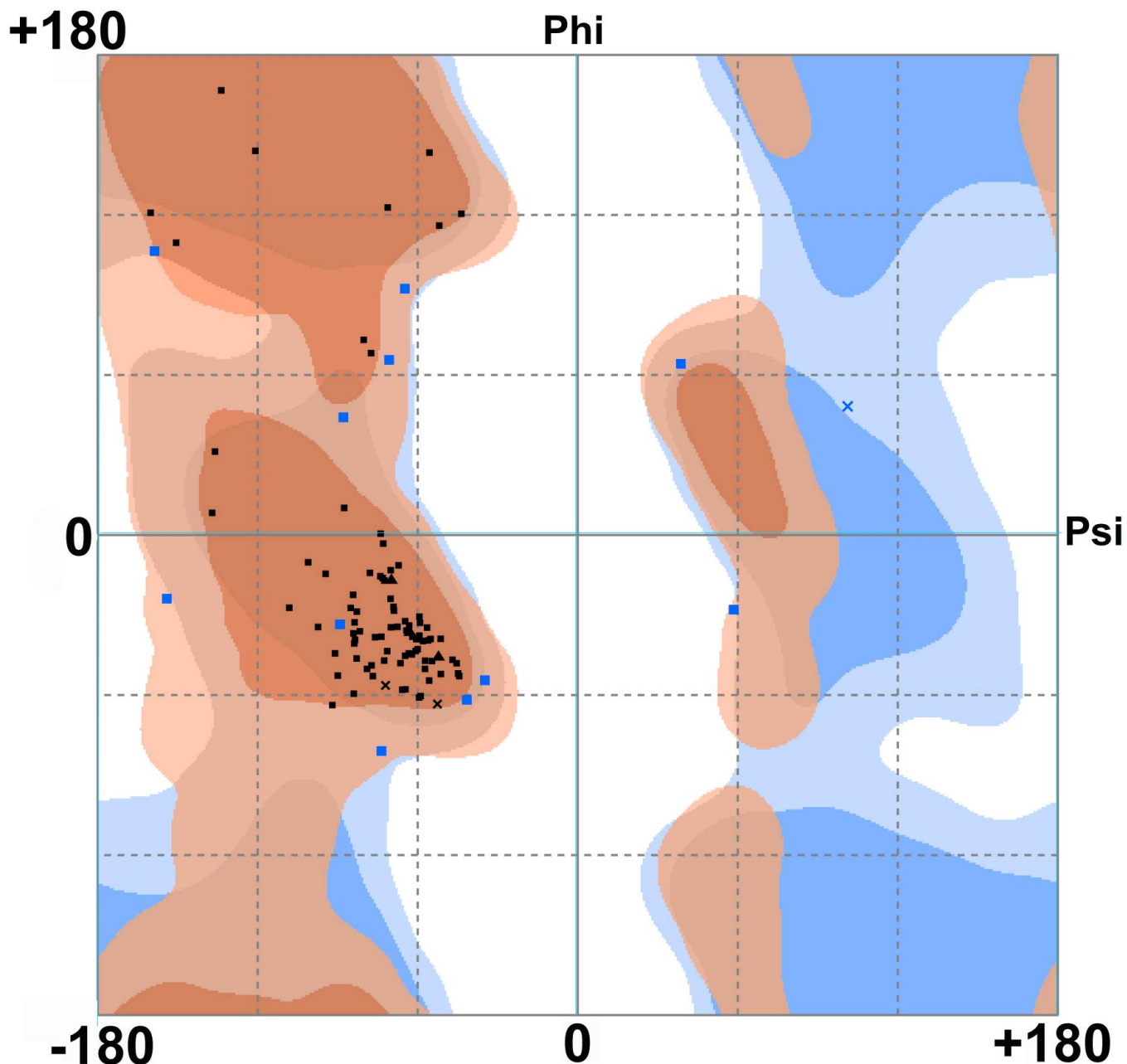


Supplementary Figure S1: Ramachandran Plot



- ▲ General/Pre-Pro/Proline favoured
- × Glycine favoured
- ▲ General/Pre-Pro/Proline allowed
- × Glycine allowed

