Supporting information for

On the Validation of Protein Force Fields Based on Structural Criteria

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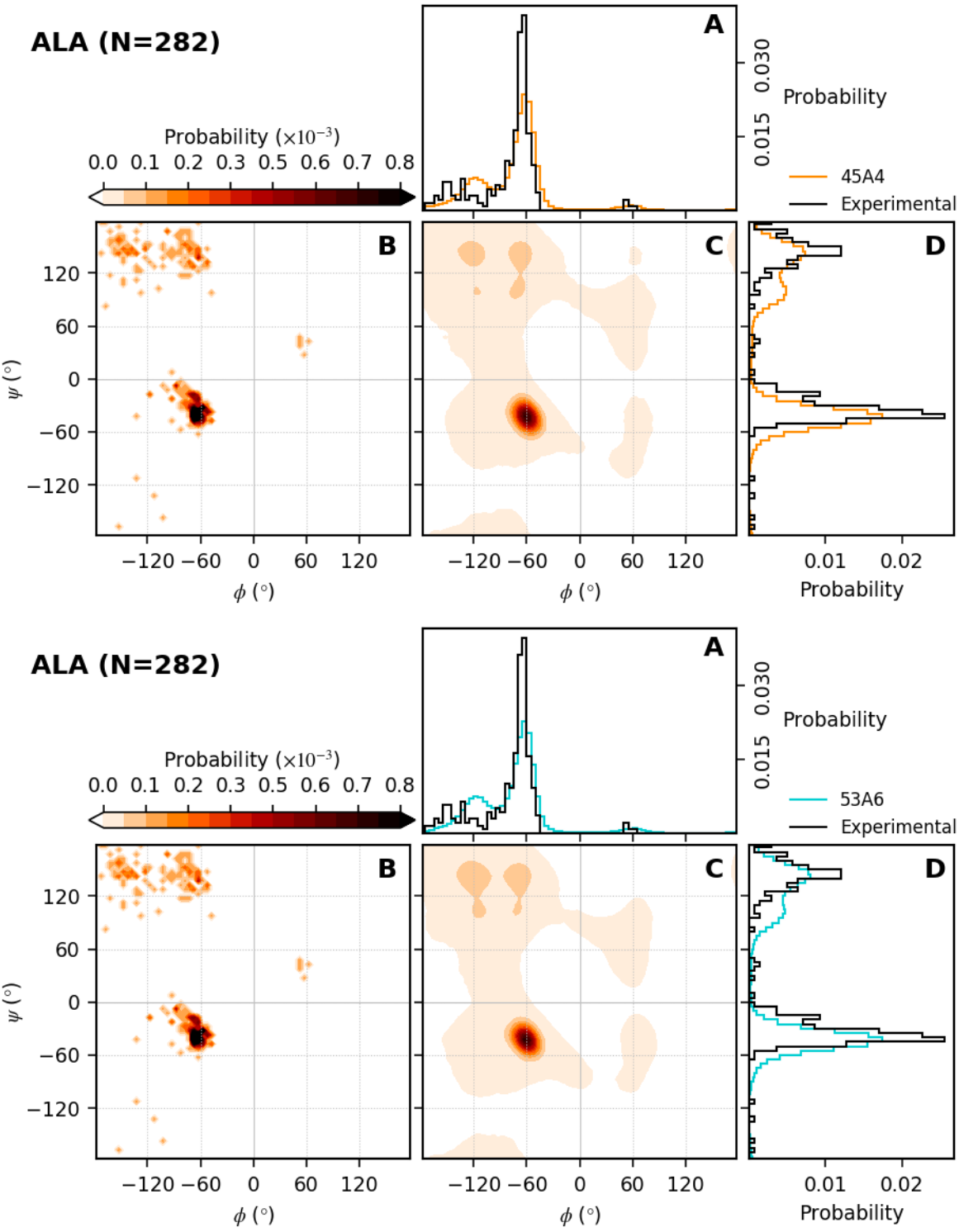

ALA (N=282)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.015 0.030
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.01 0.02
Probability
ALA (N=282)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.015 0.030
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.01 0.02
Probability

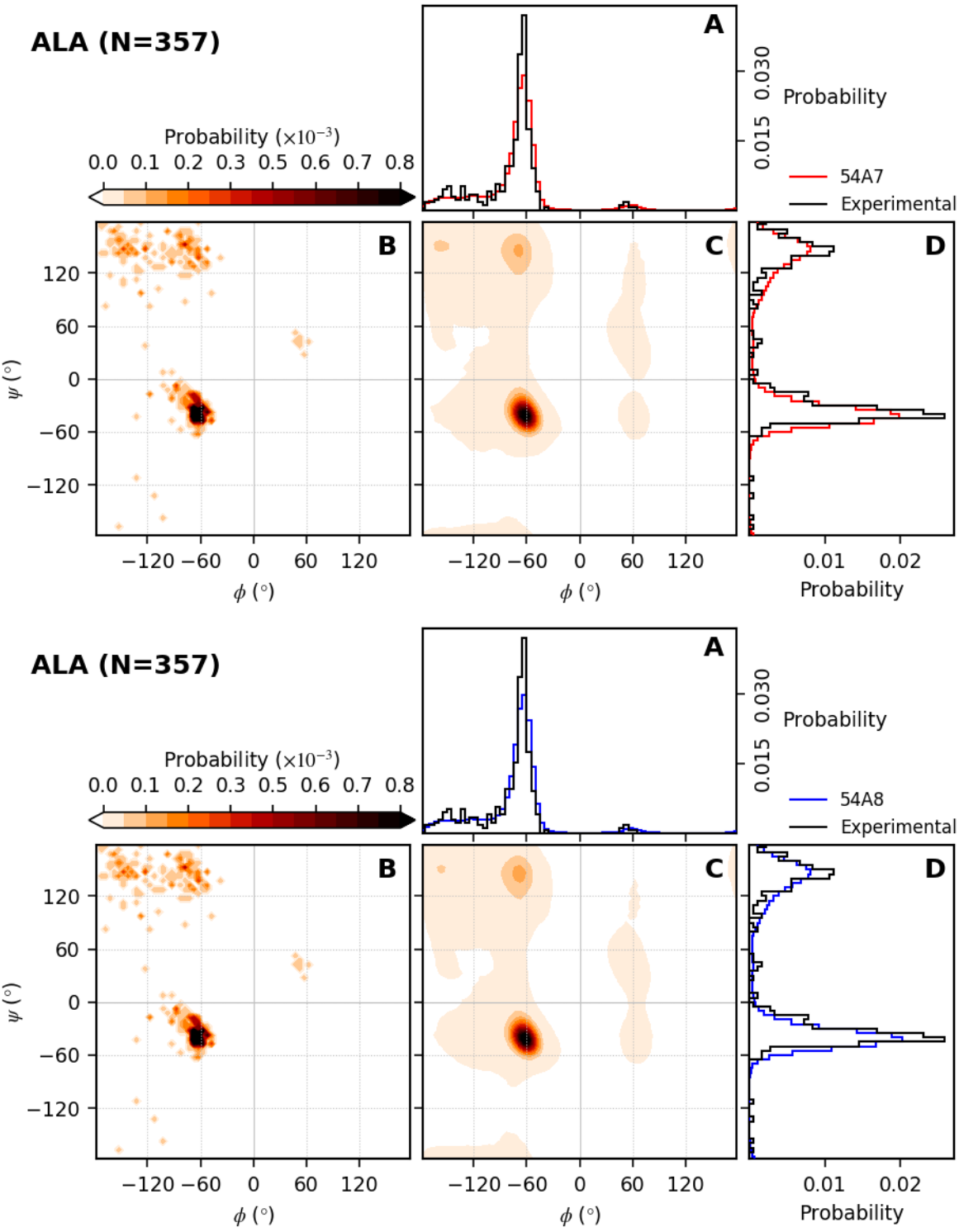
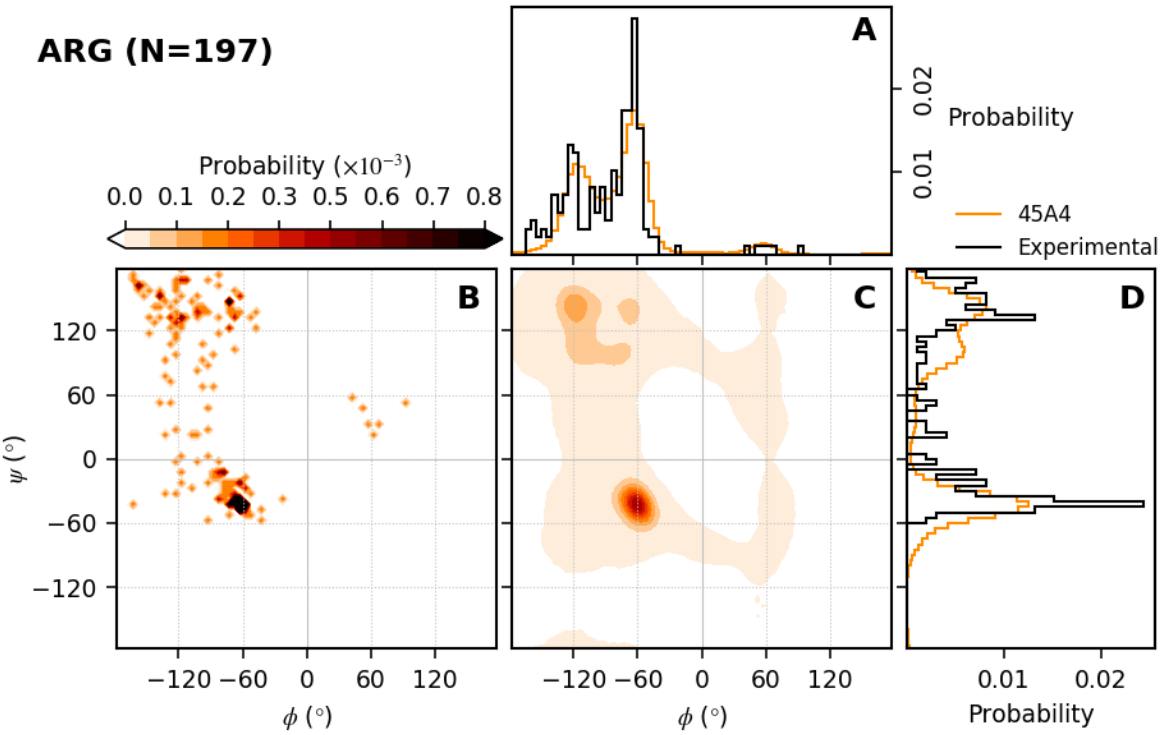
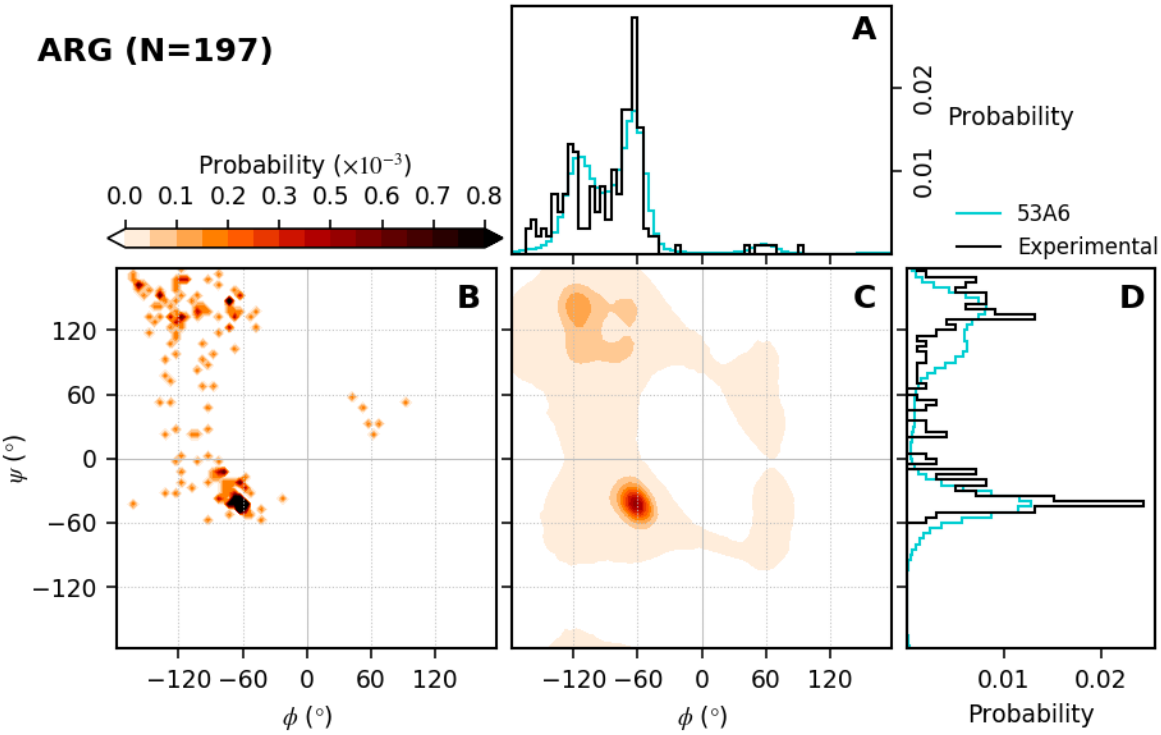


Figure S2. Distribution of alanine (ALA) backbone dihedral angles.


ARG (N=197)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.01 0.02
Probability


ARG (N=197)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.01 0.02
Probability

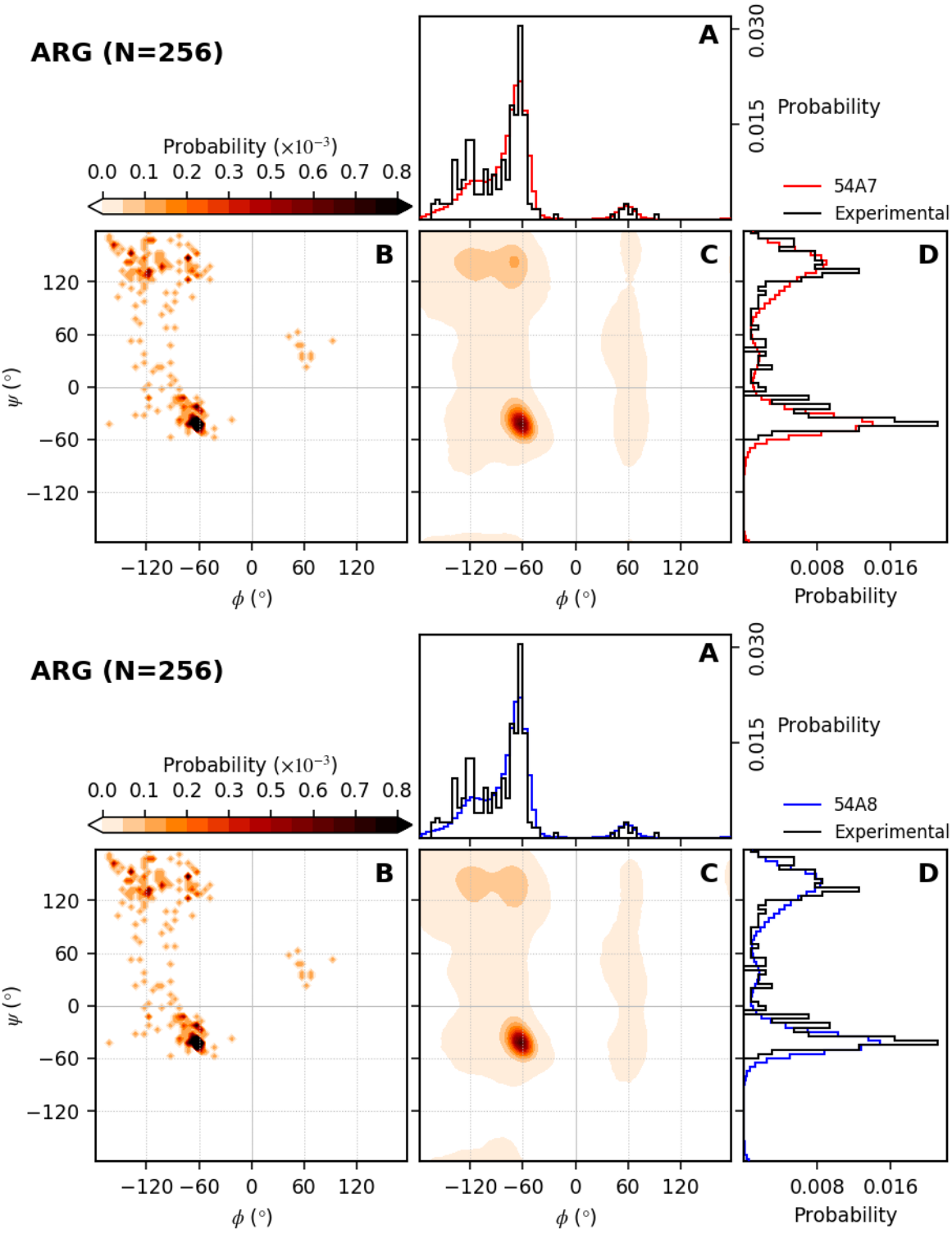
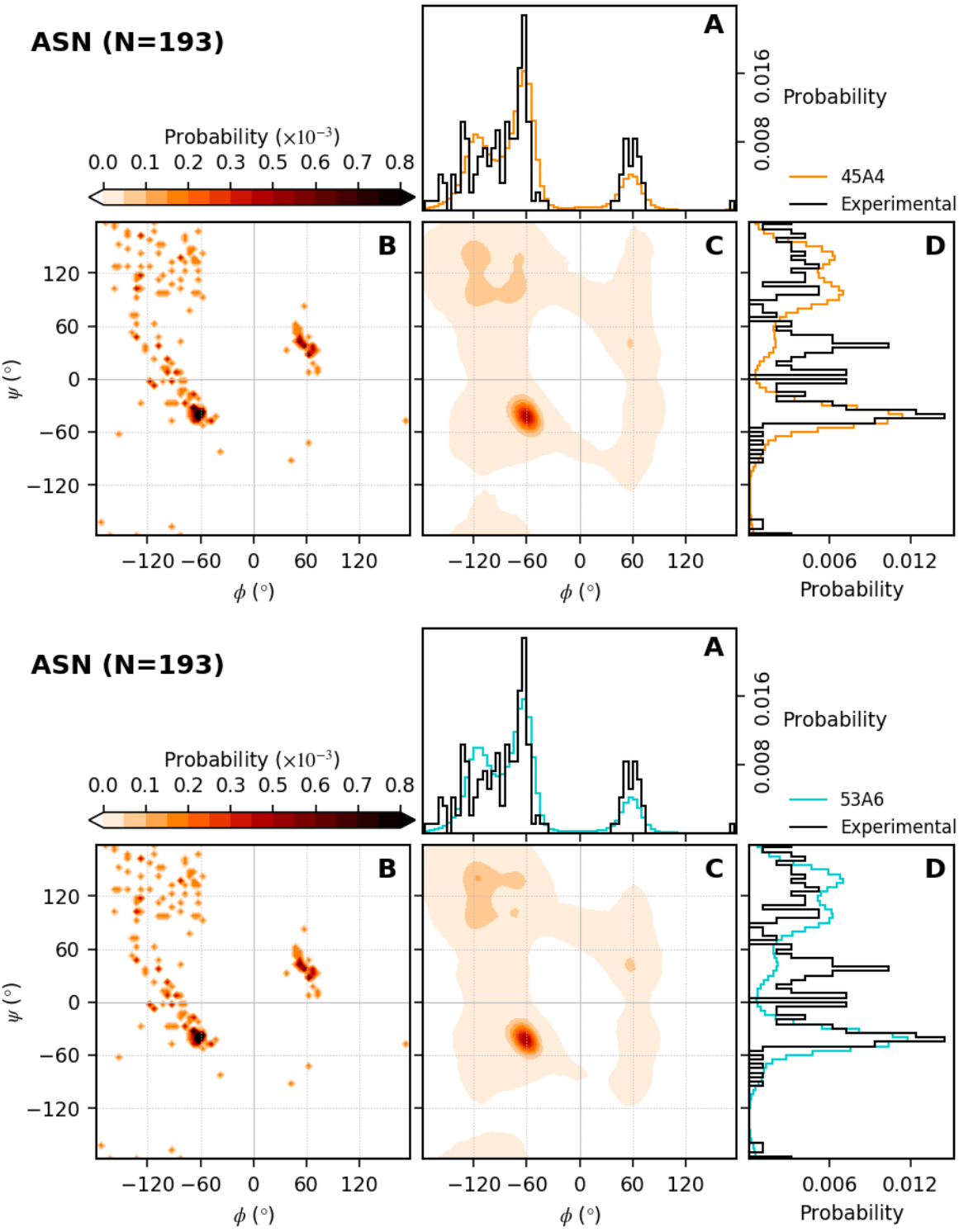


Figure S3. Distribution of arginine (ARG) backbone dihedral angles.


ASN (N=193)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.008 0.016
45A4
Experimental
ψ (°)
ϕ (°)
−120 −60 0 60 120
0.006 0.012
Probability
ASN (N=193)
53A6
Experimental

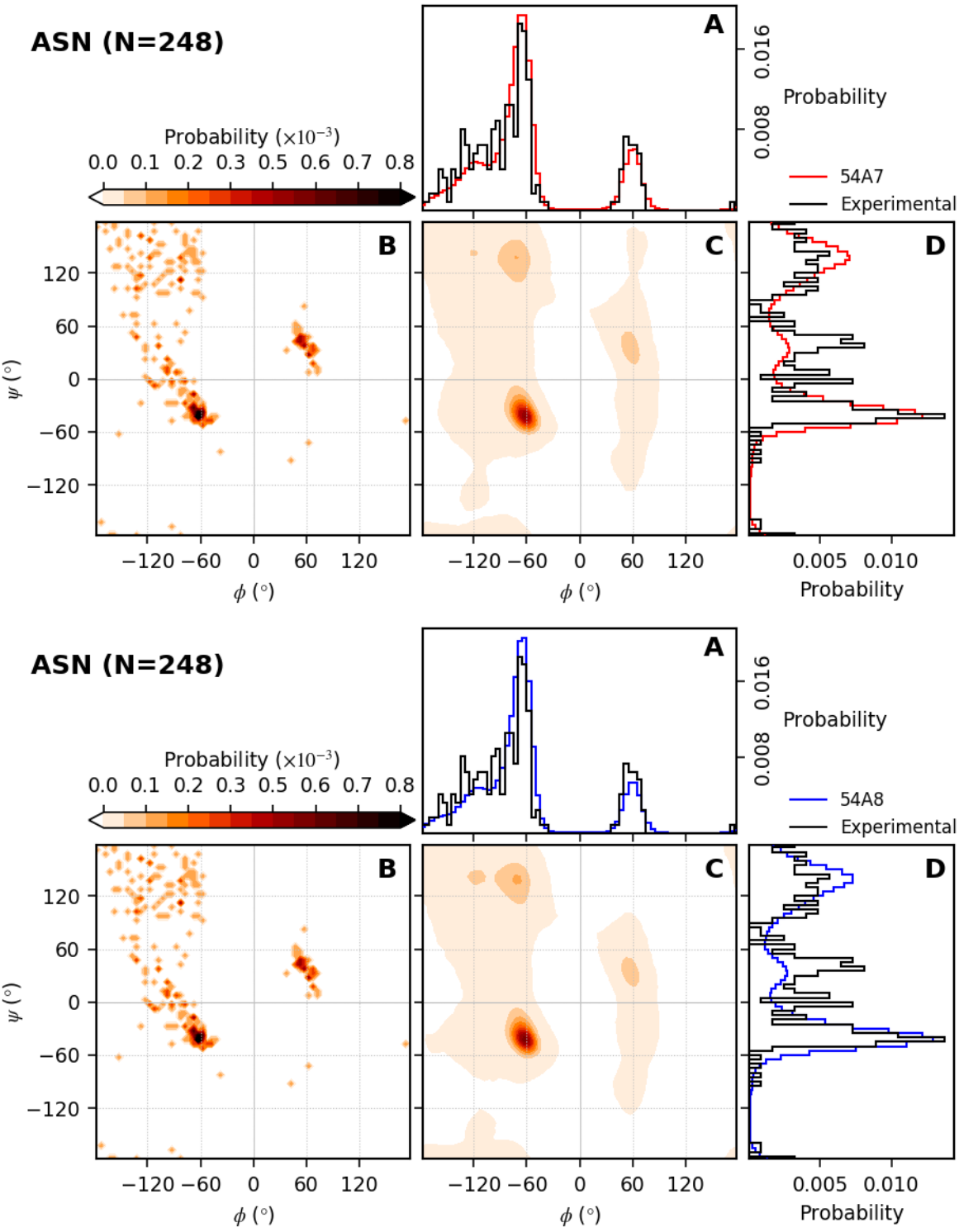
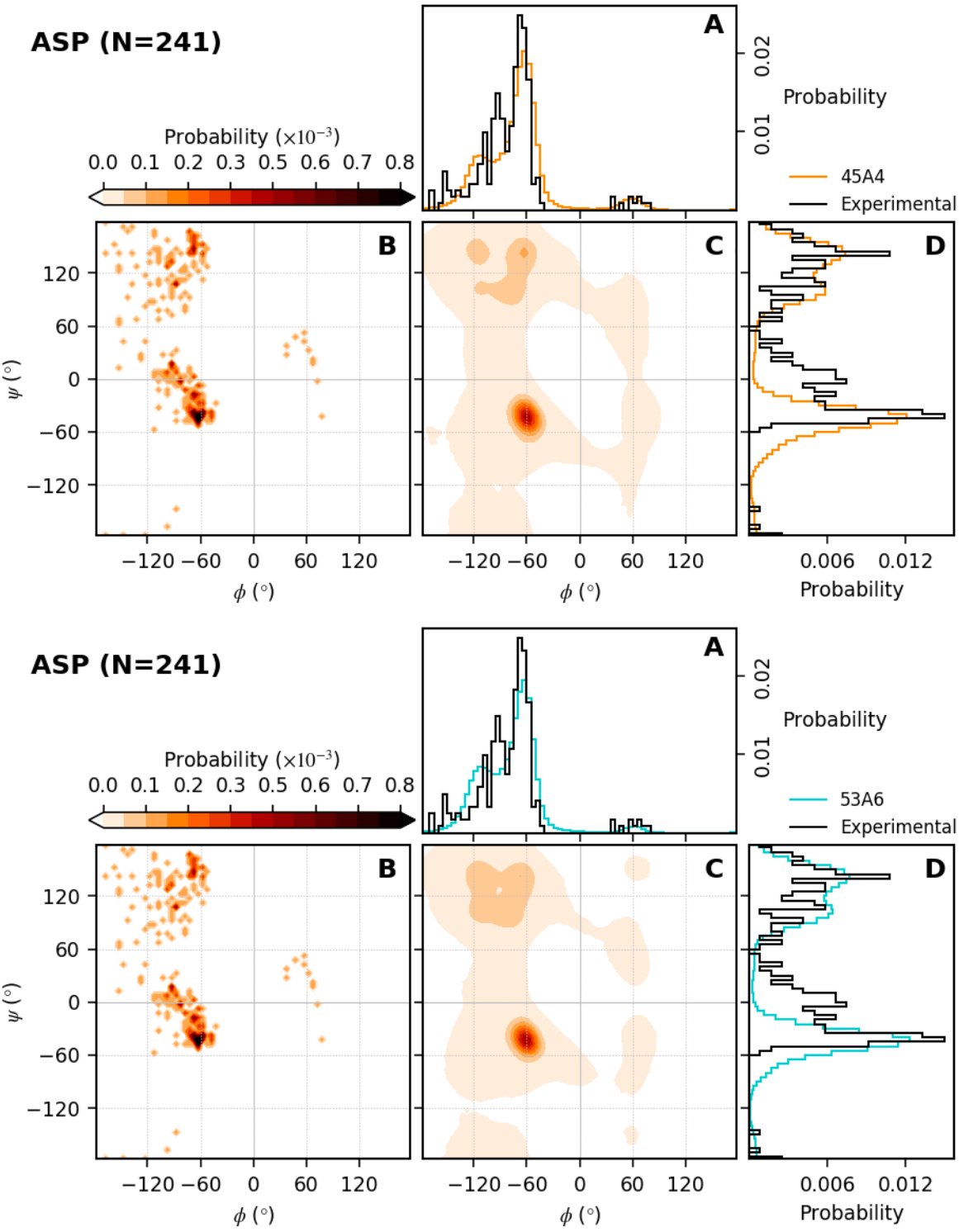


Figure S4. Distribution of asparagine (ASN) backbone dihedral angles.


