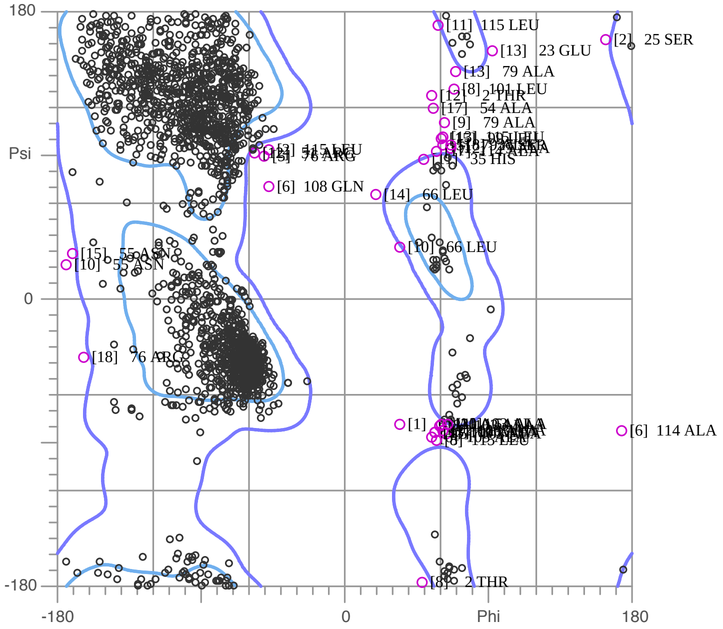
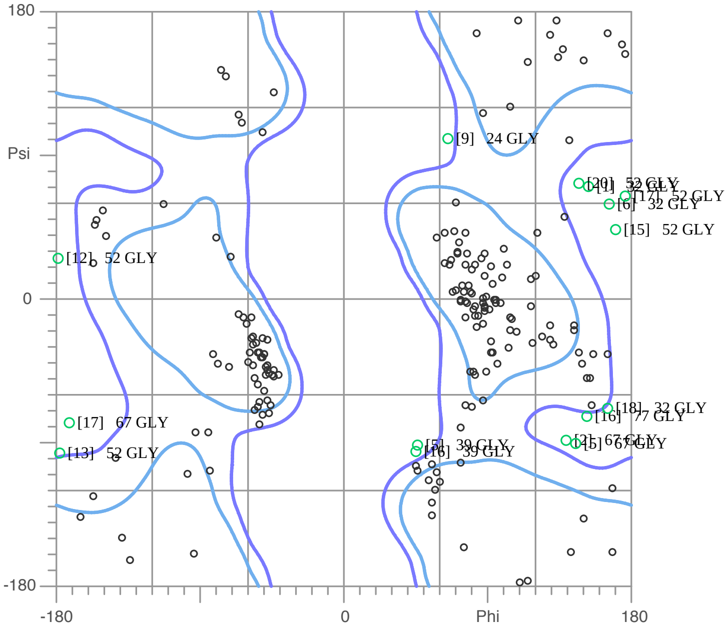
MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, all models

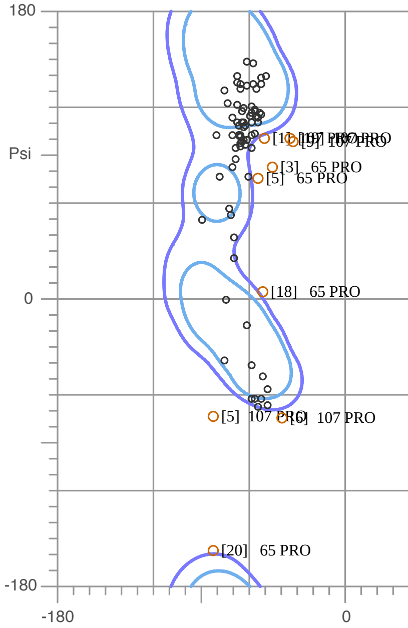
General case



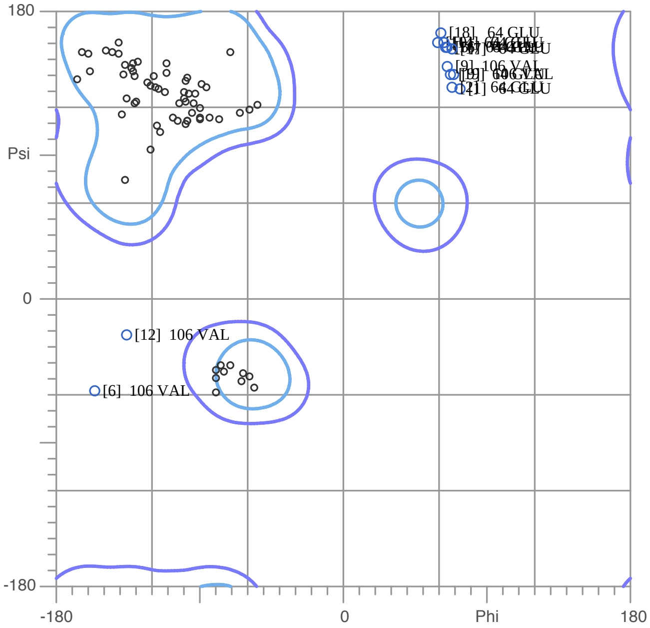
Glycine



Proline



Pre-proline



86.6% (1974/2280) of all residues were in favored (98%) regions.
96.8% (2206/2280) of all residues were in allowed (>99.8%) regions.

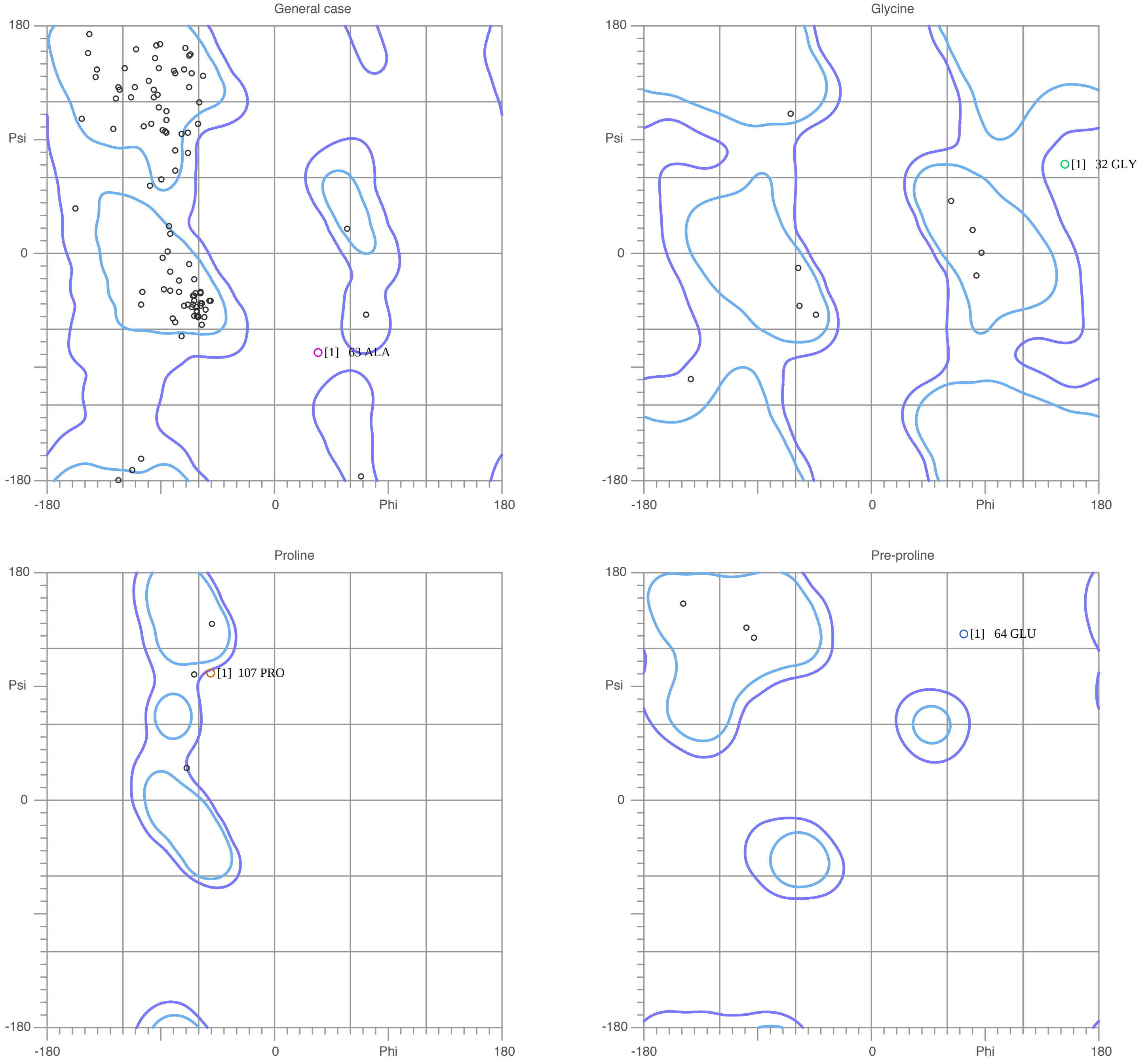
There were 74 outliers (phi, psi):
[1] 32 GLY (153.5, 71.4)
[1] 63 ALA (34.2, -78.4)
[1] 64 GLU (73.2, 132.7)
[1] 107 PRO (-51.7, 101.3)
[2] 25 SER (164.0, 163.3)
[2] 64 GLU (69.0, 133.8)
[2] 67 GLY (139.5, -88.7)
[2] 115 LEU (-48.9, 94.8)
[3] 65 PRO (-46.3, 83.3)
[4] 103 ALA (56.6, -83.5)
[5] 39 GLY (46.7, -91.9)
[5] 64 GLU (65.7, 158.9)
[5] 65 PRO (-55.9, 76.5)
[5] 67 GLY (145.5, -90.6)
[5] 76 ARG (-51.4, 90.9)
[5] 79 ALA (61.4, 97.0)
[5] 103 ALA (63.4, -85.0)
[5] 107 PRO (-83.6, -73.9)
[6] 32 GLY (166.3, 60.3)
[6] 103 ALA (54.8, -86.4)
[6] 106 VAL (-156.1, -57.8)
[6] 107 PRO (-40.7, -74.5)
[6] 108 GLN (-48.7, 71.5)
[6] 114 ALA (173.9, -82.1)
[7] 103 ALA (61.1, -82.2)
[8] 2 THR (49.0, -177.7)
[8] 101 LEU (68.3, 132.8)
[8] 103 ALA (59.2, -79.8)
[8] 115 LEU (57.1, -88.3)
[9] 24 GLY (66.0, 101.6)
[9] 64 GLU (69.4, 141.5)
[9] 79 ALA (62.9, 111.4)
[9] 106 VAL (65.7, 146.0)
[9] 107 PRO (-33.3, 99.4)
[10] 55 ASN (-175.4, 22.6)
[10] 64 GLU (59.2, 161.5)
[10] 66 LEU (34.6, 33.7)
[11] 35 HIS (49.6, 88.7)
[11] 103 ALA (60.8, -78.2)
[11] 115 LEU (58.4, 172.6)
[12] 2 THR (55.0, 128.2)
[12] 51 ARG (-58.0, 93.0)
[12] 52 GLY (-179.4, 26.9)
[12] 79 ALA (66.1, 95.9)
[12] 103 ALA (61.5, -82.9)
[12] 106 VAL (-136.4, -22.1)
[13] 23 GLU (92.5, 156.1)
[13] 52 GLY (-178.6, -96.8)
[13] 79 ALA (69.7, 143.9)
[13] 103 ALA (56.6, -83.0)
[13] 115 LEU (61.1, 102.5)
[14] 64 GLU (63.4, 161.9)
[14] 66 LEU (19.0, 66.0)
[15] 52 GLY (170.8, 45.0)
[15] 55 ASN (-171.8, 29.9)
[15] 99 LEU (60.1, 101.6)
[16] 39 GLY (45.9, -96.0)
[16] 64 GLU (64.7, 158.3)
[16] 77 GLY (152.9, -73.2)
[17] 52 GLY (176.9, 65.9)
[17] 54 ALA (55.5, 120.8)
[17] 64 GLU (68.7, 157.4)
[17] 67 GLY (-172.2, -77.6)
[17] 114 ALA (57.6, 93.5)
[18] 32 GLY (165.1, -68.9)
[18] 37 SER (66.5, 97.1)
[18] 64 GLU (61.2, 168.0)
[18] 65 PRO (-52.2, 6.0)
[18] 76 ARG (-164.3, -36.4)
[19] 106 VAL (67.1, 141.1)
[19] 107 PRO (-35.0, 101.8)
[20] 52 GLY (147.9, 73.6)
[20] 54 ALA (64.5, -78.6)
[20] 65 PRO (-83.8, -157.2)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 1



