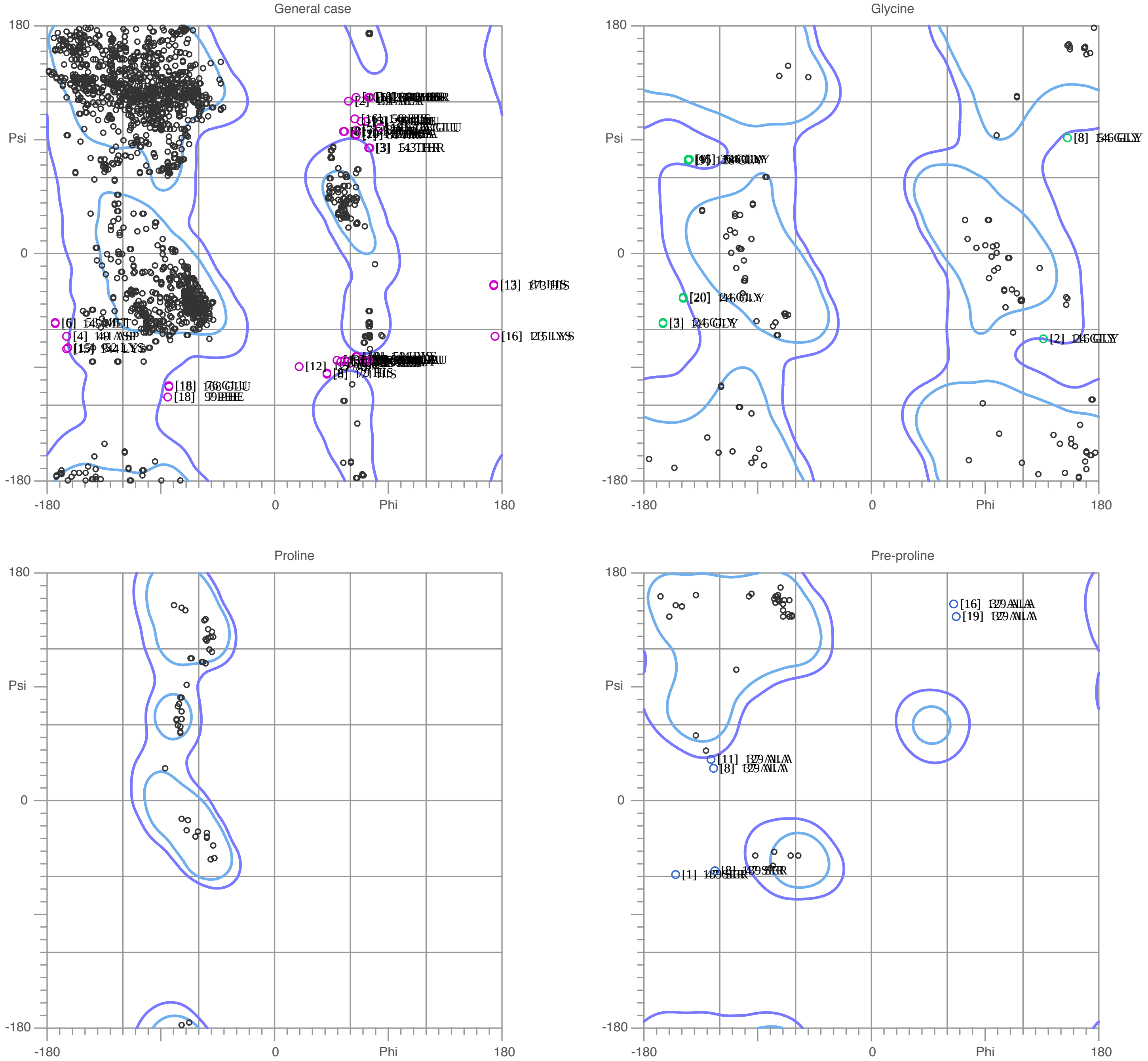
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, all models



88.4% (2829/3200) of all residues were in favored (98%) regions.
97.2% (3110/3200) of all residues were in allowed (>99.8%) regions.

There were 90 outliers (phi, psi):

```
  [1]   47 SER (-155.0, -58.2)
  [1]  139 SER (-155.0, -58.3)
  [2]   24 GLY (136.8, -67.9)
  [2]   39 ALA (58.8, 121.0)
  [2]  116 GLY (136.7, -67.8)
  [2]  131 ALA (58.7, 121.1)
  [3]    5 ALA (71.5, -85.0)
  [3]   24 GLY (-165.1, -54.9)
  [3]   51 THR (74.9, 85.0)
  [3]   97 ALA (71.5, -85.0)
  [3]  116 GLY (-165.1, -55.1)
  [3]  143 THR (75.1, 85.0)
  [4]   49 ASP (-165.0, -65.1)
  [4]  141 ASP (-165.0, -65.0)
  [5]    7 PHE (72.1, 105.0)
  [5]   50 HIS (75.1, 124.9)
  [5]   99 PHE (72.2, 105.1)
  [5]  142 HIS (75.0, 125.0)
  [6]   53 MET (-175.0, -54.9)
  [6]  145 MET (-175.0, -55.0)
  [7]   22 GLU (57.5, -85.3)
  [7]   39 ALA (64.9, 98.3)
  [7]   81 HIS (65.0, 94.9)
  [7]  114 GLU (57.4, -85.2)
  [7]  131 ALA (65.0, 98.3)
  [7]  173 HIS (65.0, 95.1)
  [8]    5 ALA (73.0, -84.9)
  [8]   37 ALA (-125.1, 26.4)
  [8]   47 SER (-124.8, -55.5)
  [8]   51 THR (55.0, 97.7)
  [8]   54 GLY (155.0, 92.3)
  [8]   79 HIS (41.7, -94.9)
  [8]   97 ALA (73.1, -85.0)
  [8]  129 ALA (-125.1, 26.4)
  [8]  139 SER (-124.9, -55.5)
  [8]  143 THR (55.0, 97.6)
  [8]  146 GLY (155.0, 92.2)
  [8]  171 HIS (41.8, -95.0)
  [9]   35 ASN (60.9, -86.5)
  [9]   36 GLY (-145.0, 75.0)
  [9]  127 ASN (60.9, -86.4)
  [9]  128 GLY (-145.0, 75.0)
  [10]   23 LYS (65.0, 125.0)
  [10]   52 LYS (64.9, -81.3)
  [10]   81 HIS (74.8, 125.0)
  [10]  115 LYS (64.9, 125.0)
  [10]  144 LYS (65.0, -81.3)
  [10]  173 HIS (74.8, 125.0)
  [11]   37 ALA (-127.6, 33.6)
  [11]  129 ALA (-127.7, 33.6)
  [12]   35 ASN (19.9, -89.6)
  [12]  127 ASN (20.0, -89.6)
  [13]    6 GLU (68.5, 105.1)
  [13]   22 GLU (49.2, -84.9)
  [13]   81 HIS (173.6, -25.0)
  [13]   98 GLU (68.6, 105.0)
  [13]  114 GLU (49.2, -84.9)
  [13]  173 HIS (173.6, -25.0)
  [14]   22 GLU (52.4, -85.0)
  [14]   51 THR (75.1, 125.0)
  [14]  114 GLU (52.4, -85.0)
  [14]  143 THR (75.0, 125.0)
  [15]    6 GLU (74.9, -84.9)
  [15]   22 GLU (55.4, -85.0)
  [15]   52 LYS (-165.0, -74.9)
  [15]   54 GLY (-145.0, 75.0)
  [15]   98 GLU (74.9, -85.0)
  [15]  114 GLU (55.5, -85.0)
  [15]  144 LYS (-165.1, -75.0)
  [15]  146 GLY (-145.0, 75.1)
  [16]   23 LYS (175.0, -65.1)
  [16]   37 ALA (65.3, 156.1)
  [16]   50 HIS (63.3, 107.3)
  [16]  115 LYS (174.9, -65.0)
  [16]  129 ALA (65.3, 156.2)
  [16]  142 HIS (63.3, 107.1)
  [18]    7 PHE (-85.0, -113.5)
  [18]   76 GLU (-85.0, -104.9)
  [18]   99 PHE (-85.0, -113.5)
  [18]  168 GLU (-85.0, -105.0)
  [19]   37 ALA (67.8, 146.0)
  [19]   39 ALA (64.9, 95.0)
  [19]   76 GLU (83.5, 100.8)
  [19]  129 ALA (67.7, 146.0)
  [19]  131 ALA (65.0, 95.1)
  [19]  168 GLU (83.4, 100.8)
  [20]   24 GLY (-149.2, -35.0)
  [20]   79 HIS (65.0, 95.1)
  [20]  116 GLY (-149.2, -35.0)
  [20]  171 HIS (65.0, 95.1)
```

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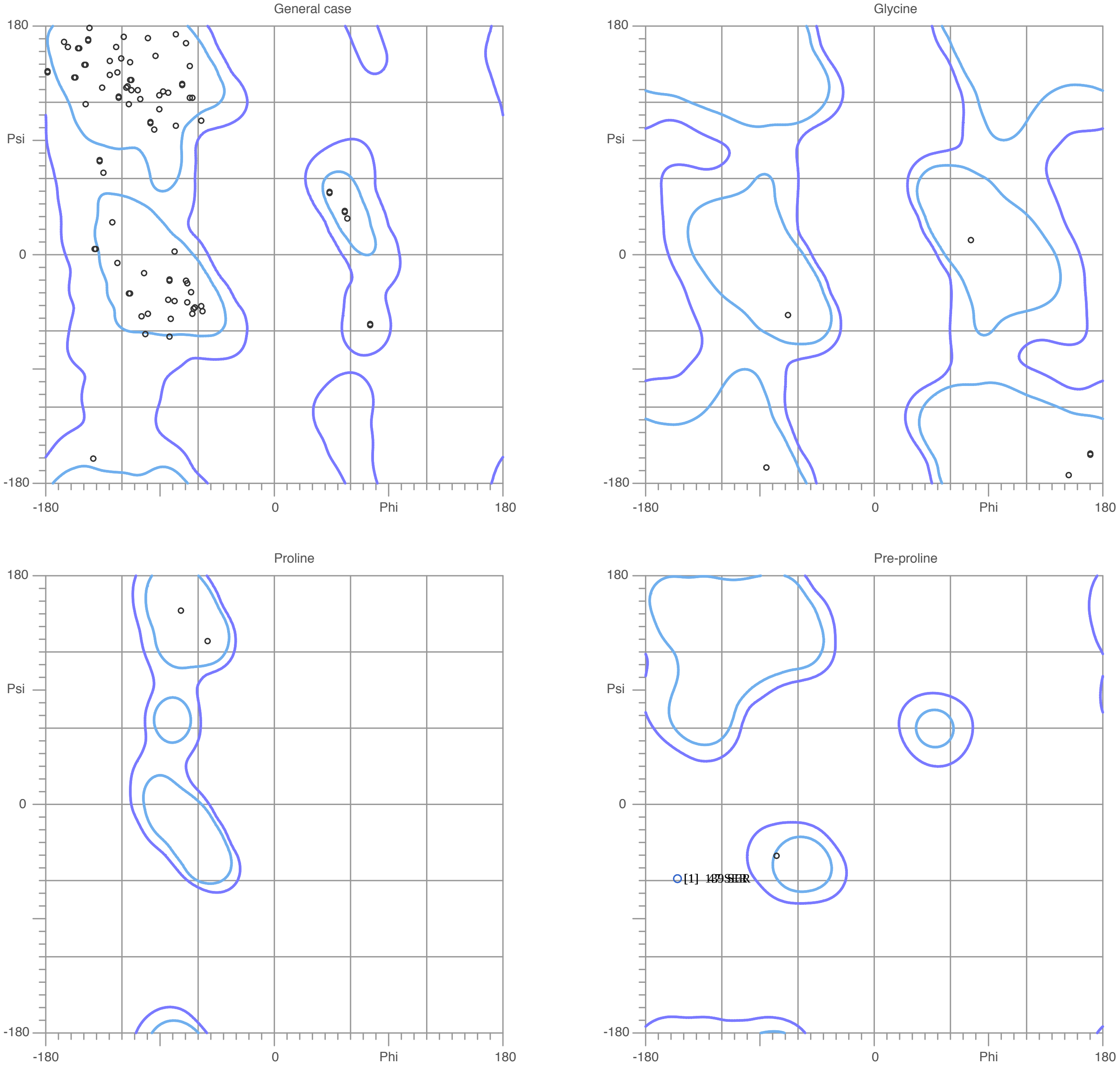
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 1



