molecules

MDPI

Supporting Information

Naive Prediction of Protein Backbone Phi and Psi Dihedral Angles Using Deep Learning

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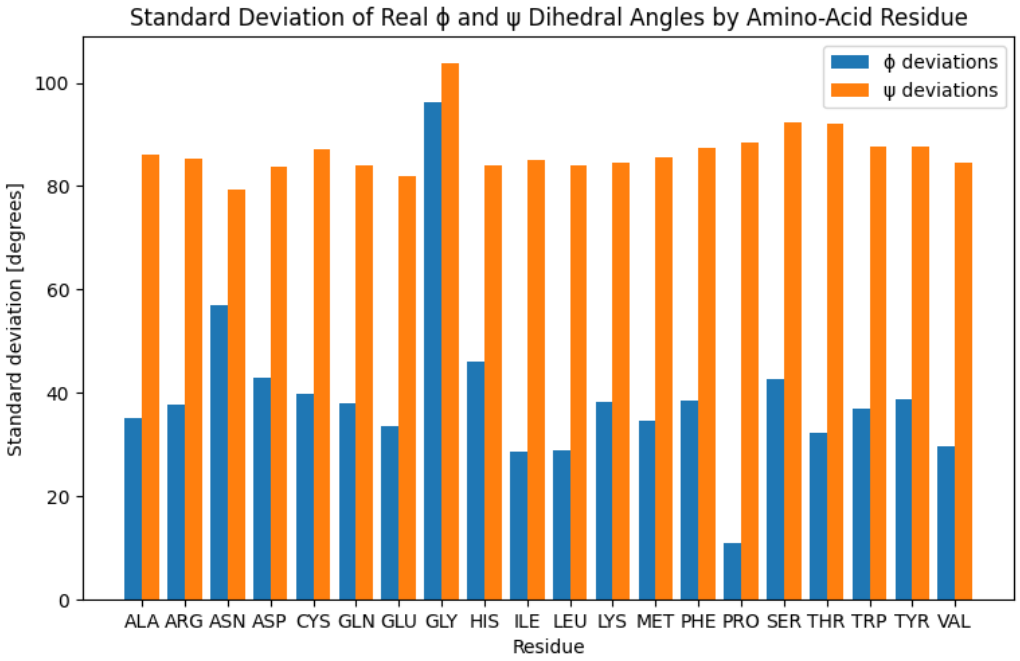
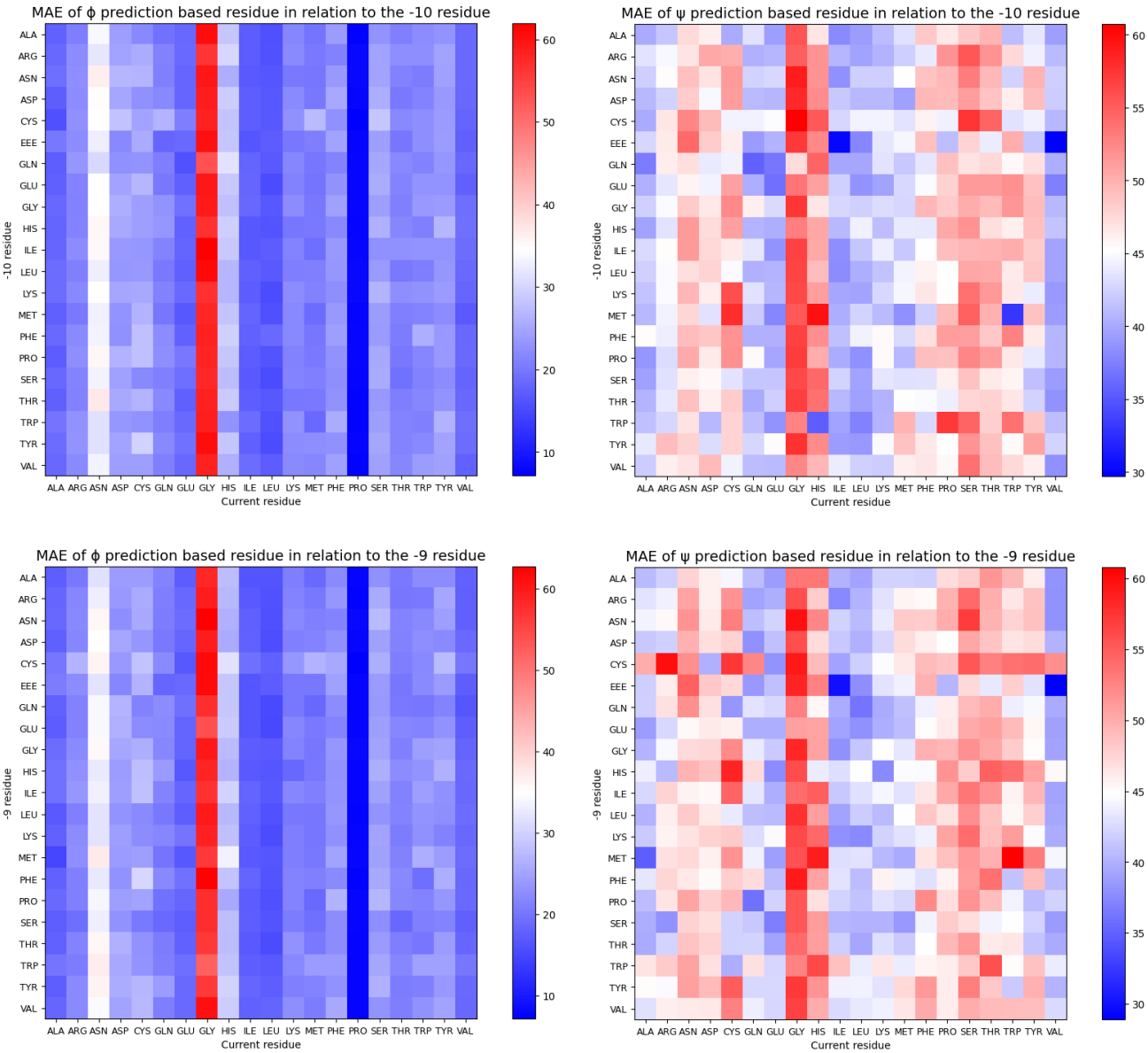


