MolProbity Ramachandran analysis

2KIW_NMR.pdb, all models

General case

Glycine

Proline

Pre-proline
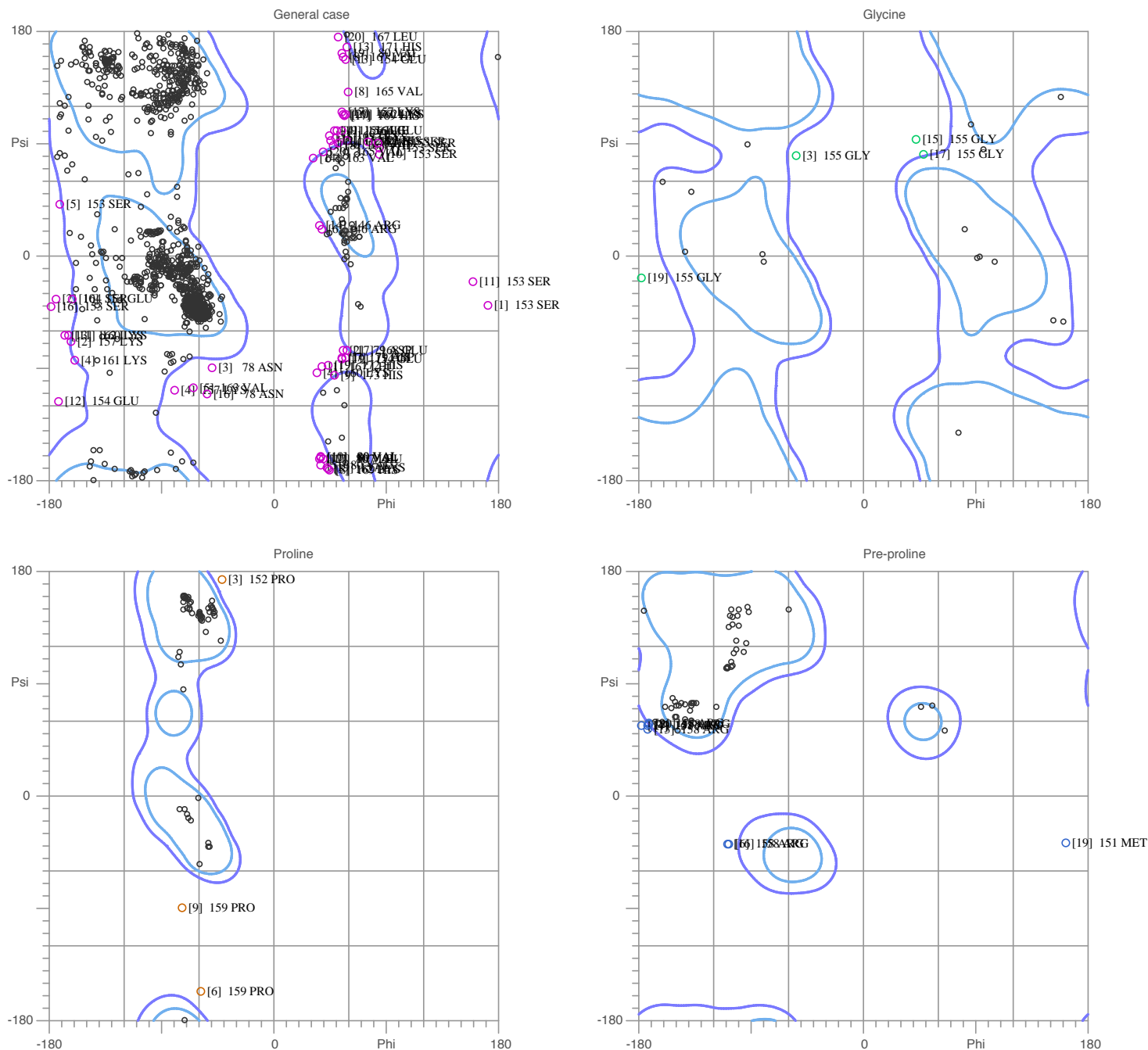
91.3% (1990/2180) of all residues were in favored (98%) regions.
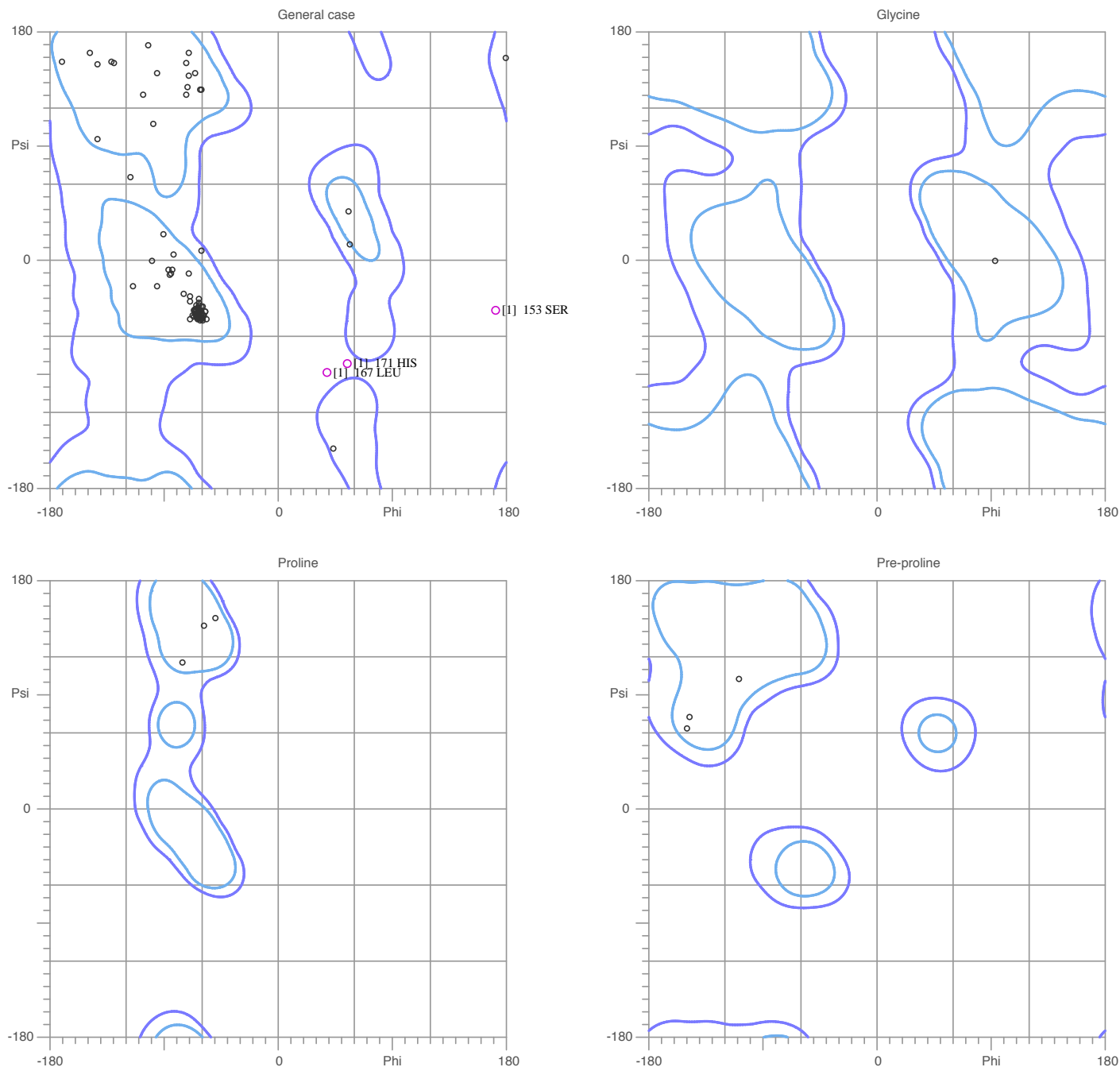96.6% (2106/2180) of all residues were in allowed (>99.8%) regions.

There were 74 outliers (phi, psi):
[1] 153 SER (171.0, -39.9)
[1] 167 LEU (38.0, -88.6)
[1] 171 HIS (54.1, -81.1)
[2] 79 ASP (55.8, -75.5)
[2] 157 LYS (-164.0, -68.3)
[2] 164 SER (-175.3, -34.4)
[3] 78 ASN (-50.8, -89.2)
[3] 152 PRO (-43.0, 174.2)
[3] 155 GLY (-54.2, 81.5)
[3] 162 LYS (43.5, -170.3)
[3] 169 HIS (44.4, 97.3)
[4] 151 MET (-173.9, 57.8)
[4] 156 ILE (50.6, 101.7)
[4] 157 LYS (-80.5, -107.9)
[4] 160 LYS (35.0, -93.1)
[4] 161 LYS (-161.0, -83.2)
[5] 80 VAL (37.7, -167.4)
[5] 153 SER (-172.5, 42.2)
[5] 163 VAL (-65.1, -105.4)
[6] 146 ARG (38.4, 22.6)
[6] 157 LYS (49.2, 95.8)
[6] 158 ARG (-108.3, -38.1)
[6] 159 PRO (-59.6, -156.5)
[7] 79 ASP (58.0, -81.3)
[7] 153 SER (84.4, 87.1)
[8] 165 VAL (89.4, 133.0)
[8] 167 LEU (55.6, 160.5)
[8] 169 HIS (44.3, -171.3)
[9] 158 ARG (-172.8, 59.2)
[9] 159 PRO (-74.9, -89.6)
[9] 173 HIS (48.3, -95.1)
[10] 80 VAL (37.3, -160.2)
[10] 153 SER (84.7, 82.3)
[10] 154 GLU (-162.8, -34.6)
[11] 80 VAL (37.1, -161.3)