ASP (N=241)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.006 0.012
Probability
ASP (N=241)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.006 0.012
Probability

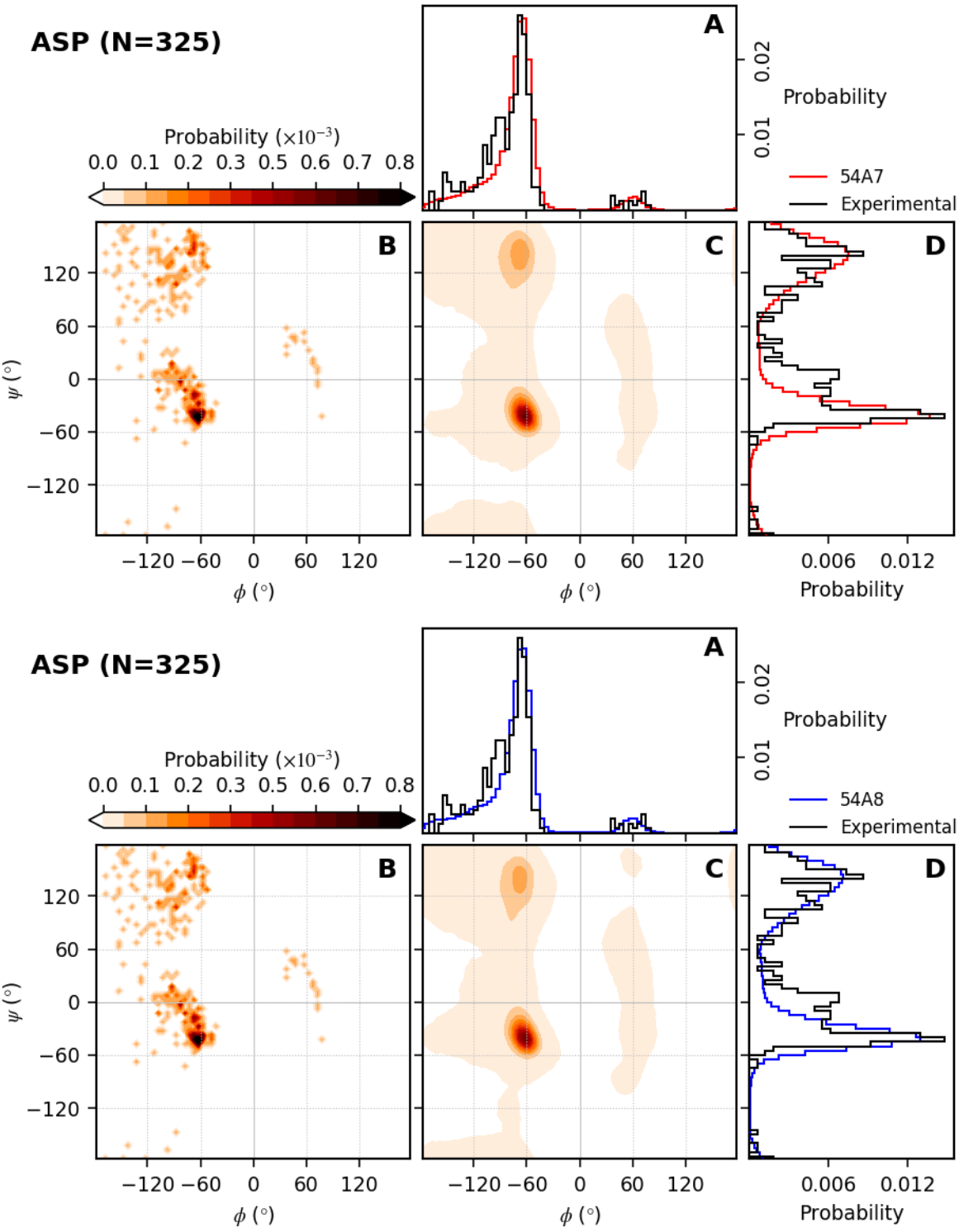
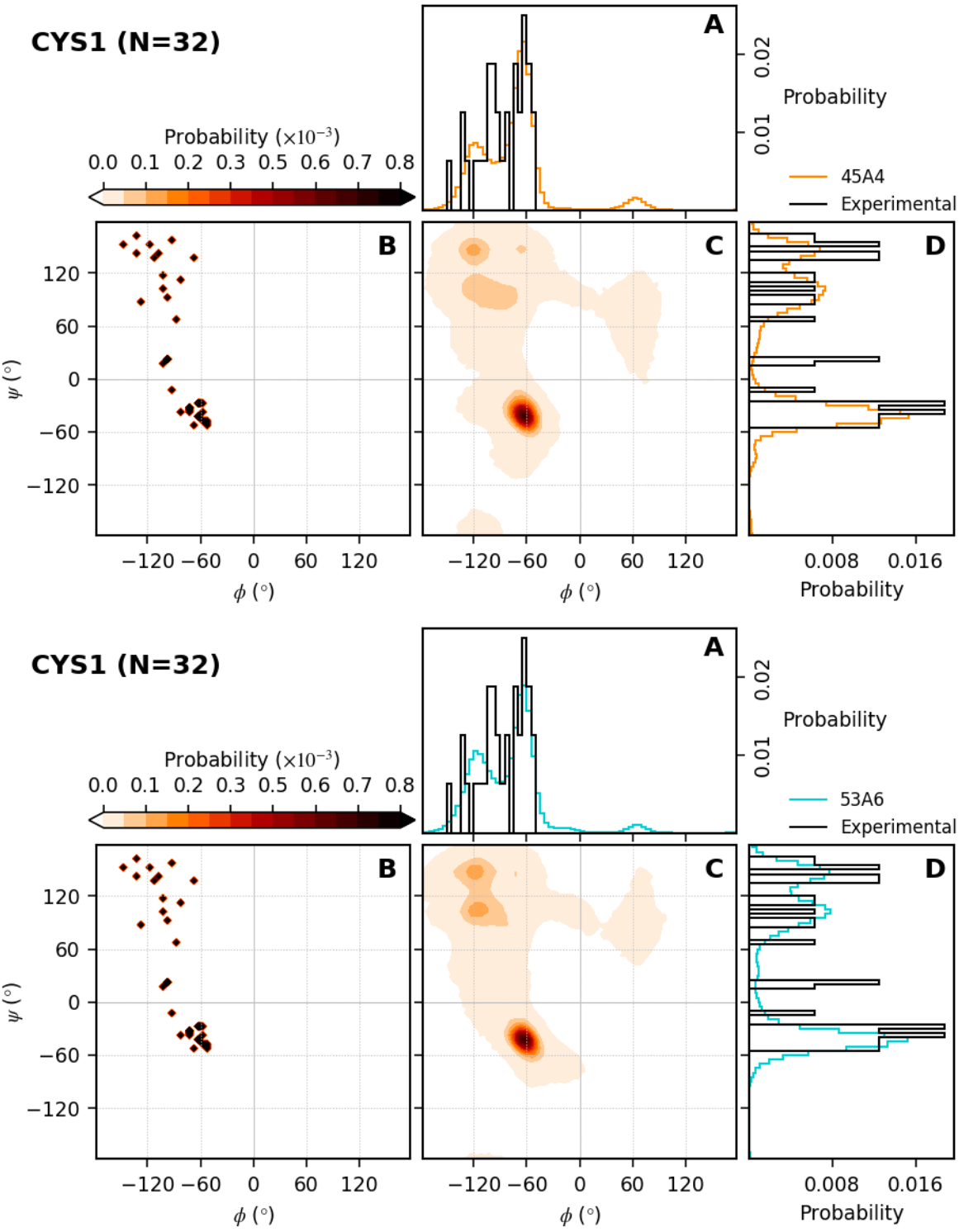


Figure S5. Distribution of aspartic acid (ASP) backbone dihedral angles.


CYS1 (N=32)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability
CYS1 (N=32)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability

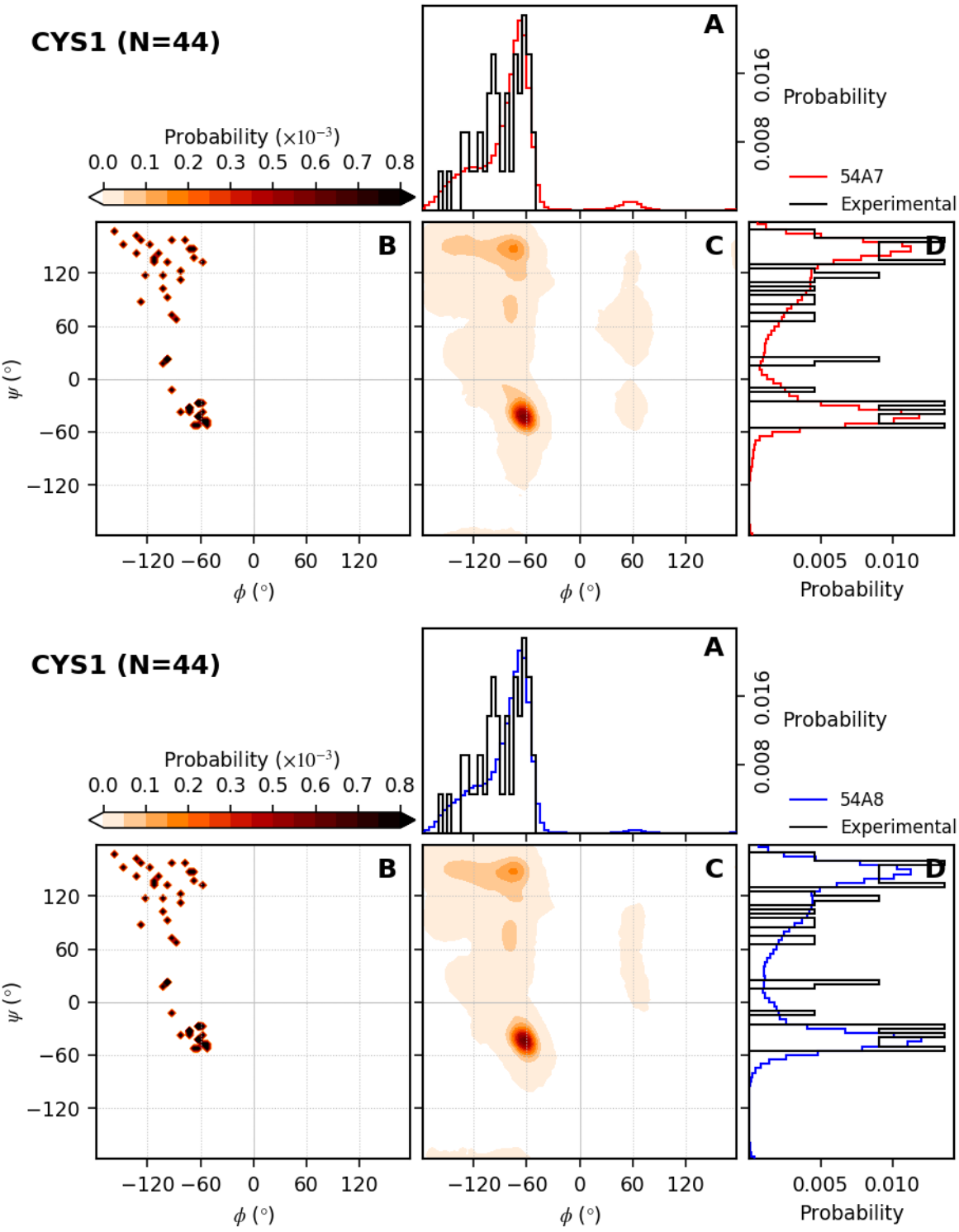
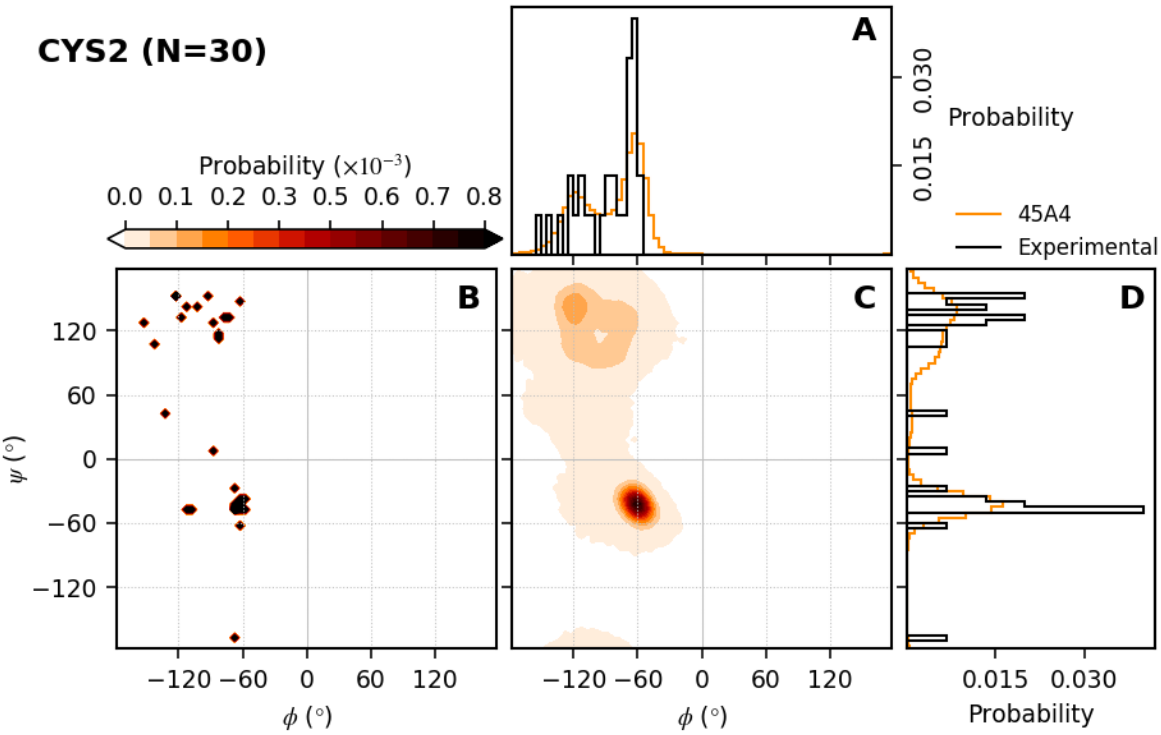
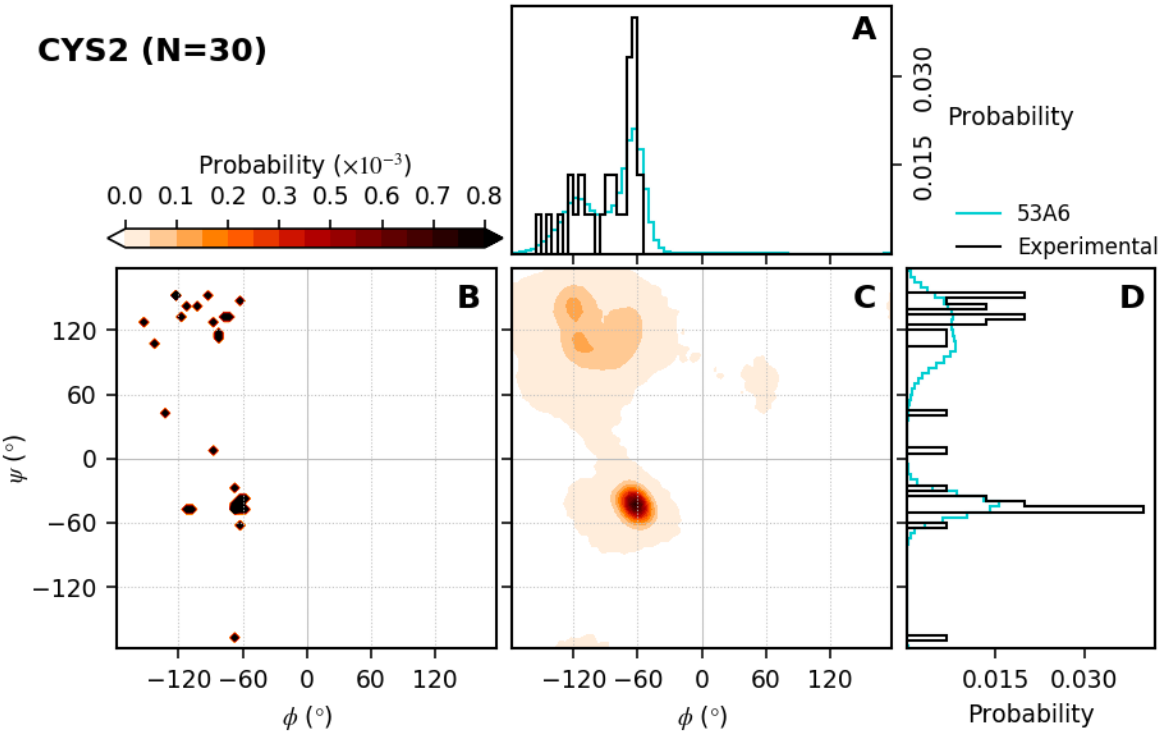


Figure S6. Distribution of first cysteine in S-S bridge (CYS1) backbone dihedral angles.


CYS2 (N=30)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.015 0.030
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.015 0.030
Probability


CYS2 (N=30)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.015 0.030
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.015 0.030
Probability

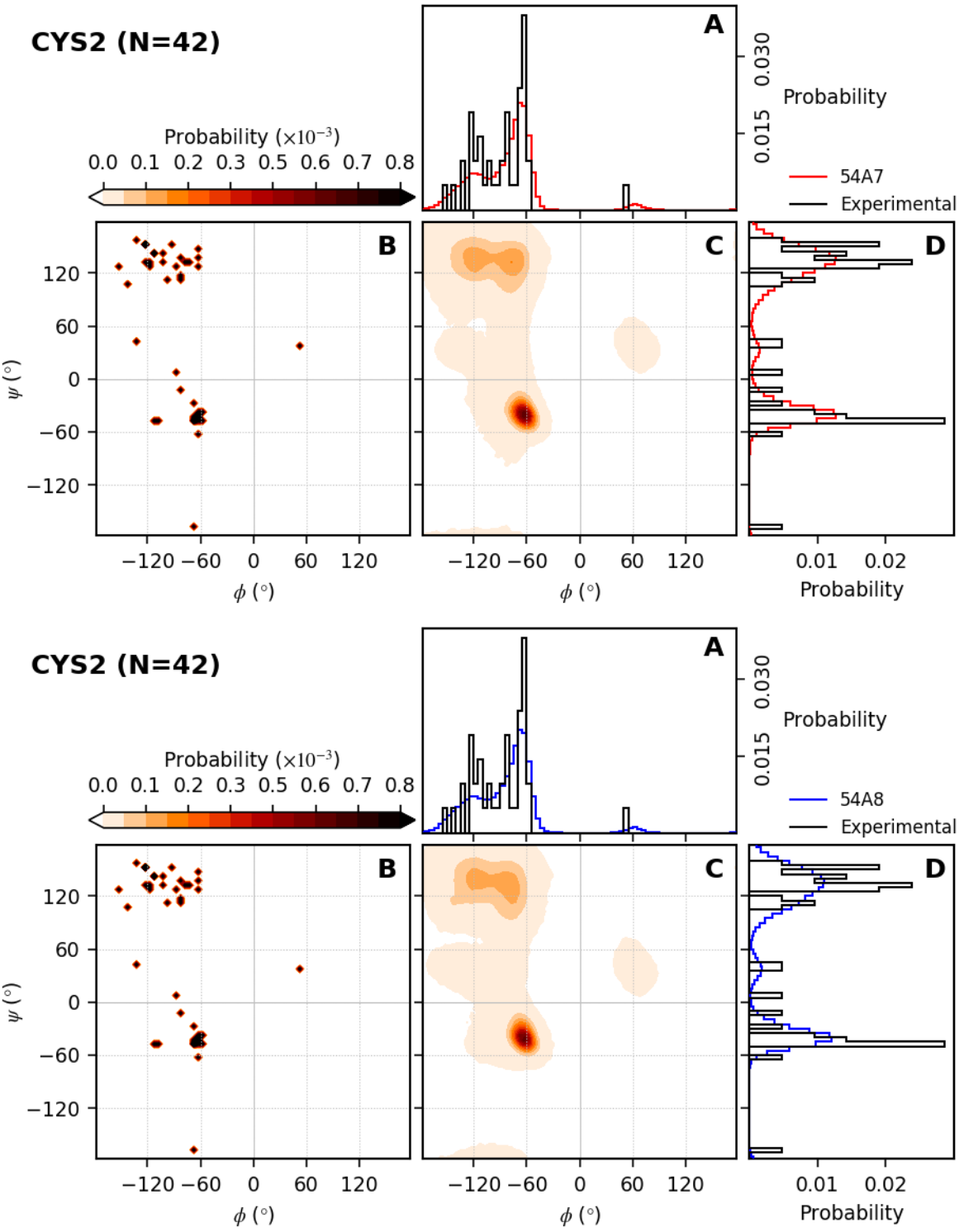
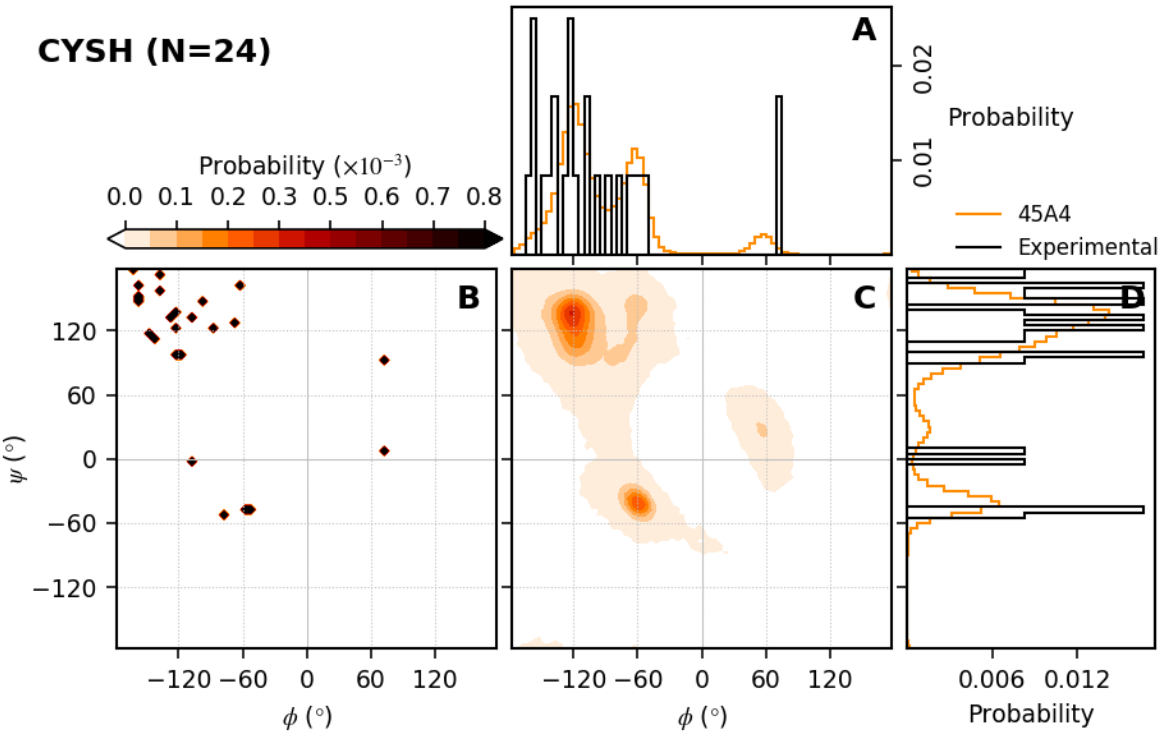
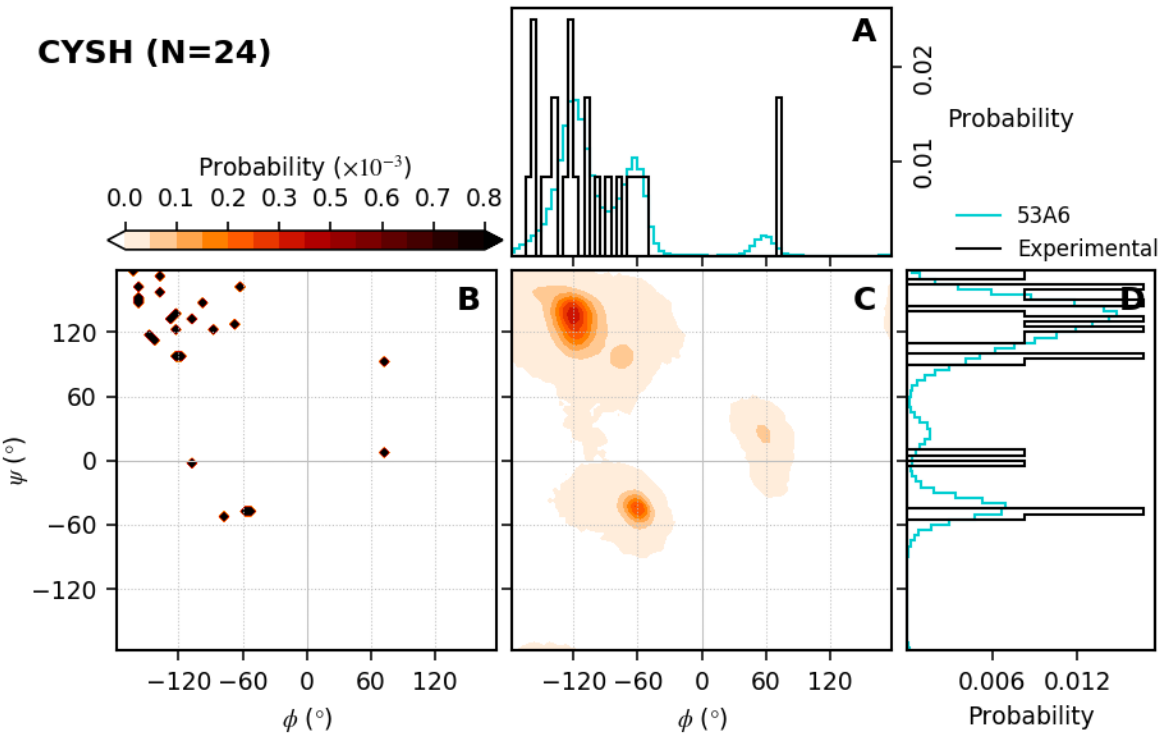


