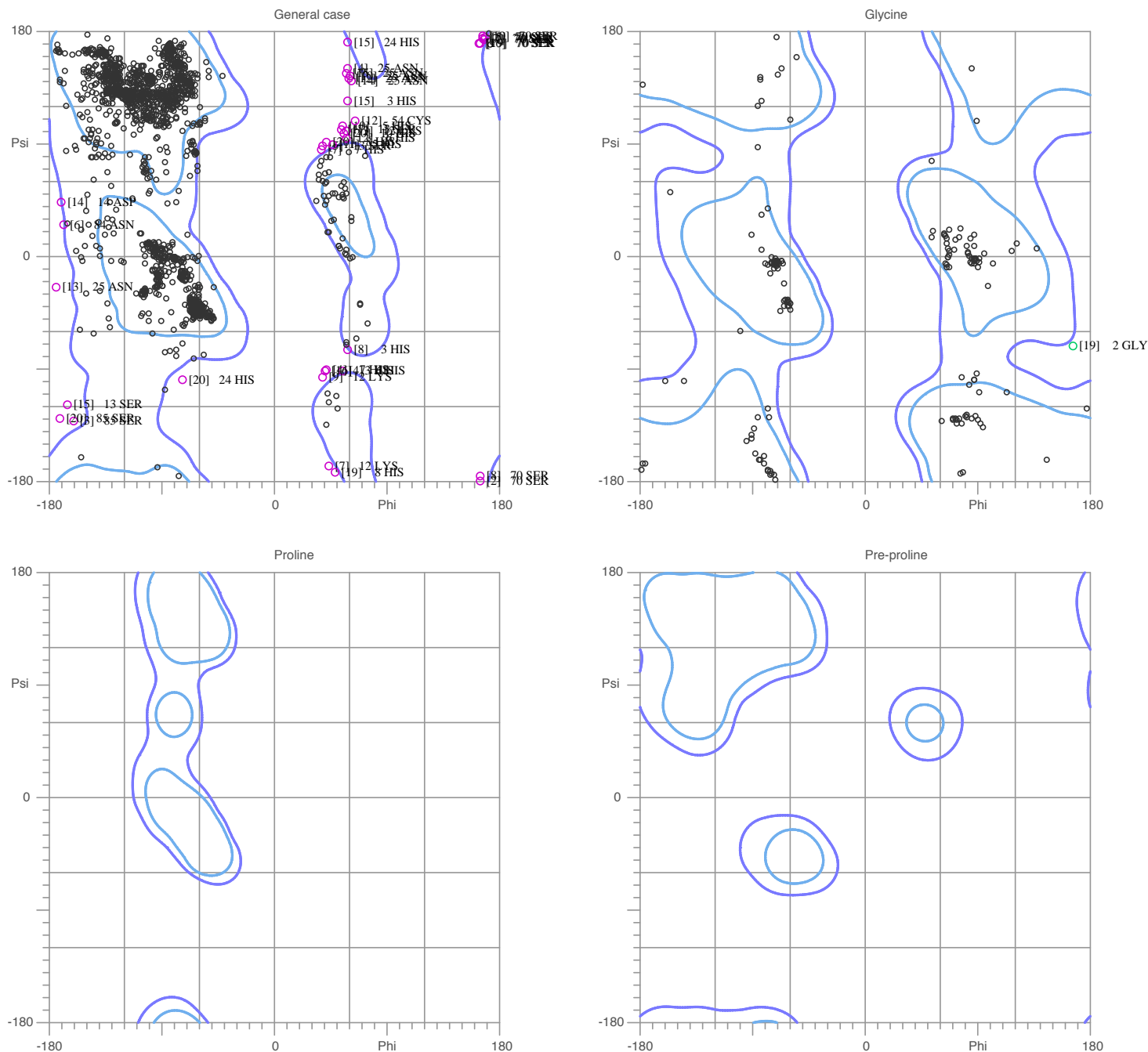# MolProbity Ramachandran analysis

2KJR_NMR.pdb, all models
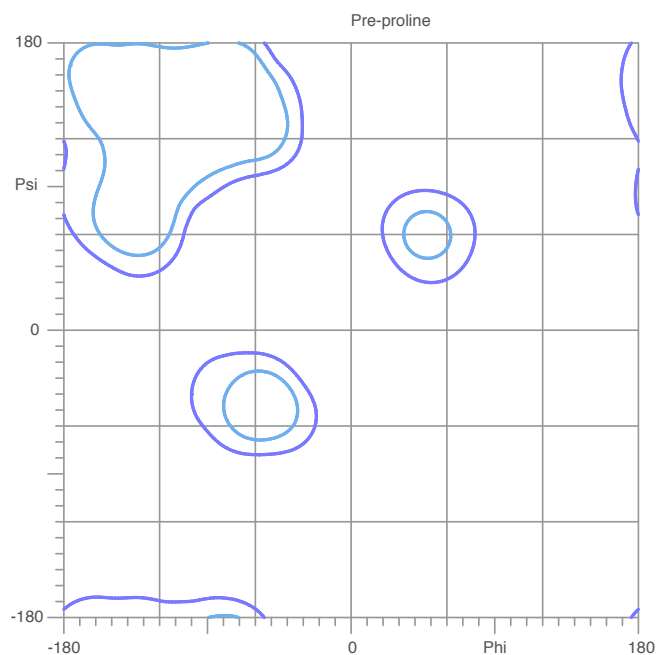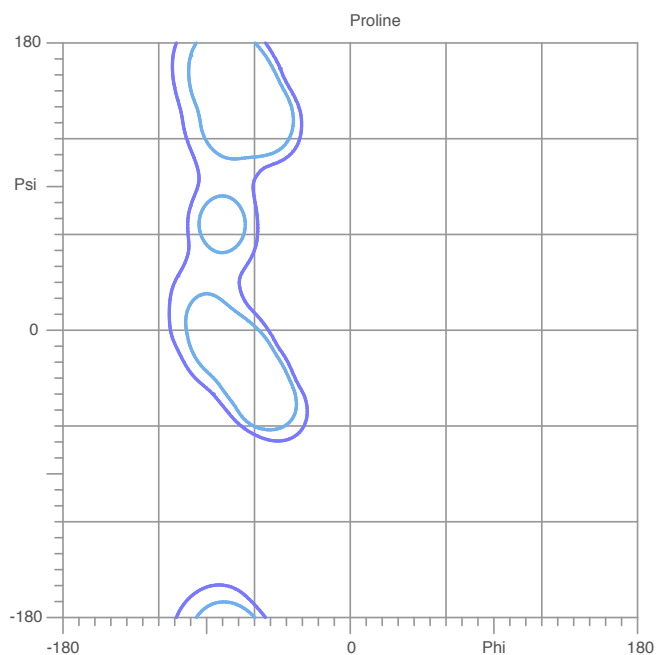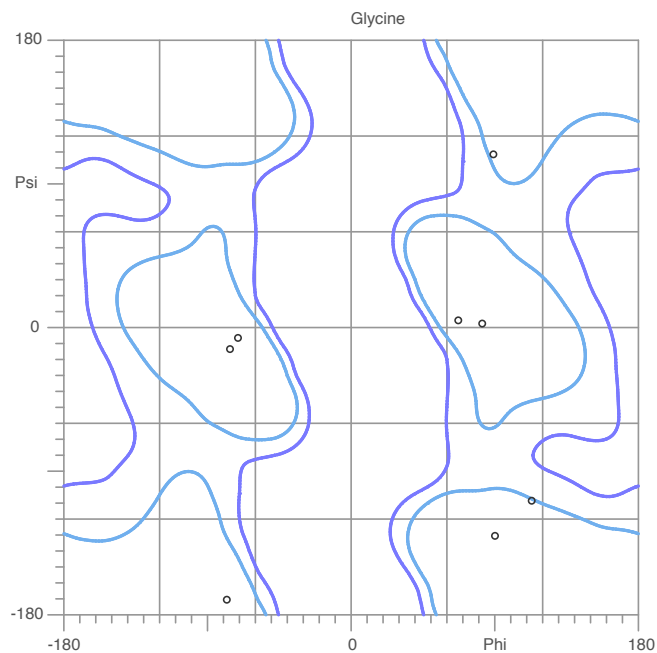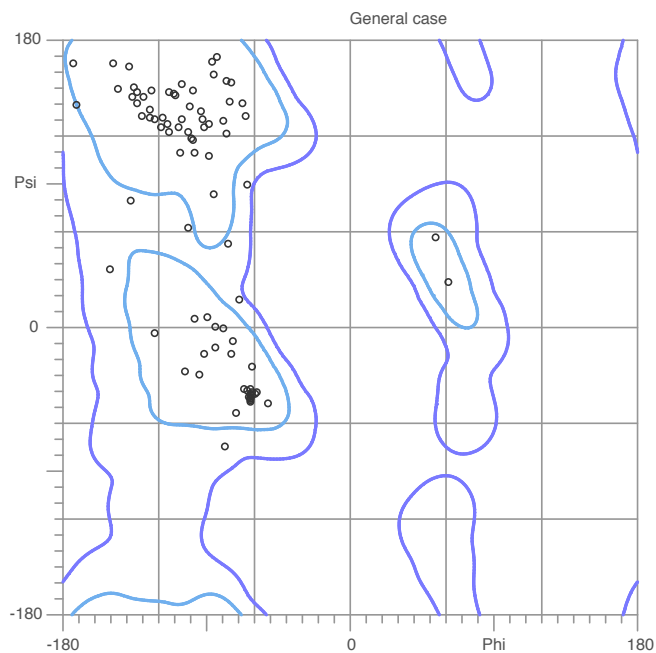

General case

Glycine

Proline

Pre-proline

89.7% (1669/1860) of all residues were in favored (98%) regions.
97.8% (1820/1860) of all residues were in allowed (>99.8%) regions.

There were 40 outliers (phi, psi):
[2]   70 SER (164.7, -179.3)
[3]   85 SER (-161.5, -131.8)
[4]   6 HIS (54.8, -91.2)
[4]   7 HIS (41.8, -90.2)
[4]   25 ASN (58.6, 151.2)
[4]   70 SER (167.5, 174.4)
[5]   13 SER (38.7, 89.4)
[5]   70 SER (168.4, 176.5)
[6]   84 ASN (-169.6, 26.9)
[7]   7 HIS (37.8, 86.4)
[7]   12 LYS (43.0, -167.7)
[7]   70 SER (166.0, 175.9)
[8]   3 HIS (58.7, -75.0)
[8]   70 SER (164.8, -175.9)
[9]   12 LYS (38.1, -96.4)
[10]   5 HIS (54.5, 105.8)
[10]   25 ASN (60.6, 145.2)
[10]   70 SER (166.7, 177.0)

[11]   5 HIS (46.6, 90.1)
[12]   6 HIS (57.9, 95.4)
[12]   25 ASN (59.1, 143.2)
[12]   54 CYS (65.0, 109.5)
[13]   12 LYS (57.2, 101.9)
[13]   25 ASN (-175.2, -24.0)
[14]   14 ASP (-171.5, 44.5)
[14]   25 ASN (61.2, 141.9)
[15]   3 HIS (58.7, 125.5)
[15]   13 SER (-166.3, -118.7)
[15]   24 HIS (58.9, 172.8)
[15]   25 ASN (58.0, 147.2)
[16]   3 HIS (40.9, -91.3)
[16]   70 SER (163.9, 171.8)
[17]   13 SER (53.0, 102.6)
[19]   2 GLY (166.2, -71.2)
[19]   8 HIS (48.3, -172.6)
[19]   70 SER (164.2, 171.6)
[20]   8 HIS (41.5, 92.6)
[20]   10 HIS (55.1, 99.9)
[20]   24 HIS (-74.9, -98.3)
[20]   85 SER (-172.7, -129.8)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 1