[11] 153 SER (159.2, -20.6)
[11] 160 LYS (-165.4, -63.8)
[11] 166 GLU (54.7, 101.2)
[11] 172 HIS (58.7, 93.6)
[12] 80 VAL (36.9, -162.6)
[12] 154 GLU (-173.2, -116.7)
[12] 162 LYS (45.5, 93.8)
[13] 154 GLU (57.2, 158.9)
[13] 158 ARG (-173.7, 54.1)
[13] 162 LYS (-168.5, -63.6)
[13] 171 HIS (58.6, 168.4)
[14] 146 ARG (36.6, 25.5)
[14] 153 SER (75.9, 92.9)
[14] 158 ARG (-178.9, 57.9)
[14] 163 VAL (31.6, 79.3)
[14] 170 HIS (51.6, 91.7)
[15] 155 GLY (42.5, 94.6)
[16] 78 ASN (-54.4, -110.7)
[16] 153 SER (-179.7, -40.1)
[16] 158 ARG (-109.0, -38.1)
[16] 161 LYS (55.8, 114.4)
[17] 155 GLY (48.8, 82.4)
[17] 157 LYS (54.9, 116.9)
[17] 167 LEU (39.9, -163.0)
[17] 168 GLU (58.8, -75.7)
[17] 169 HIS (56.6, 113.0)
[18] 163 VAL (47.3, 90.0)
[19] 80 VAL (54.7, 163.1)
[19] 151 MET (162.5, -37.9)
[19] 154 GLU (54.1, -82.6)
[19] 155 GLY (-178.4, -17.7)
[19] 156 ILE (48.7, 101.0)
[19] 157 LYS (42.1, -169.1)
[19] 172 HIS (44.0, -97.8)
[20] 153 SER (83.3, 91.9)
[20] 158 ARG (-172.3, 58.5)
[20] 162 LYS (57.2, 114.6)
[20] 165 VAL (40.0, 84.1)
[20] 167 LEU (51.0, 176.2)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 1
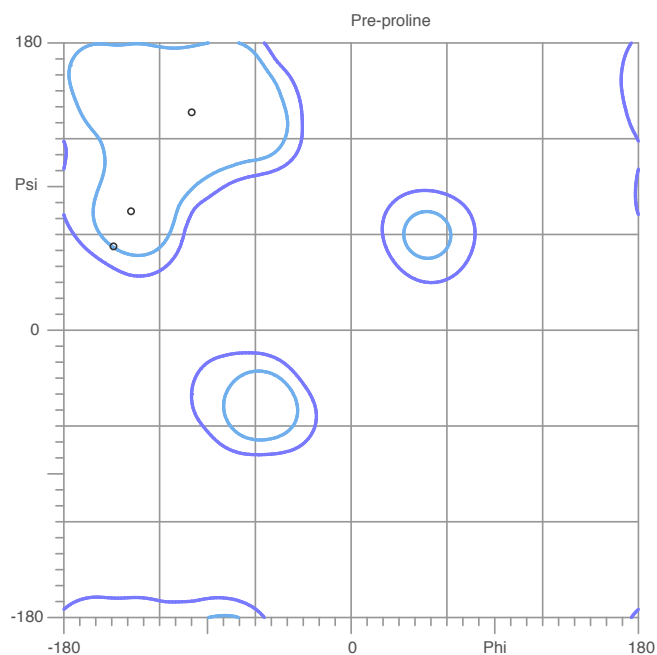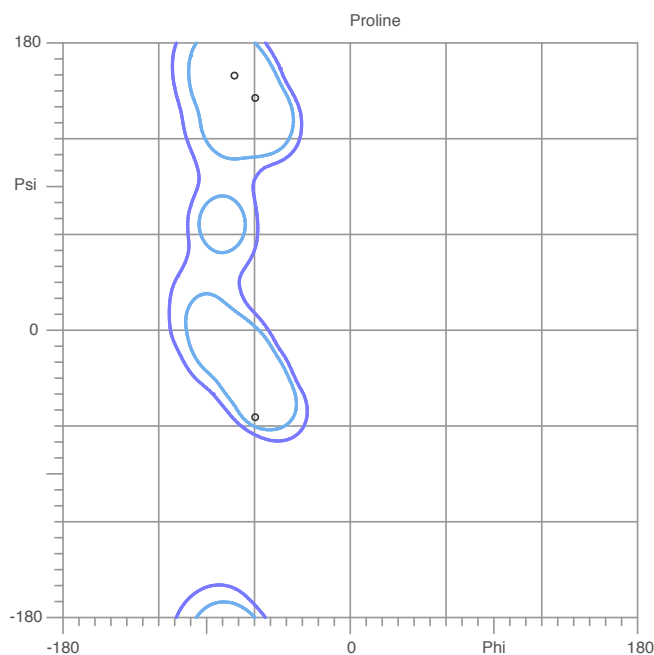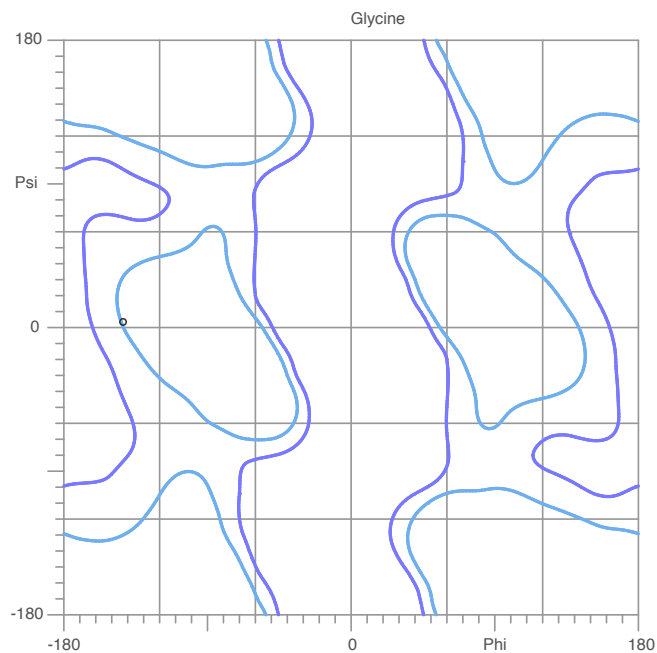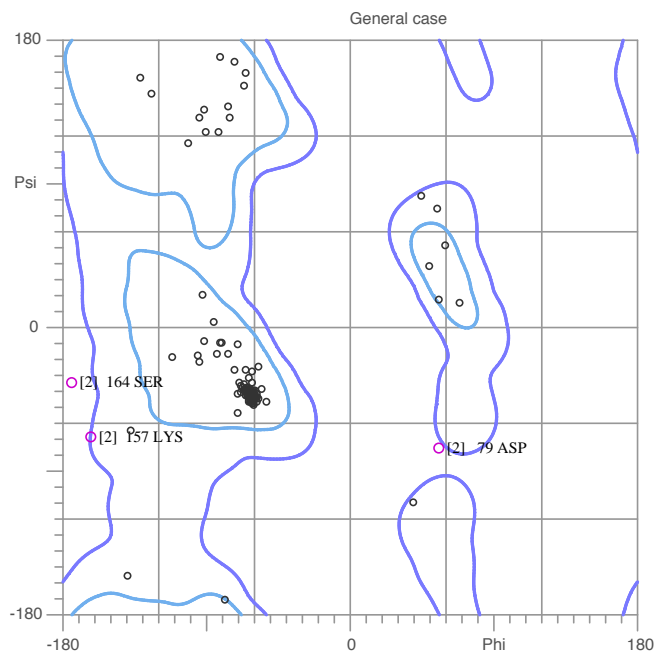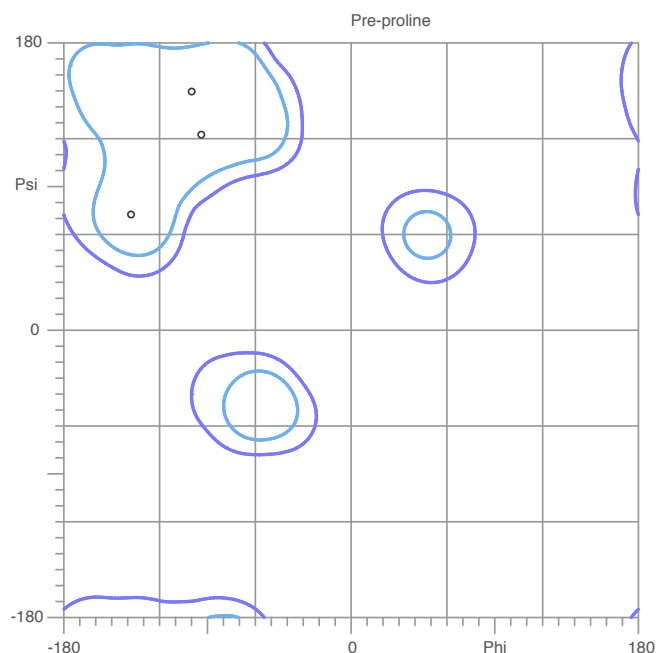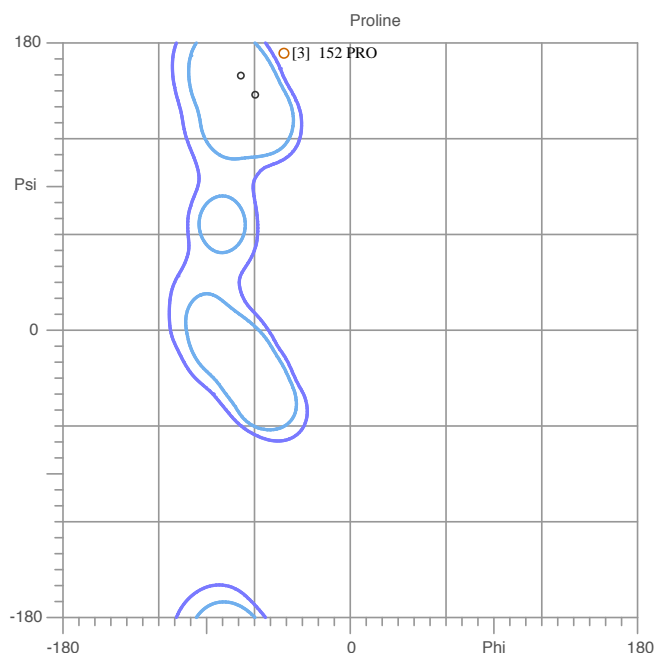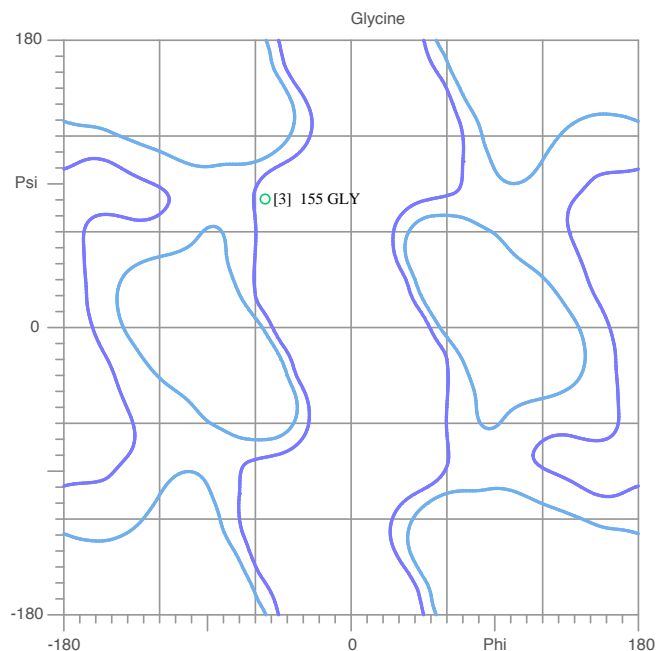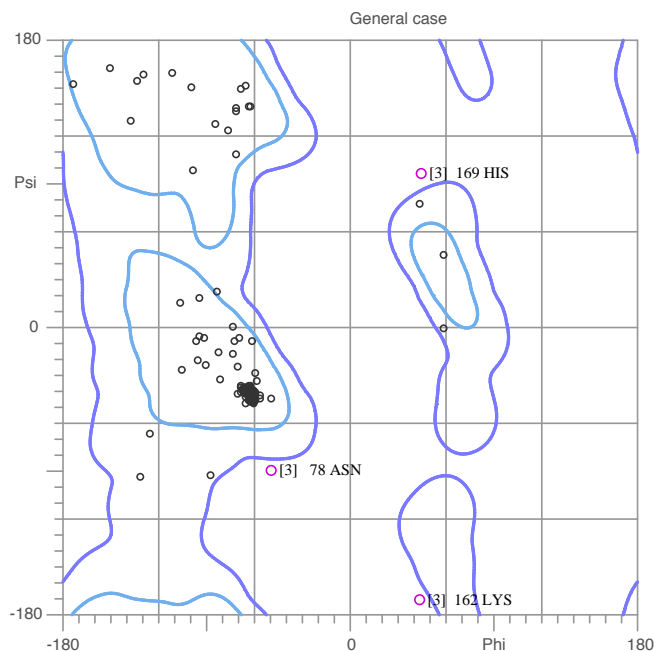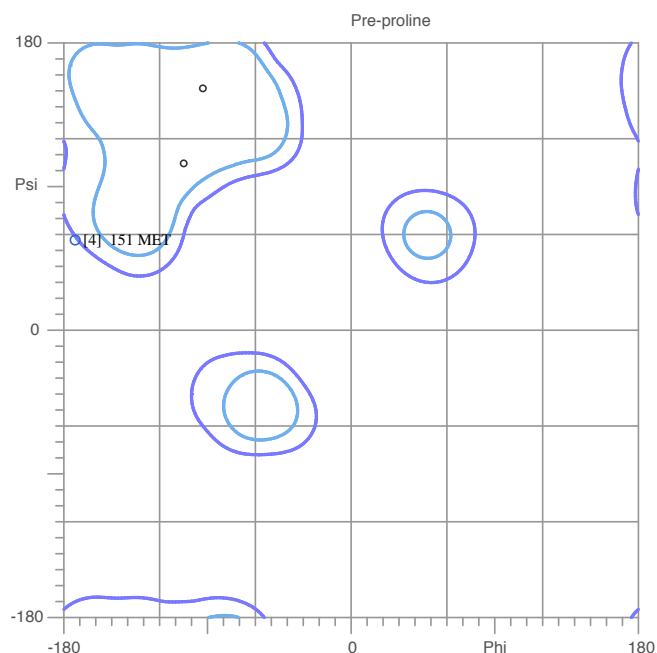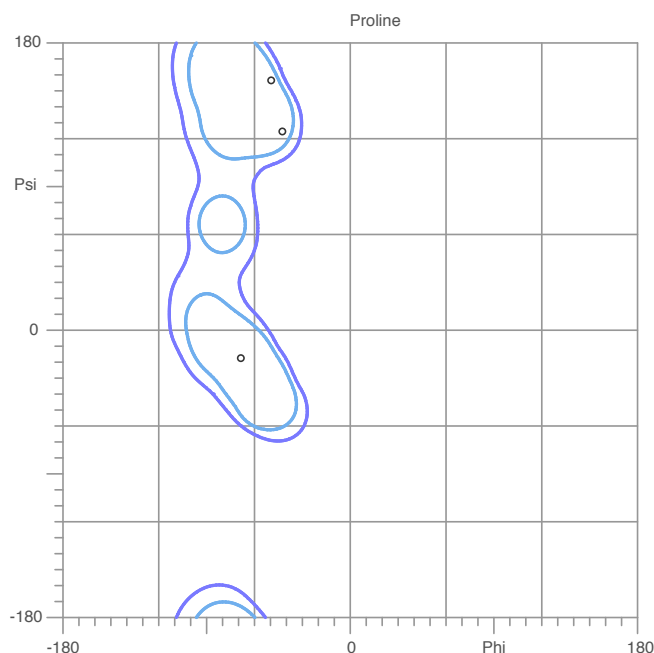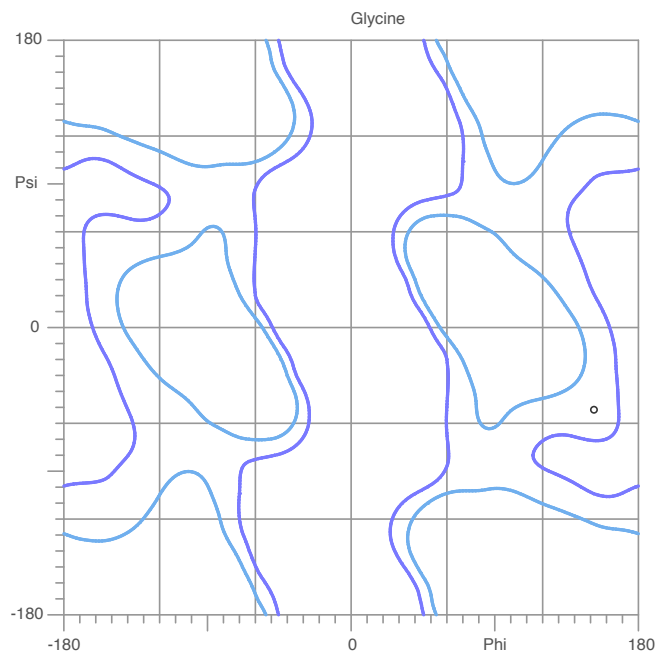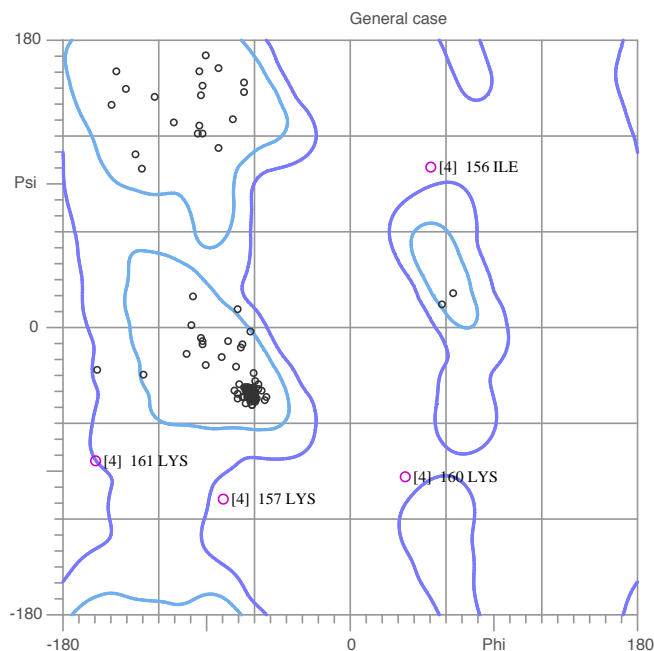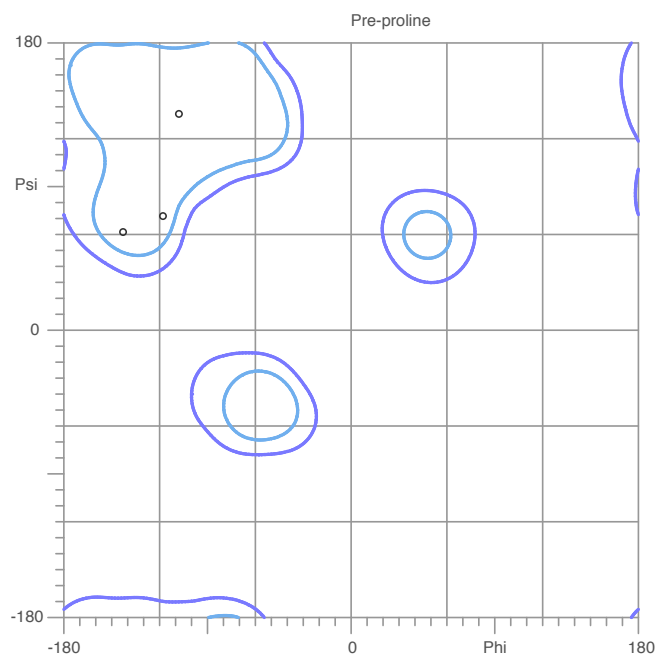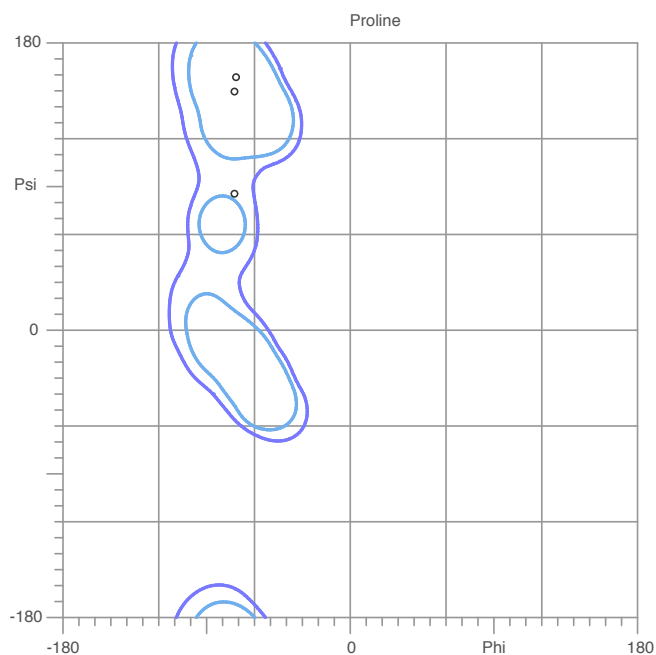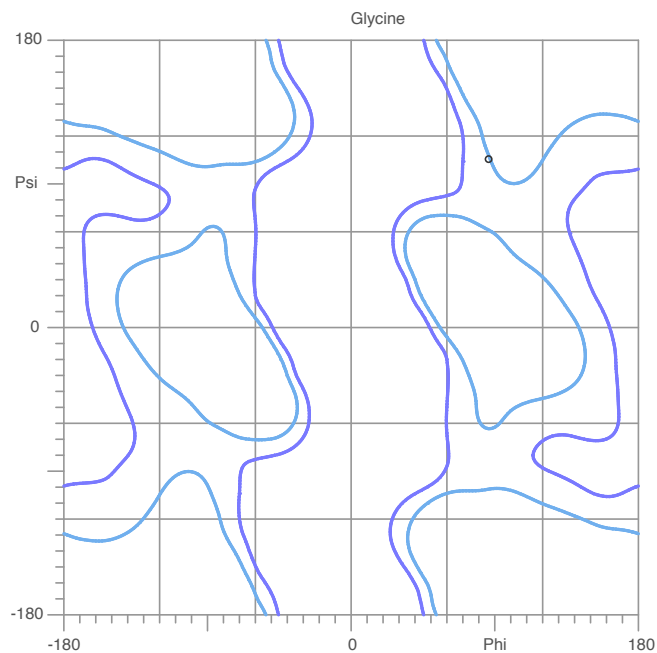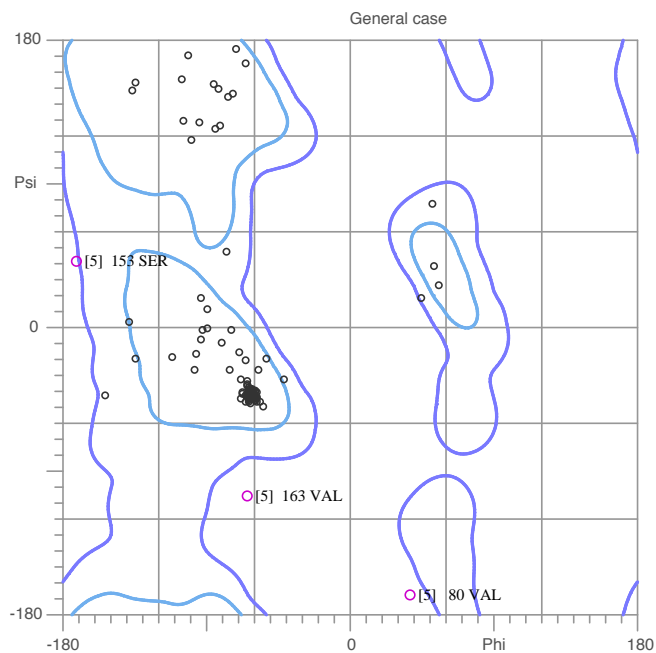
General case