Figure S7. Distribution of second cysteine in S-S bridge (CYS2) backbone dihedral angles.


CYSH (N=24)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.006 0.012
Probability


CYSH (N=24)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.006 0.012
Probability

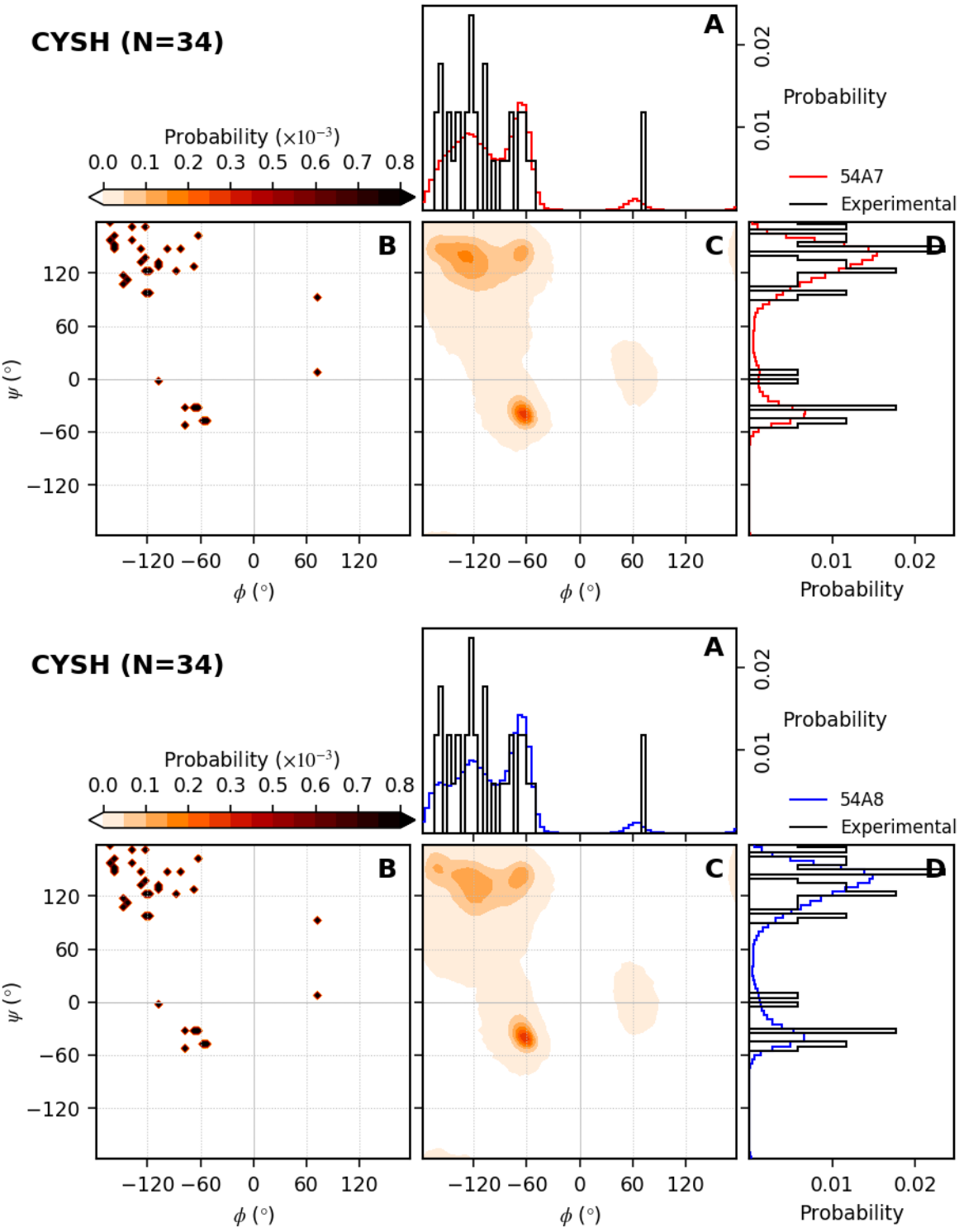
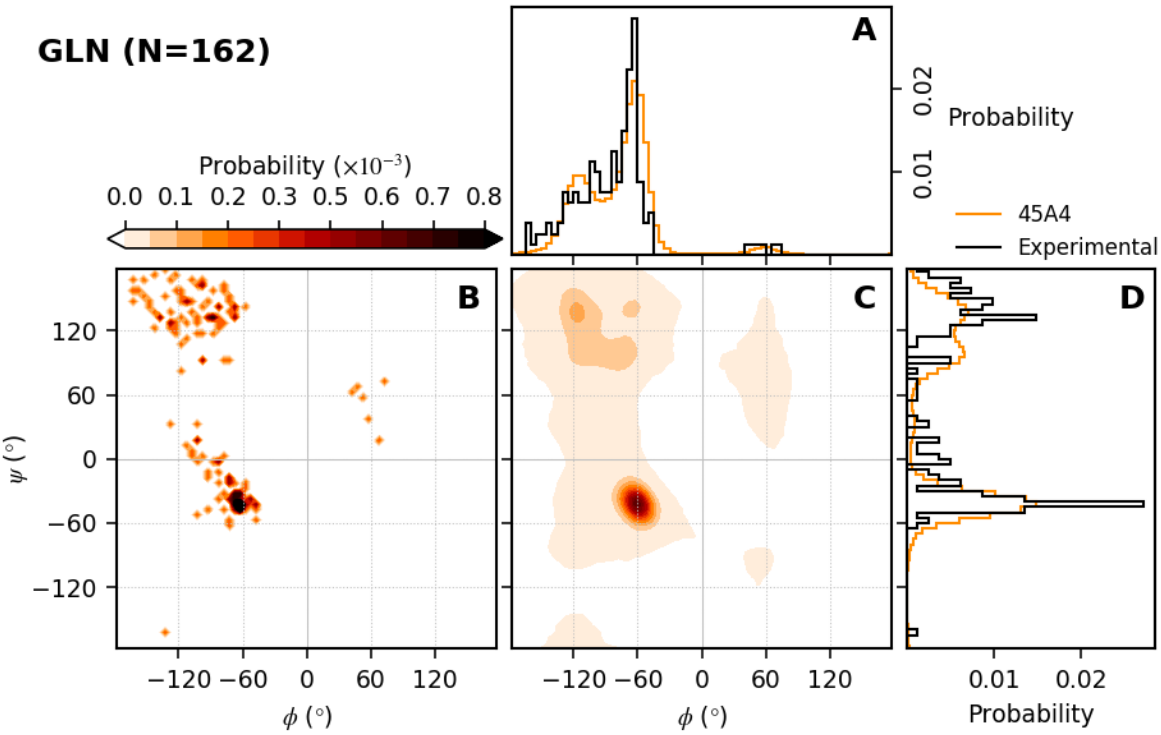
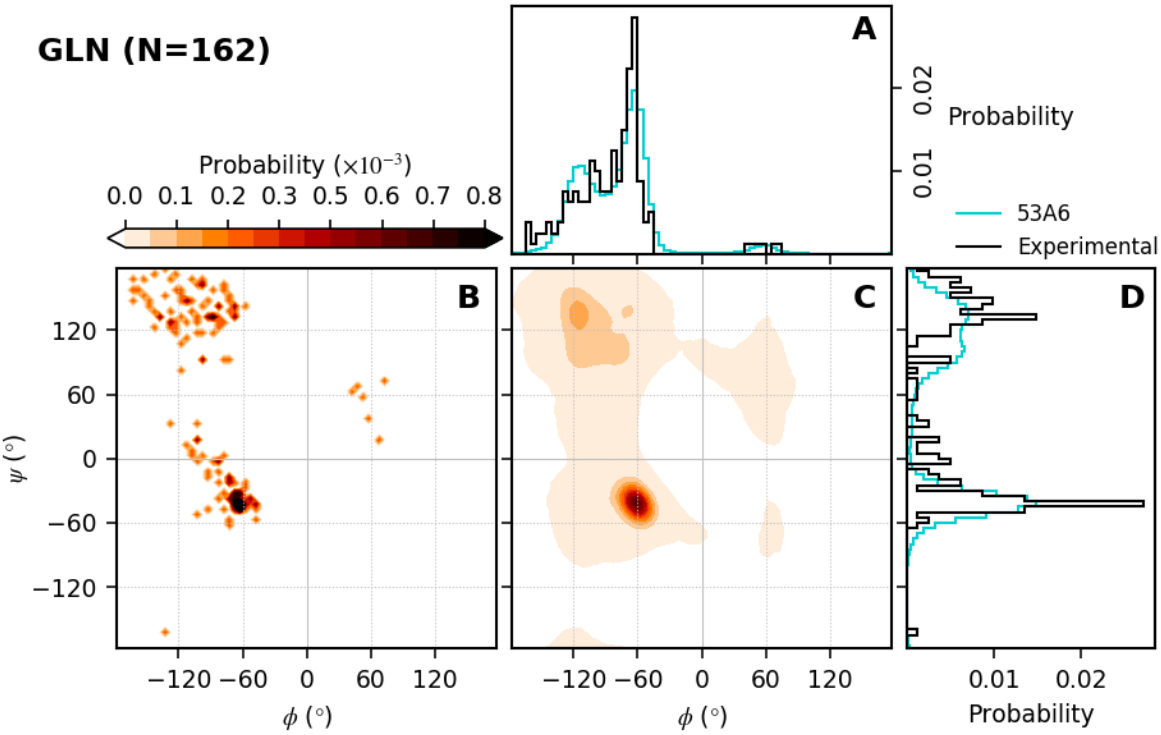


Figure S8. Distribution of neutral cysteine (CYSH) backbone dihedral angles.


GLN (N=162)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.01 0.02
Probability


GLN (N=162)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.01 0.02
Probability

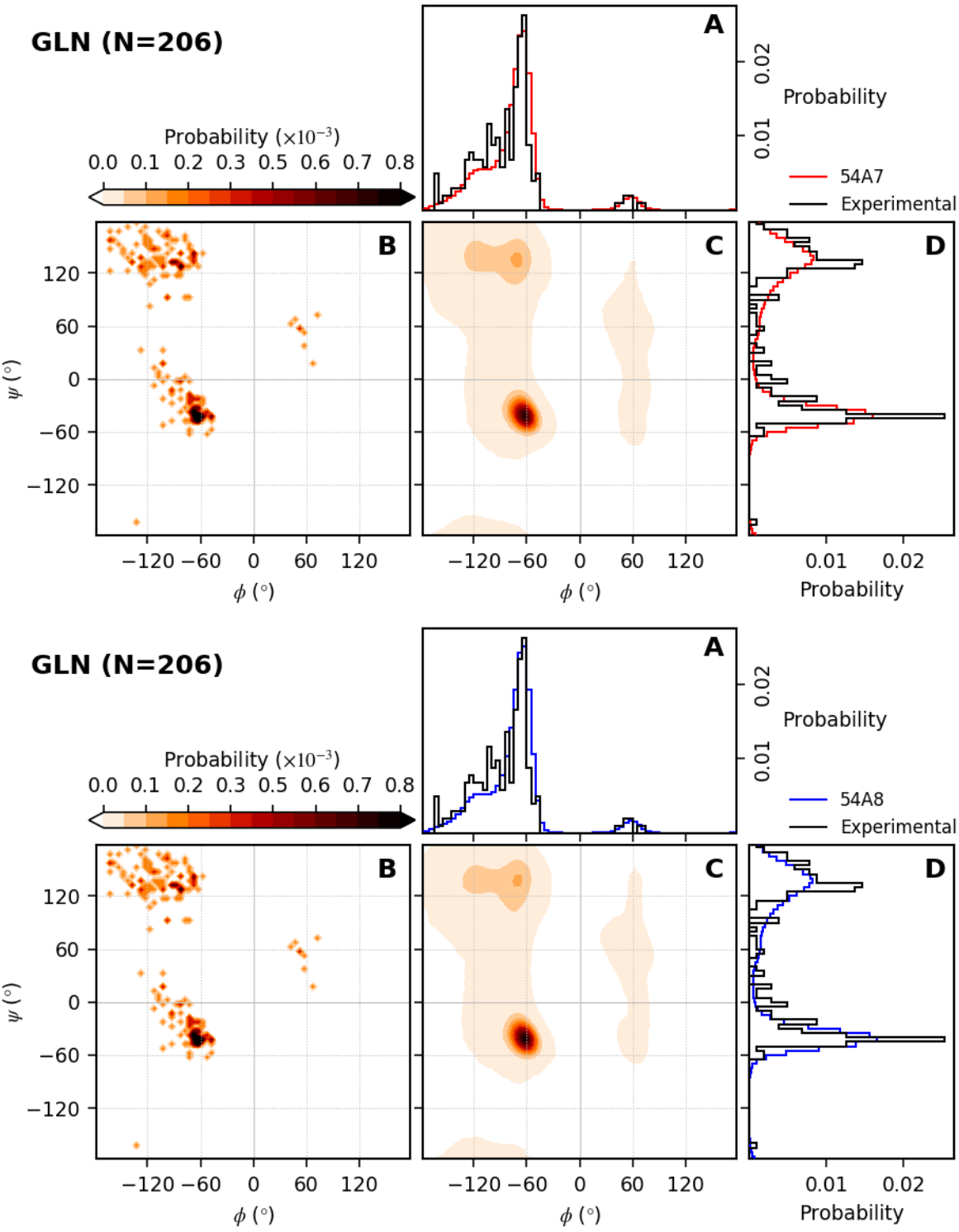
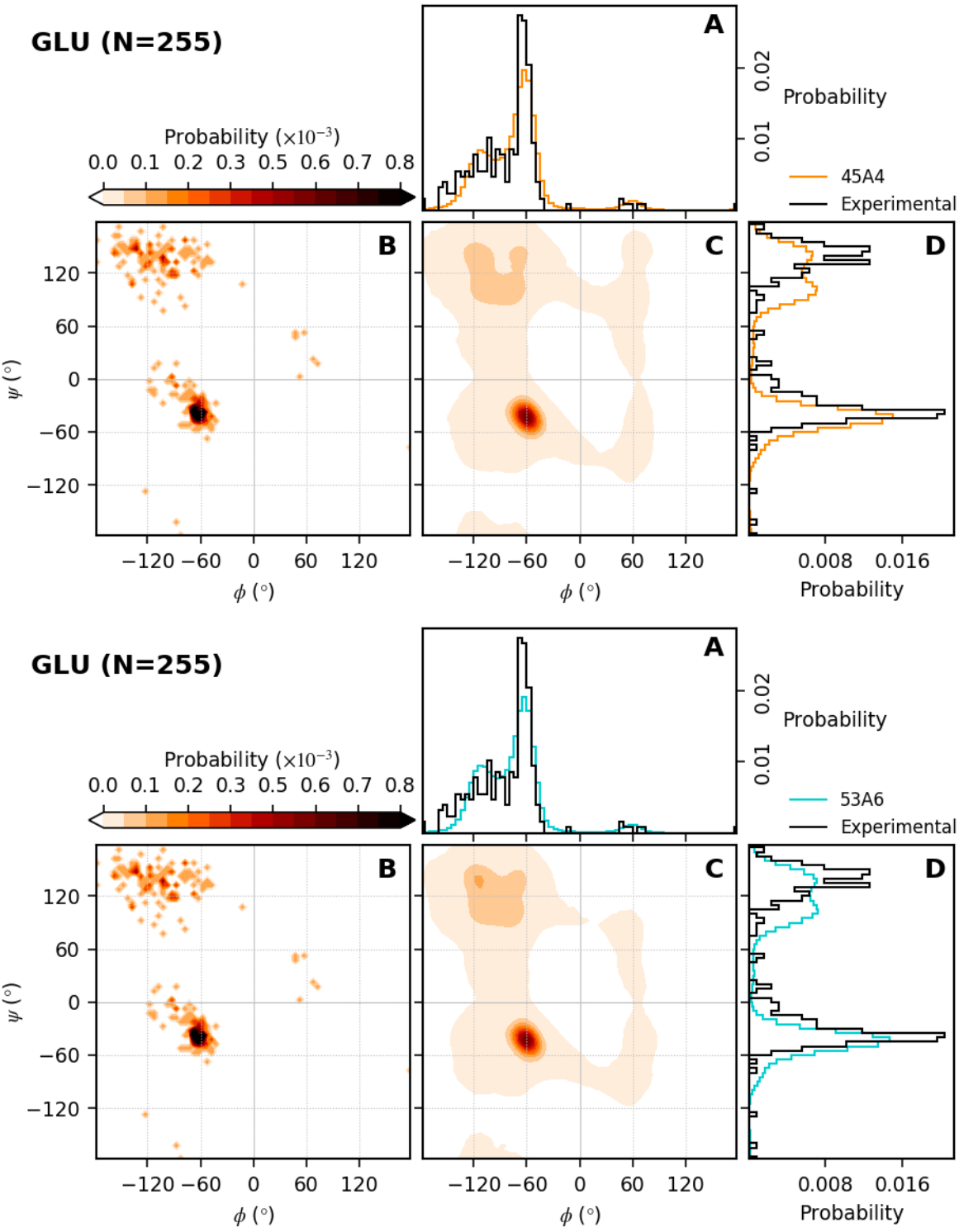


Figure S9. Distribution of glutamine (GLN) backbone dihedral angles.


GLU (N=255)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability
GLU (N=255)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability

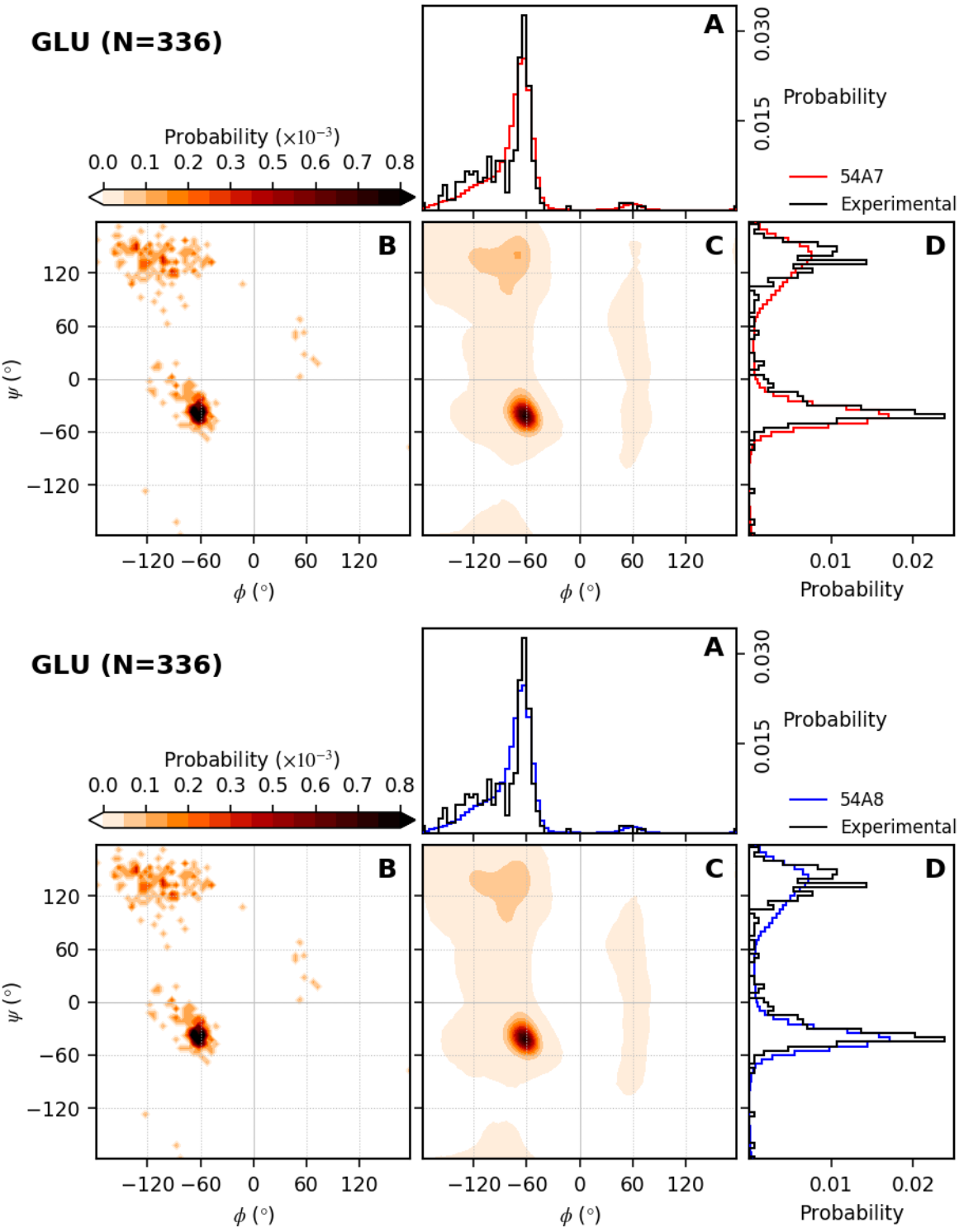
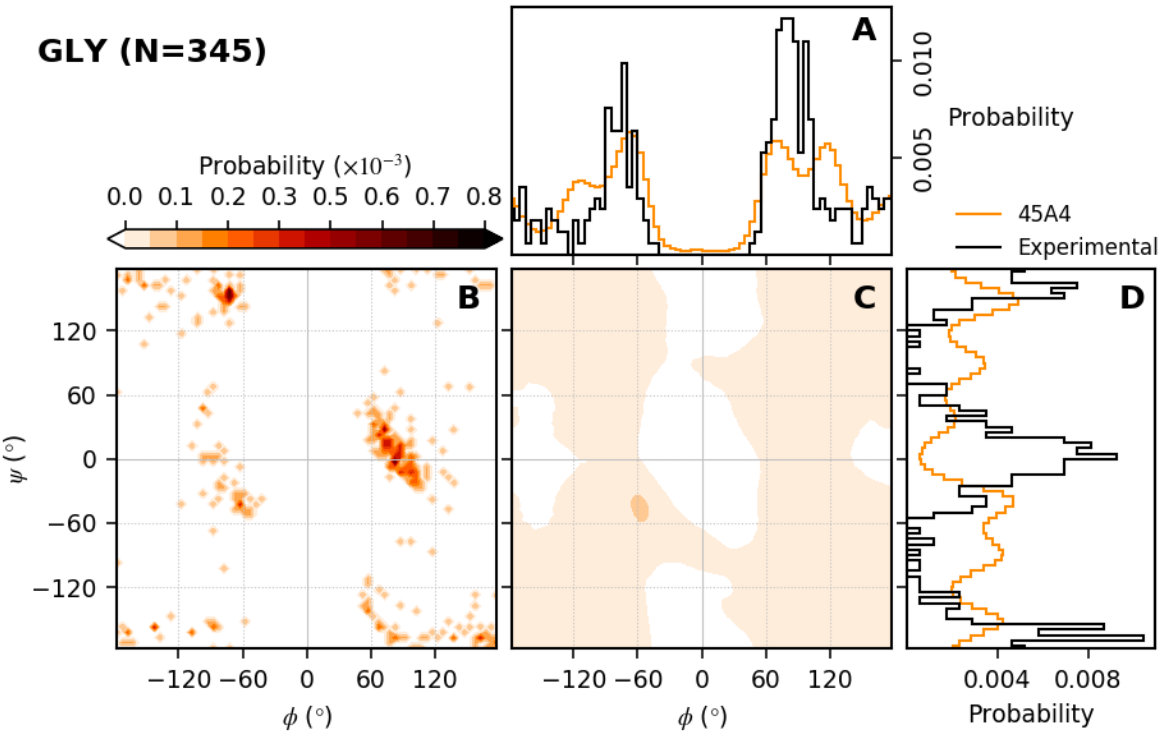
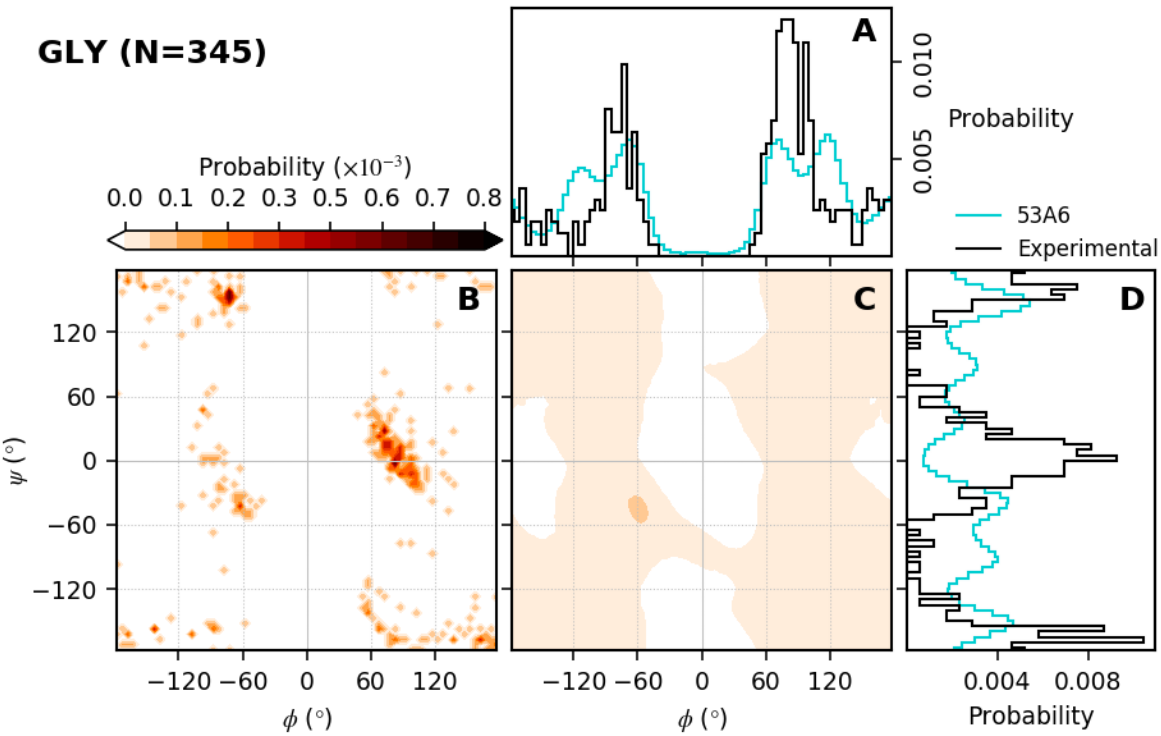


Figure S10. Distribution of glutamic acid (GLU) backbone dihedral angles.


GLY (N=345)
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
A
B
C
D
Probability
0.005 0.010
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.004 0.008
Probability


GLY (N=345)
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
A
B
C
D
Probability
0.005 0.010
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.004 0.008
Probability

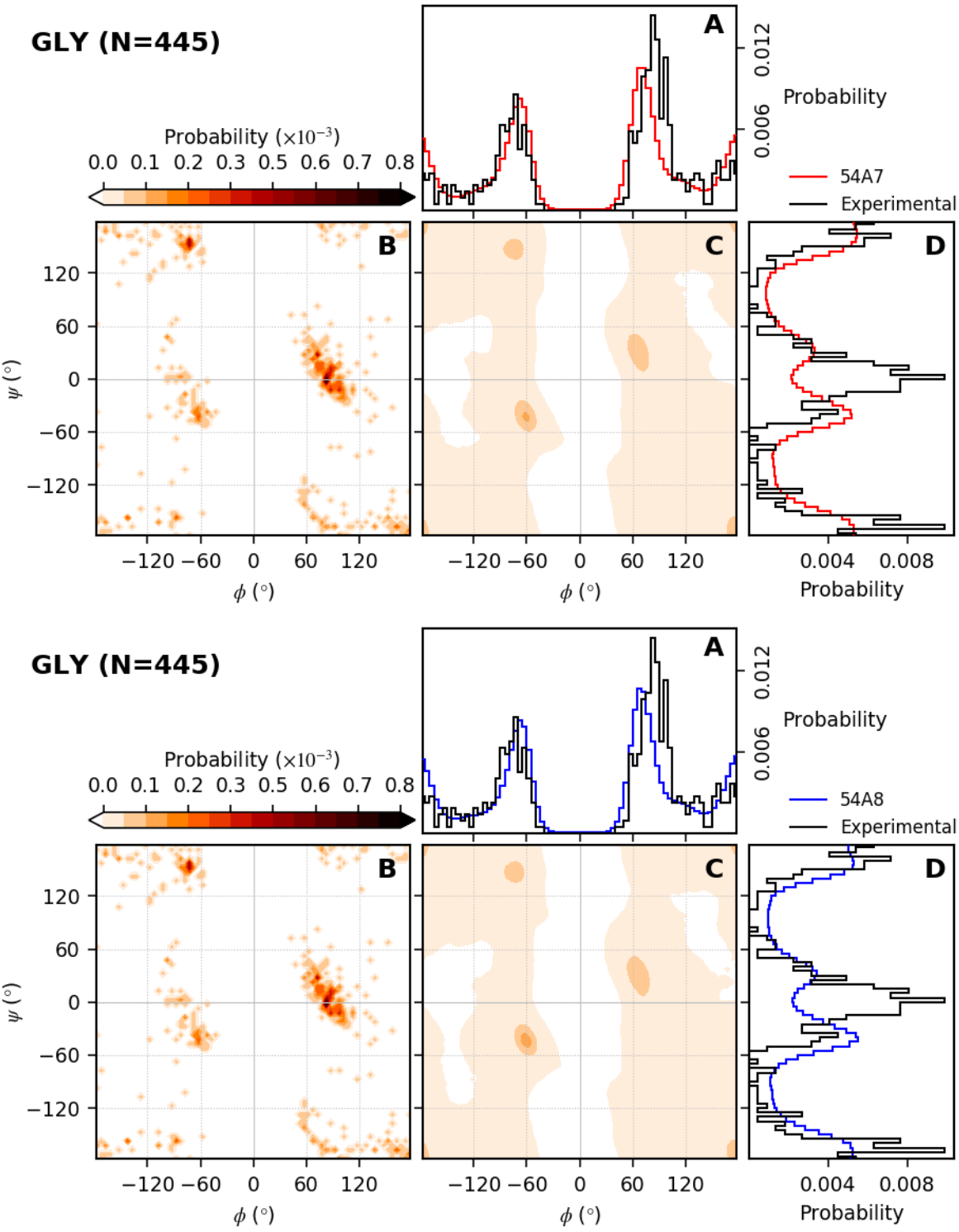
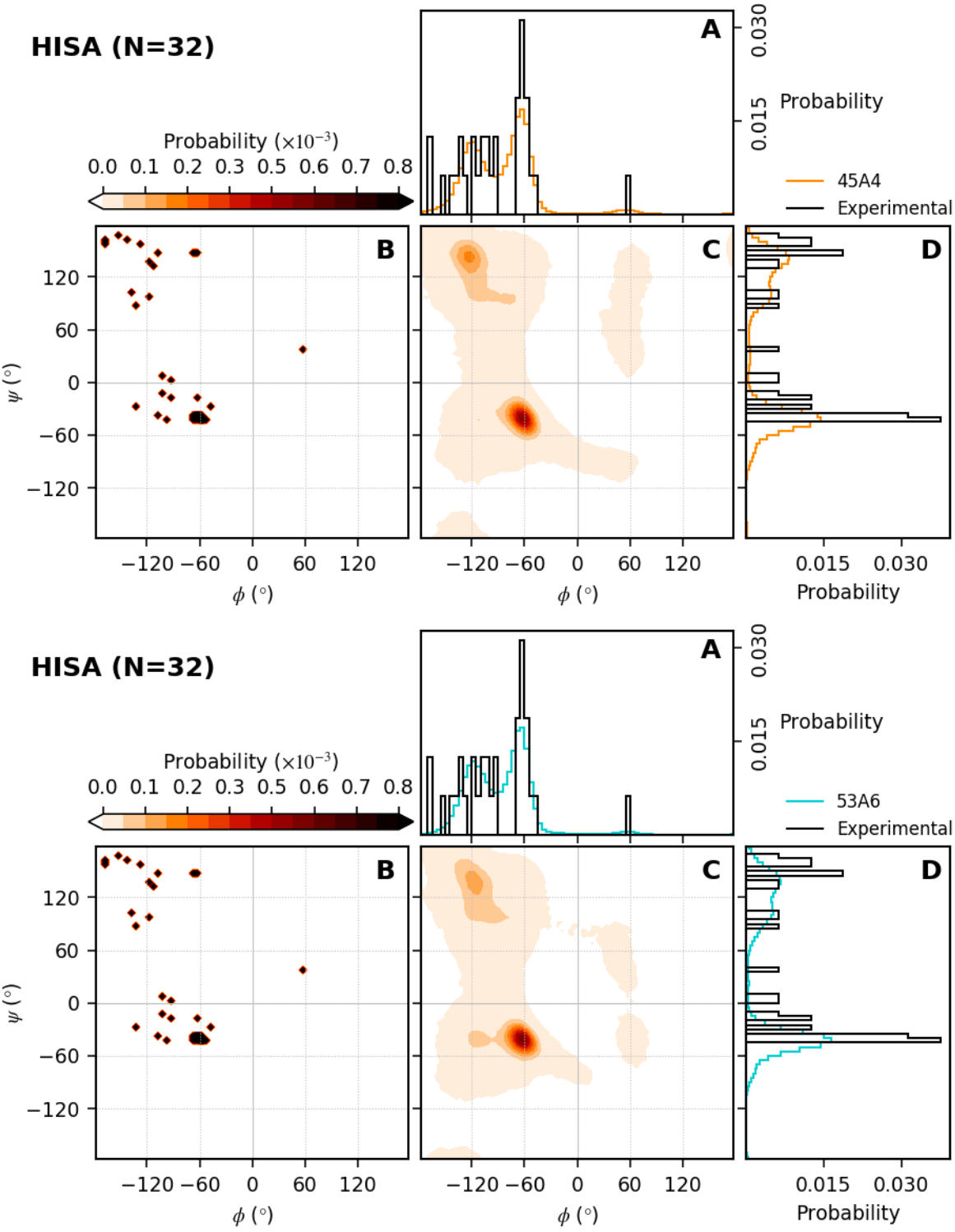


Figure S11. Distribution of glycine (GLY) backbone dihedral angles.


HISA (N=32)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.015
0.030
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.015 0.030
Probability
HISA (N=32)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.015
0.030
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.015 0.030
Probability

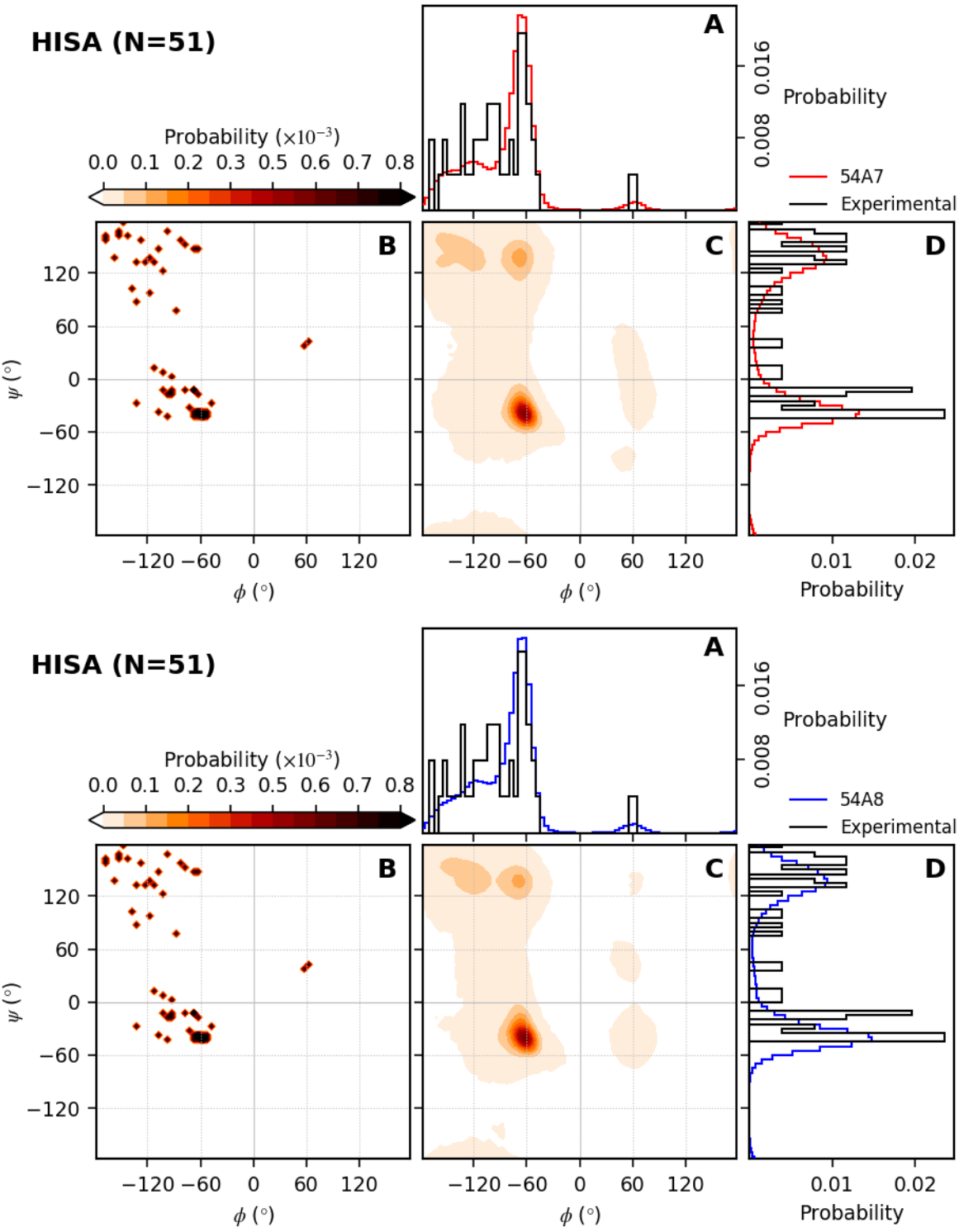
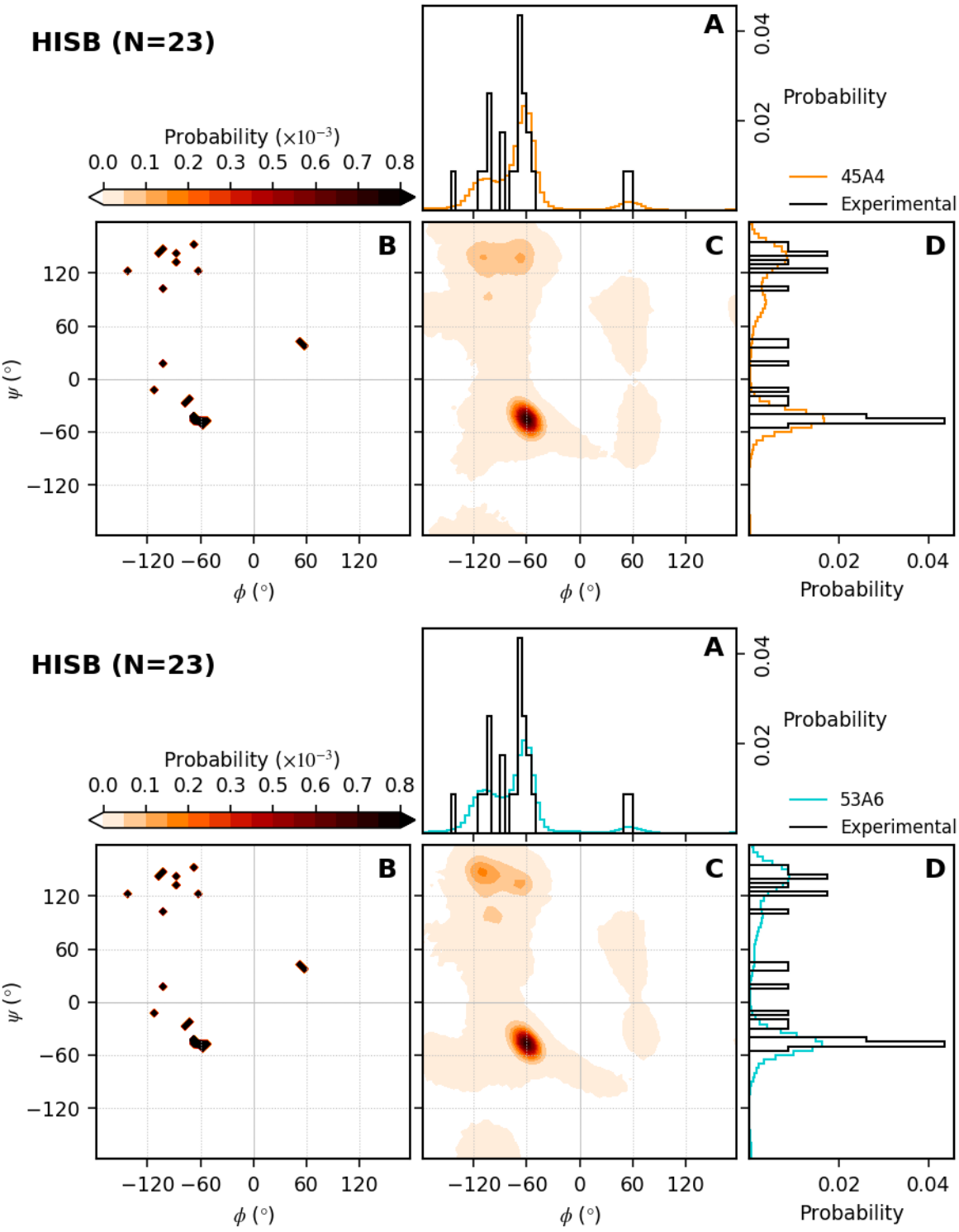


Figure S12. Distribution of histidine protonated at ND1 (HISA) backbone dihedral angles.


HISB (N=23)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.02
0.04
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.02 0.04
Probability
HISB (N=23)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.02
0.04
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.02 0.04
Probability

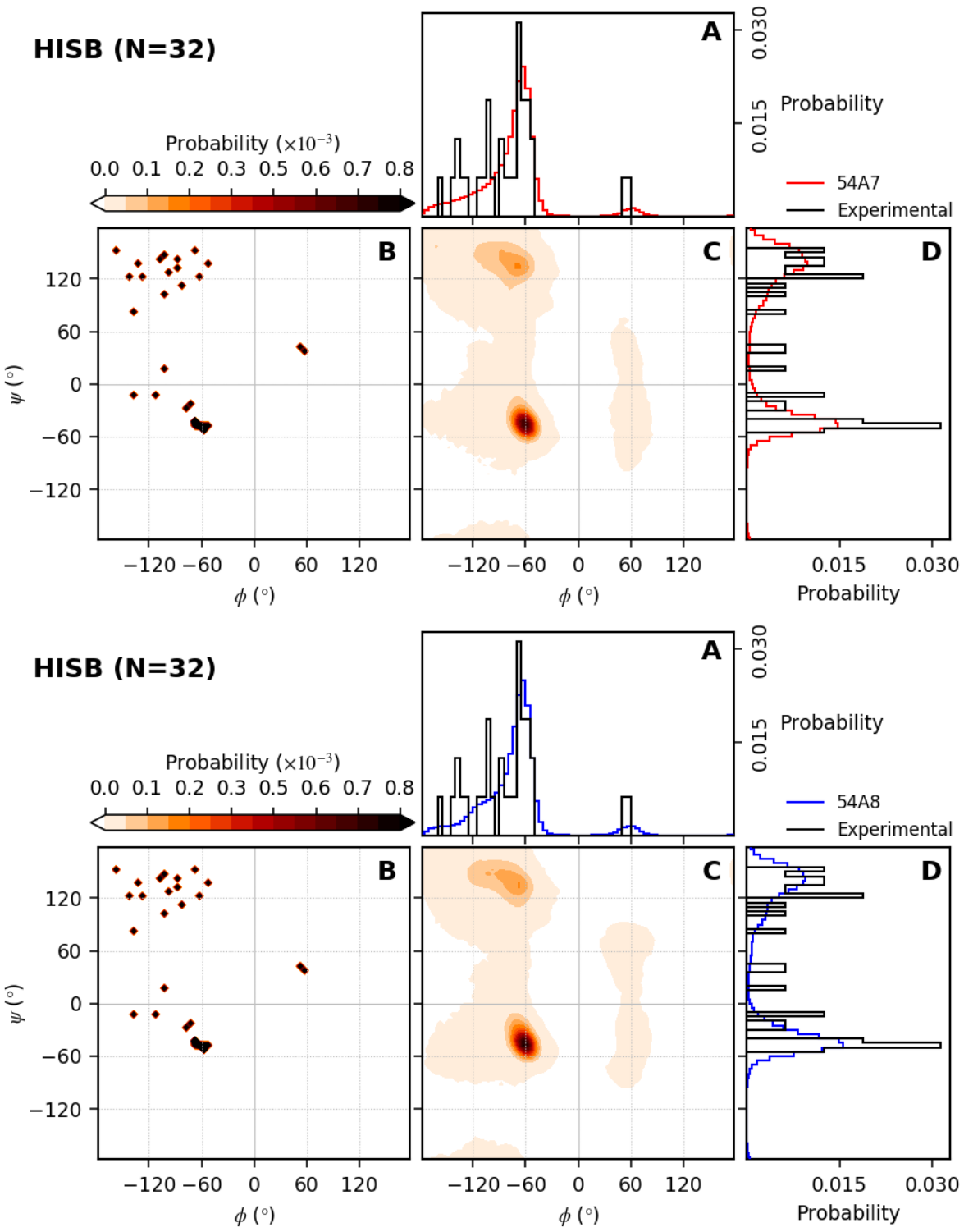
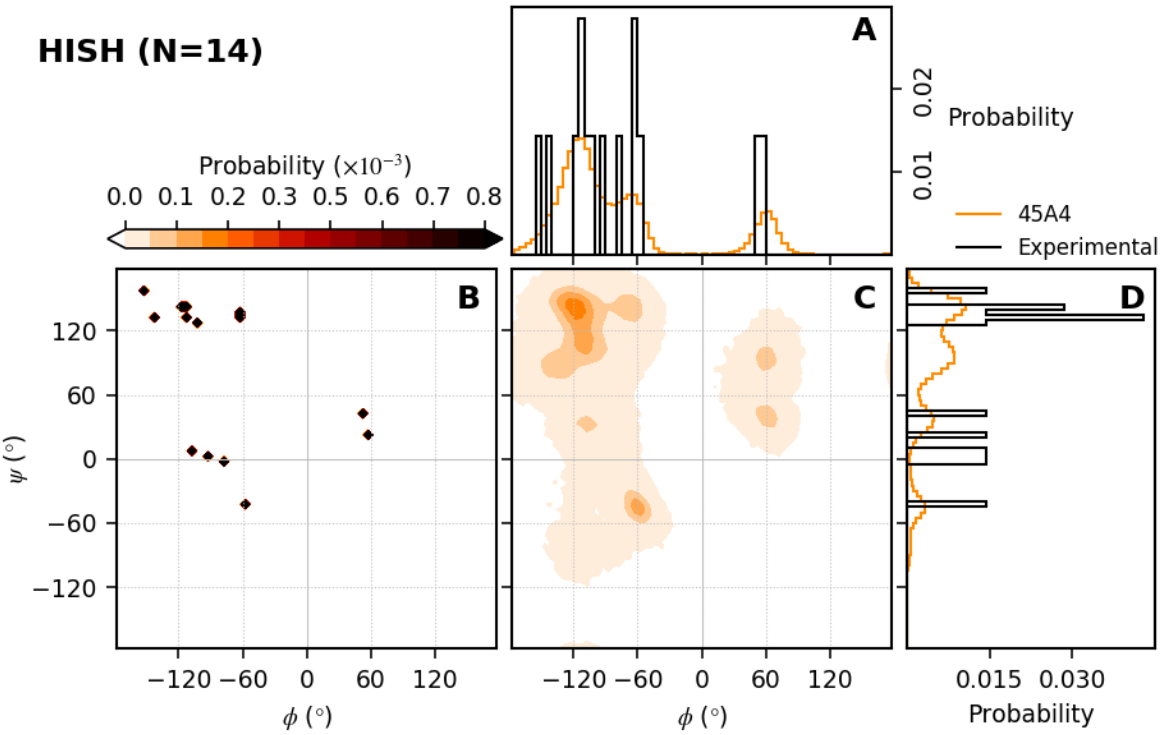
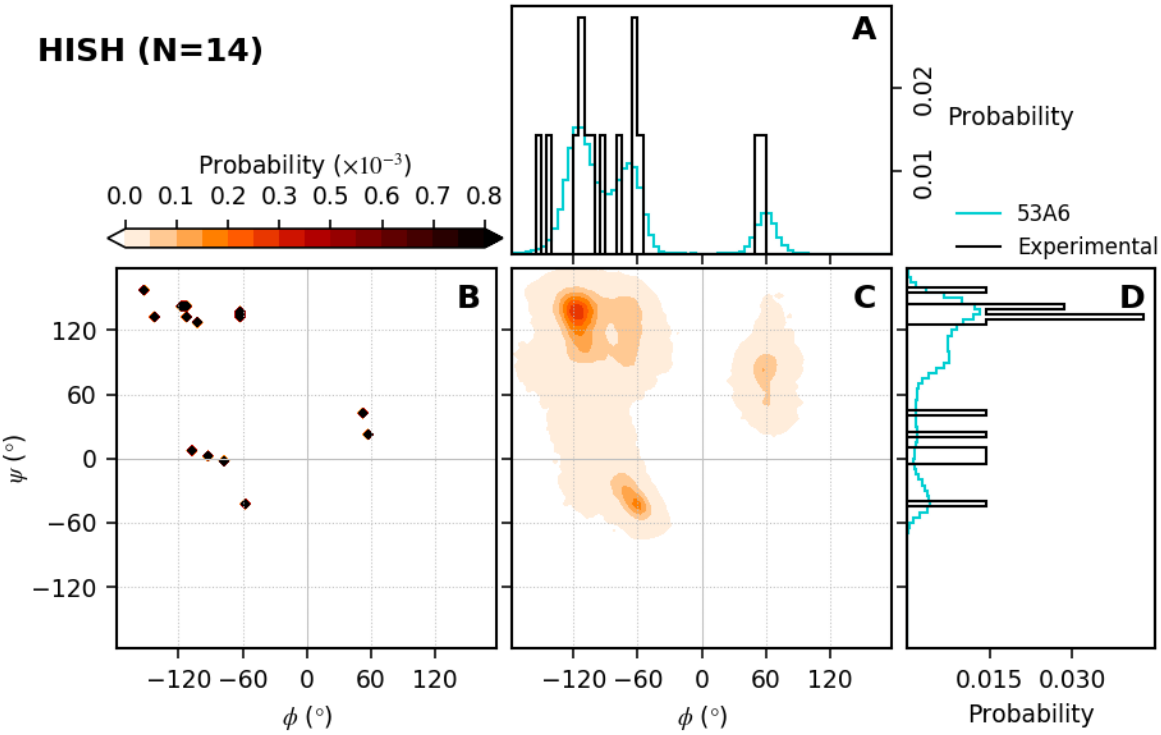