91.4% (85/93) of all residues were in favored (98%) regions.
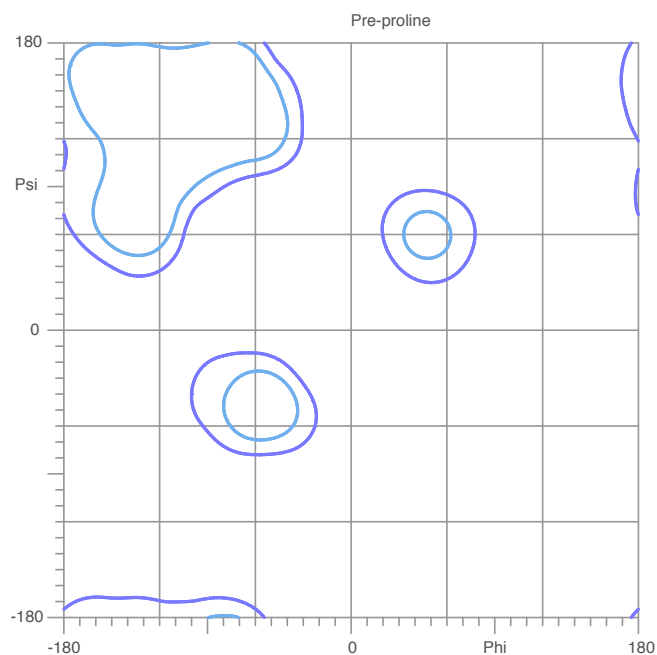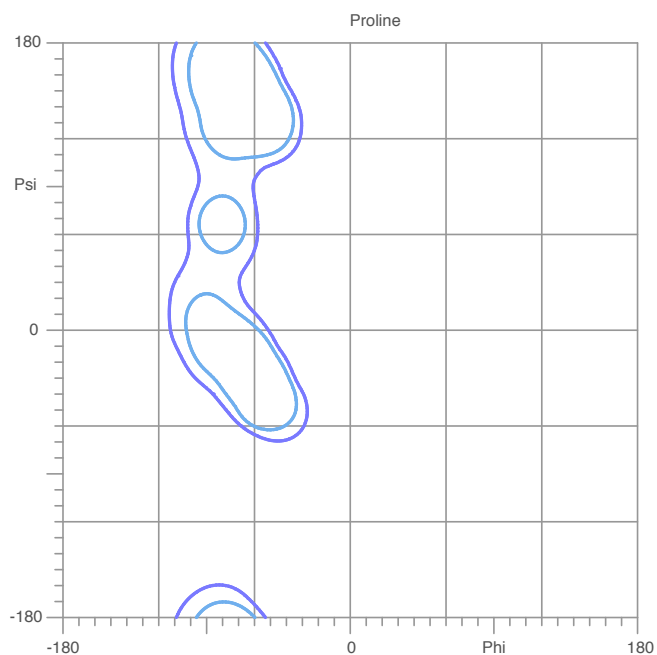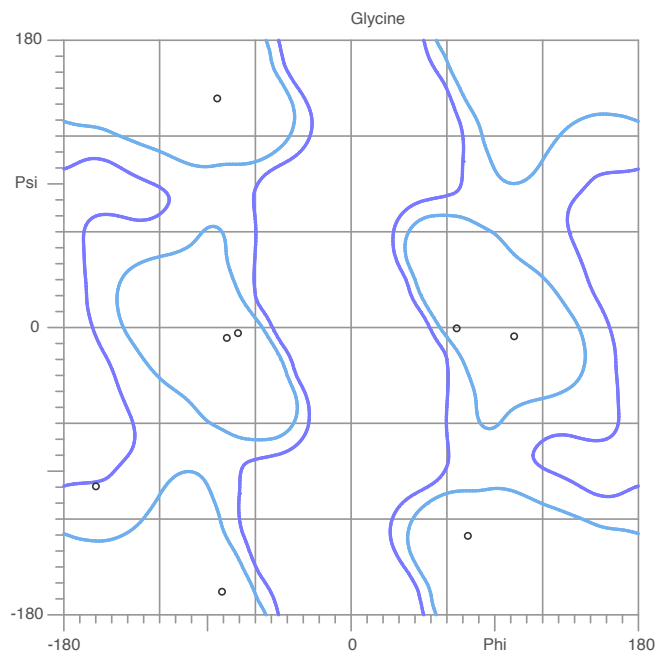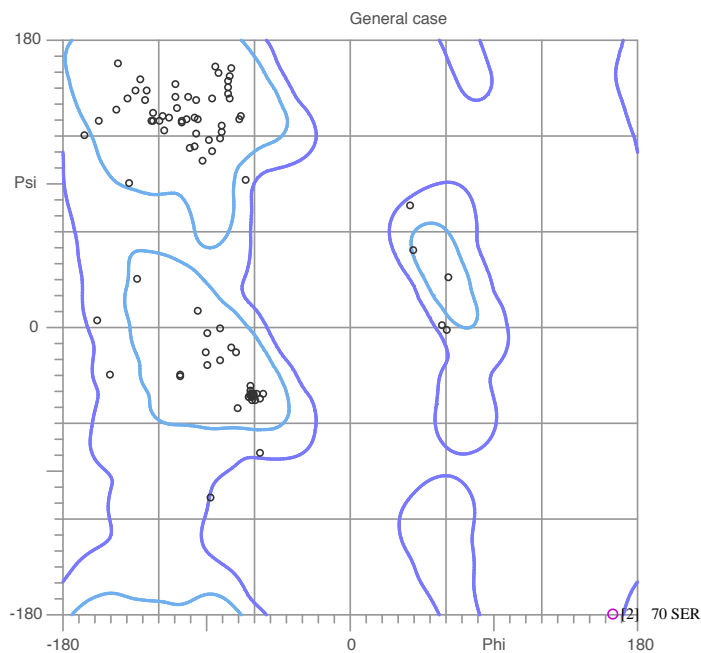100.0% (93/93) of all residues were in allowed (>99.8%) regions.

There were no outliers.

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 2

88.2% (82/93) of all residues were in favored (98%) regions.
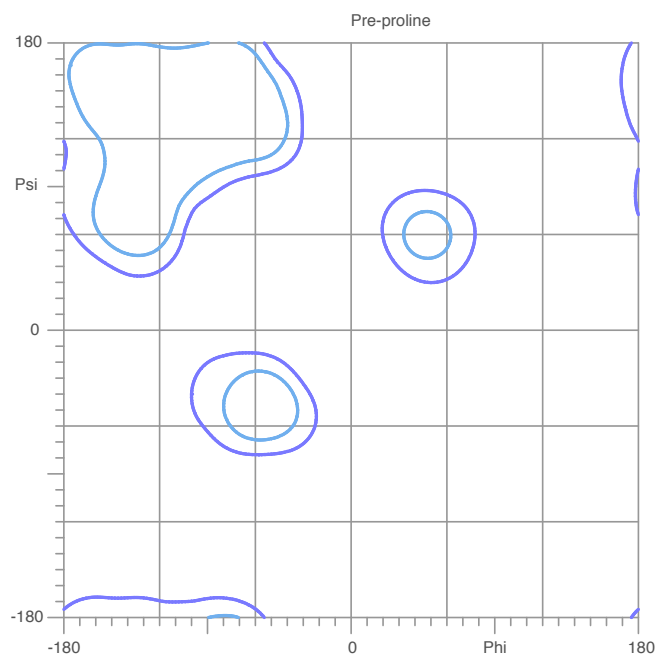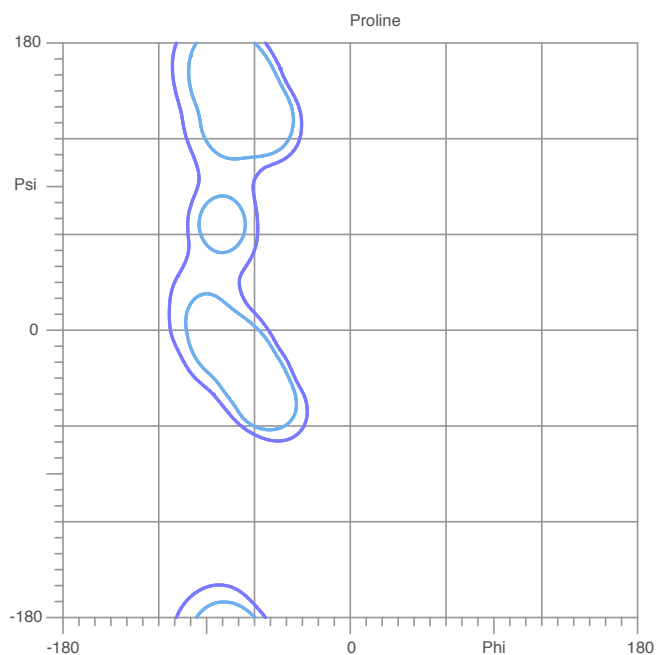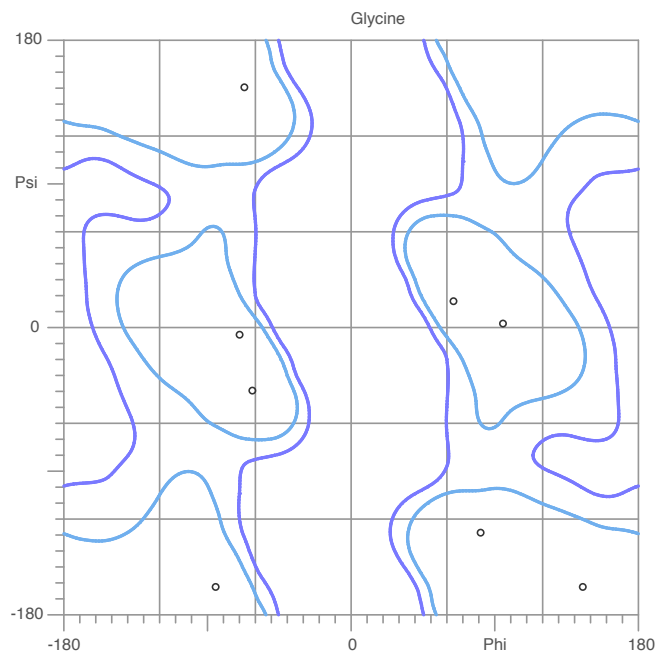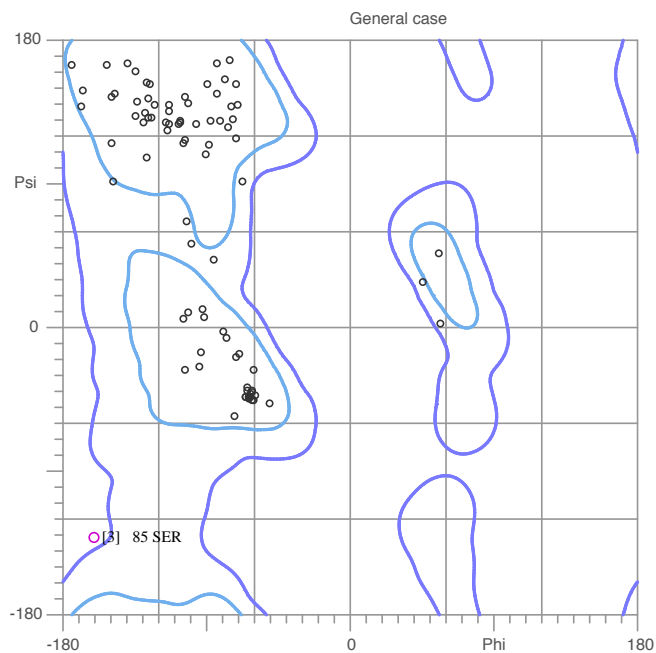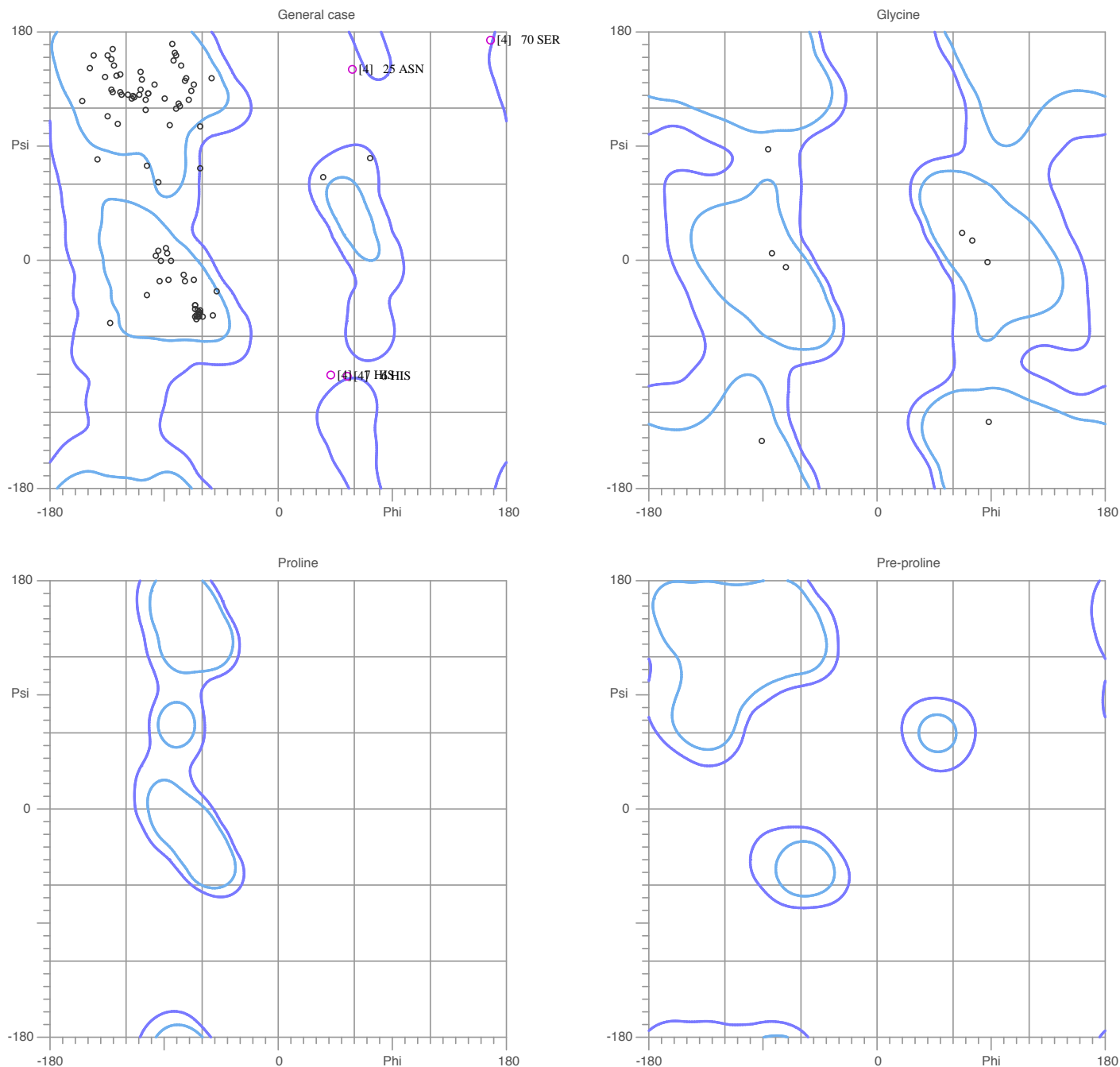98.9% (92/93) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
[2]   70 SER (164.7, -179.3)

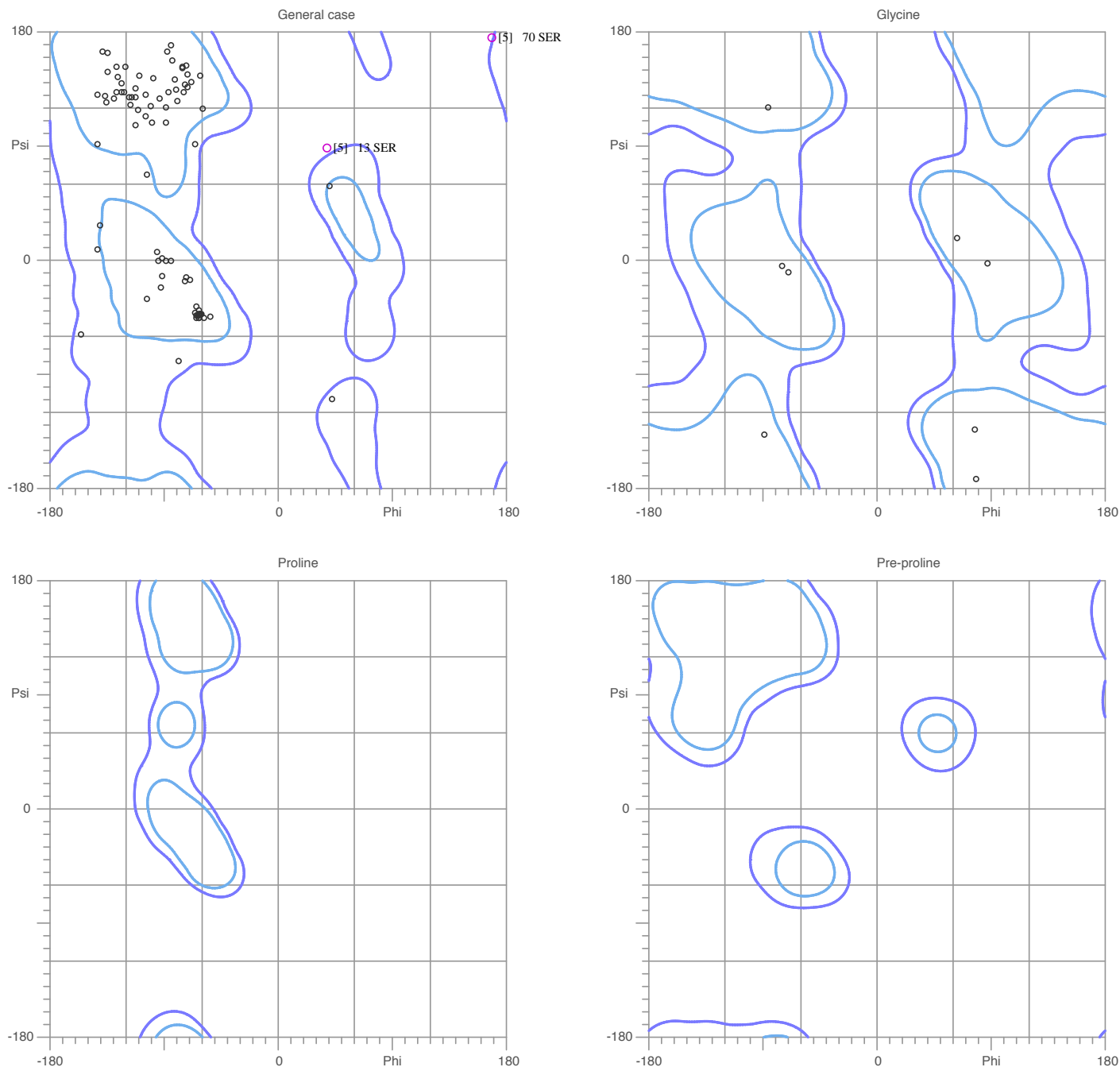# MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 3

