MolProbity Ramachandran analysis

2HEQ_NMR.pdb, all models

General case

[20] 77 LEU
[19] 80 HIS
[10] 86 HIS
[15] 2 ALA / [5] 2 TRP
[8] [15] 22 ASN
[15] 22 ASN
[10] 79 HIS
[15] 9 TYR
[18] 75 LEU
[3] 2 ALA
[8] 2 ALA
[15] 73 LEU
[20] 10 TRP
[26] 25 TYR
[14] 25 ARG
[11] 8 LYS

Glycine

[7] 71 GLY
[13] 33 GLY
[14] 3 GLY
[18] 71 GLY
[14] 71 GLY
[10] 3 GLY
[13] 71 GLY
[7] 72 GLY
[5] 27 GLY
[16] 3 GLY

Proline

[11] 7 PRO
[2] 7 PRO
[1] [2] PRO
[9] 29 PRO
[14] [17] 29 PRO / 5 PRO

Pre-proline

[14] 6 LEU
[5] 6 LEU
[17] 6 LEU
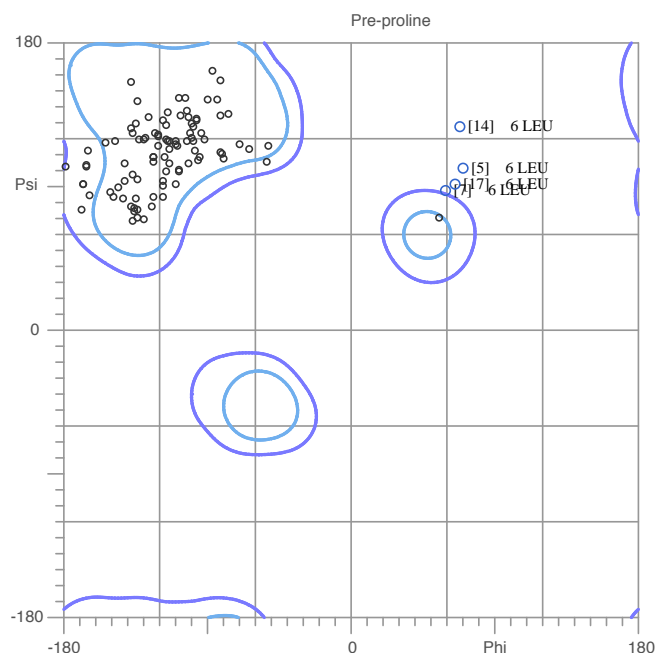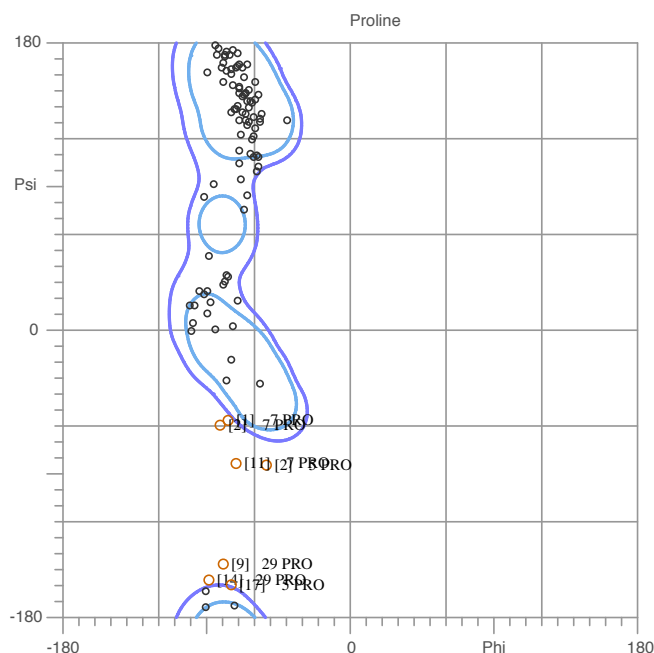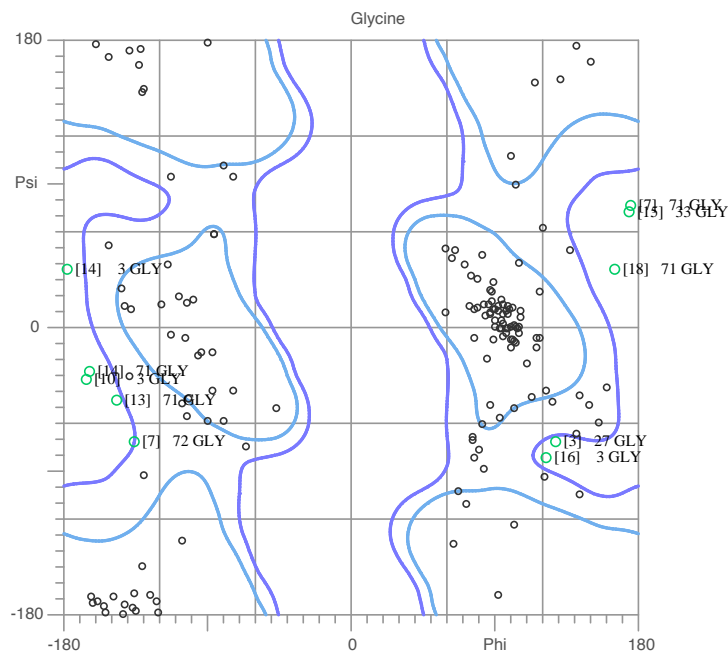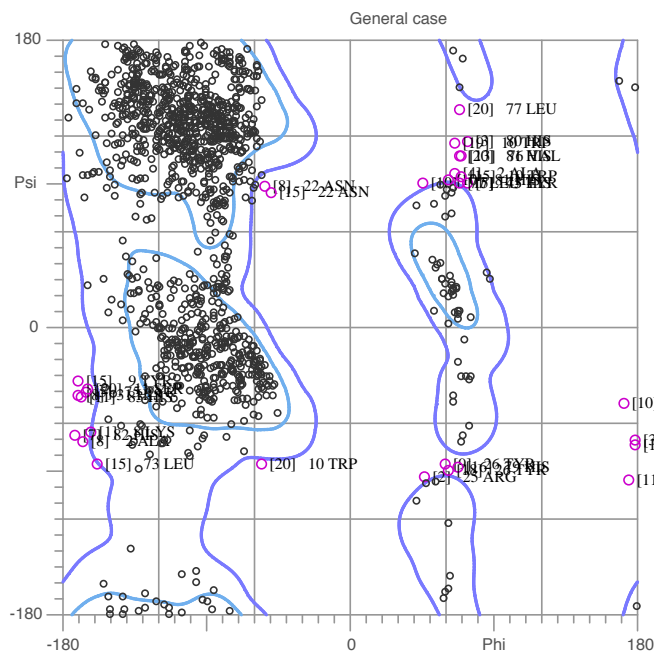
85.2% (1398/1640) of all residues were in favored (98%) regions.
96.8% (1588/1640) of all residues were in allowed (>99.8%) regions.

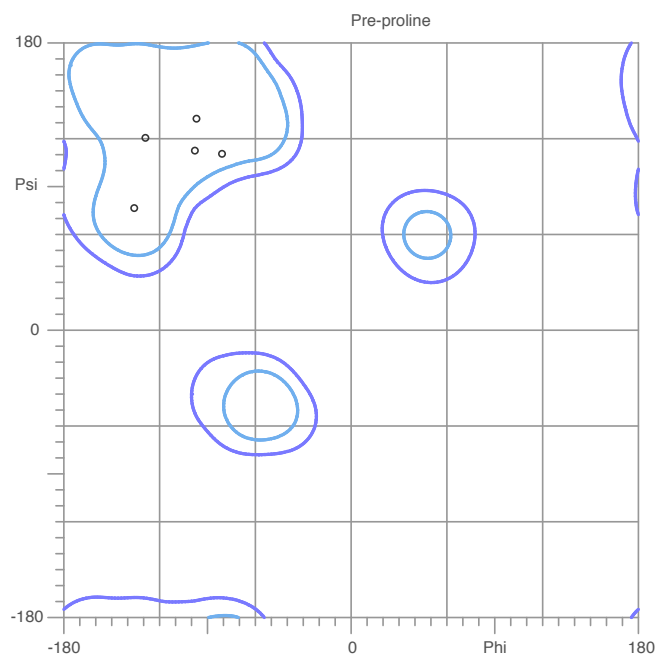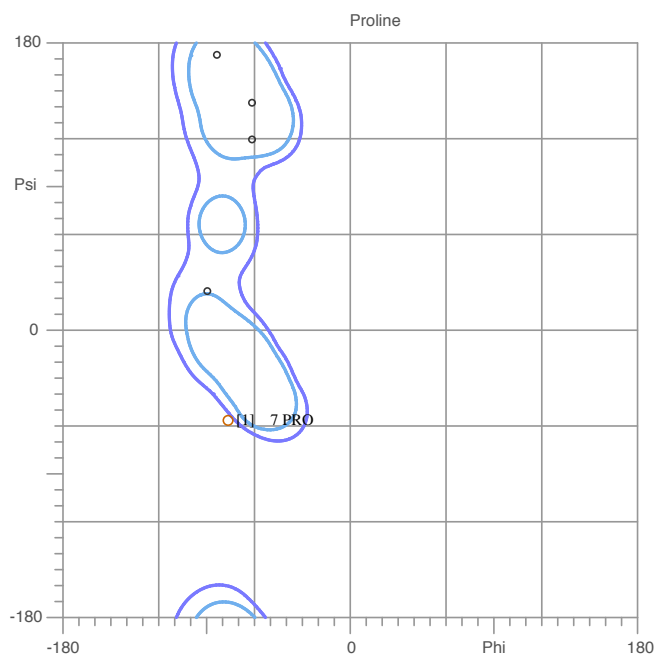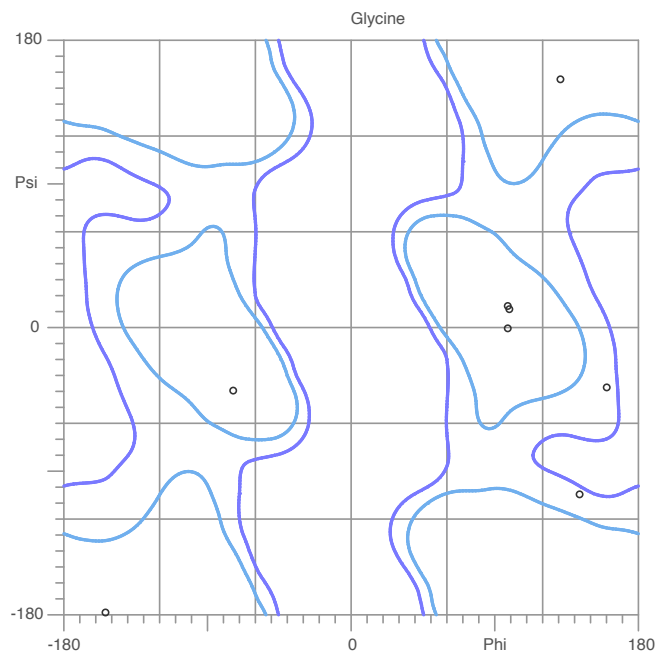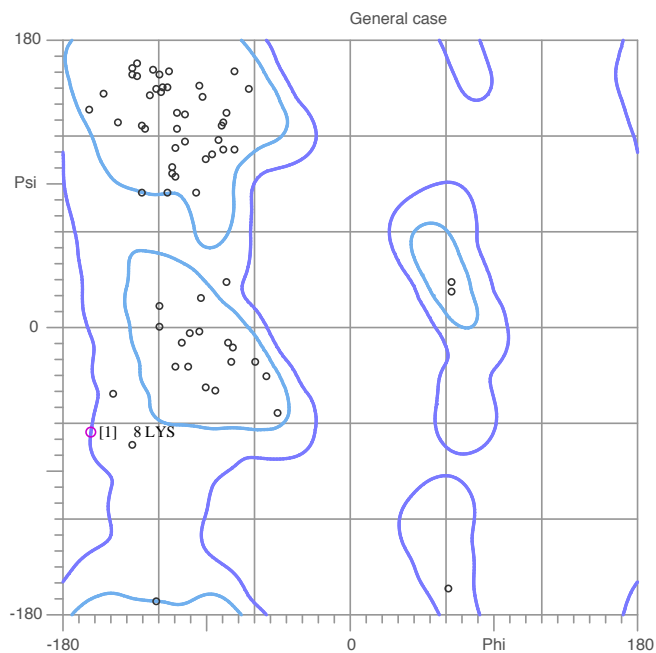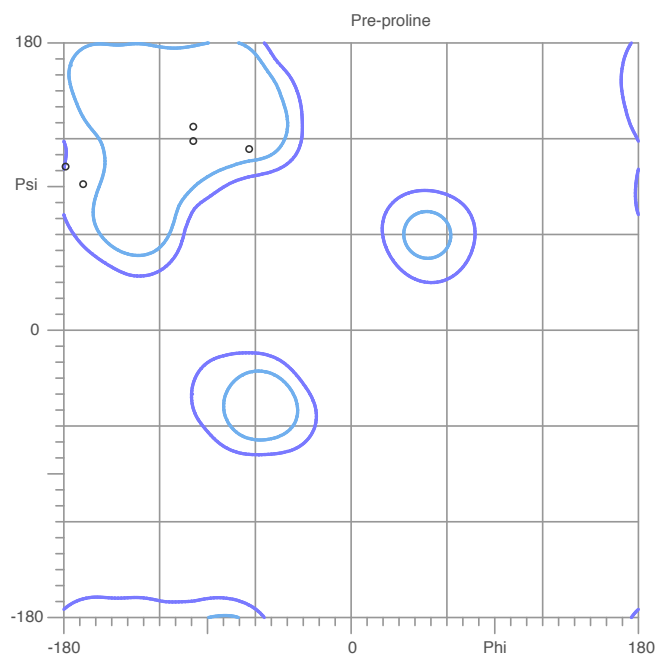There were 52 outliers (phi, psi):
[1] 7 PRO (-77.1, -56.0)
[1] 8 LYS (-163.1, -65.0)
[2] 5 PRO (-53.4, -84.9)
[2] 7 PRO (-82.7, -59.2)
[2] 25 ARG (46.2, -93.9)
[3] 2 ALA (178.1, -70.9)
[3] 27 GLY (128.5, -71.0)
[3] 80 HIS (73.6, 117.8)
[4] 2 ALA (65.7, 97.7)
[5] 6 LEU (70.1, 102.5)
[5] 75 TYR (-166.7, -40.1)
[7] 6 LEU (59.6, 88.4)
[7] 71 GLY (175.6, 77.1)
[7] 72 GLY (-136.6, -71.1)
[7] 75 TYR (73.9, 91.9)
[7] 82 HIS (-173.8, -67.0)
[8] 2 ALA (-168.9, -71.1)
[8] 22 ASN (-54.2, 89.4)
[8] 31 HIS (-171.6, -42.9)
[9] 26 TYR (59.0, -85.1)
[9] 29 PRO (-80.0, -146.2)
[10] 3 GLY (-166.3, -32.9)
[10] 77 LEU (45.5, 91.2)
[10] 79 HIS (171.8, -47.6)

