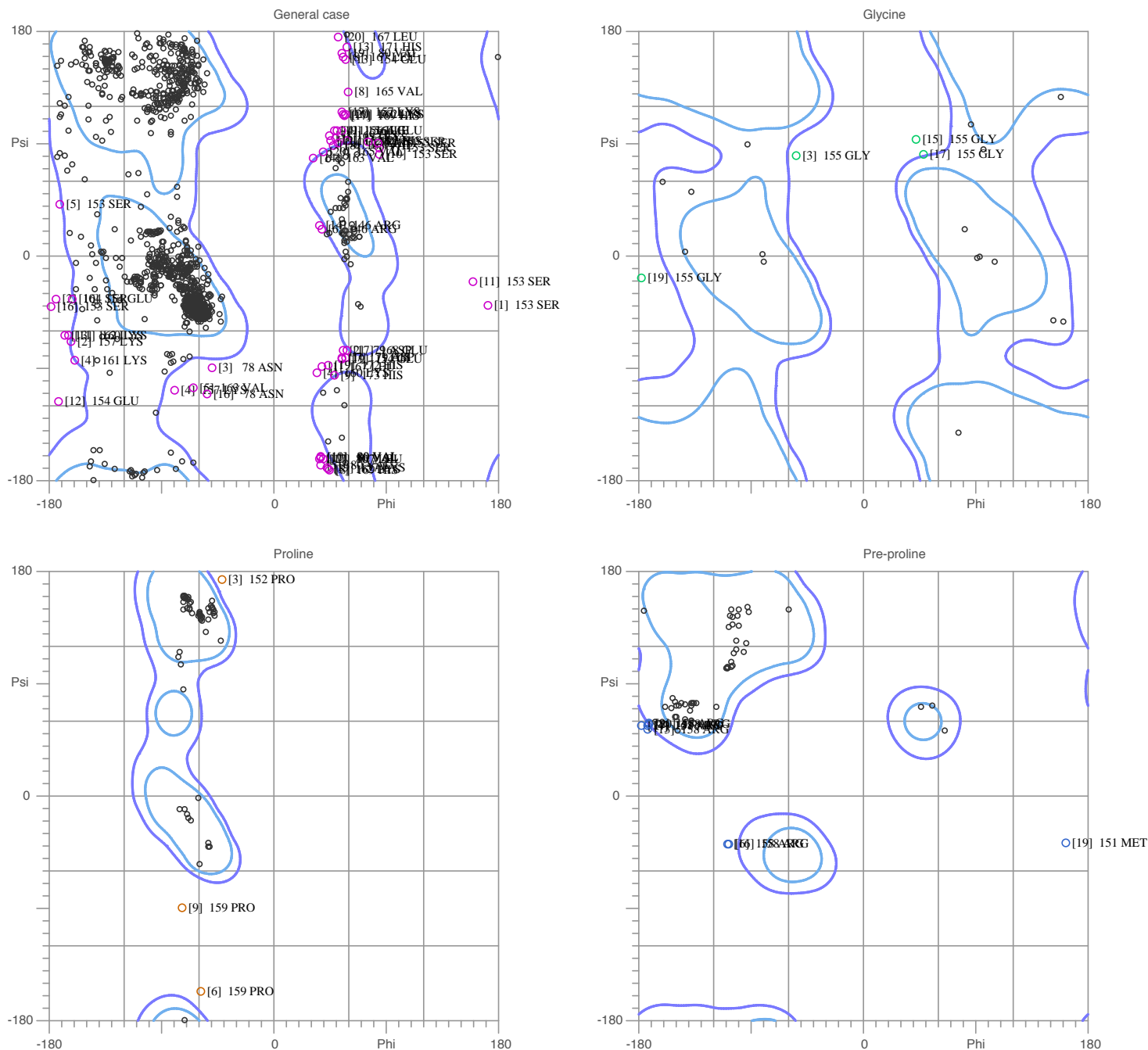


MolProbity Ramachandran analysis

2KIW_NMR.pdb, all models



91.3% (1590/2180) of all residues were in favored (98%) regions.
96.6% (2106/2180) of all residues were in allowed (1-99.9%) regions.

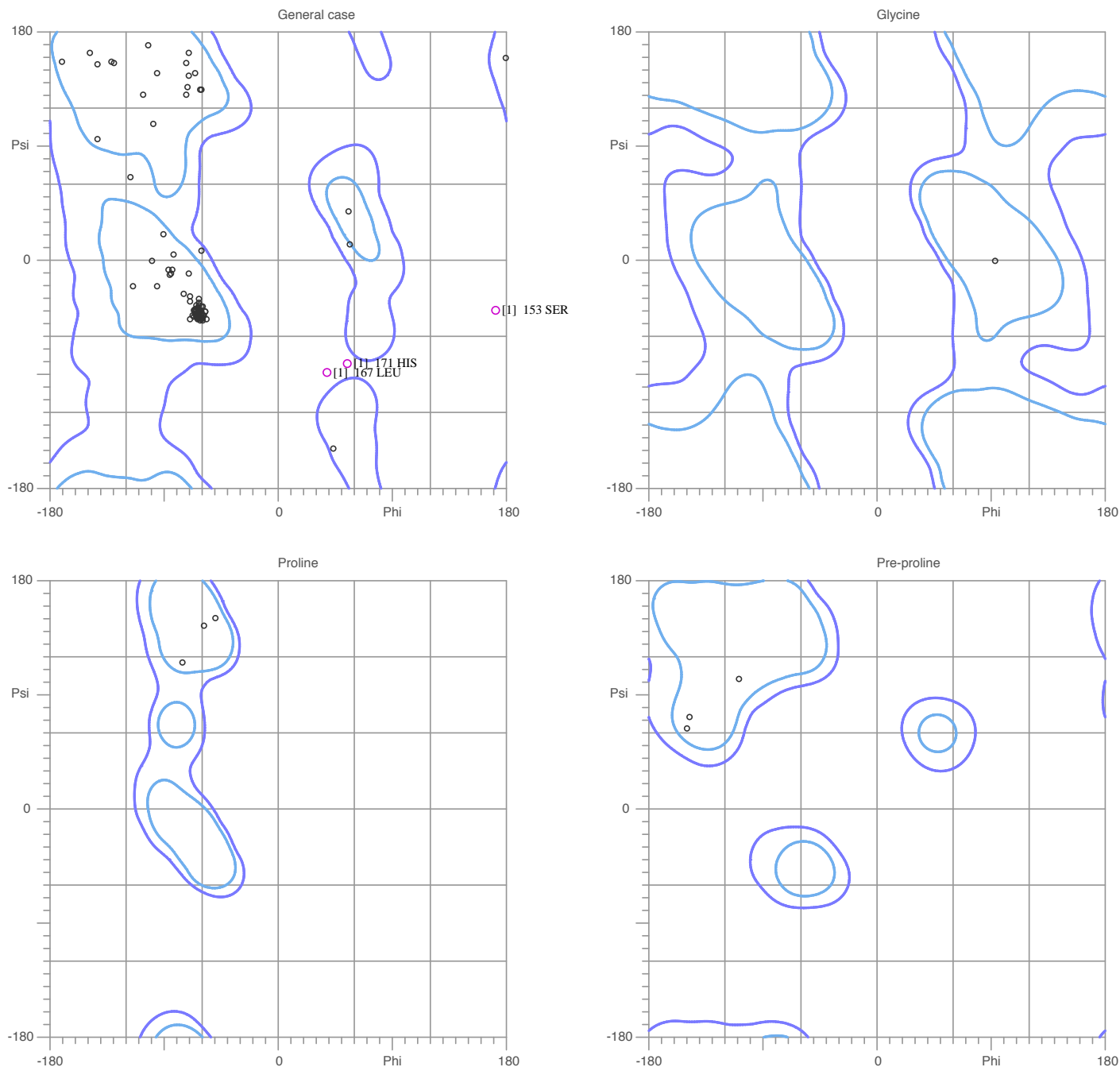
There were 74 outliers (phi, psi):

(1) 151 SER (171.0, 39.9)
(2) 167 LEU (30.0, 88.6)
(3) 171 HIS (34.1, 81.1)
(4) 79 ASP (55.4, 75.9)
(5) 157 LYS (-160.6, 68.3)
(6) 164 SER (179.3, 34.4)
(7) 78 ASN (-80.4, -80.2)
(8) 152 PRO (-43.0, 174.2)
(9) 155 GLY (-54.2, 81.5)
(10) 162 LYS (43.5, -170.3)
(11) 169 HIS (44.4, 97.3)
(12) 151 MET (-173.9, 57.8)
(13) 156 LEU (50.1, 101.7)
(14) 157 LYS (-80.2, -107.9)
(15) 160 LYS (33.0, -93.1)
(16) 161 LYS (-161.6, -84.2)
(17) 80 VAL (77.7, -167.4)
(18) 153 SER (-172.5, -62.3)
(19) 161 VAL (-65.1, -105.4)
(20) 146 ARG (34.2, 22.6)
(21) 157 LYS (69.2, 95.8)
(22) 156 ARG (108.3, 38.1)
(23) 159 PRO (-59.6, -156.5)
(24) 79 ASP (50.1, -81.3)
(25) 151 SER (84.4, 87.1)
(26) 165 VAL (59.4, 133.0)
(27) 167 LEU (55.4, 160.5)
(28) 169 HIS (44.3, -171.3)
(29) 156 ARG (-172.8, 59.2)
(30) 159 PRO (-74.9, 30.8)
(31) 171 HIS (86.5, 98.1)
(32) 80 VAL (37.5, -160.2)
(33) 151 SER (84.2, 82.3)
(34) 154 GLY (-142.8, -34.0)
(35) 80 VAL (37.1, -161.3)

(11) 153 SER (19.2, -20.0)
(12) 160 LYS (-145.4, -43.8)
(13) 166 GLY (44.7, 101.2)
(14) 172 HIS (38.7, 75.4)
(15) 80 VAL (36.9, -102.4)
(16) 154 GLY (-173.2, -116.7)
(17) 162 LYS (65.5, 93.8)
(18) 154 GLY (97.2, 158.9)
(19) 158 ARG (-175.1, 54.1)
(20) 162 LYS (-185.5, -43.6)
(21) 171 HIS (58.6, 168.4)
(22) 146 ARG (36.6, 25.5)
(23) 153 SER (55.9, 92.9)
(24) 158 ARG (-178.5, 57.9)
(25) 161 VAL (-51.6, 79.2)
(26) 170 HIS (51.4, 91.7)
(27) 155 GLY (42.5, 94.0)
(28) 78 ASN (-54.4, -110.7)
(29) 153 SER (-179.7, -40.1)
(30) 158 ARG (-109.6, -38.1)
(31) 161 LYS (58.8, 114.4)
(32) 155 GLY (68.8, 82.4)
(33) 157 LYS (54.9, 116.9)
(34) 167 LEU (19.9, -103.0)
(35) 168 GLY (38.8, 75.7)
(36) 169 HIS (36.9, 113.0)
(37) 161 VAL (-7.3, 90.0)
(38) 80 VAL (54.7, 161.1)
(39) 81 MET (-62.5, -37.9)
(40) 154 GLY (54.1, -82.6)
(41) 155 GLY (-178.4, -17.7)
(42) 156 LEU (48.7, 101.0)
(43) 157 LYS (42.1, -149.1)
(44) 172 HIS (44.0, -87.8)
(45) 153 SER (43.5, 91.9)
(46) 158 ARG (-172.5, 58.5)
(47) 162 LYS (97.2, 114.6)
(48) 165 VAL (60.0, 84.1)
(49) 167 LEU (51.0, 176.2)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 1



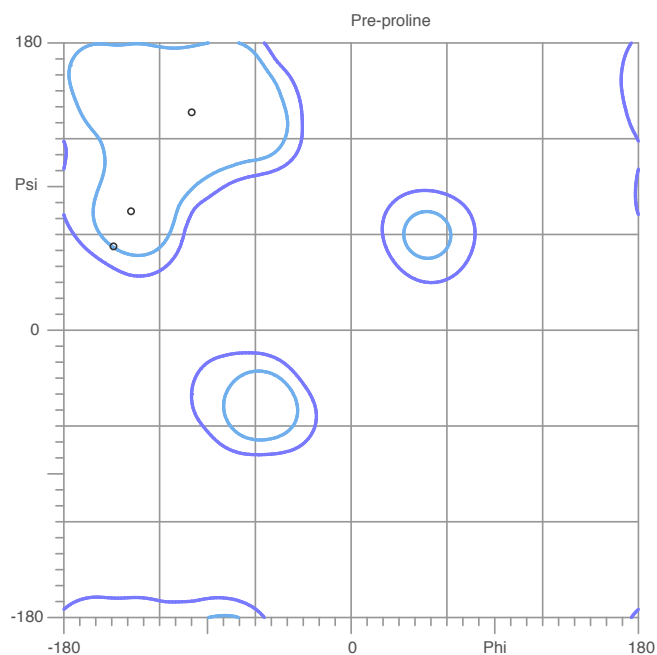
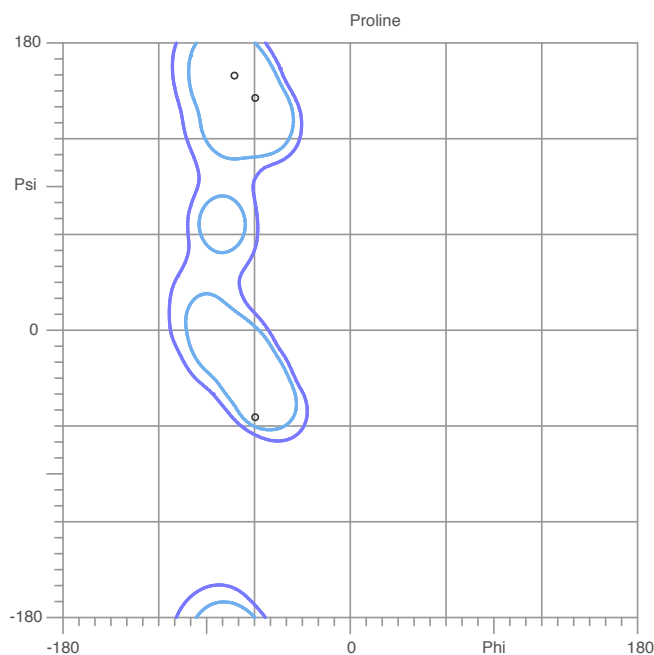
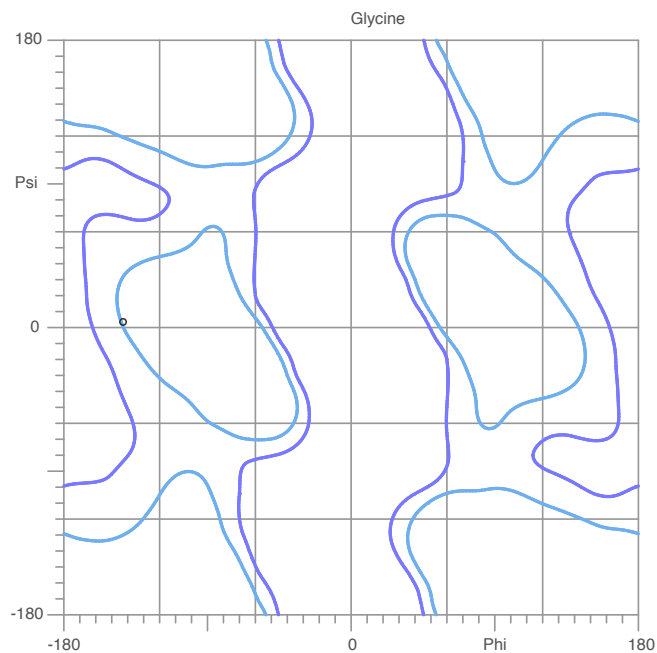
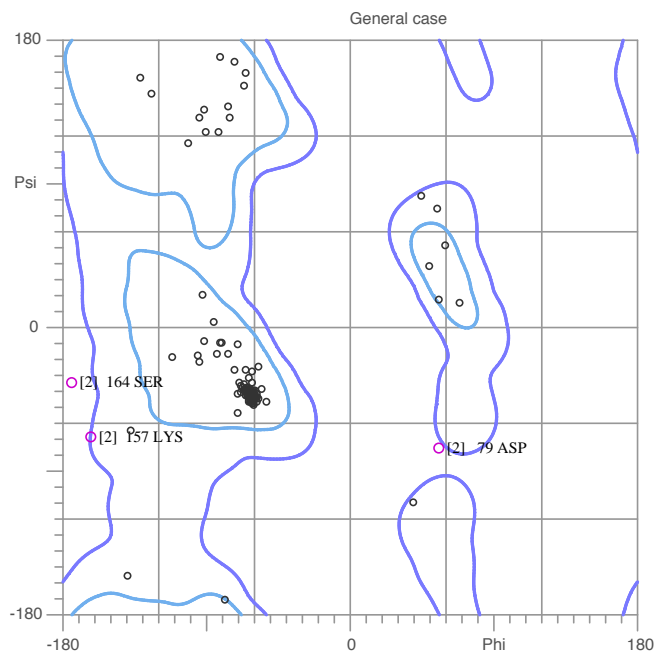
92.7% (101/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