Glycine

Proline

Pre-proline

92.7% (101/109) of all residues were in favored (98%) regions.

97.2% (106/109) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
    [1] 153 SER (171.0, -39.9)
    [1] 167 LEU (38.0, -88.6)
    [1] 171 HIS (54.1, -81.1)

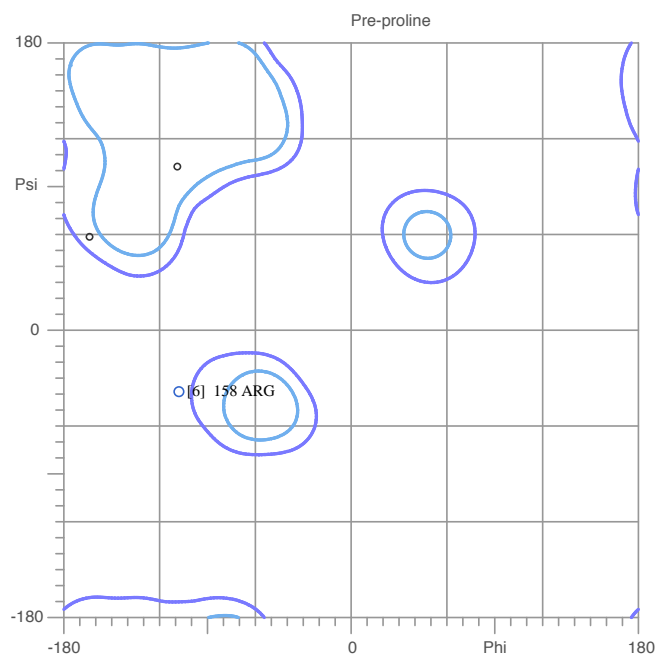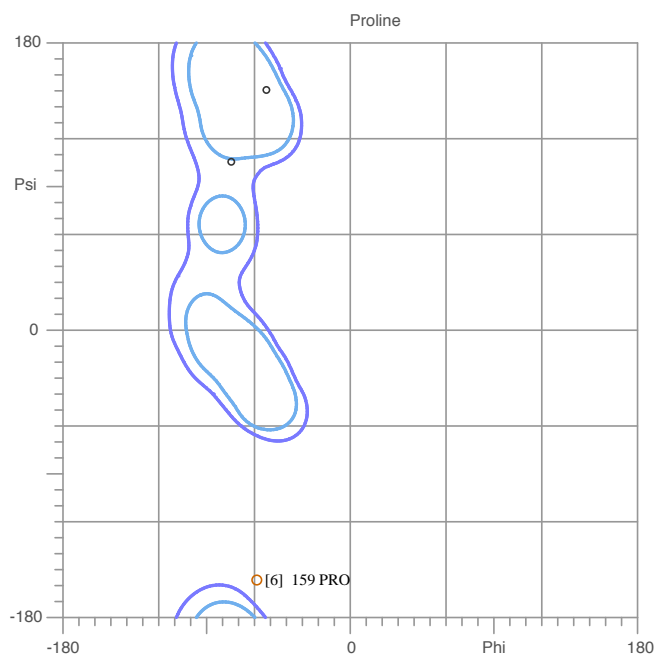# MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 2

92.7% (101/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
  [2] 79 ASP (55.8, -75.5)
  [2] 157 LYS (-164.0, -68.3)
  [2] 164 SER (-175.3, -34.4)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 3

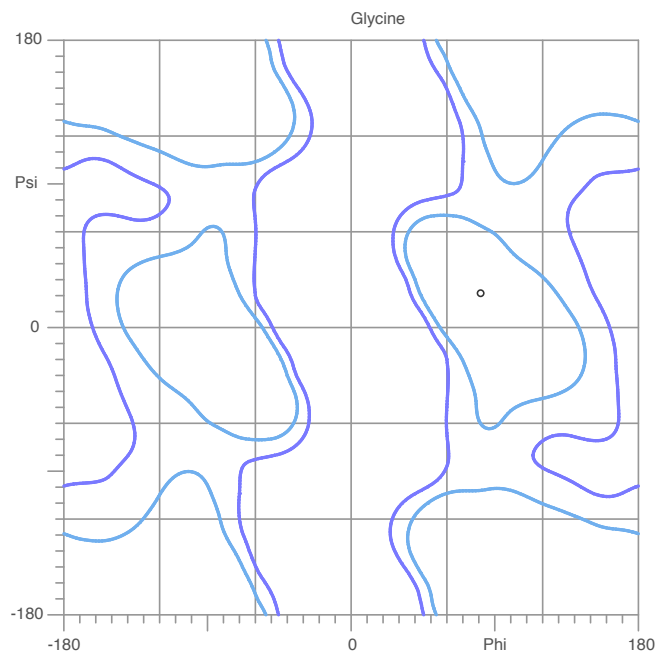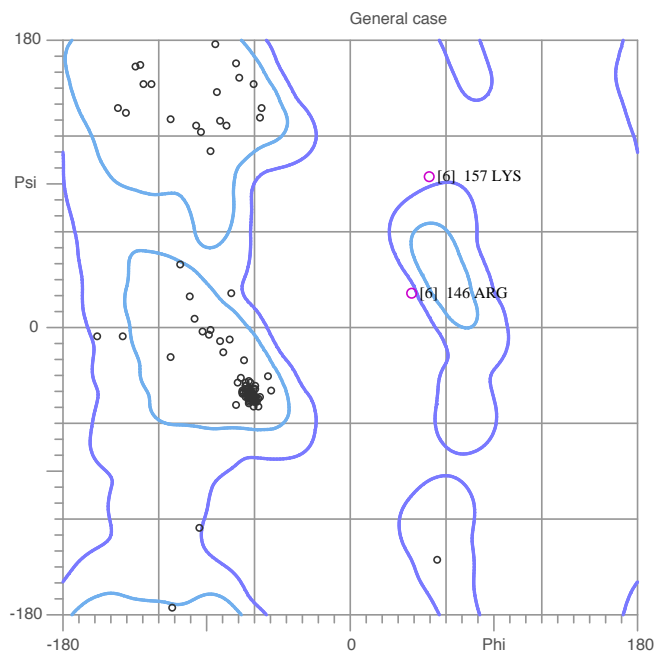General case

Glycine
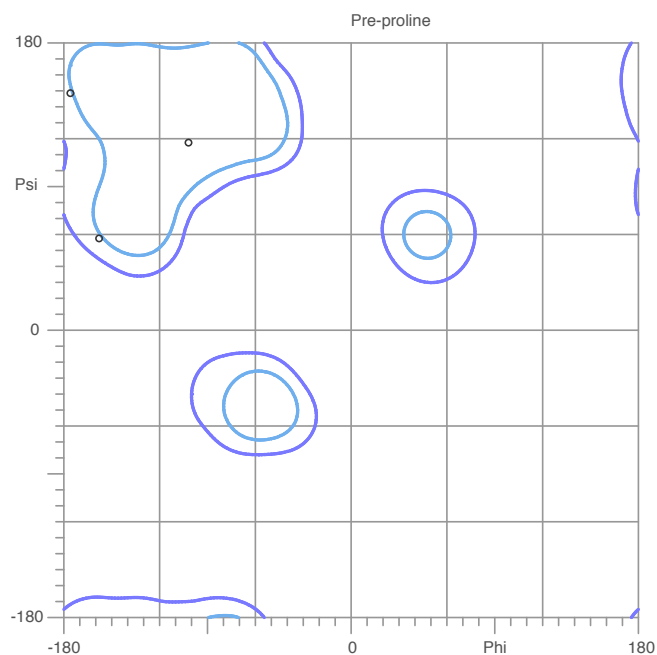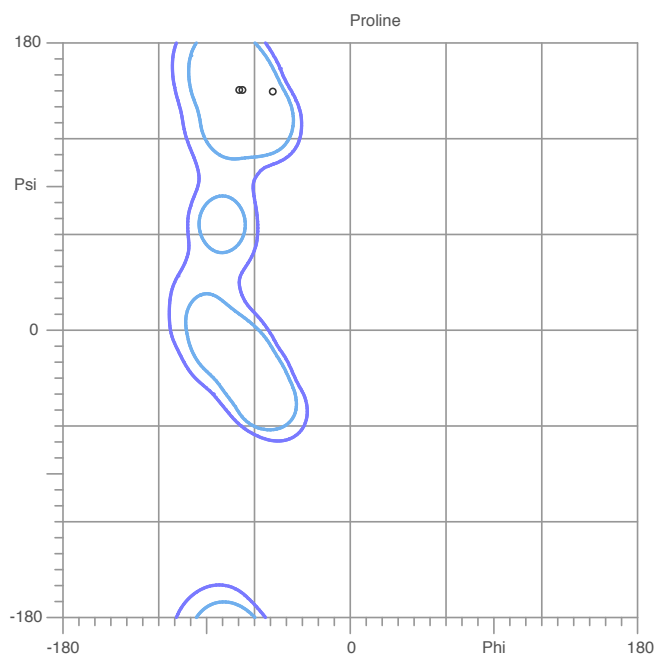

Proline

Pre-proline

89.9% (98/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[3] 78 ASN (-50.8, -89.2)
[3] 152 PRO (-43.0, 174.2)
[3] 155 GLY (-54.2, 81.5)
[3] 162 LYS (43.5, -170.3)
[3] 169 HIS (44.4, 97.3)

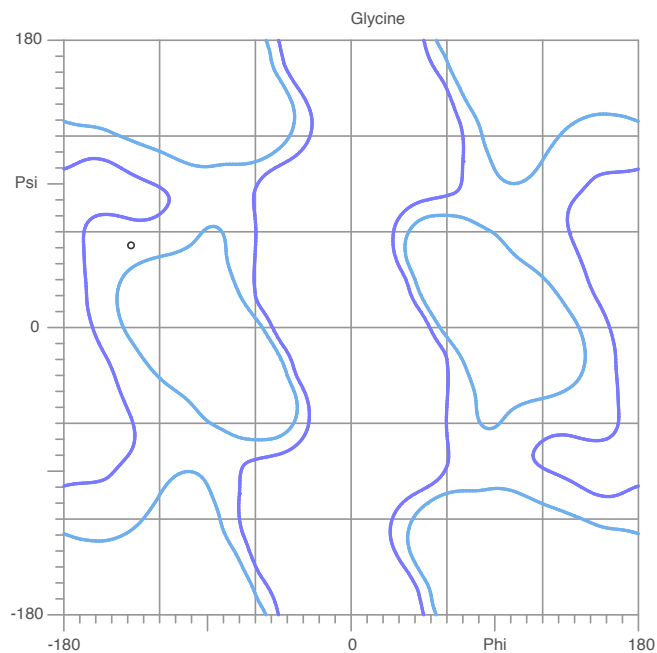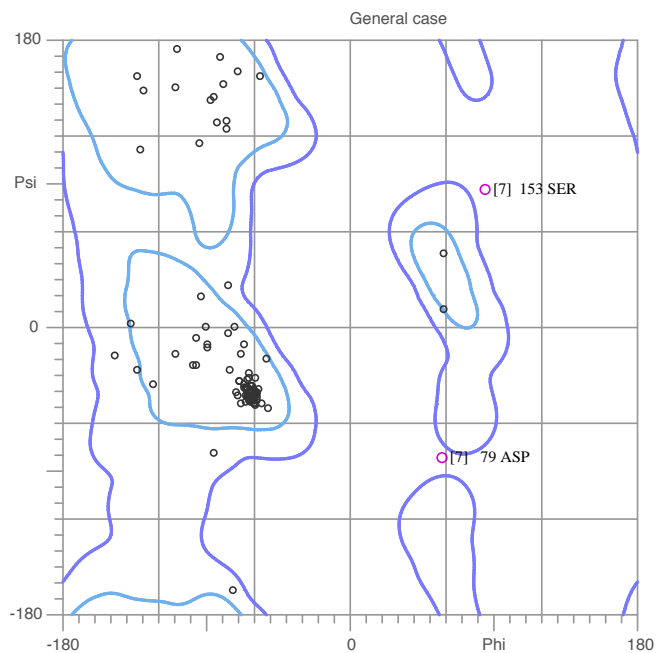# MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 4

92.7% (101/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[4] 151 MET (-173.9, 57.8)
[4] 156 ILE (50.6, 101.7)
[4] 157 LYS (-80.5, -107.9)
[4] 160 LYS (35.0, -93.1)
[4] 161 LYS (-161.0, -83.2)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 5

89.9% (98/109) of all residues were in favored (98%) regions.