87.5% (140/160) of all residues were in favored (98%) regions.
98.8% (158/160) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):

[1] 47 SER (-155.0, -58.2)
[1] 139 SER (-155.0, -58.3)

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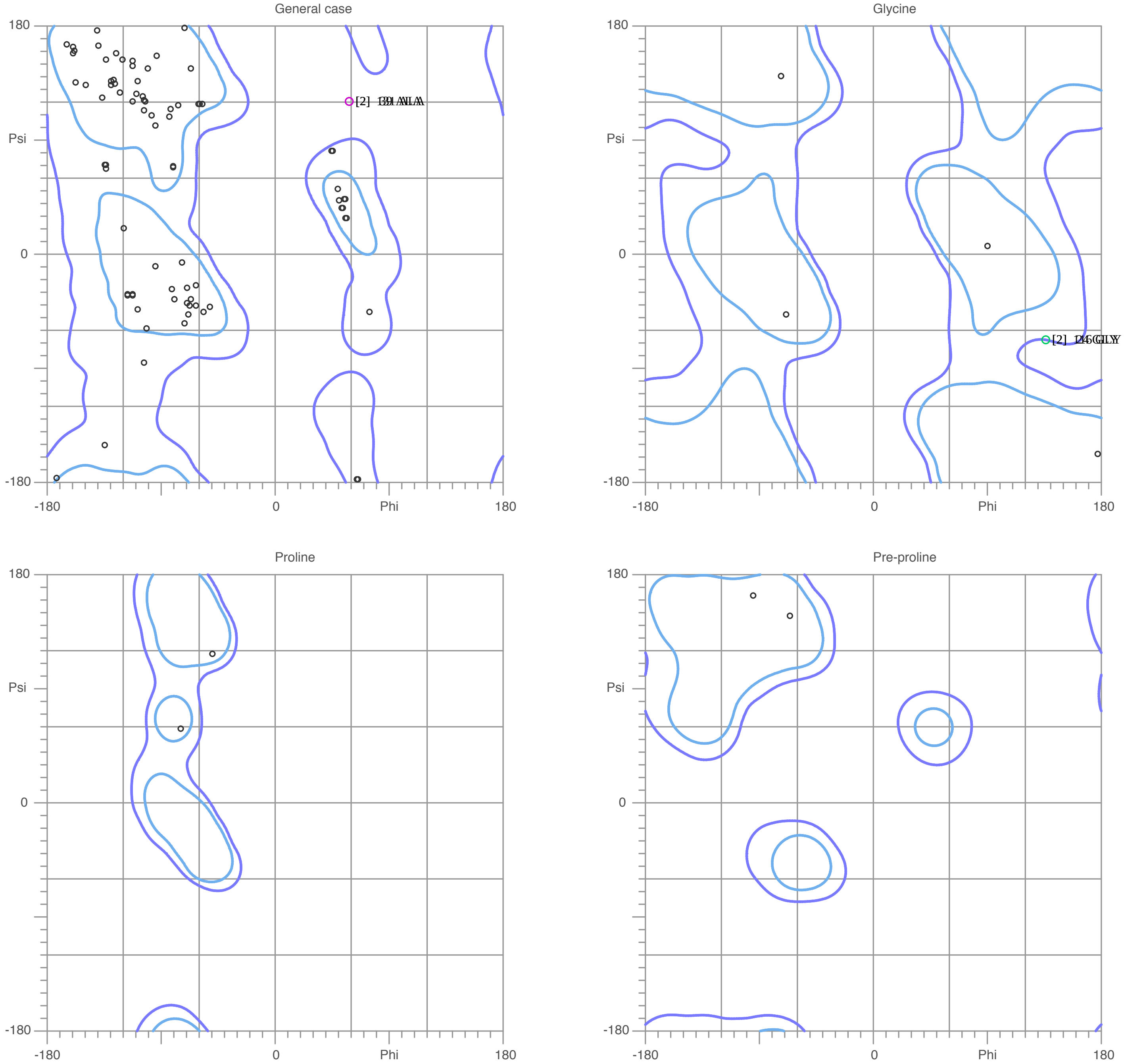
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 2



87.5% (140/160) of all residues were in favored (98%) regions.
97.5% (156/160) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
- [2] 24 GLY (136.8, -67.9)
- [2] 39 ALA (58.8, 121.0)
- [2] 116 GLY (136.7, -67.8)
- [2] 131 ALA (58.7, 121.1)

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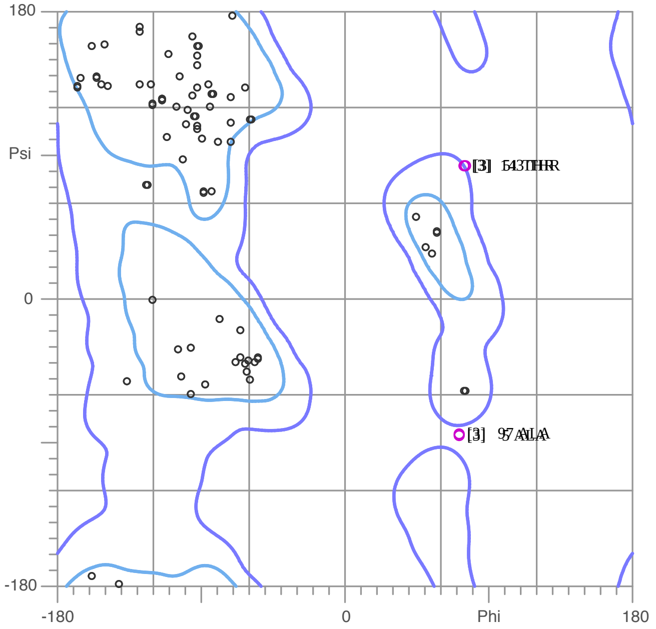
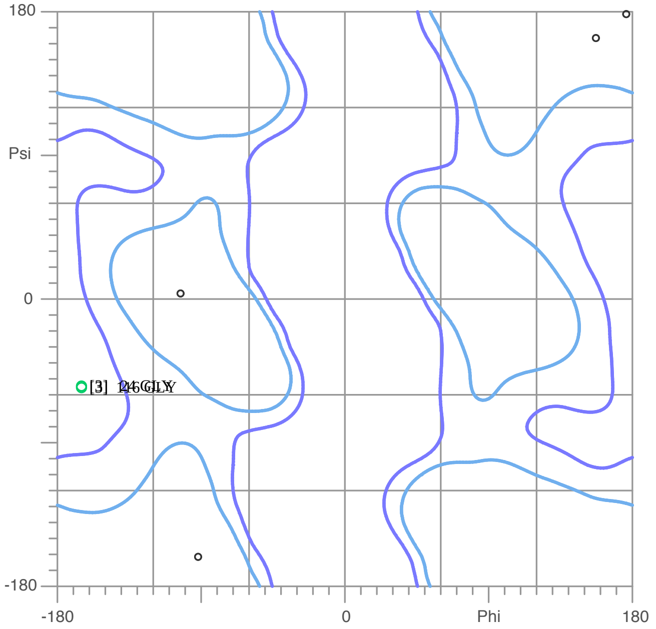
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 3

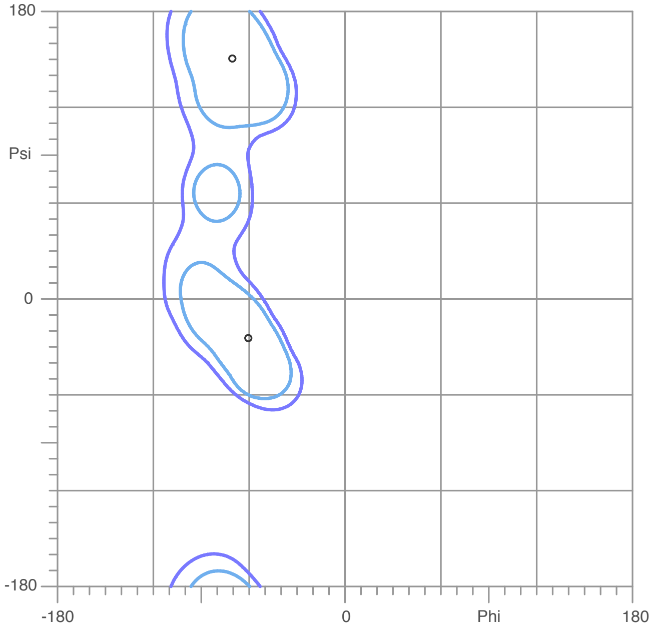
General case



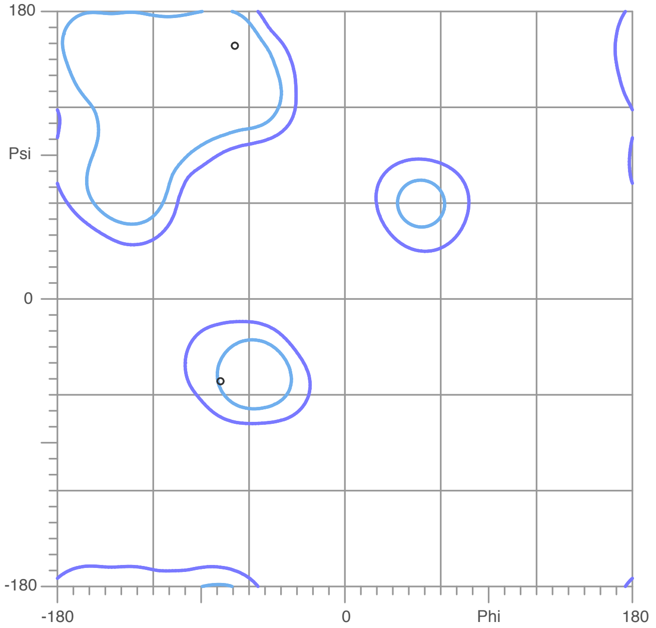
Glycine



Proline



Pre-proline



92.5% (148/160) of all residues were in favored (98%) regions.
96.2% (154/160) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):
[3] 5 ALA (71.5, -85.0)
[3] 24 GLY (-165.1, -54.9)
[3] 51 THR (74.9, 85.0)
[3] 97 ALA (71.5, -85.0)
[3] 116 GLY (-165.1, -55.1)
[3] 143 THR (75.1, 85.0)