84.2% (96/114) of all residues were in favored (98%) regions.
96.5% (110/114) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):

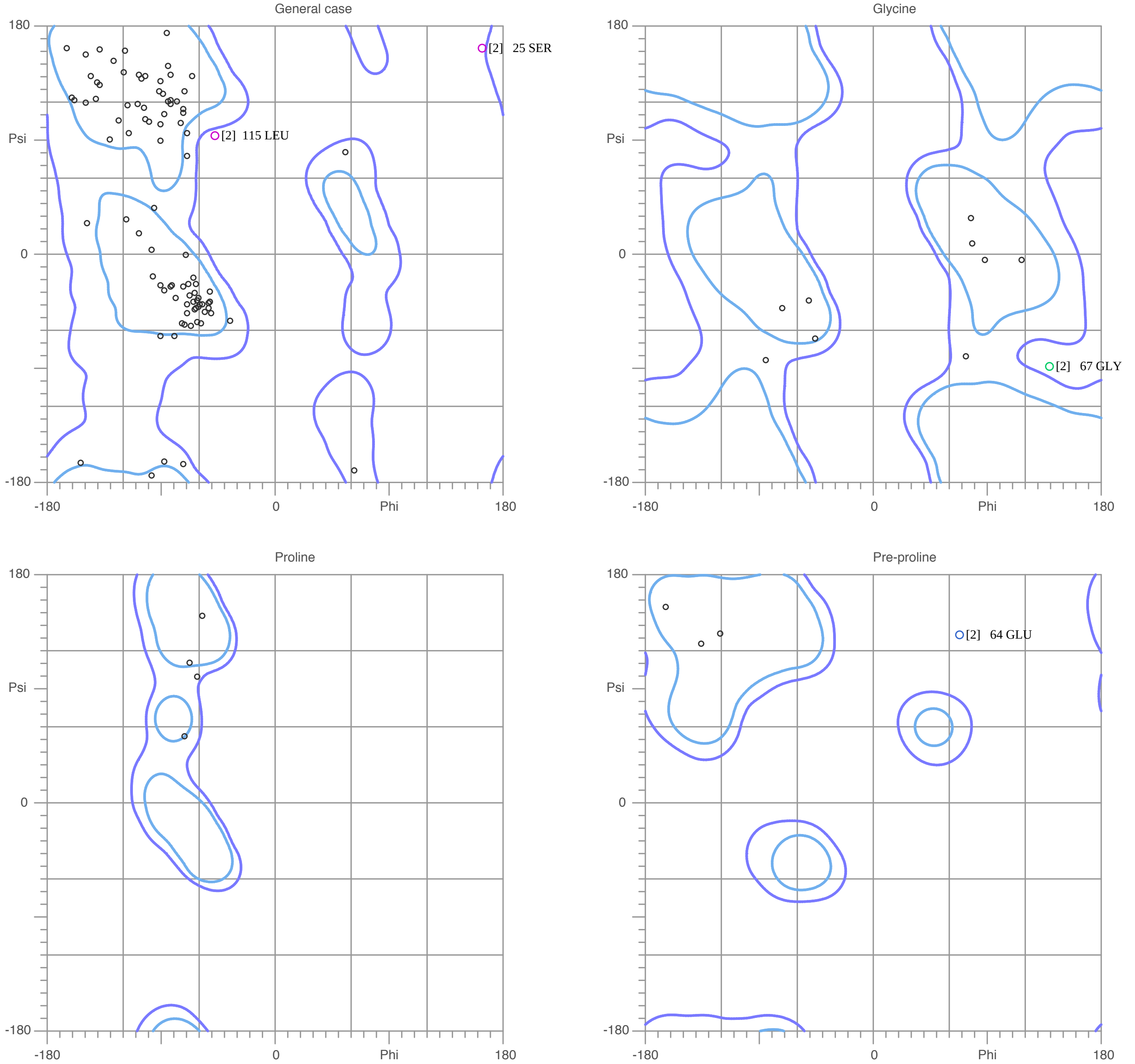
[1] 32 GLY (153.5, 71.4)
[1] 63 ALA (34.2, -78.4)
[1] 64 GLU (73.2, 132.7)
[1] 107 PRO (-51.7, 101.3)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 2



83.3% (95/114) of all residues were in favored (98%) regions.
96.5% (110/114) of all residues were in allowed (>99.8%) regions.

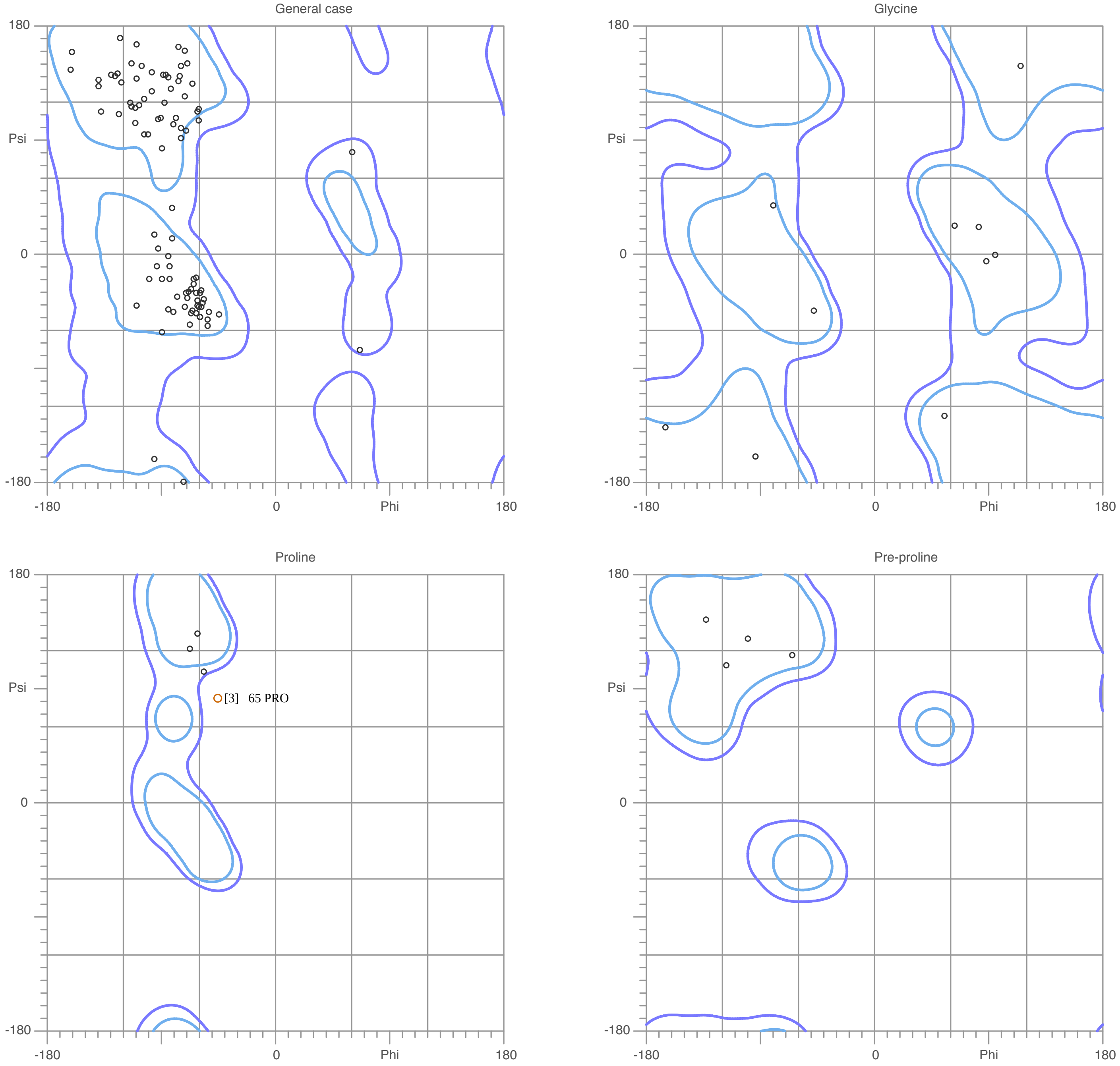
There were 4 outliers (phi, psi):
[2] 25 SER (164.0, 163.3)
[2] 64 GLU (69.0, 133.8)
[2] 67 GLY (139.5, -88.7)
[2] 115 LEU (-48.9, 94.8)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 3



93.9% (107/114) of all residues were in favored (98%) regions.
99.1% (113/114) of all residues were in allowed (>99.8%) regions.

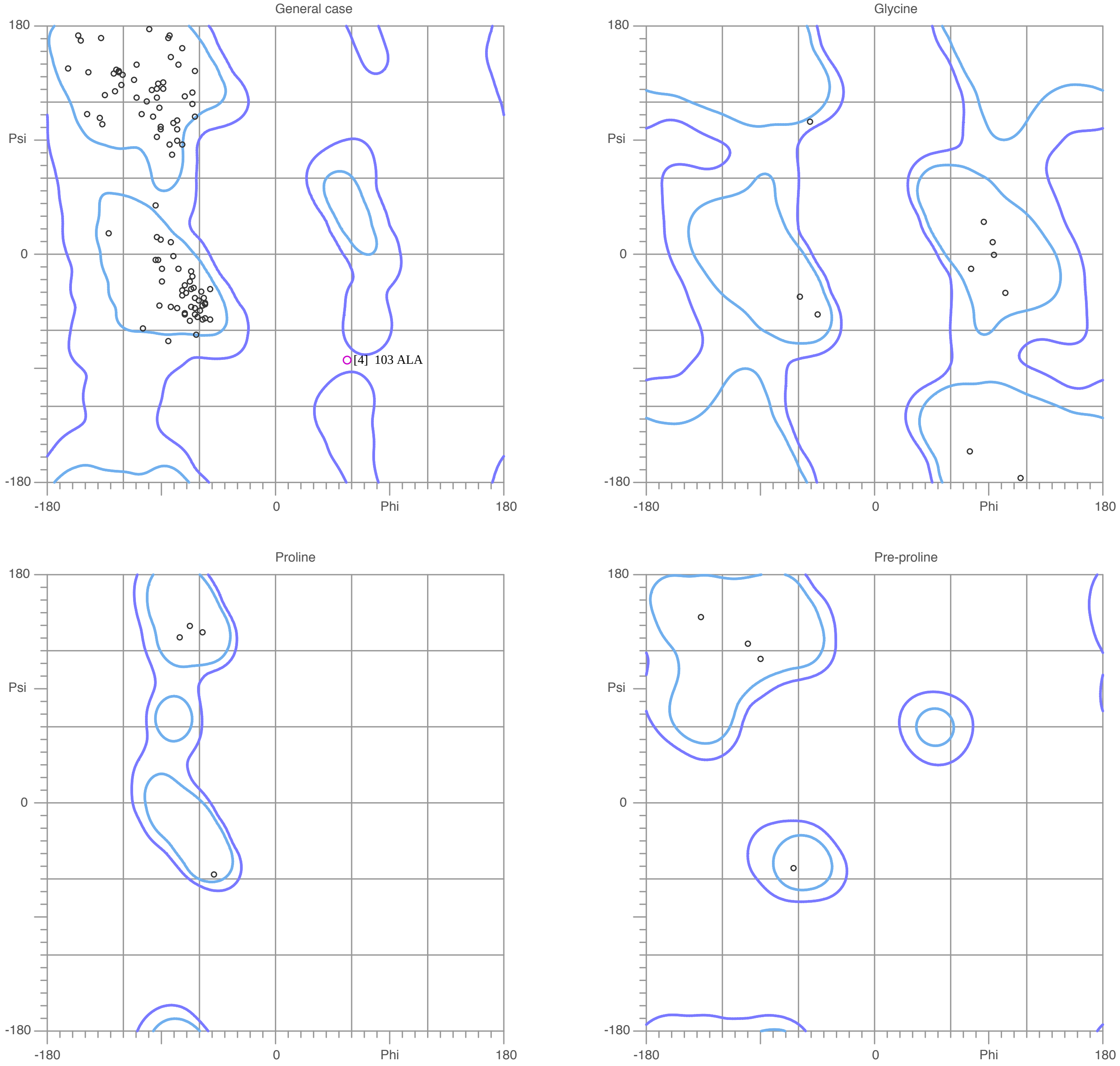
There were 1 outliers (phi, psi):
[3] 65 PRO (-46.3, 83.3)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 4



95.6% (109/114) of all residues were in favored (98%) regions.
99.1% (113/114) of all residues were in allowed (>99.8%) regions.