91.4% (85/93) of all residues were in favored (98%) regions.
98.9% (92/93) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
   [3]   85 SER (-161.5, -131.8)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 4

87.1% (81/93) of all residues were in favored (98%) regions.
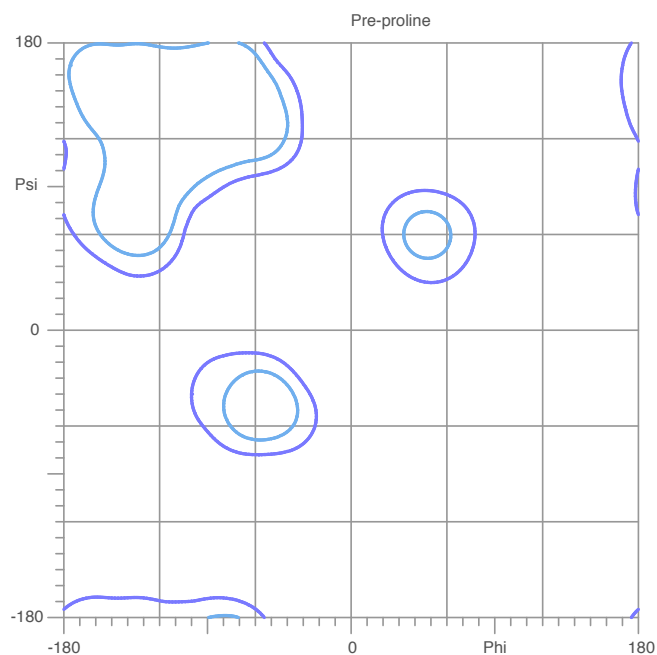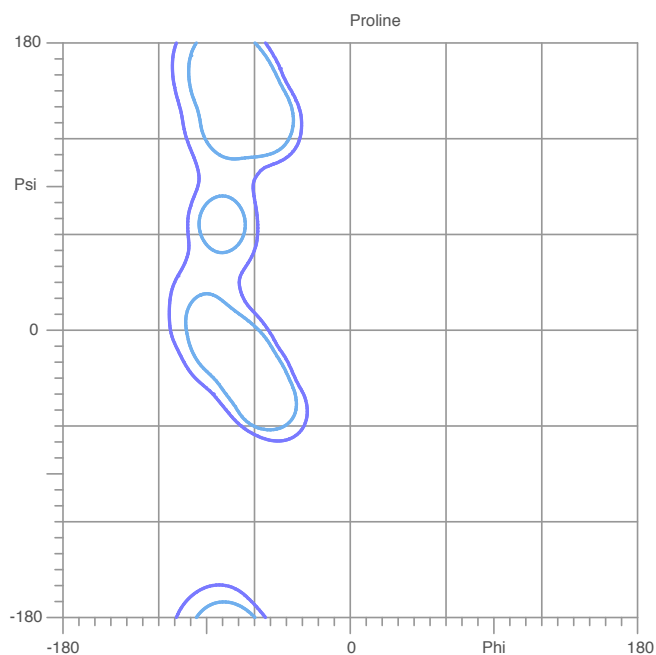95.7% (89/93) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
    [4]   6 HIS (54.8, -91.2)
    [4]   7 HIS (41.8, -90.2)
    [4]   25 ASN (58.6, 151.2)
    [4]   70 SER (167.5, 174.4)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 5

90.3% (84/93) of all residues were in favored (98%) regions.
97.8% (91/93) of all residues were in allowed (>99.8%) regions.
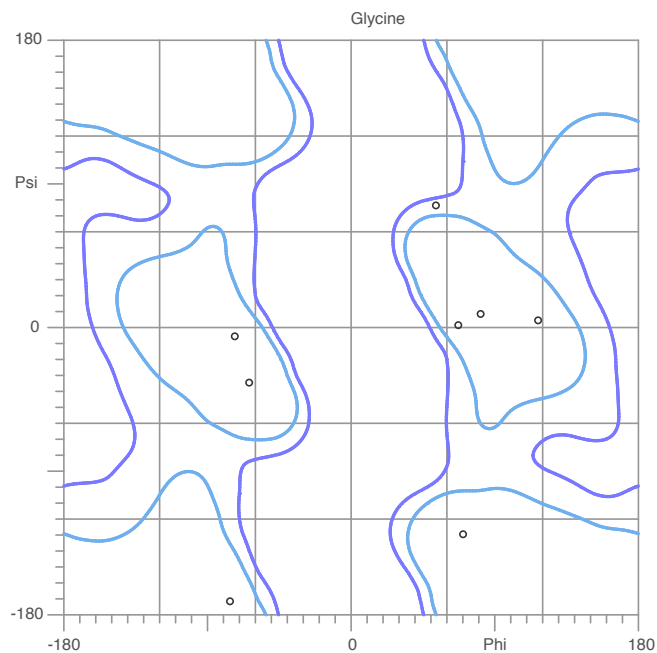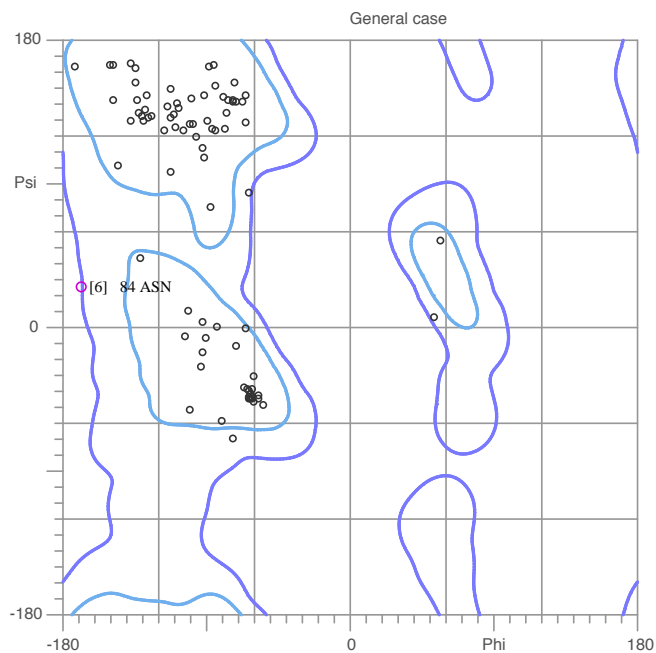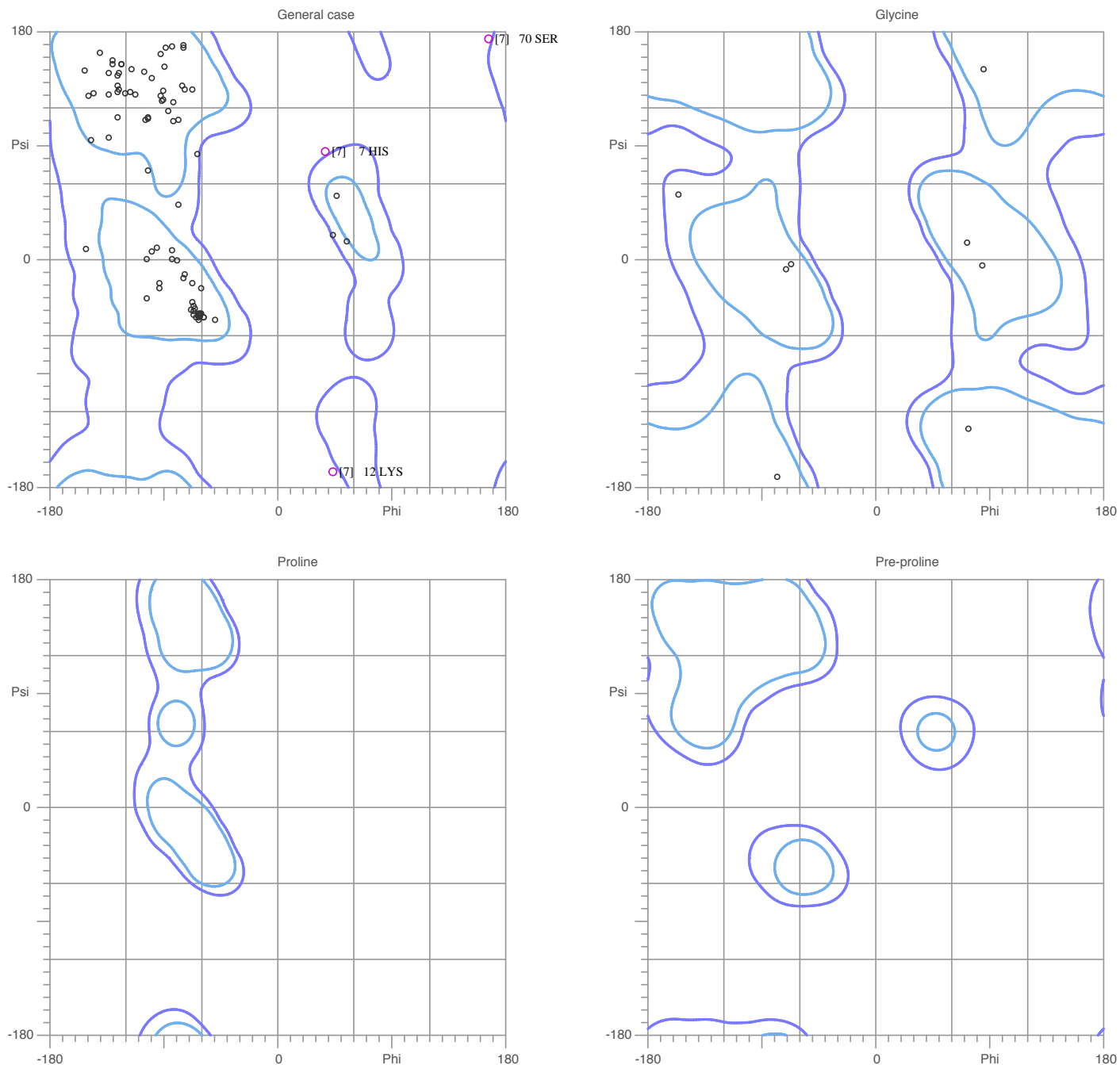
There were 2 outliers (phi, psi):
   [5]   13 SER (38.7, 89.4)
   [5]   70 SER (168.4, 176.5)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 6

94.6% (88/93) of all residues were in favored (98%) regions.
98.9% (92/93) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
   [6]   84 ASN (-169.6, 26.9)