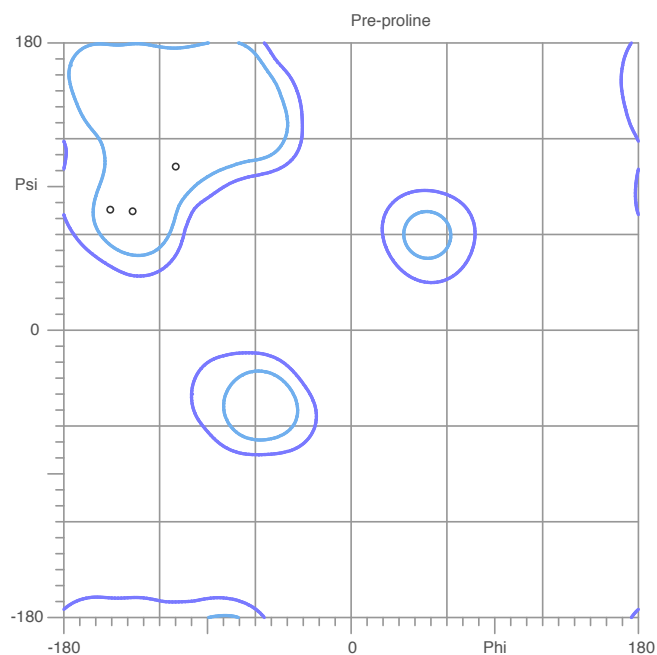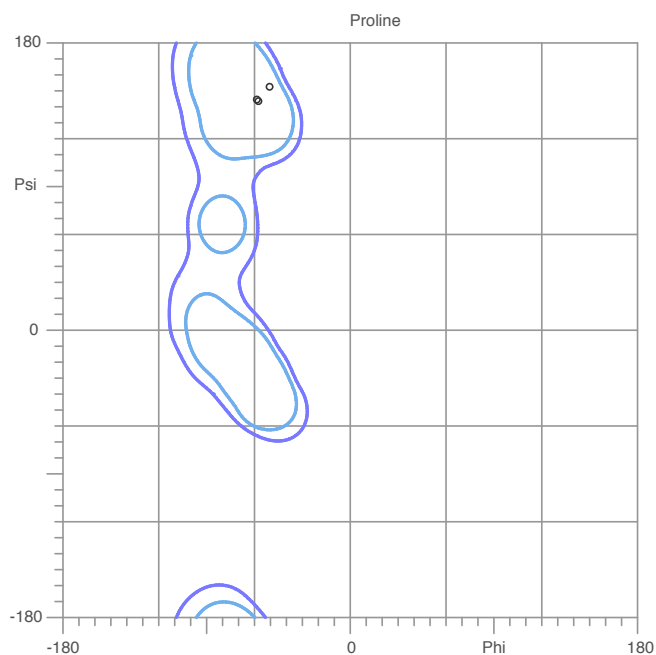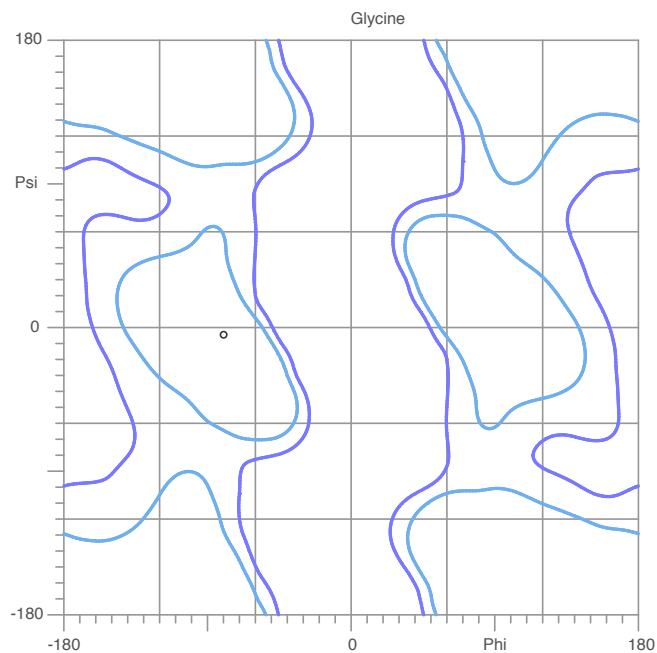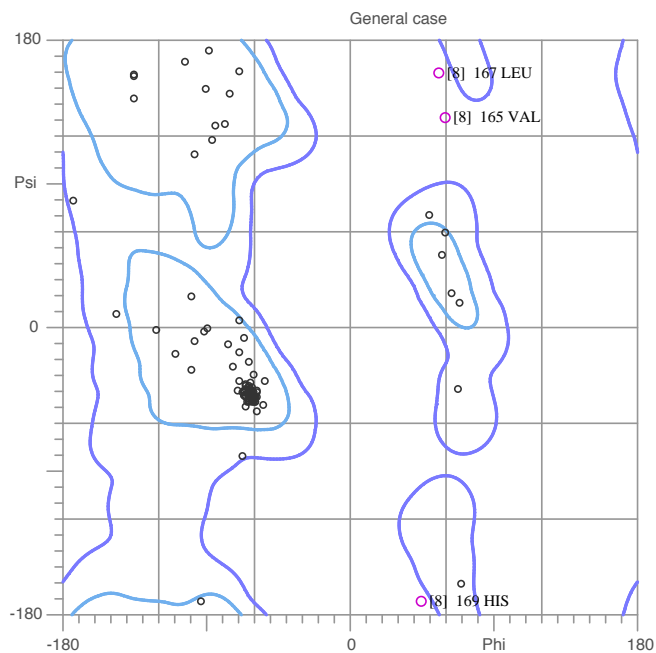97.2% (106/109) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):

    [5]   80 VAL (37.7, -167.4)

    [5] 153 SER (-172.5, 42.2)

    [5] 163 VAL (-65.1, -105.4)

MolProbity Ramachandran analysis

89.9% (98/109) of all residues were in favored (98%) regions.
96.3% (105/109) of all residues were in allowed (>99.8%) regions.
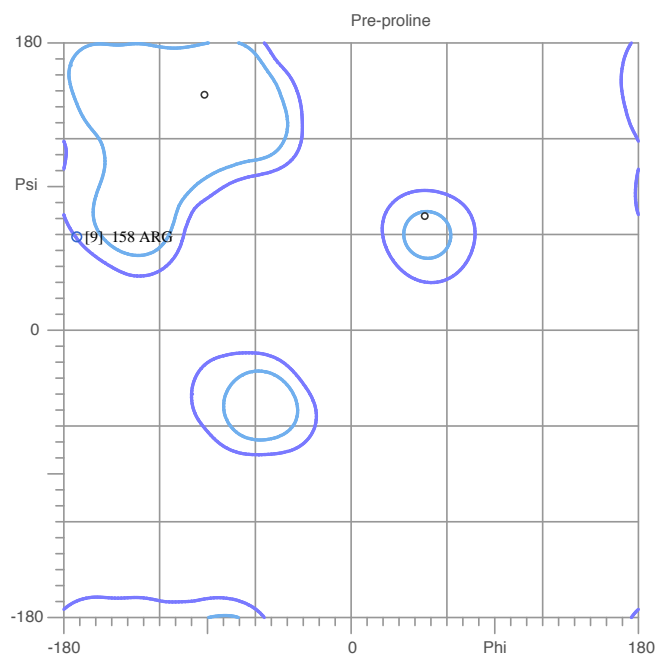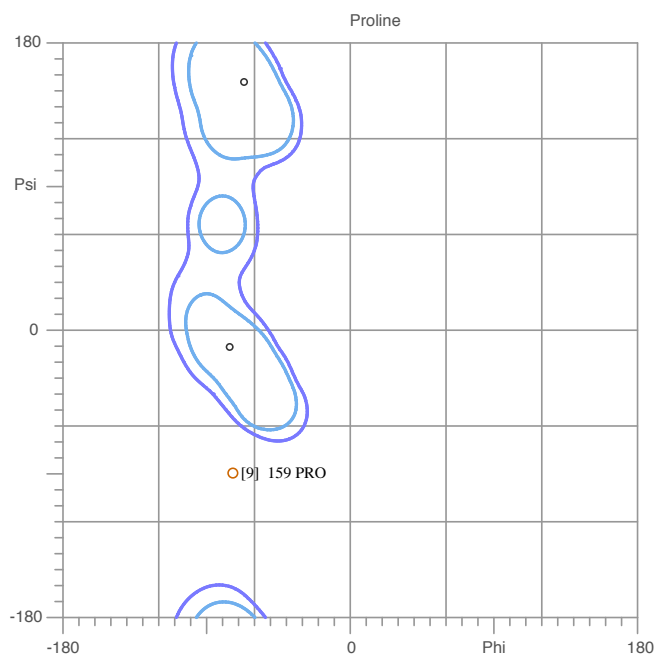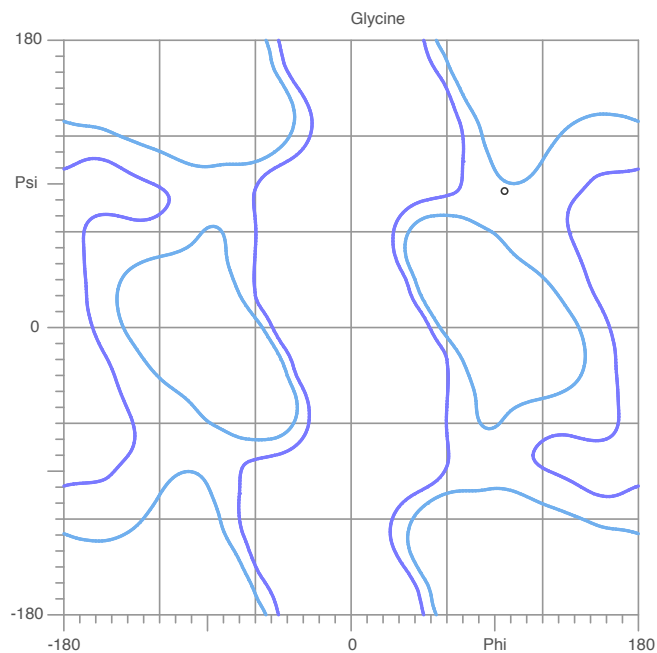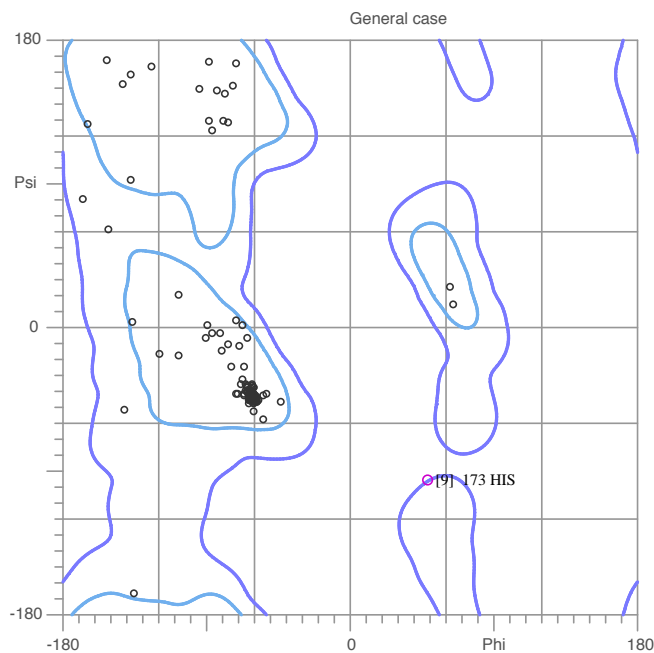
There were 4 outliers (phi, psi):
    [6] 146 ARG (38.4, 22.6)
    [6] 157 LYS (49.2, 95.8)
    [6] 158 ARG (-108.3, -38.1)
    [6] 159 PRO (-59.6, -156.5)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 7

89.9% (98/109) of all residues were in favored (98%) regions.
98.2% (107/109) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
    [7]   79 ASP (58.0, -81.3)
    [7] 153 SER (84.4, 87.1)

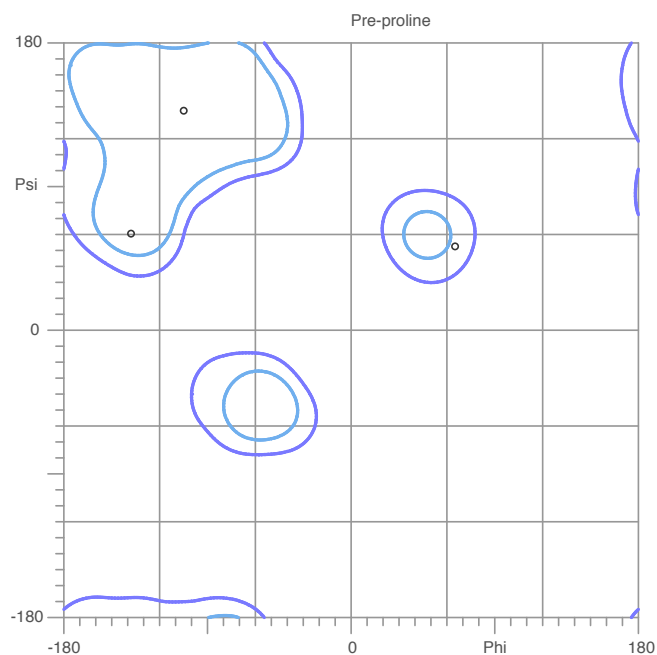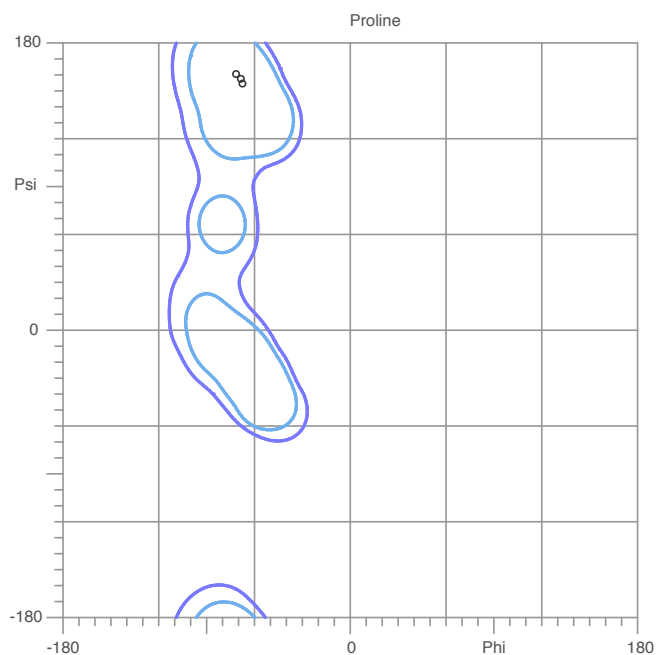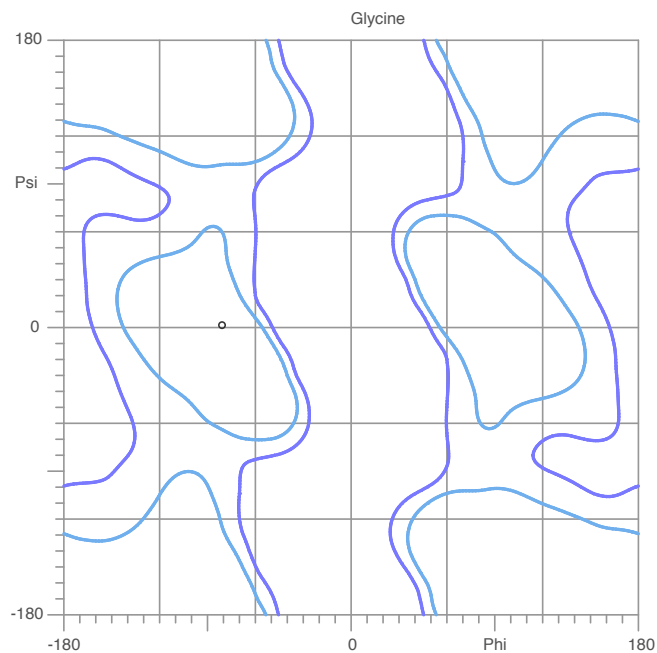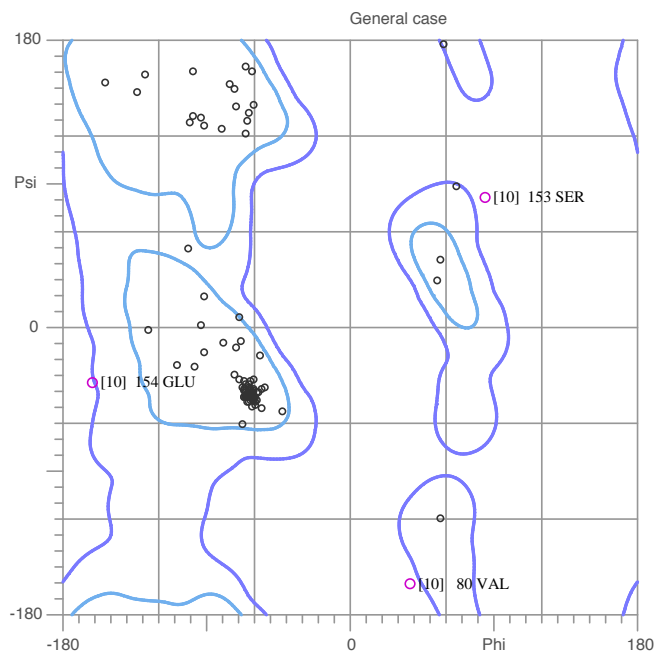# MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 8

91.7% (100/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
  [8] 165 VAL (59.4, 133.0)
  [8] 167 LEU (55.6, 160.5)
  [8] 169 HIS (44.3, -171.3)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 9

92.7% (101/109) of all residues were in favored (98%) regions.