[10] 81 HIS (61.0, 93.4)
[11] 7 PRO (-72.3, -83.4)
[11] 8 LYS (174.0, -95.7)
[11] 83 HIS (-169.1, -43.8)
[13] 71 GLY (-147.3, -45.5)
[13] 76 VAL (69.0, 108.5)
[14] 3 GLY (-178.2, 37.1)
[14] 6 LEU (68.1, 128.6)
[14] 29 PRO (-89.1, -156.6)
[14] 71 GLY (-164.5, -27.3)
[15] 9 TYR (-171.9, -33.4)
[15] 10 TRP (69.9, 95.9)
[15] 22 ASN (-50.7, 85.9)
[15] 33 GLY (175.0, 74.0)
[15] 43 HIS (68.1, 92.0)
[15] 73 LEU (-159.8, -85.4)
[16] 3 GLY (123.0, -81.7)
[16] 79 HIS (67.9, -87.8)
[17] 5 PRO (-75.3, -159.4)
[17] 6 LEU (65.8, 92.3)
[18] 26 TYR (61.3, -89.1)
[18] 71 GLY (165.3, 37.6)
[18] 73 LEU (178.0, -73.9)
[19] 10 TRP (65.9, 116.5)
[20] 10 TRP (-56.8, -85.6)
[20] 11 SER (-165.3, -38.4)
[20] 77 LEU (68.2, 137.9)
[20] 81 HIS (68.2, 108.3)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 1

General case

Glycine

Proline

Pre-proline

89.0% (73/82) of all residues were in favored (98%) regions.
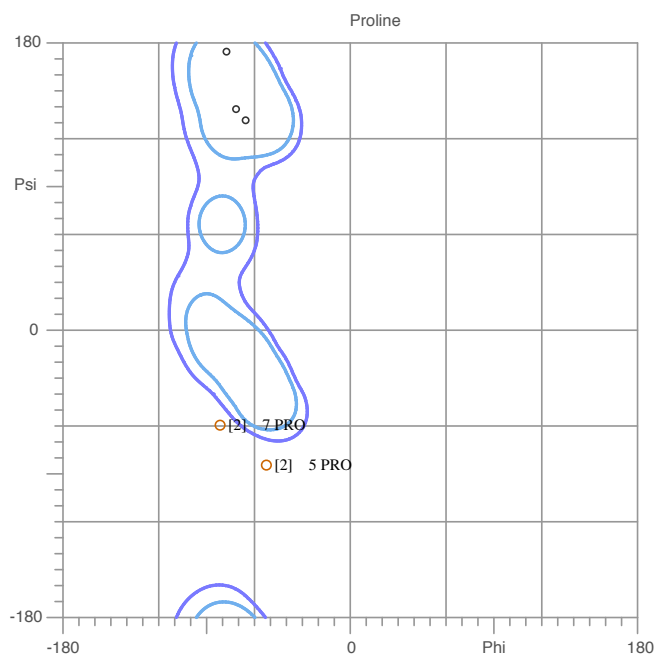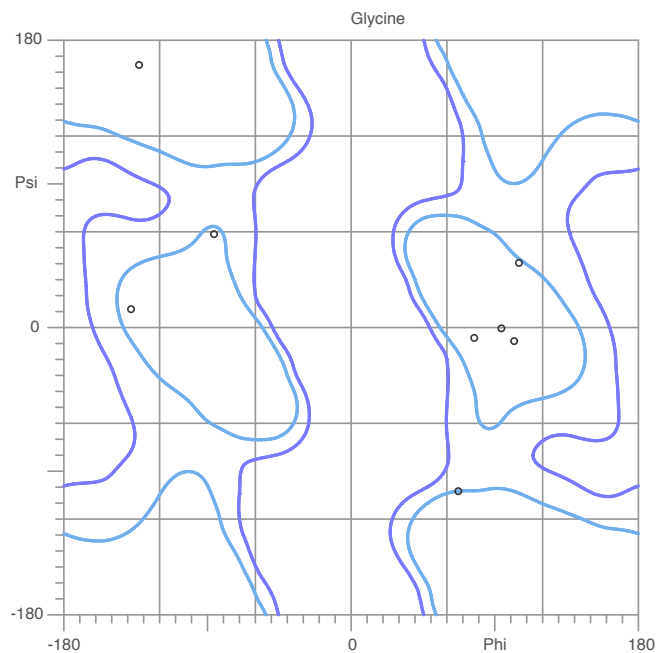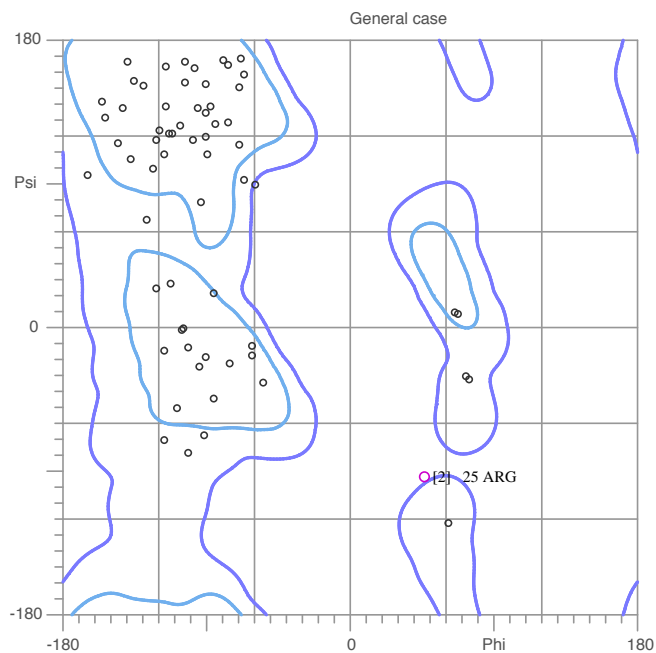97.6% (80/82) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
    [1]   7 PRO (-77.1, -56.0)
    [1]   8 LYS (-163.1, -65.0)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 2
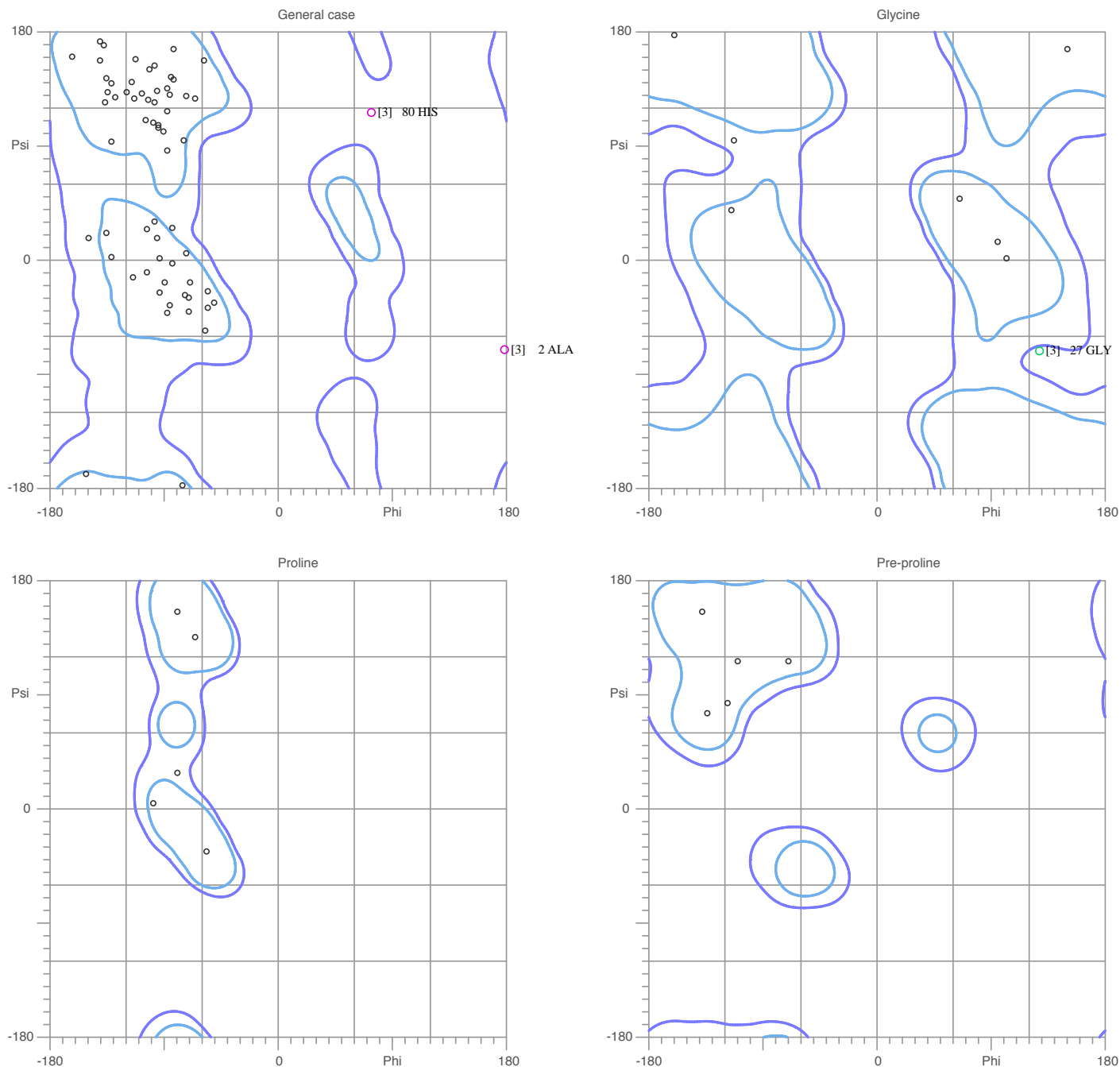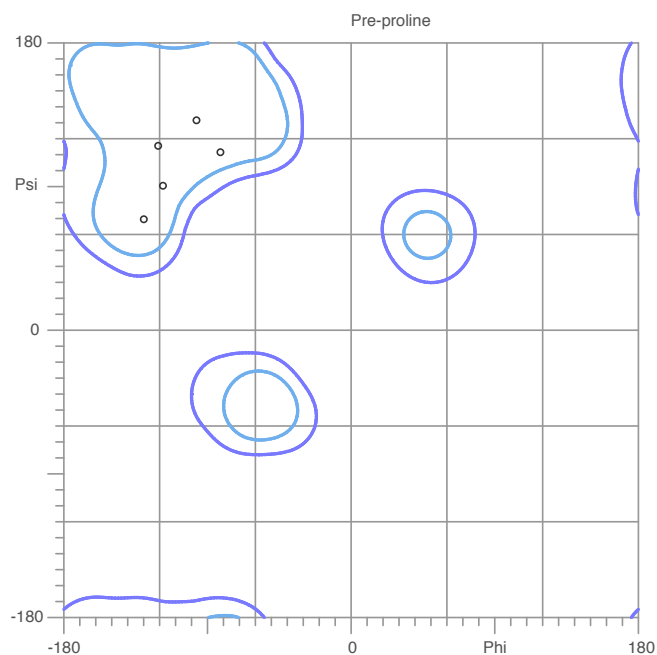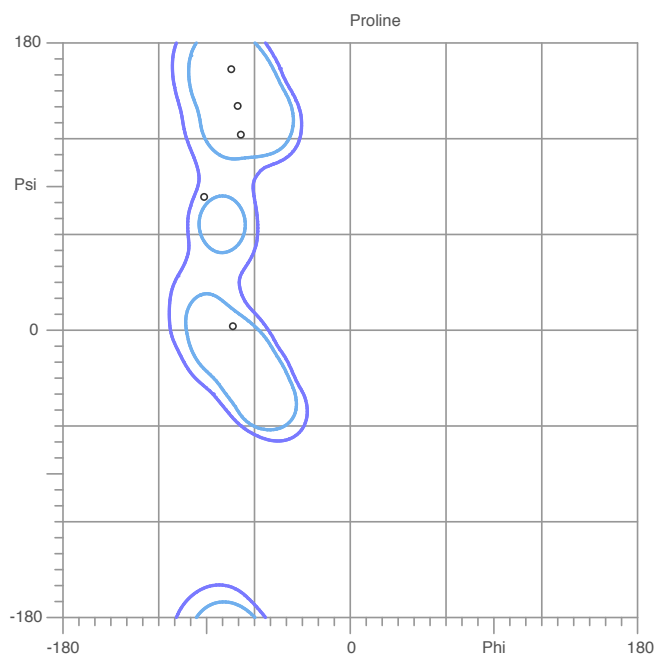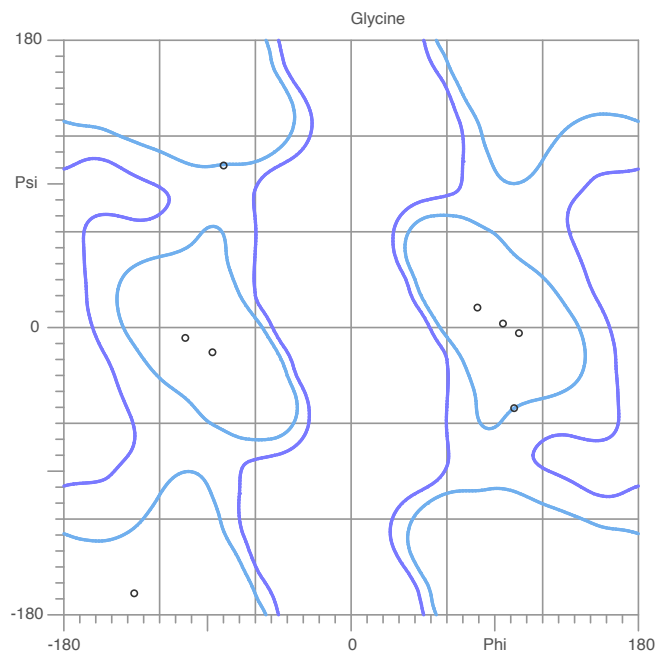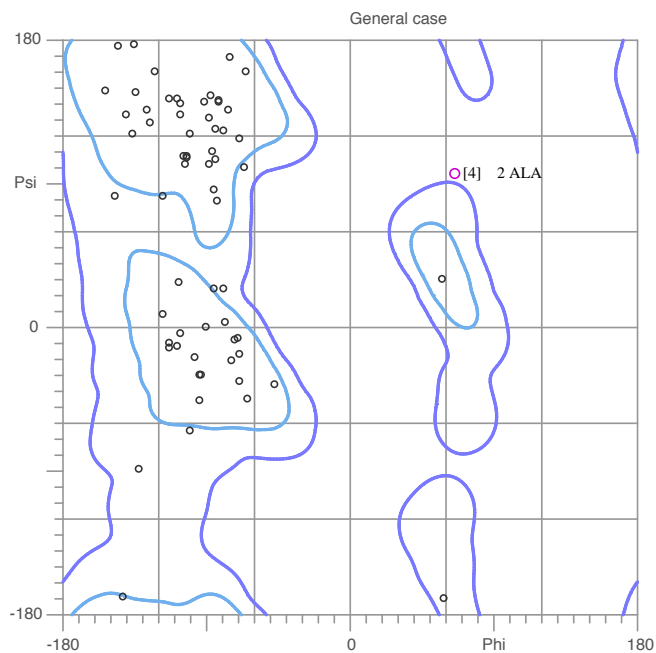