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



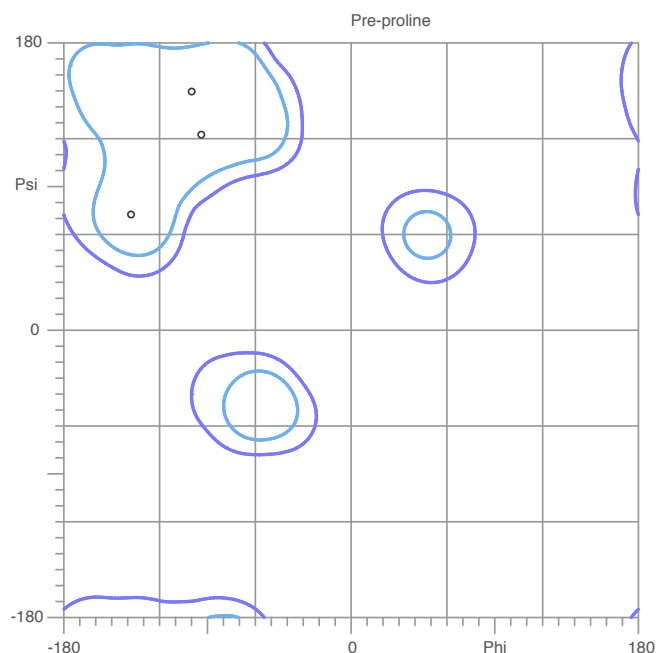
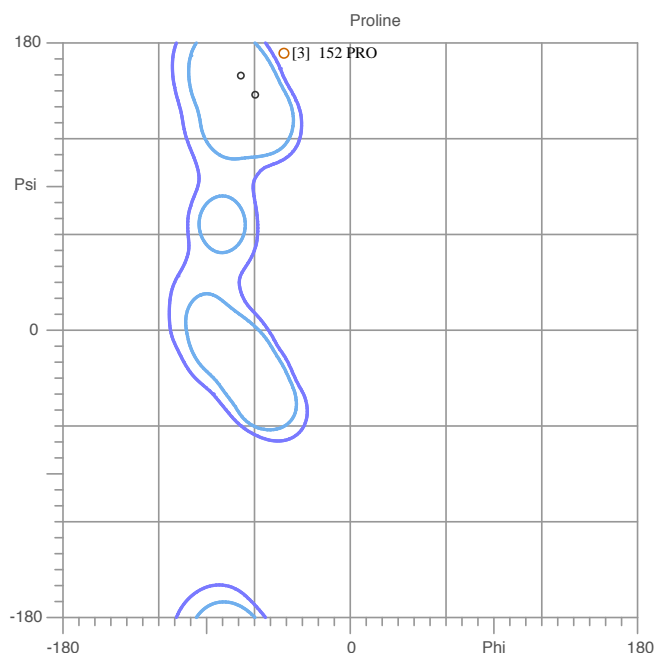
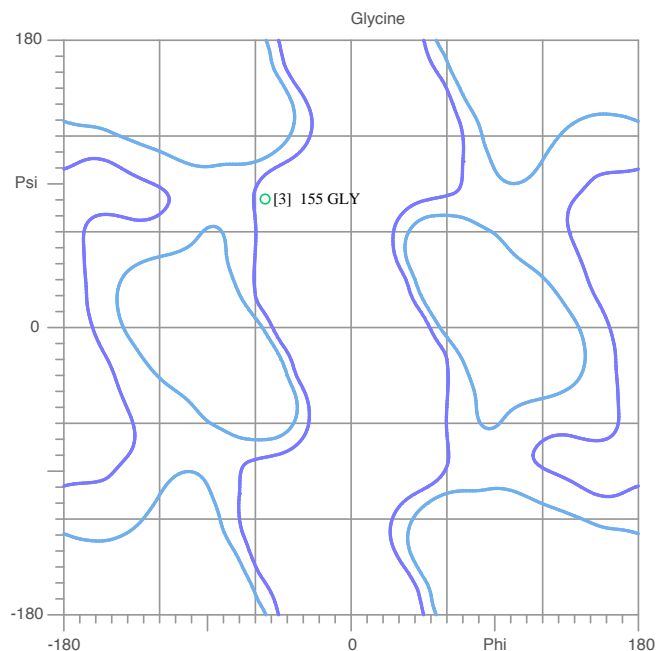
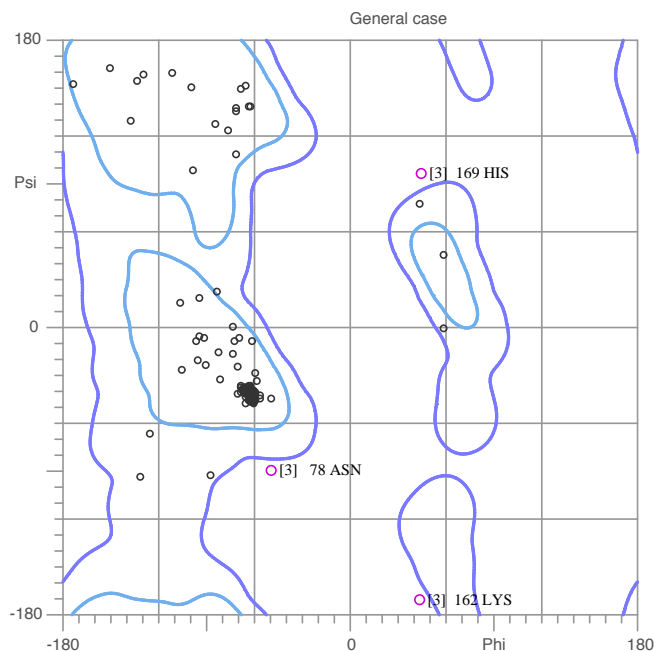
92.7% (101/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

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



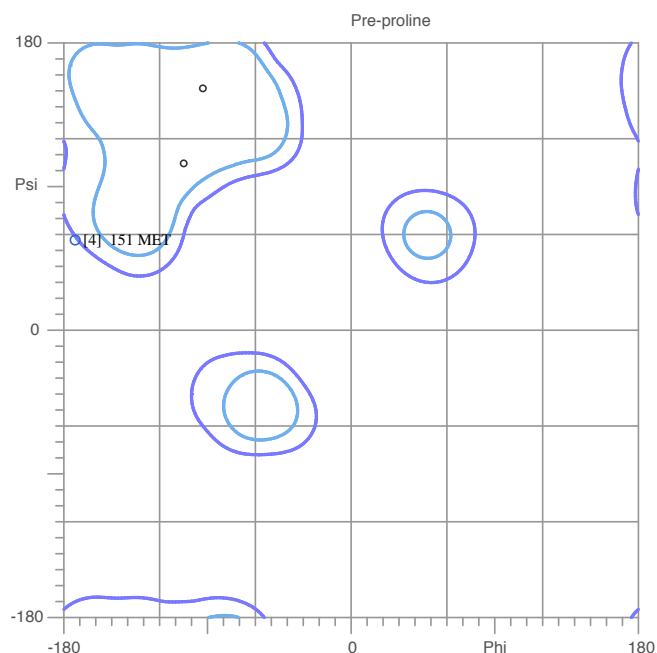
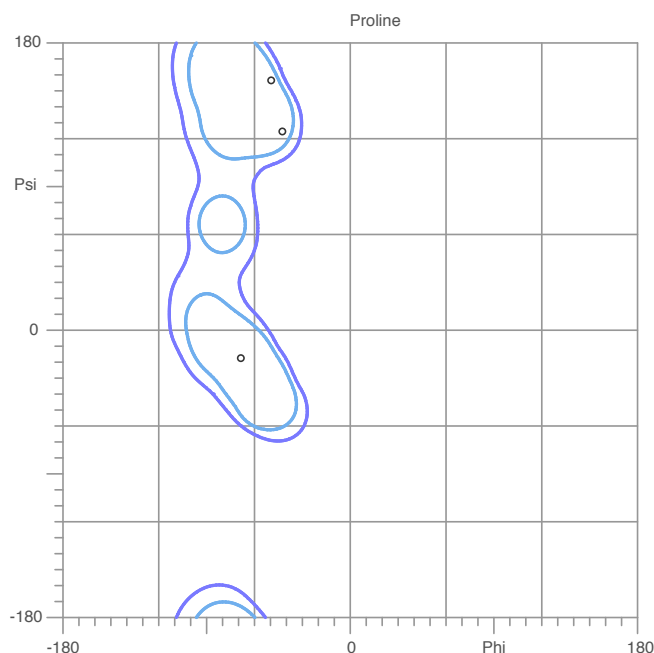
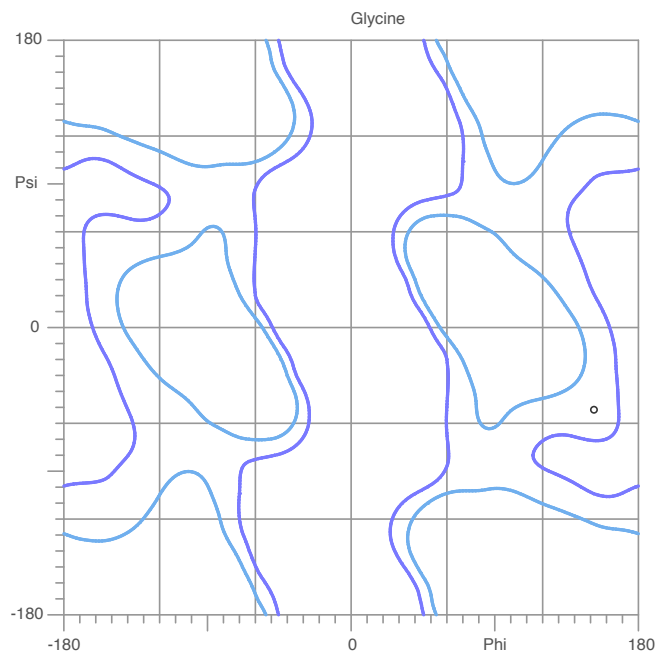
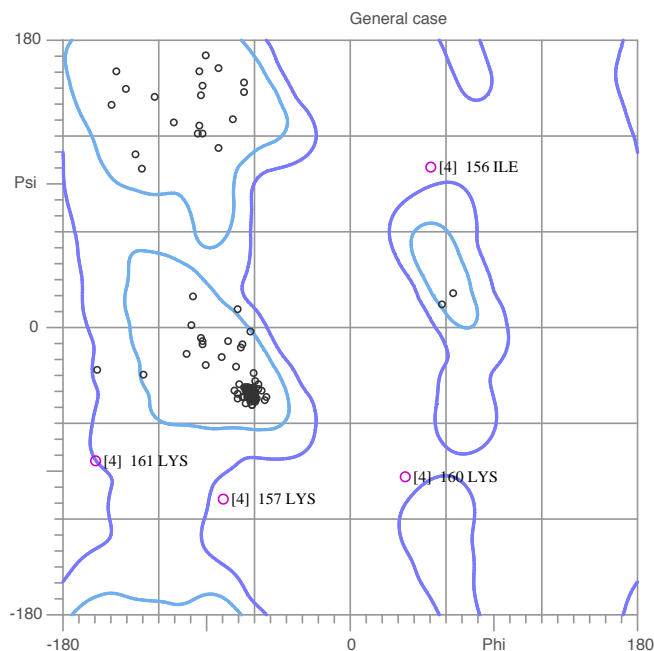
89.9% (98/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