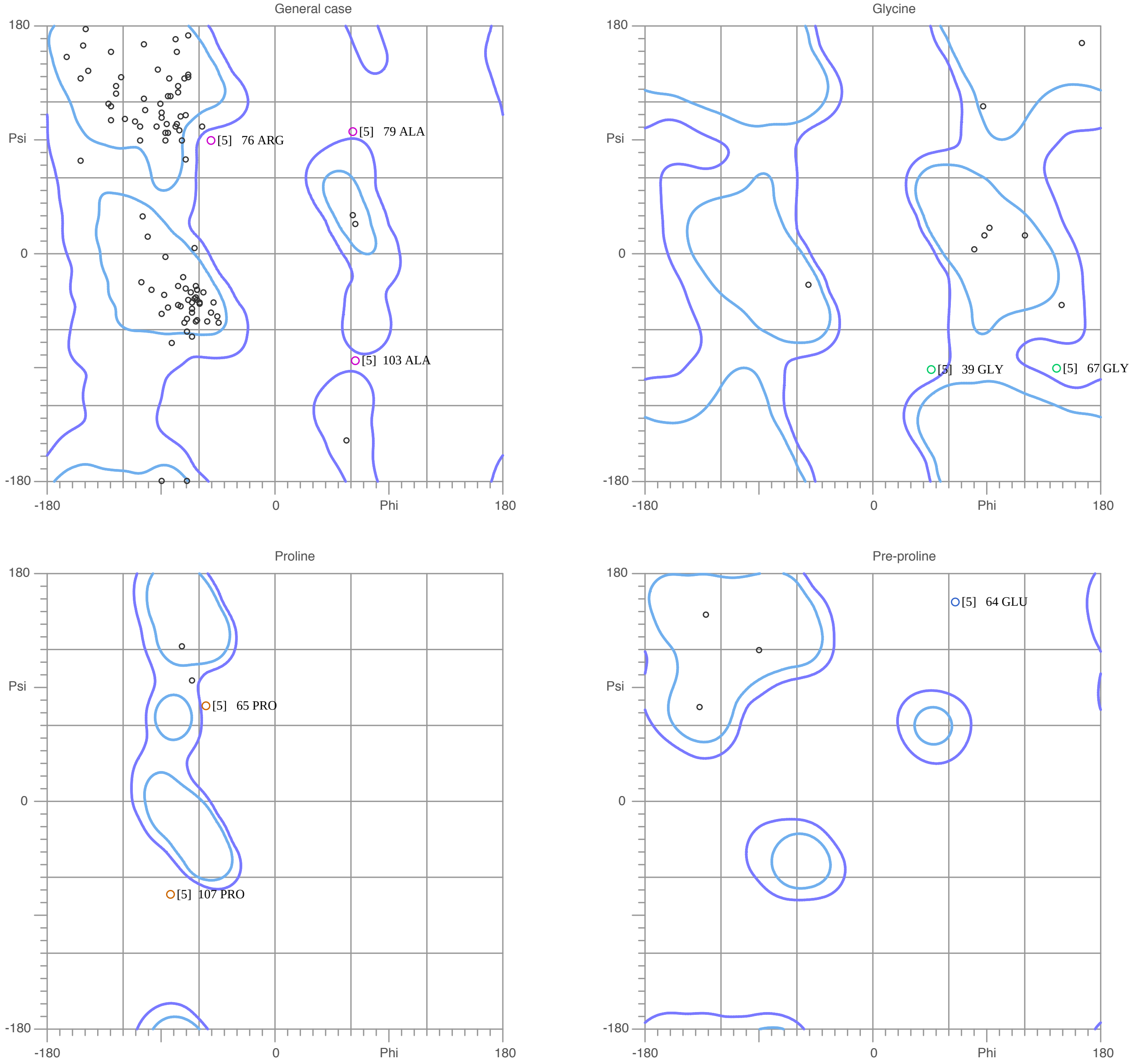
There were 1 outliers (phi, psi):
[4] 103 ALA (56.6, -83.5)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 5



85.1% (97/114) of all residues were in favored (98%) regions.
93.0% (106/114) of all residues were in allowed (>99.8%) regions.

There were 8 outliers (phi, psi):

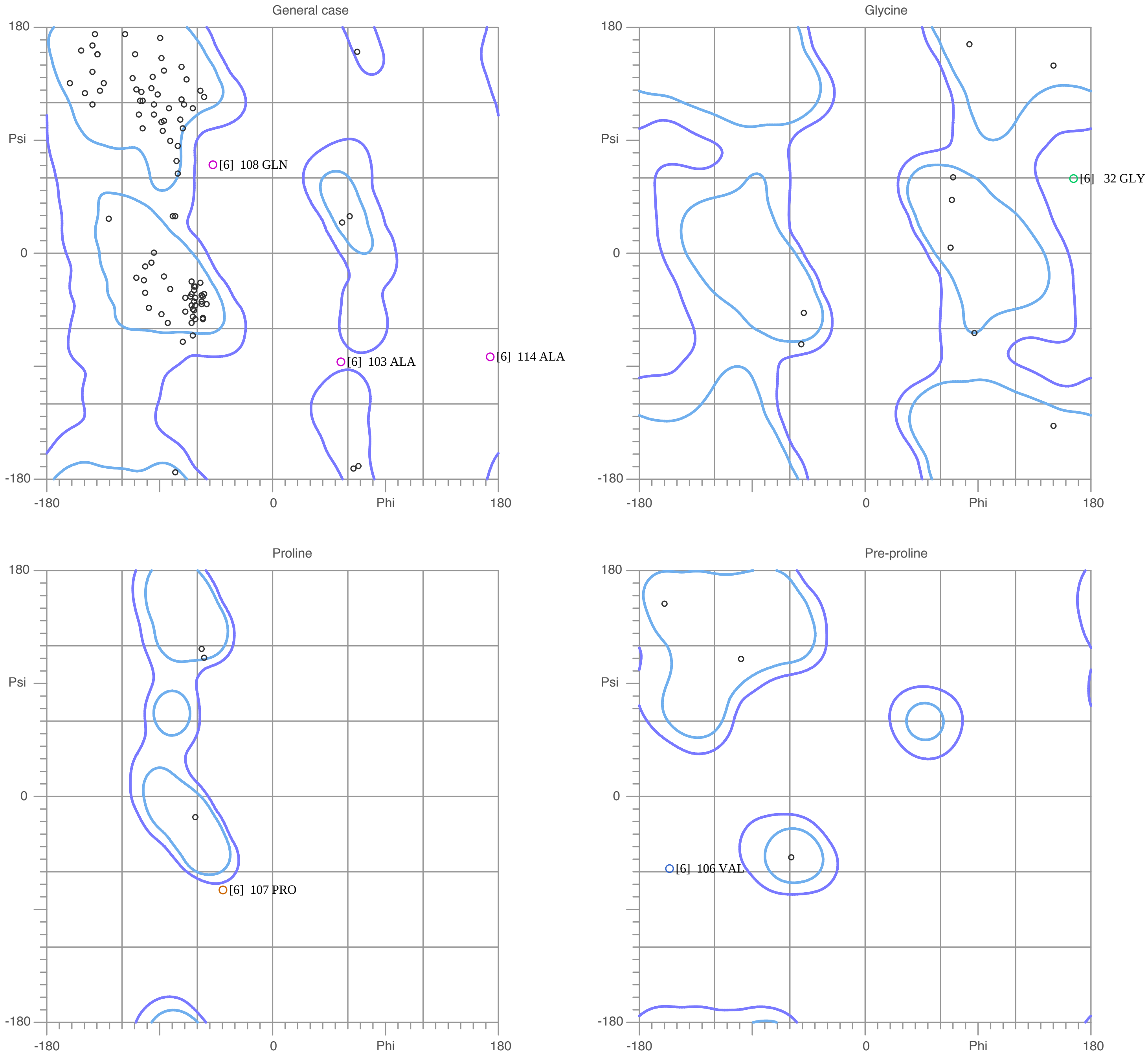
[5] 39 GLY (46.7, -91.9)
[5] 64 GLU (65.7, 158.9)
[5] 65 PRO (-55.9, 76.5)
[5] 67 GLY (145.5, -90.6)
[5] 76 ARG (-51.4, 90.9)
[5] 79 ALA (61.4, 97.0)
[5] 103 ALA (63.4, -85.0)
[5] 107 PRO (-83.6, -73.9)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 6



87.7% (100/114) of all residues were in favored (98%) regions.
94.7% (108/114) of all residues were in allowed (>99.8%) regions.

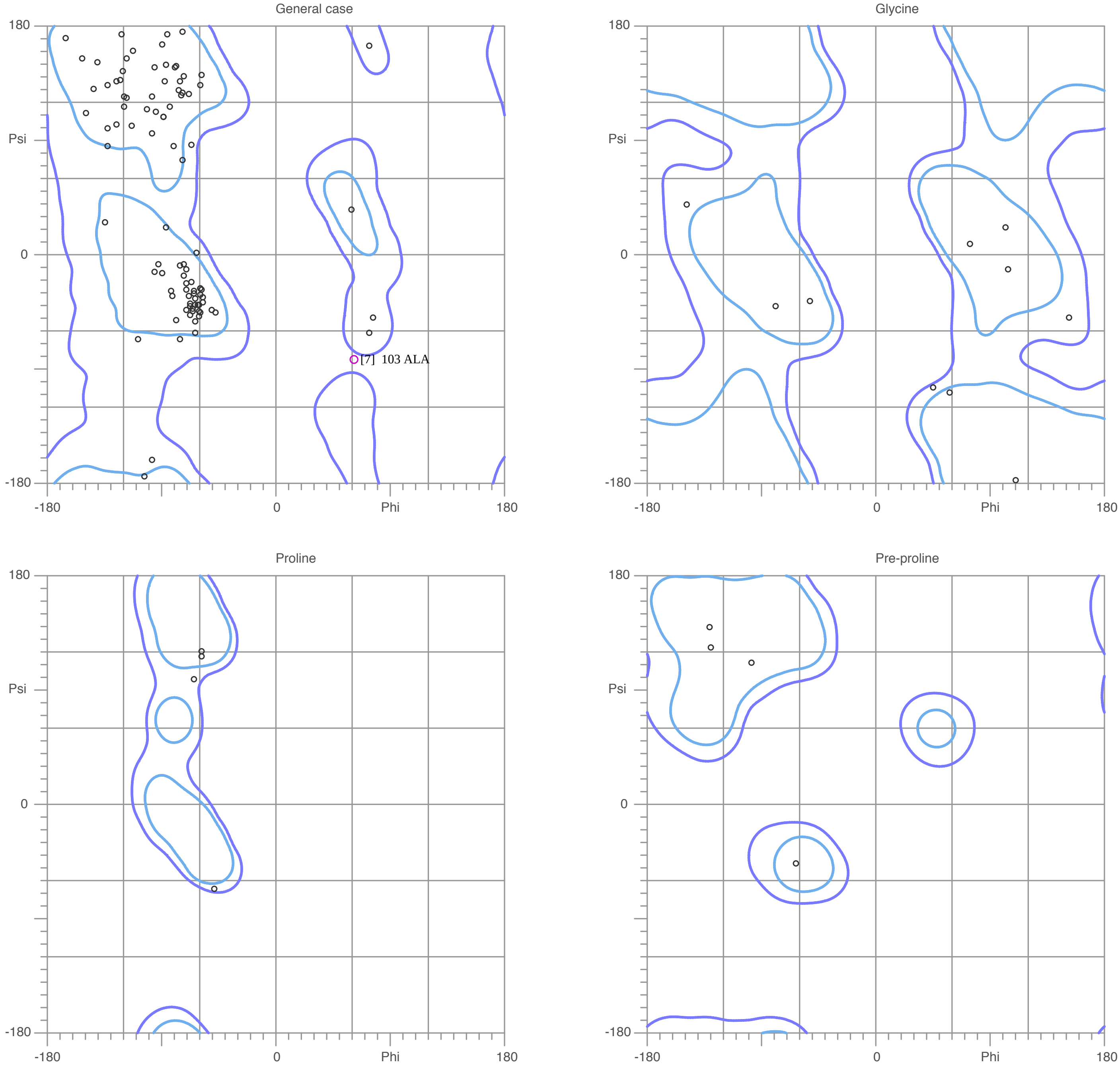
There were 6 outliers (phi, psi):
[6] 32 GLY (166.3, 60.3)
[6] 103 ALA (54.8, -86.4)
[6] 106 VAL (-156.1, -57.8)
[6] 107 PRO (-40.7, -74.5)
[6] 108 GLN (-48.7, 71.5)
[6] 114 ALA (173.9, -82.1)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 7