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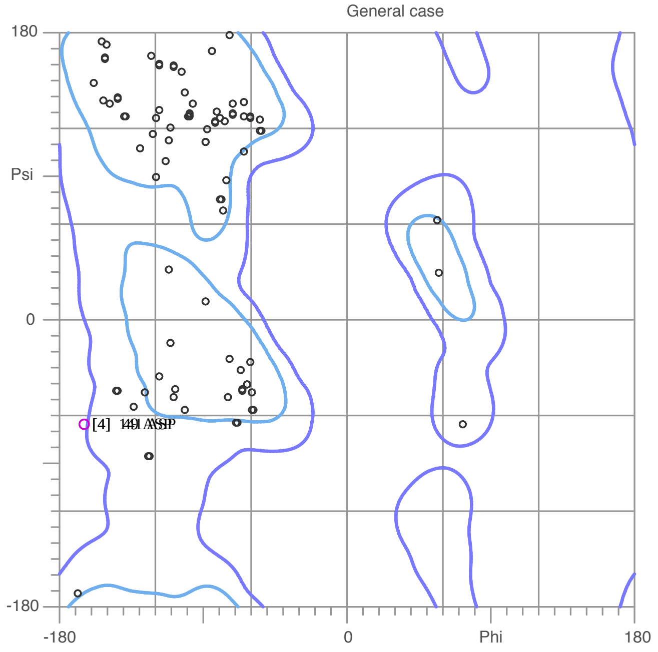
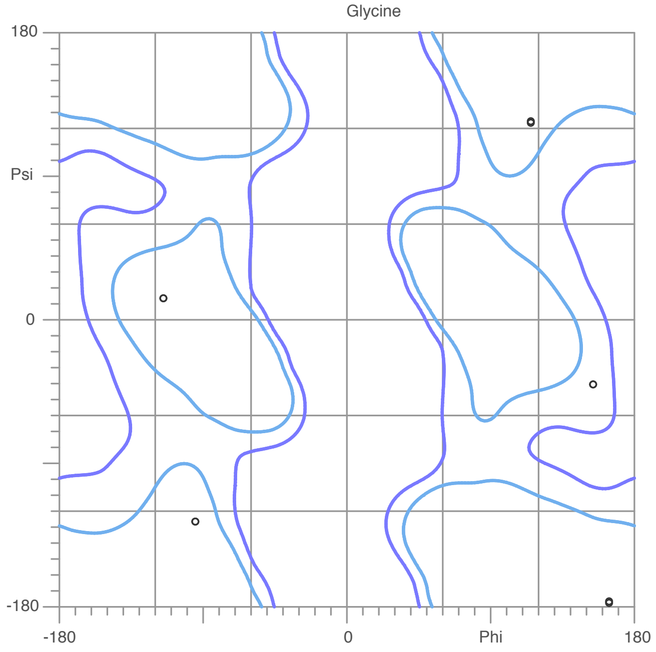
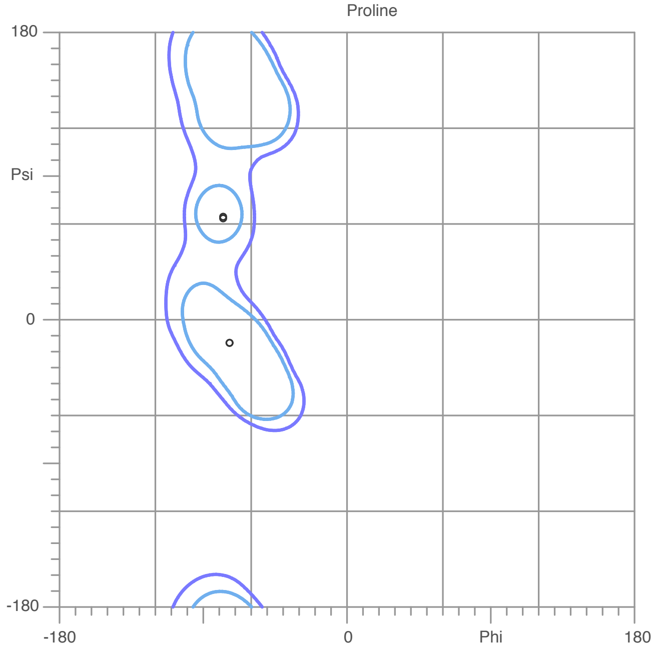
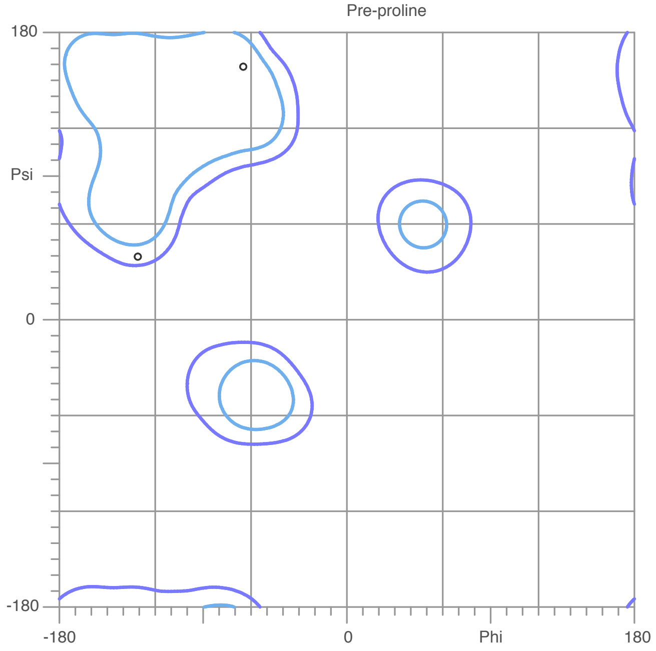
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 4


General case


Glycine


Proline


Pre-proline

87.5% (140/160) of all residues were in favored (98%) regions.
98.8% (158/160) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):

[4] 49 ASP (-165.0, -65.1)
[4] 141 ASP (-165.0, -65.0)

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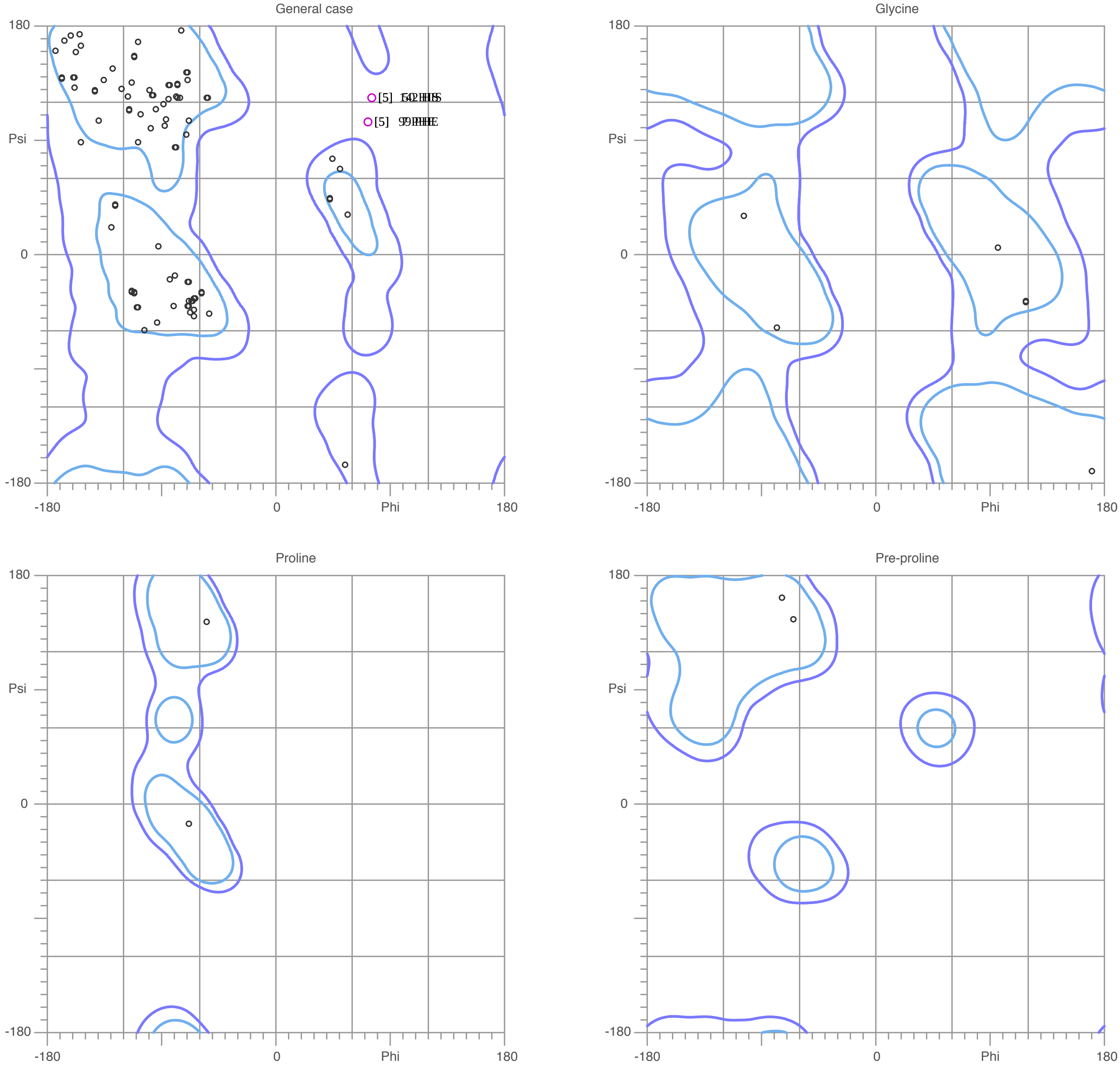
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 5



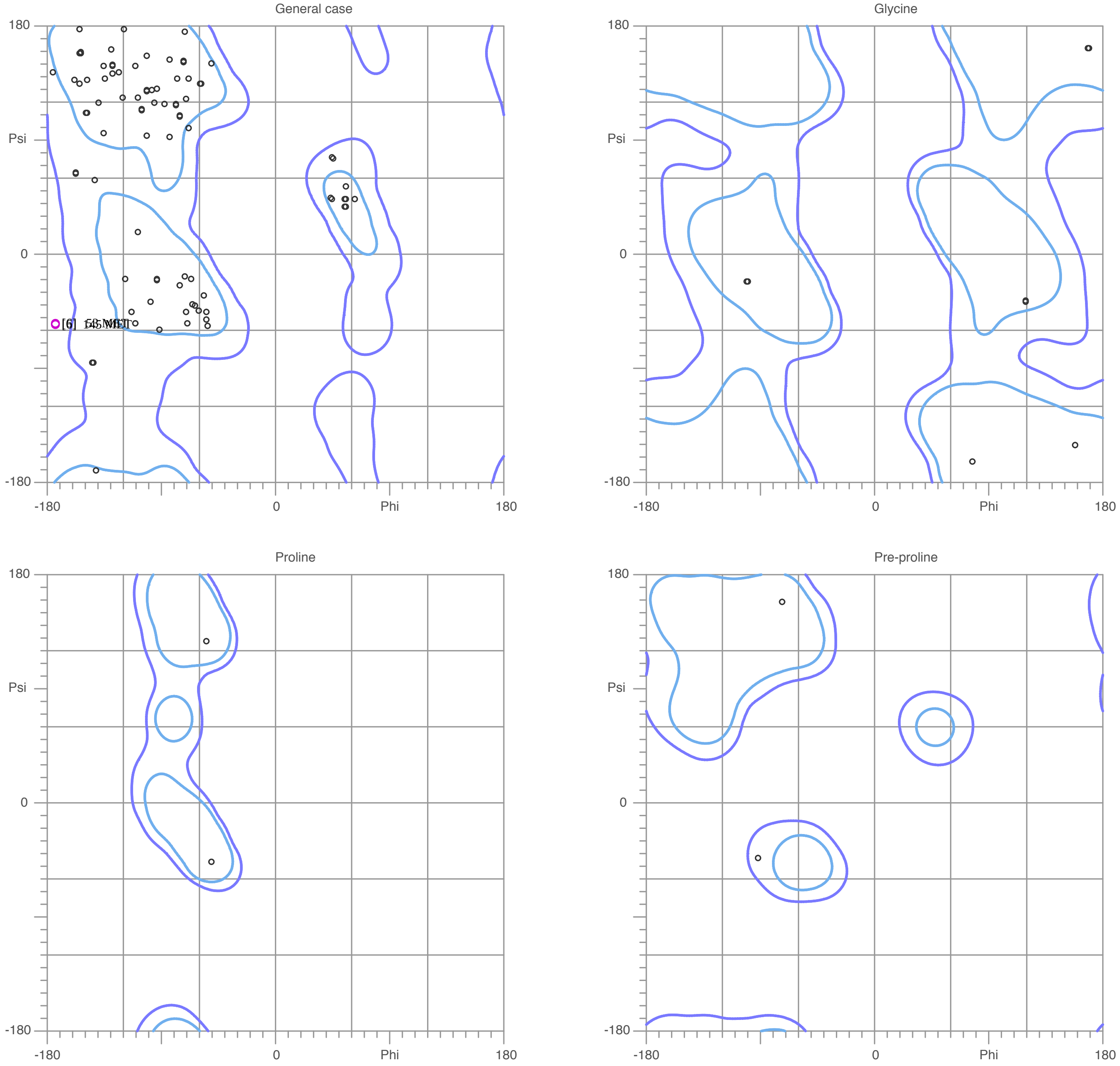
91.2% (146/160) of all residues were in favored (98%) regions.
97.5% (156/160) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):