MolProbity Ramachandran analysis
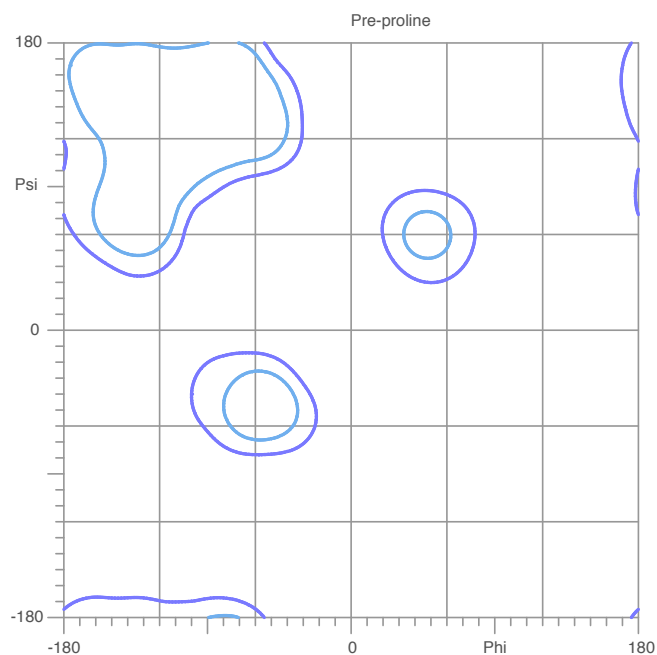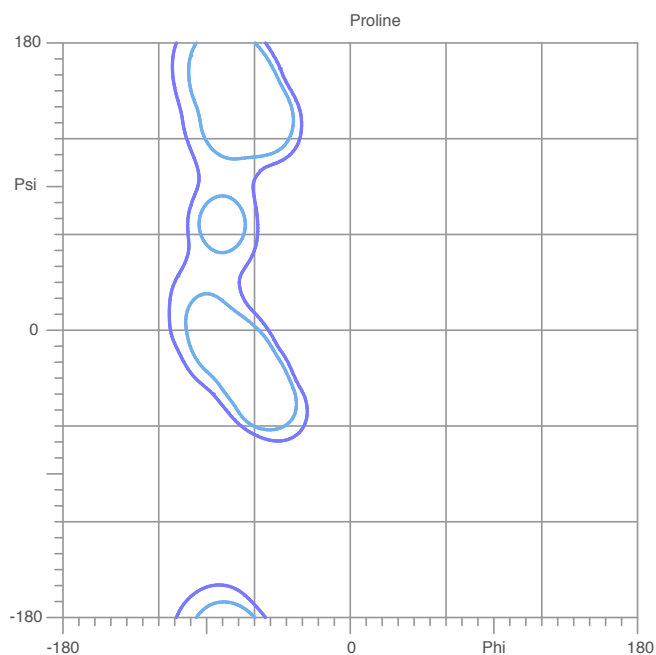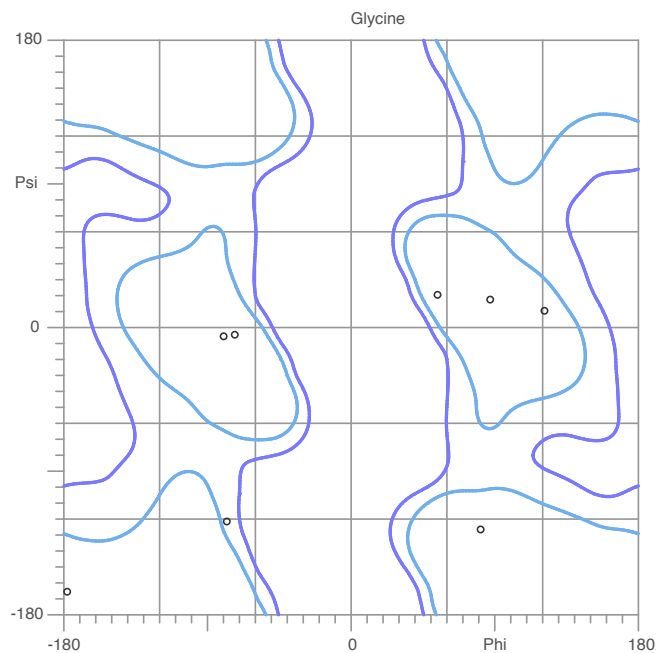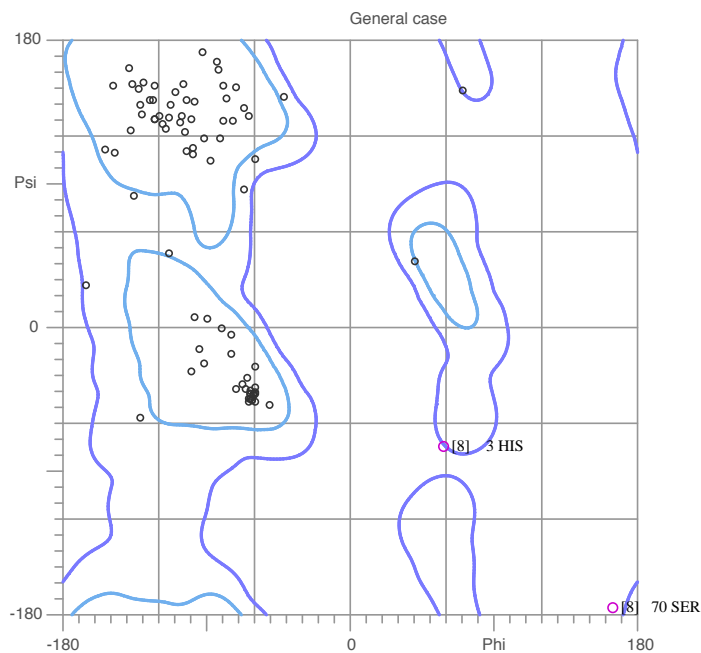
2KJR_NMR.pdb, model 7

89.2% (83/93) of all residues were in favored (98%) regions.
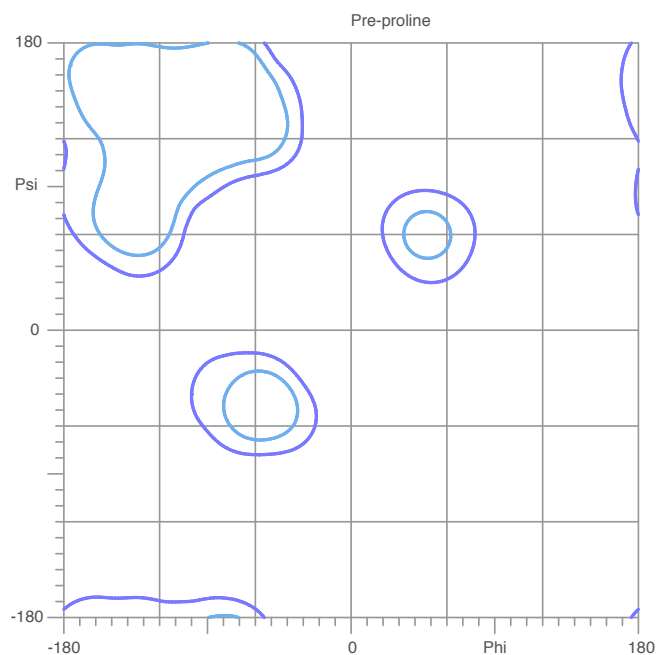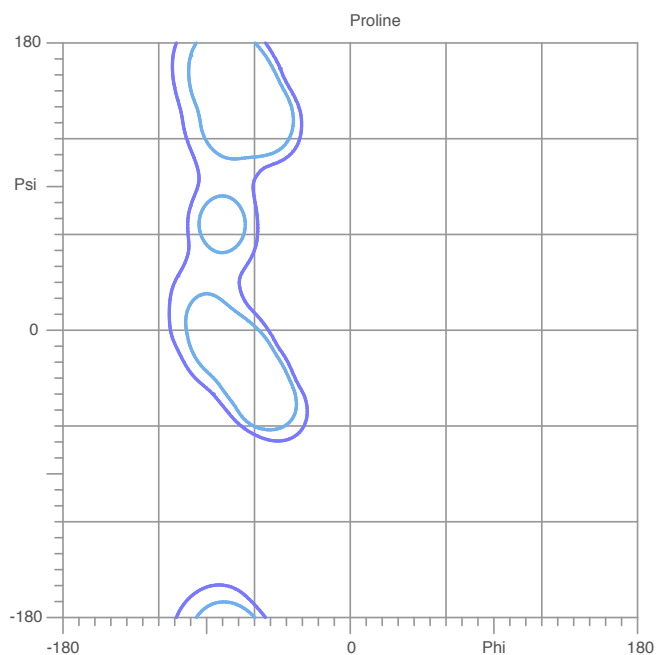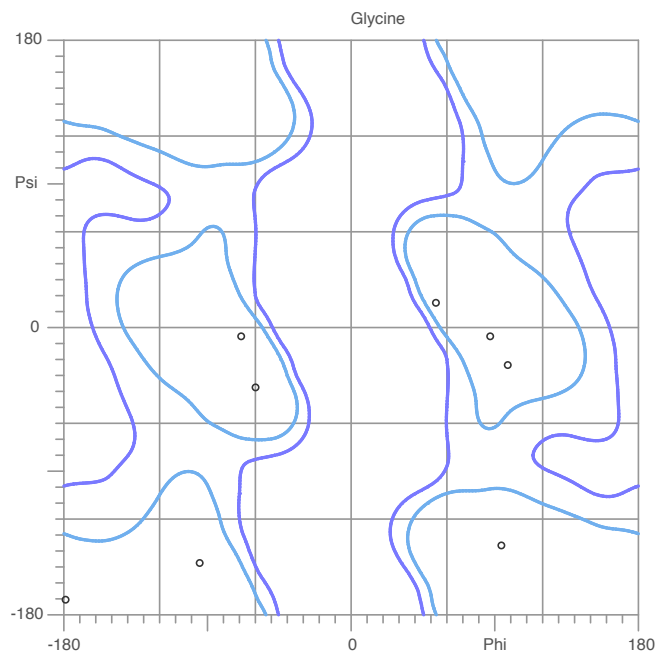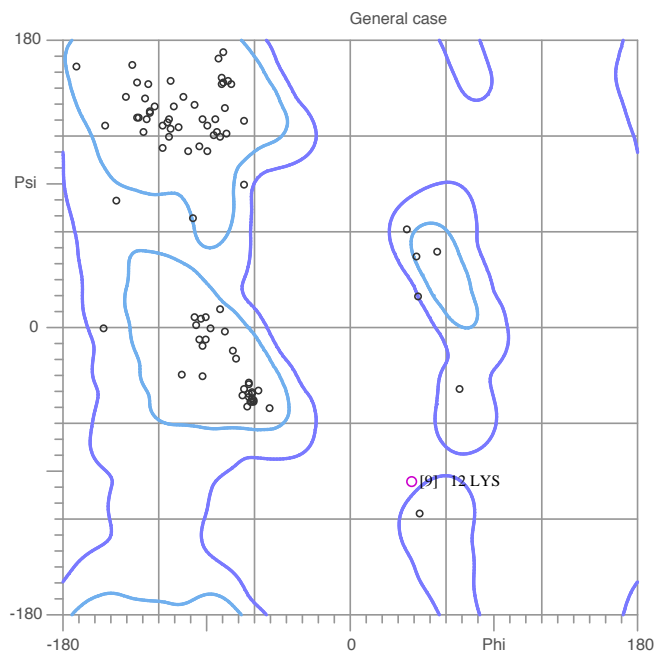96.8% (90/93) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
    [7]   7 HIS (37.8, 86.4)
    [7]   12 LYS (43.0, -167.7)
    [7]   70 SER (166.0, 175.9)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 8

88.2% (82/93) of all residues were in favored (98%) regions.
97.8% (91/93) of all residues were in allowed (>99.8%) regions.
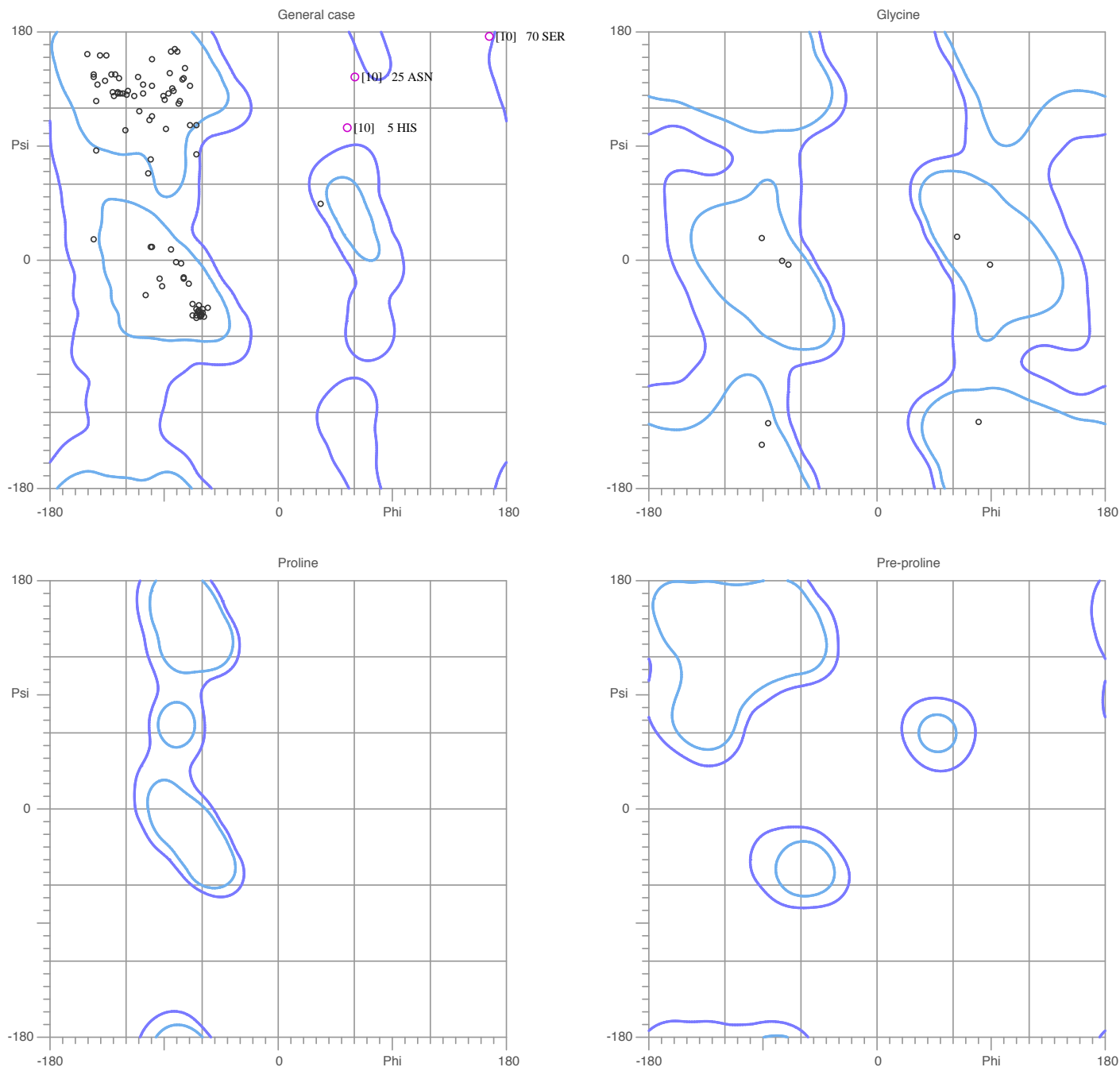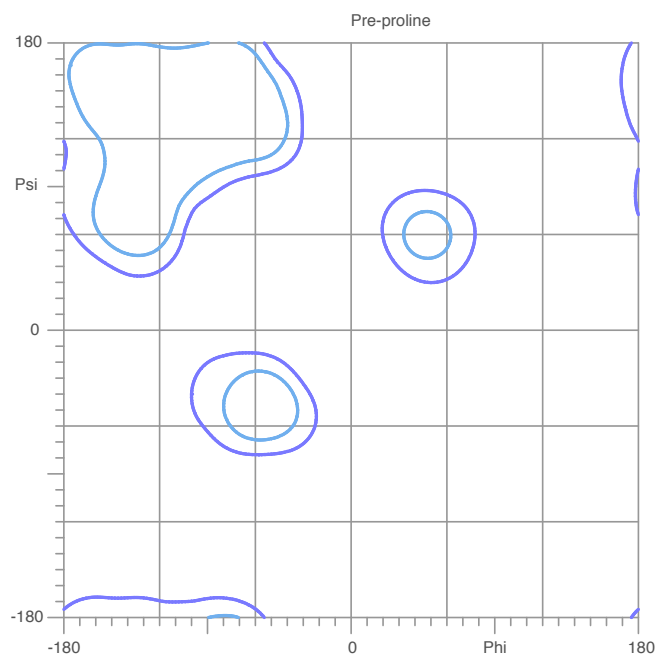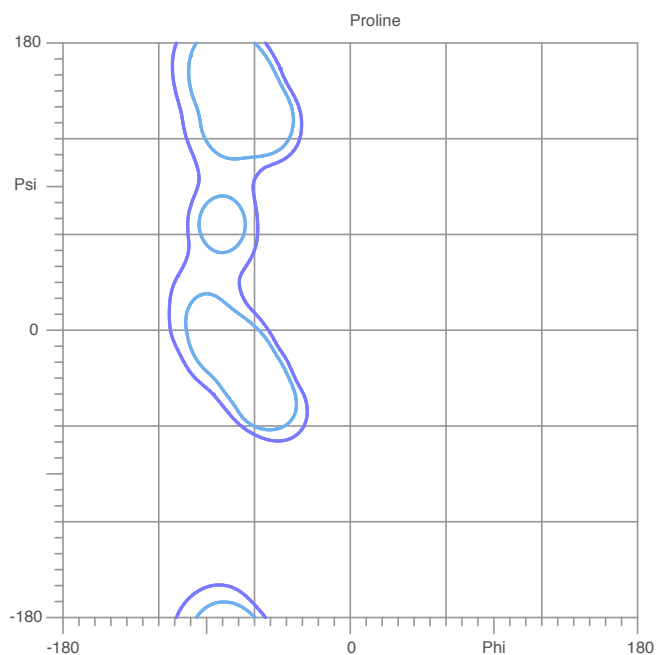
There were 2 outliers (phi, psi):
   [8]   3 HIS (58.7, -75.0)
   [8] 70 SER (164.8, -175.9)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 9