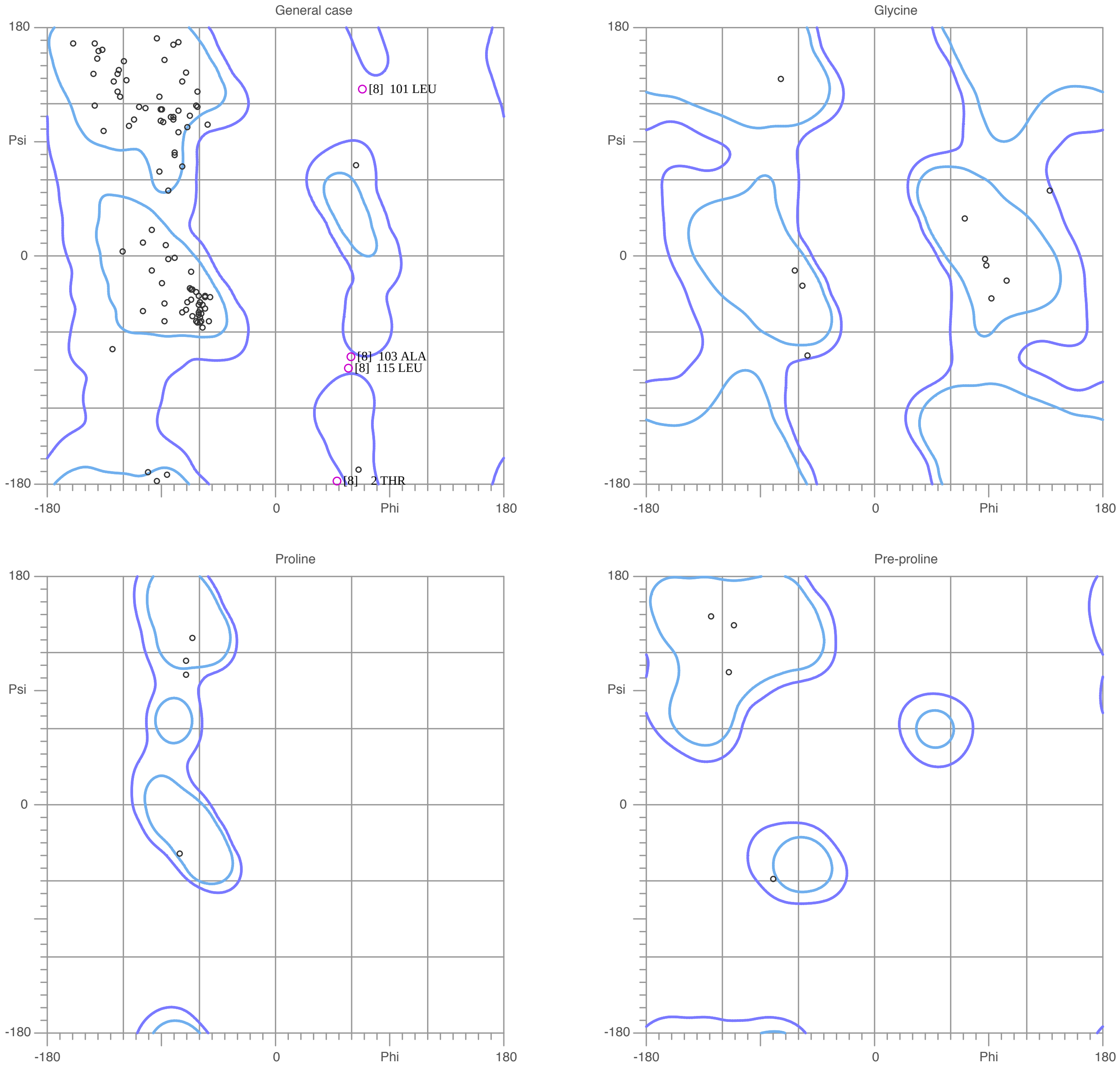


87.7% (100/114) of all residues were in favored (98%) regions.
99.1% (113/114) of all residues were in allowed (>99.8%) regions.

There were 1 outliers (phi, psi):
[7] 103 ALA (61.1, -82.2)

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 8



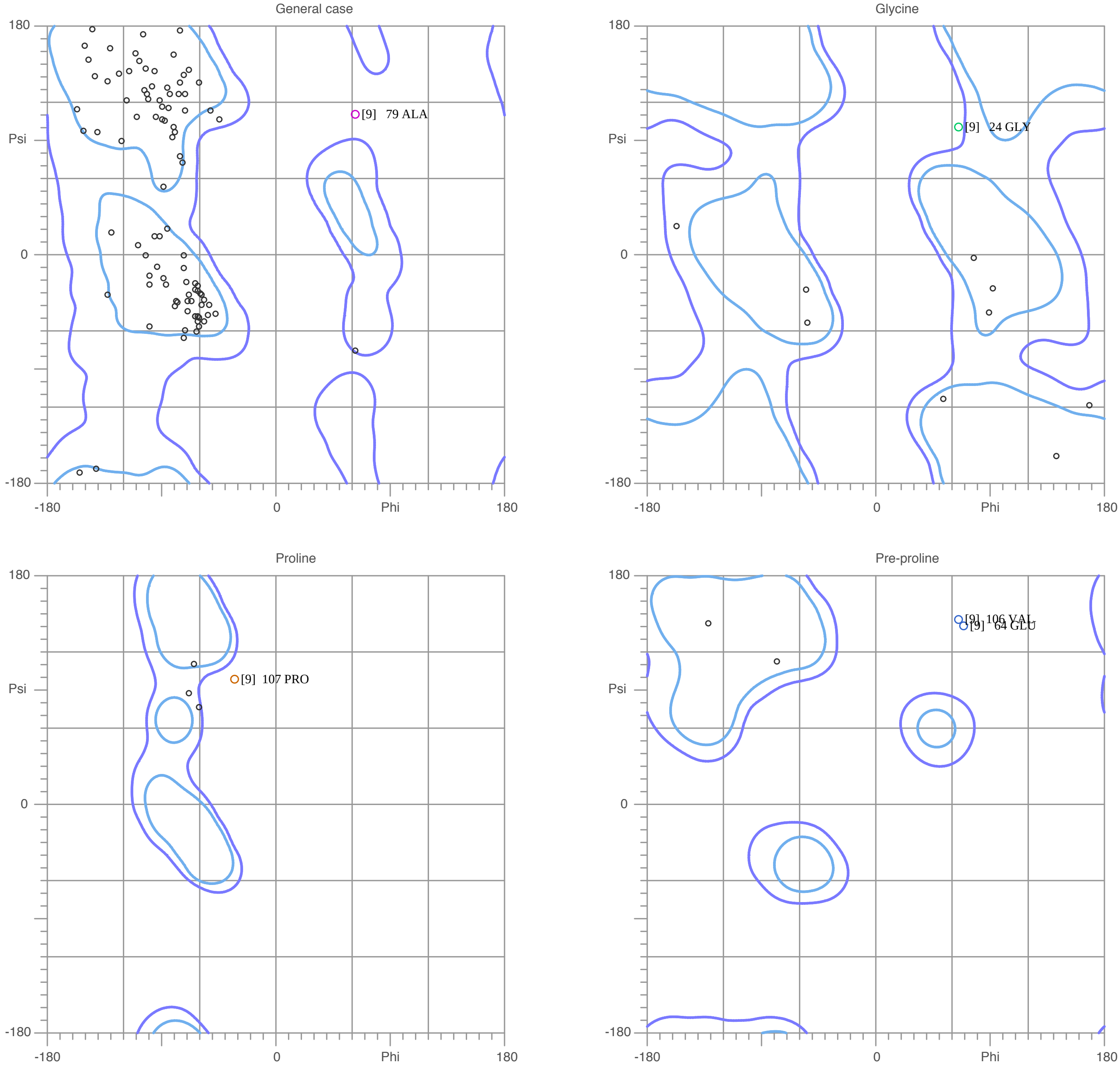
88.6% (101/114) of all residues were in favored (98%) regions.
96.5% (110/114) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):

[8] 2 THR (49.0, -177.7)
[8] 101 LEU (68.3, 132.8)
[8] 103 ALA (59.2, -79.8)
[8] 115 LEU (57.1, -88.3)

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 9



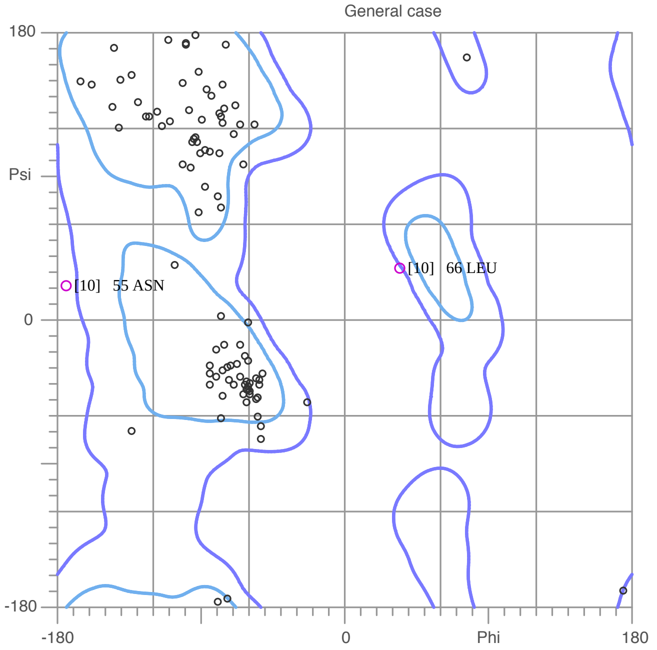
87.7% (100/114) of all residues were in favored (98%) regions.
95.6% (109/114) of all residues were in allowed (>99.8%) regions.