81.7% (67/82) of all residues were in favored (98%) regions.
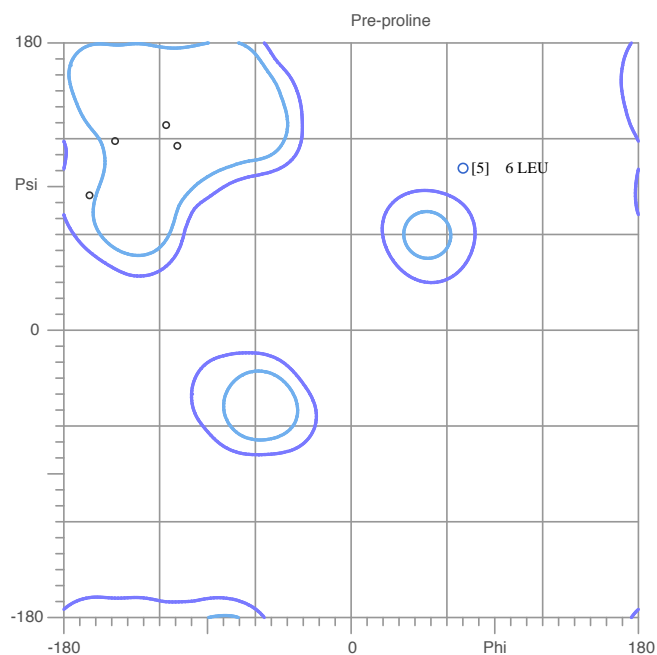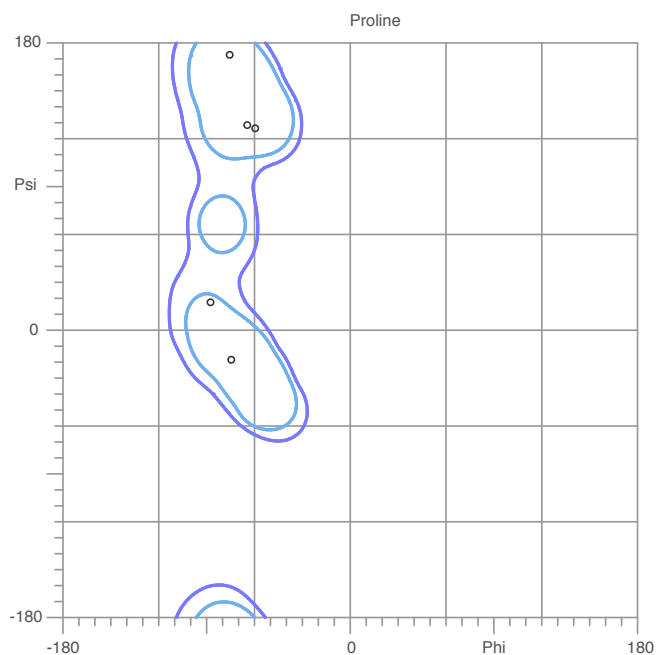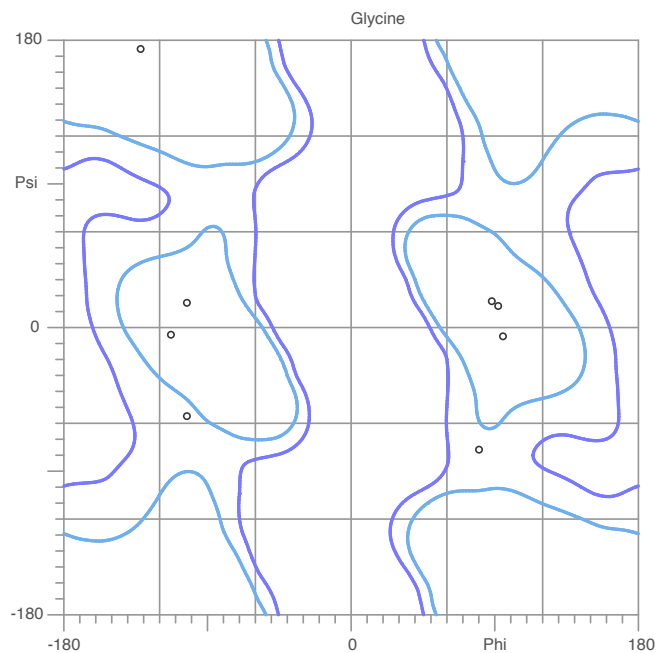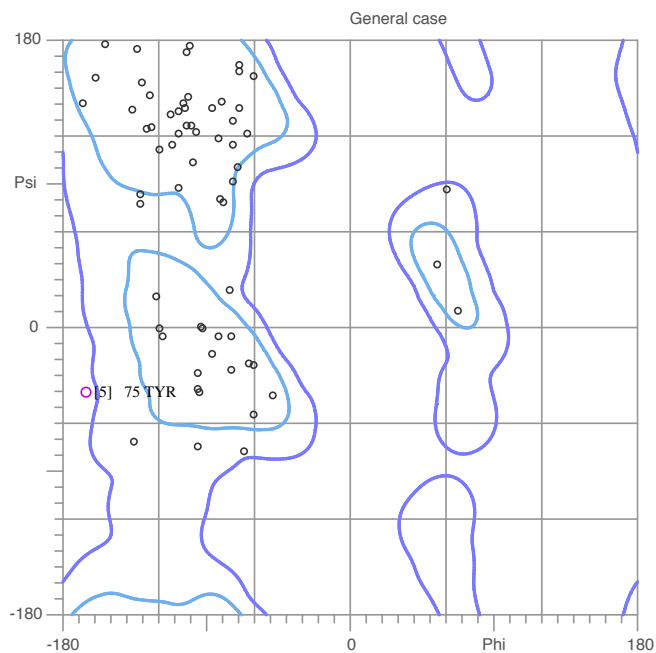96.3% (79/82) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
  [2]   5 PRO (-53.4, -84.9)
  [2]   7 PRO (-82.7, -59.2)
  [2]   25 ARG (46.2, -93.9)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 3

91.5% (75/82) of all residues were in favored (98%) regions.
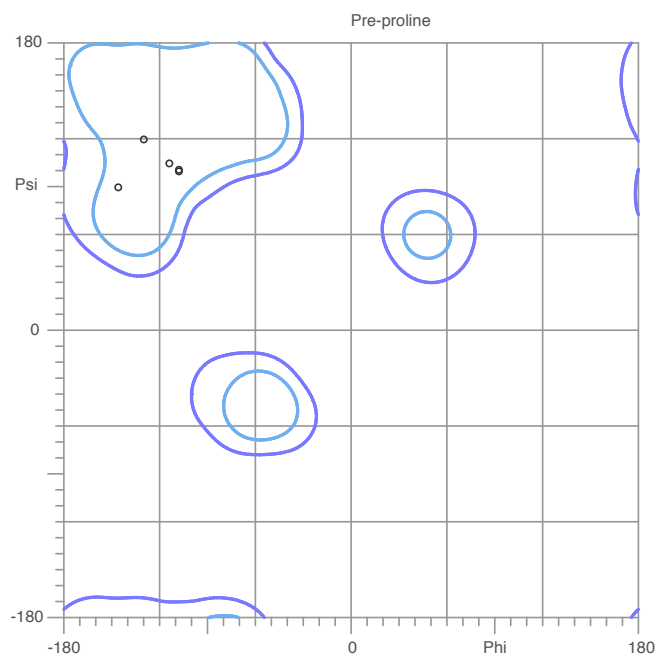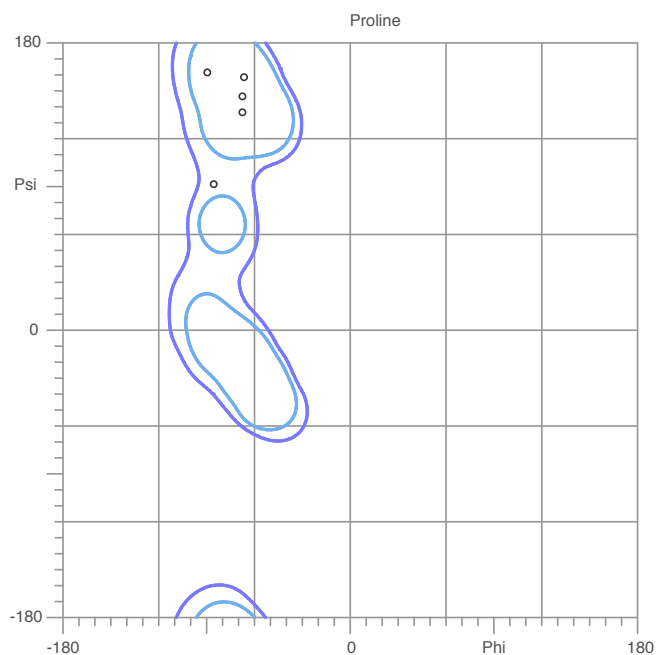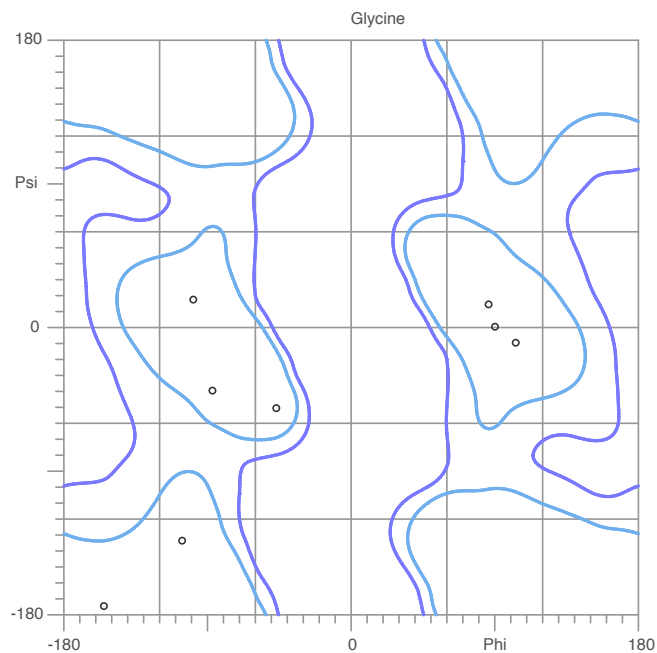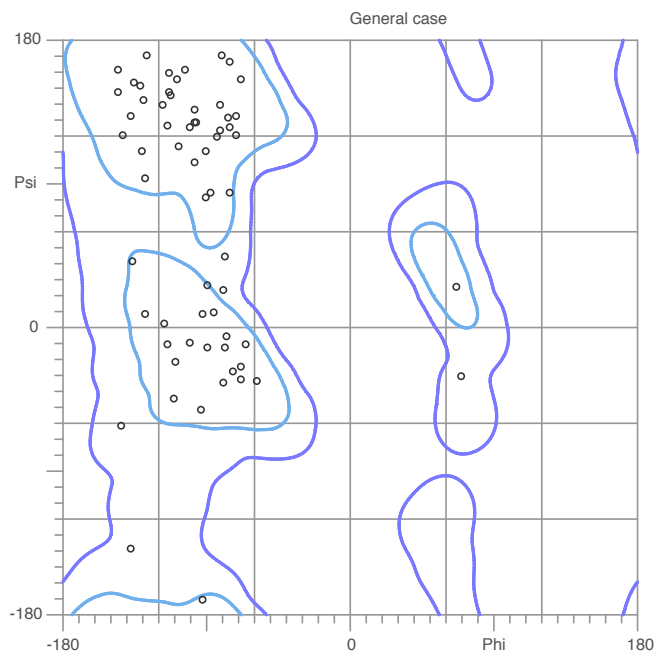96.3% (79/82) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
    [3]   2 ALA (178.1, -70.9)
    [3] 27 GLY (128.5, -71.0)
    [3] 80 HIS (73.6, 117.8)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 4

87.8% (72/82) of all residues were in favored (98%) regions.
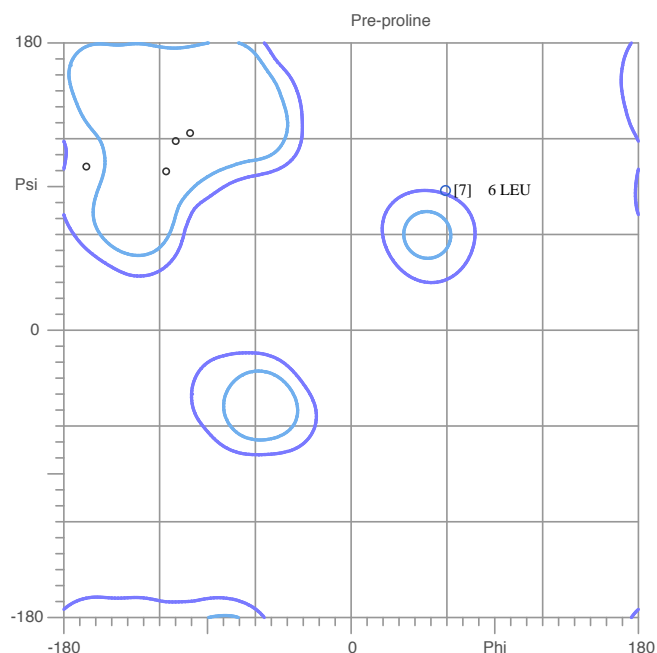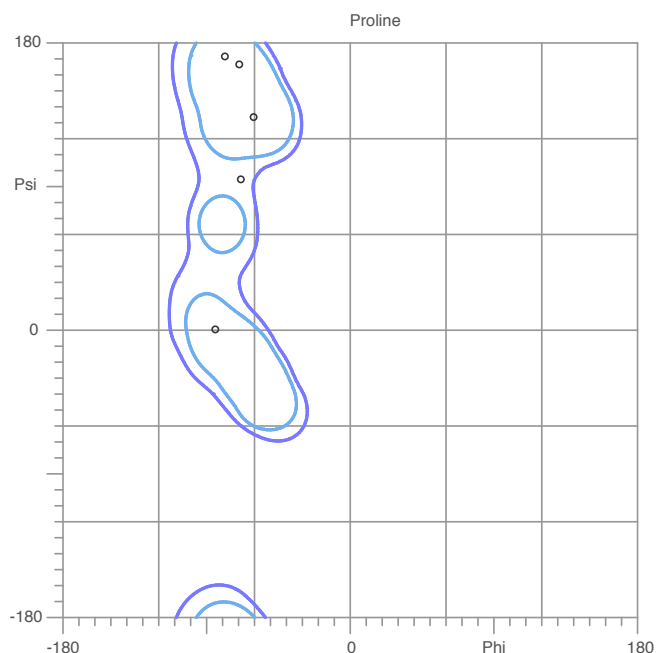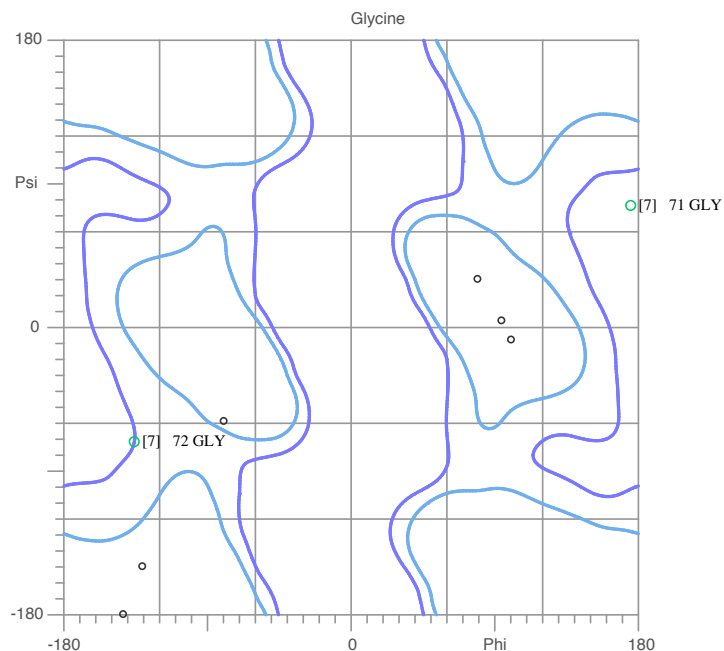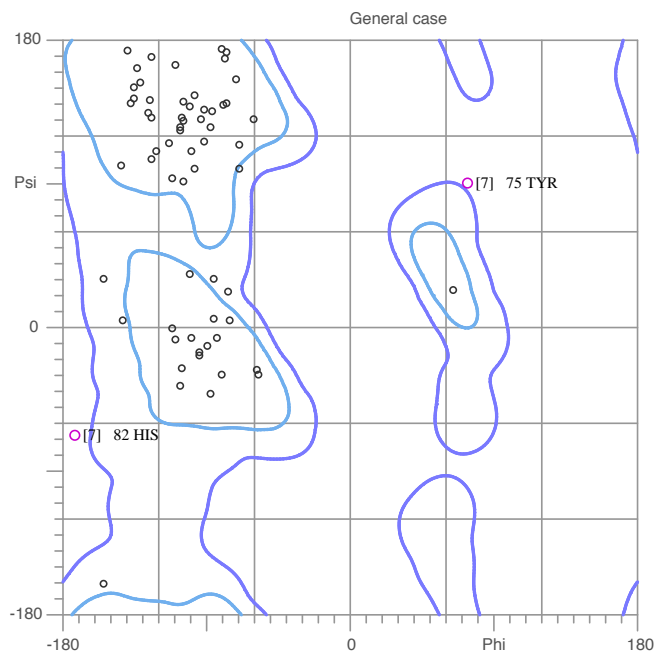98.8% (81/82) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
    [4]   2 ALA (65.7, 97.7)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 5