Figure S13. Distribution of histidine protonated at NE2 (HISB) backbone dihedral angles.


HISH (N=14)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.015 0.030
Probability


HISH (N=14)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.015 0.030
Probability

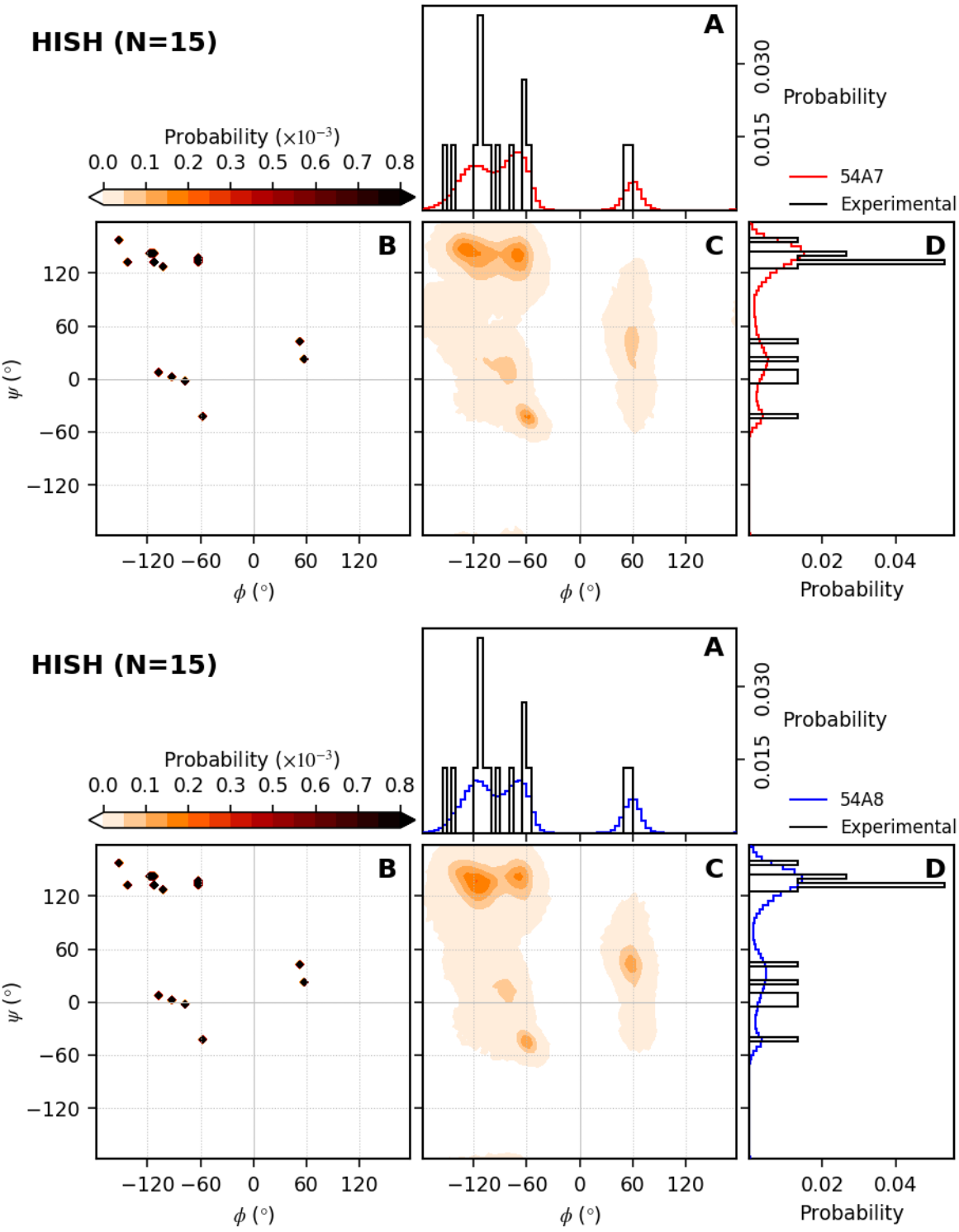
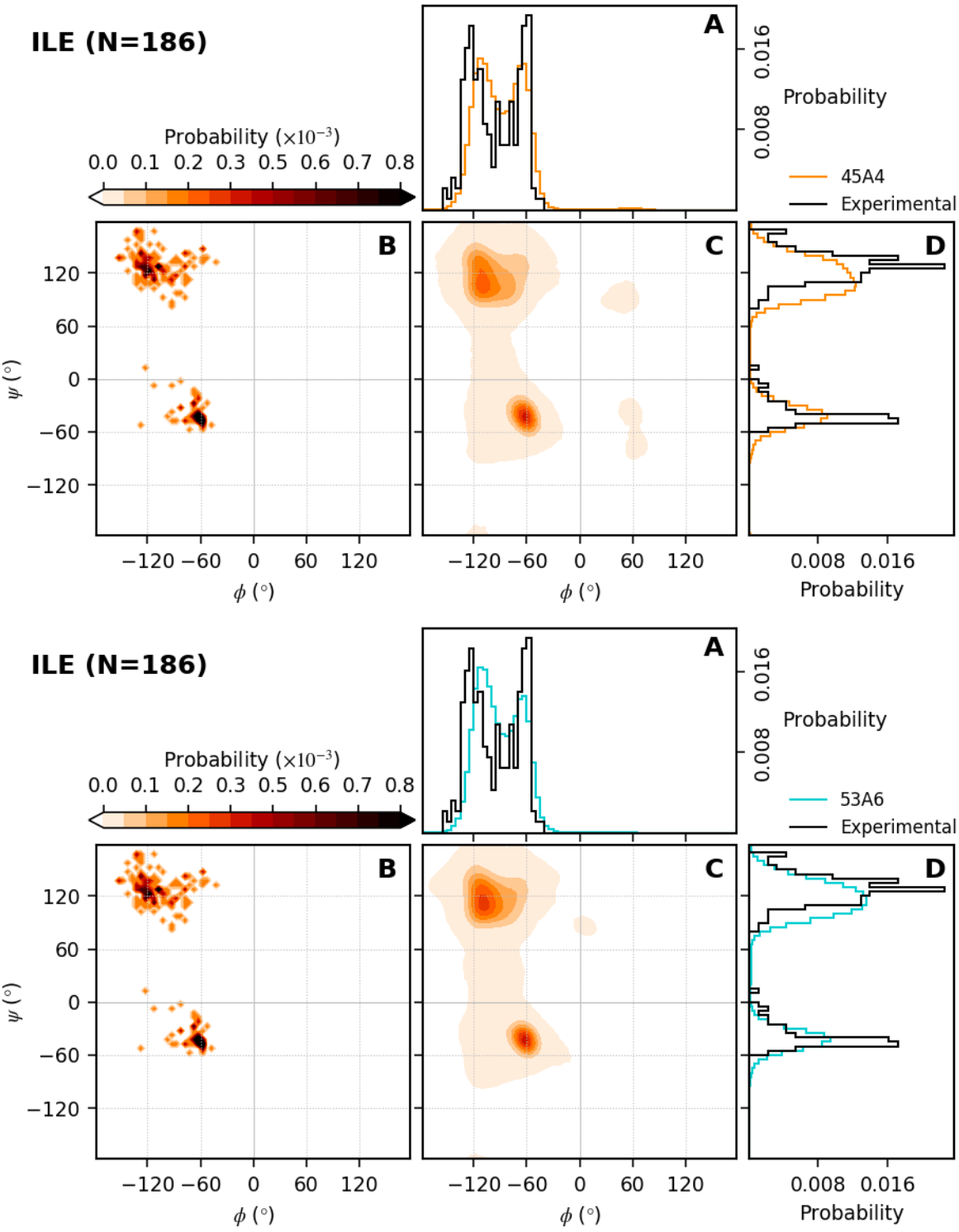


Figure S14. Distribution of histidine with +1 formal charge (HISH) backbone dihedral angles.


ILE (N=186)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.008 0.016
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability
ILE (N=186)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.008 0.016
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability

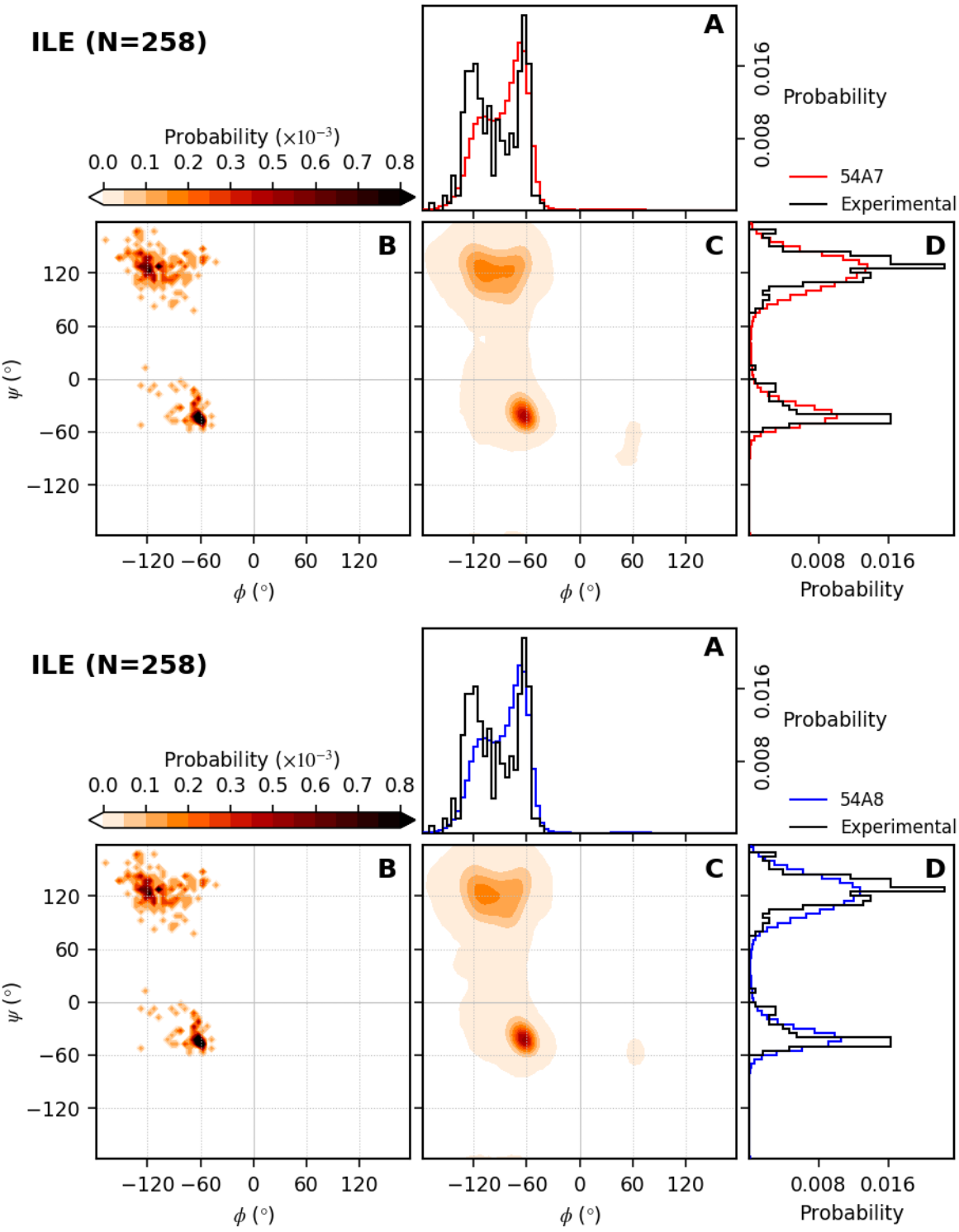
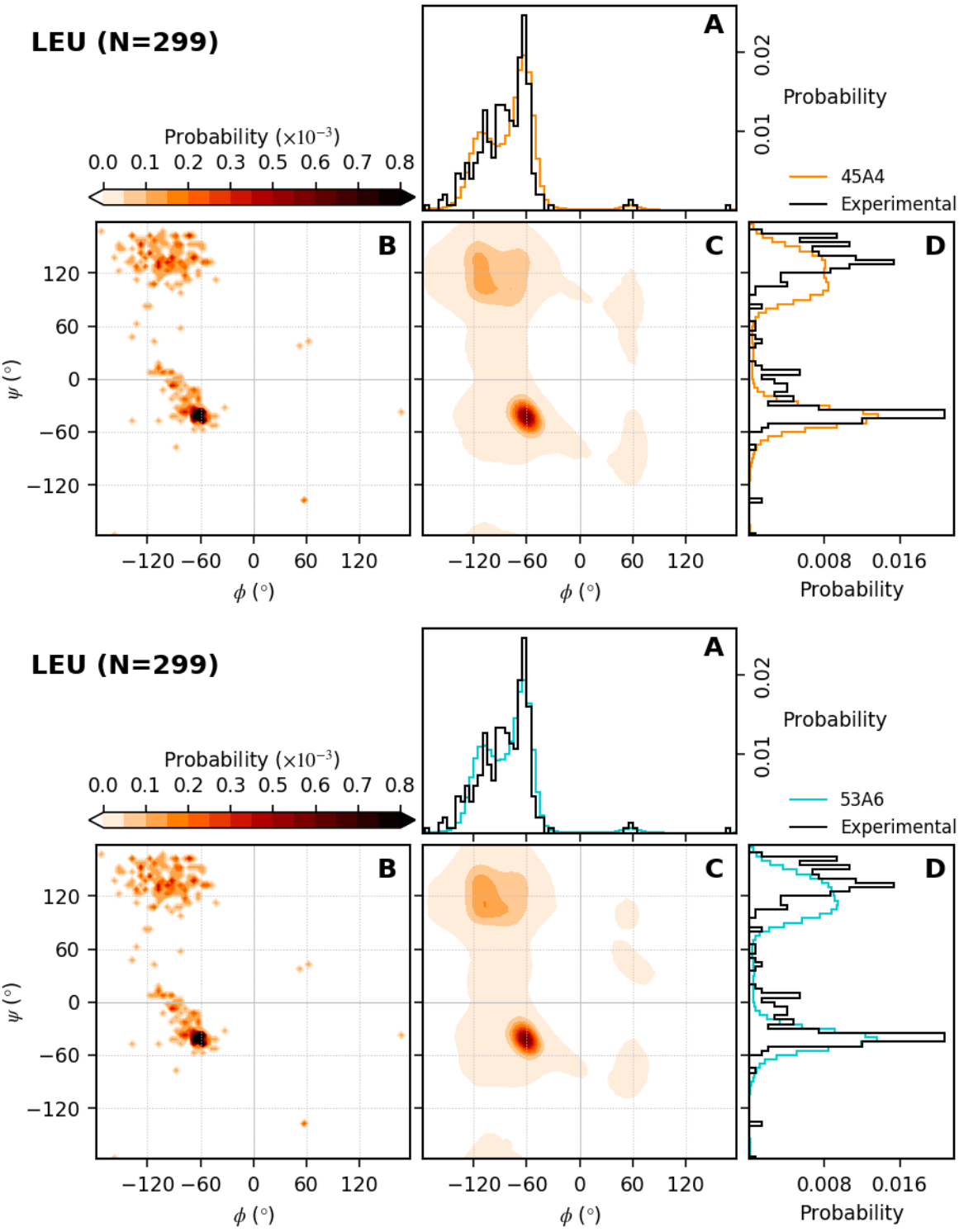


Figure S15. Distribution of isoleucine (ILE) backbone dihedral angles.


LEU (N=299)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability
LEU (N=299)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability

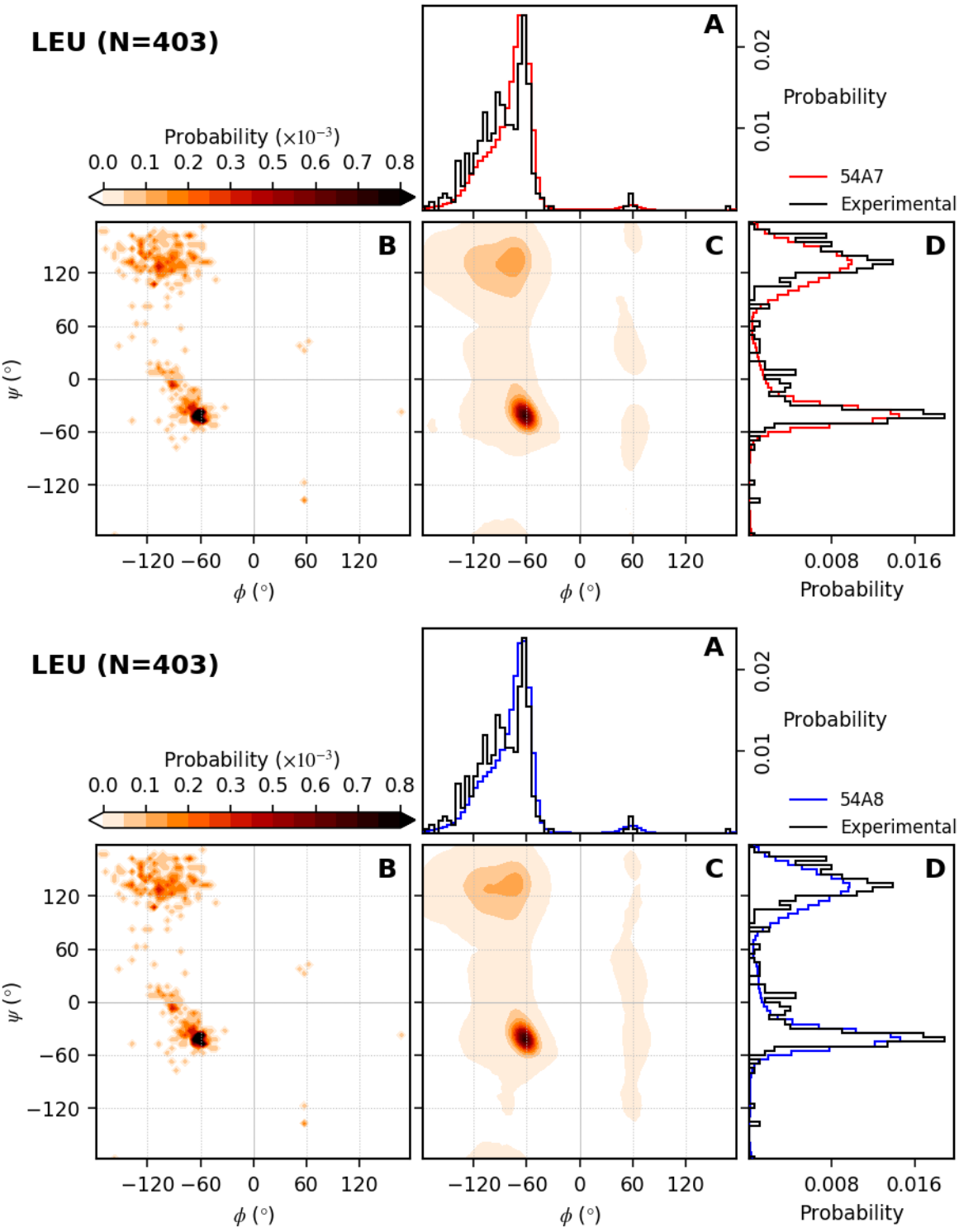
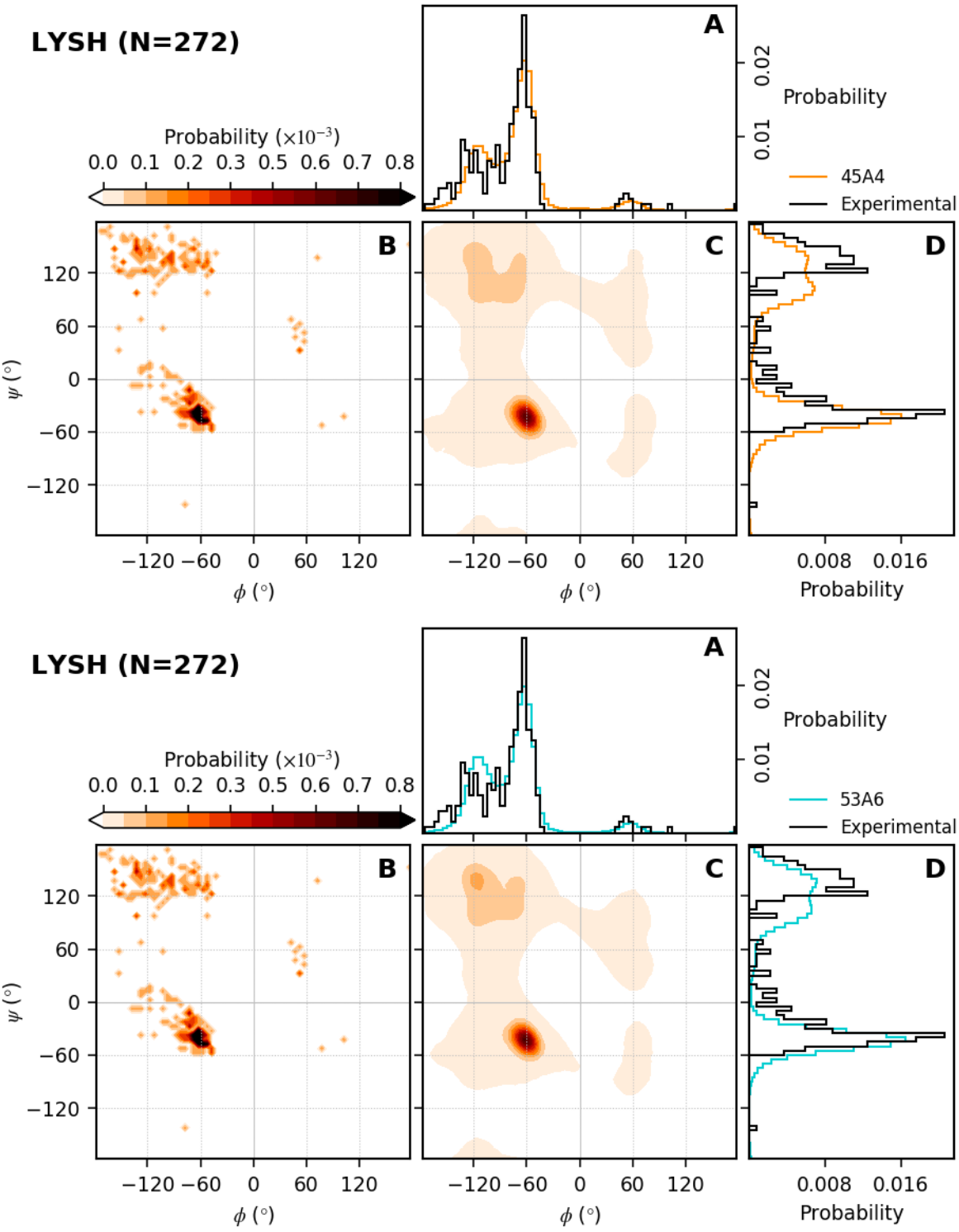


Figure S16. Distribution of leucine (LEU) backbone dihedral angles.