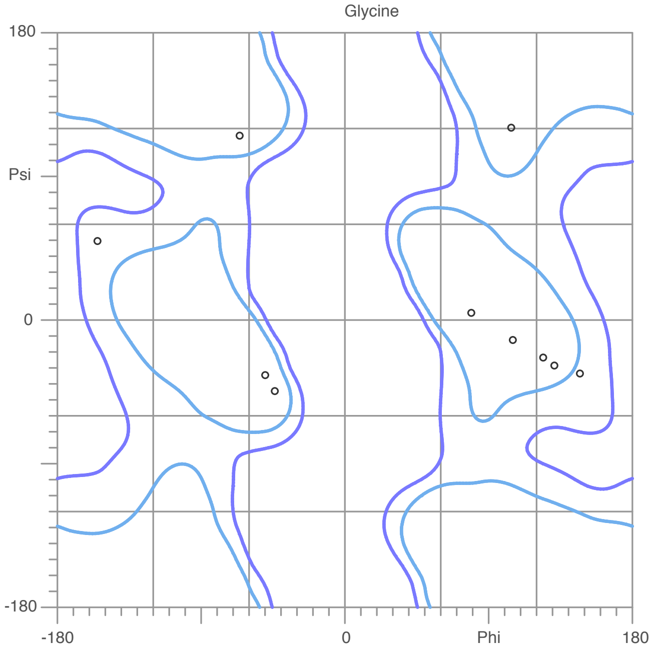
There were 5 outliers (phi, psi):

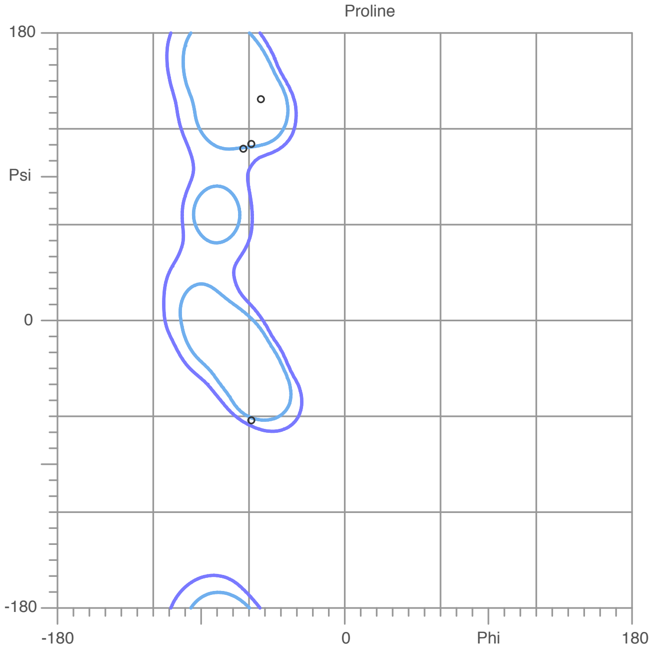
[9] 24 GLY (66.0, 101.6)
[9] 64 GLU (69.4, 141.5)
[9] 79 ALA (62.9, 111.4)
[9] 106 VAL (65.7, 146.0)
[9] 107 PRO (-33.3, 99.4)

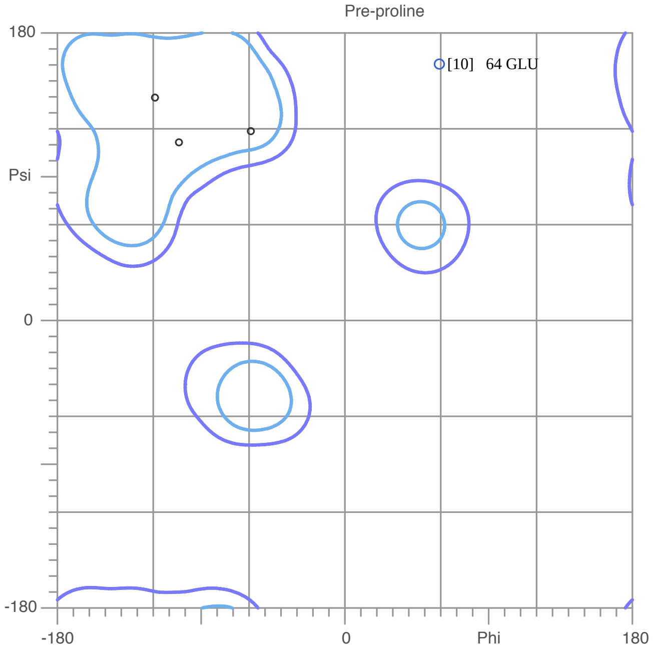
MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 10









87.7% (100/114) of all residues were in favored (98%) regions.
97.4% (111/114) of all residues were in allowed (>99.8%) regions.

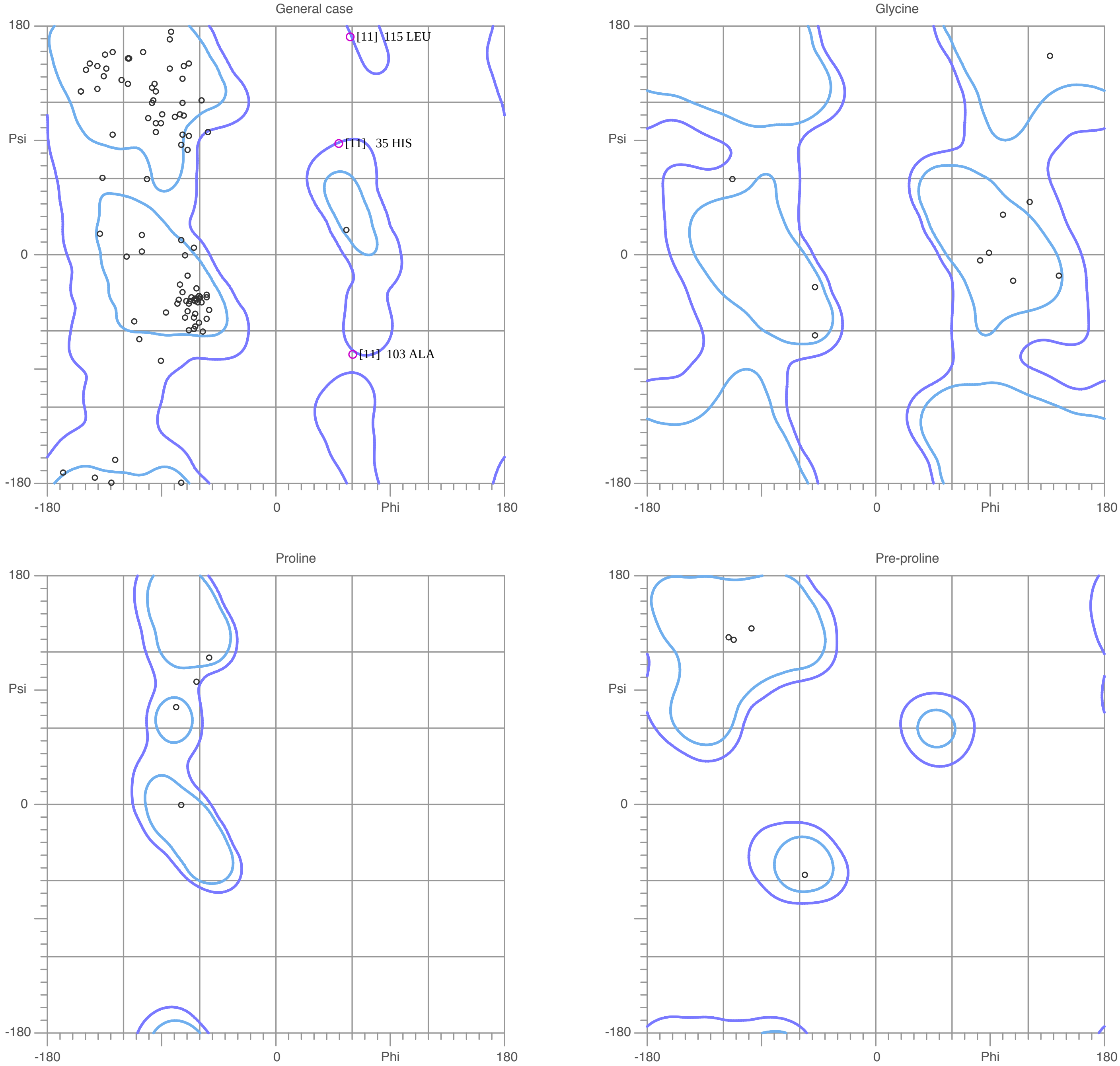
There were 3 outliers (phi, psi):
[10] 55 ASN (-175.4, 22.6)
[10] 64 GLU (59.2, 161.5)
[10] 66 LEU (34.6, 33.7)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 11



86.0% (98/114) of all residues were in favored (98%) regions.
97.4% (111/114) of all residues were in allowed (>99.8%) regions.

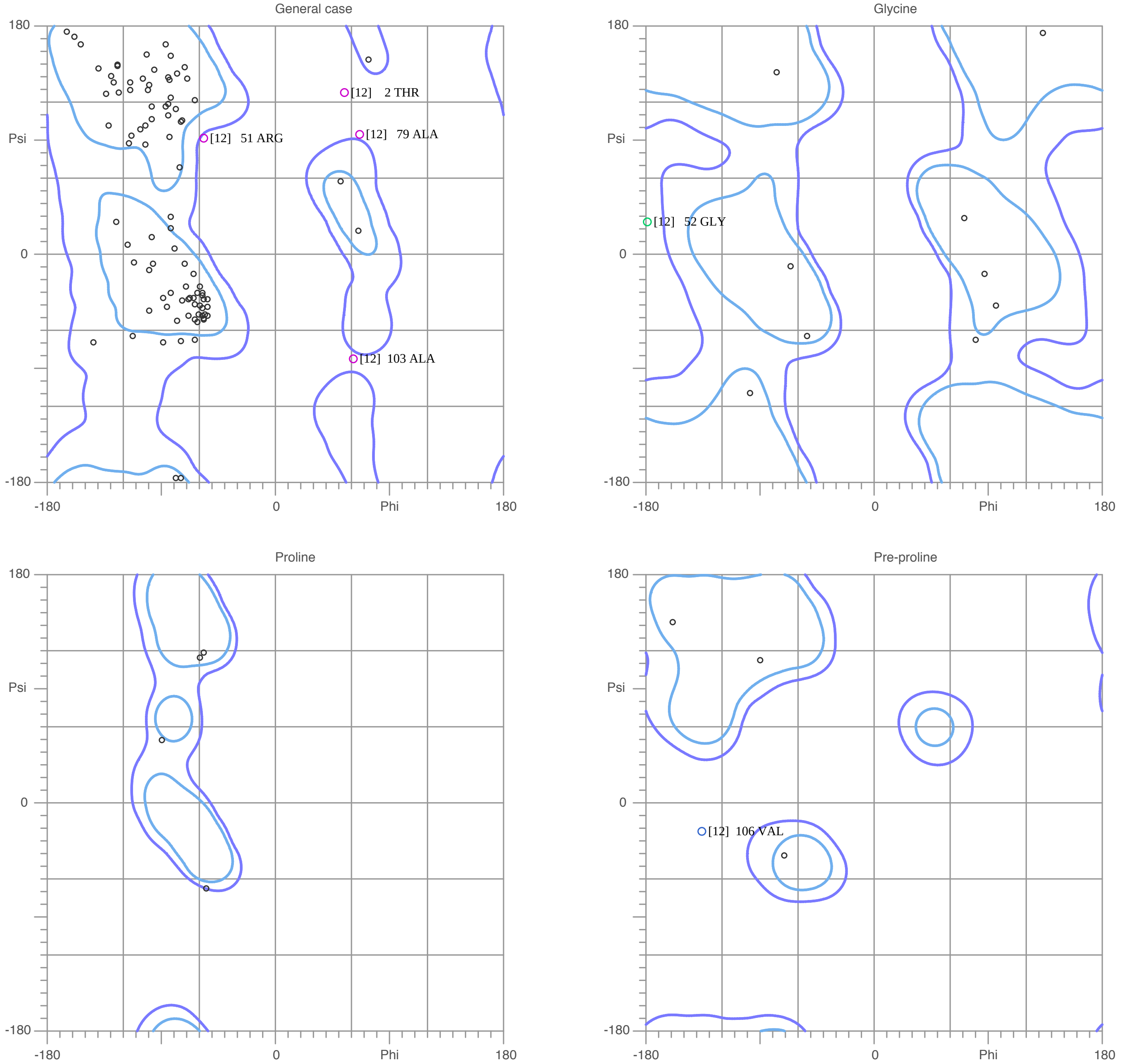
There were 3 outliers (phi, psi):
[11] 35 HIS (49.6, 88.7)
[11] 103 ALA (60.8, -78.2)
[11] 115 LEU (58.4, 172.6)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 12