97.2% (106/109) of all residues were in allowed (>99.8%) regions.
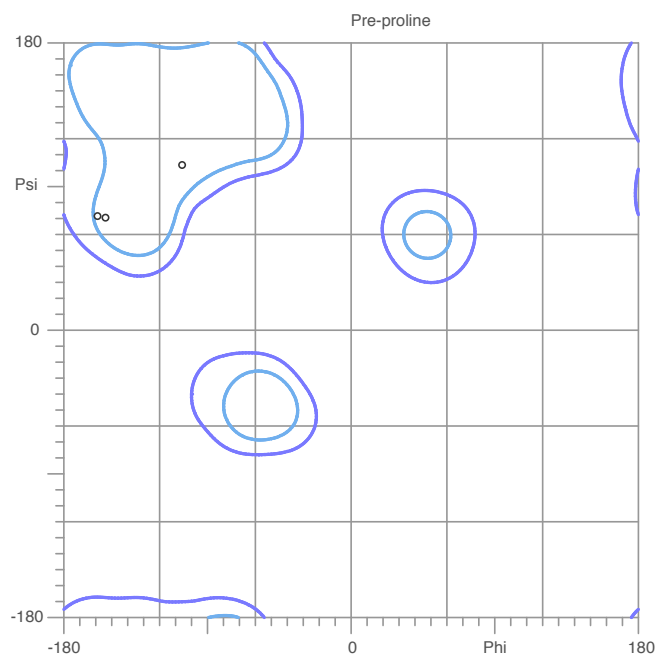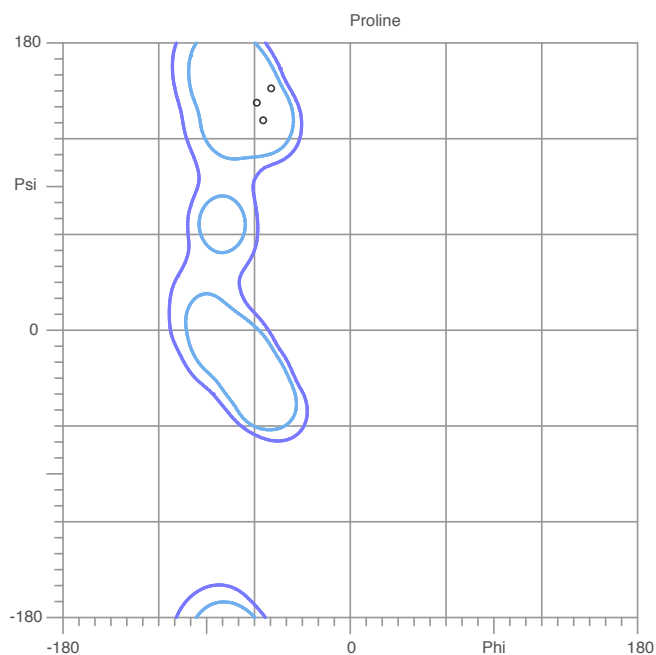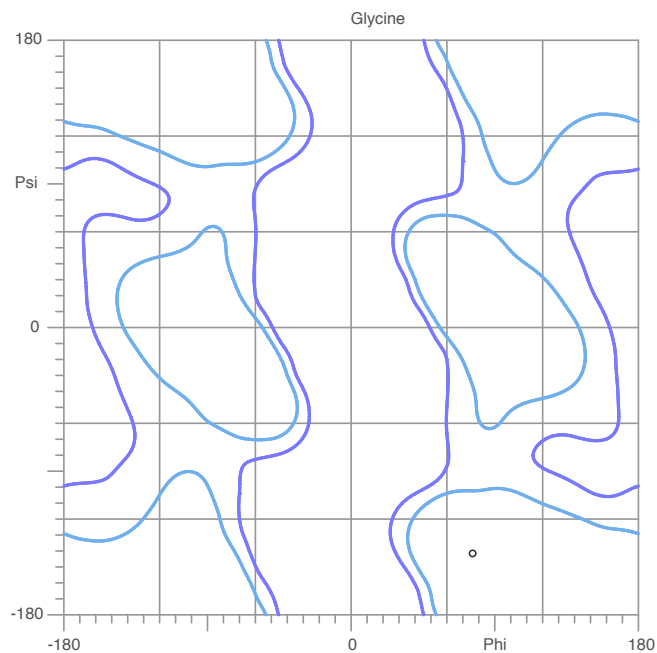
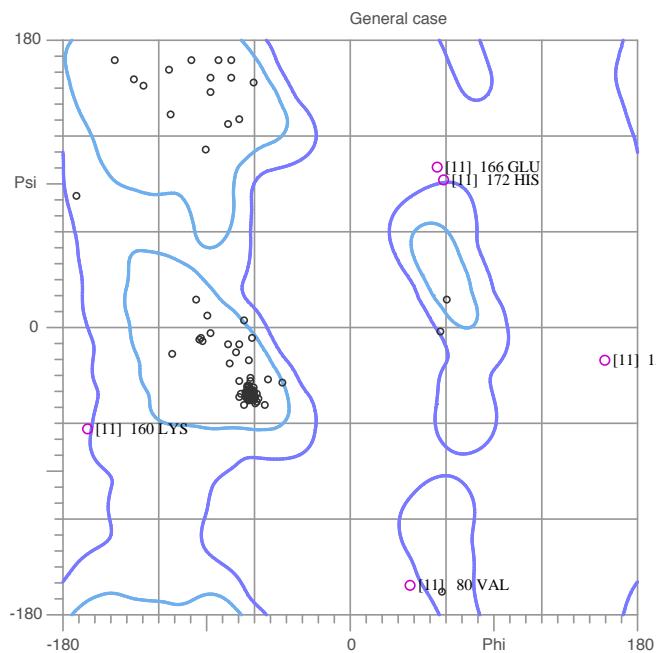There were 3 outliers (phi, psi):

    [9] 158 ARG (-172.8, 59.2)

    [9] 159 PRO (-74.9, -89.8)

    [9] 173 HIS (48.3, -95.1)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 10

92.7% (101/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
    [10]   80 VAL (37.3, -160.2)
    [10] 153 SER (84.7, 82.3)
    [10] 154 GLU (-162.8, -34.6)

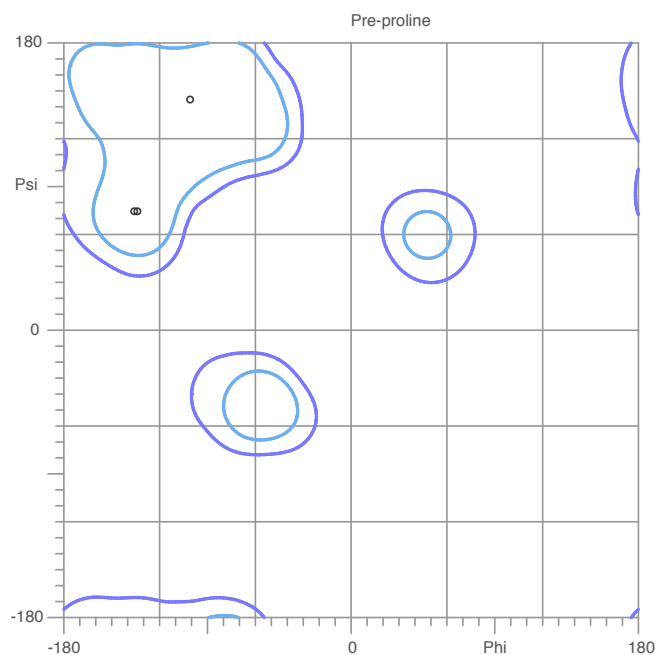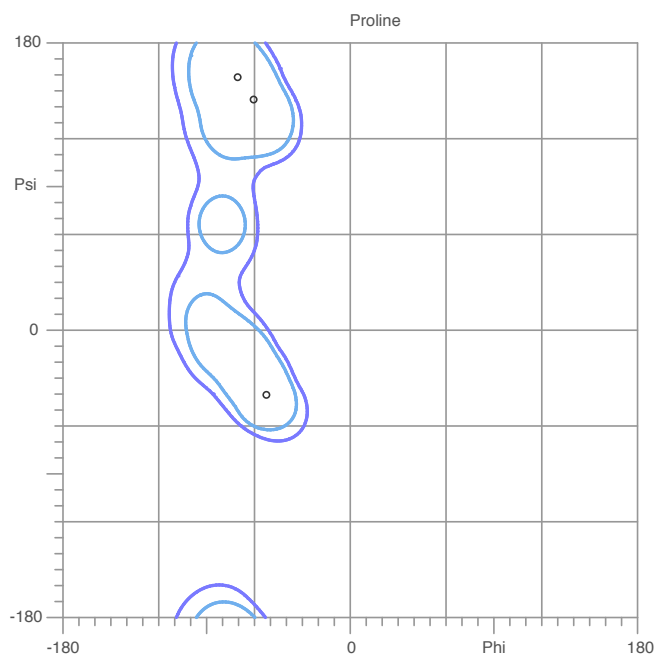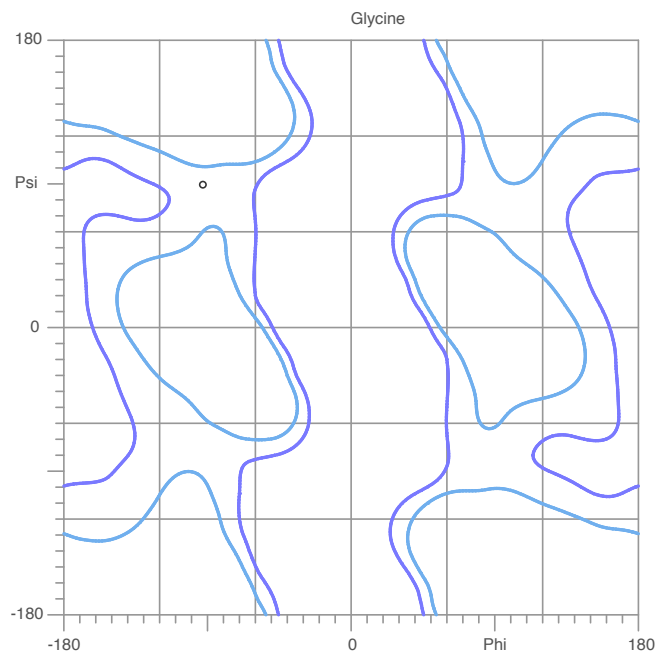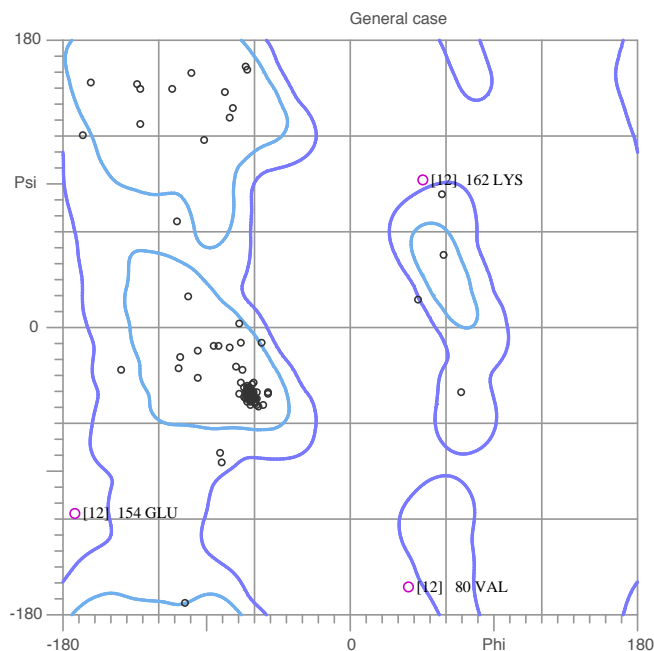# MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 11

91.7% (100/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[11]   80 VAL (37.1, -161.3)
[11] 153 SER (159.2, -20.6)
[11] 160 LYS (-165.4, -63.8)
[11] 166 GLU (54.7, 101.2)
[11] 172 HIS (58.7, 93.6)