General case

Glycine

Proline

Pre-proline

85.4% (70/82) of all residues were in favored (98%) regions.
97.6% (80/82) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
    [5]   6 LEU (70.1, 102.5)
    [5]   75 TYR (-166.7, -40.1)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 6

92.7% (76/82) of all residues were in favored (98%) regions.
100.0% (82/82) of all residues were in allowed (>99.8%) regions.

There were no outliers.

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 7

General case
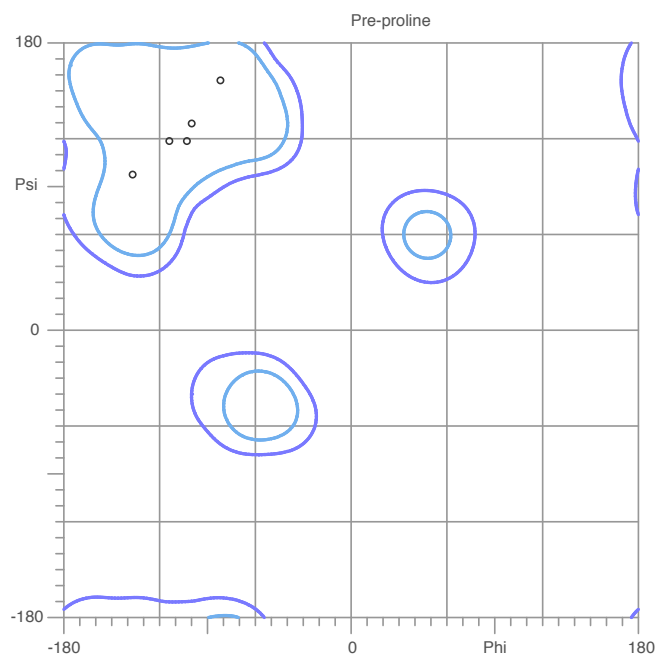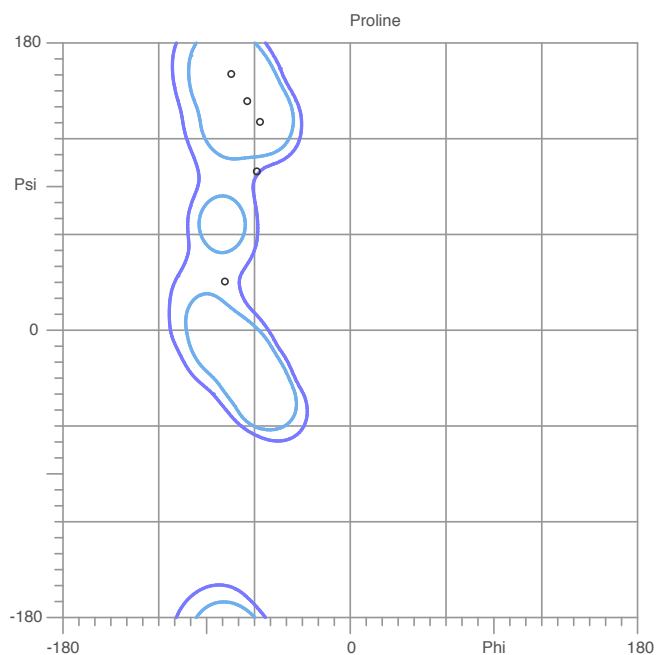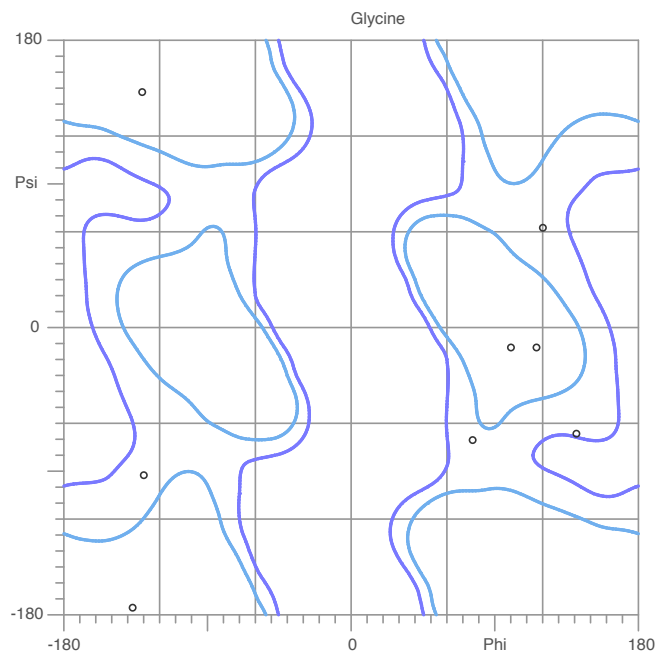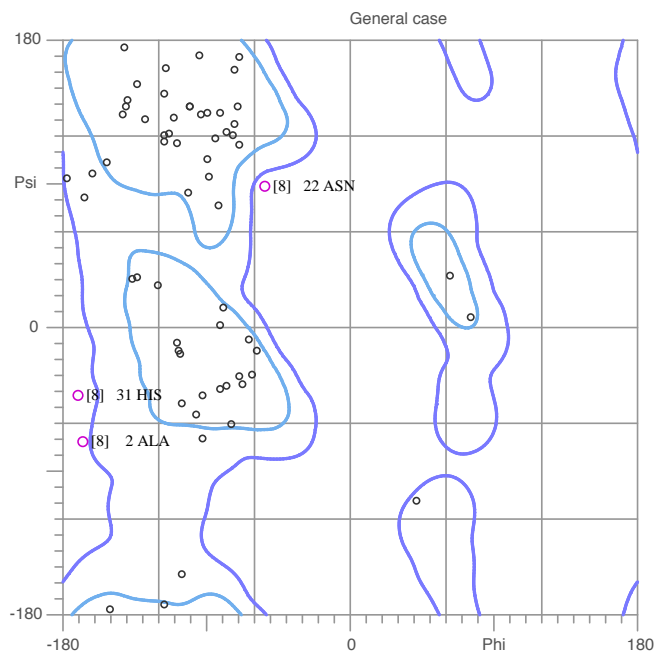

Glycine

Proline

Pre-proline

85.4% (70/82) of all residues were in favored (98%) regions.
93.9% (77/82) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[7]　 6 LEU (59.6, 88.4)
[7]　71 GLY (175.6, 77.1)
[7]　72 GLY (-136.6, -71.1)
[7]　75 TYR (73.9, 91.9)
[7]　82 HIS (-173.8, -67.0)
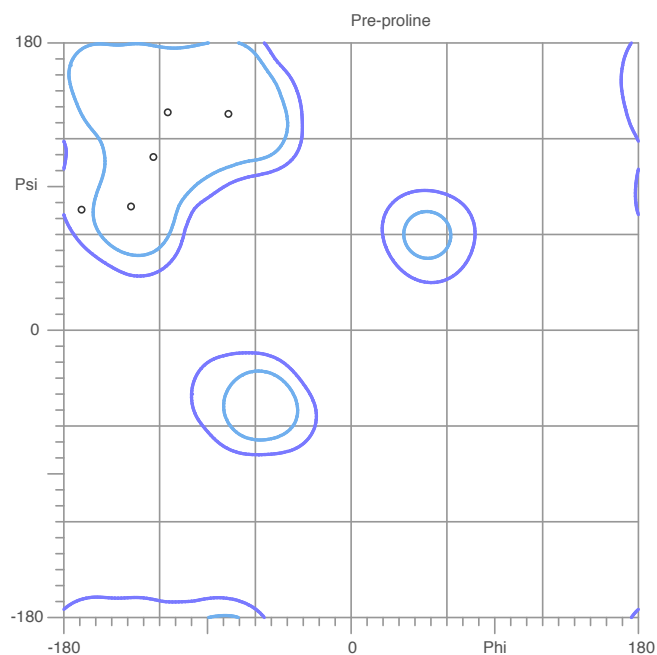
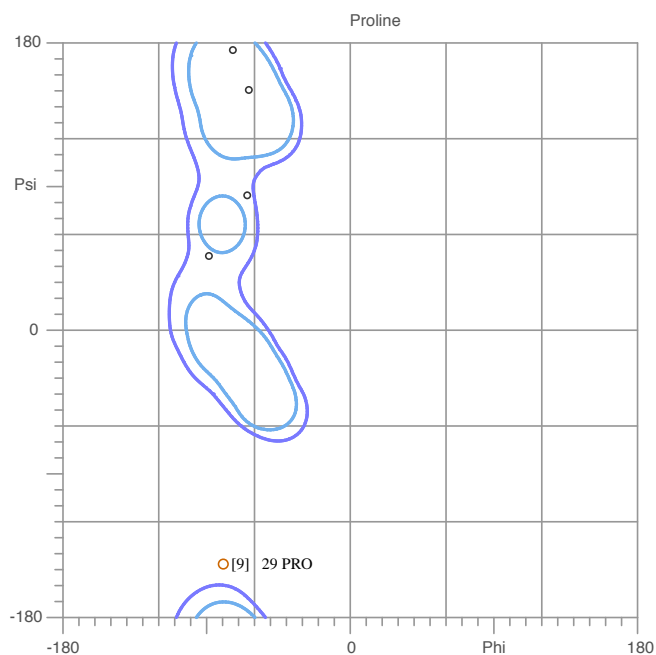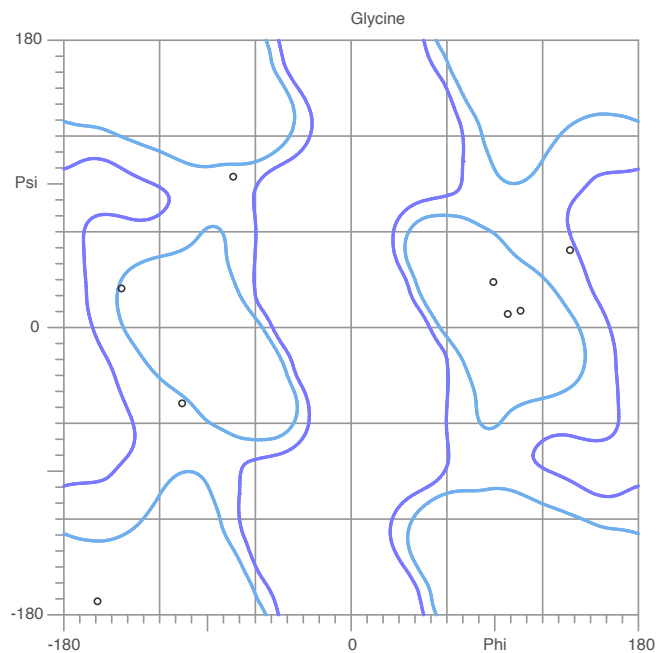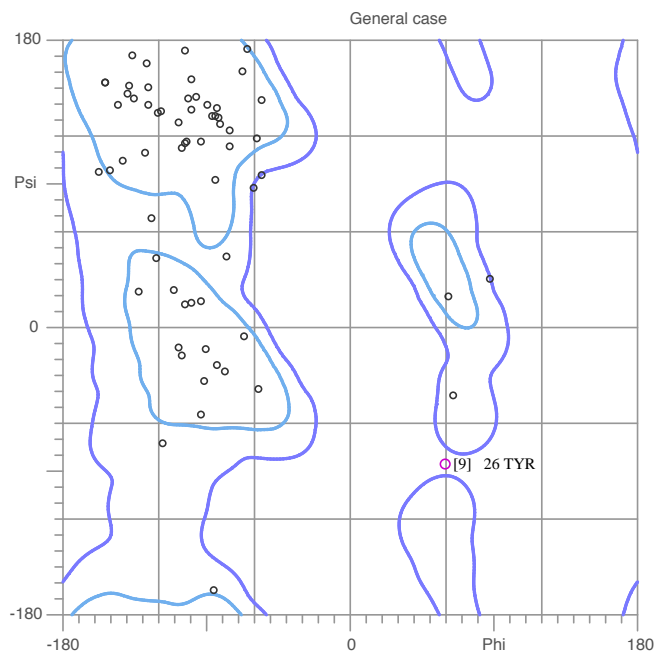# MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 8

81.7% (67/82) of all residues were in favored (98%) regions.
96.3% (79/82) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
   [8]   2 ALA (-168.9, -71.1)
   [8]   22 ASN (-54.2, 89.4)
   [8]   31 HIS (-171.6, -42.9)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 9