85.1% (97/114) of all residues were in favored (98%) regions.
94.7% (108/114) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):

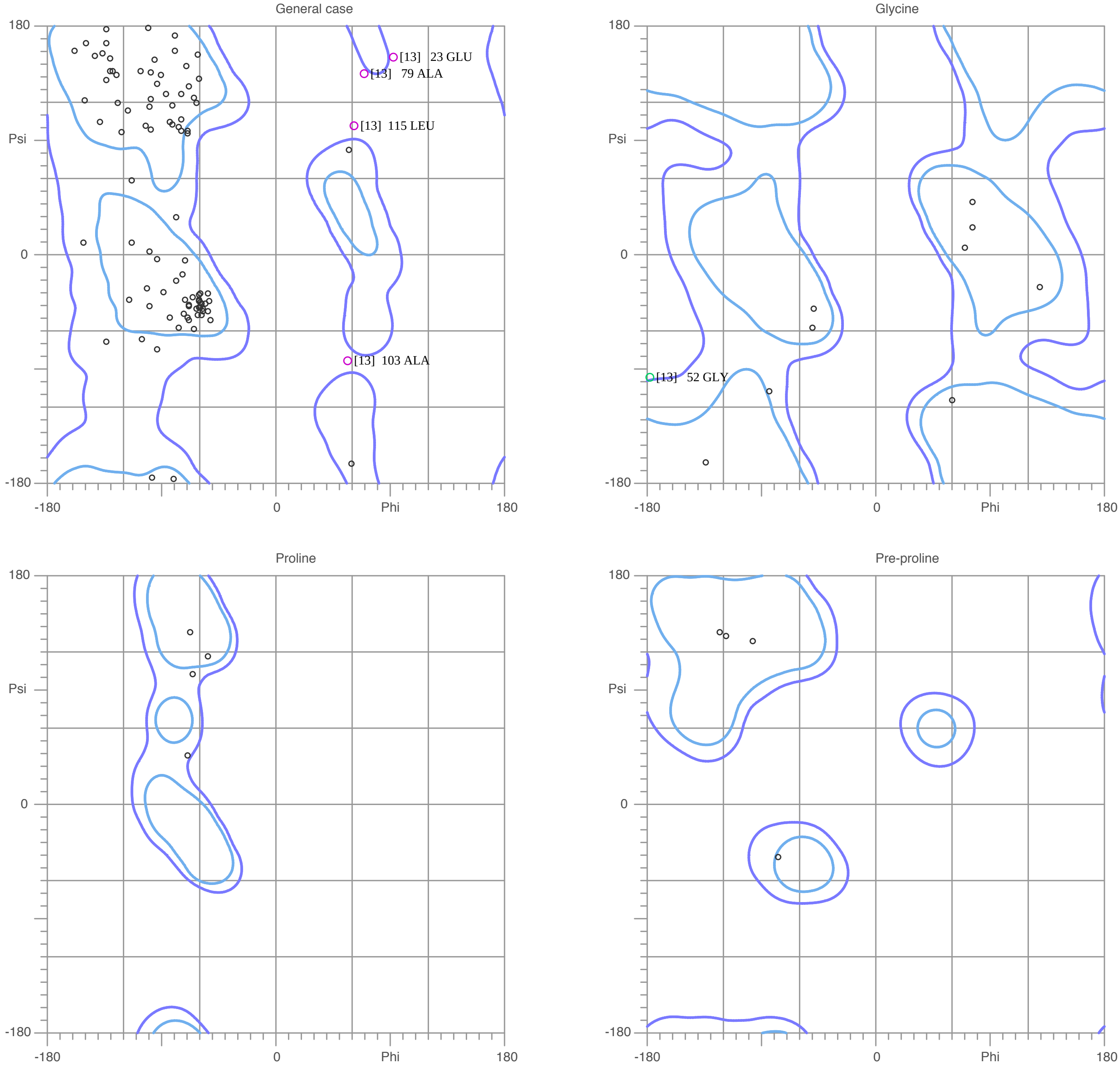
[12] 2 THR (55.0, 128.2)
[12] 51 ARG (-58.0, 93.0)
[12] 52 GLY (-179.4, 26.9)
[12] 79 ALA (66.1, 95.9)
[12] 103 ALA (61.5, -82.9)
[12] 106 VAL (-136.4, -22.1)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 13



84.2% (96/114) of all residues were in favored (98%) regions.
95.6% (109/114) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

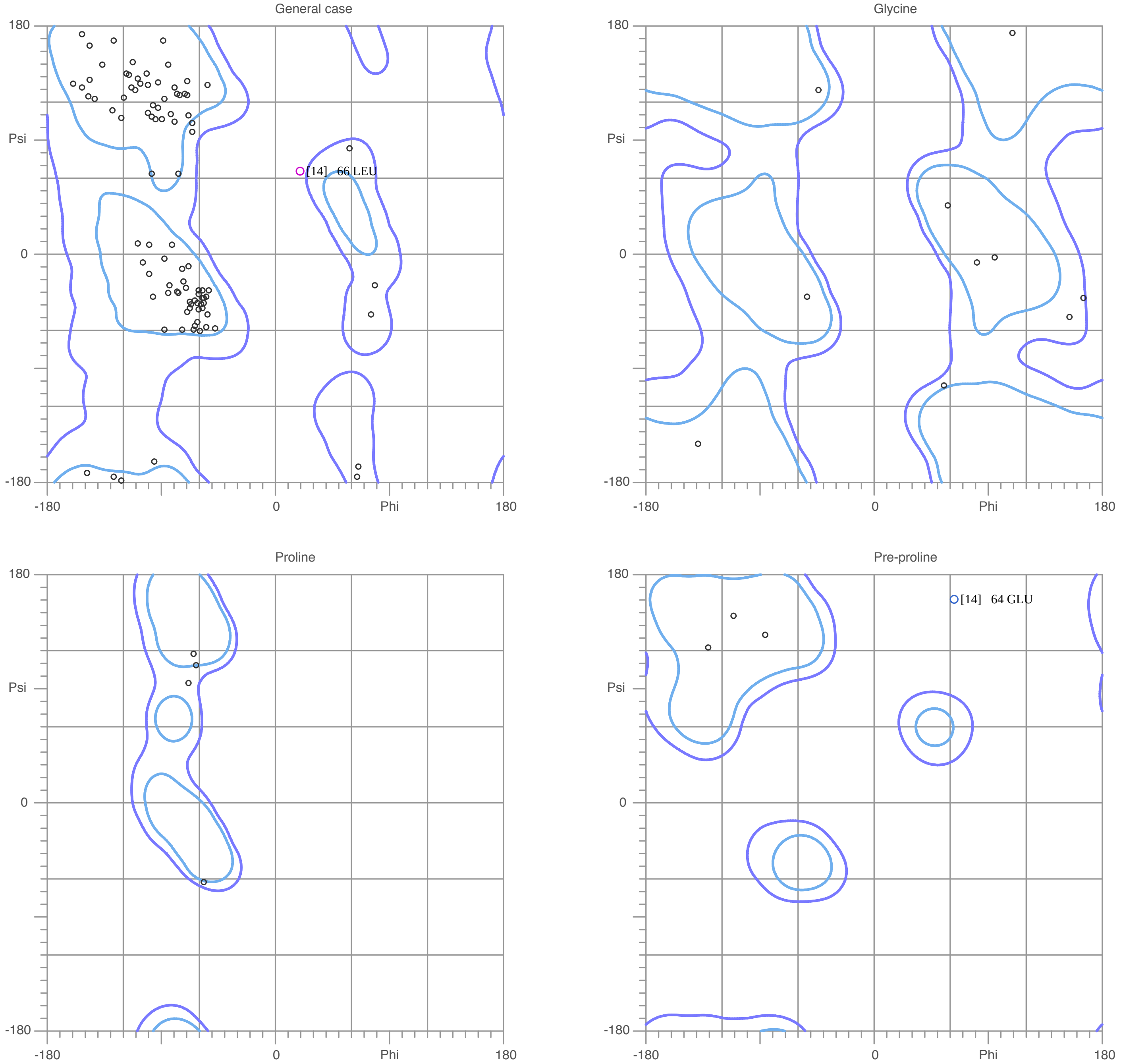
[13] 23 GLU (92.5, 156.1)
[13] 52 GLY (-178.6, -96.8)
[13] 79 ALA (69.7, 143.9)
[13] 103 ALA (56.6, -83.0)
[13] 115 LEU (61.1, 102.5)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 14

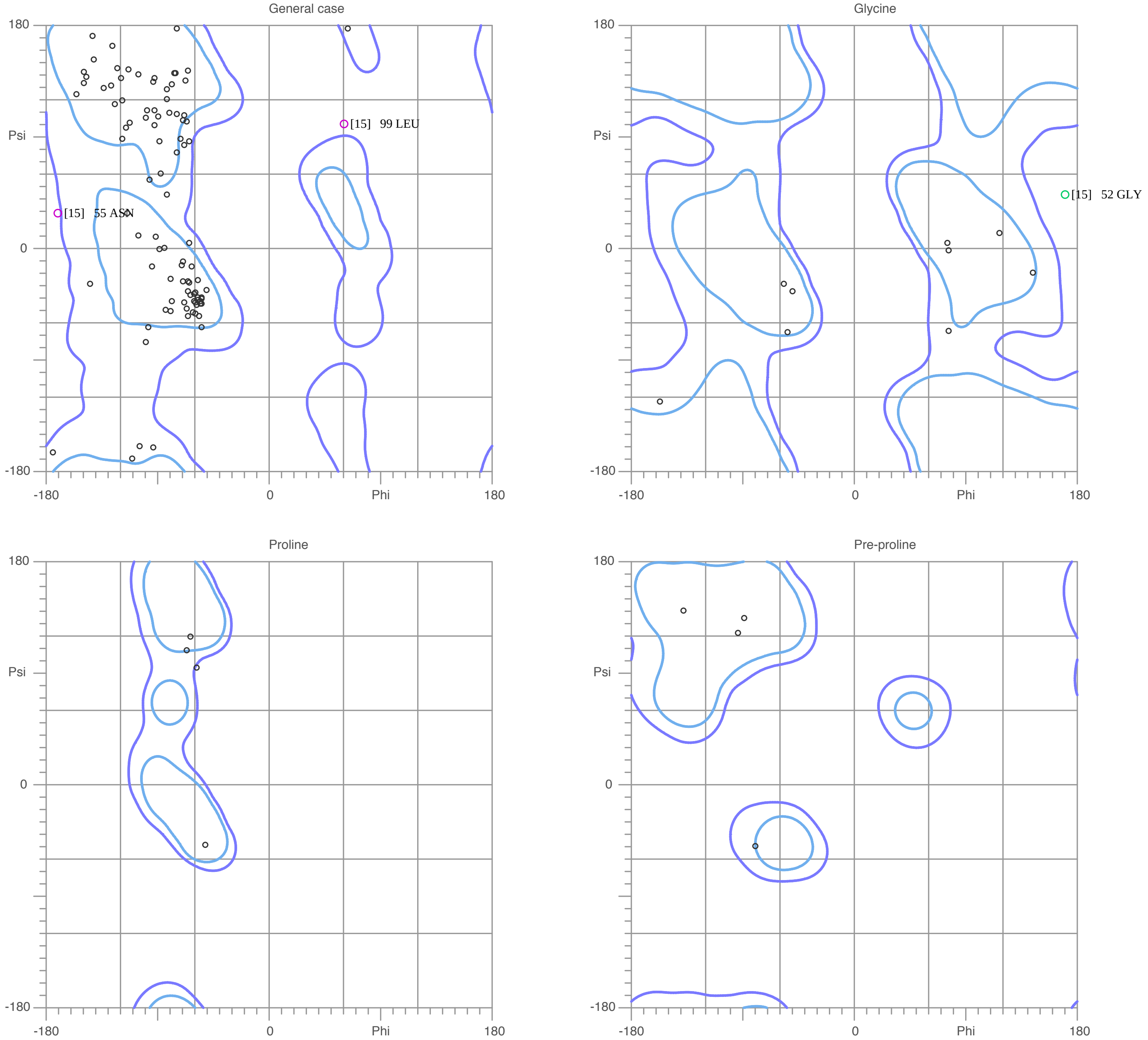


86.0% (98/114) of all residues were in favored (98%) regions.
98.2% (112/114) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
[14] 64 GLU (63.4, 161.9)
[14] 66 LEU (19.0, 66.0)