LYSH (N=272)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability
LYSH (N=272)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability

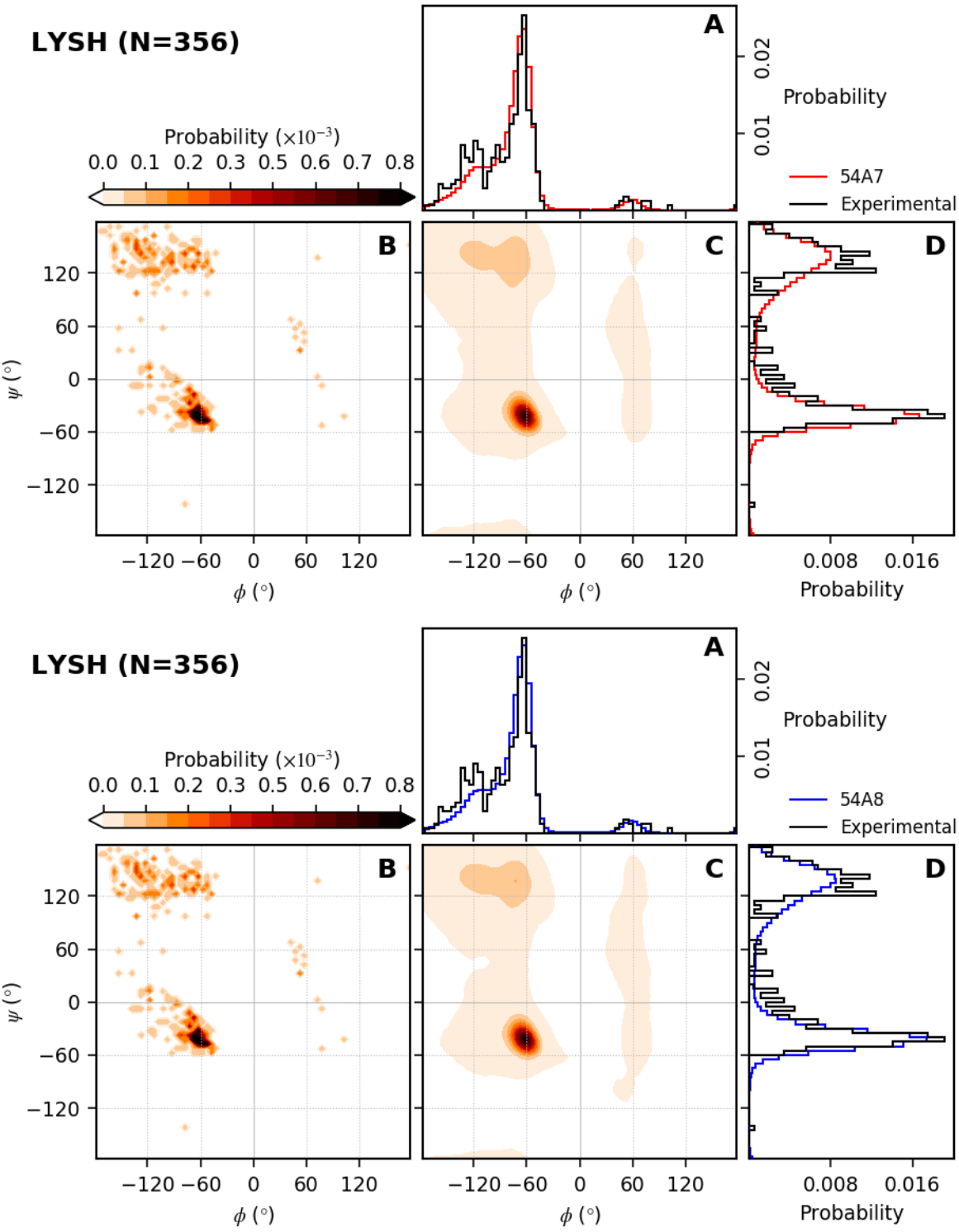
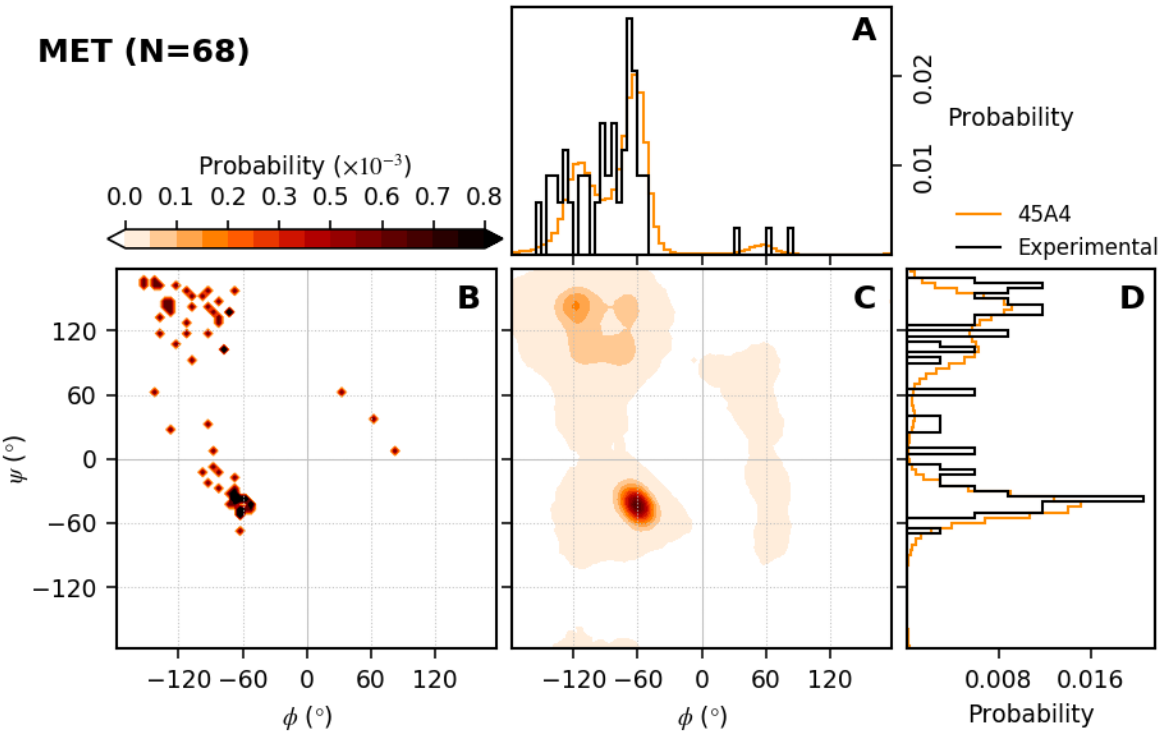
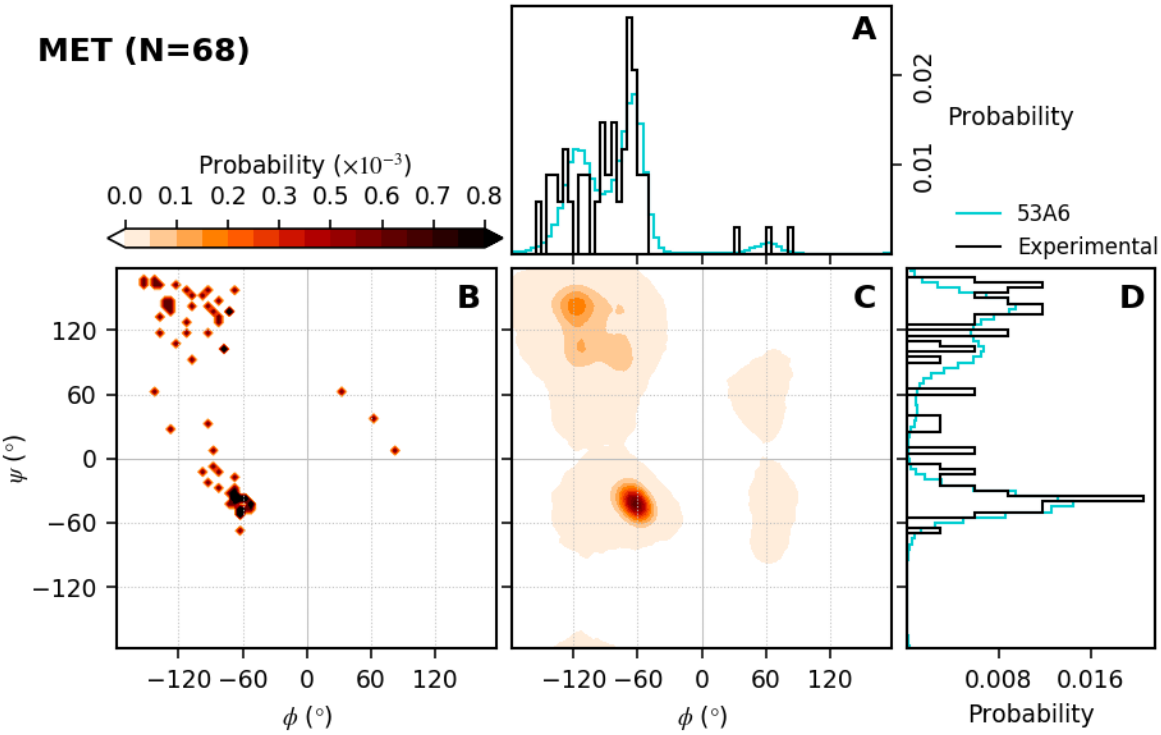


Figure S17. Distribution of lysine with +1 formal charge (LYSH) backbone dihedral angles.


MET (N=68)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability


MET (N=68)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability

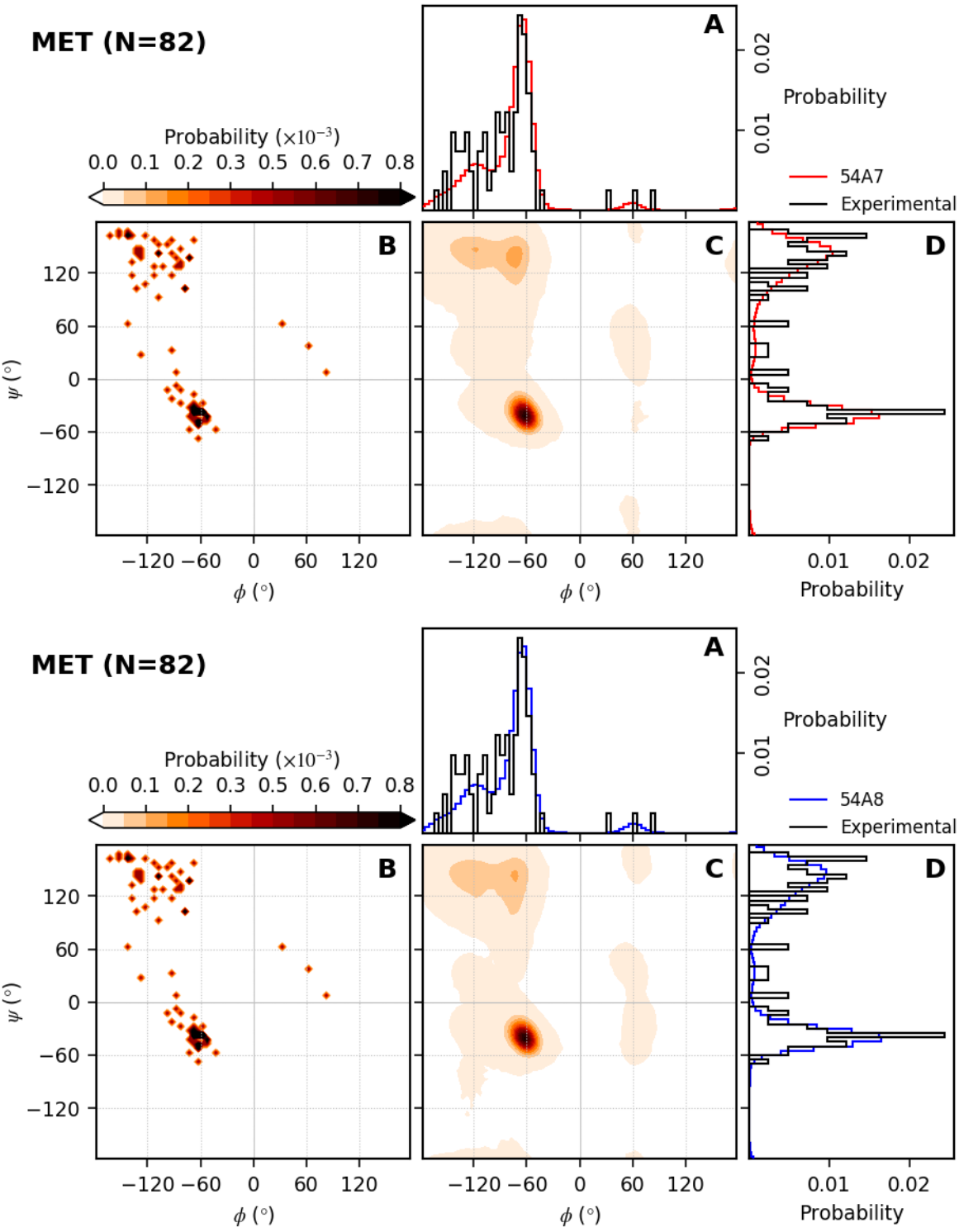
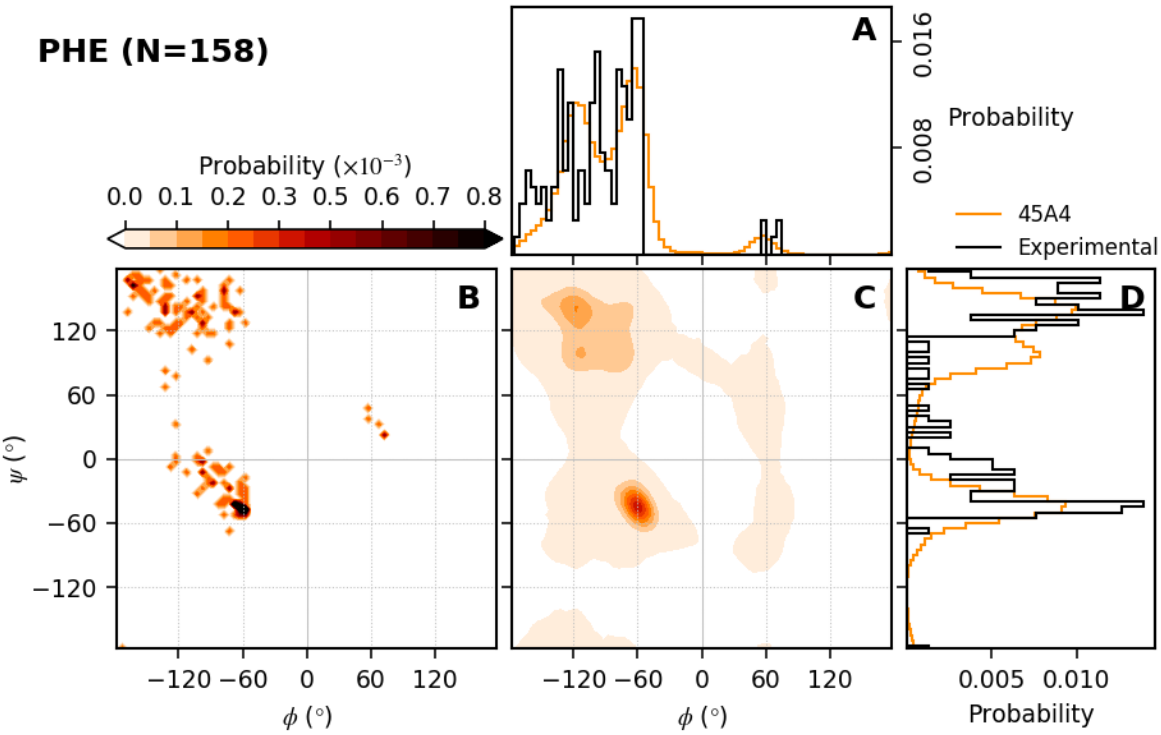
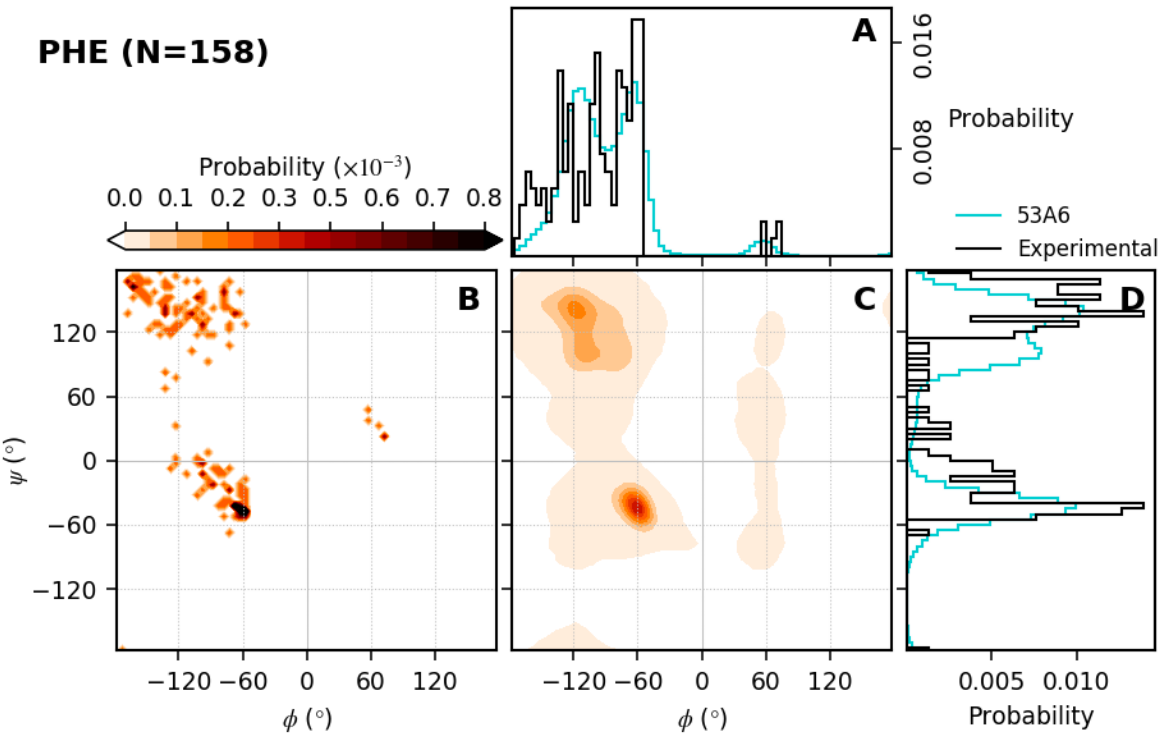


Figure S18. Distribution of methionine (MET) backbone dihedral angles.


PHE (N=158)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.016
0.008
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.005 0.010
Probability


PHE (N=158)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.016
0.008
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.005 0.010
Probability