79.3% (65/82) of all residues were in favored (98%) regions.
97.6% (80/82) of all residues were in allowed (>99.8%) regions.
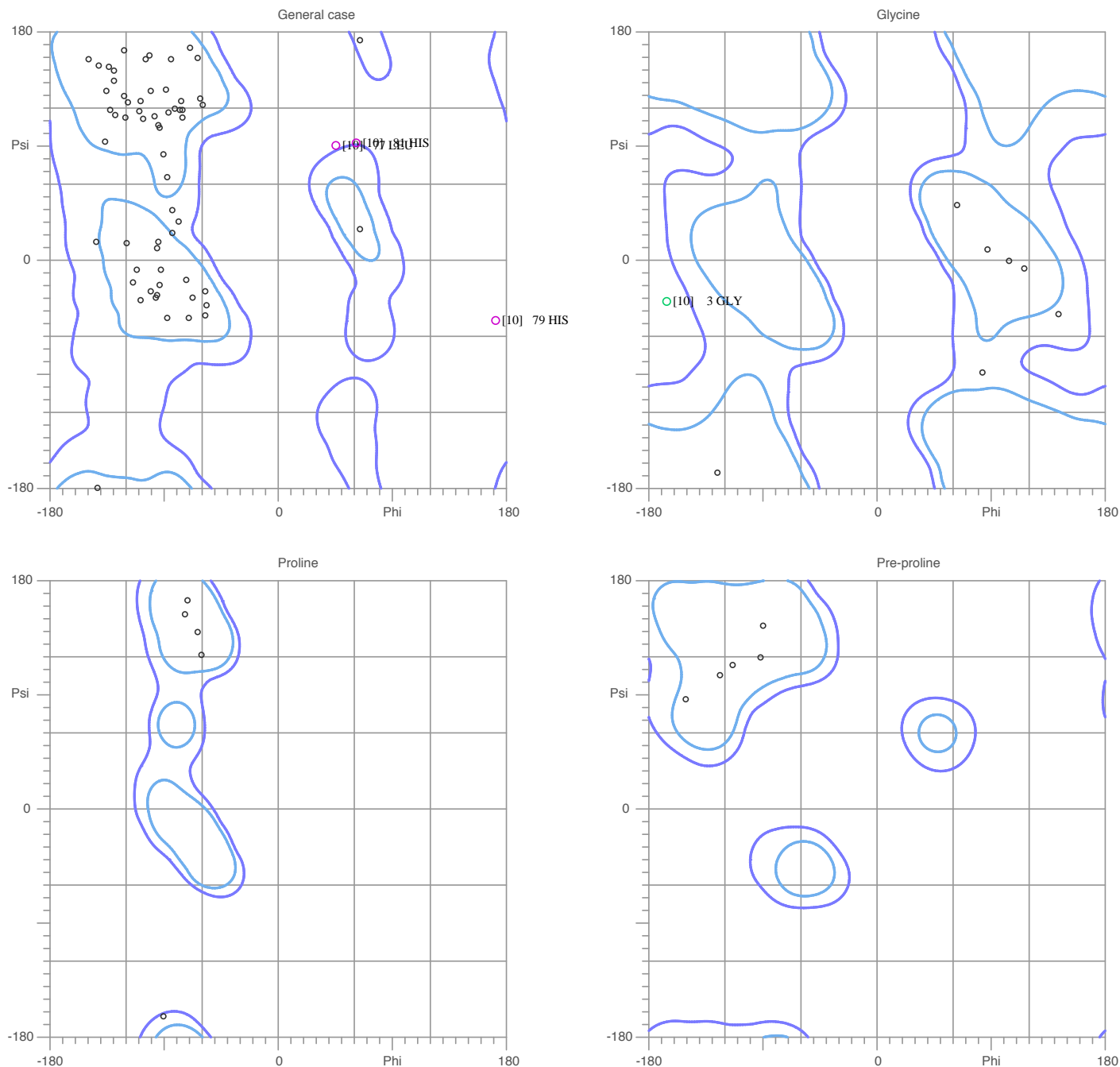
There were 2 outliers (phi, psi):
   [9]   26 TYR (59.0, -85.1)
   [9]   29 PRO (-80.0, -146.2)

MolProbity Ramachandran analysis
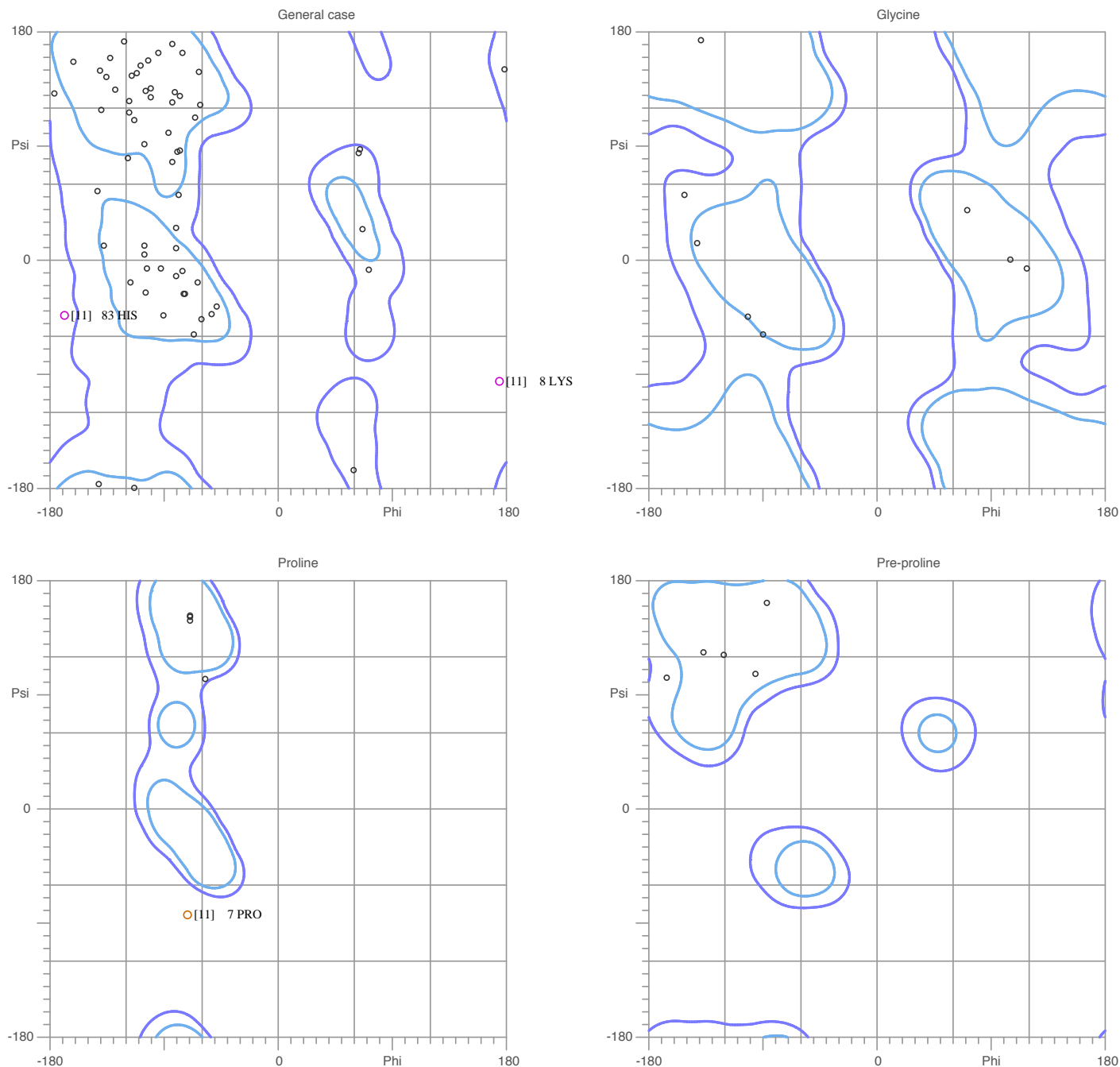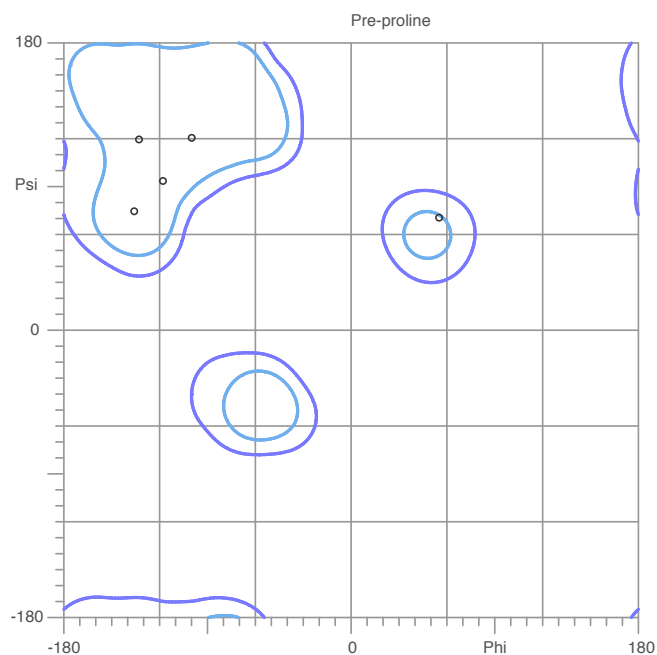
2HEQ_NMR.pdb, model 10
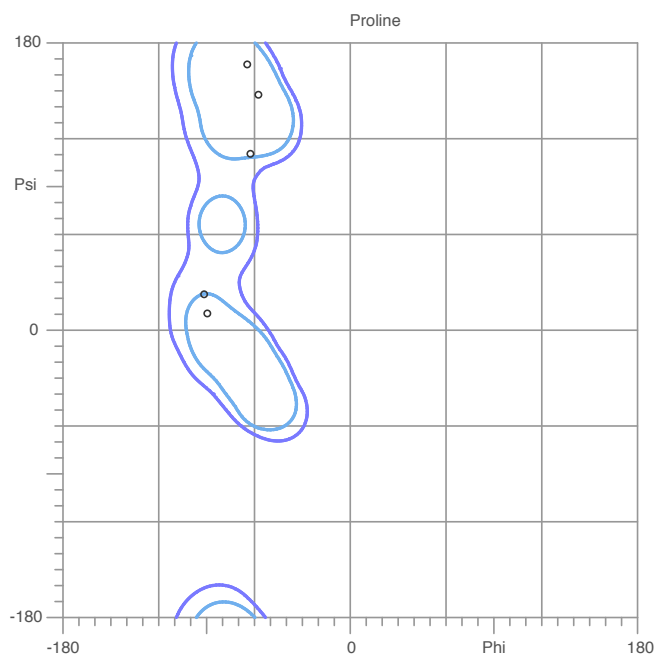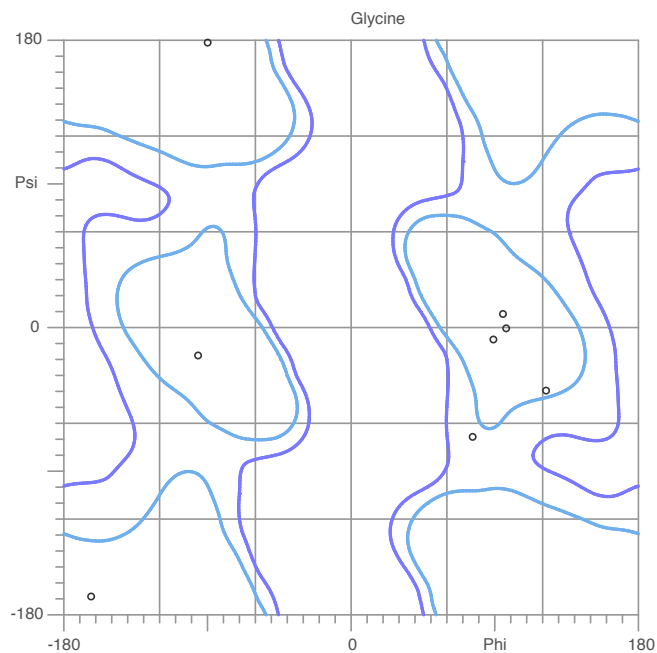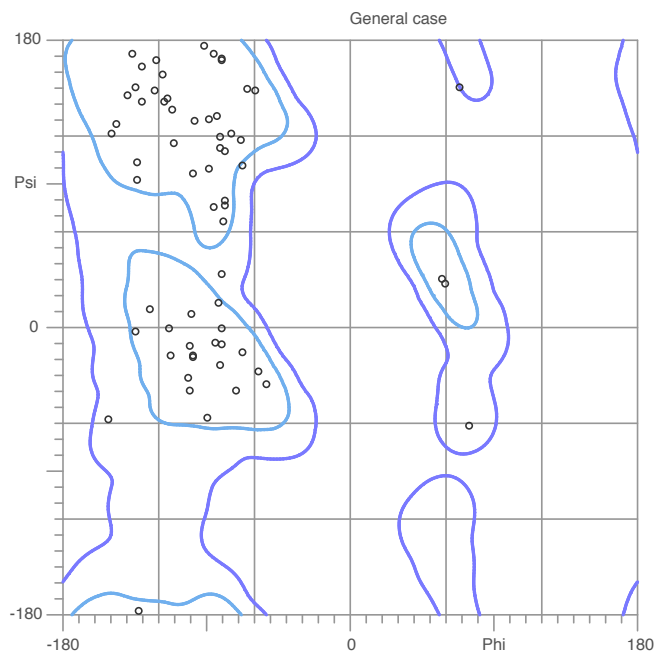

85.4% (70/82) of all residues were in favored (98%) regions.
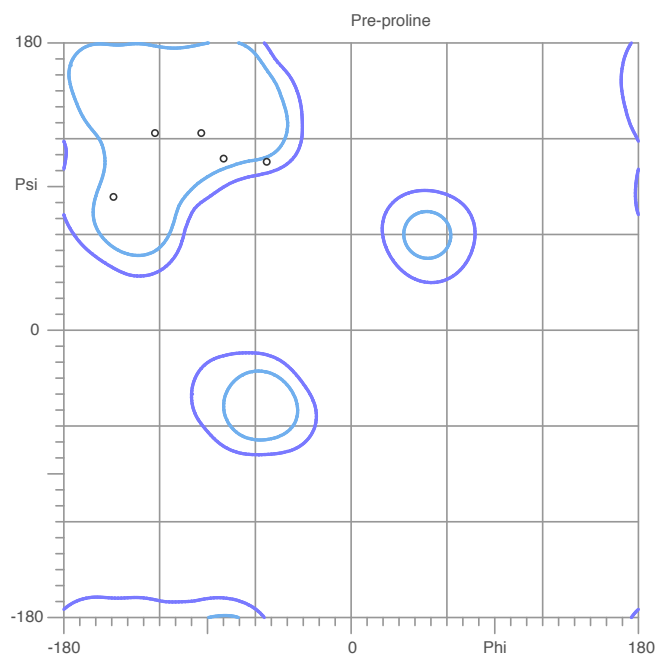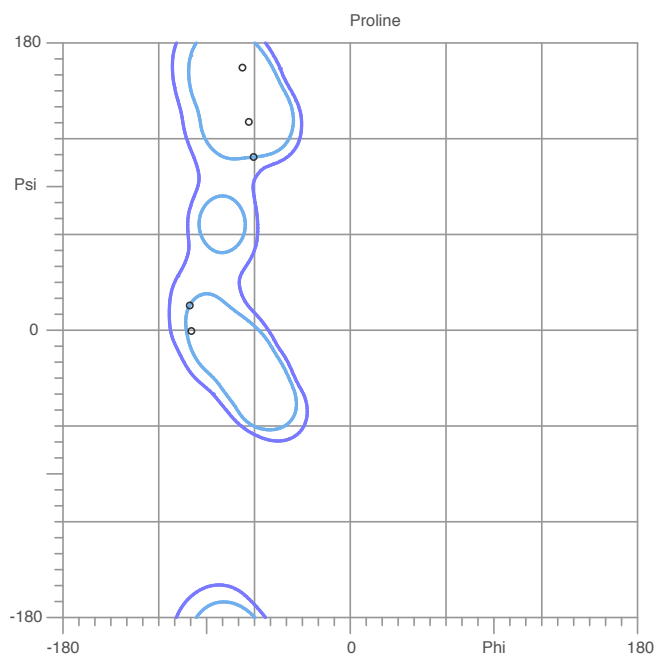95.1% (78/82) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
    [10]   3 GLY (-166.3, -32.9)
    [10]   77 LEU (45.5, 91.2)
    [10]   79 HIS (171.8, -47.6)
    [10]   81 HIS (61.0, 93.4)

MolProbity Ramachandran analysis

General case

Glycine

Proline

Pre-proline

80.5% (66/82) of all residues were in favored (98%) regions.