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 15



81.6% (93/114) of all residues were in favored (98%) regions.
97.4% (111/114) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):

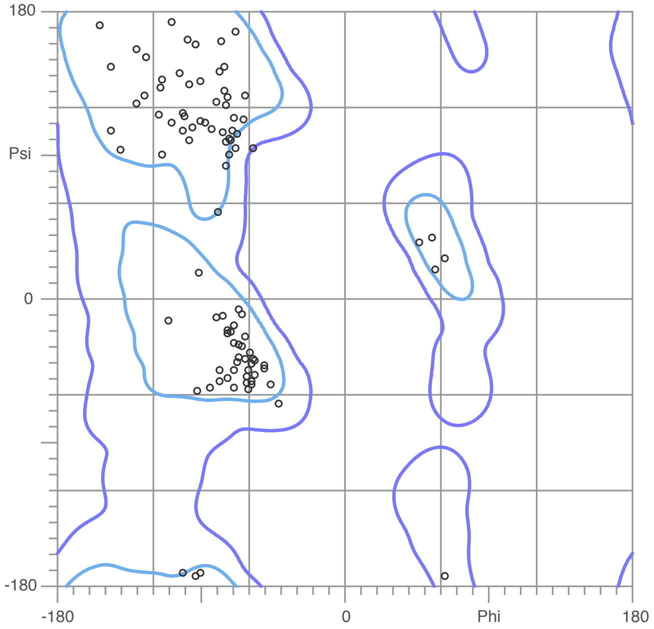
[15] 52 GLY (170.8, 45.0)
[15] 55 ASN (-171.8, 29.9)
[15] 99 LEU (60.1, 101.6)

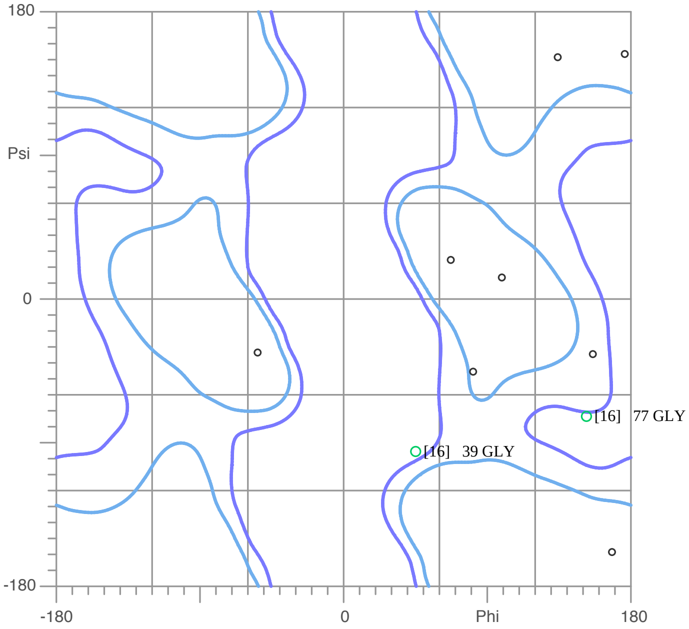
http://kinemage.biochem.duke.edu

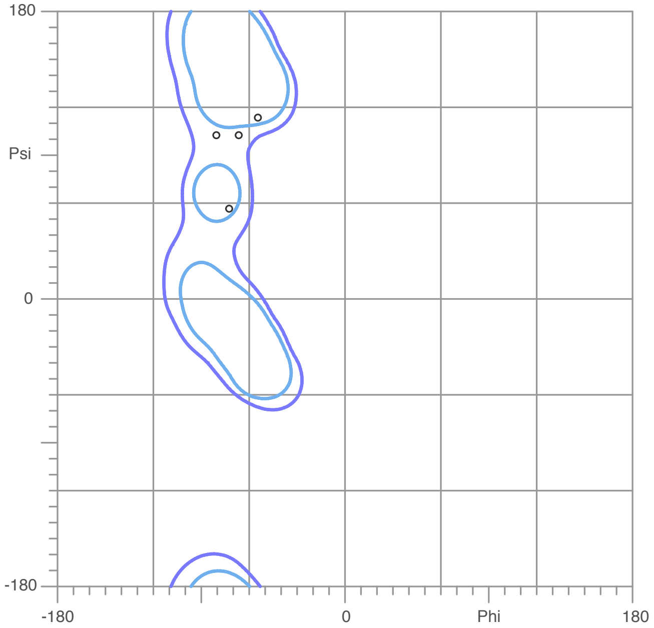
Lovell, Davis, et al. Proteins 50:437 (2003)

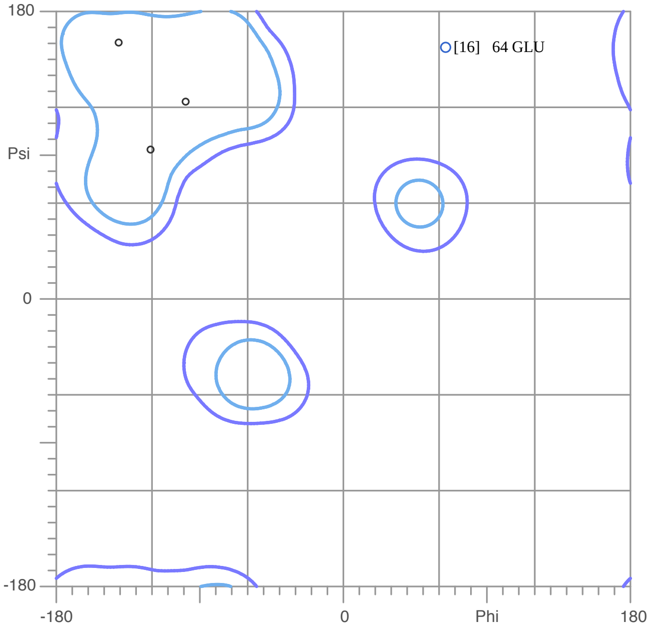
MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 16


General case


Glycine


Proline


Pre-proline

90.4% (103/114) of all residues were in favored (98%) regions.
97.4% (111/114) of all residues were in allowed (>99.8%) regions.

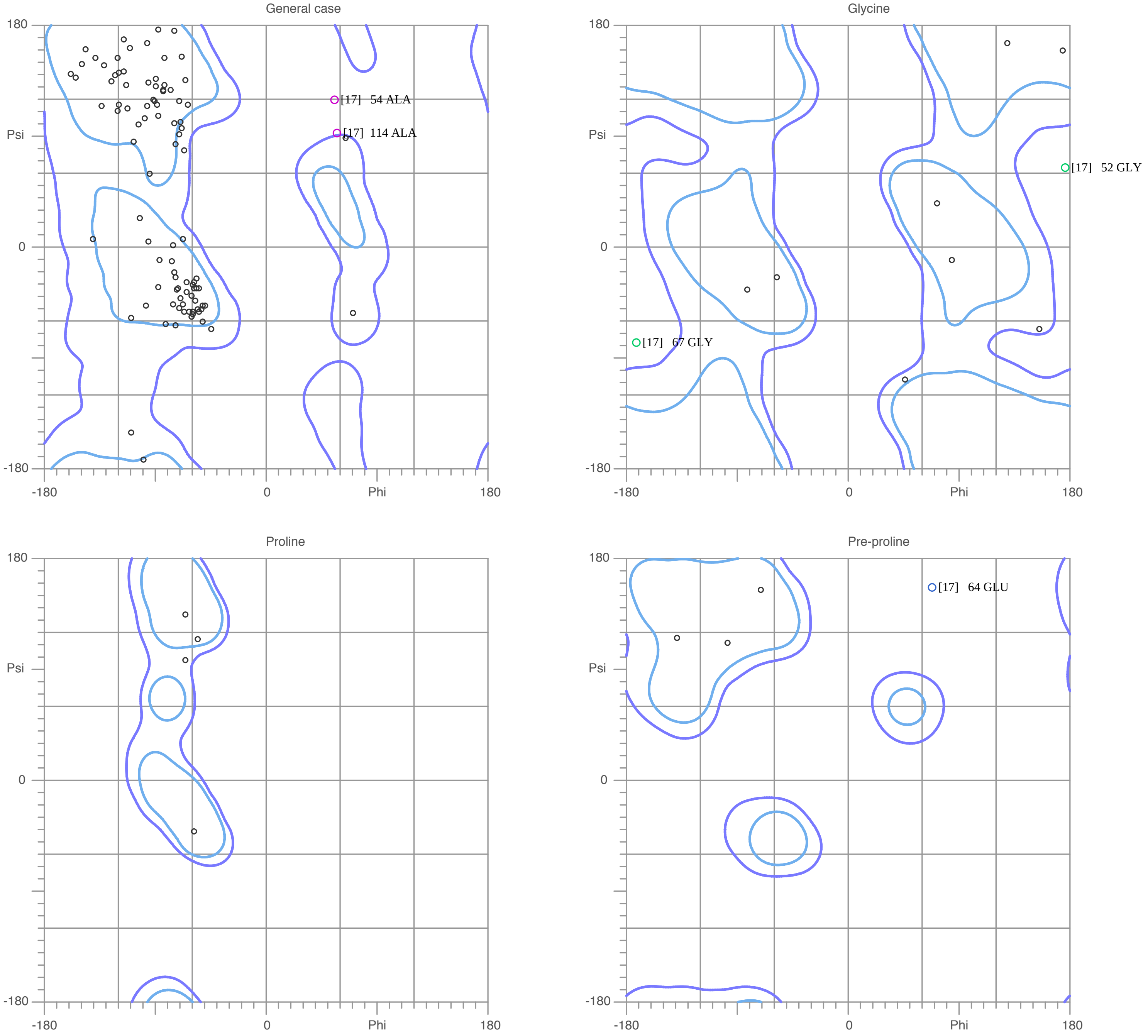
There were 3 outliers (phi, psi):
[16] 39 GLY (45.9, -96.0)
[16] 64 GLU (64.7, 158.3)
[16] 77 GLY (152.9, -73.2)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 17



84.2% (96/114) of all residues were in favored (98%) regions.
95.6% (109/114) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