General case
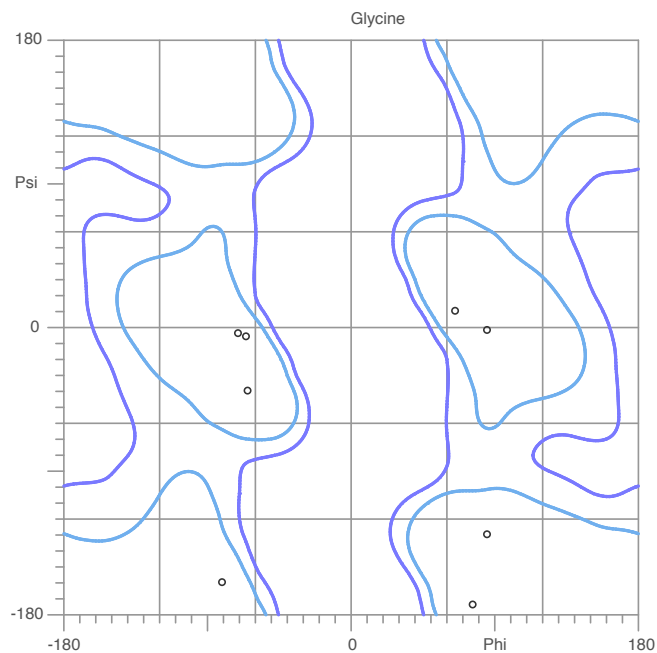
Glycine

Proline

Pre-proline

90.3% (84/93) of all residues were in favored (98%) regions.
98.9% (92/93) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
  [9]   12 LYS (38.1, -96.4)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 10
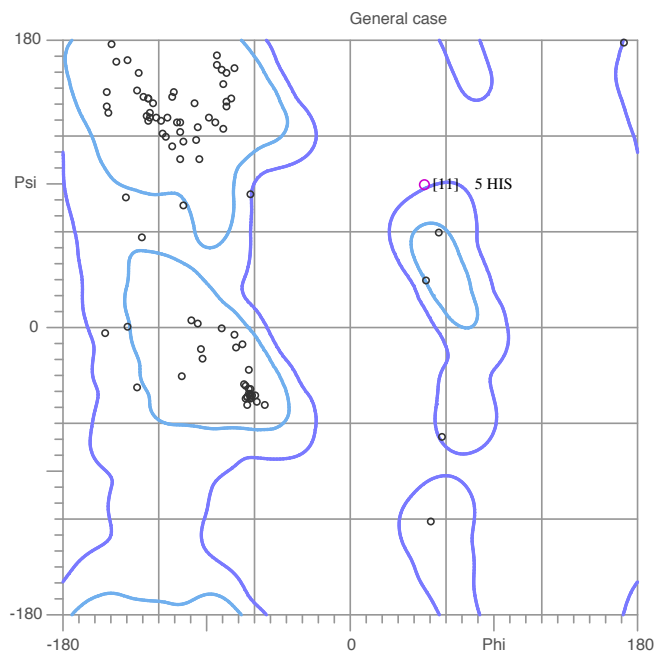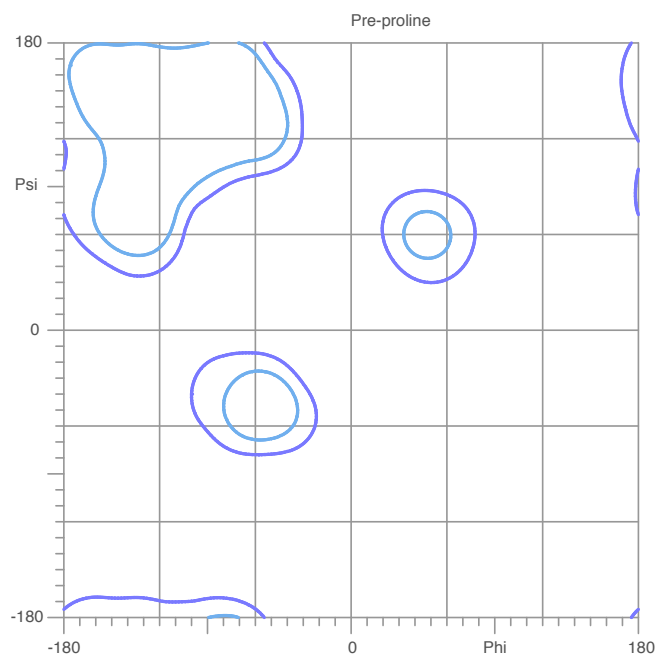
General case

Glycine

Proline

Pre-proline

91.4% (85/93) of all residues were in favored (98%) regions.
96.8% (90/93) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
  [10]   5 HIS (54.5, 105.8)
  [10]   25 ASN (60.6, 145.2)
  [10]   70 SER (166.7, 177.0)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 11

88.2% (82/93) of all residues were in favored (98%) regions.
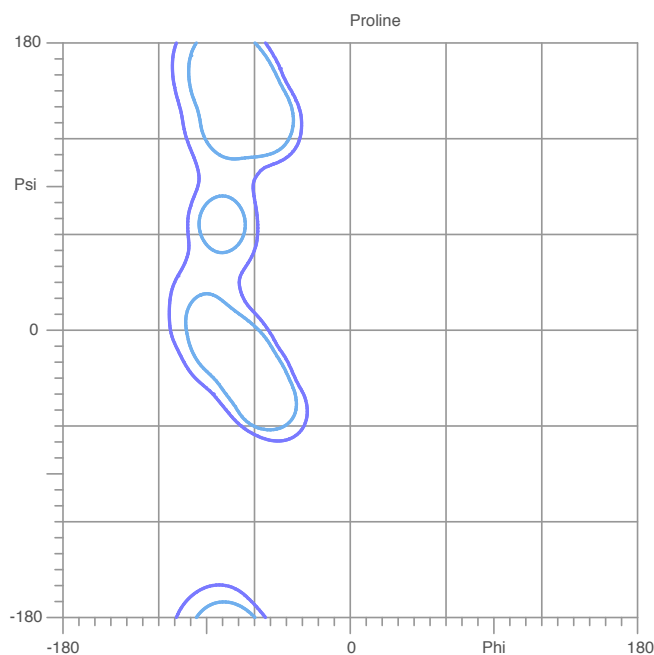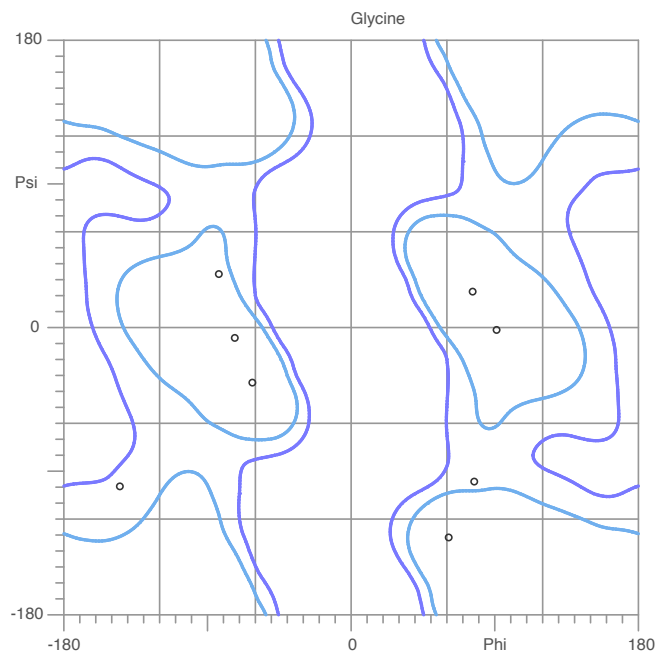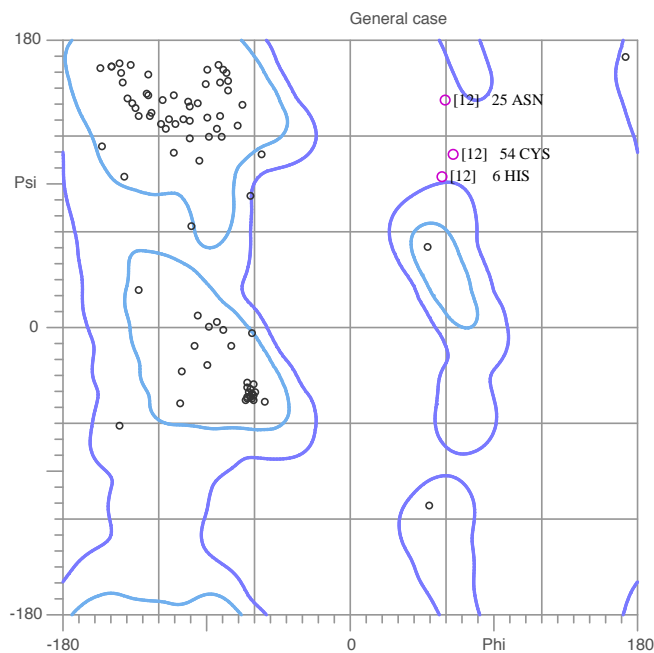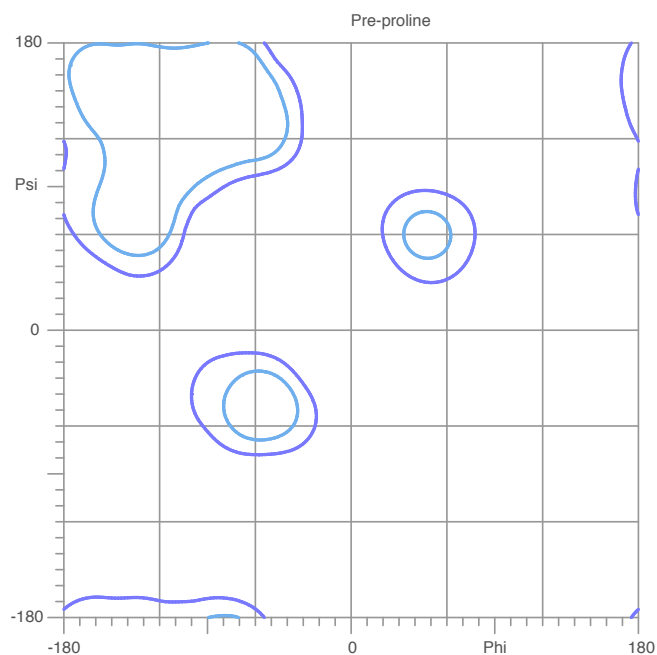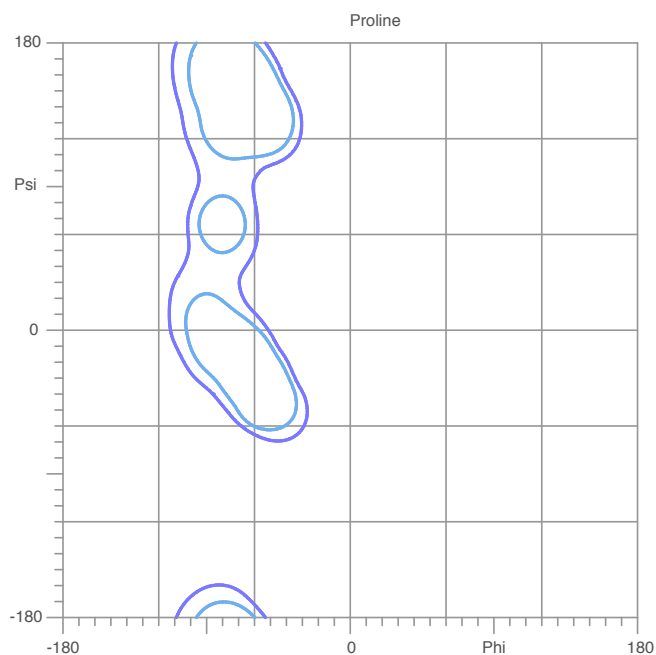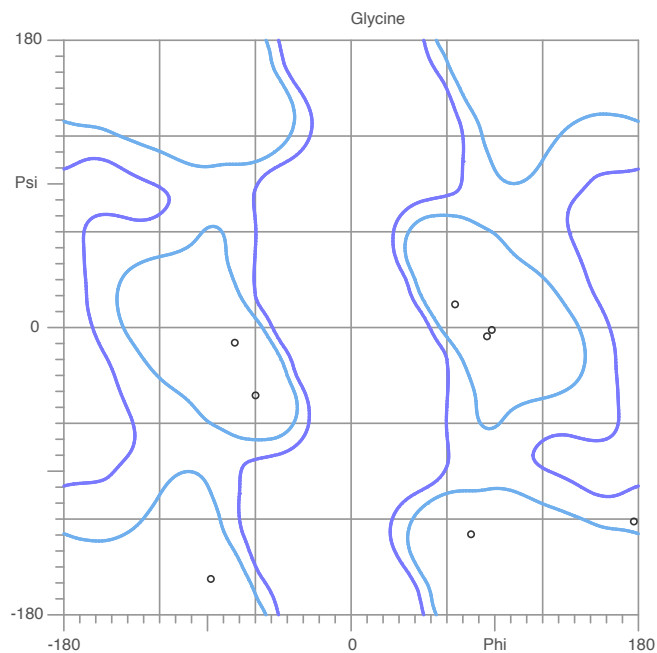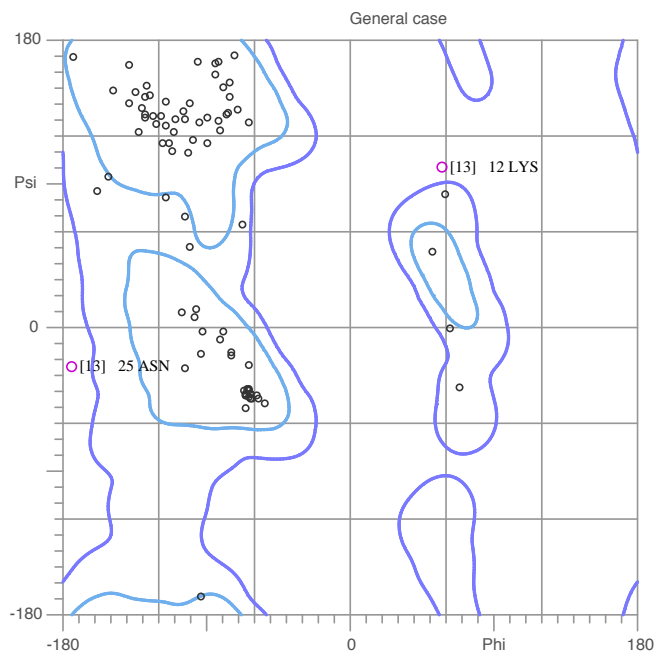98.9% (92/93) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
   [11]   5 HIS (46.6, 90.1)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 12