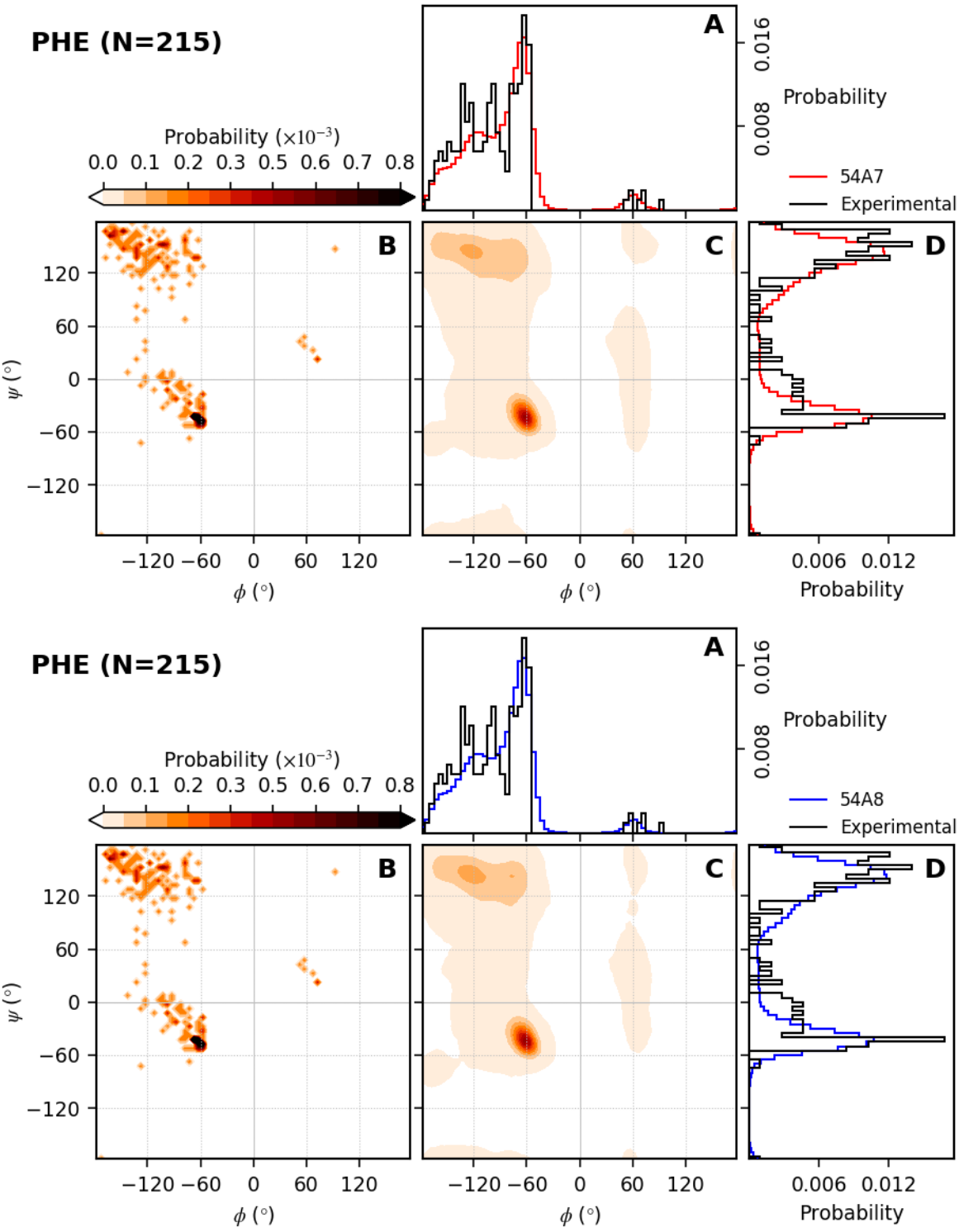
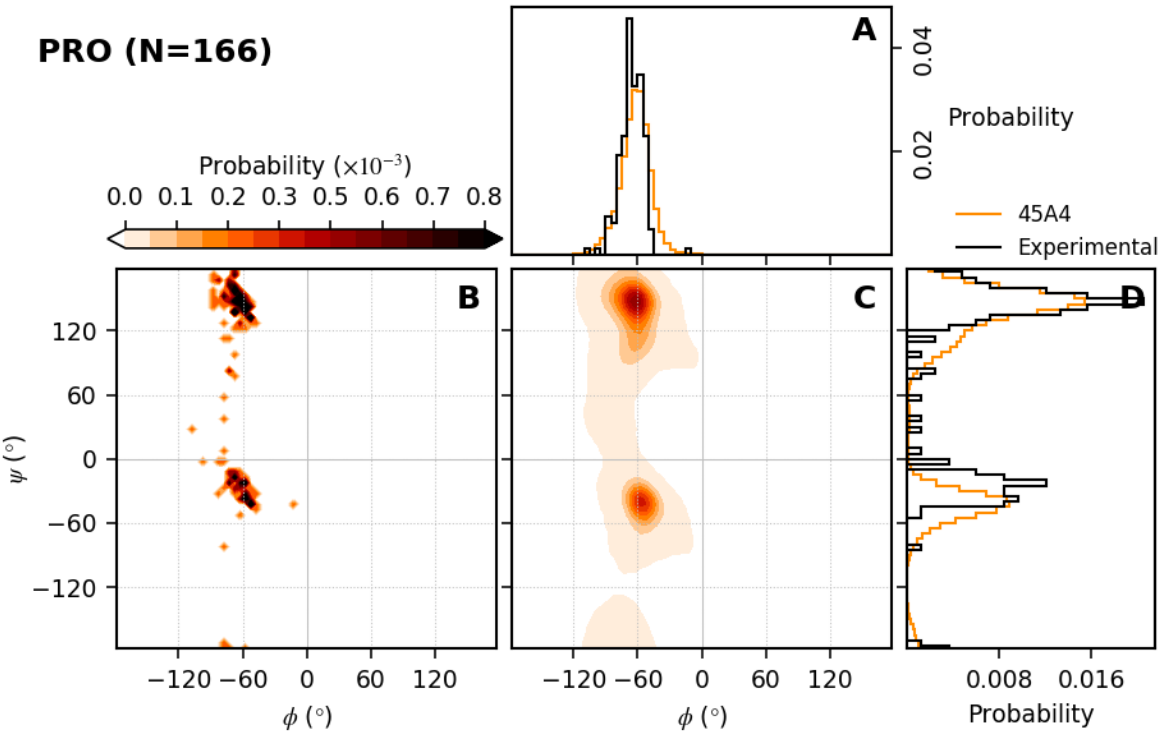
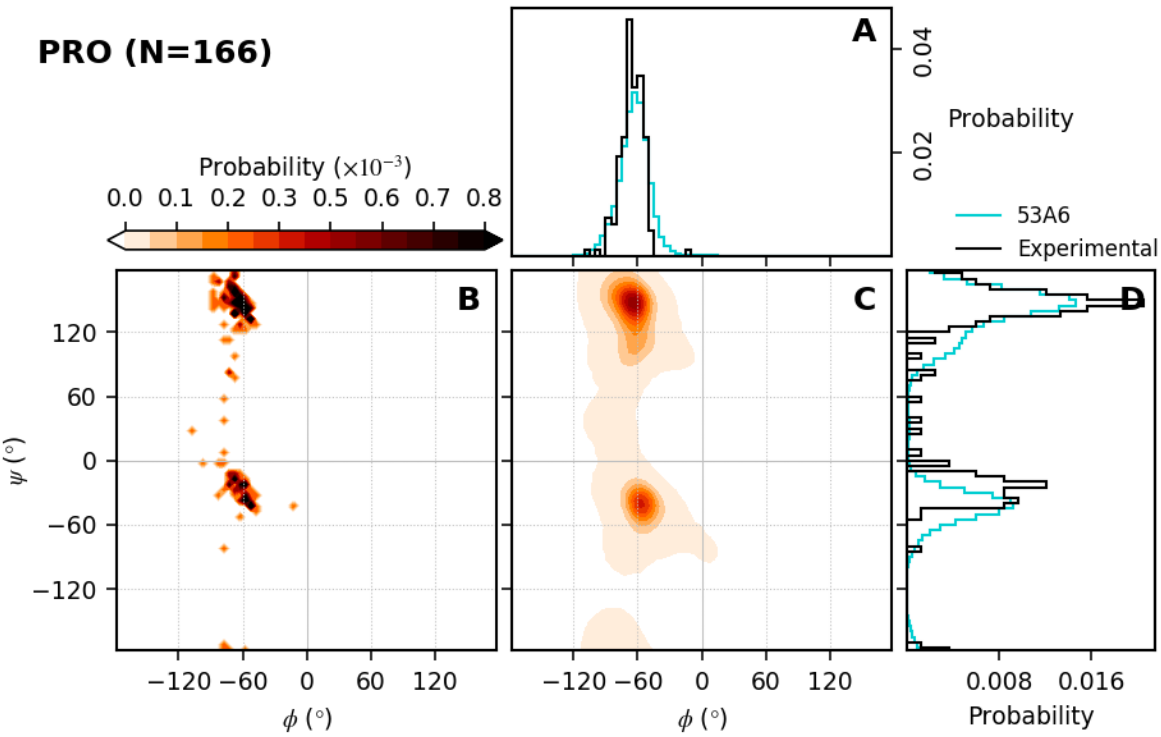


Figure S19. Distribution of phenylalanine (PHE) backbone dihedral angles.


PRO (N=166)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.04
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability


PRO (N=166)
A
B
C
D
Probability ($\times 10^{-3}$)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.04
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability

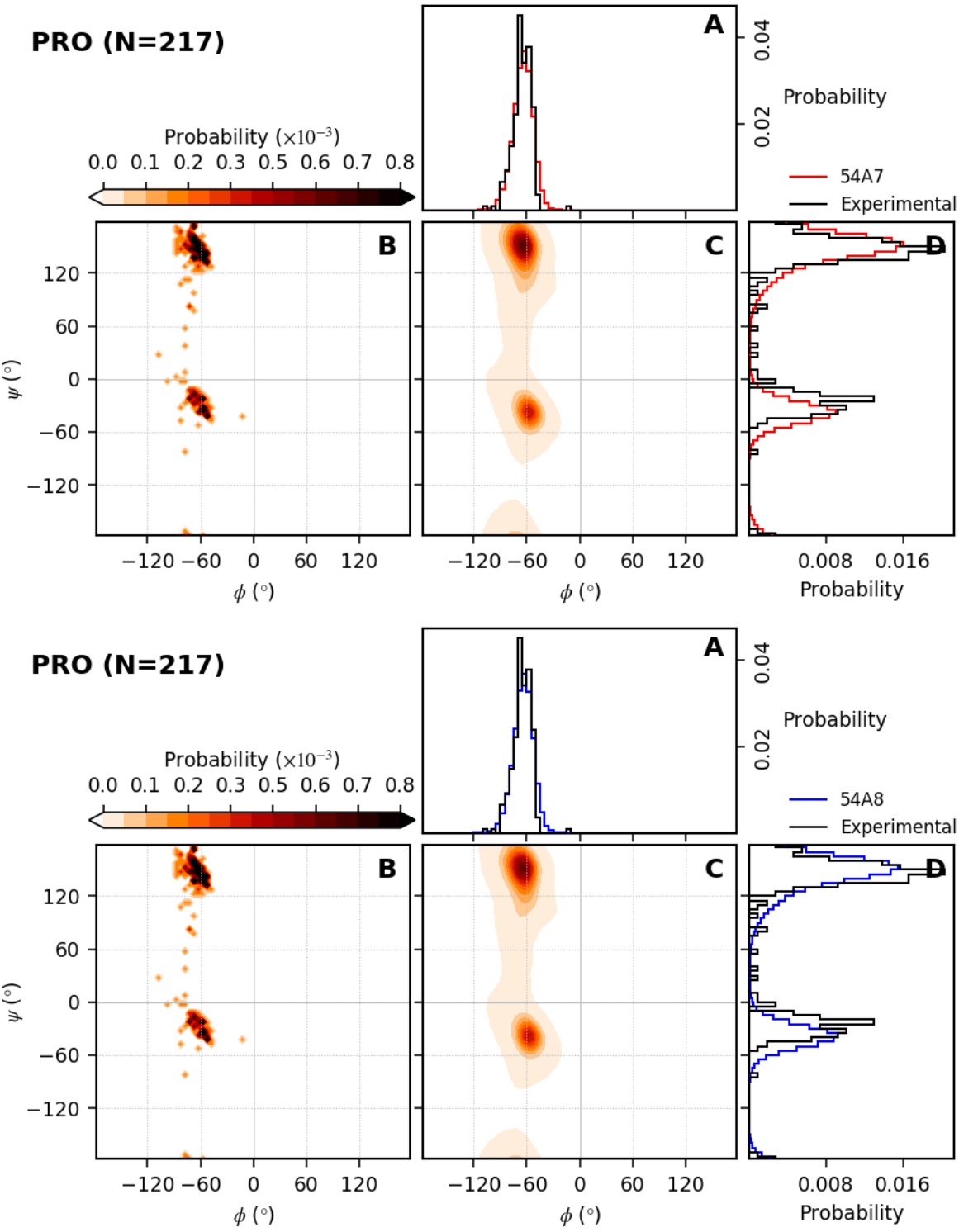
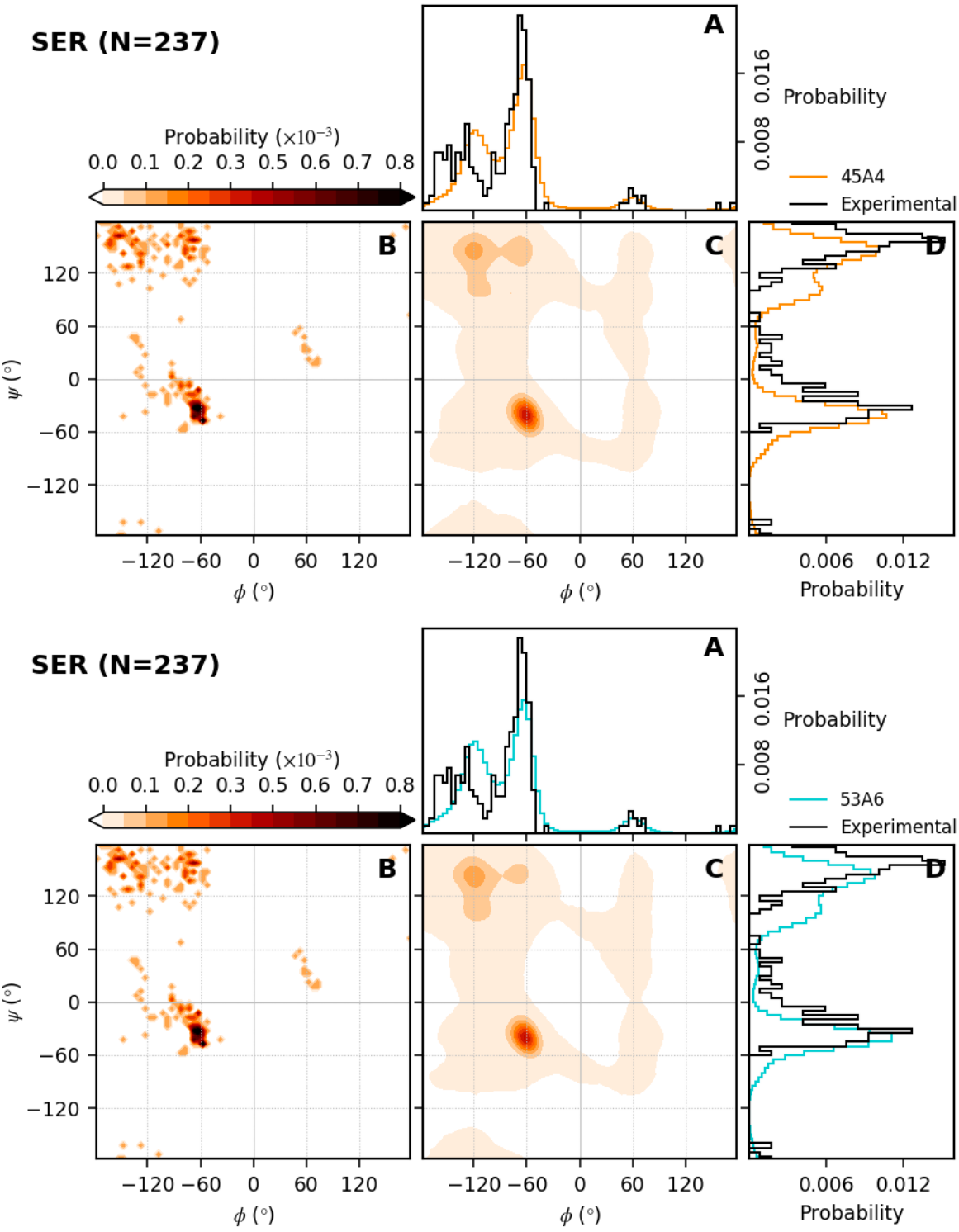


Figure S20. Distribution of proline (PRO) backbone dihedral angles.


SER (N=237)
A
Probability
0.008 0.016
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
45A4
Experimental
B
C
D
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.006 0.012
Probability
SER (N=237)
A
Probability
0.008 0.016
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
53A6
Experimental
B
C
D
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.006 0.012
Probability

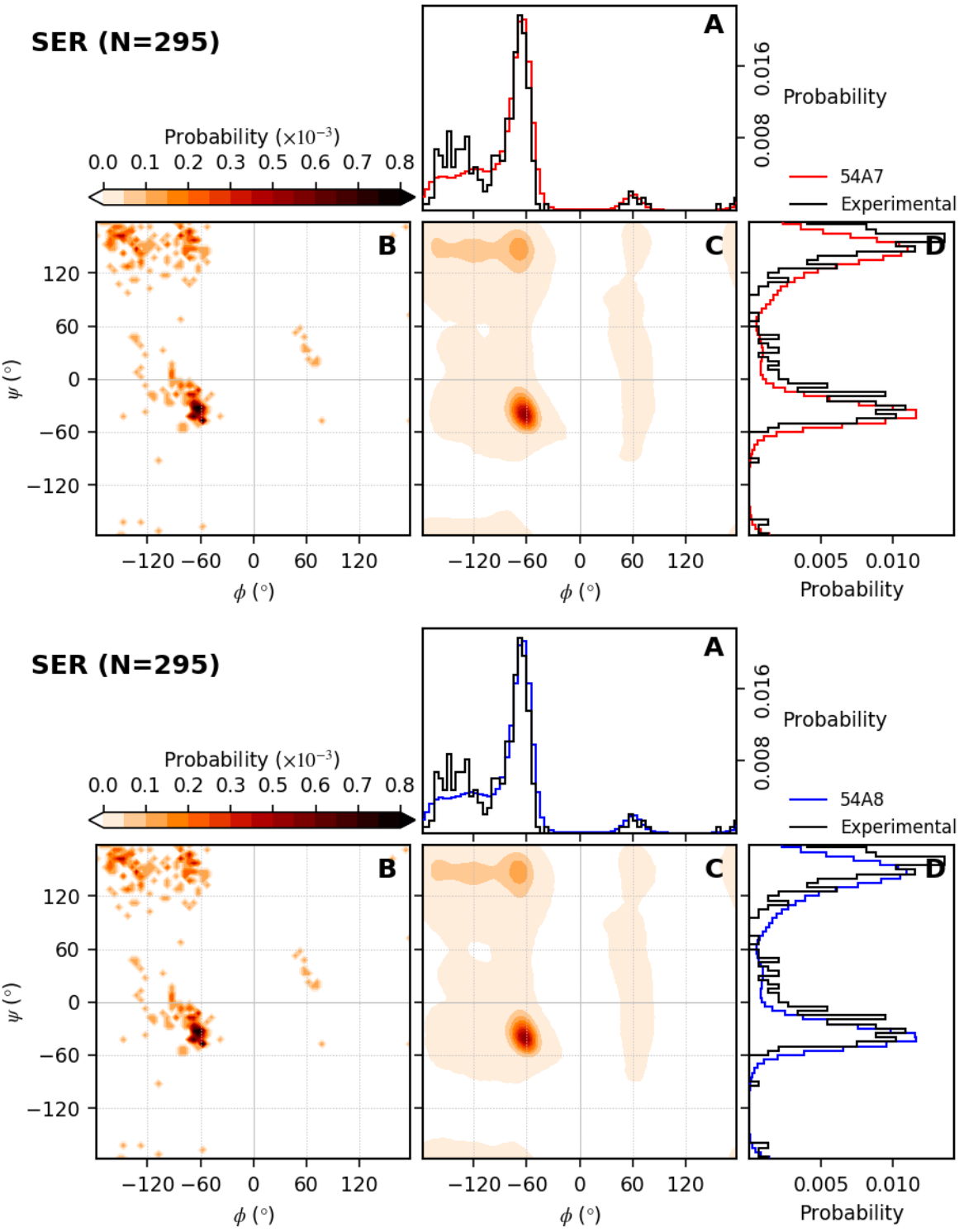
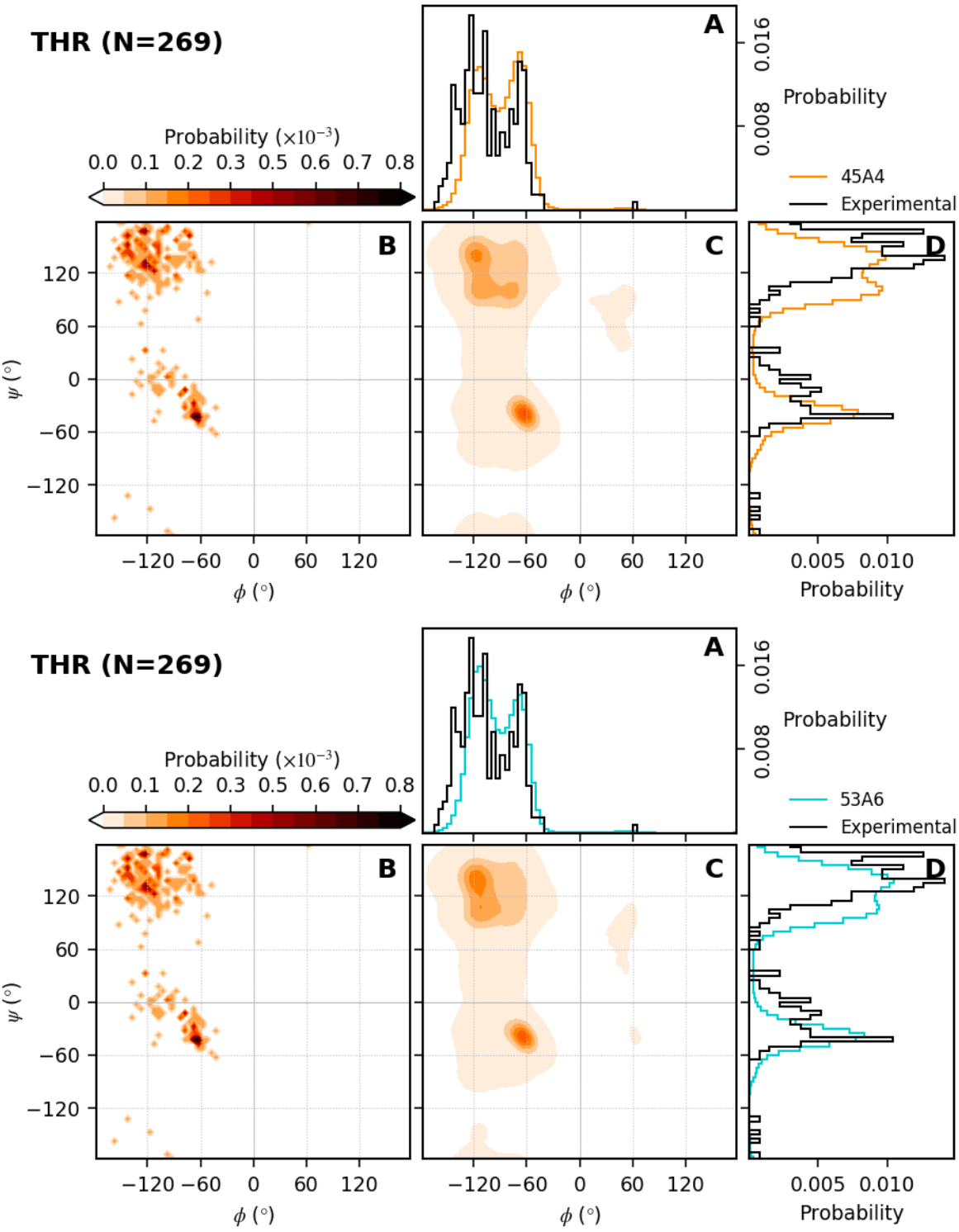


Figure S21. Distribution of serine (SER) backbone dihedral angles.


THR (N=269)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.008
0.016
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.005 0.010
Probability
THR (N=269)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.008
0.016
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.005 0.010
Probability

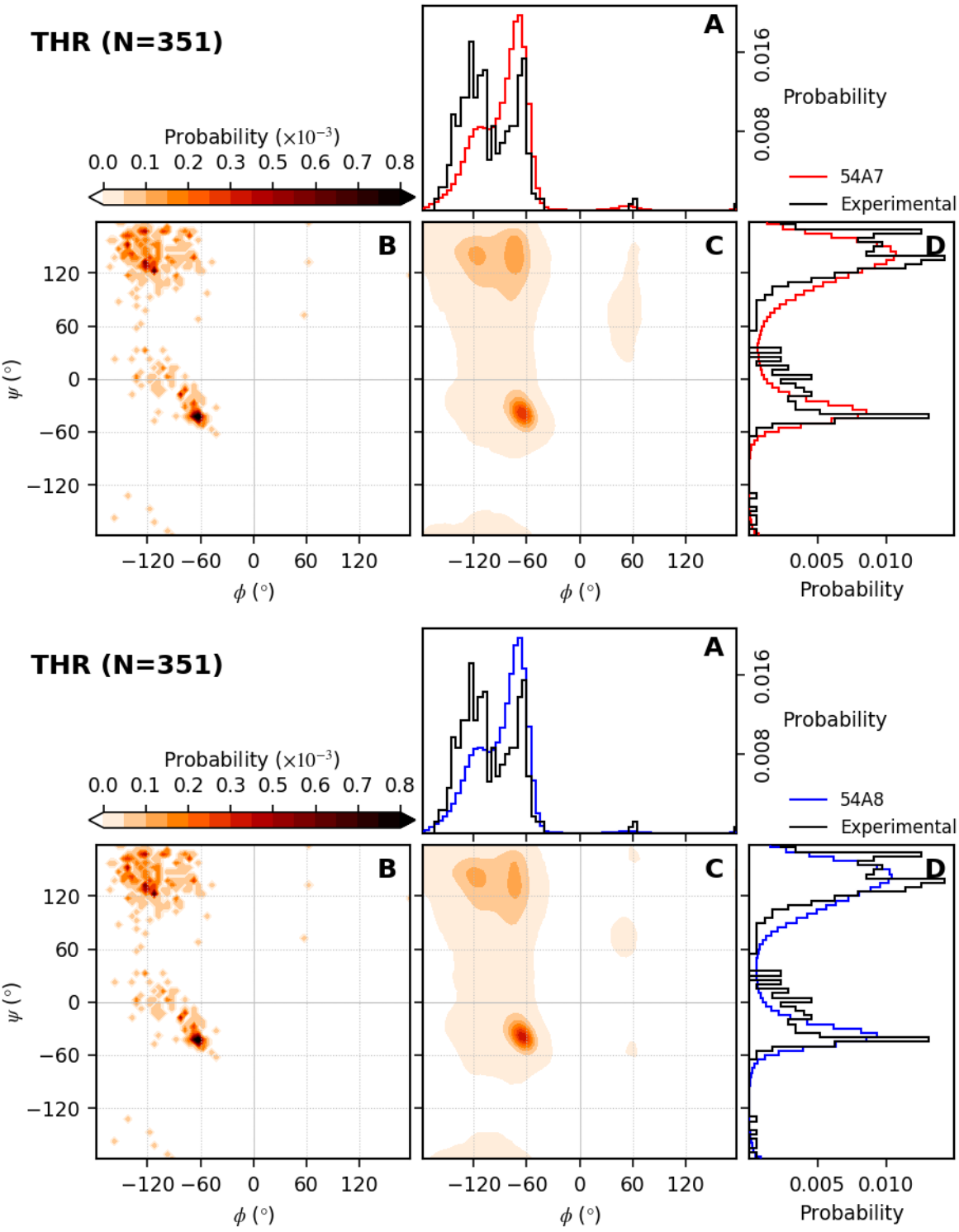
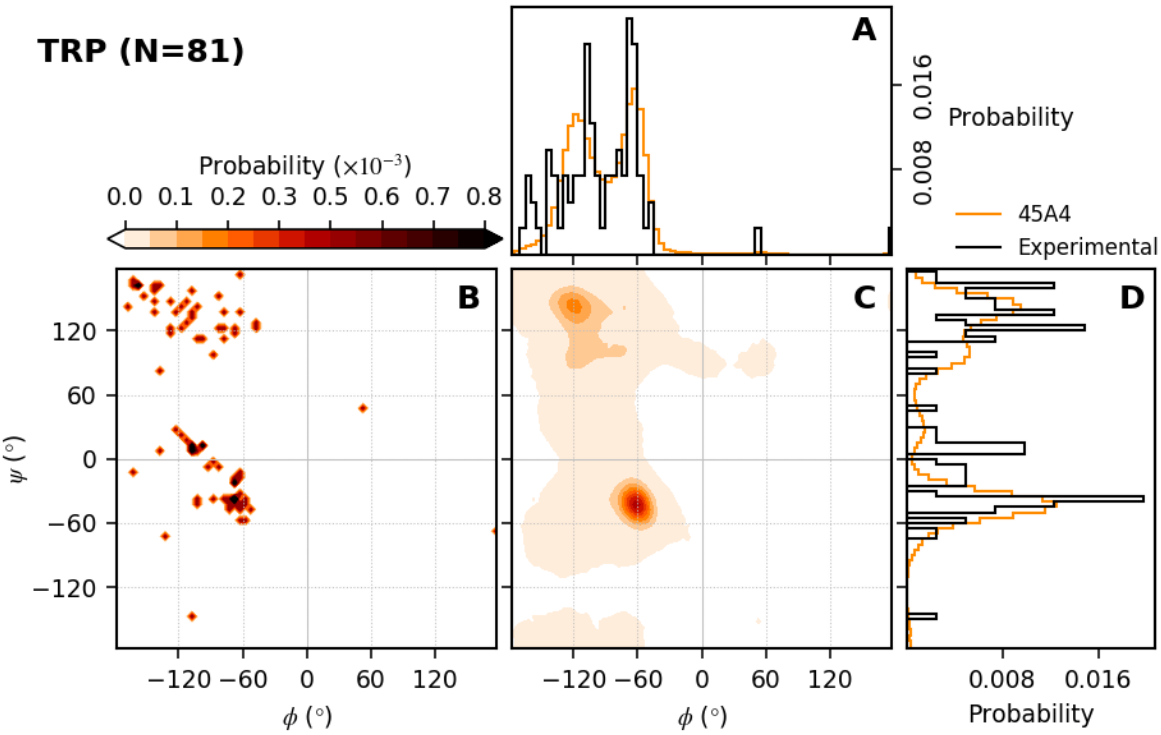
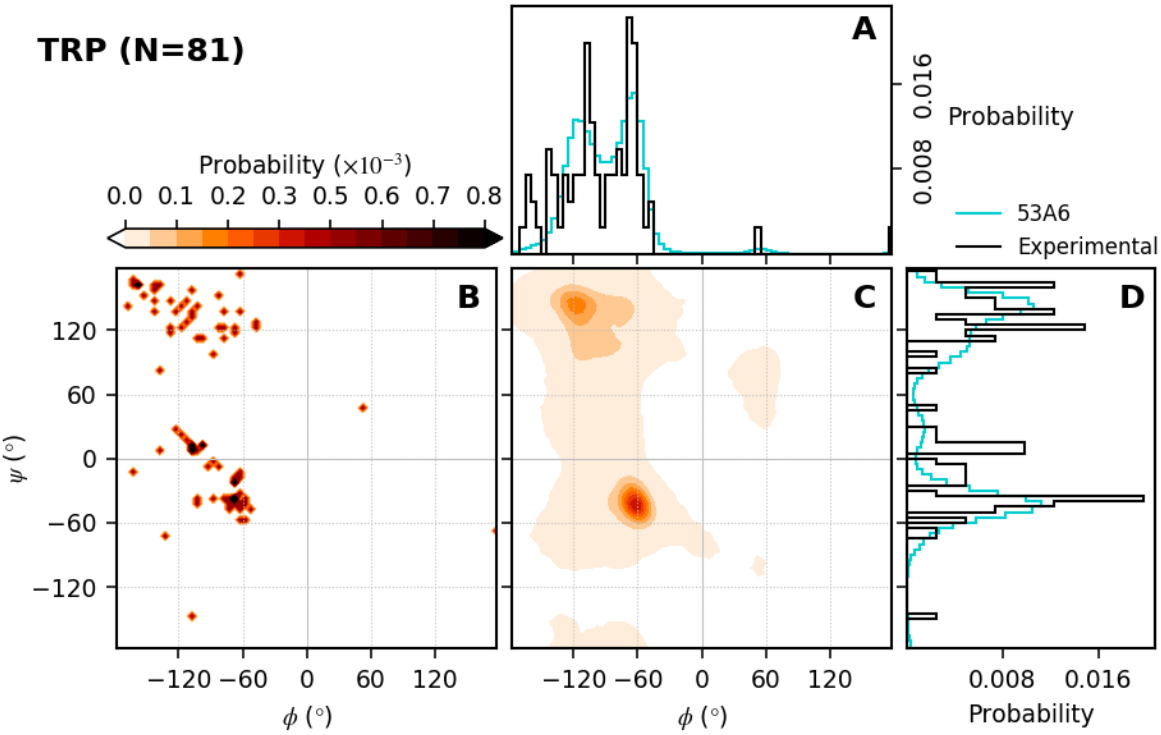