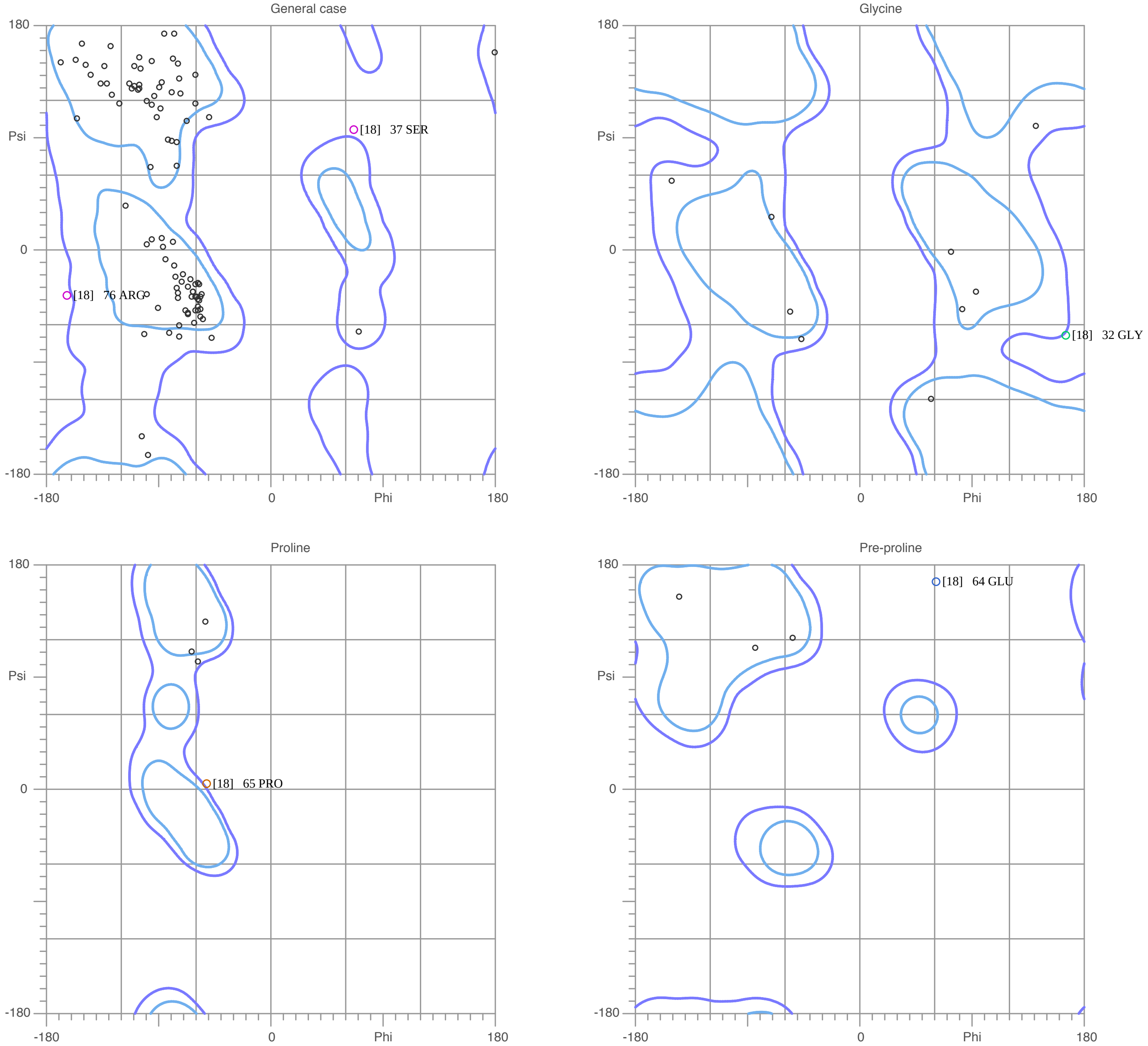
[17] 52 GLY (176.9, 65.9)
[17] 54 ALA (55.5, 120.8)
[17] 64 GLU (68.7, 157.4)
[17] 67 GLY (-172.2, -77.6)
[17] 114 ALA (57.6, 93.5)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 18



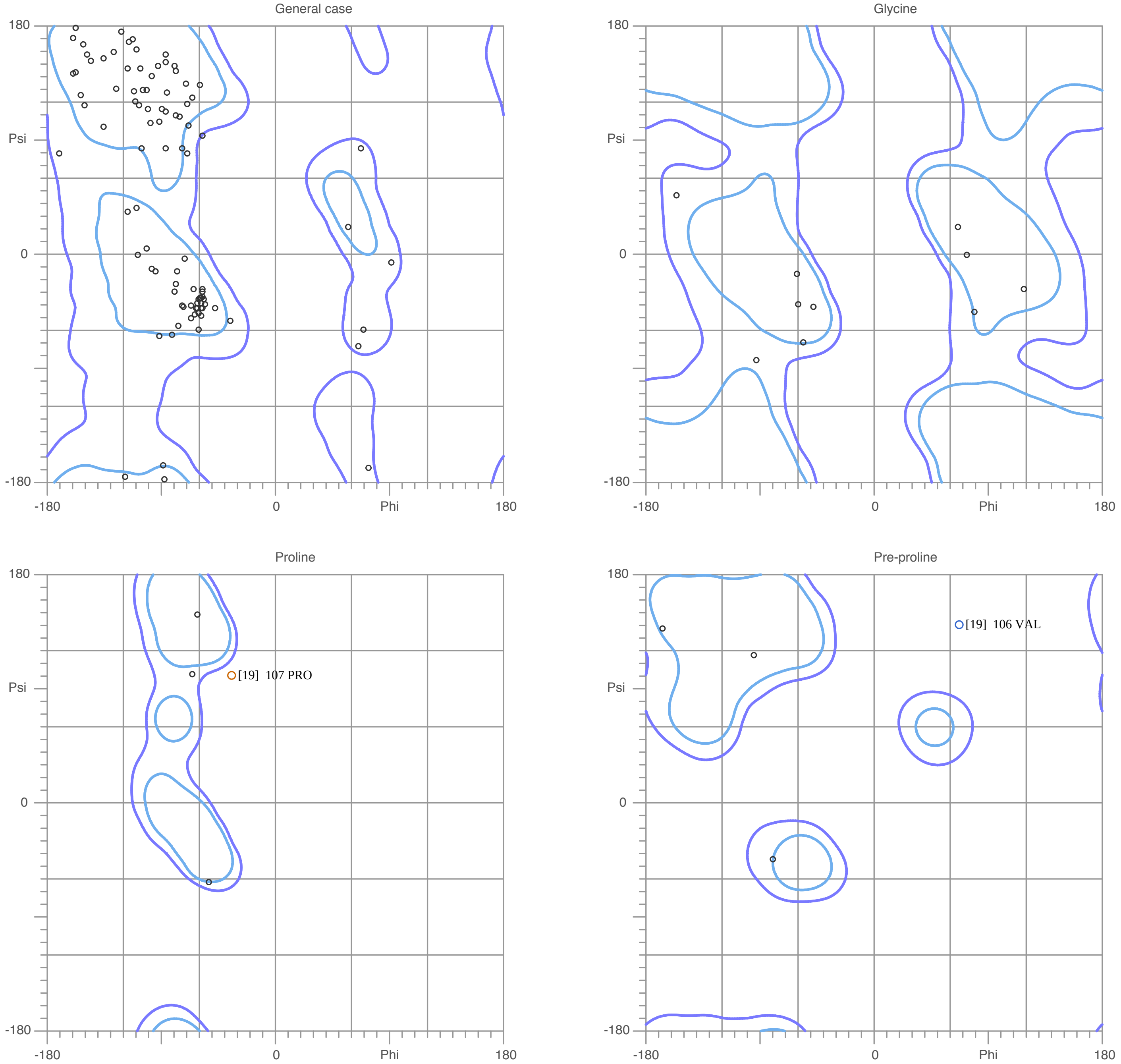
83.3% (95/114) of all residues were in favored (98%) regions.
95.6% (109/114) of all residues were in allowed (>99.8%) regions.

There were 5 outliers (phi, psi):

[18] 32 GLY (165.1, -68.9)
[18] 37 SER (66.5, 97.1)
[18] 64 GLU (61.2, 168.0)
[18] 65 PRO (-52.2, 6.0)
[18] 76 ARG (-164.3, -36.4)

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 19



84.2% (96/114) of all residues were in favored (98%) regions.
98.2% (112/114) of all residues were in allowed (>99.8%) regions.

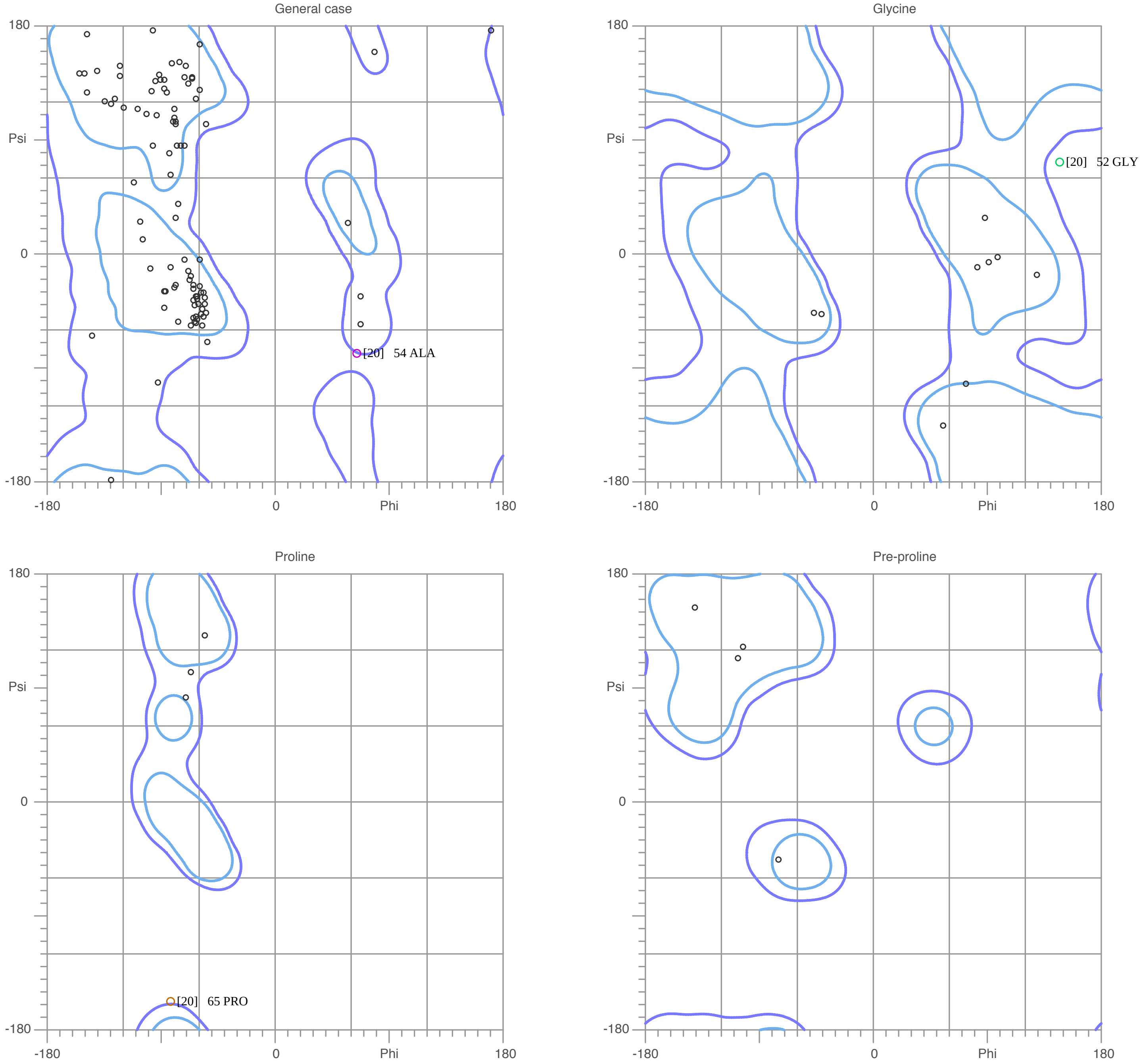
There were 2 outliers (phi, psi):
[19] 106 VAL (67.1, 141.1)
[19] 107 PRO (-35.0, 101.8)

http://kinemage.biochem.duke.edu

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

MolProbity Ramachandran analysis

CCR55_NMR_em_bcr3.pdb, model 20



85.1% (97/114) of all residues were in favored (98%) regions.
97.4% (111/114) of all residues were in allowed (>99.8%) regions.

There were 3 outliers (phi, psi):
[20] 52 GLY (147.9, 73.6)
[20] 54 ALA (64.5, -78.6)
[20] 65 PRO (-83.8, -157.2)

http://kinemage.biochem.duke.edu

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