[5] 7 PHE (72.1, 105.0)
[5] 50 HIS (75.1, 124.9)
[5] 99 PHE (72.2, 105.1)
[5] 142 HIS (75.0, 125.0)

MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 6

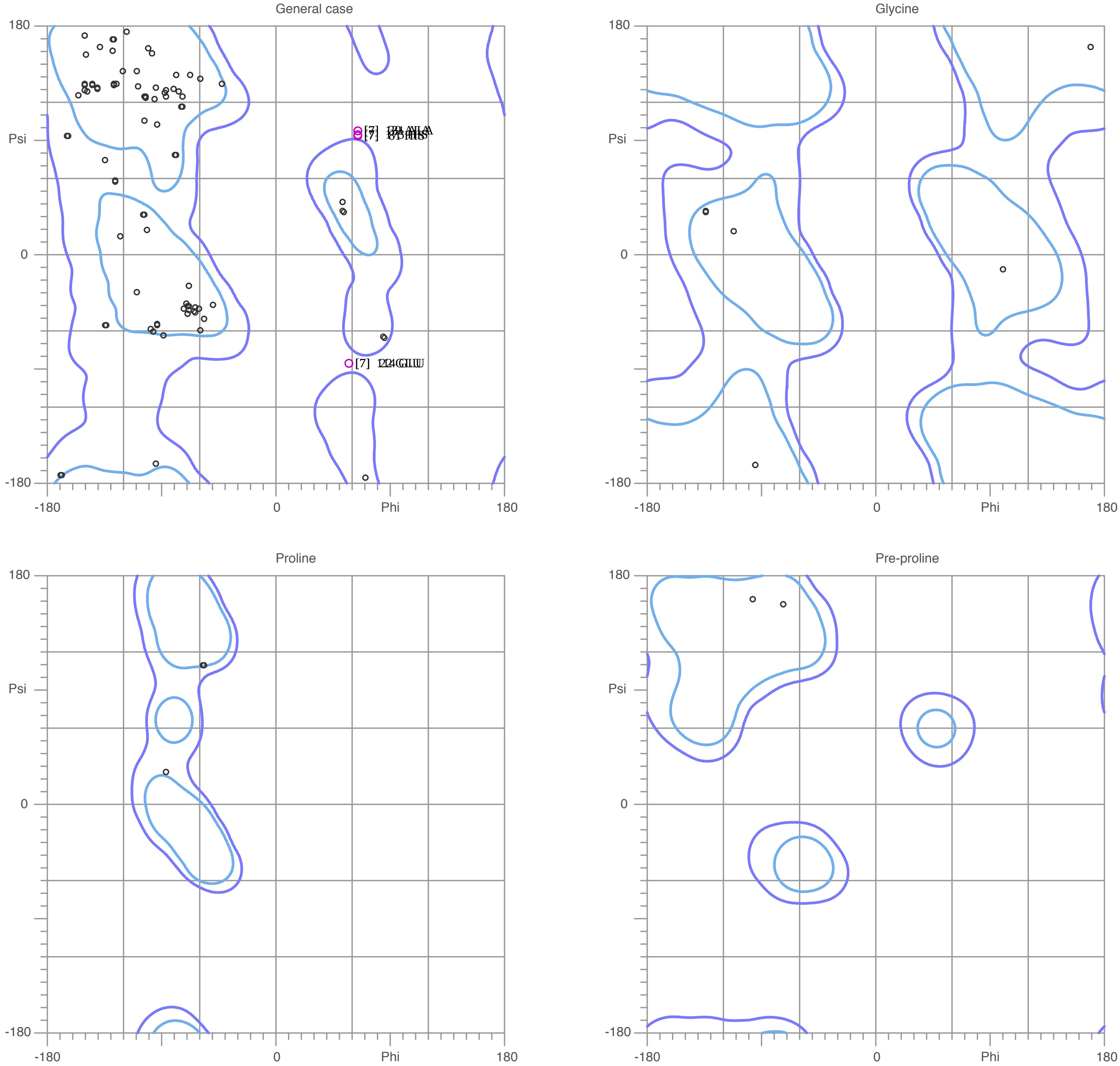


90.0% (144/160) of all residues were in favored (98%) regions.
98.8% (158/160) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
[6] 53 MET (-175.0, -54.9)
[6] 145 MET (-175.0, -55.0)

MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 7



83.8% (134/160) of all residues were in favored (98%) regions.
96.2% (154/160) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):

[7] 22 GLU (57.5, -85.3)
[7] 39 ALA (64.9, 98.3)
[7] 81 HIS (65.0, 94.9)
[7] 114 GLU (57.4, -85.2)
[7] 131 ALA (65.0, 98.3)
[7] 173 HIS (65.0, 95.1)

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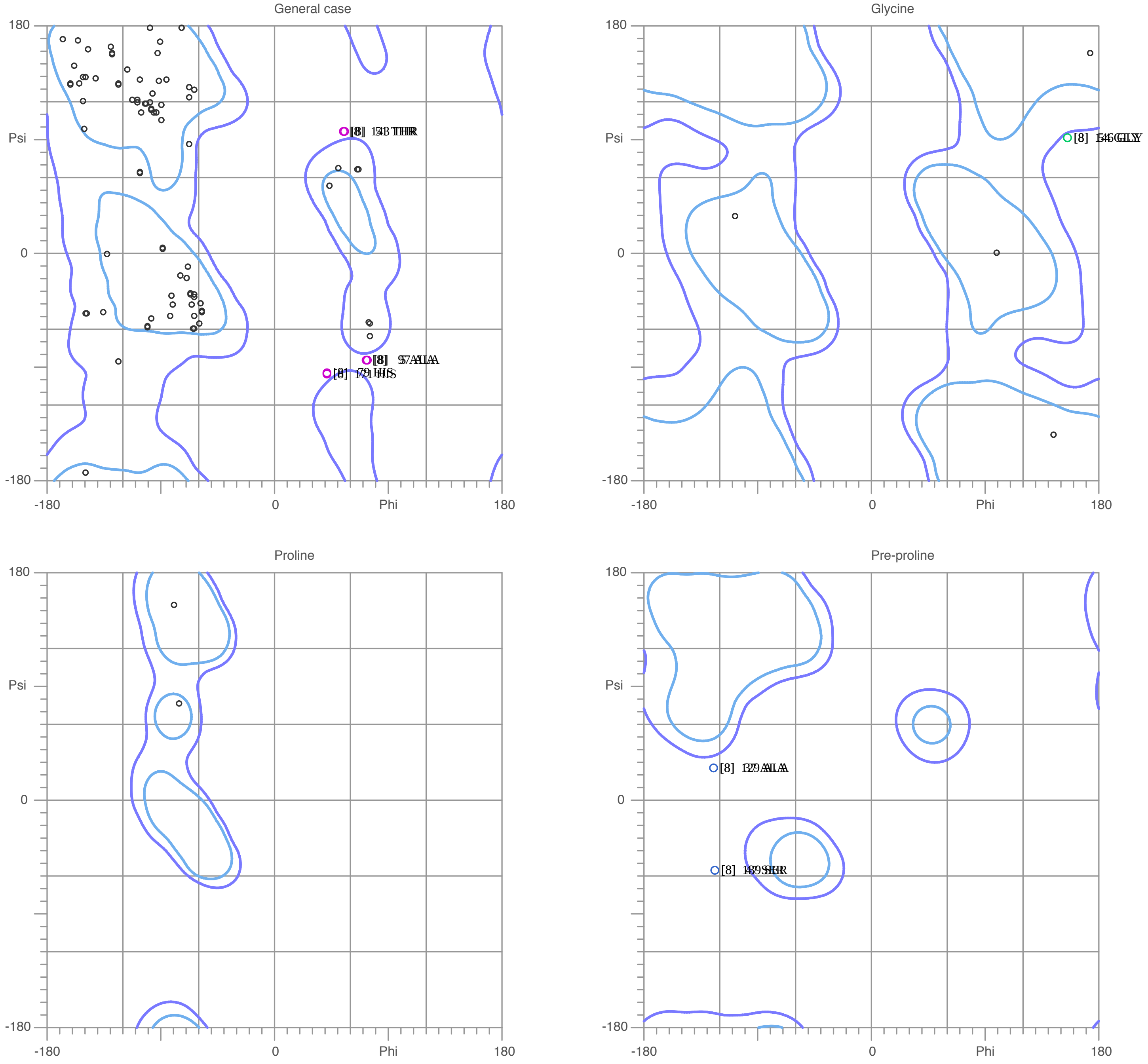
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 8



81.2% (130/160) of all residues were in favored (98%) regions.
92.5% (148/160) of all residues were in allowed (>99.8%) regions.

There were 12 outliers (phi, psi):

[8] 5 ALA (73.0, -84.9)
[8] 37 ALA (-125.1, 26.4)
[8] 47 SER (-124.8, -55.5)
[8] 51 THR (55.0, 97.7)
[8] 54 GLY (155.0, 92.3)
[8] 79 HIS (41.7, -94.9)
[8] 97 ALA (73.1, -85.0)
[8] 129 ALA (-125.1, 26.4)
[8] 139 SER (-124.9, -55.5)
[8] 143 THR (55.0, 97.6)
[8] 146 GLY (155.0, 92.2)
[8] 171 HIS (41.8, -95.0)

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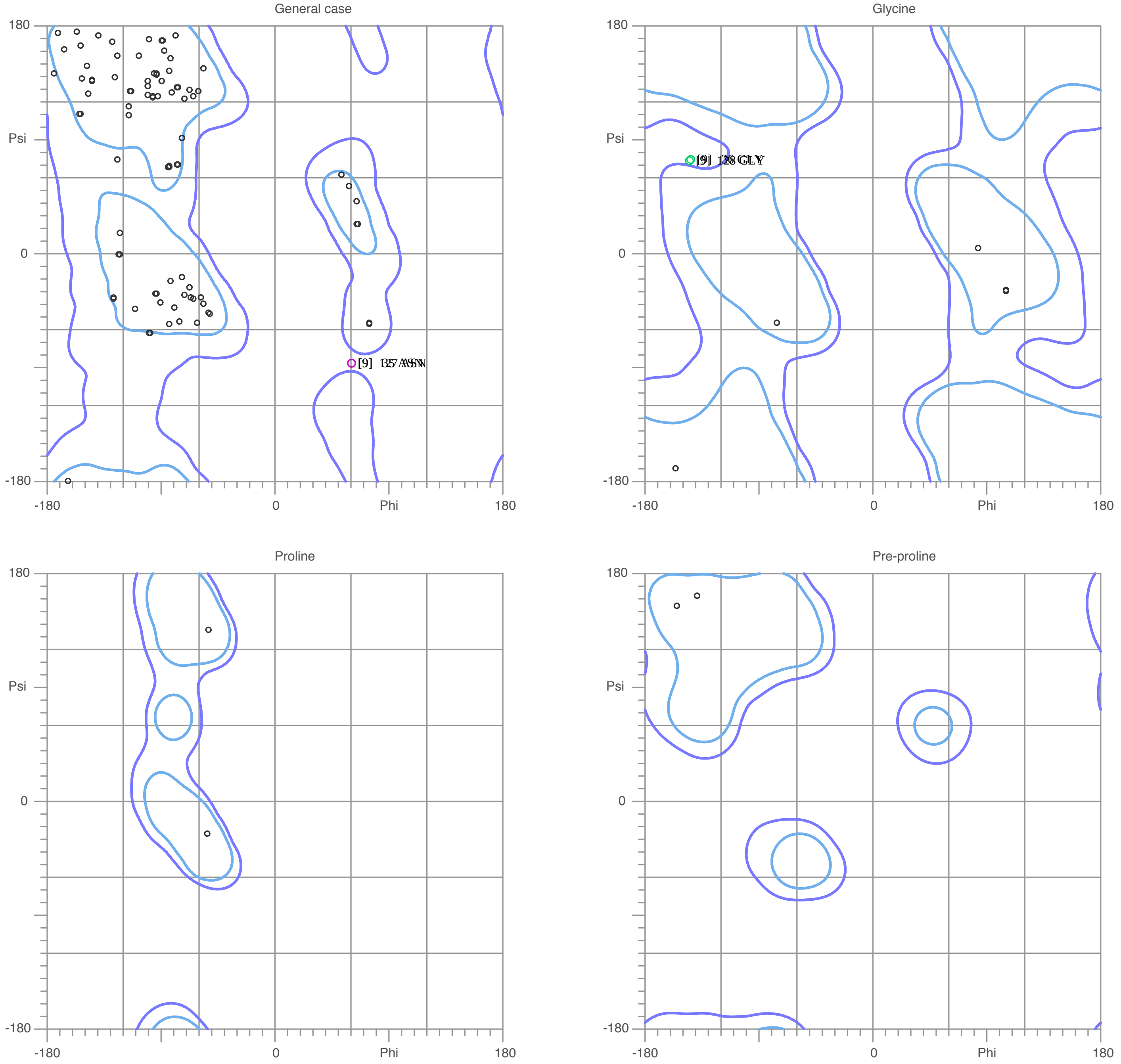
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 9