96.3% (79/82) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
  [11]   7 PRO (-72.3, -83.4)
  [11]   8 LYS (174.0, -95.7)
  [11]   83 HIS (-169.1, -43.8)

MolProbity Ramachandran analysis

92.7% (76/82) of all residues were in favored (98%) regions.
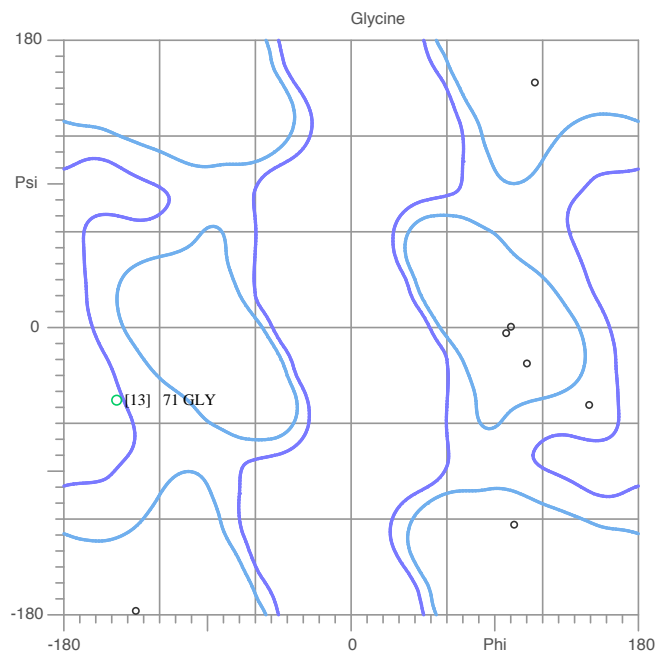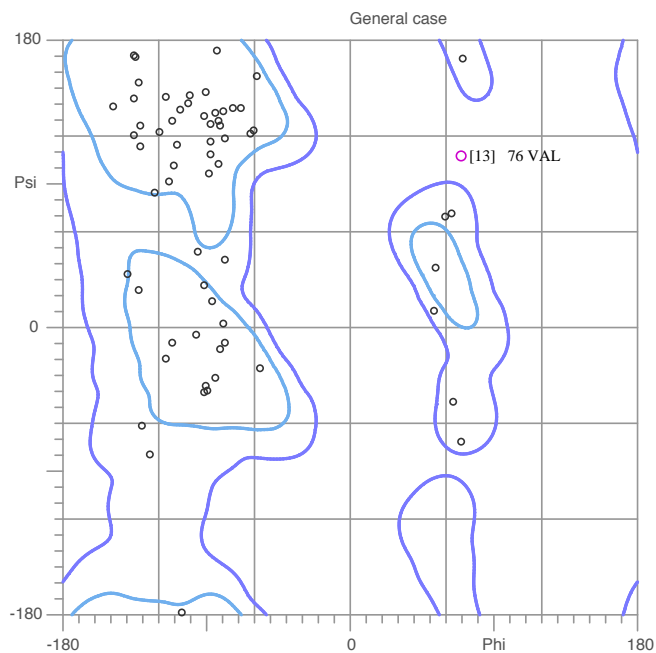100.0% (82/82) of all residues were in allowed (>99.8%) regions.

There were no outliers.

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 13

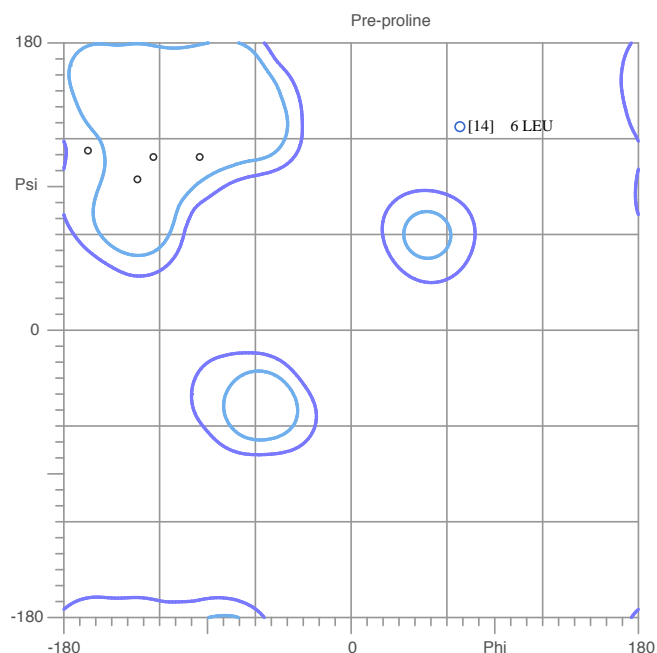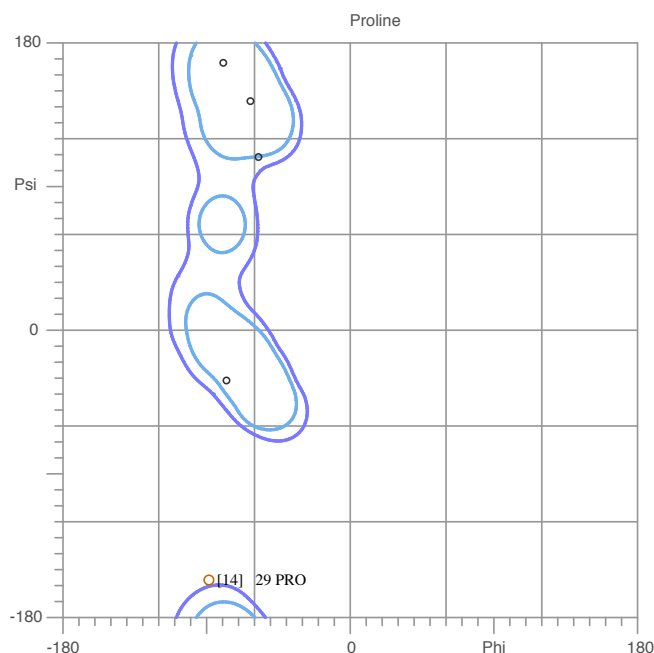General case
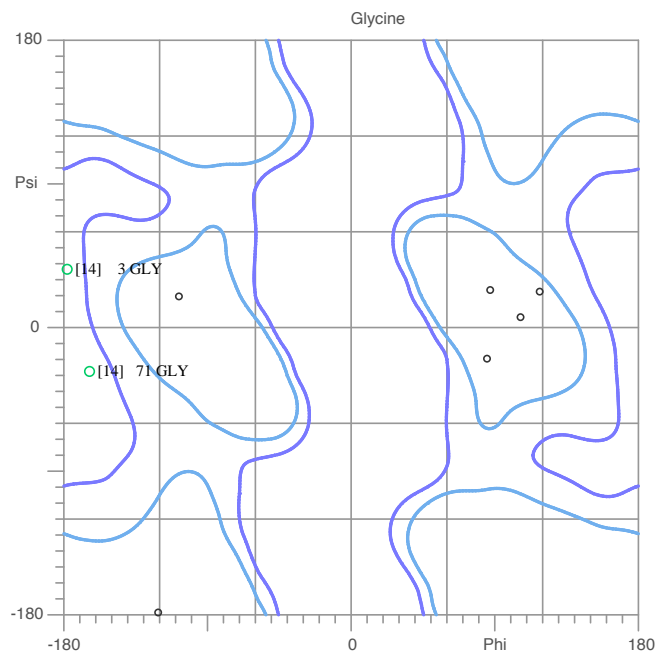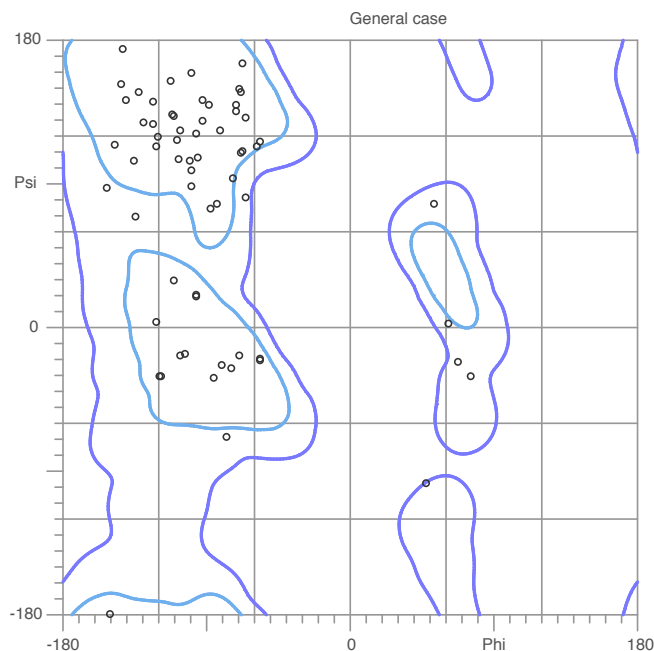

Glycine

Proline

Pre-proline

80.5% (66/82) of all residues were in favored (98%) regions.
97.6% (80/82) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
    [13]   71 GLY (-147.3, -45.5)
    [13]   76 VAL (69.0, 108.5)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 14

General case
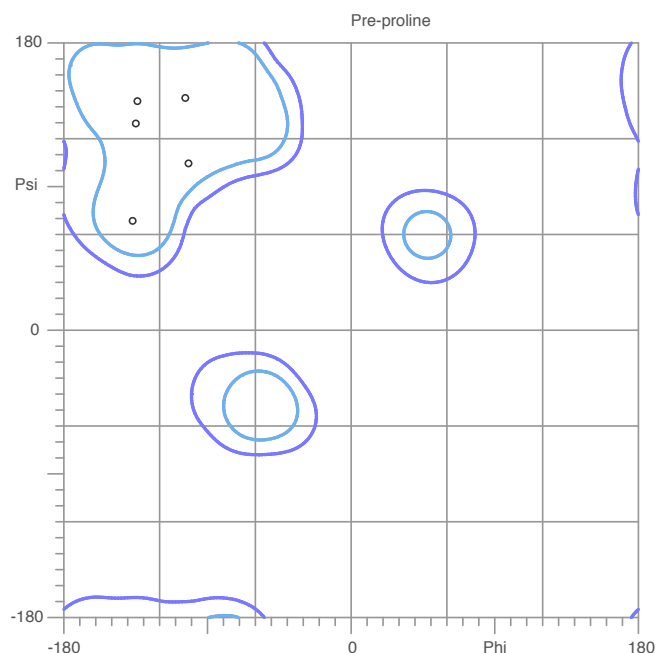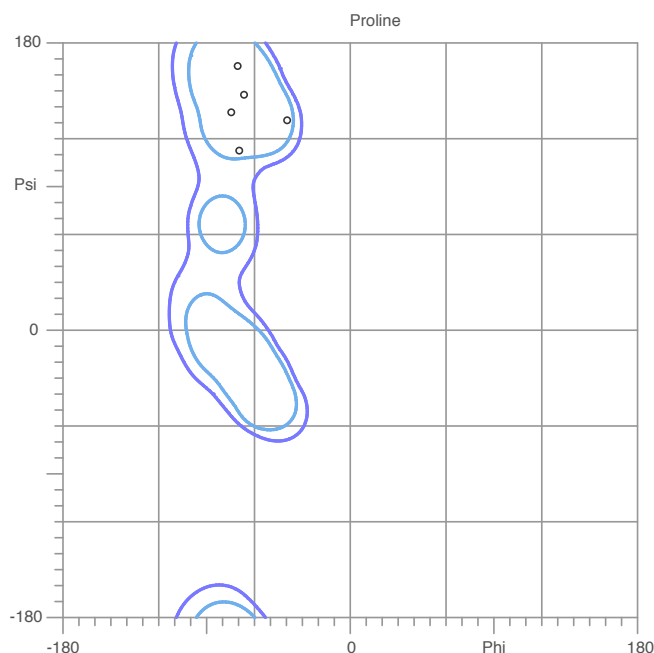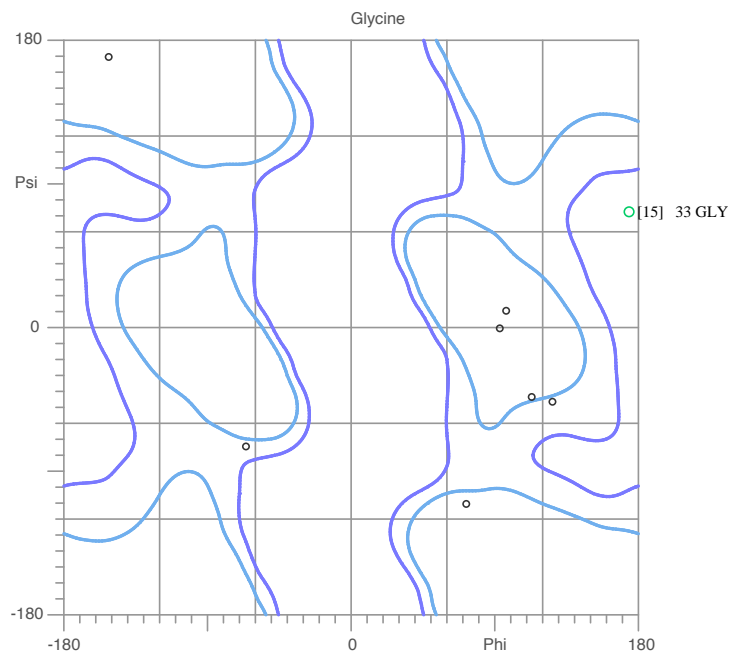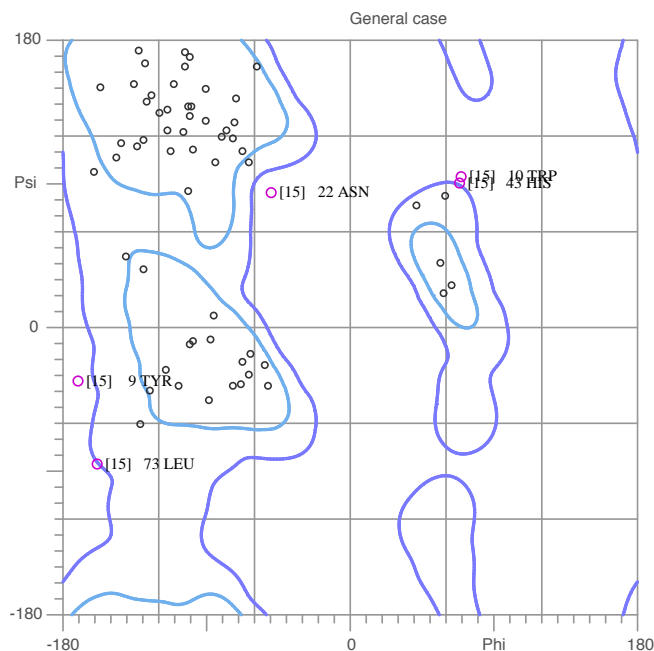
Glycine