88.2% (82/93) of all residues were in favored (98%) regions.
96.8% (90/93) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
   [12]   6 HIS (57.9, 95.4)
   [12]   25 ASN (59.1, 143.2)
   [12]   54 CYS (65.0, 109.5)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 13

86.0% (80/93) of all residues were in favored (98%) regions.
97.8% (91/93) of all residues were in allowed (>99.8%) regions.
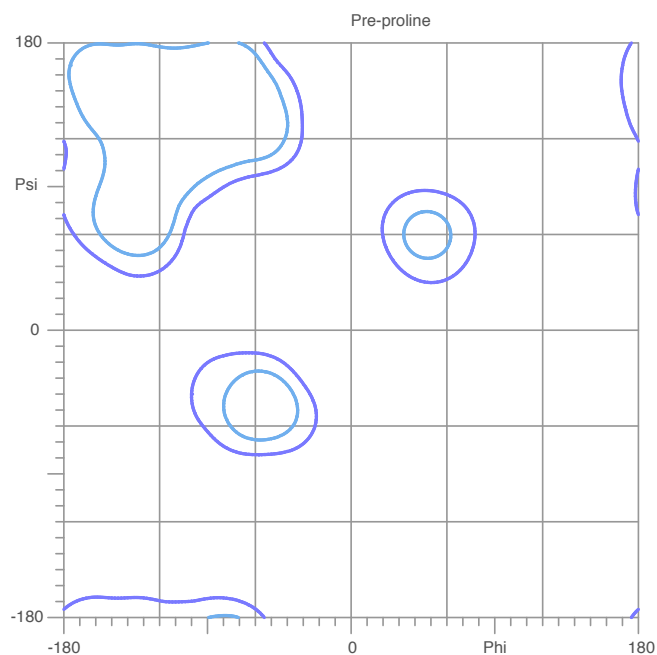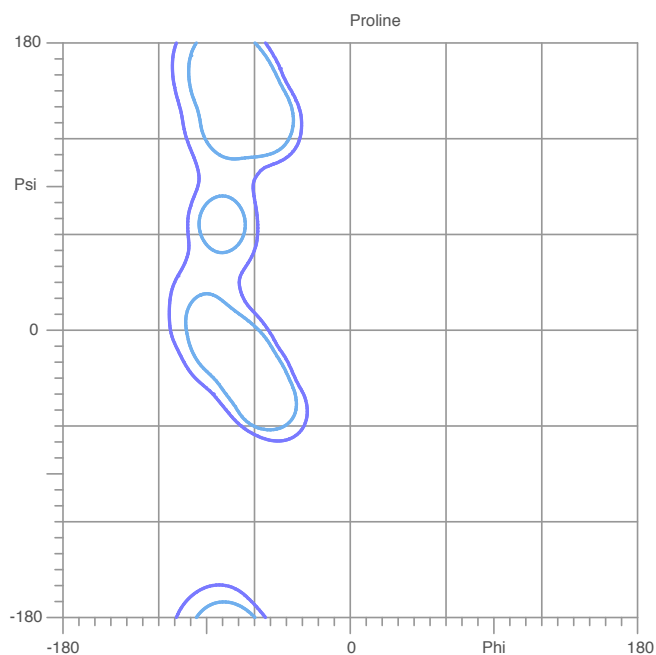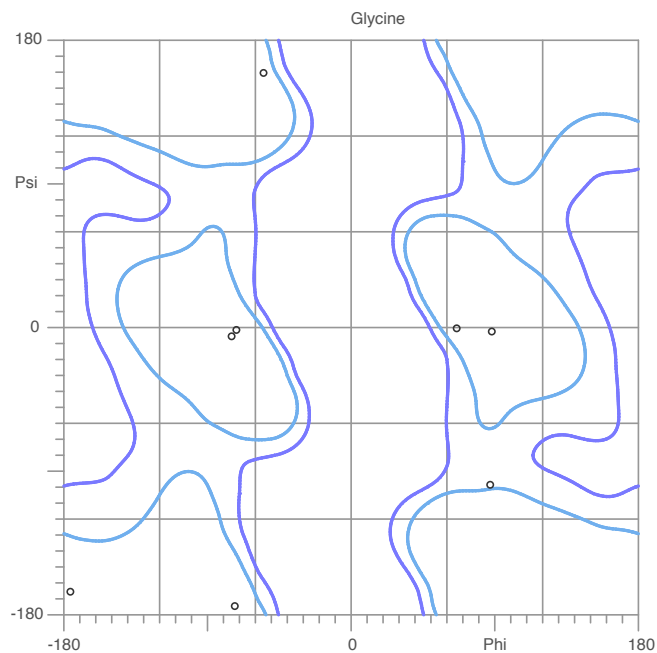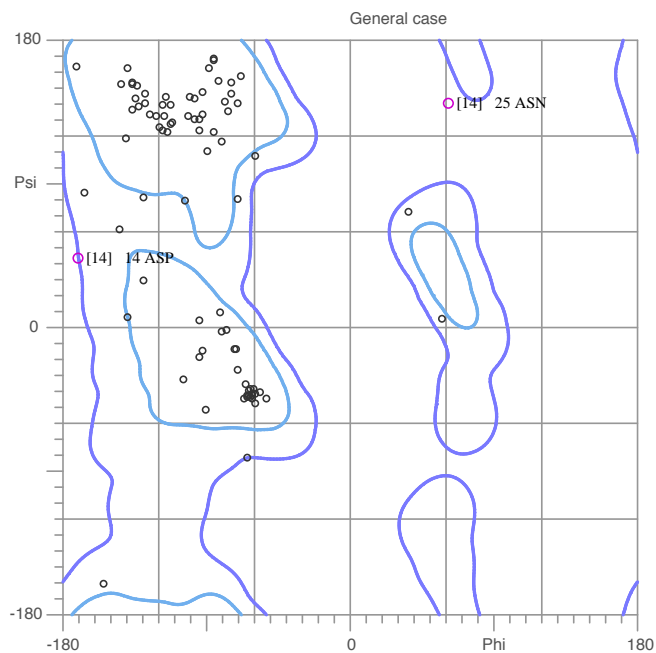
There were 2 outliers (phi, psi):
   [13]   12 LYS (57.2, 101.9)
   [13]   25 ASN (-175.2, -24.0)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 14

86.0% (80/93) of all residues were in favored (98%) regions.
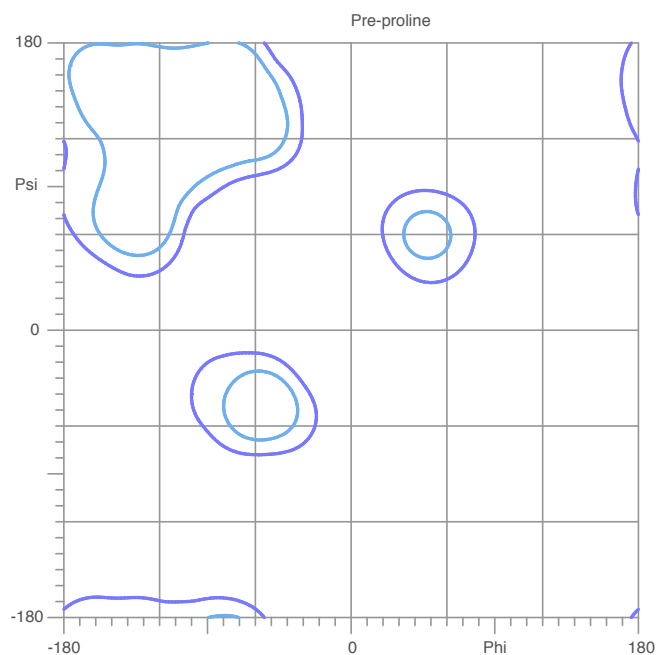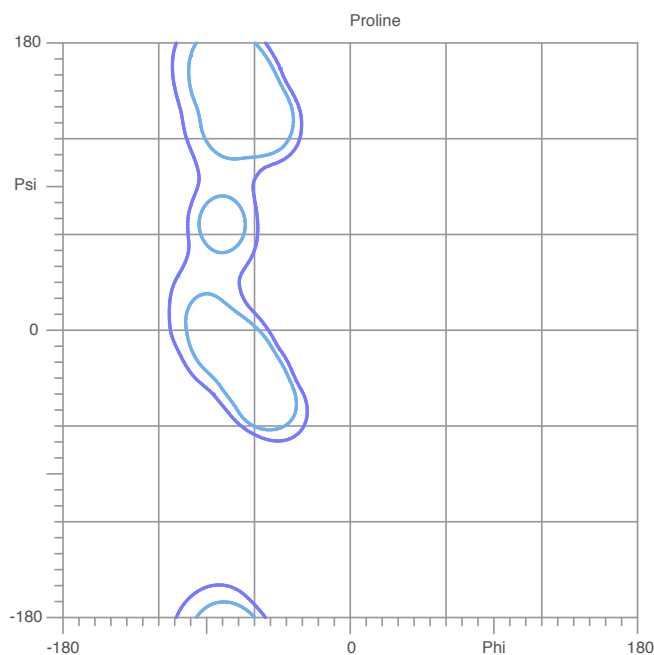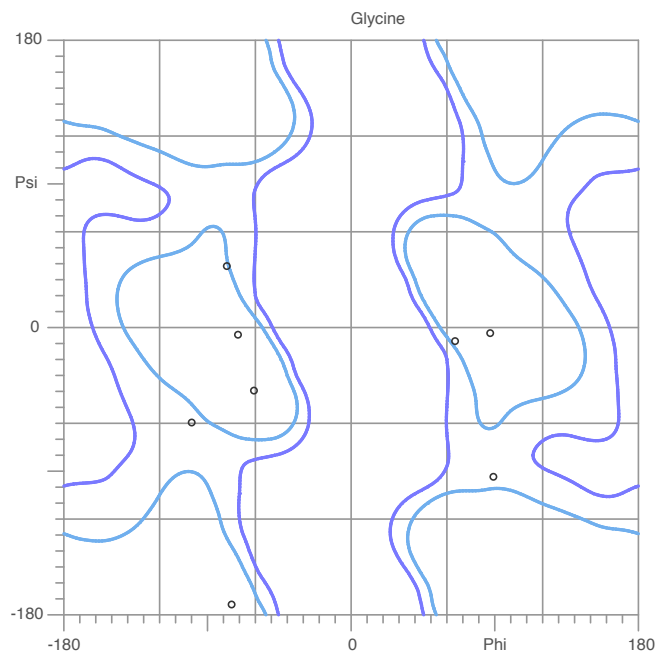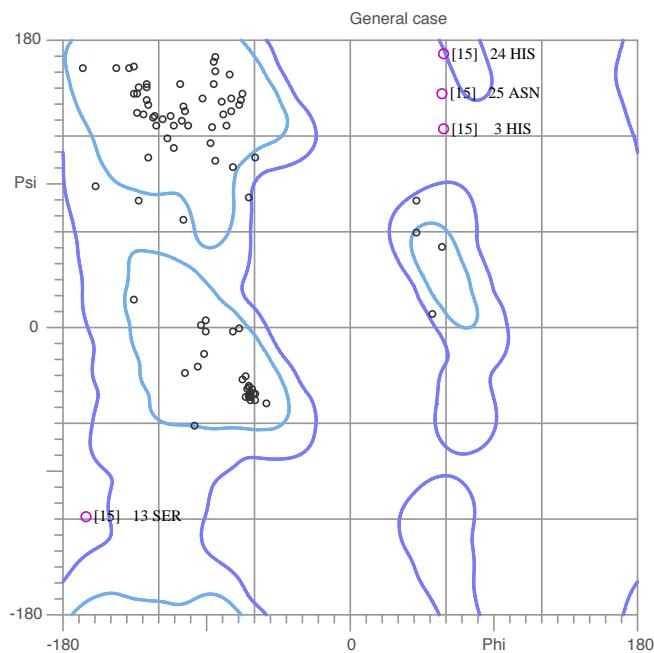97.8% (91/93) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
    [14]   14 ASP (-171.5, 44.5)
    [14]   25 ASN (61.2, 141.9)