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



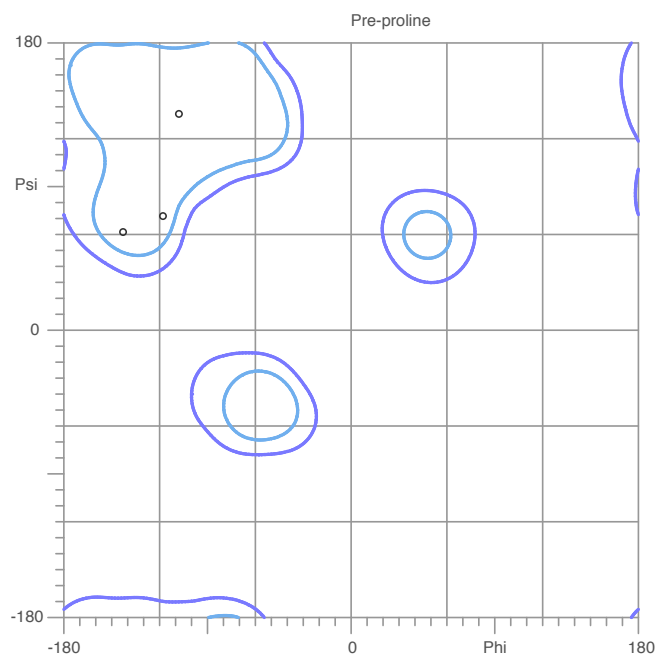
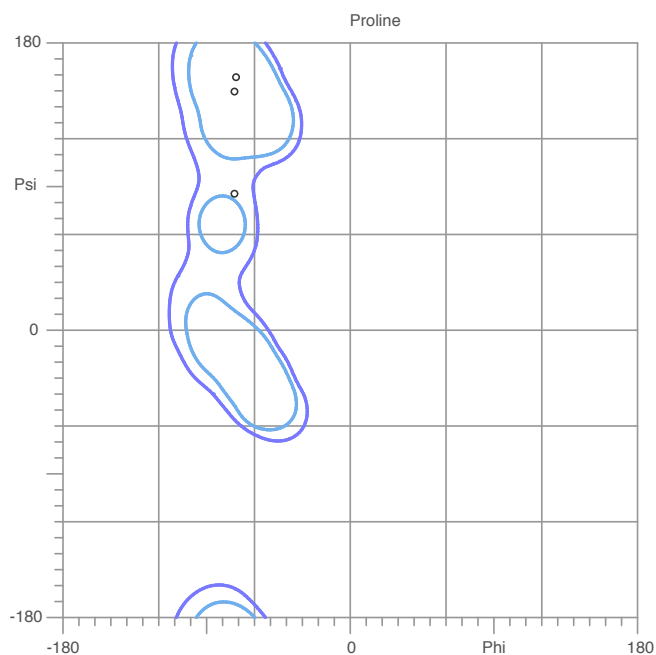
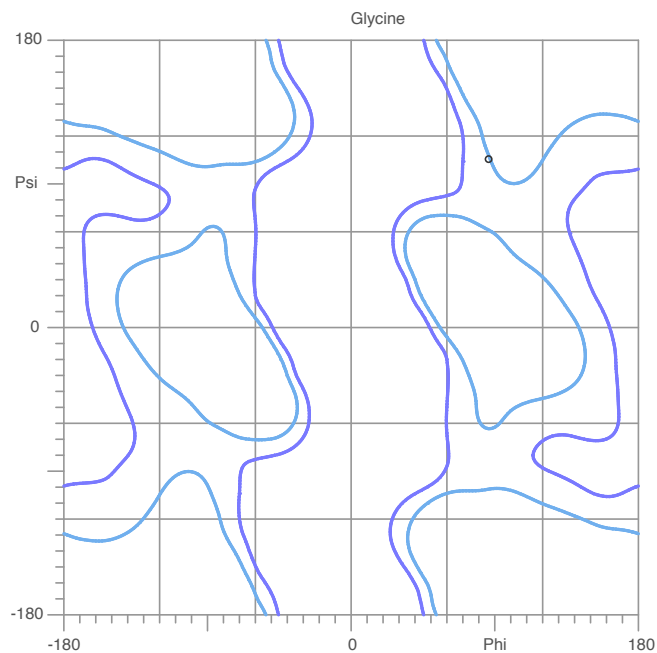
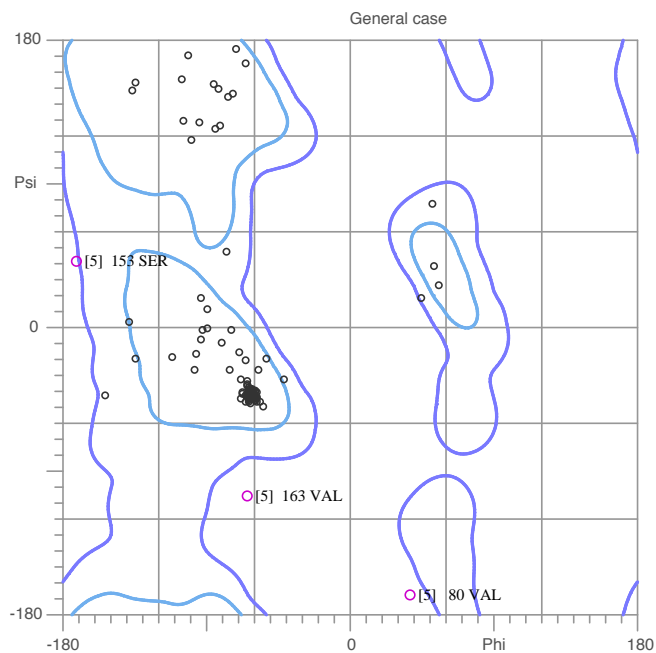
92.7% (101/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

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



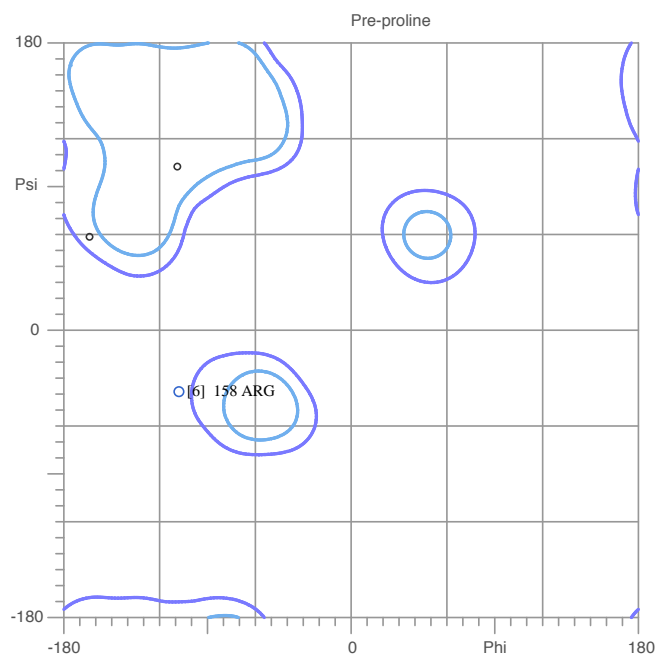
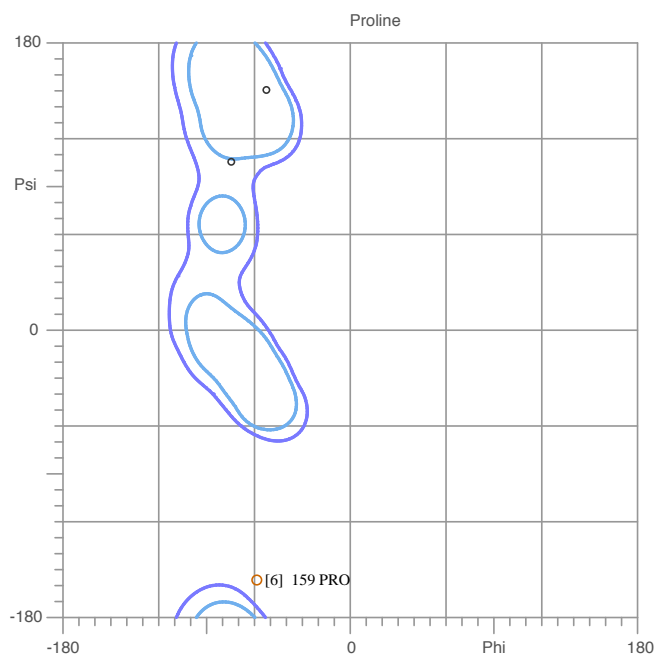
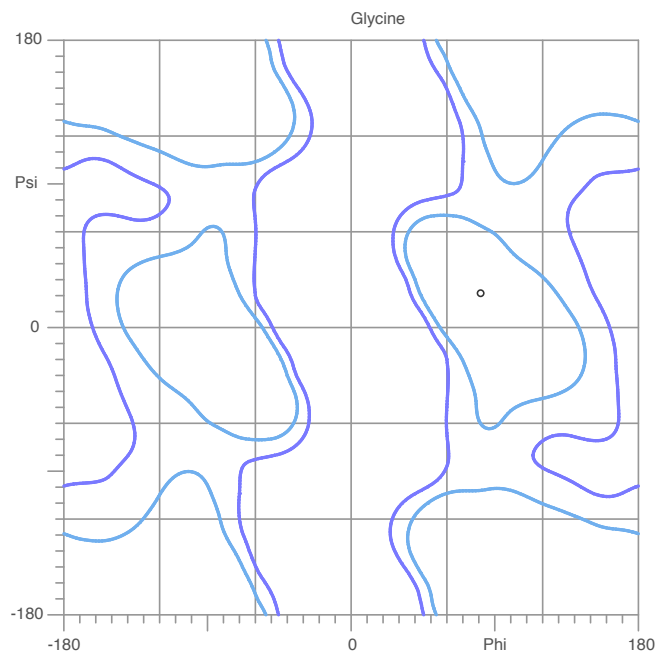
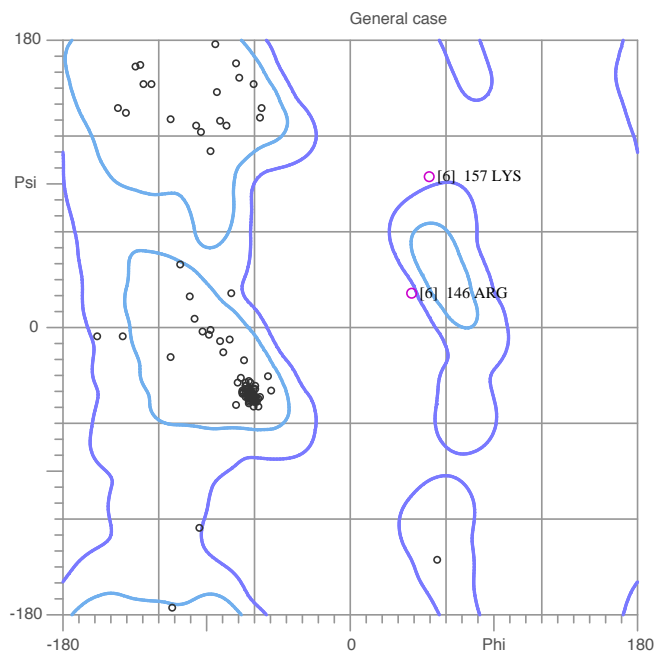
89.9% (98/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

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

2KIW_NMR.pdb, model 6



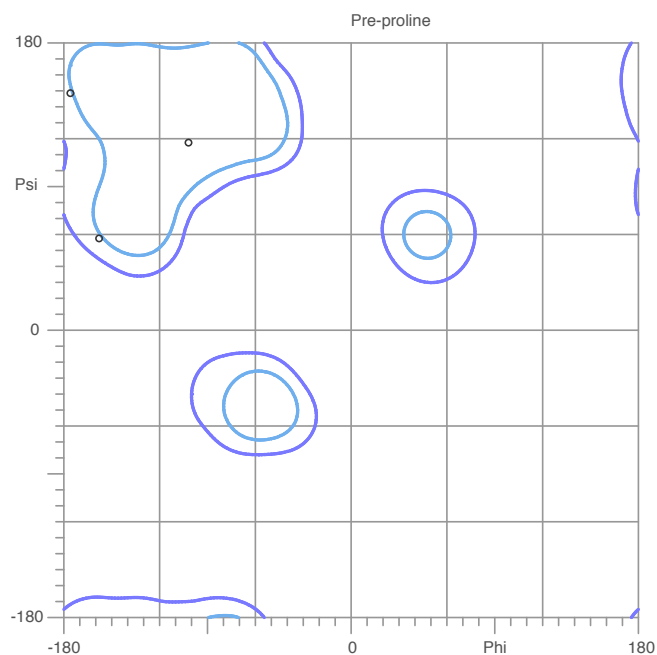
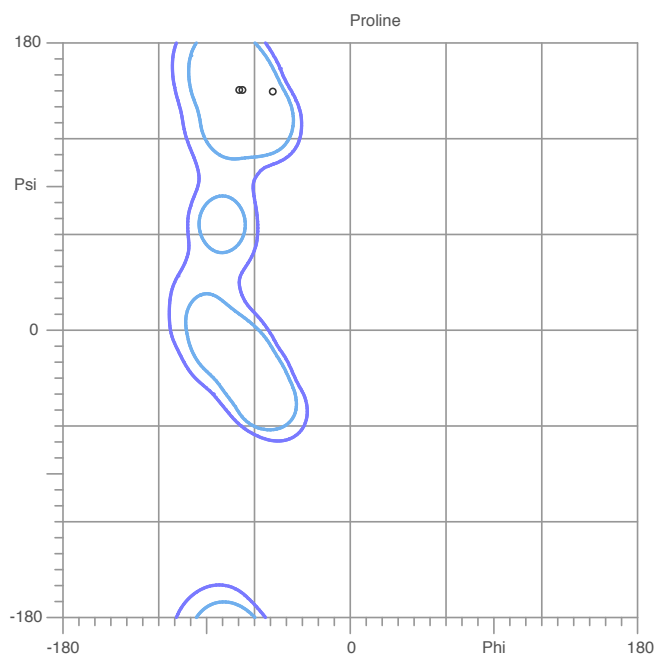
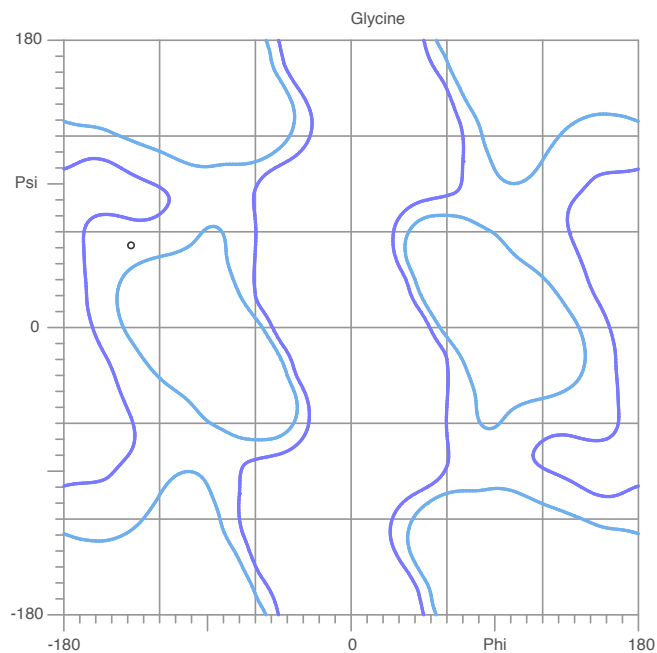
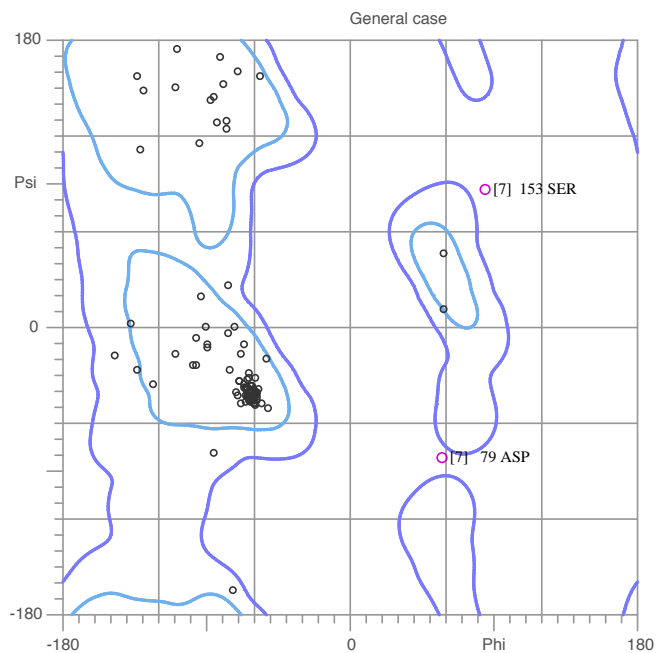
89.9% (98/109) of all residues were in favored (98%) regions.
96.3% (105/109) of all residues were in allowed (>99.8%) regions.