Proline

Pre-proline

82.9% (68/82) of all residues were in favored (98%) regions.
95.1% (78/82) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
    [14]   3 GLY (-178.2, 37.1)
    [14]   6 LEU (68.1, 128.6)
    [14] 29 PRO (-89.1, -156.6)
    [14] 71 GLY (-164.5, -27.3)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 15

82.9% (68/82) of all residues were in favored (98%) regions.
92.7% (76/82) of all residues were in allowed (>99.8%) regions.
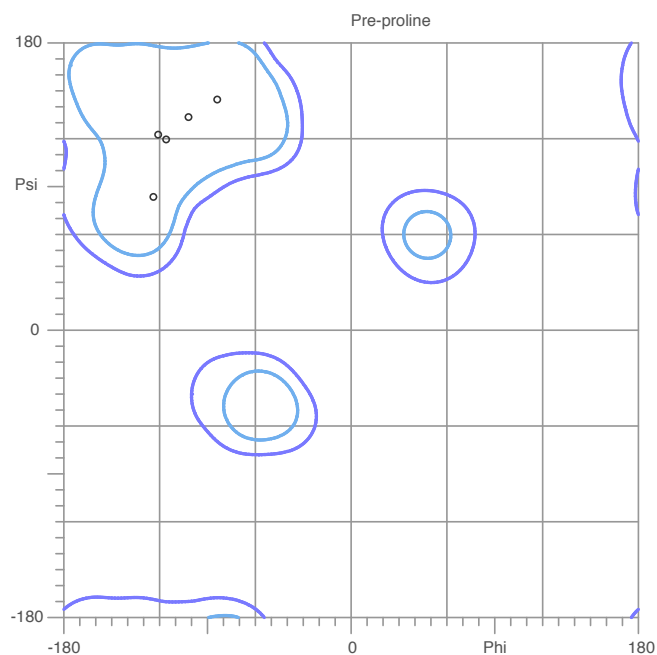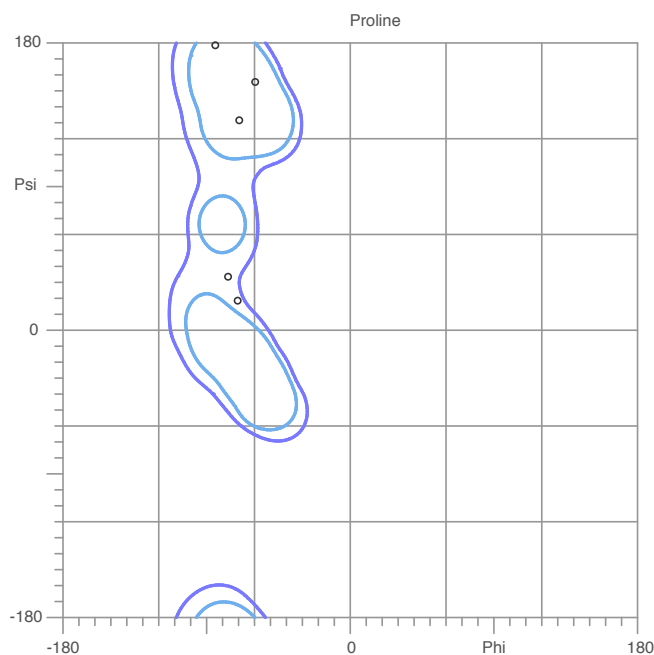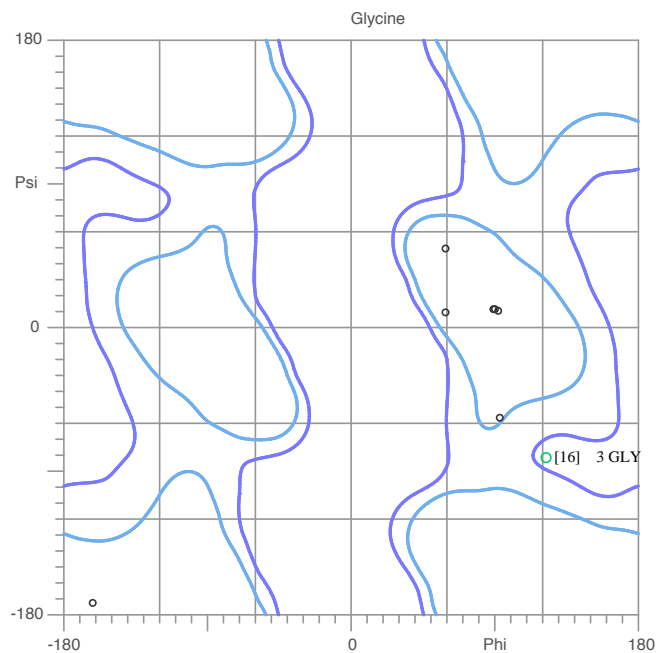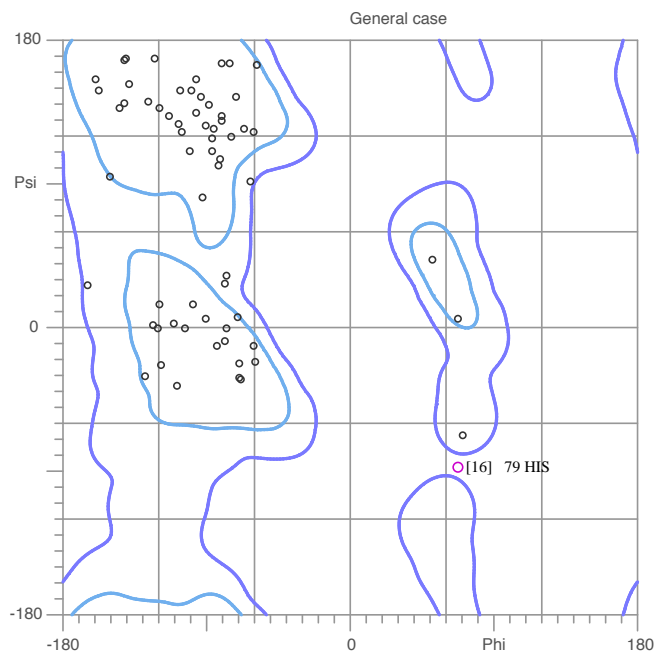
There were 6 outliers (phi, psi):

   [15]   9 TYR (-171.9, -33.4)

[15]   10 TRP (69.9, 95.9)
[15]   22 ASN (-50.7, 85.9)
[15]   33 GLY (175.0, 74.0)
[15]   43 HIS (68.1, 92.0)
[15]   73 LEU (-159.8, -85.4)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 16

87.8% (72/82) of all residues were in favored (98%) regions.
97.6% (80/82) of all residues were in allowed (>99.8%) regions.
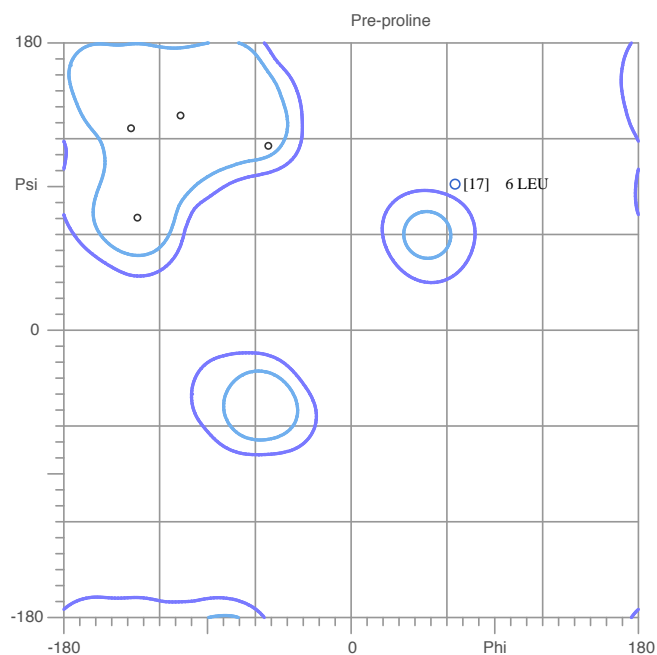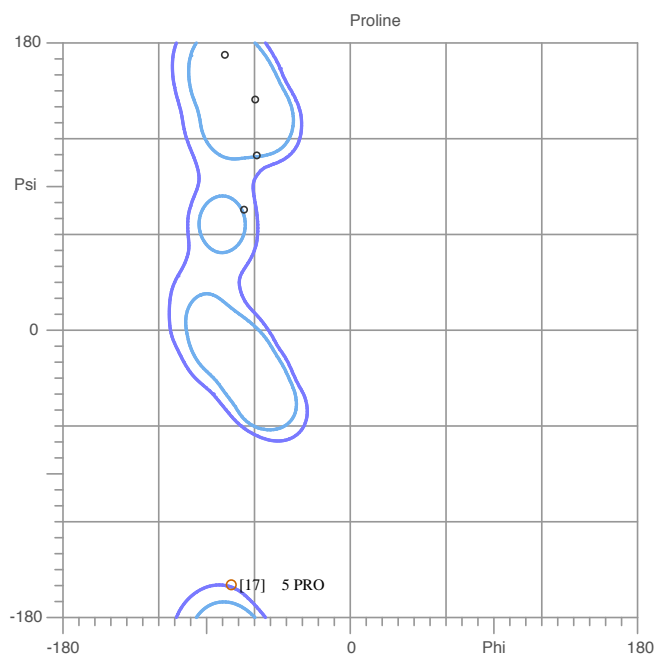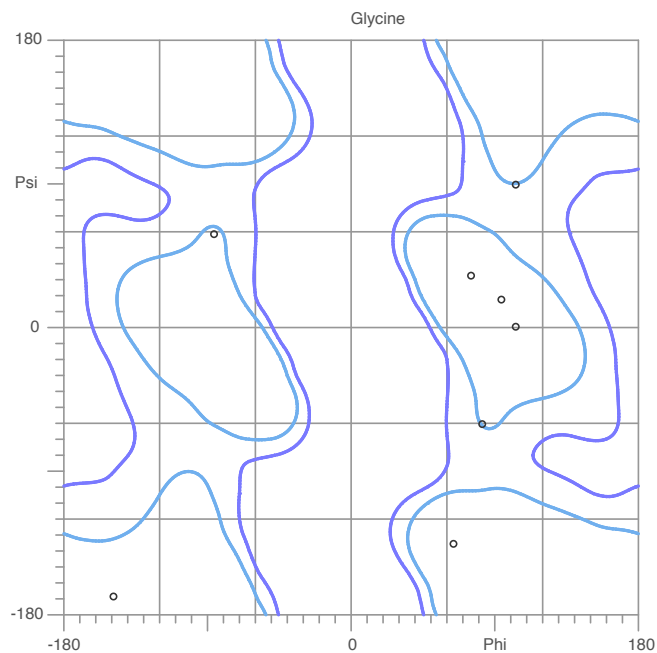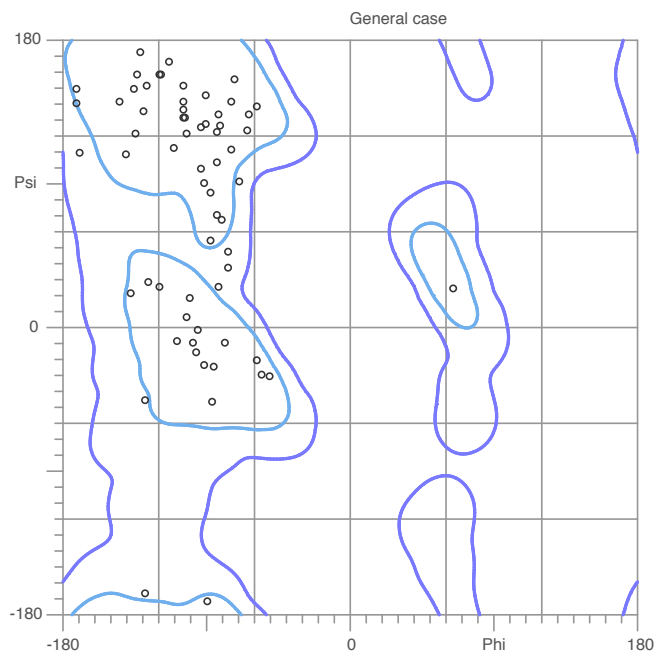
There were 2 outliers (phi, psi):
    [16]   3 GLY (123.0, -81.7)
    [16]   79 HIS (67.9, -87.8)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 17