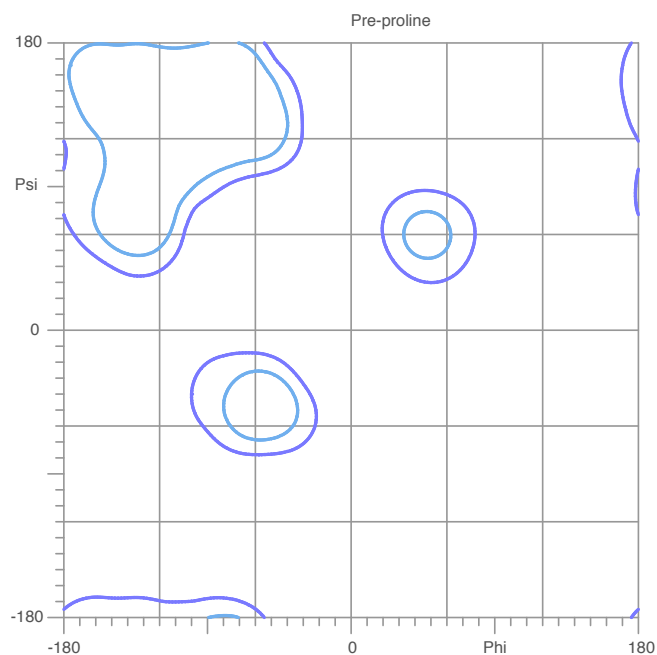# MolProbity Ramachandran analysis
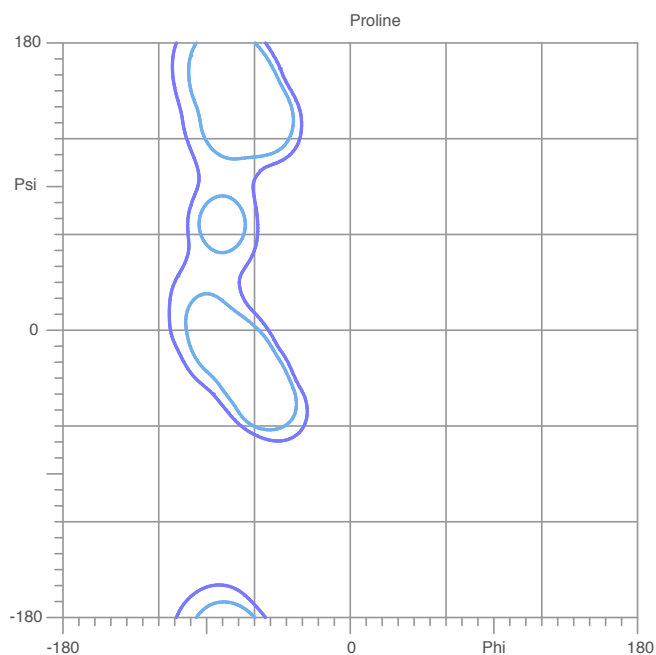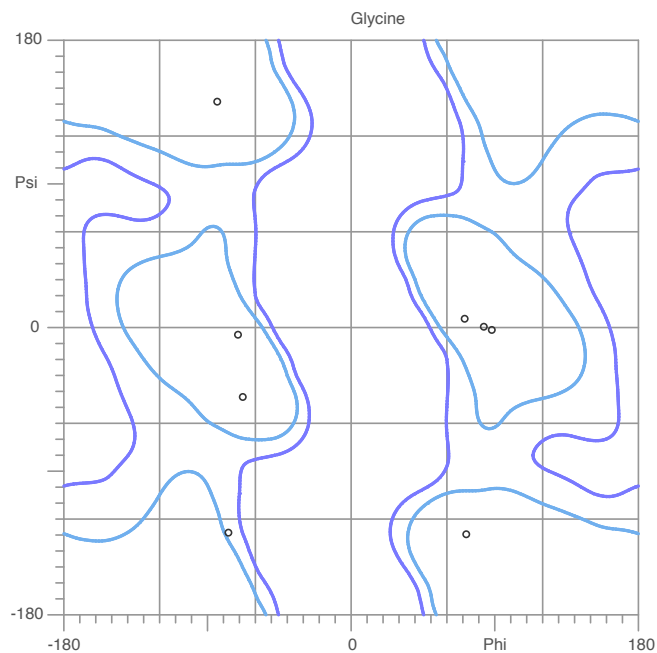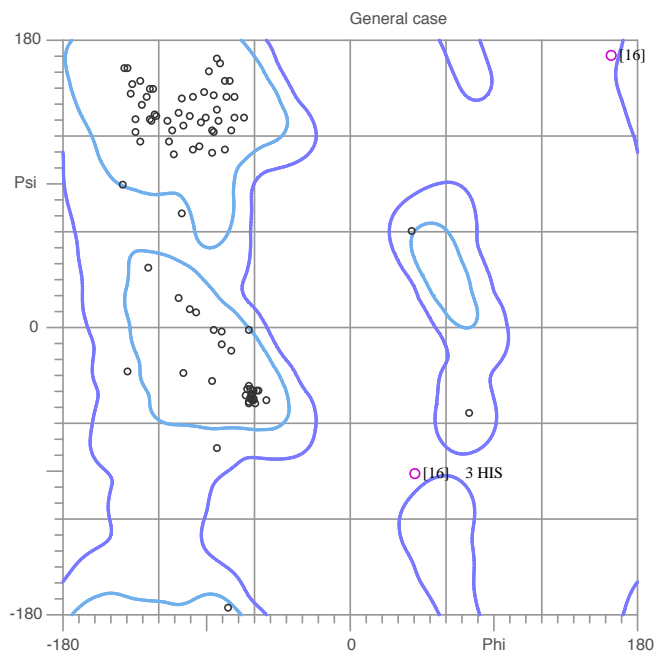
2KJR_NMR.pdb, model 15

84.9% (79/93) of all residues were in favored (98%) regions.
95.7% (89/93) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
     [15]   3 HIS (58.7, 125.5)
     [15]   13 SER (-166.3, -118.7)
     [15]   24 HIS (58.9, 172.8)
     [15]   25 ASN (58.0, 147.2)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 16

91.4% (85/93) of all residues were in favored (98%) regions.
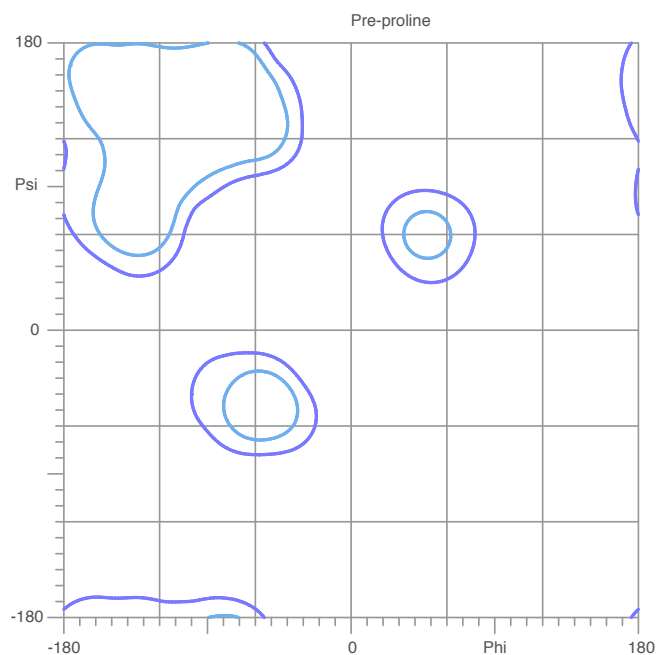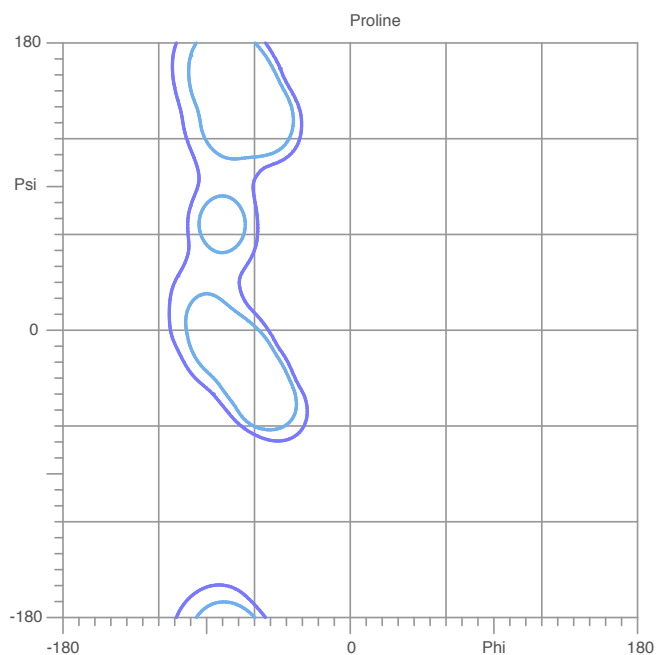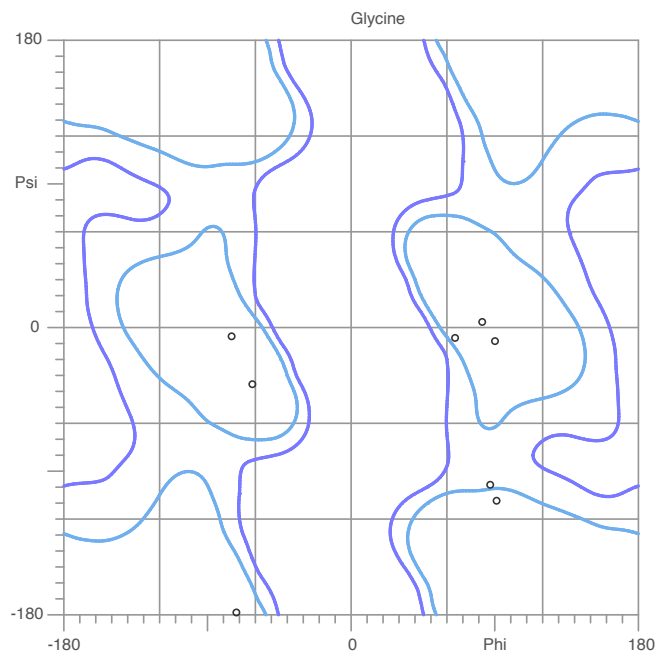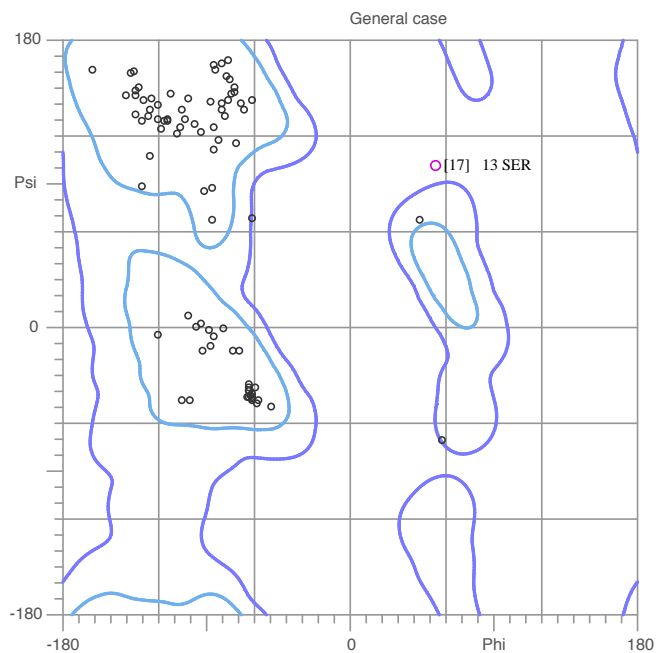97.8% (91/93) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
   [16]   3 HIS (40.9, -91.3)
   [16] 70 SER (163.9, 171.8)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 17

94.6% (88/93) of all residues were in favored (98%) regions.
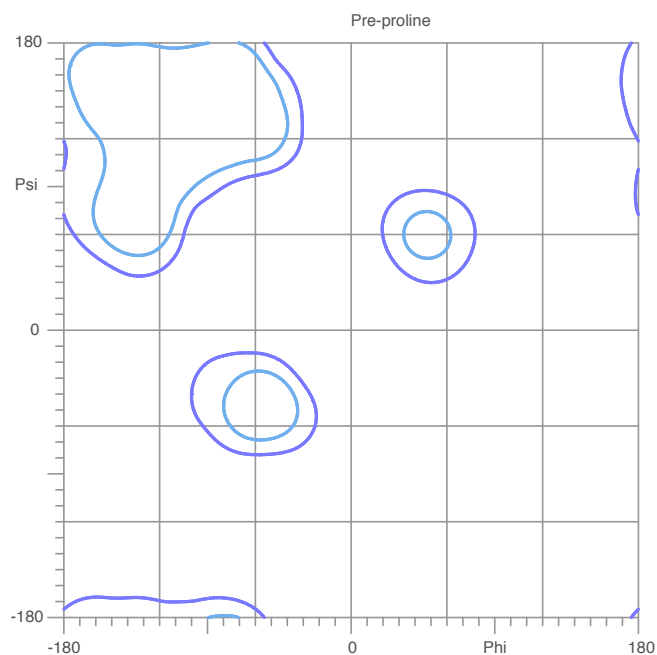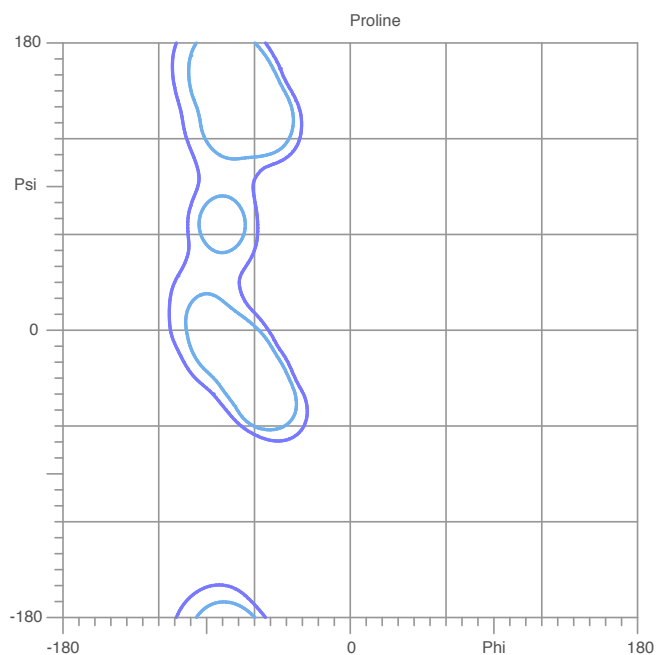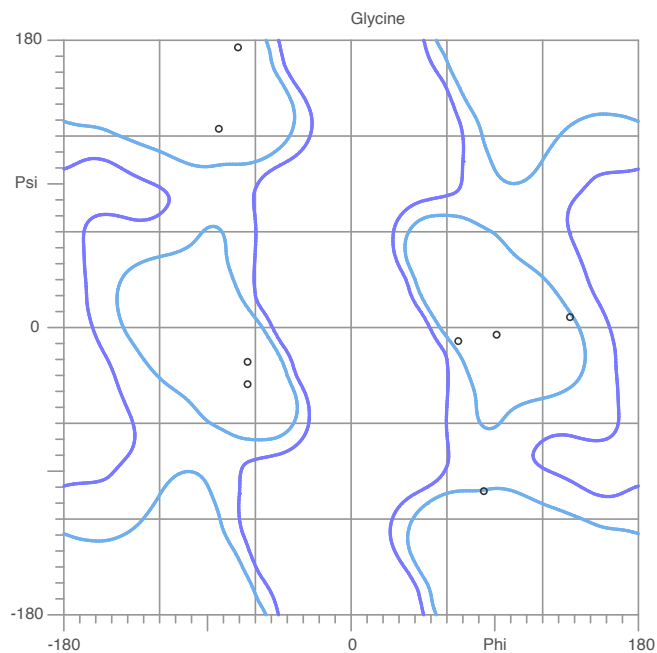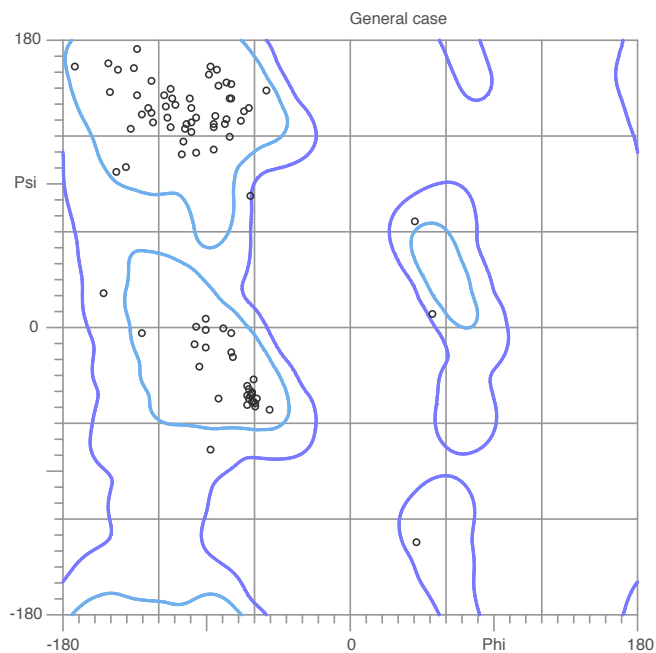98.9% (92/93) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
    [17]   13 SER (53.0, 102.6)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 18