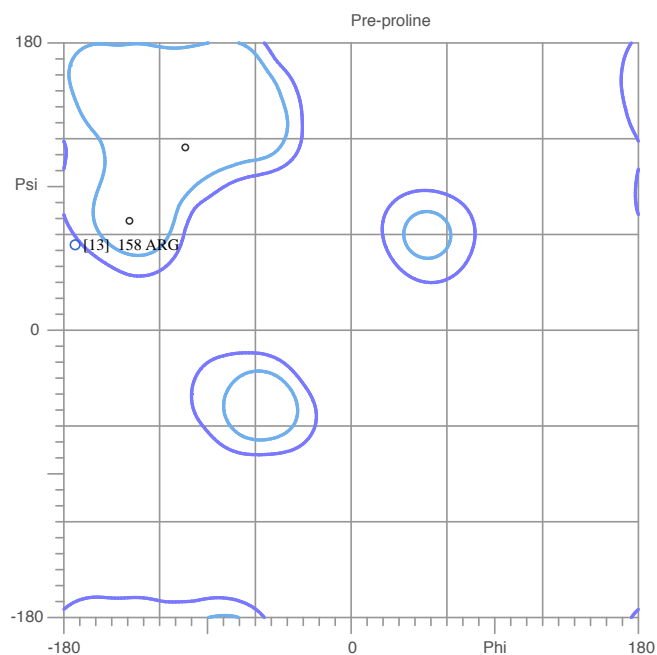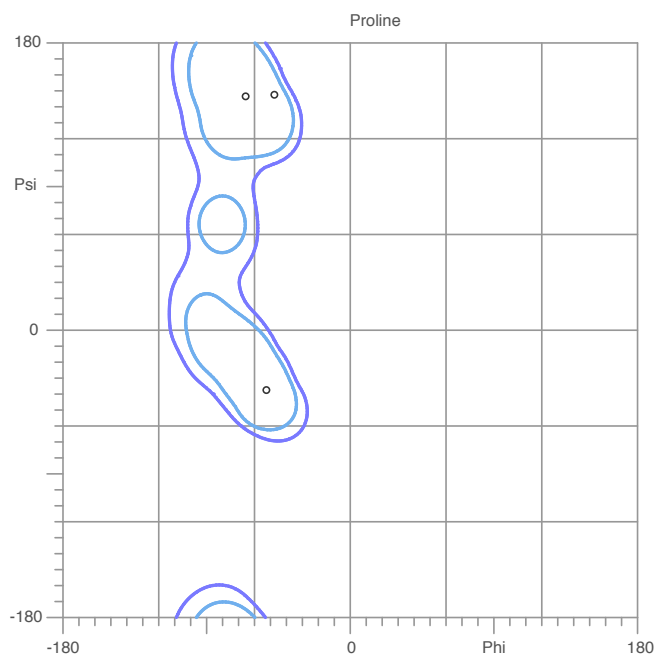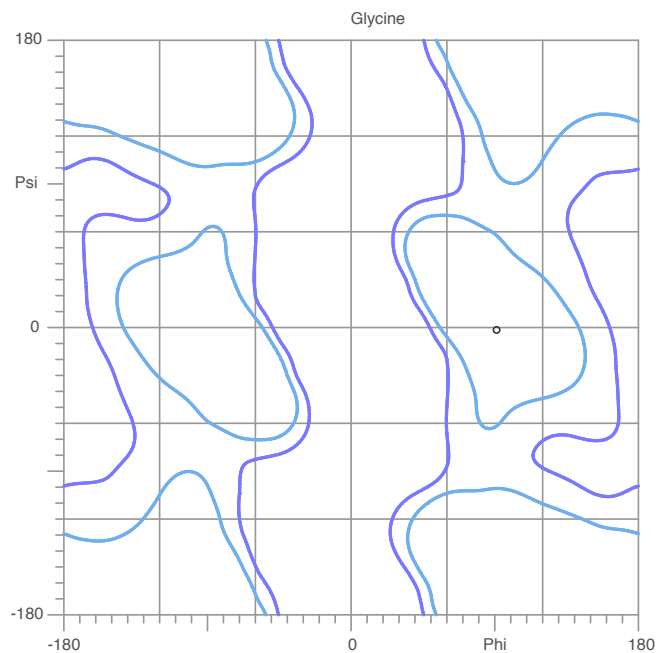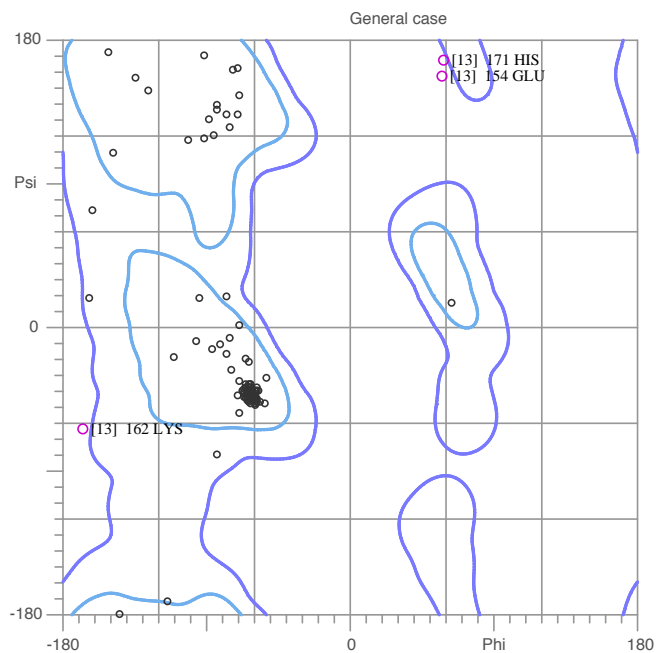# MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 12

87.2% (95/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
    [12]   80 VAL (36.9, -162.6)
    [12] 154 GLU (-173.2, -116.7)
    [12] 162 LYS (45.5, 93.8)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 13
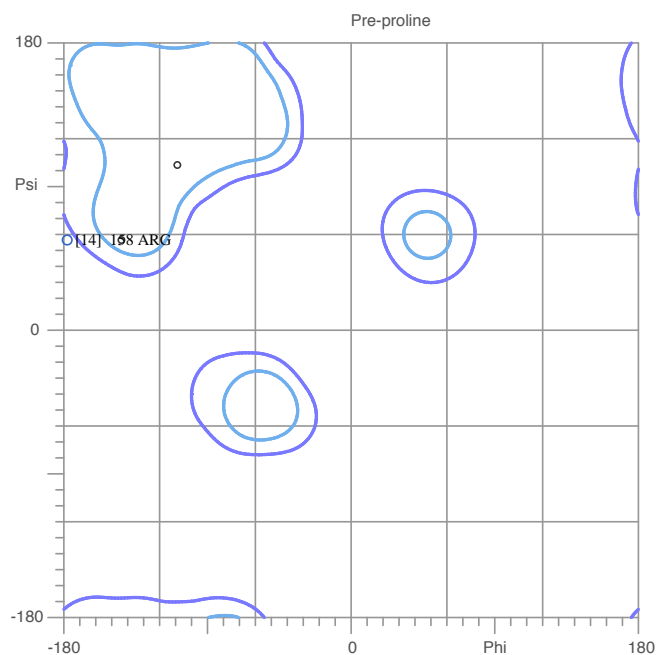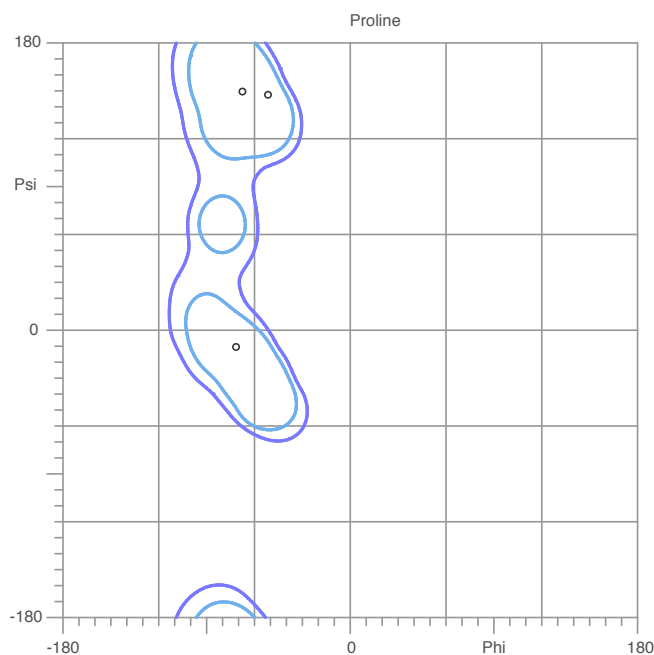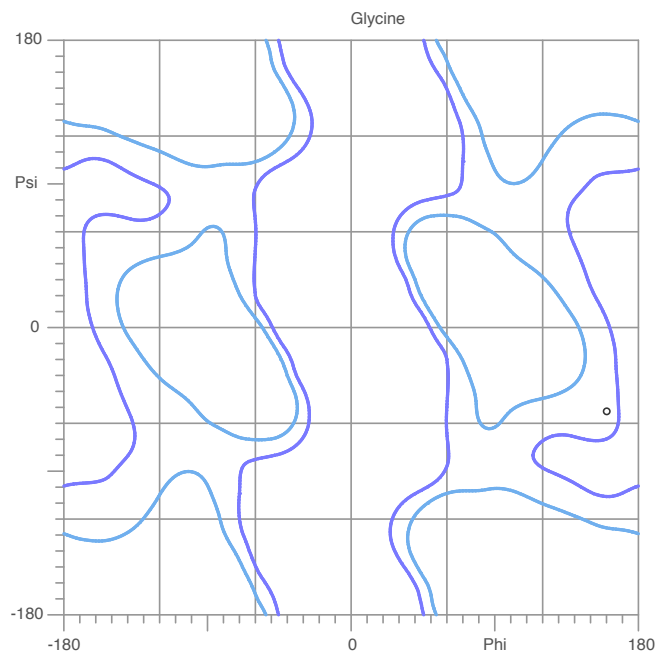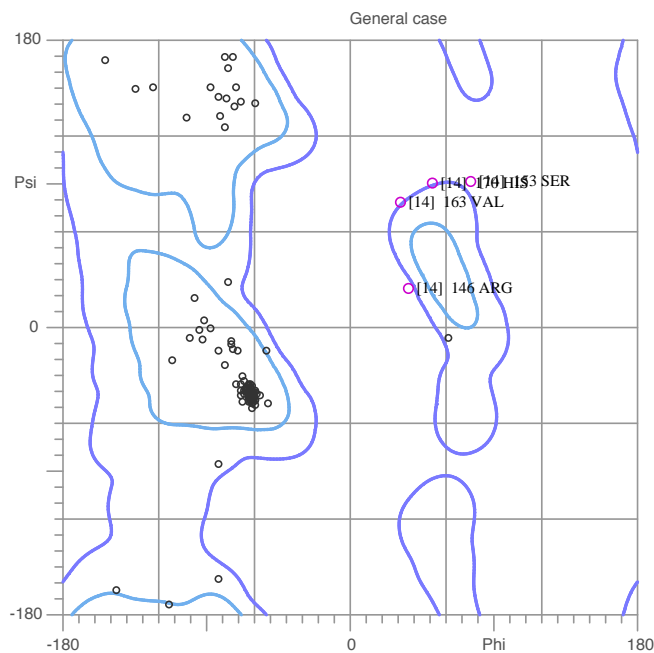

General case

Glycine

Proline

Pre-proline

91.7% (100/109) of all residues were in favored (98%) regions.
96.3% (105/109) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
    [13] 154 GLU (57.2, 158.9)
    [13] 158 ARG (-173.7, 54.1)
    [13] 162 LYS (-168.5, -63.6)
    [13] 171 HIS (58.6, 168.4)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 14

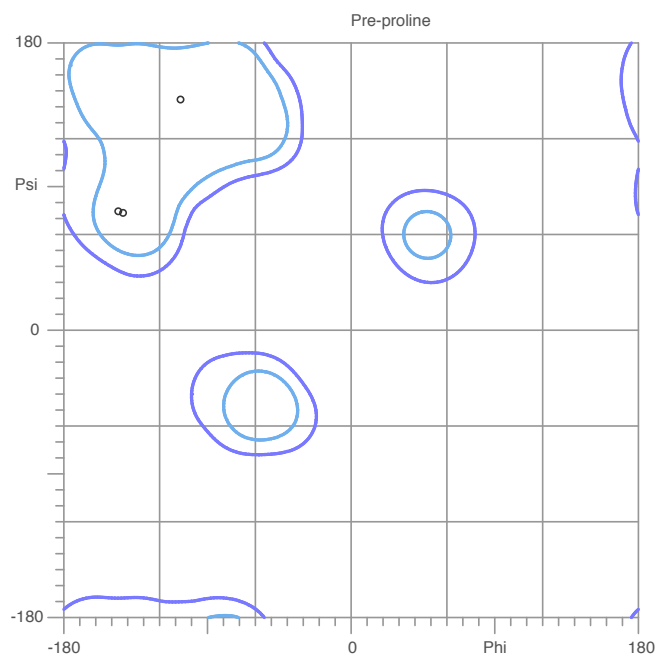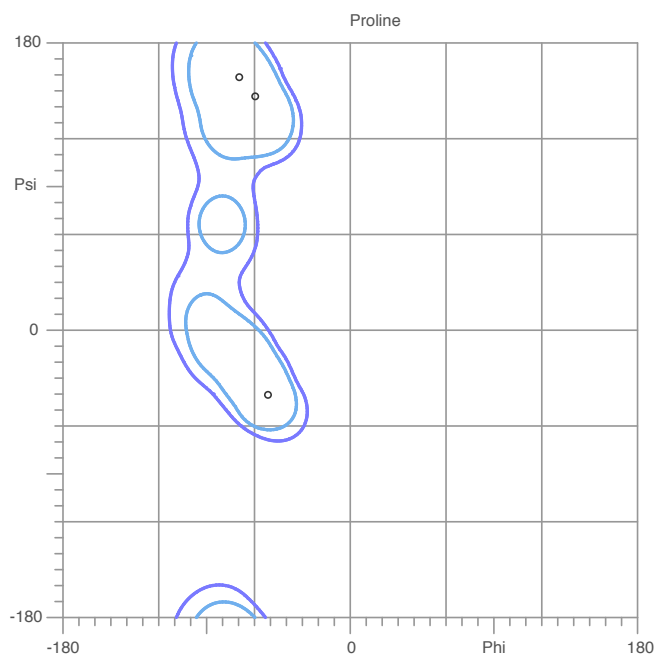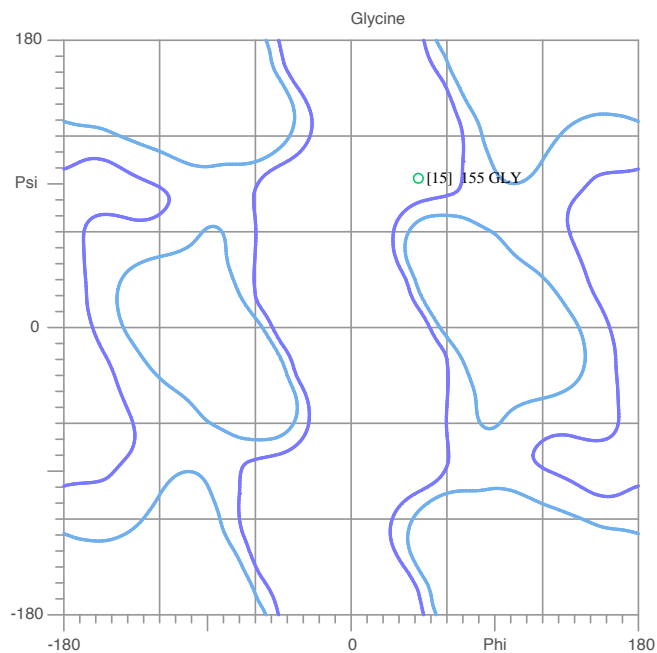General case

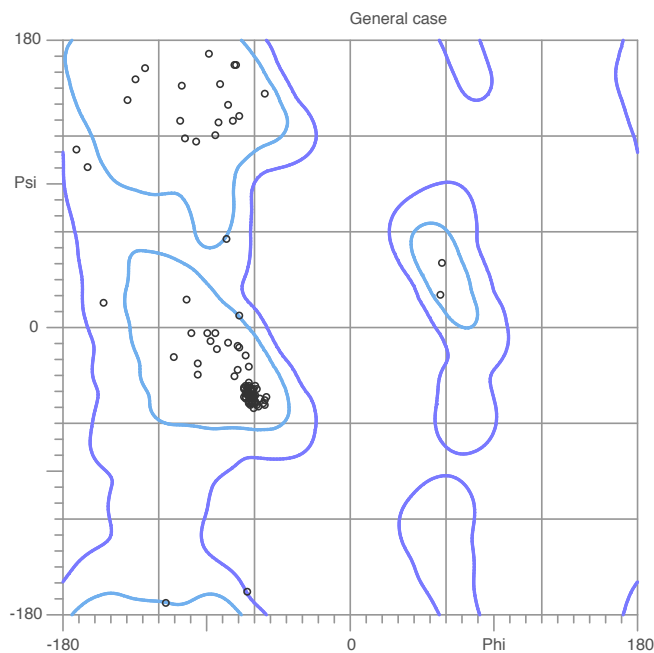Glycine

Proline

Pre-proline

89.9% (98/109) of all residues were in favored (98%) regions.