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.

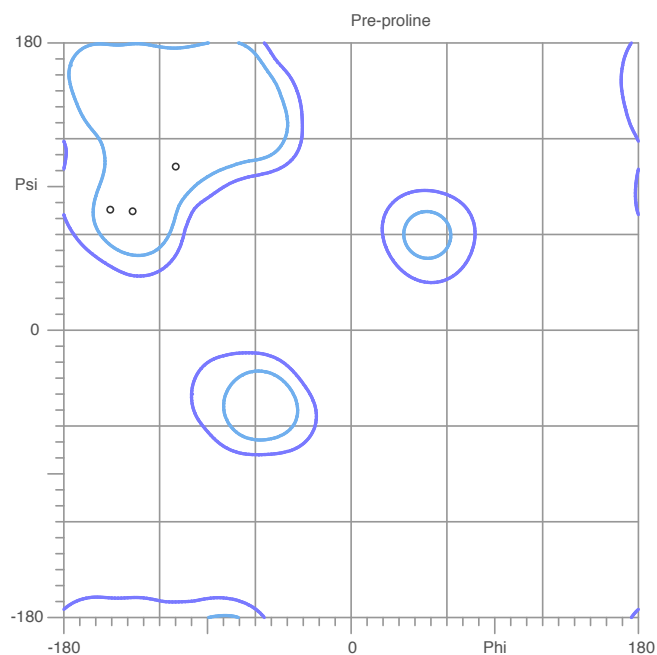
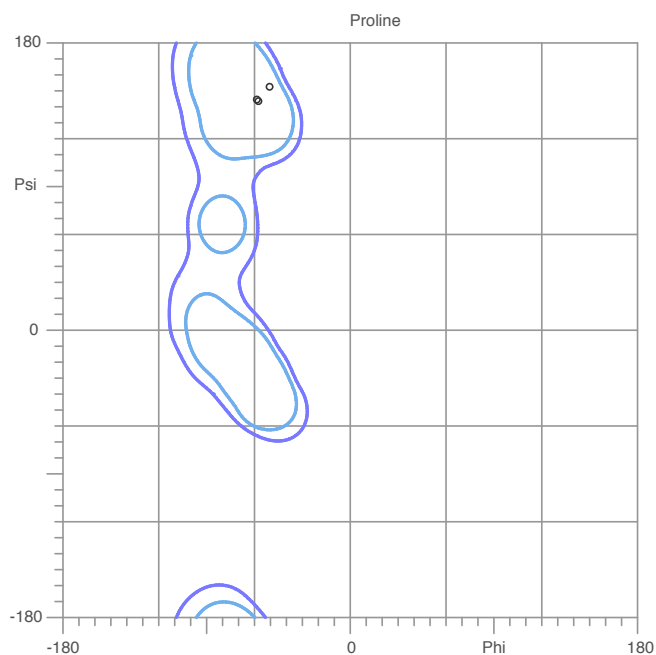
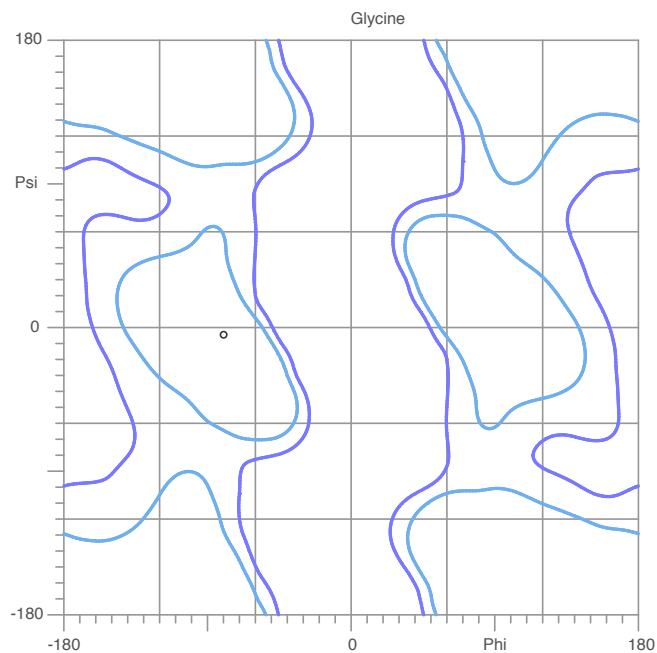
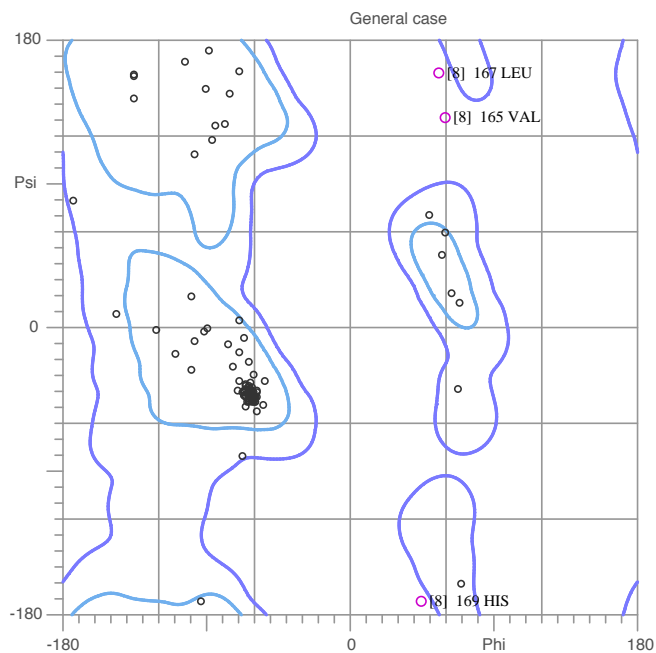
There were 2 outliers (phi, psi):

[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):

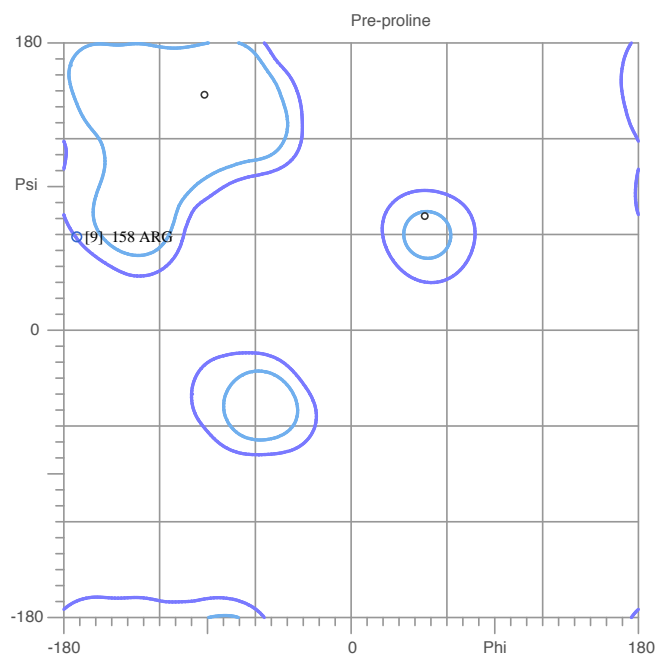
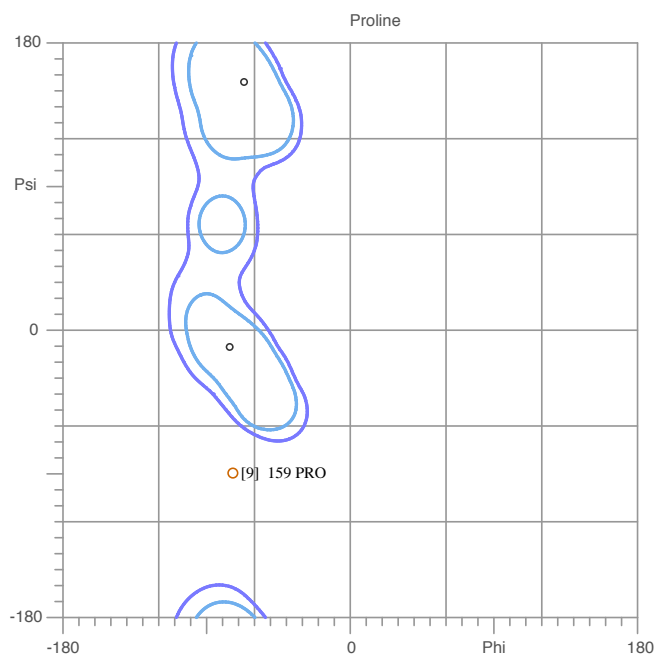
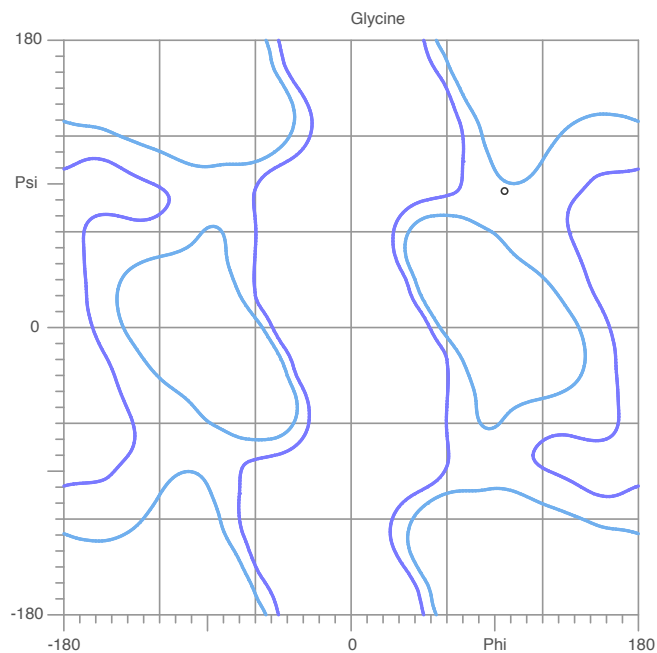
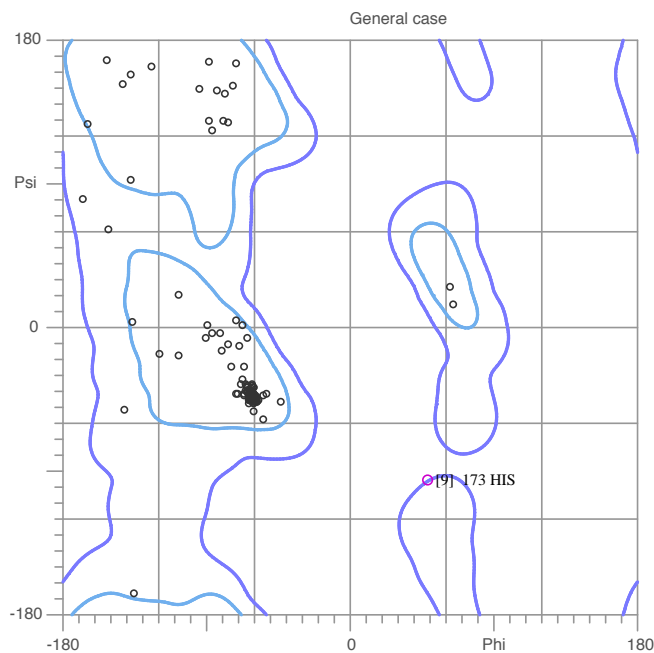
[8] 165 VAL (59.4, 133.0)

[8] 167 LEU (55.6, 160.5)

[8] 169 HIS (44.3, -171.3)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 9



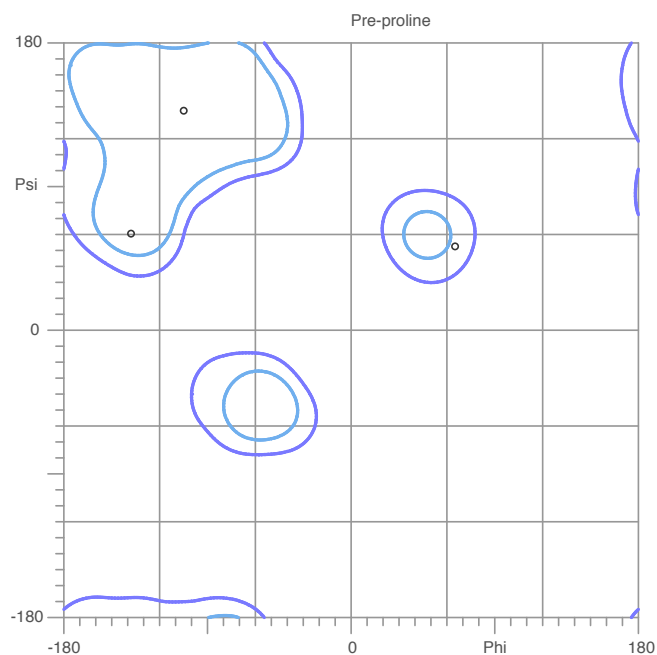
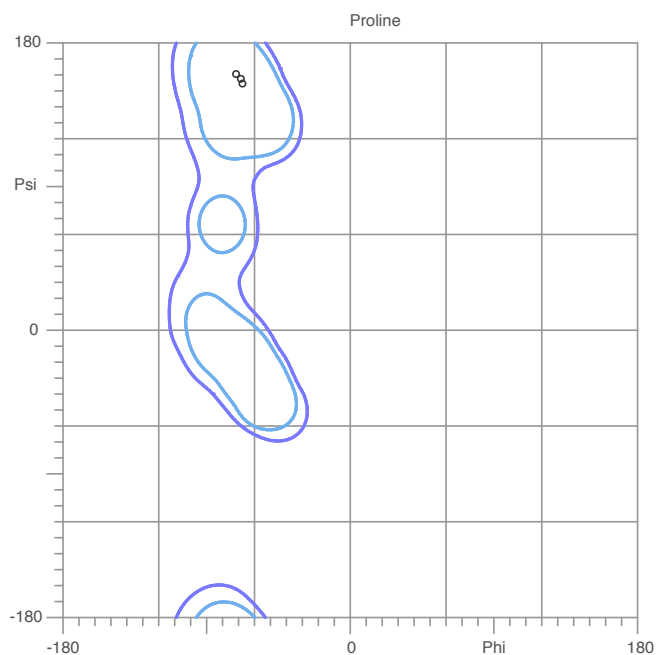
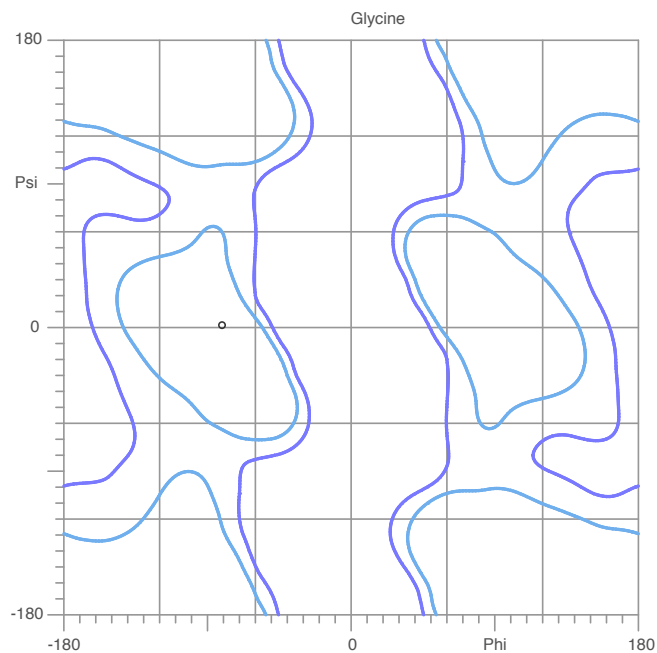
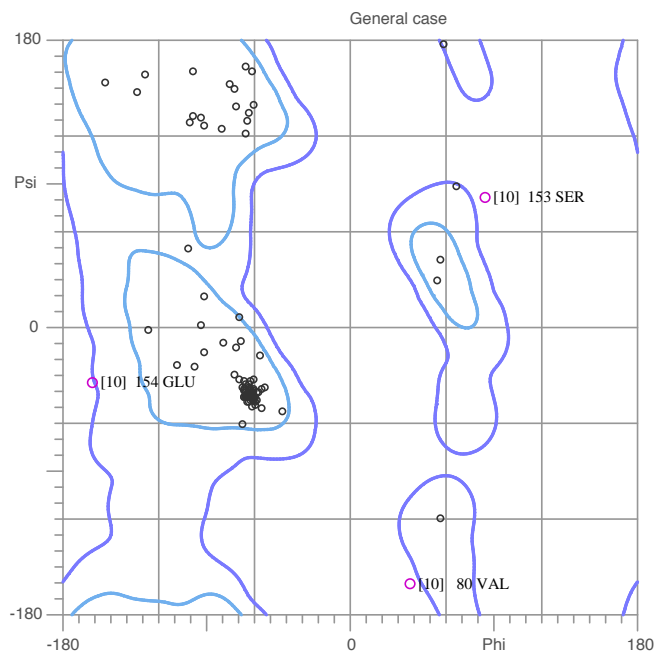
92.7% (101/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