Supplementary information

The parameter file for DIMBOA in .off format which is a library format to be used with 'tleap' program of AmberTools18.

```
!!index array str
"DIM"
!entry.DIM.unit.atoms table str name str type int typex int resx int flags int seq int elmnt dbl chg
"01" "os" 0 1 131072 1 8 -0.355900
"02" "oh" 0 1 131072 2 8 -0.594800
"03" "oh" 0 1 131072 3 8 -0.420100
"04" "os" 0 1 131072 4 8 -0.321900
"05" "o" 0 1 131072 5 8 -0.554500
"N1" "n" 0 1 131072 6 7 -0.154500
"C1" "ca" 0 1 131072 7 6 -0.070400
"C2" "ca" 0 1 131072 8 6 0.139100
"C3" "c3" 0 1 131072 9 6 0.275900
"C4" "c" 0 1 131072 10 6 0.646500
"C5" "ca" 0 1 131072 11 6 -0.166000
"C6" "ca" 0 1 131072 12 6 -0.057000
"C7" "ca" 0 1 131072 13 6 0.147100
"C8" "ca" 0 1 131072 14 6 -0.216000
"C9" "c3" 0 1 131072 15 6 0.112700
"H1" "h2" 0 1 131072 16 1 0.107700
"H2" "ha" 0 1 131072 17 1 0.170000
"H3" "ha" 0 1 131072 18 1 0.156000
"H4" "ha" 0 1 131072 19 1 0.146000
"H5" "ho" 0 1 131072 20 1 0.432000
"H6" "ho" 0 1 131072 21 1 0.435000
"H7" "h1" 0 1 131072 22 1 0.048033
"H8" "h1" 0 1 131072 23 1 0.048033
"H9" "h1" 0 1 131072 24 1 0.048033
!entry.DIM.unit.atoms pertinfo table str pname str ptype int ptypex int pelmnt dbl pchg
"01" "os" 0 -1 0.0
"02" "oh" 0 -1 0.0
"03" "oh" 0 -1 0.0
"04" "os" 0 -1 0.0
"05" "o" 0 -1 0.0
"N1" "n" 0 -1 0.0
"C1" "ca" 0 -1 0.0
"C2" "ca" 0 -1 0.0
"C3" "c3" 0 -1 0.0
"C4" "c" 0 -1 0.0
"C5" "ca" 0 -1 0.0
"C6" "ca" 0 -1 0.0
"C7" "ca" 0 -1 0.0
"C8" "ca" 0 -1 0.0
"C9" "c3" 0 -1 0.0
"H1" "h2" 0 -1 0.0
"H2" "ha" 0 -1 0.0
"H3" "ha" 0 -1 0.0
"H4" "ha" 0 -1 0.0
"H5" "ho" 0 -1 0.0
"H6" "ho" 0 -1 0.0
"H7" "h1" 0 -1 0.0
"H8" "h1" 0 -1 0.0
"H9" "h1" 0 -1 0.0
!entry.DIM.unit.boundbox array dbl
-1.000000
0.0
0.0
0.0
0.0
!entry.DIM.unit.childsequence single int
2
```

```

!entry.DIM.unit.connect array int
0
0
!entry.DIM.unit.connectivity table int atom1x int atom2x int flags
1 8 1
1 9 1
2 9 1
2 20 1
3 6 1
3 21 1
4 13 1
4 15 1
5 10 2
6 7 1
6 10 1
7 8 4
7 12 4
8 11 4
9 10 1
9 16 1
11 13 4
11 17 1
12 14 4
12 18 1
13 14 4
14 19 1
15 22 1
15 23 1
15 24 1
!entry.DIM.unit.hierarchy table str abovetype int abovex str belowtype int belowx
"U" 0 "R" 1
"R" 1 "A" 1
"R" 1 "A" 2
"R" 1 "A" 3
"R" 1 "A" 4
"R" 1 "A" 5
"R" 1 "A" 6
"R" 1 "A" 7
"R" 1 "A" 8
"R" 1 "A" 9
"R" 1 "A" 10
"R" 1 "A" 11
"R" 1 "A" 12
"R" 1 "A" 13
"R" 1 "A" 14
"R" 1 "A" 15
"R" 1 "A" 16
"R" 1 "A" 17
"R" 1 "A" 18
"R" 1 "A" 19
"R" 1 "A" 20
"R" 1 "A" 21
"R" 1 "A" 22
"R" 1 "A" 23
"R" 1 "A" 24
!entry.DIM.unit.name single str
"DIM"
!entry.DIM.unit.positions table dbl x dbl y dbl z
0.916000 -1.632000 -0.135000
3.220000 -1.973000 -0.137000
1.683000 2.482000 -0.129000
-3.759000 -0.828000 -0.022000
3.711000 0.658000 -0.013000
1.448000 1.104000 -0.023000
0.124000 0.657000 0.014000
-0.103000 -0.722000 -0.035000
2.159000 -1.163000 0.356000
2.542000 0.287000 0.069000
-1.406000 -1.222000 -0.058000
-0.964000 1.536000 0.052000

```