92.5% (148/160) of all residues were in favored (98%) regions.
97.5% (156/160) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
- [9] 35 ASN (60.9, -86.5)
- [9] 36 GLY (-145.0, 75.0)
- [9] 127 ASN (60.9, -86.4)
- [9] 128 GLY (-145.0, 75.0)

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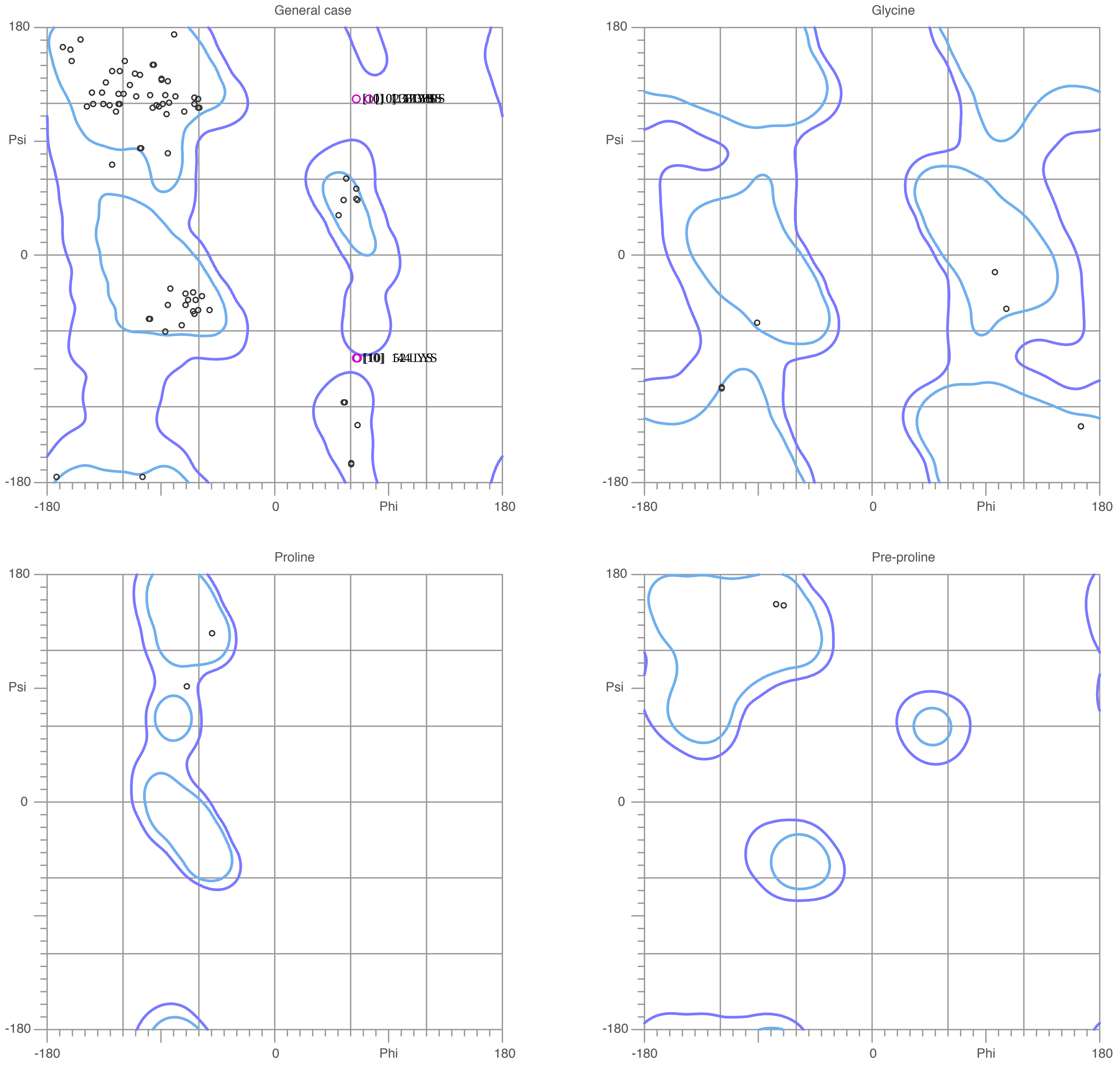
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 10



88.8% (142/160) of all residues were in favored (98%) regions.
96.2% (154/160) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):
[10] 23 LYS (65.0, 125.0)
[10] 52 LYS (64.9, -81.3)
[10] 81 HIS (74.8, 125.0)
[10] 115 LYS (64.9, 125.0)
[10] 144 LYS (65.0, -81.3)
[10] 173 HIS (74.8, 125.0)

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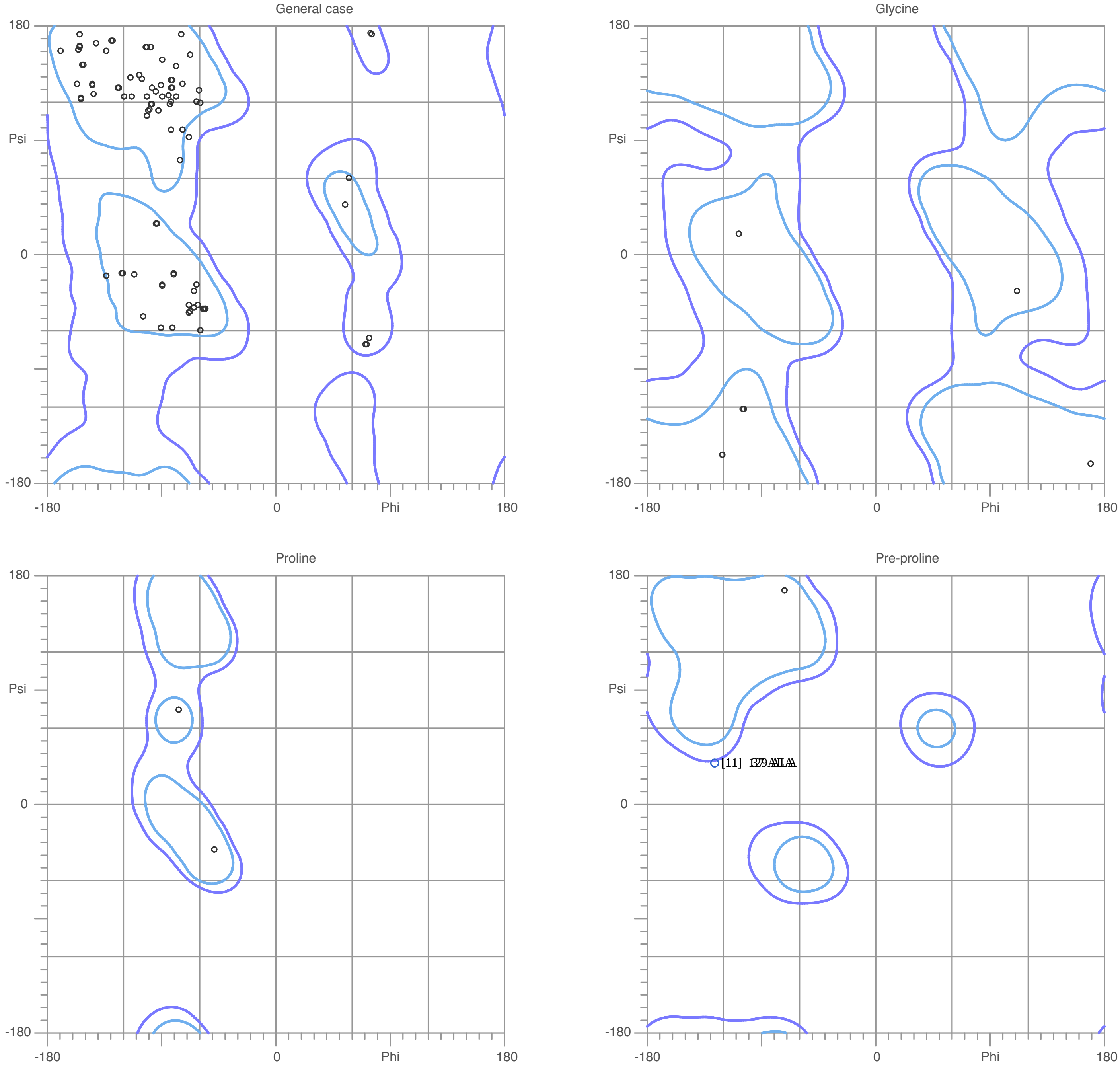
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 11



92.5% (148/160) of all residues were in favored (98%) regions.
98.8% (158/160) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
[11] 37 ALA (-127.6, 33.6)
[11] 129 ALA (-127.7, 33.6)