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):

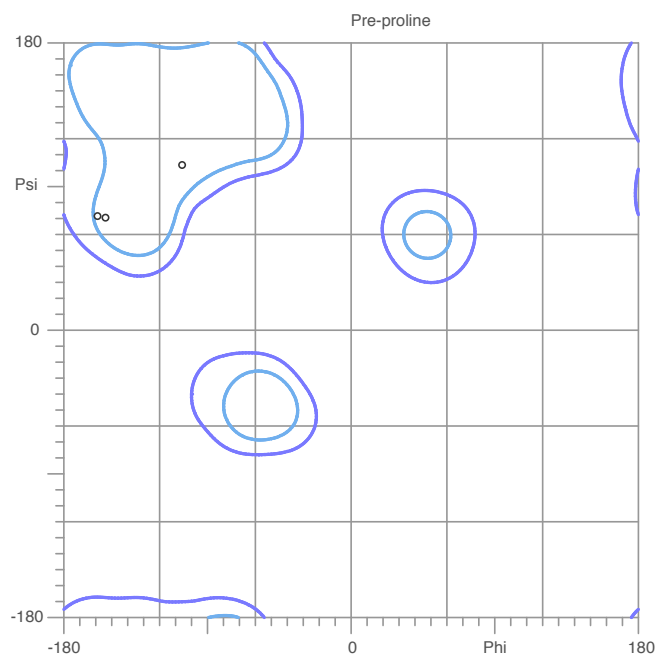
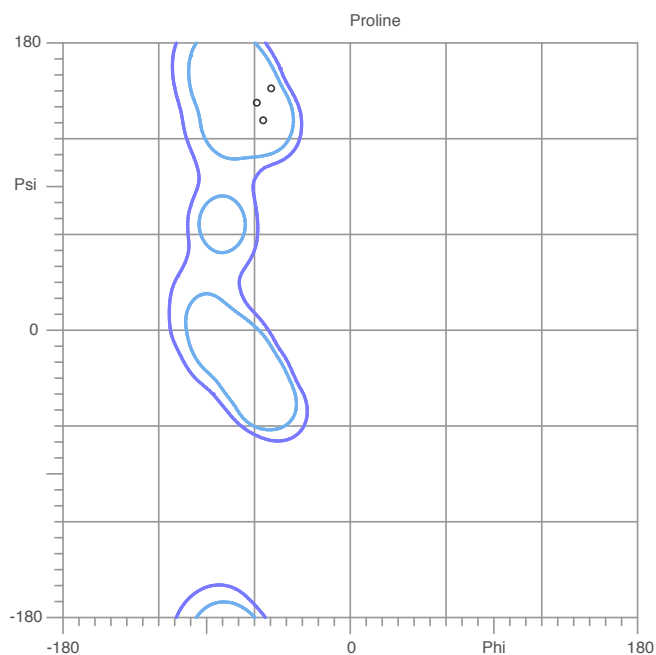
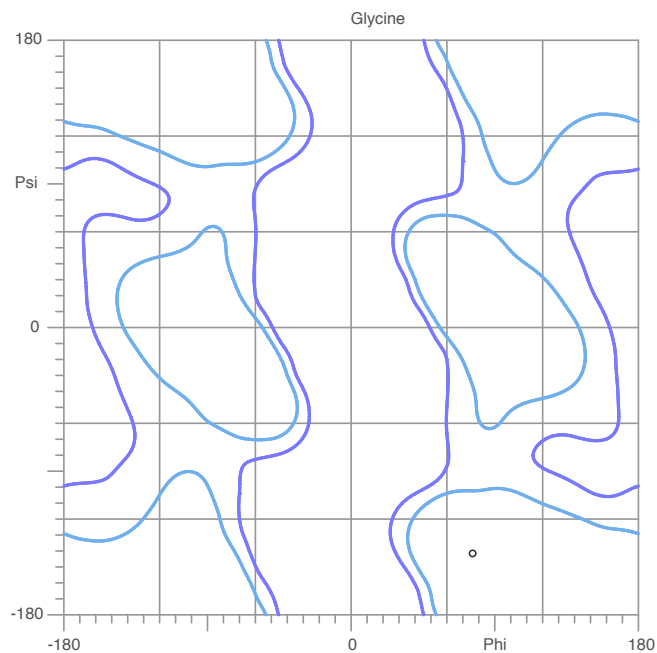
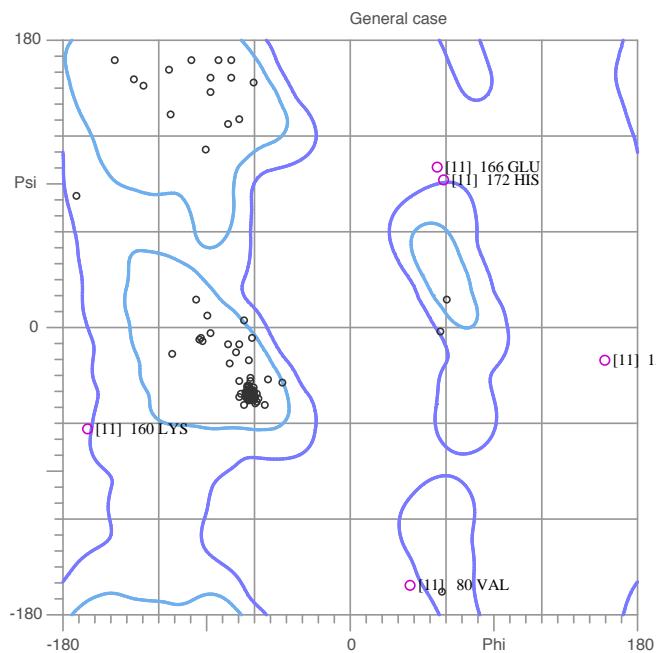
[10] 80 VAL (37.3, -160.2)

[10] 153 SER (84.7, 82.3)

[10] 154 GLU (-162.8, -34.6)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 11



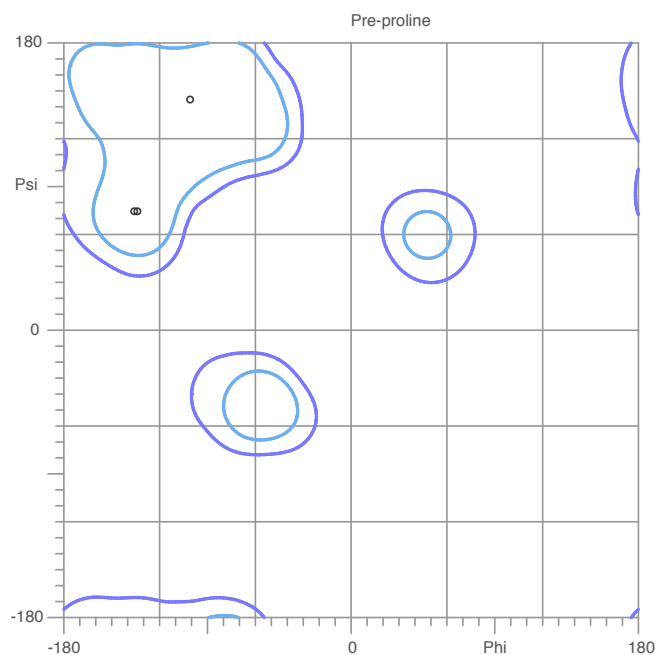
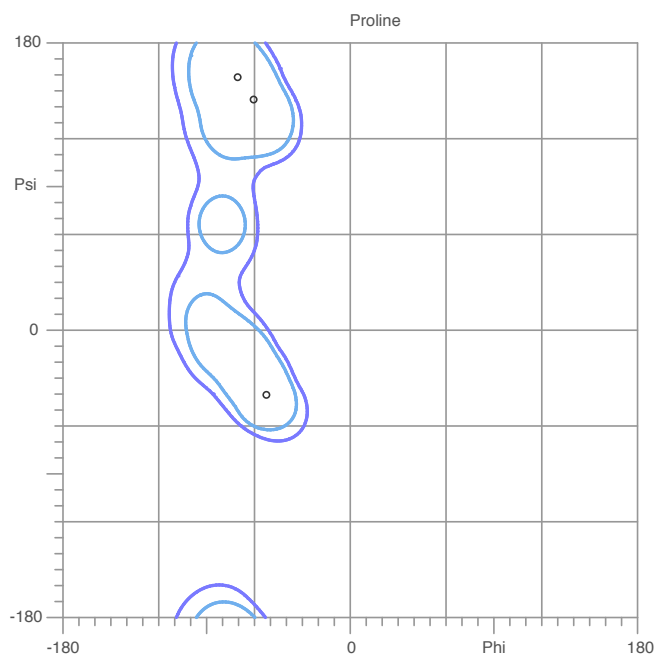
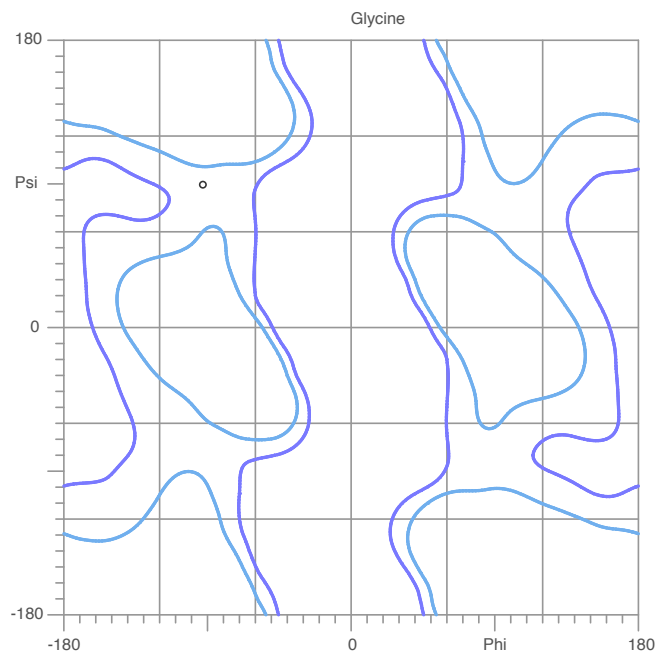
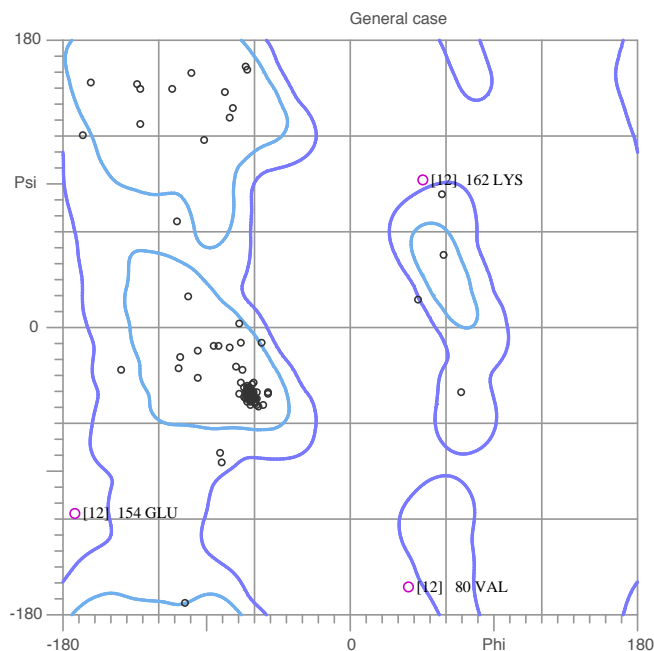
91.7% (100/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