86.6% (71/82) of all residues were in favored (98%) regions.
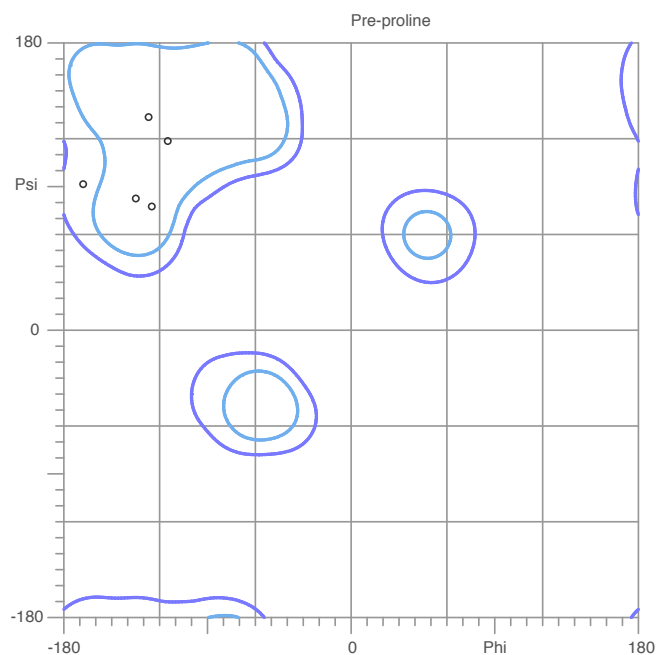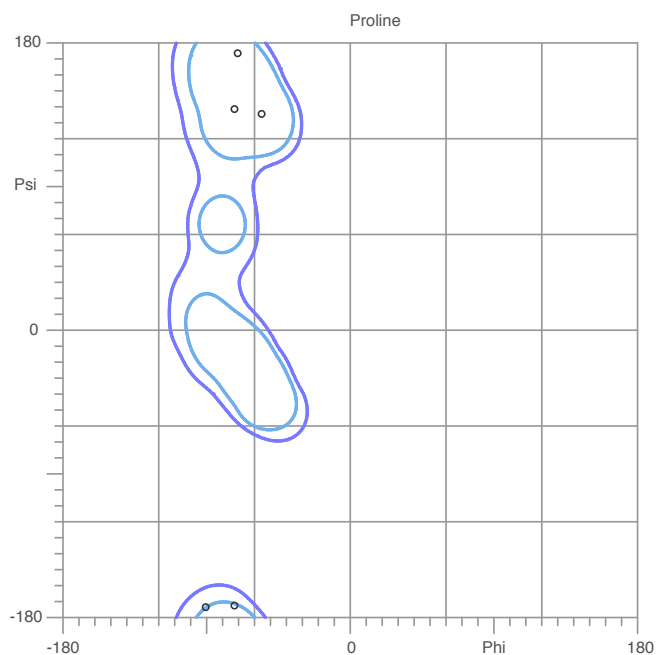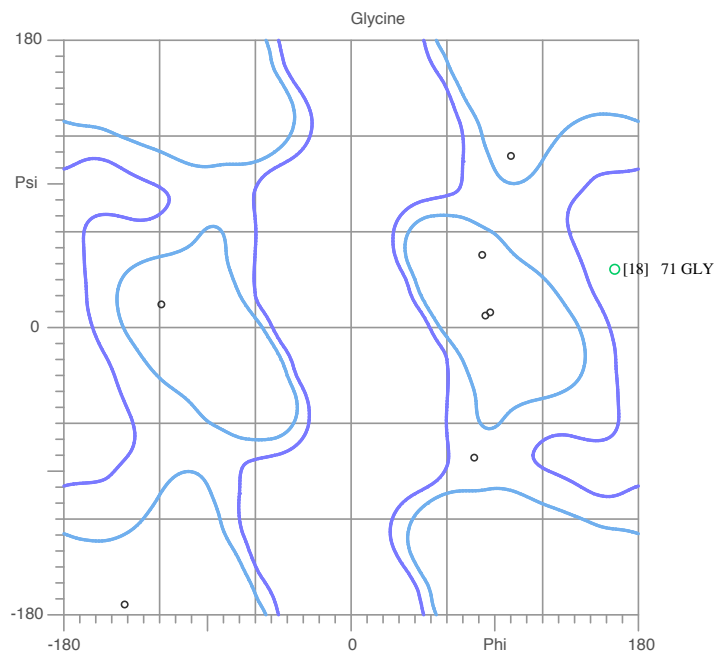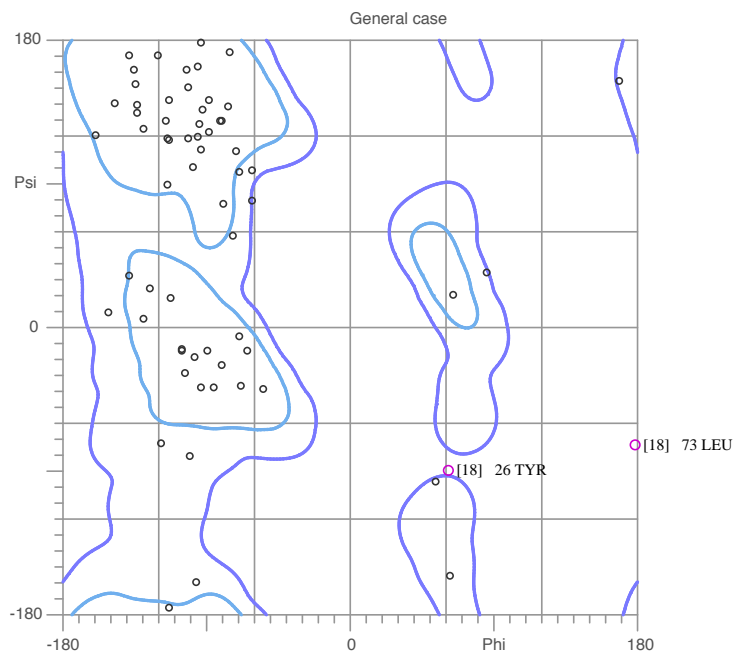97.6% (80/82) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
   [17]   5 PRO (-75.3, -159.4)
   [17]   6 LEU (65.8, 92.3)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 18

General case

Glycine

O[18] 71 GLY

O[18] 73 LEU
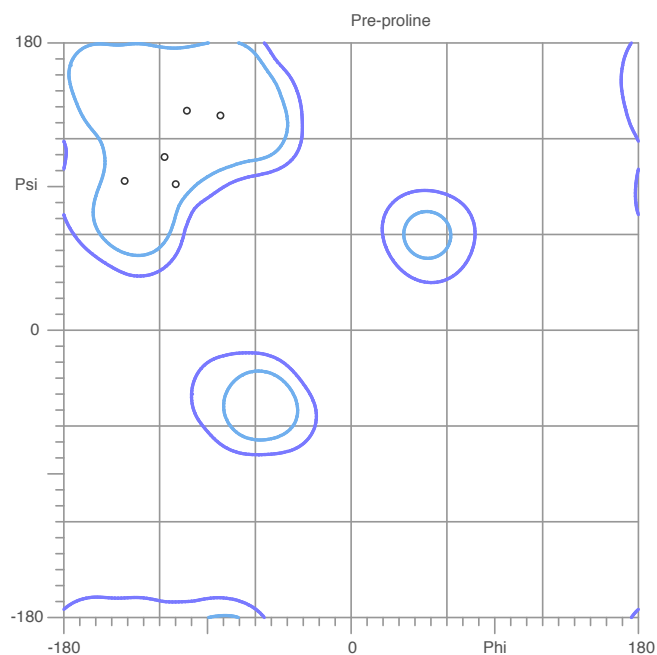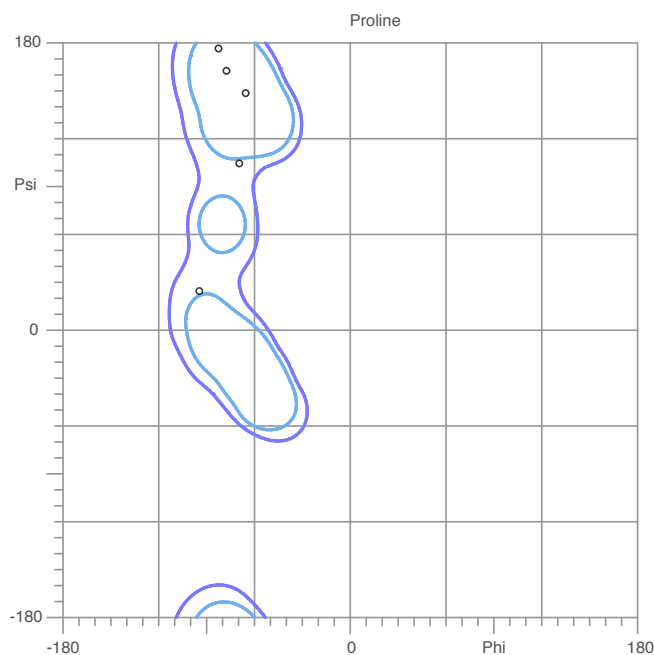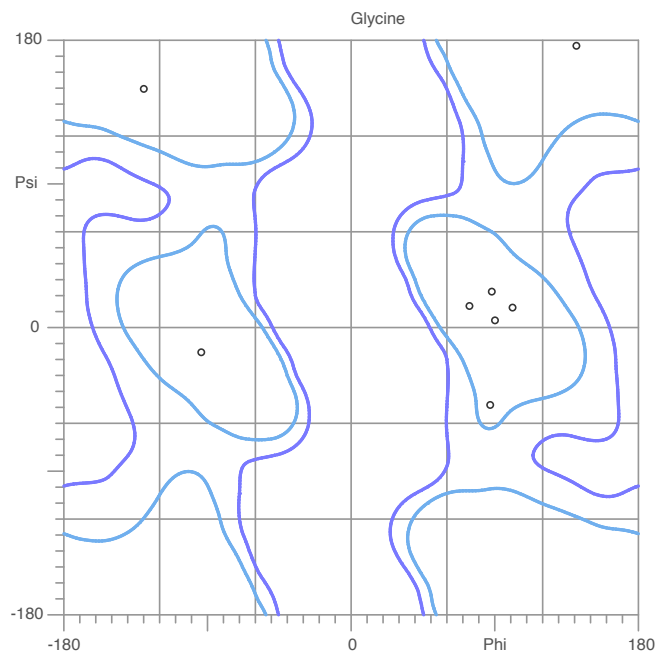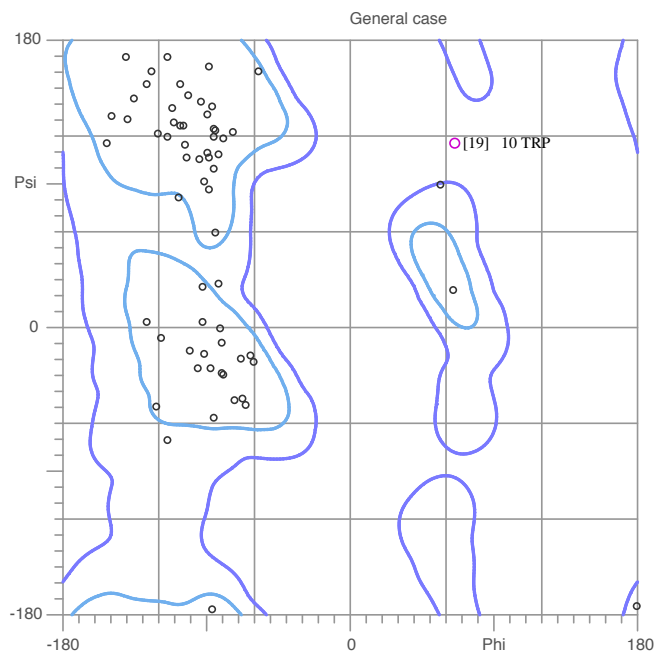
O[18] 26 TYR

Proline

Pre-proline

76.8% (63/82) of all residues were in favored (98%) regions.
96.3% (79/82) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
   [18]   26 TYR (61.3, -89.1)
   [18]   71 GLY (165.3, 37.6)
   [18]   73 LEU (178.0, -73.9)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 19

90.2% (74/82) of all residues were in favored (98%) regions.
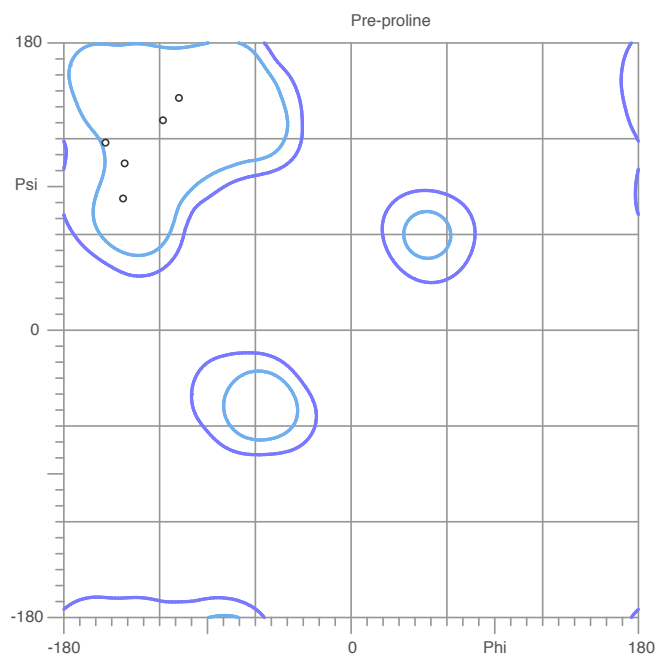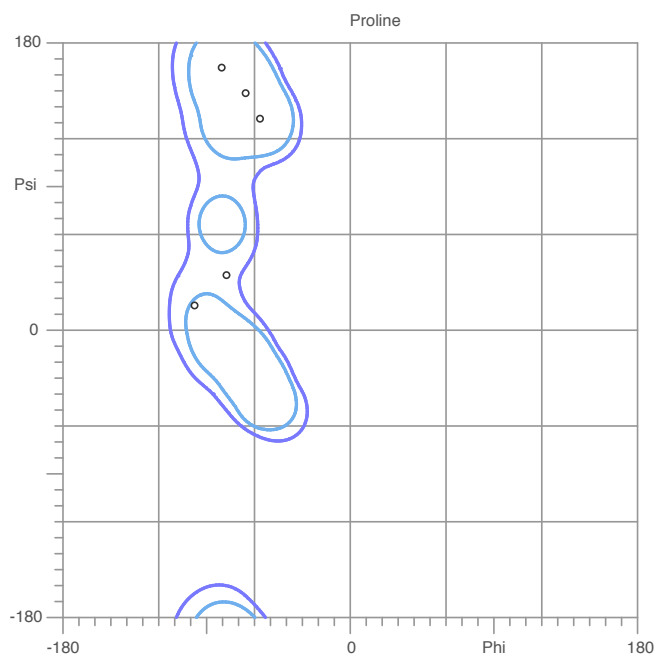98.8% (81/82) of all residues were in allowed (>99.8%) regions.
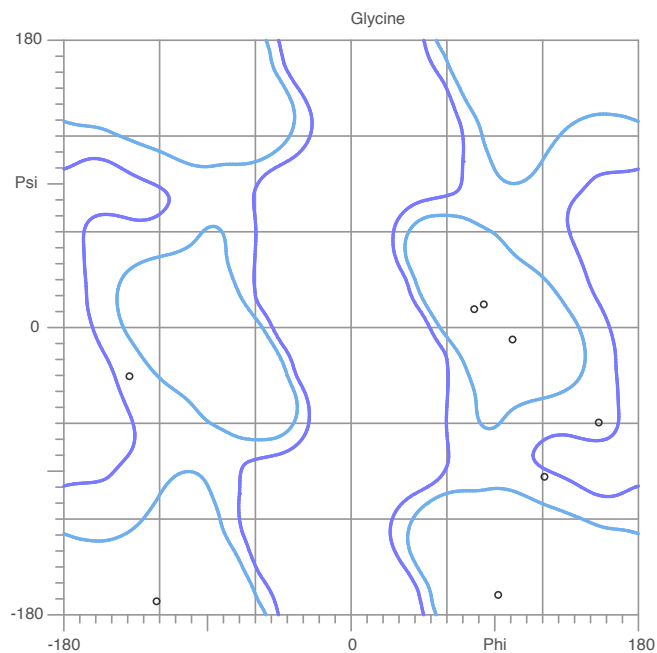
There were 1 outliers (phi, psi):
   [19]   10 TRP (65.9, 116.5)

MolProbity Ramachandran analysis

2HEQ_NMR.pdb, model 20

General case

Glycine

Proline

Pre-proline

84.1% (69/82) of all residues were in favored (98%) regions.
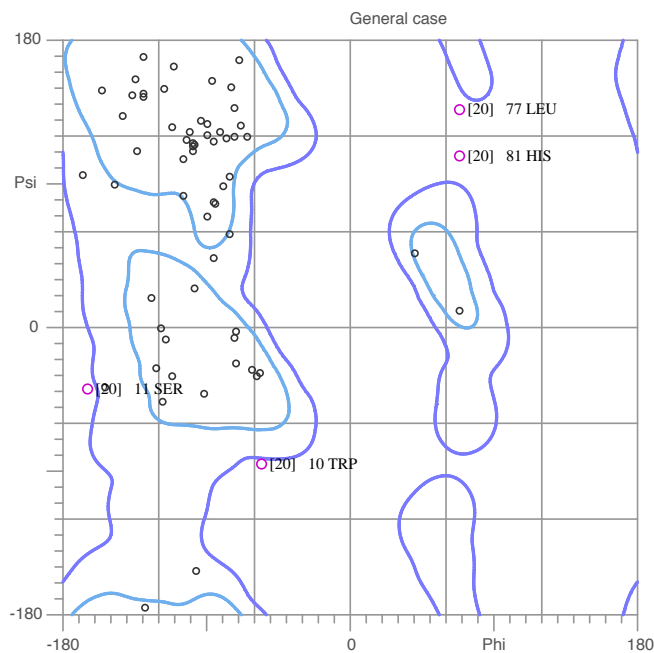95.1% (78/82) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
   [20]   10 TRP (-56.8, -85.6)
   [20]   11 SER (-165.3, -38.4)
   [20]   77 LEU (68.2, 137.9)
   [20]   81 HIS (68.2, 108.3)