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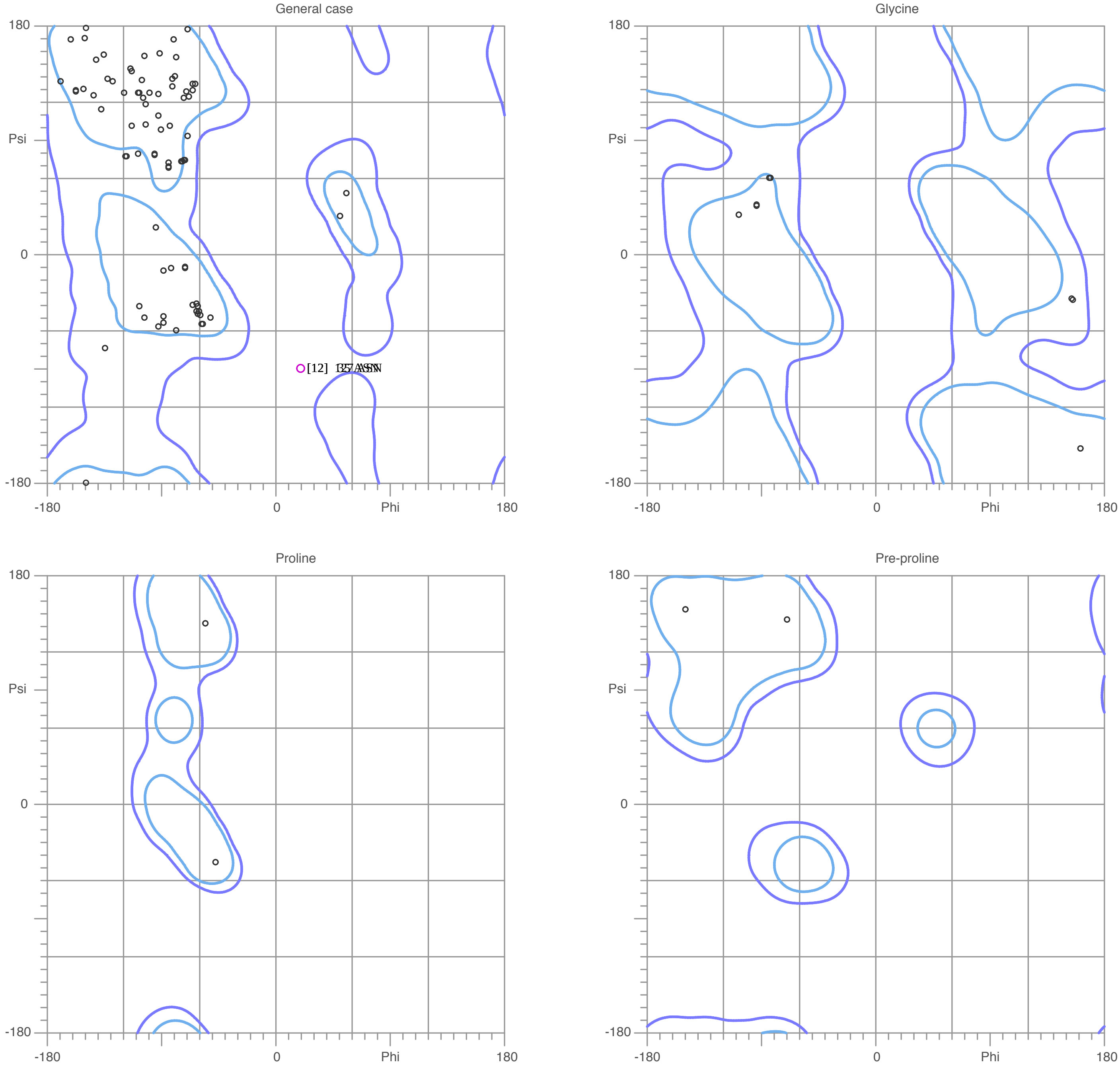
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 12



90.6% (145/160) of all residues were in favored (98%) regions.
98.8% (158/160) of all residues were in allowed (>99.8%) regions.

There were 2 outliers (phi, psi):
[12] 35 ASN (19.9, -89.6)
[12] 127 ASN (20.0, -89.6)

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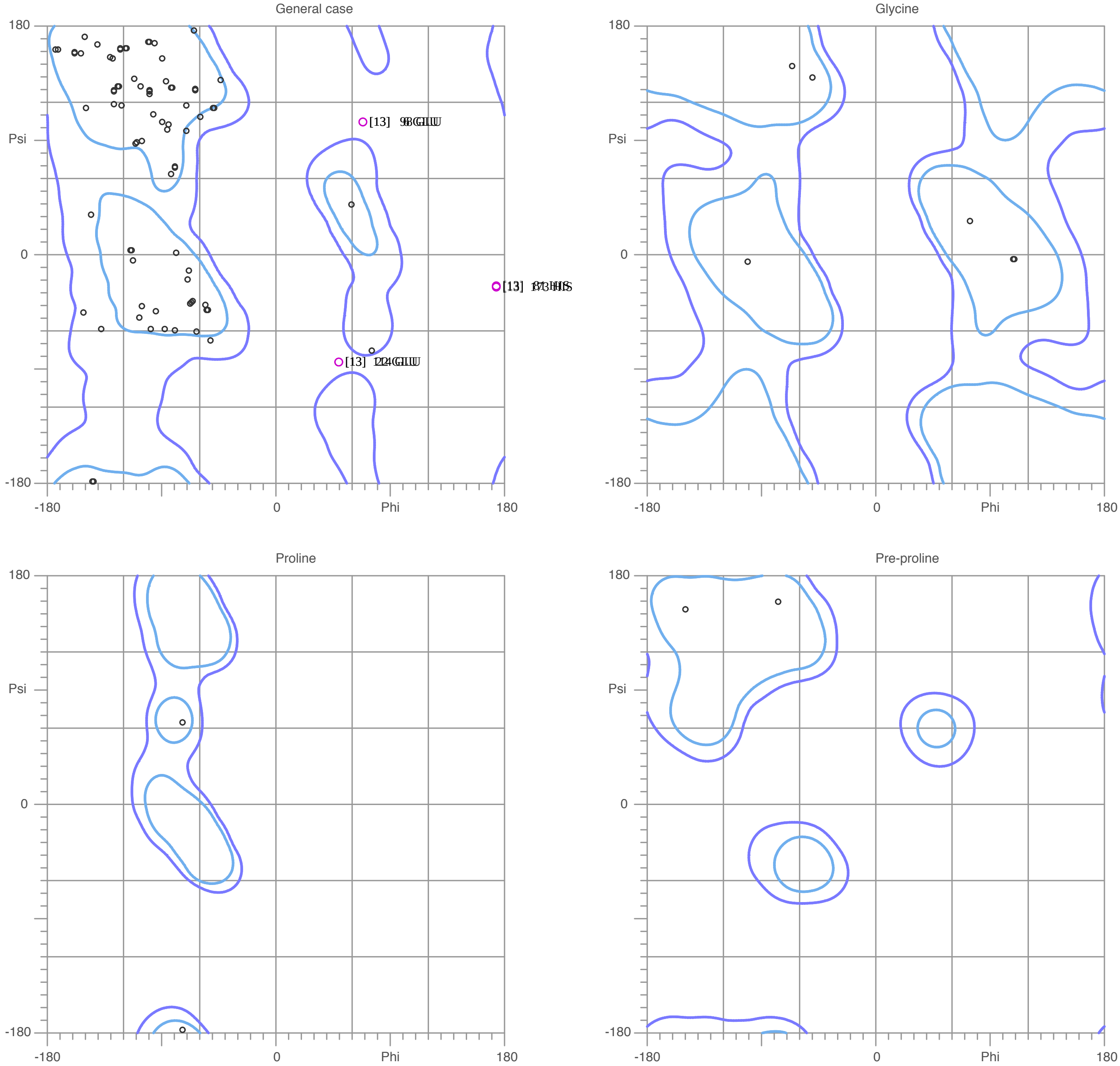
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 13



88.8% (142/160) of all residues were in favored (98%) regions.
96.2% (154/160) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):
[13] 6 GLU (68.5, 105.1)
[13] 22 GLU (49.2, -84.9)
[13] 81 HIS (173.6, -25.0)
[13] 98 GLU (68.6, 105.0)
[13] 114 GLU (49.2, -84.9)
[13] 173 HIS (173.6, -25.0)

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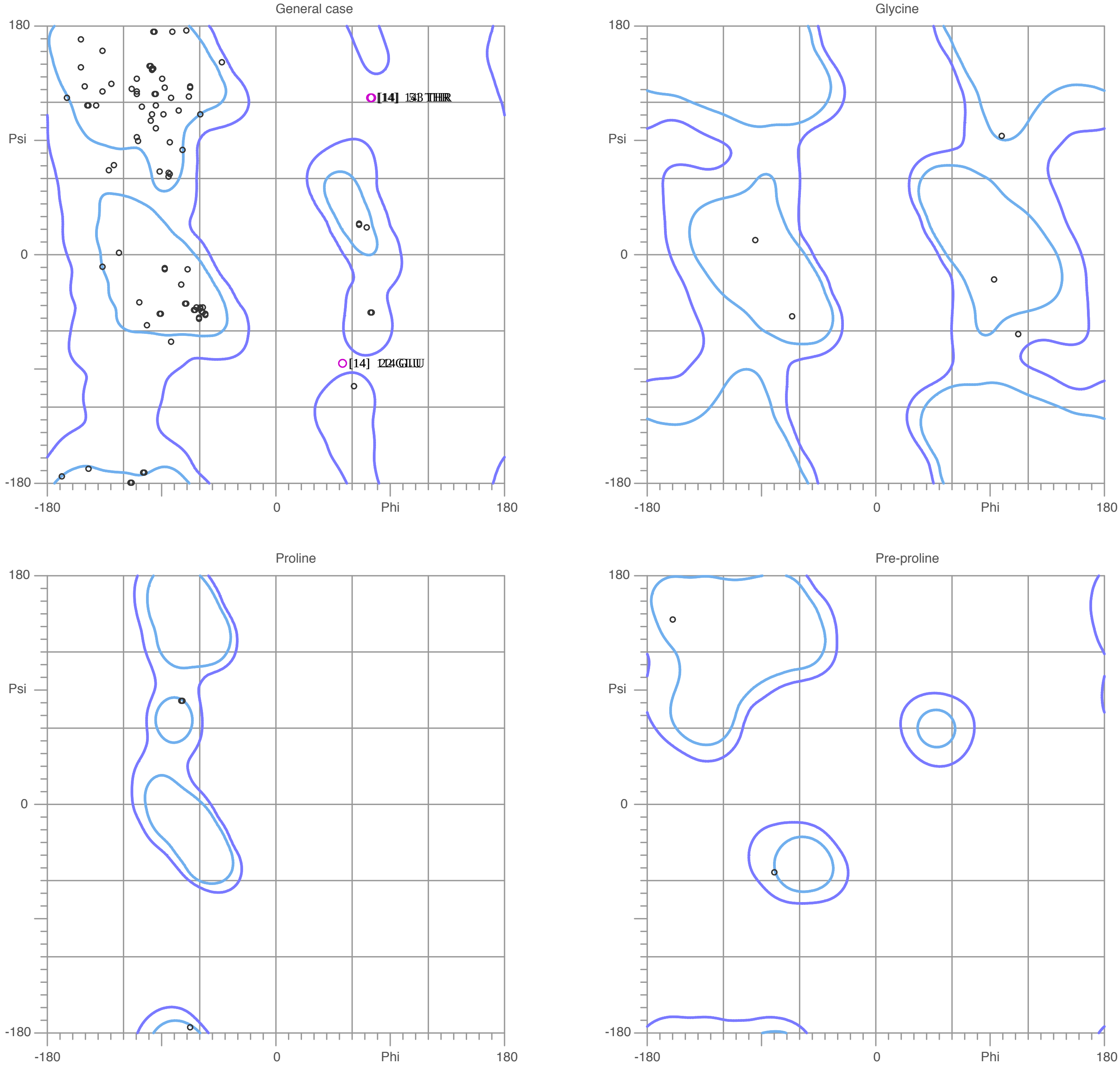
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 14



82.5% (132/160) of all residues were in favored (98%) regions.
97.5% (156/160) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
- [14] 22 GLU (52.4, -85.0)
- [14] 51 THR (75.1, 125.0)
- [14] 114 GLU (52.4, -85.0)
- [14] 143 THR (75.0, 125.0)