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



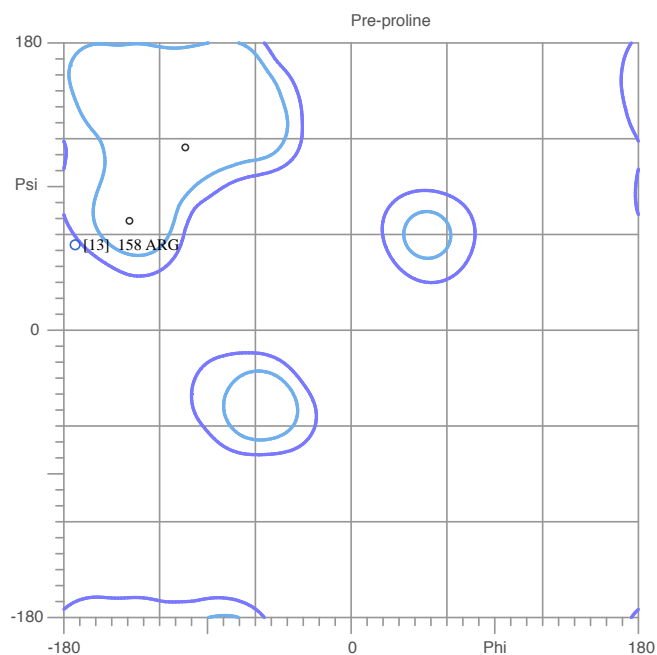
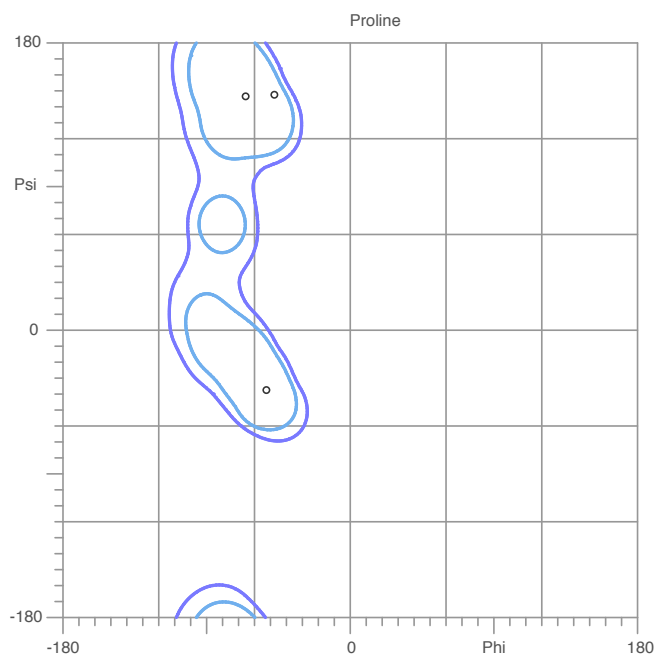
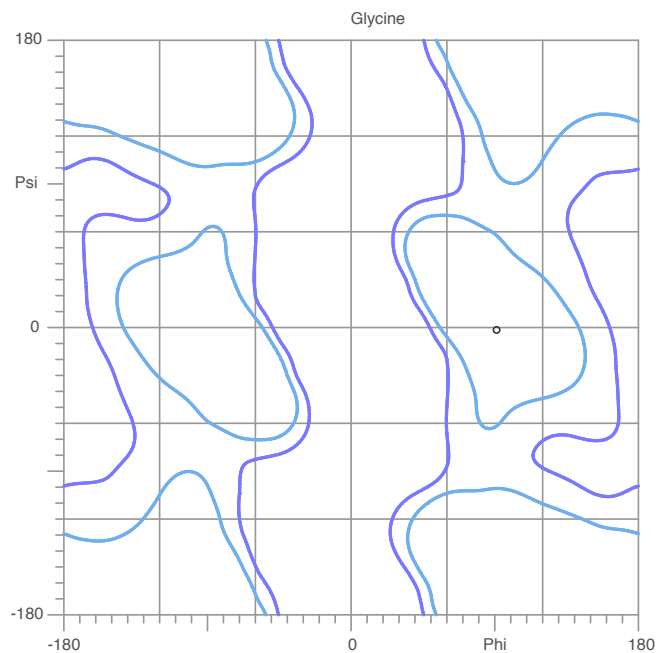
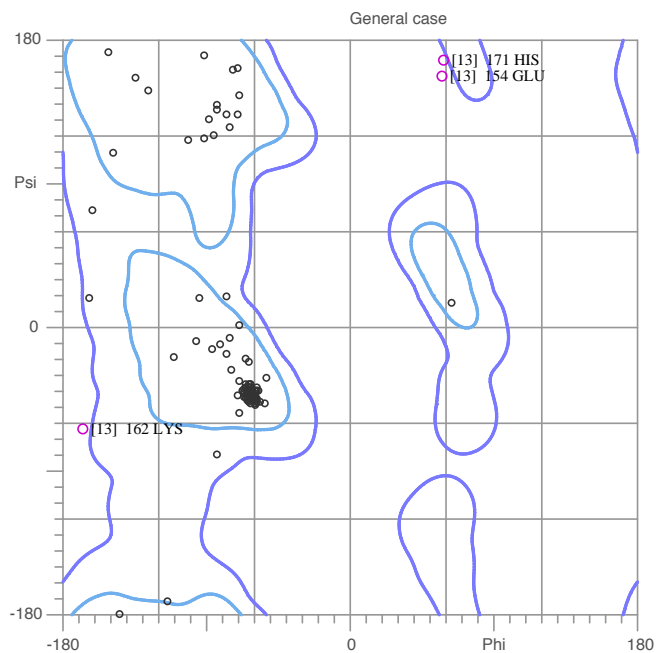
87.2% (95/109) of all residues were in favored (98%) regions.
97.2% (106/109) of all residues were in allowed (>99.8%) regions.

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



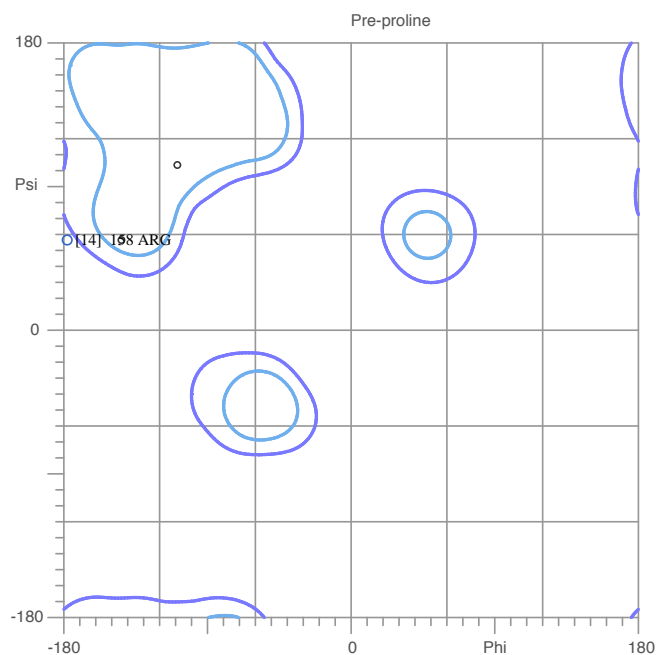
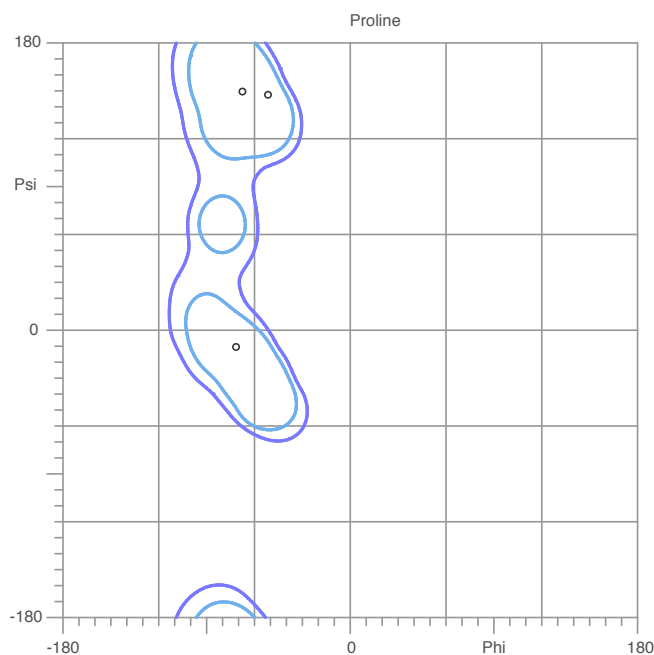
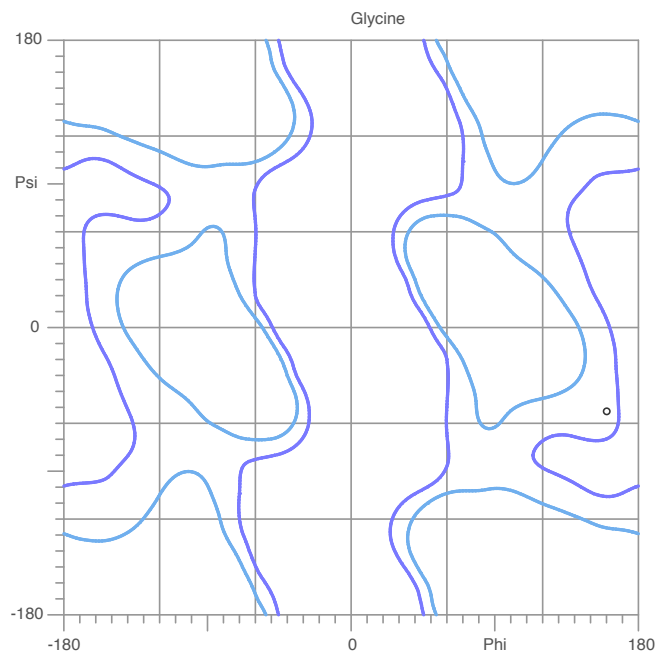
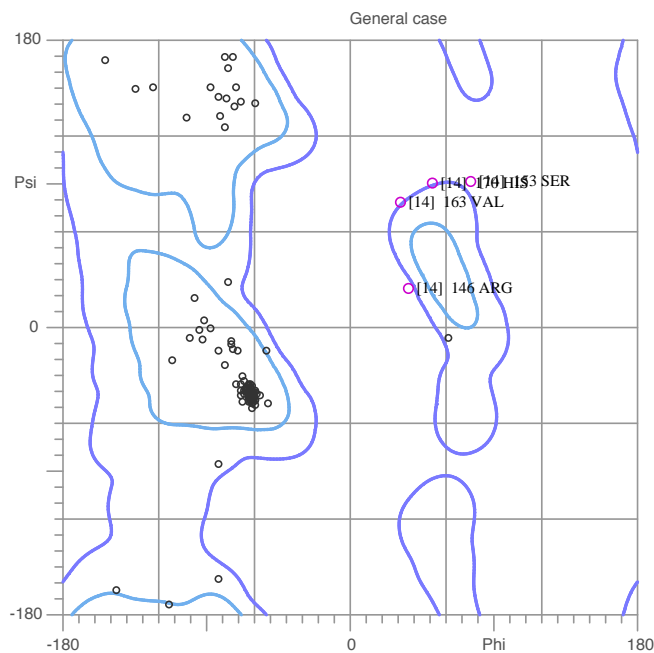
91.7% (100/109) of all residues were in favored (98%) regions.
96.3% (105/109) of all residues were in allowed (>99.8%) regions.

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



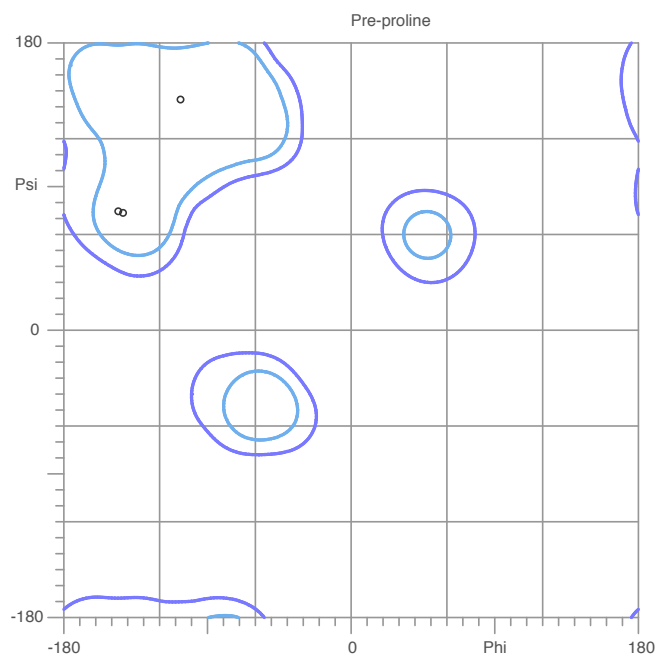
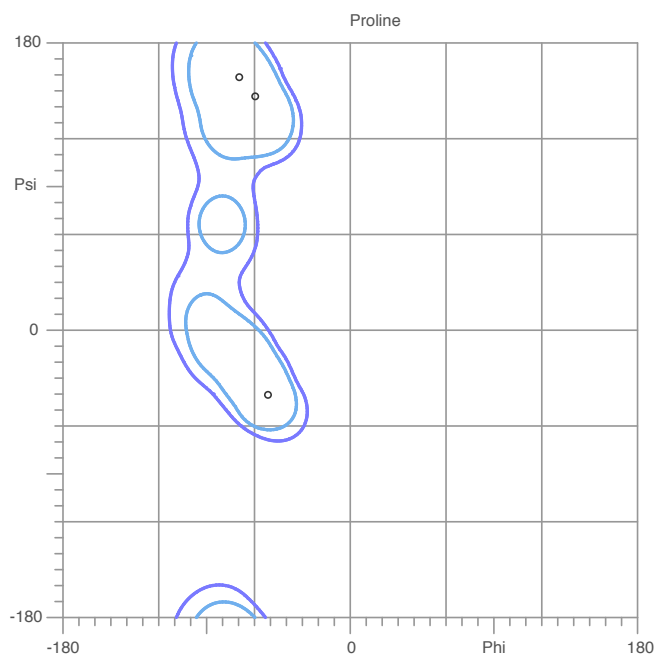
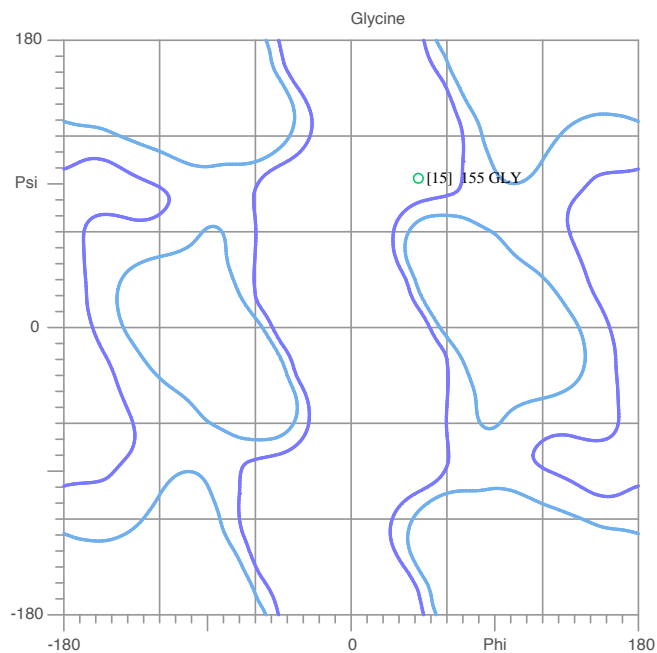
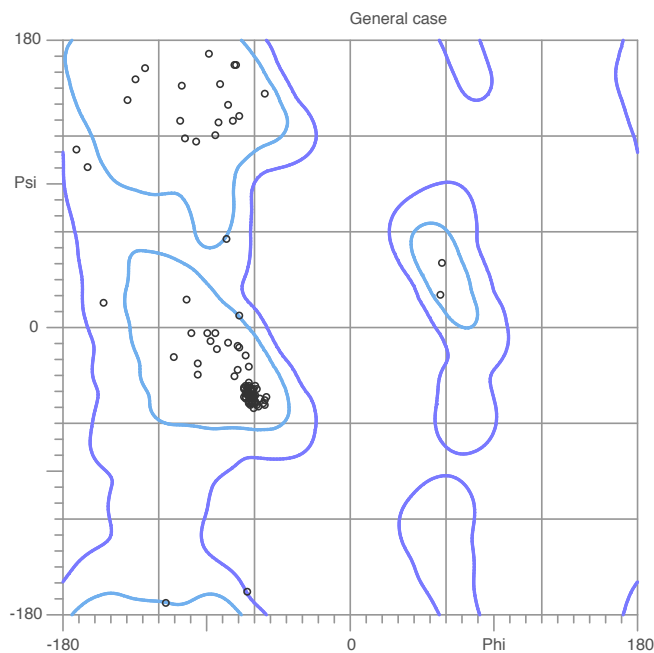
89.9% (98/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

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

2KIW_NMR.pdb, model 15



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.