93.5% (87/93) of all residues were in favored (98%) regions.
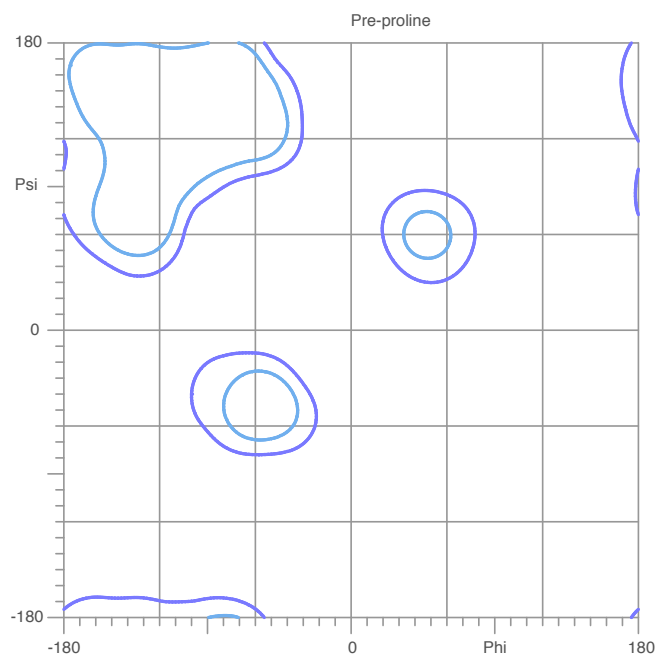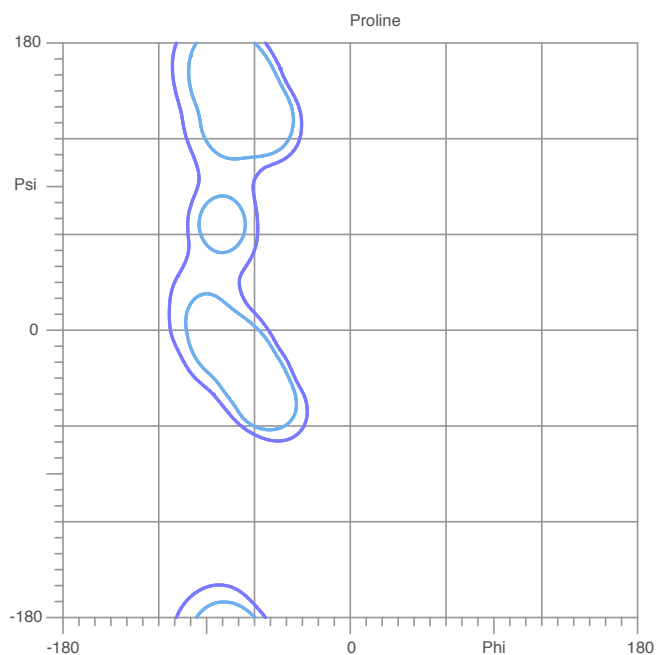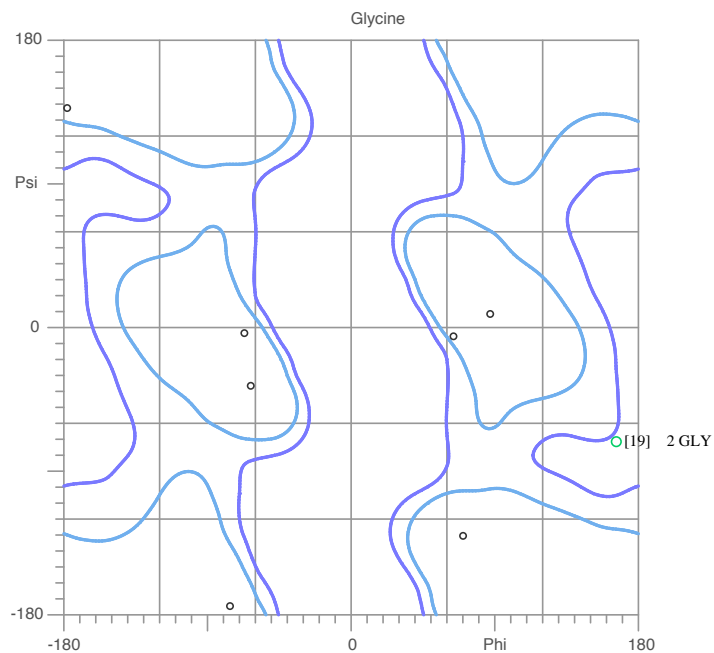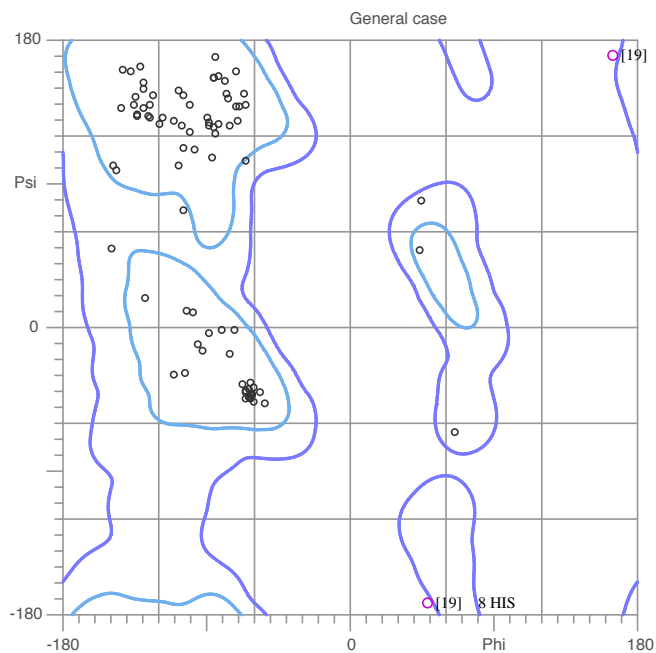100.0% (93/93) of all residues were in allowed (>99.8%) regions.

There were no outliers.

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 19

92.5% (86/93) of all residues were in favored (98%) regions.
96.8% (90/93) of all residues were in allowed (>99.8%) regions.

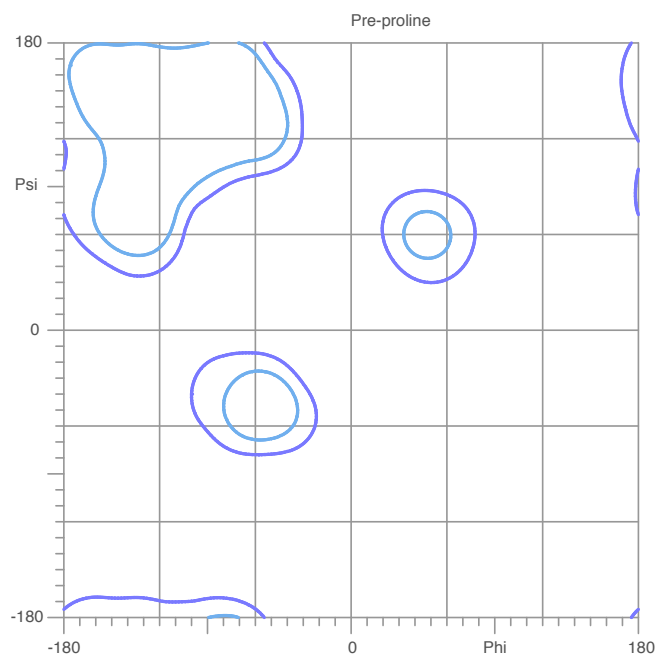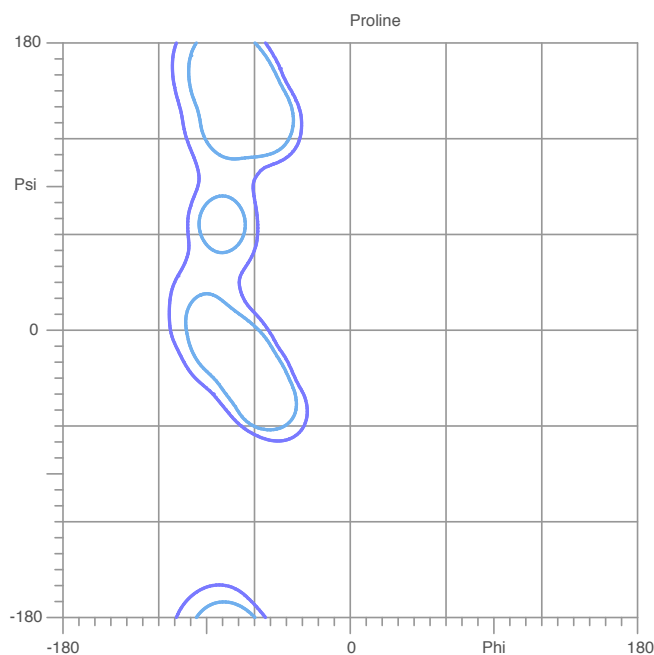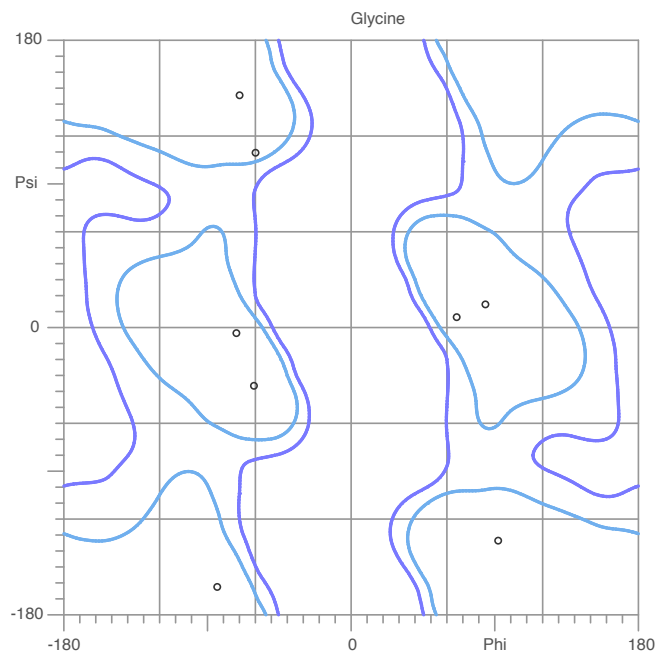There were 3 outliers (phi, psi):
    [19]   2 GLY (166.2, -71.2)
    [19]   8 HIS (48.3, -172.6)
    [19] 70 SER (164.2, 171.6)

MolProbity Ramachandran analysis

2KJR_NMR.pdb, model 20

87.1% (81/93) of all residues were in favored (98%) regions.
95.7% (89/93) of all residues were in allowed (>99.8%) regions.
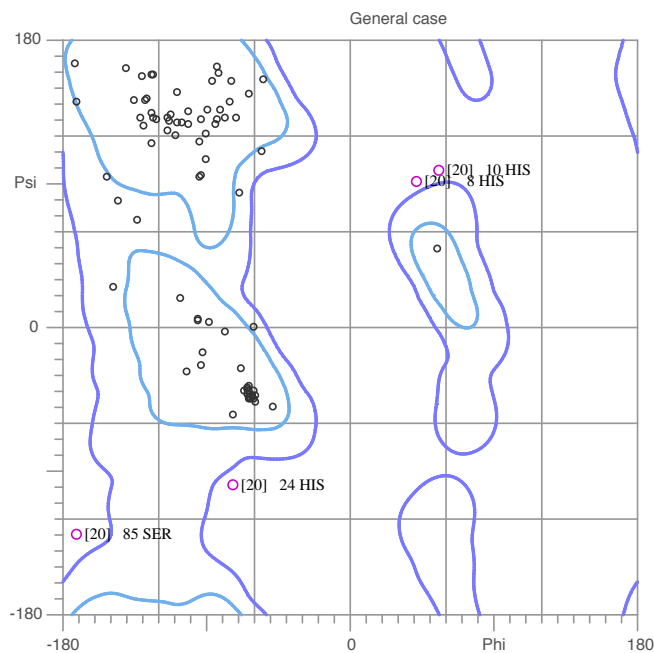
There were 4 outliers (phi, psi):
    [20]   8 HIS (41.5, 92.6)
    [20] 10 HIS (55.1, 99.9)
    [20] 24 HIS (-74.9, -98.3)
    [20] 85 SER (-172.7, -129.8)

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