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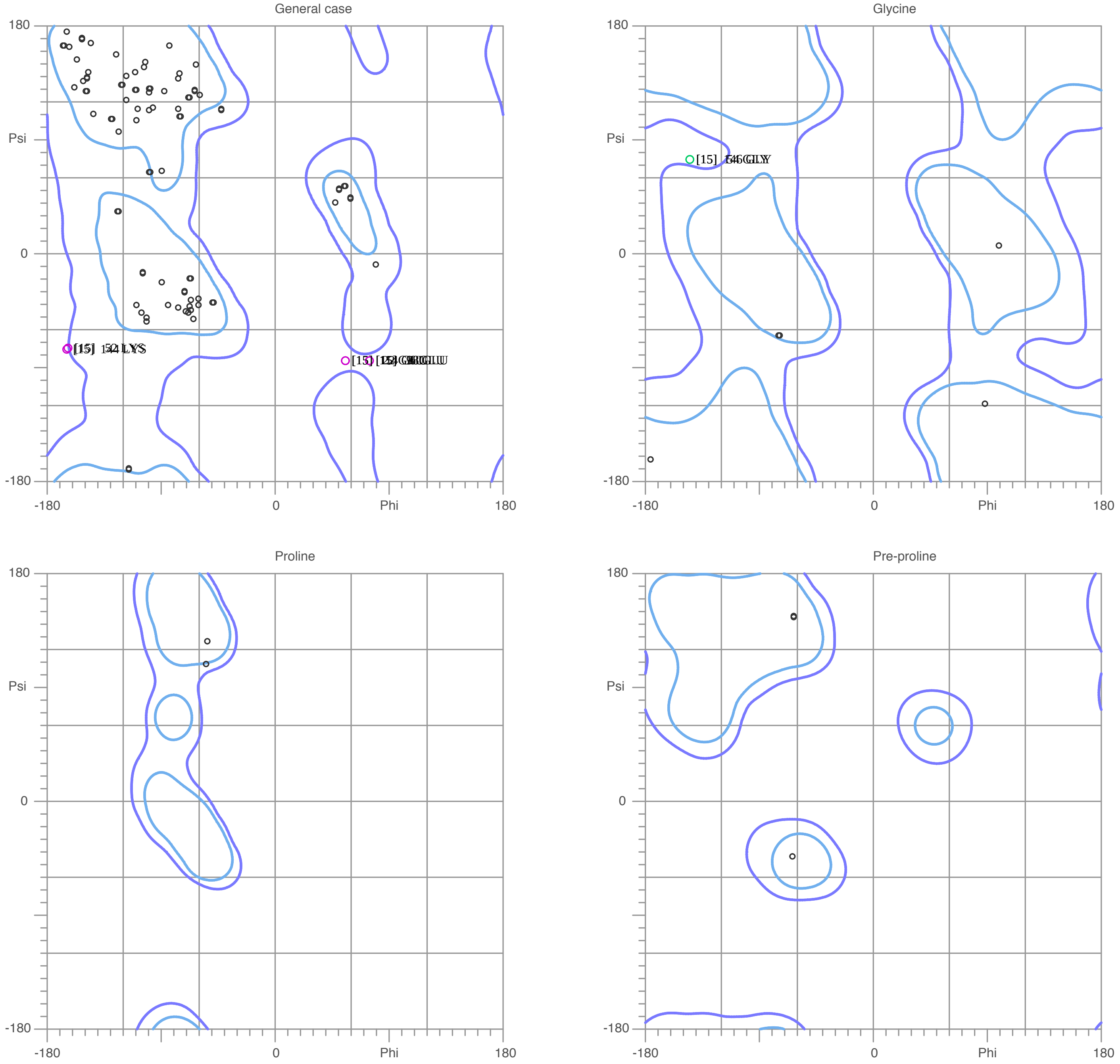
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 15



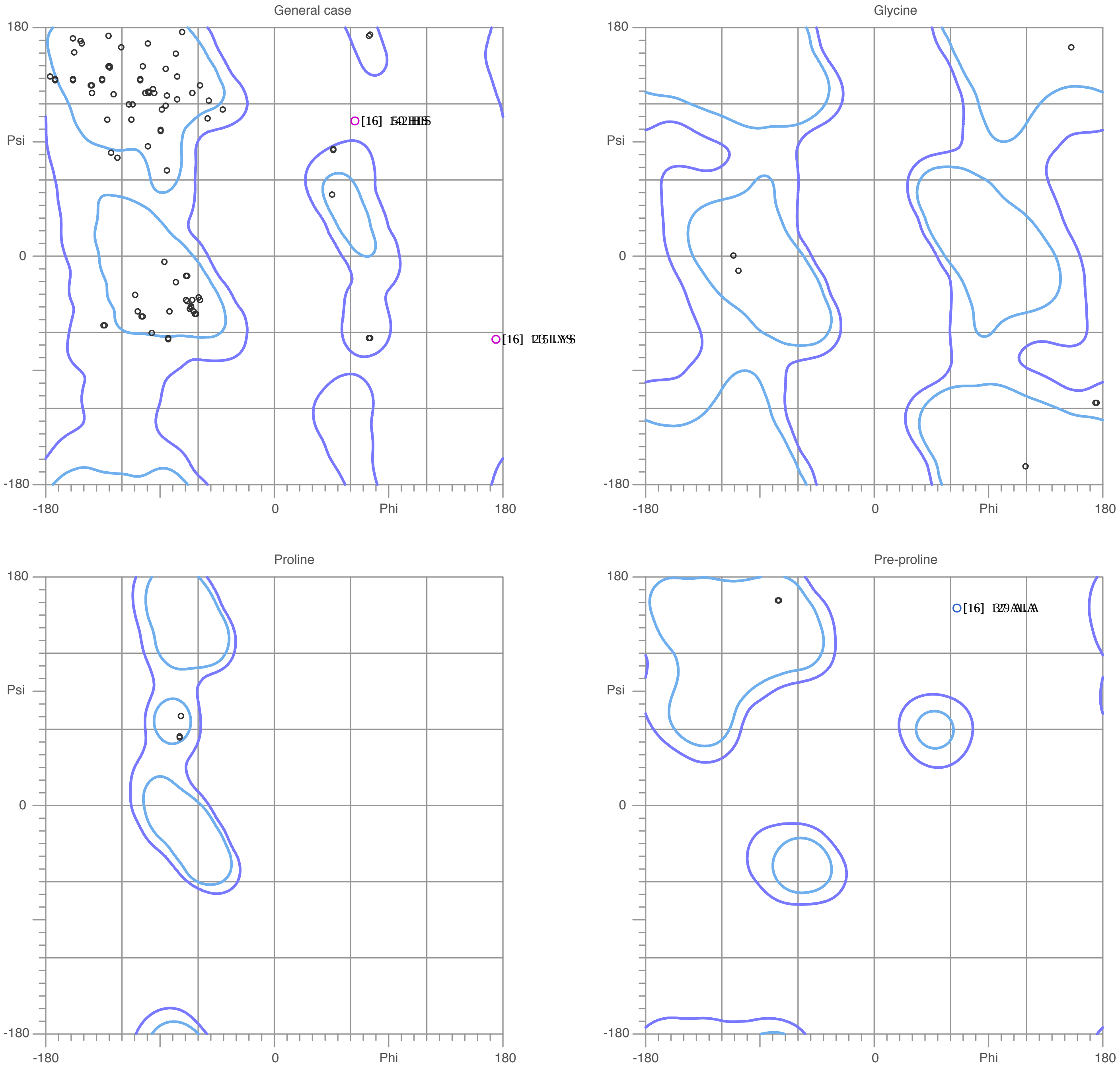
90.0% (144/160) of all residues were in favored (98%) regions.
95.0% (152/160) of all residues were in allowed (>99.8%) regions.

There were 8 outliers (phi, psi):

[15]	6 GLU	(74.9, -84.9)
[15]	22 GLU	(55.4, -85.0)
[15]	52 LYS	(-165.0, -74.9)
[15]	54 GLY	(-145.0, 75.0)
[15]	98 GLU	(74.9, -85.0)
[15]	114 GLU	(55.5, -85.0)
[15]	144 LYS	(-165.1, -75.0)
[15]	146 GLY	(-145.0, 75.1)

MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 16



81.2% (130/160) of all residues were in favored (98%) regions.

96.2% (154/160) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):

[16] 23 LYS (175.0, -65.1)

[16] 37 ALA (65.3, 156.1)

[16] 50 HIS (63.3, 107.3)

[16] 115 LYS (174.9, -65.0)

[16] 129 ALA (65.3, 156.2)

[16] 142 HIS (63.3, 107.1)

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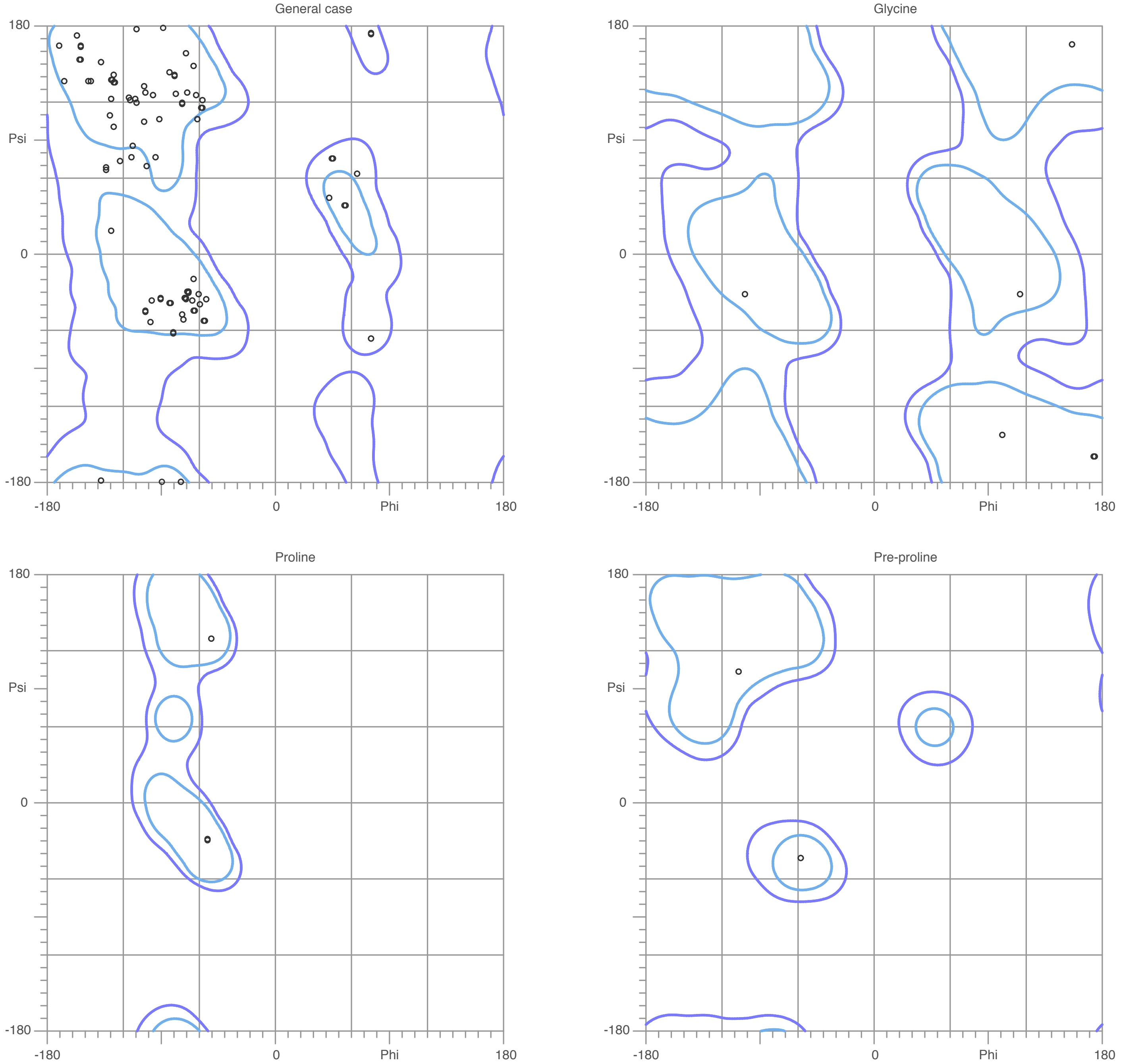
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 17



87.5% (140/160) of all residues were in favored (98%) regions.
100.0% (160/160) of all residues were in allowed (>99.8%) regions.

There were no outliers.