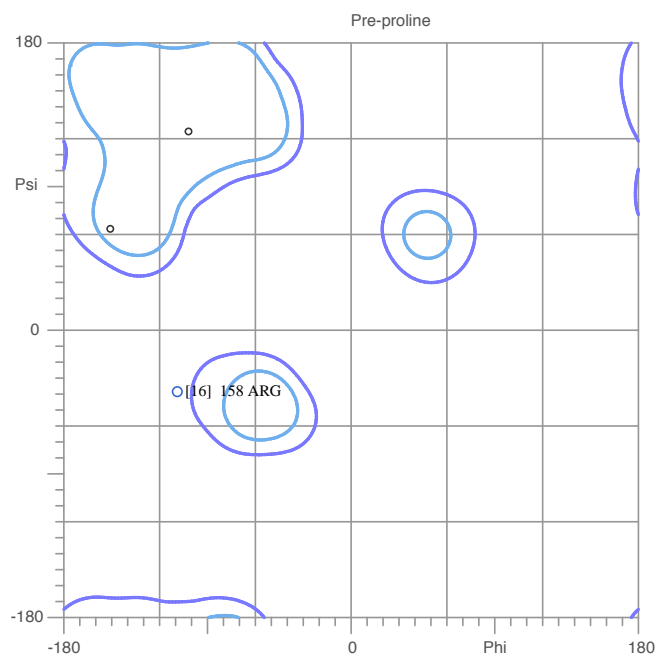
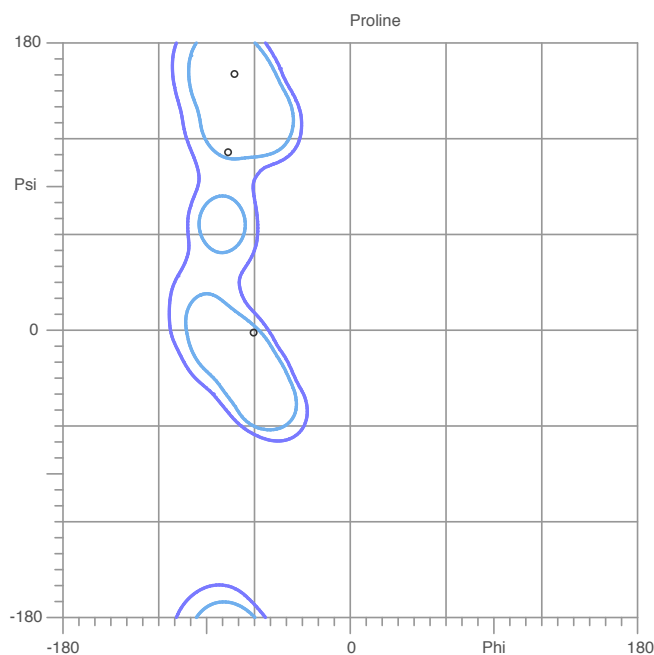
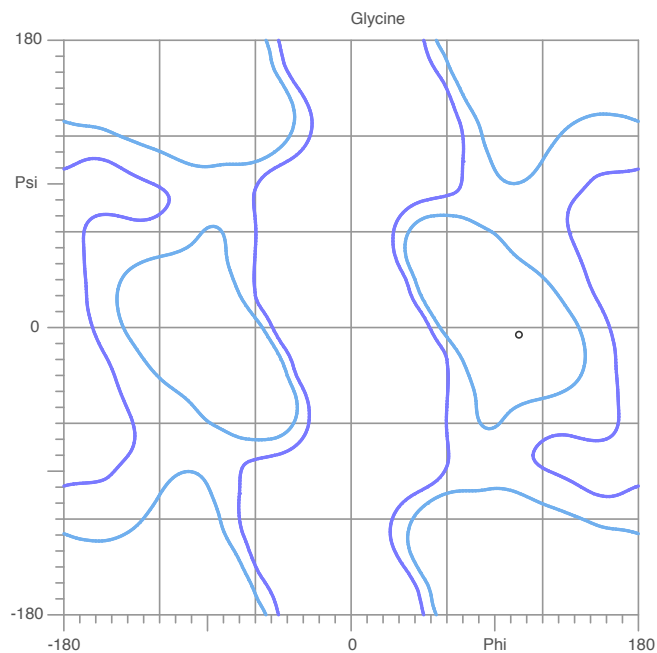
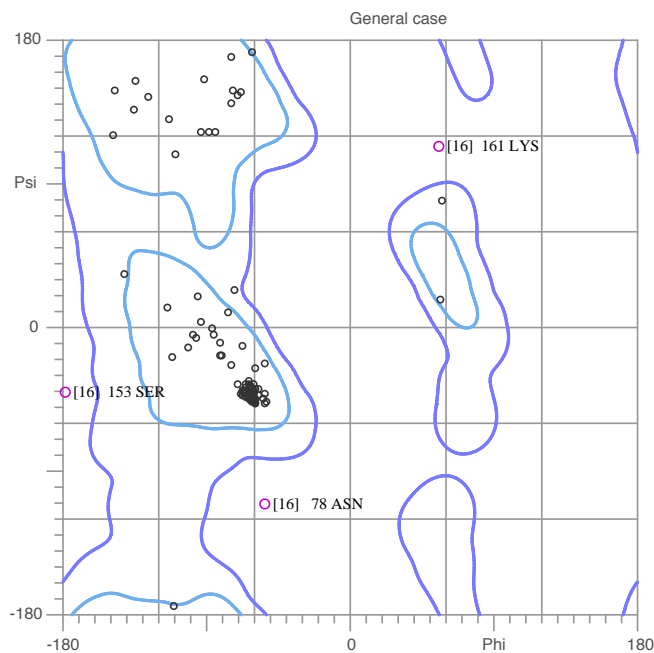
There were 1 outliers (phi, psi):
[15] 155 GLY (42.5, 94.6)

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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)

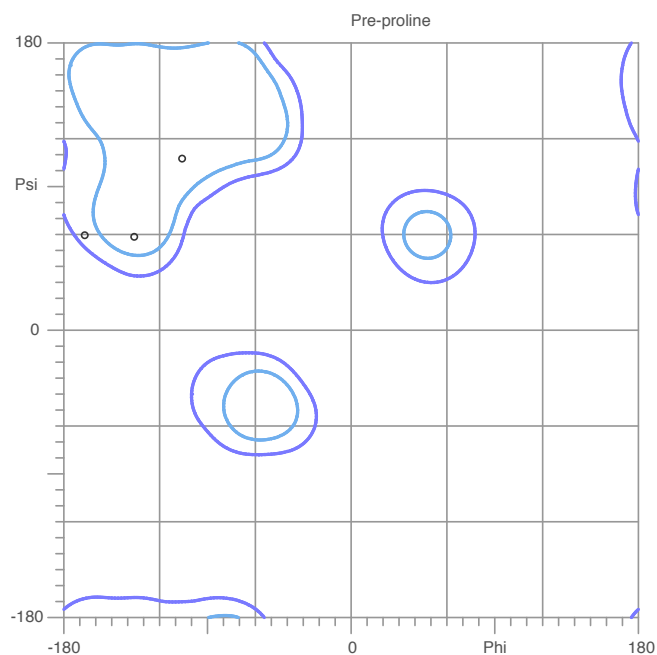
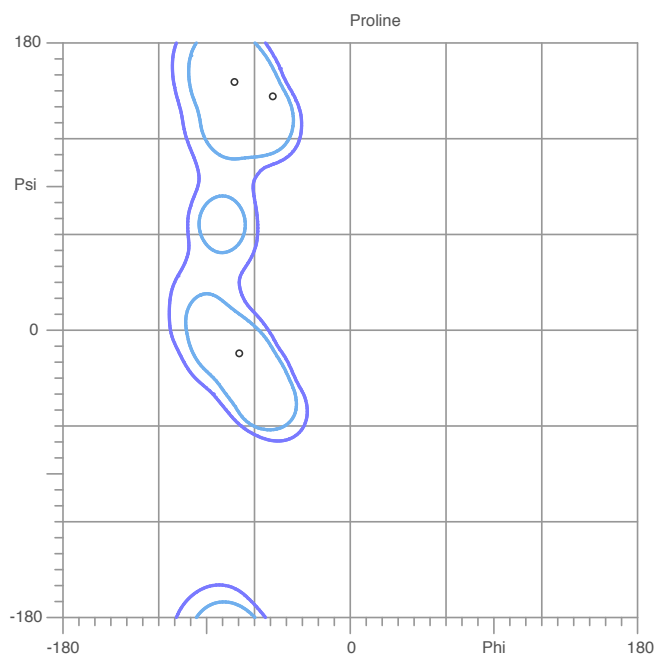
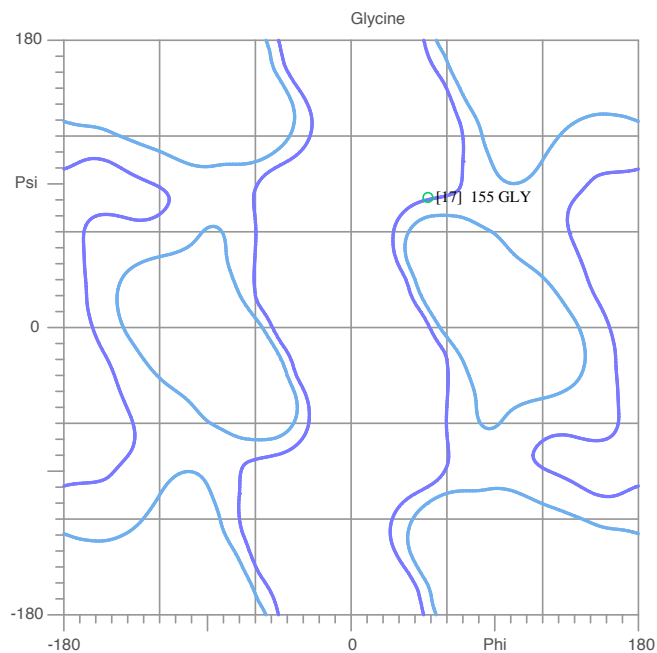
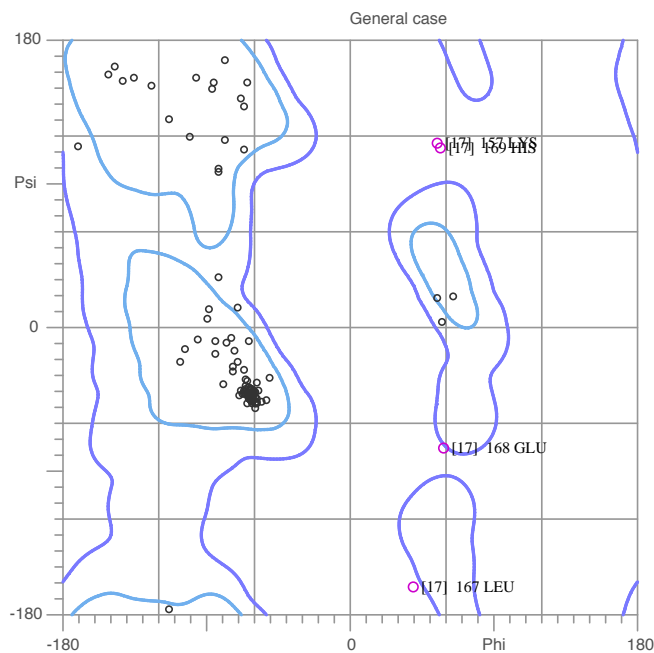
[16] 153 SER (-179.7, -40.1)

[16] 158 ARG (-109.0, -38.1)

[16] 161 LYS (55.8, 114.4)

MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 17



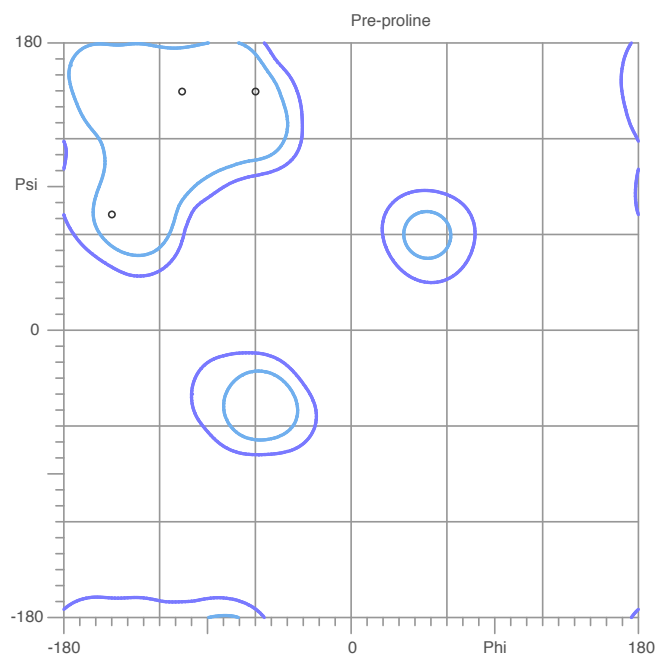
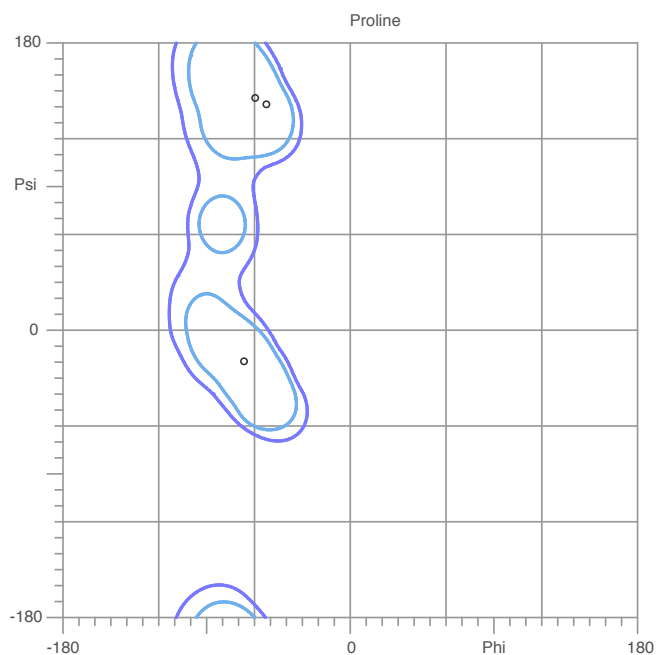
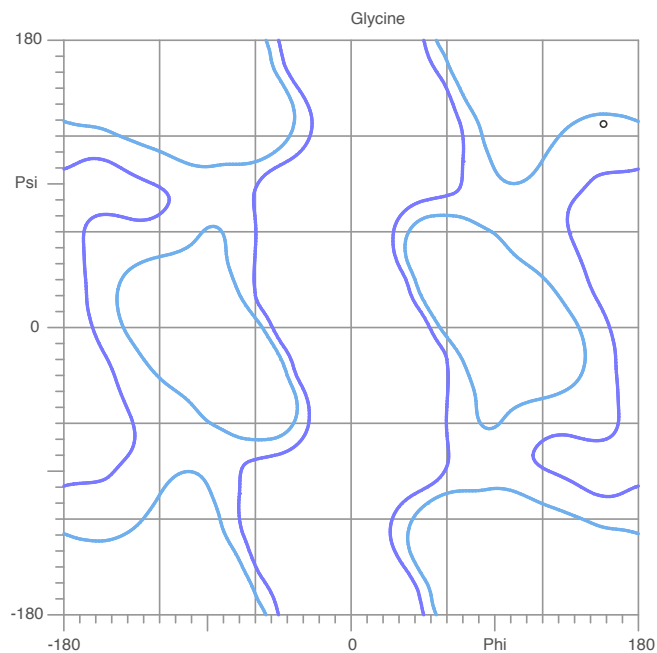
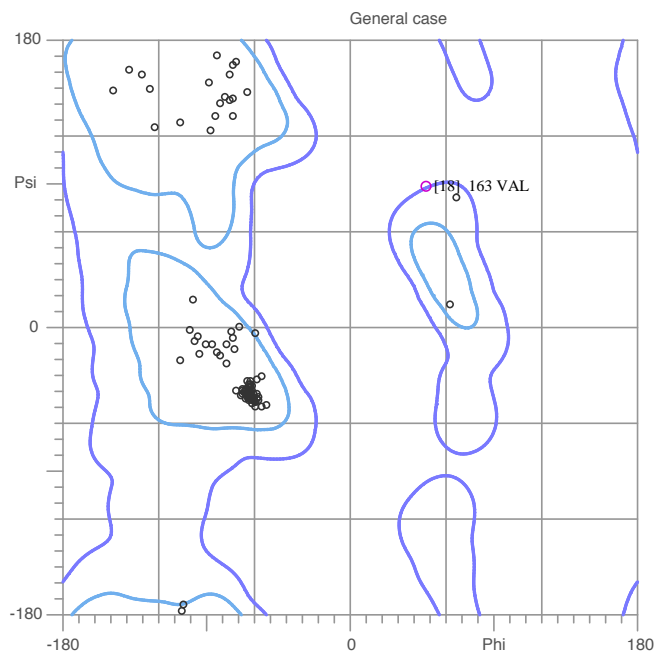
90.8% (99/109) of all residues were in favored (98%) regions.
95.4% (104/109) of all residues were in allowed (>99.8%) regions.

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.

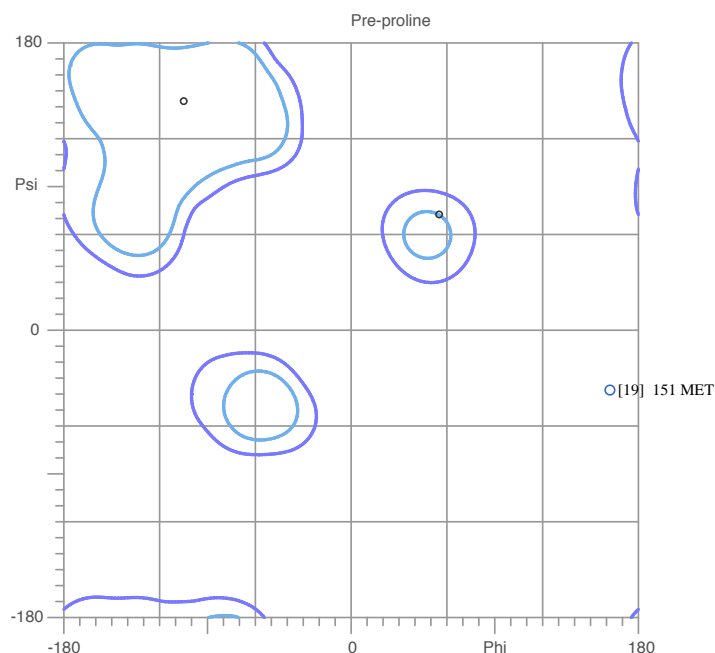
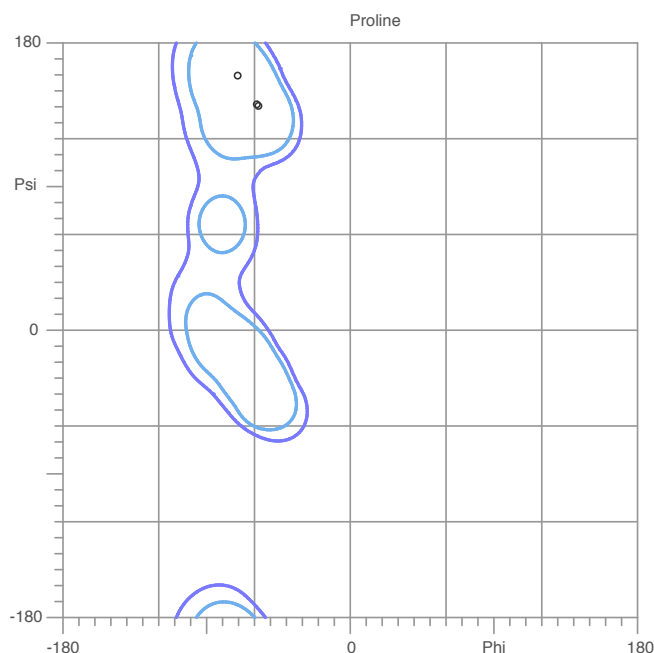
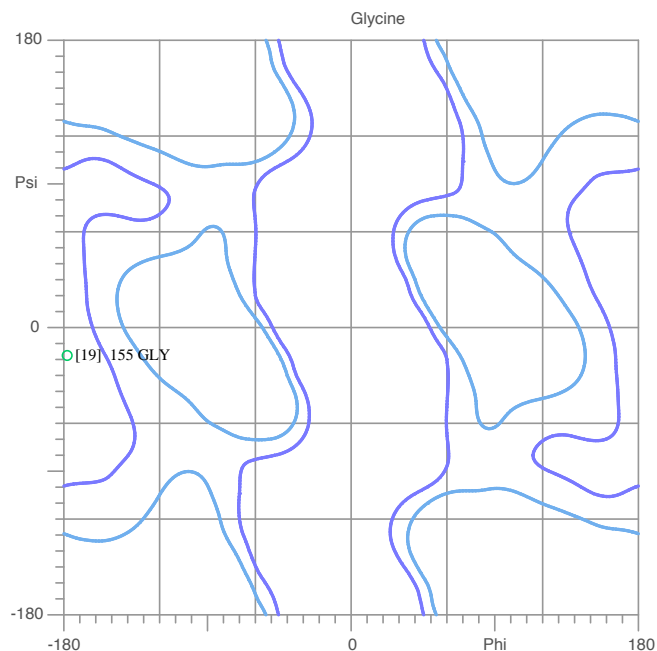
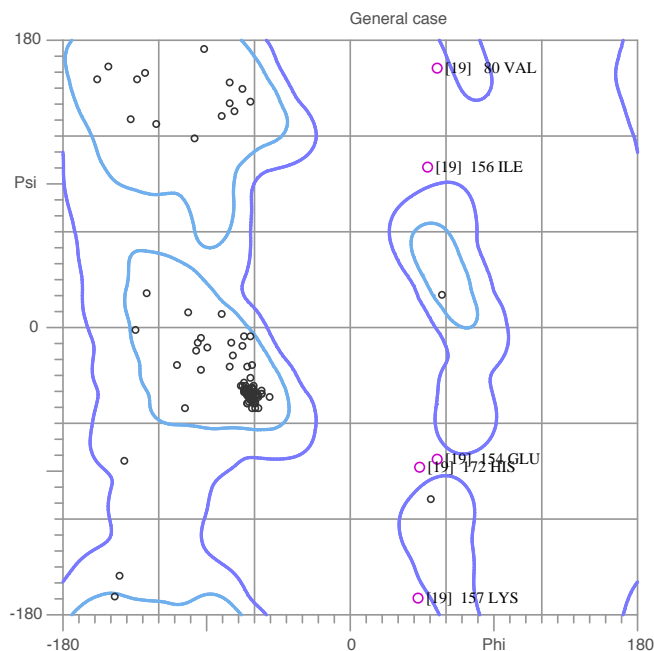
There were 1 outliers (phi, psi):
[18] 163 VAL (47.3, 90.0)

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MolProbity Ramachandran analysis

2KIW_NMR.pdb, model 19



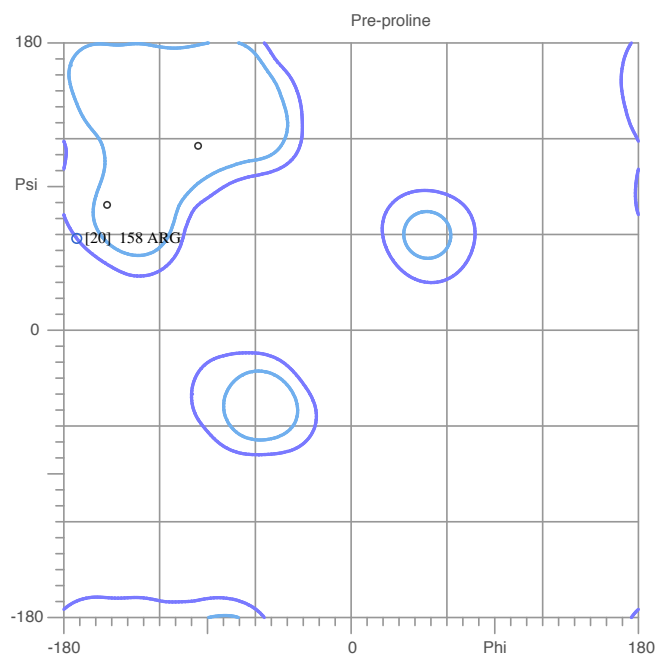
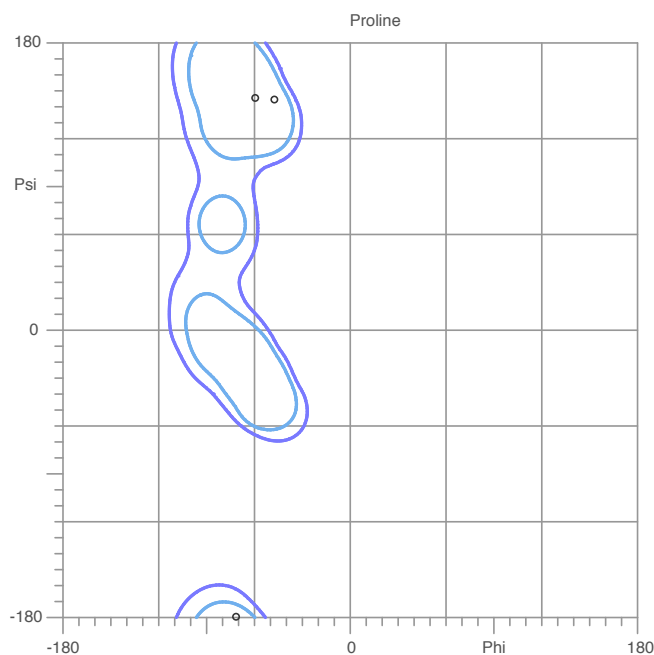
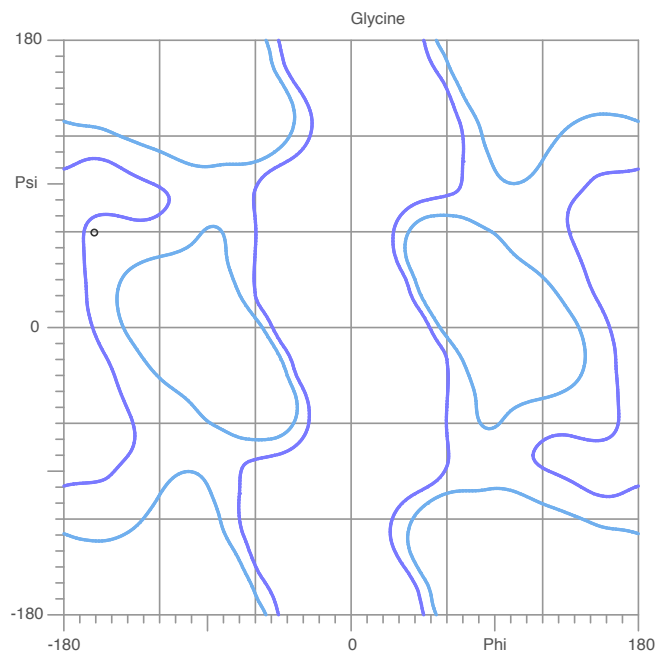
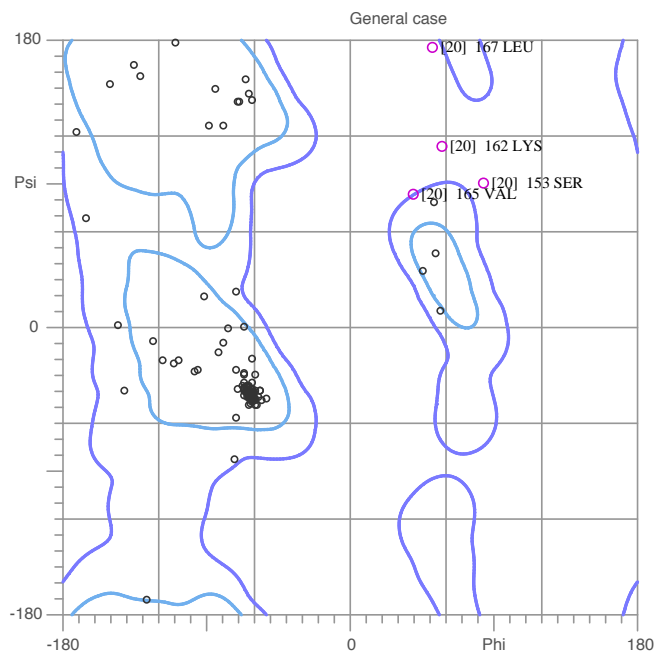
89.9% (98/109) of all residues were in favored (98%) regions.
93.6% (102/109) of all residues were in allowed (>99.8%) regions.

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



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)