95.4% (104/109) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[14] 146 ARG (36.6, 25.5)
[14] 153 SER (75.9, 92.9)
[14] 158 ARG (-178.9, 57.9)
[14] 163 VAL (31.6, 79.3)
[14] 170 HIS (51.6, 91.7)

MolProbity Ramachandran analysis

94.5% (103/109) of all residues were in favored (98%) regions.
99.1% (108/109) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
  [15] 155 GLY (42.5, 94.6)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 16

92.7% (101/109) of all residues were in favored (98%) regions.
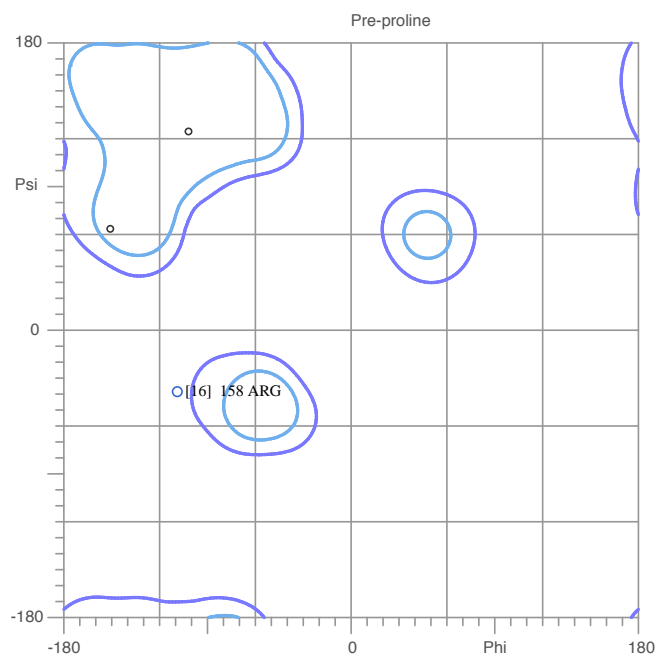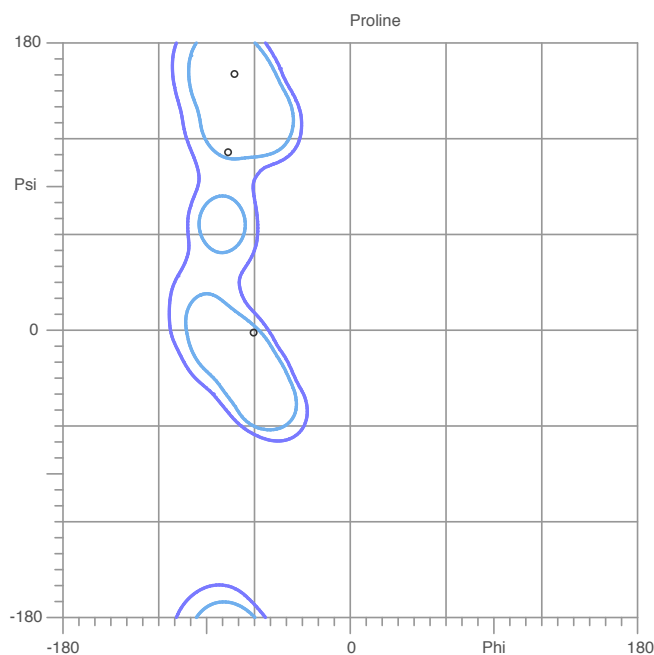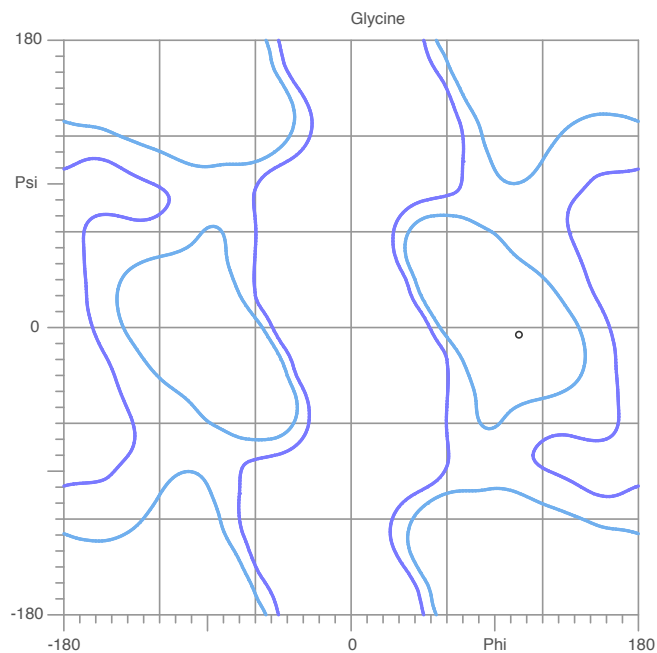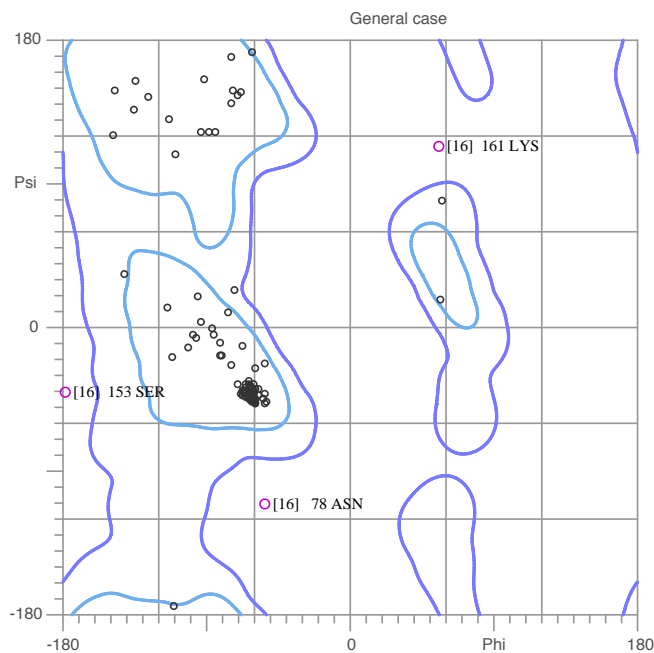96.3% (105/109) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
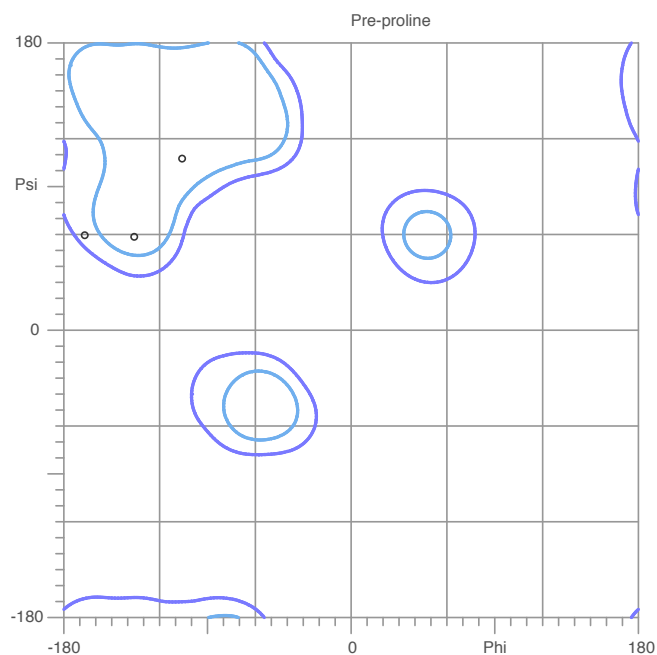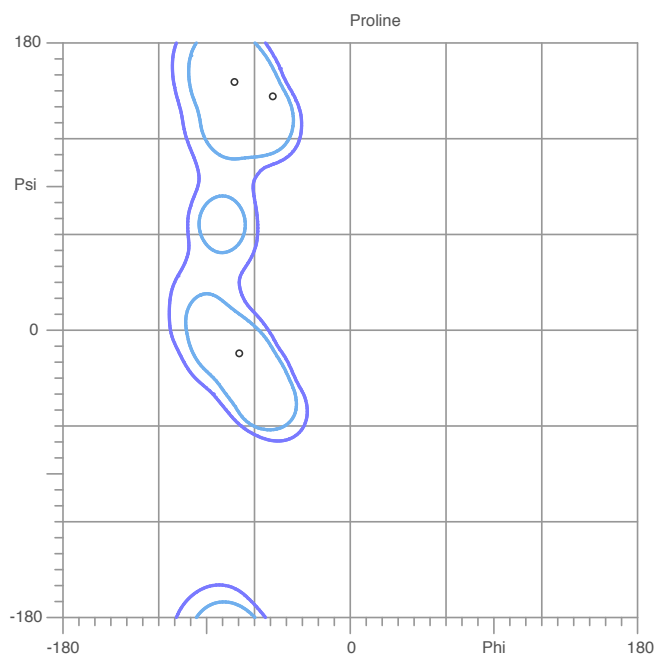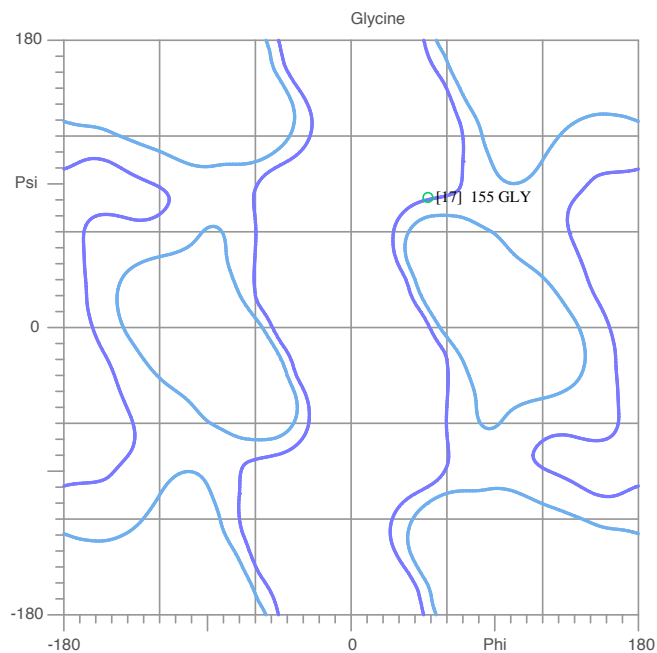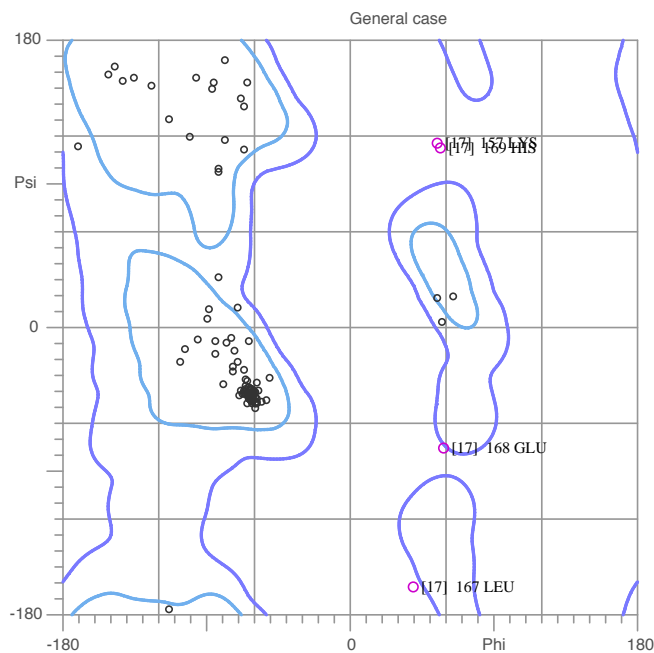   [16]   78 ASN (-54.4, -110.7)
   [16] 153 SER (-179.7, -40.1)
   [16] 158 ARG (-109.0, -38.1)
   [16] 161 LYS (55.8, 114.4)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 17

General case

Glycine

○[17] 157 LYS
○[17] 169 HIS

○[17] 168 GLU

○[17] 167 LEU
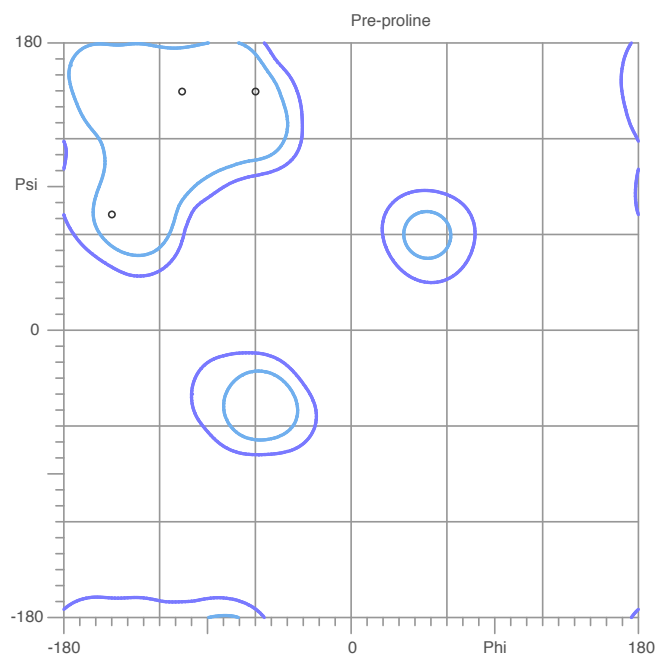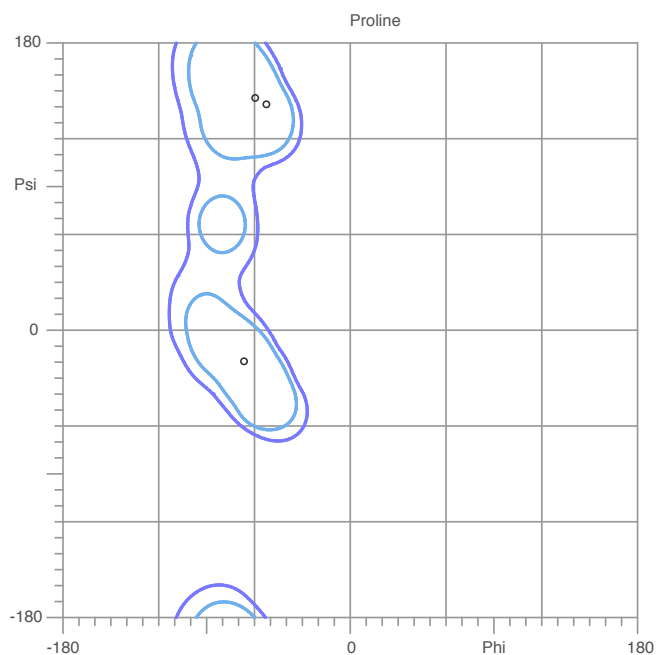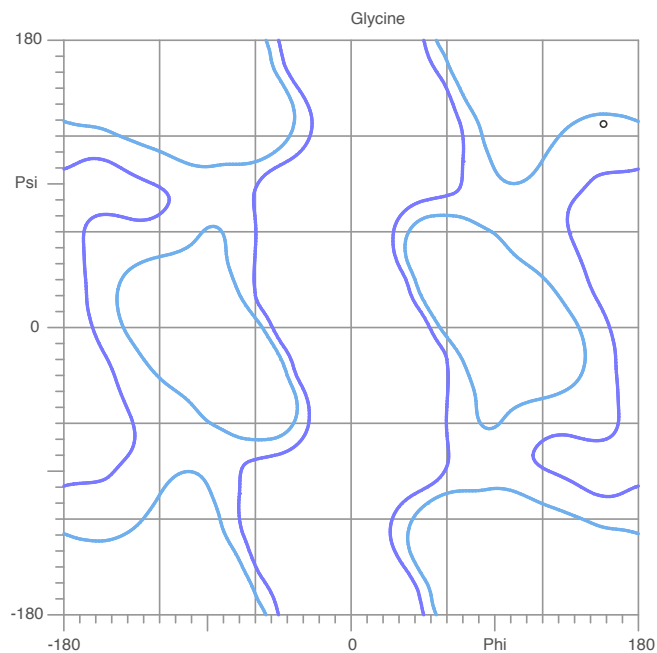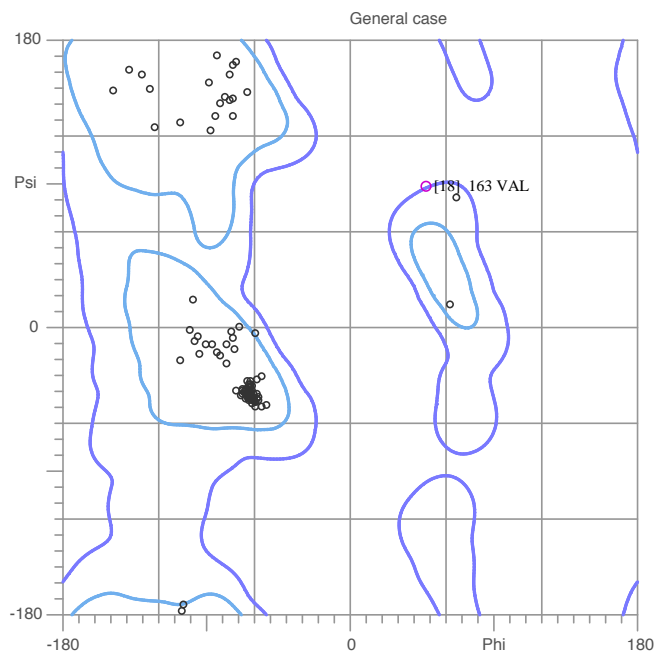
○[17] 155 GLY