Figure S22. Distribution of threonine (THR) backbone dihedral angles.


TRP (N=81)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.008 0.016
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability


TRP (N=81)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.008 0.016
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.008 0.016
Probability

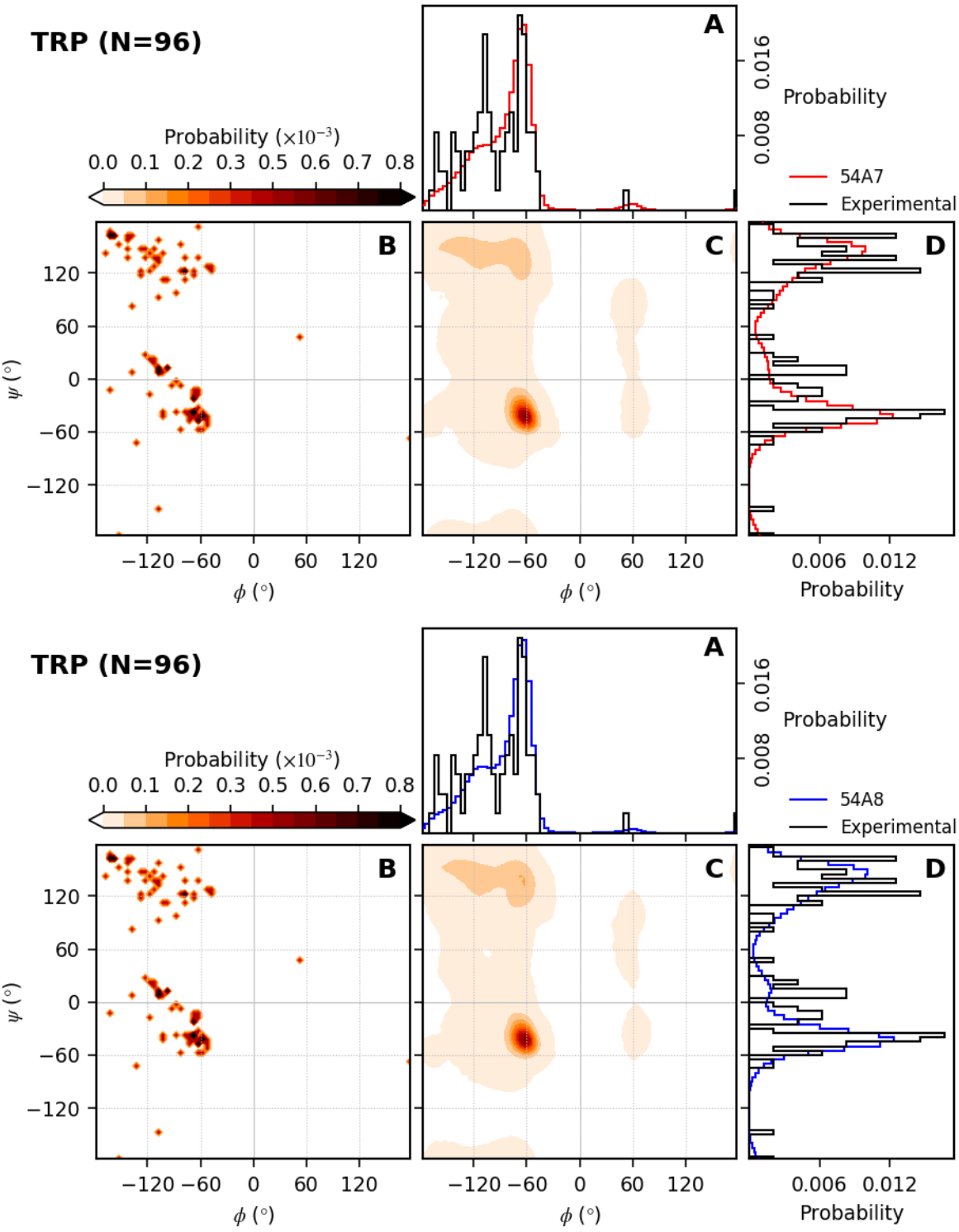
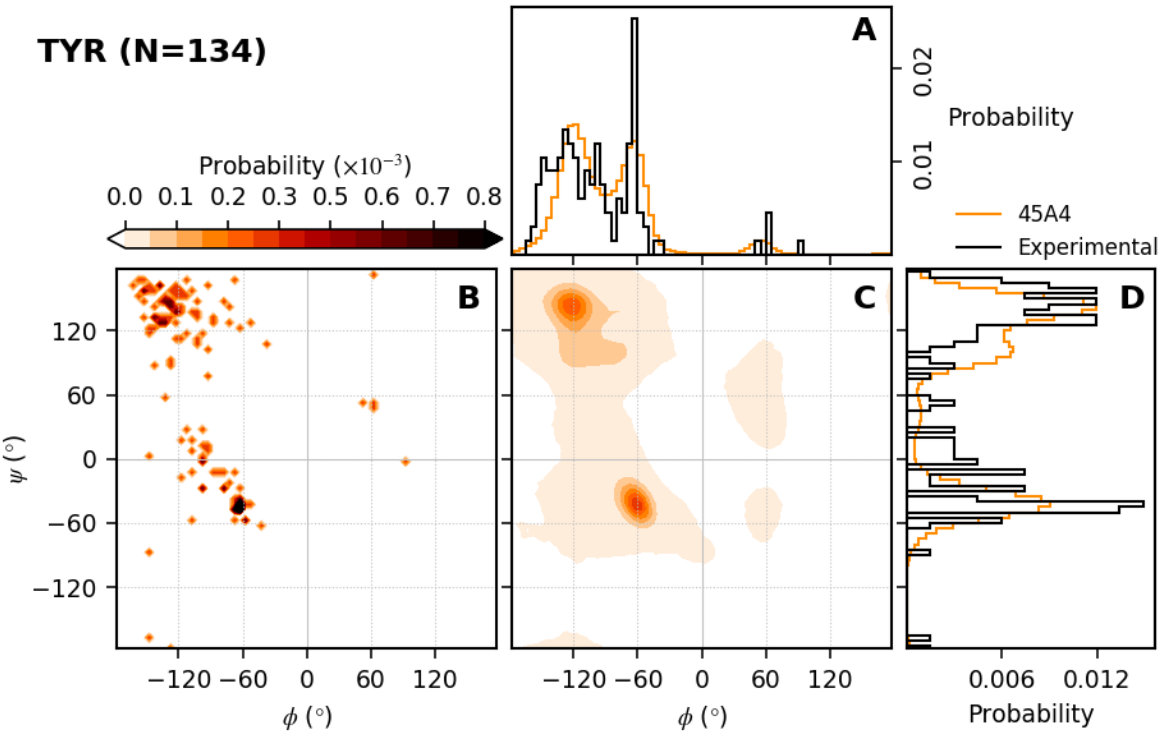
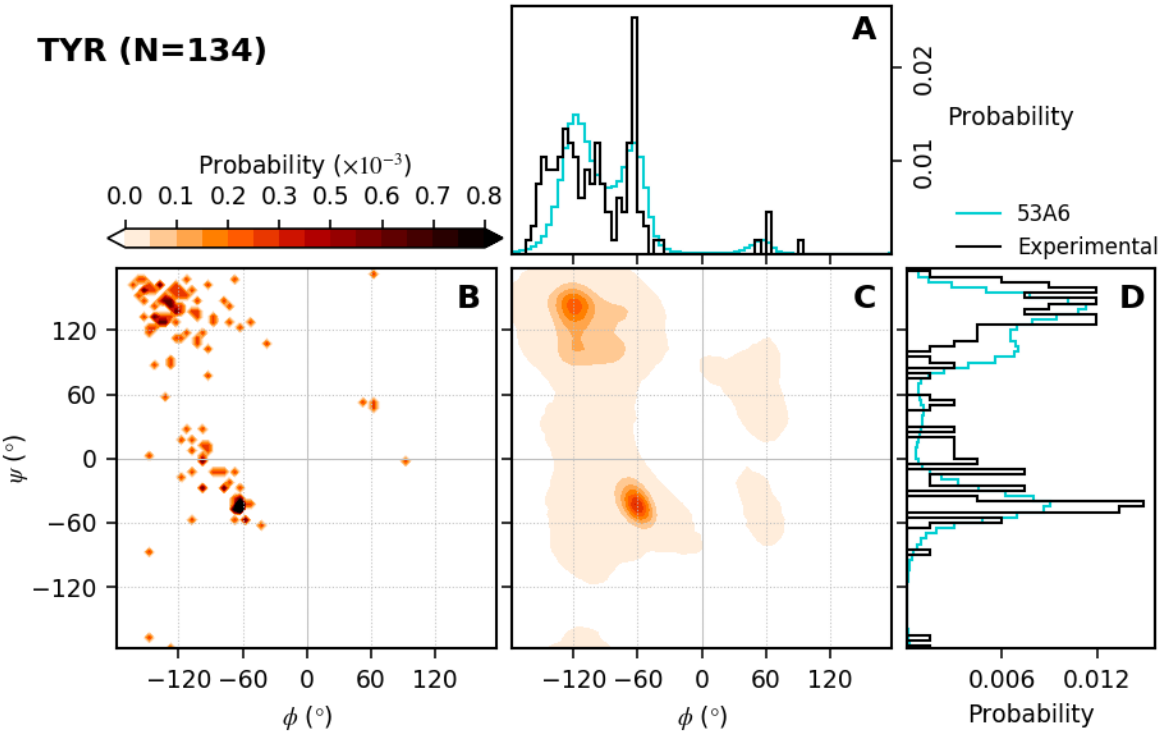


Figure S23. Distribution of tryptophan (TRP) backbone dihedral angles.


TYR (N=134)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.006 0.012
Probability


TYR (N=134)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.01
0.02
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.006 0.012
Probability

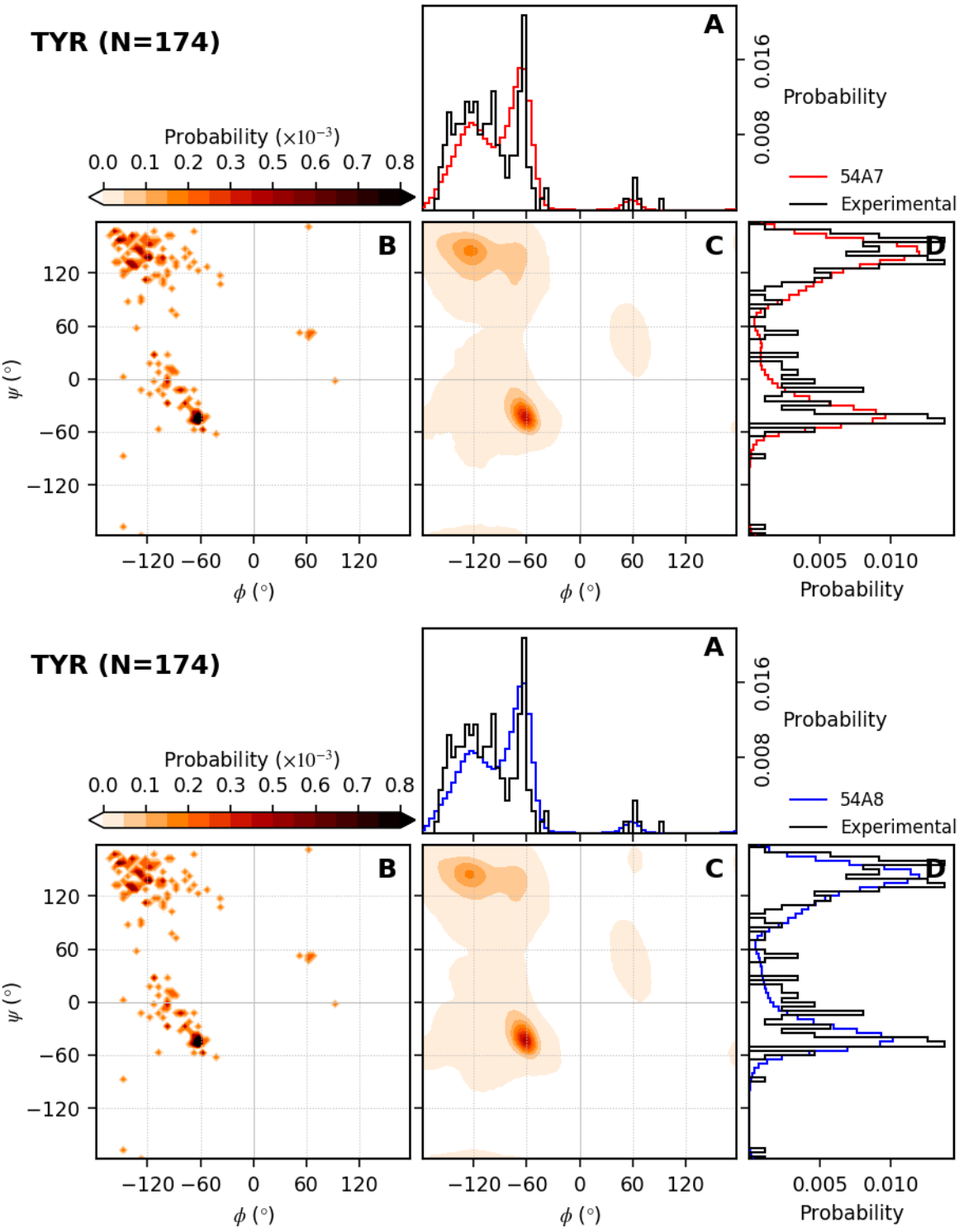
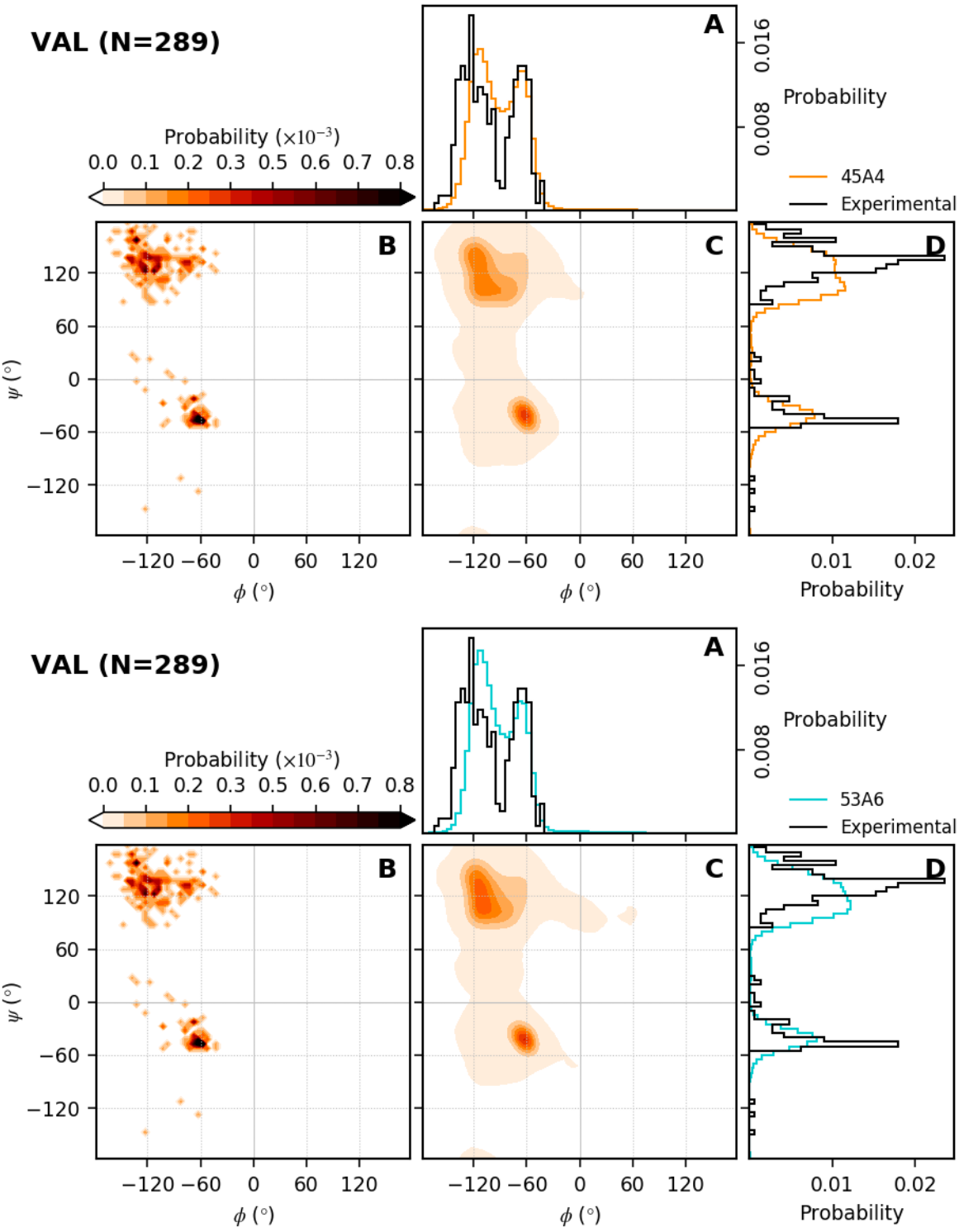


Figure S24. Distribution of tyrosine (TYR) backbone dihedral angles.


VAL (N=289)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.016
0.008
45A4
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.01 0.02
Probability
VAL (N=289)
A
B
C
D
Probability (×10⁻³)
0.0 0.1 0.2 0.3 0.5 0.6 0.7 0.8
Probability
0.016
0.008
53A6
Experimental
120
60
0
−60
−120
ψ (°)
−120 −60 0 60 120
ϕ (°)
0.01 0.02
Probability

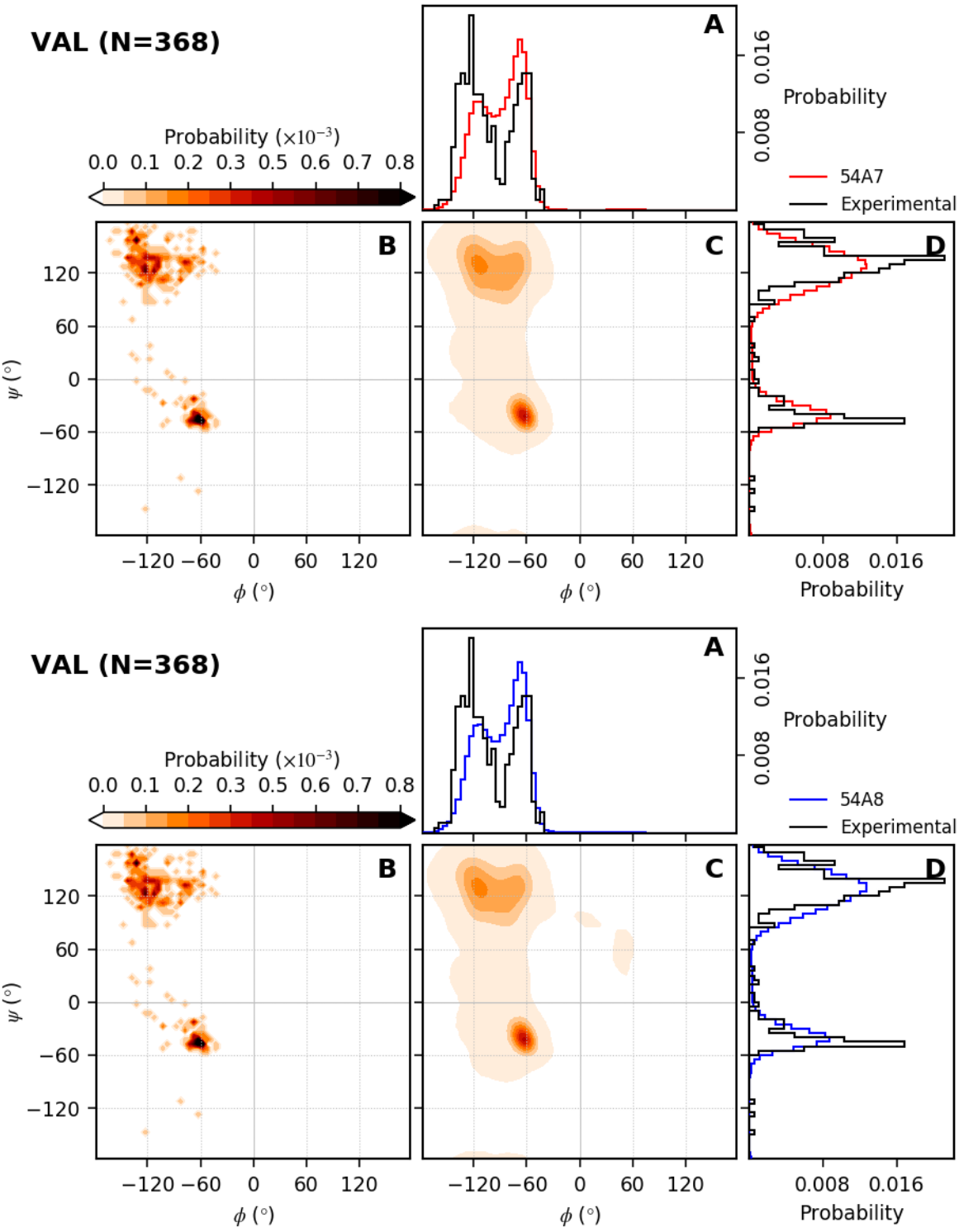


Figure S25. Distribution of valine (VAL) backbone dihedral angles.