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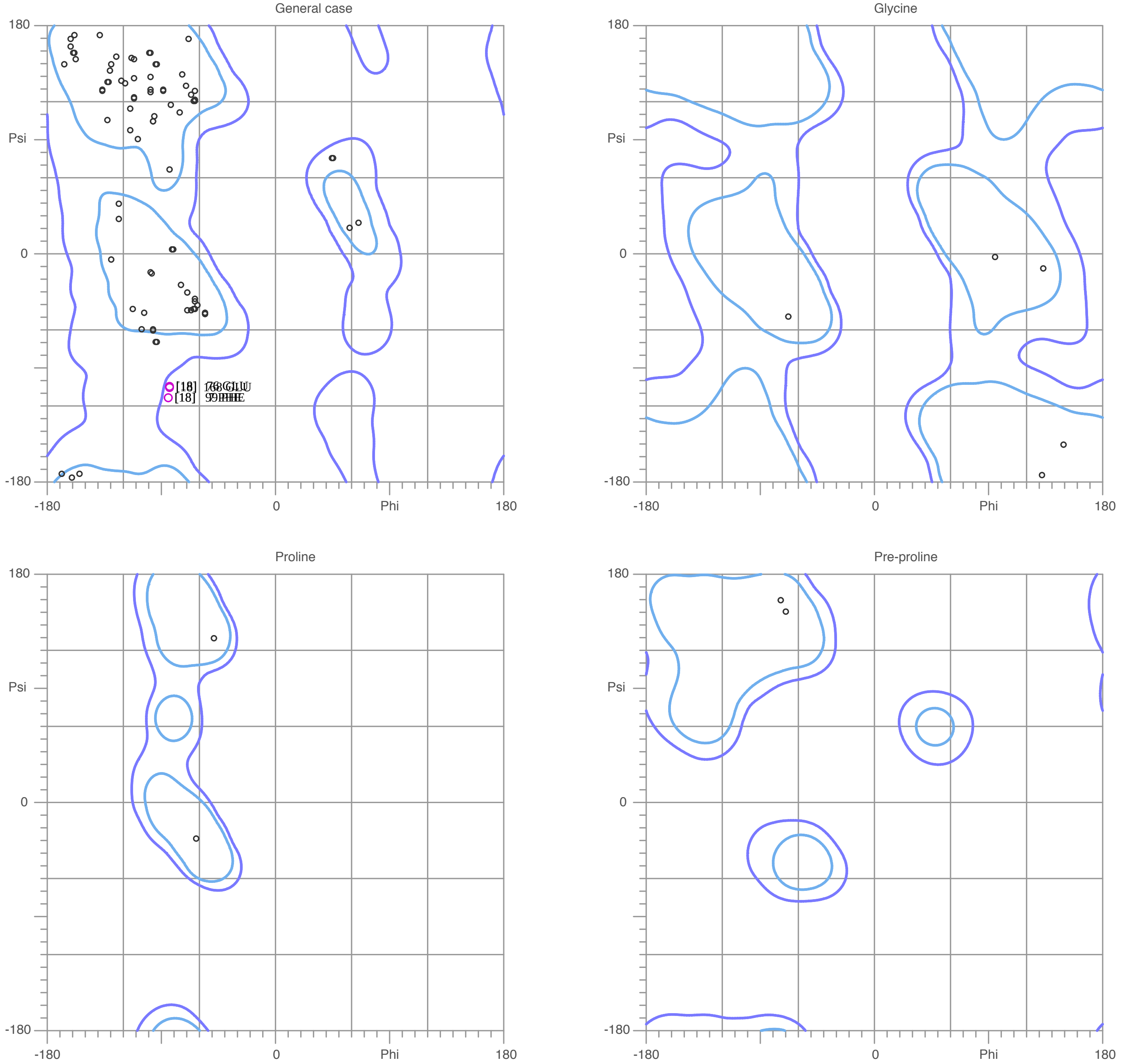
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 18



93.8% (150/160) of all residues were in favored (98%) regions.
97.5% (156/160) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
[18] 7 PHE (-85.0, -113.5)
[18] 76 GLU (-85.0, -104.9)
[18] 99 PHE (-85.0, -113.5)
[18] 168 GLU (-85.0, -105.0)

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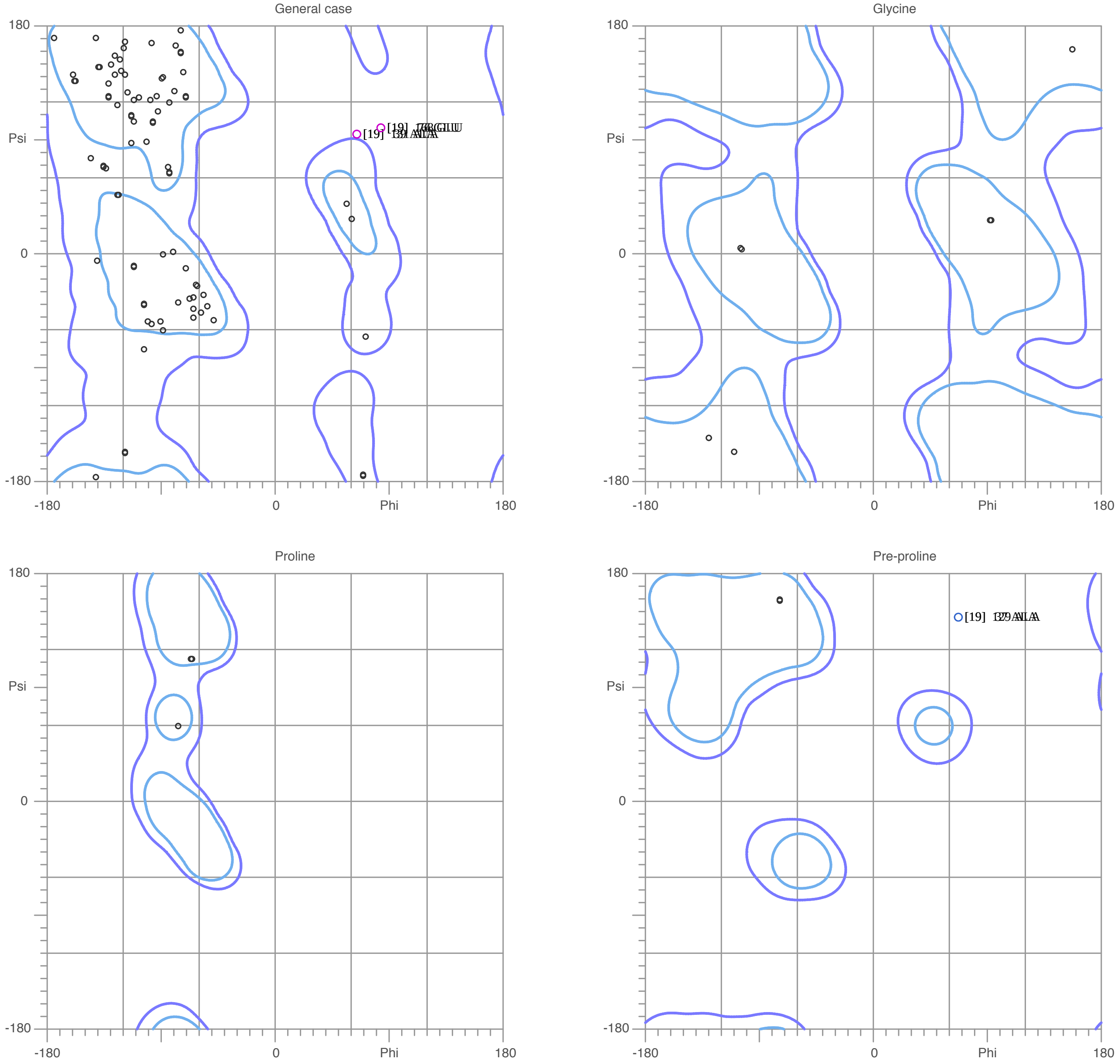
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 19



85.0% (136/160) of all residues were in favored (98%) regions.
96.2% (154/160) of all residues were in allowed (>99.8%) regions.

There were 6 outliers (phi, psi):
[19] 37 ALA (67.8, 146.0)
[19] 39 ALA (64.9, 95.0)
[19] 76 GLU (83.5, 100.8)
[19] 129 ALA (67.7, 146.0)
[19] 131 ALA (65.0, 95.1)
[19] 168 GLU (83.4, 100.8)

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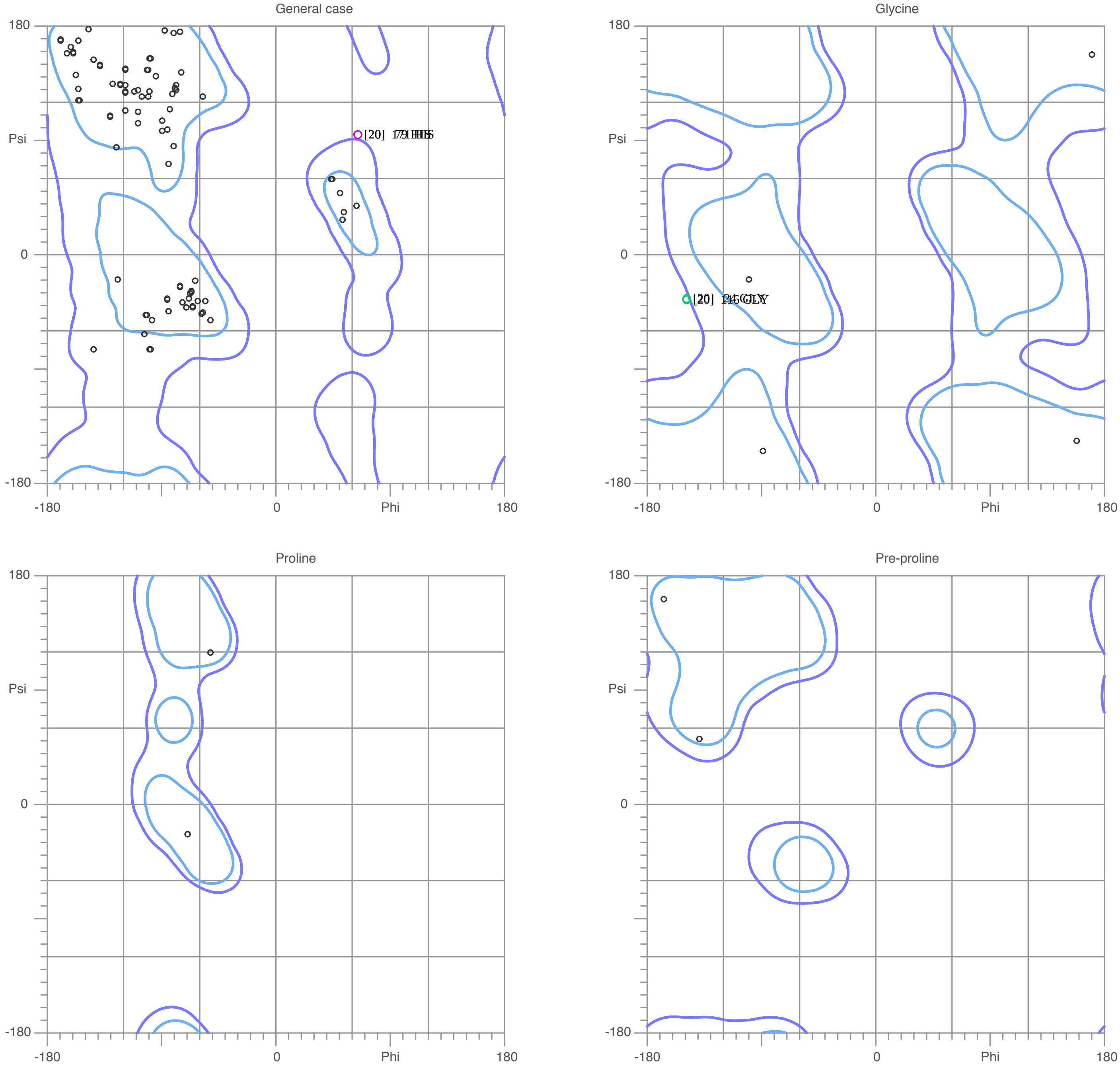
MolProbity Ramachandran analysis

SPR104_R3_em_bcr3.pdb, model 20



93.8% (150/160) of all residues were in favored (98%) regions.
97.5% (156/160) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
[20] 24 GLY (-149.2, -35.0)
[20] 79 HIS (65.0, 95.1)
[20] 116 GLY (-149.2, -35.0)
[20] 171 HIS (65.0, 95.1)

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