Proline

Pre-proline

90.8% (99/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[17] 155 GLY (48.8, 82.4)
[17] 157 LYS (54.9, 116.9)
[17] 167 LEU (39.9, -163.0)
[17] 168 GLU (58.8, -75.7)
[17] 169 HIS (56.6, 113.0)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 18

96.3% (105/109) of all residues were in favored (98%) regions.
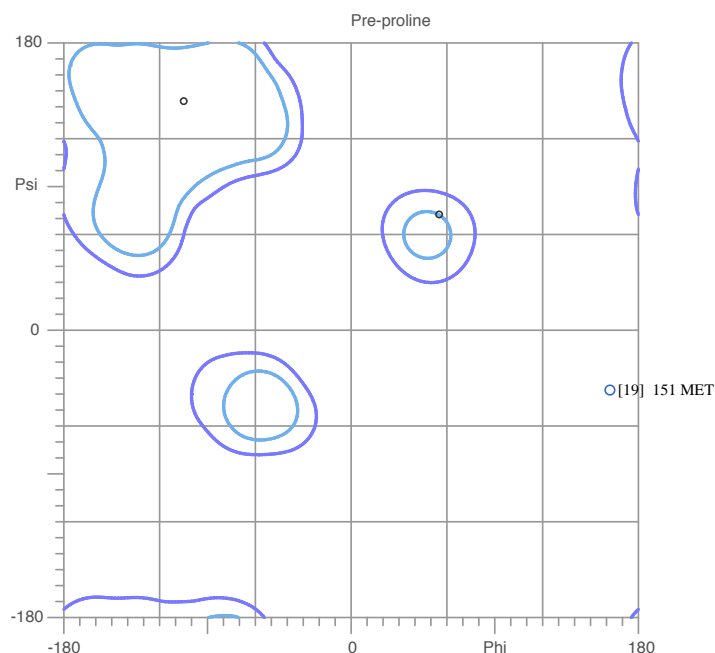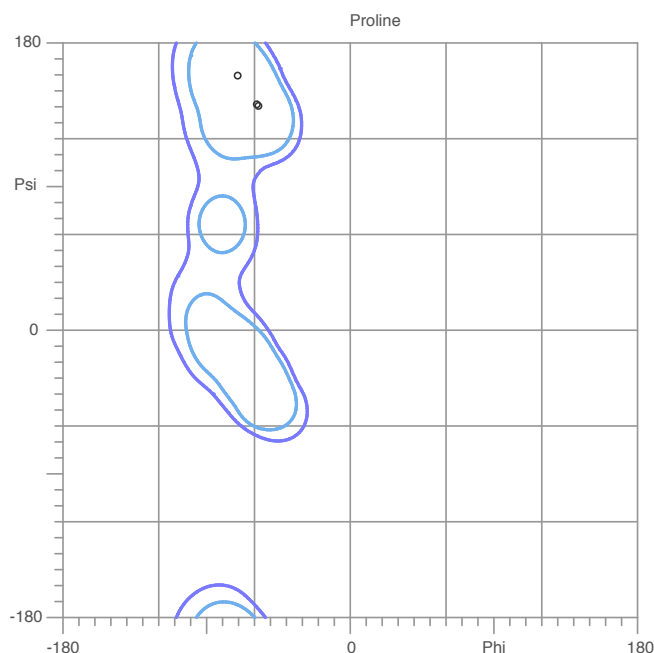99.1% (108/109) of all residues were in allowed (>99.8%) regions.
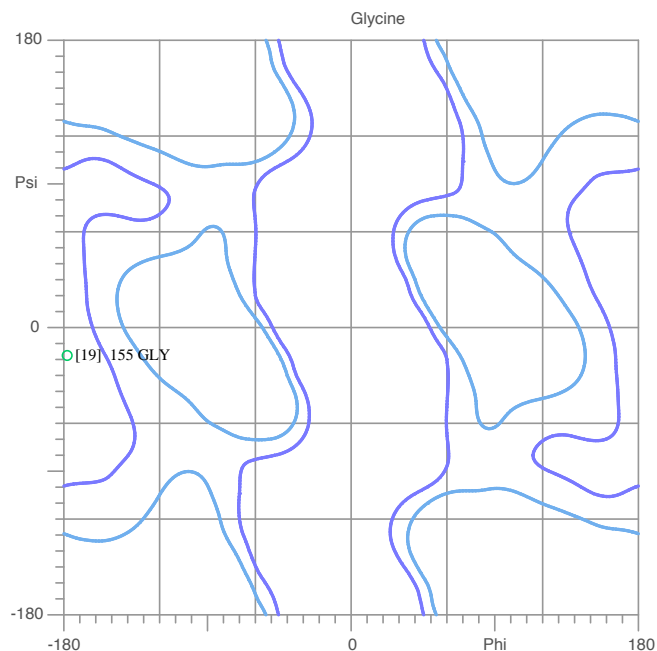
There were 1 outliers (phi, psi):
   [18] 163 VAL (47.3, 90.0)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 19

89.9% (98/109) of all residues were in favored (98%) regions.
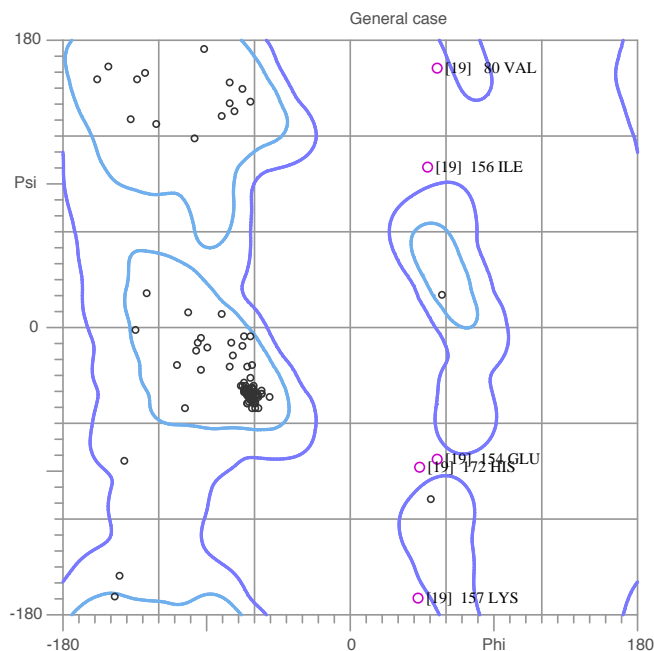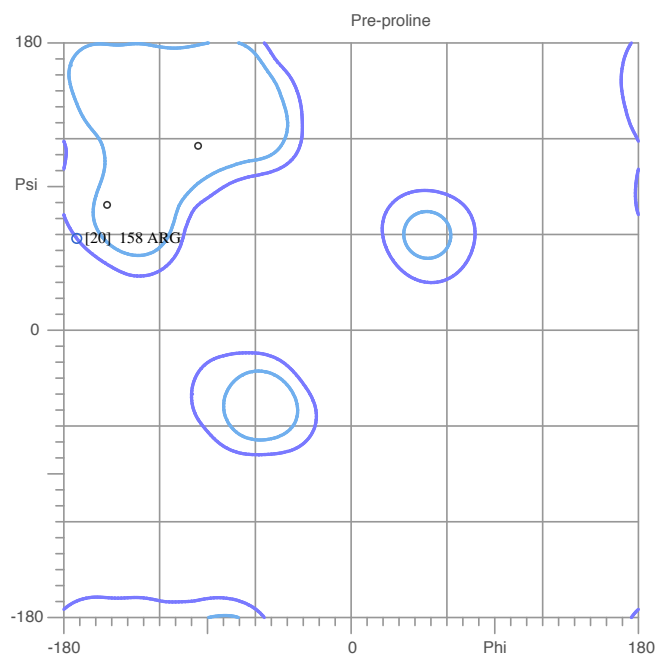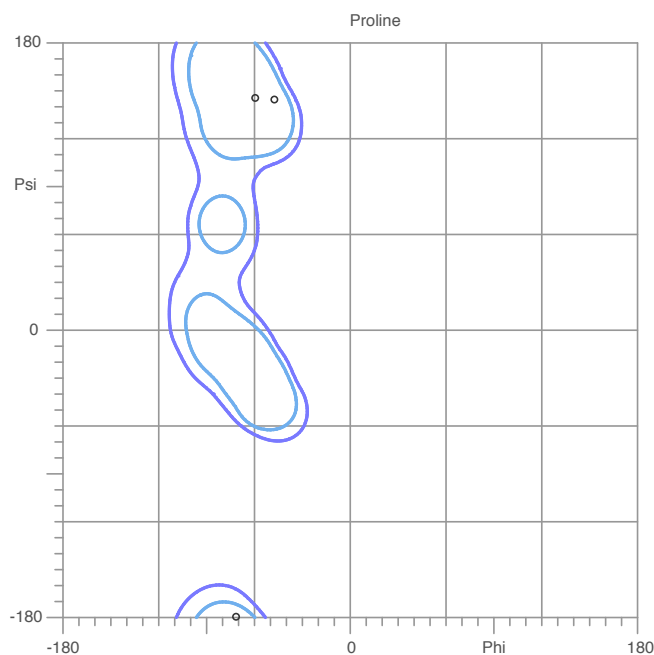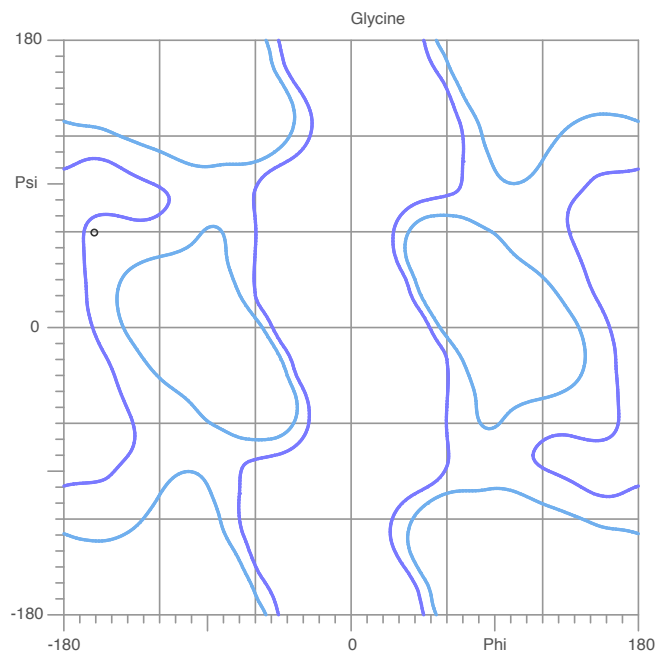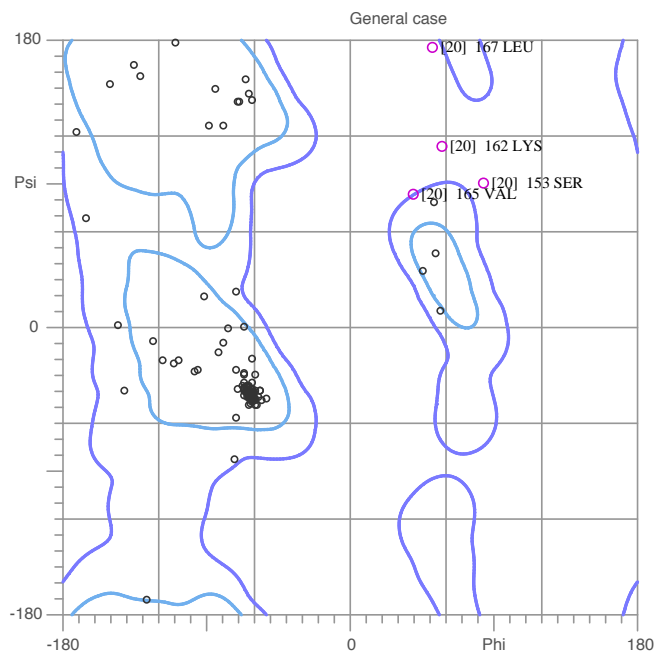93.6% (102/109) of all residues were in allowed (>99.8%) regions.

There were 7 outliers (phi, psi):
  [19] 80 VAL (54.7, 163.1)

[19] 151 MET (162.5, -37.9)
[19] 154 GLU (54.1, -82.6)
[19] 155 GLY (-178.4, -17.7)
[19] 156 ILE (48.7, 101.0)
[19] 157 LYS (42.1, -169.1)
[19] 172 HIS (44.0, -87.8)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 20

General case

Glycine

Proline

Pre-proline

86.2% (94/109) of all residues were in favored (98%) regions.

95.4% (104/109) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[20] 153 SER (83.3, 91.9)
[20] 158 ARG (-172.3, 58.5)
[20] 162 LYS (57.2, 114.6)
[20] 165 VAL (40.0, 84.1)
[20] 167 LEU (51.0, 176.2)