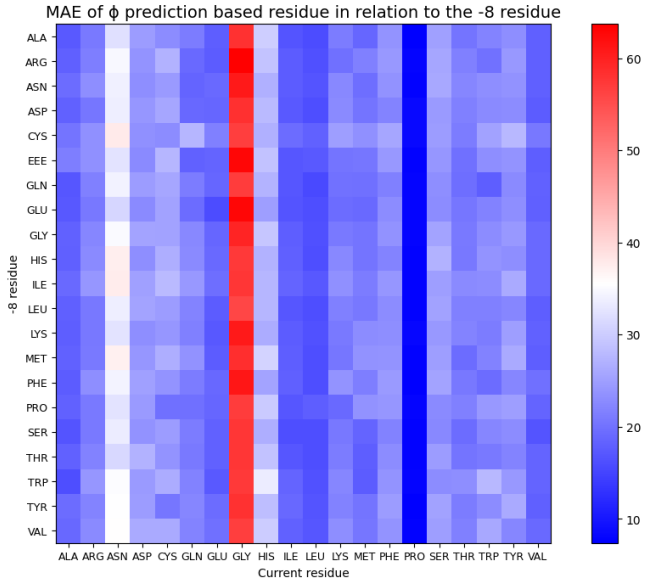
Figure S1. A bar graph of standard deviations of real ϕ and ψ angles in the entire dataset by amino-acid residue.

Table S1. Exact values of standard deviations of real ϕ and ψ angles in the train and test datasets.

Amino-acid residue	φ	Ψ
ALA	35.60	86.03
ARG	38.43	85.36
ASN	57.24	79.45
ASP	43.04	82.89
CYS	40.57	87.62
GLN	37.42	84.01
GLU	33.40	81.83
GLY	**96.21**	**103.41**
HIS	45.06	84.18
ILE	28.64	85.19
LEU	28.90	84.04
LYS	38.09	84.24

MET	34.79	85.69
PHE	38.23	87.17
PRO	**10.93**	88.23
SER	42.12	92.21
THR	31.99	92.51
TRP	36.87	87.83
TYR	38.62	87.47
VAL	29.85	84.83




MAE of ϕ prediction based residue in relation to the -8 residue
-8 residue
Current residue
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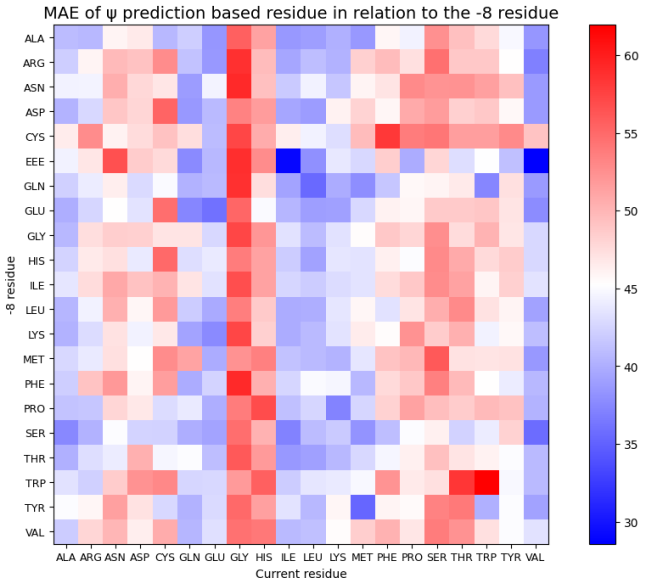
60
50
40
30
20
10


MAE of ψ prediction based residue in relation to the -8 residue
-8 residue
Current residue
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60
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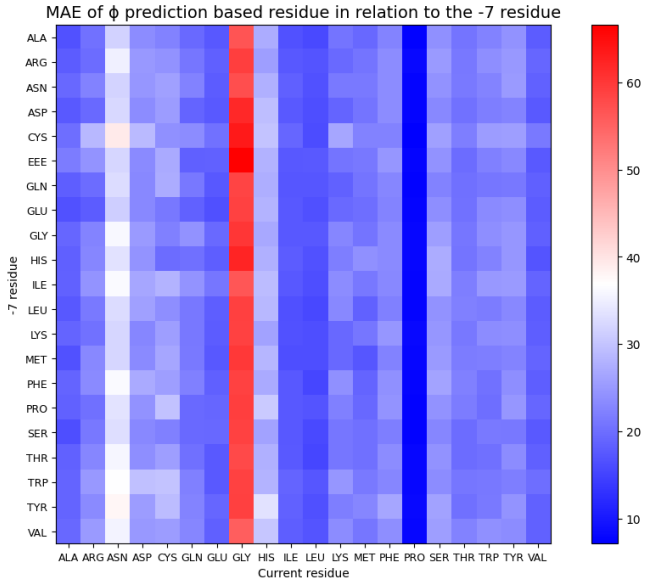
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-7 residue
Current residue
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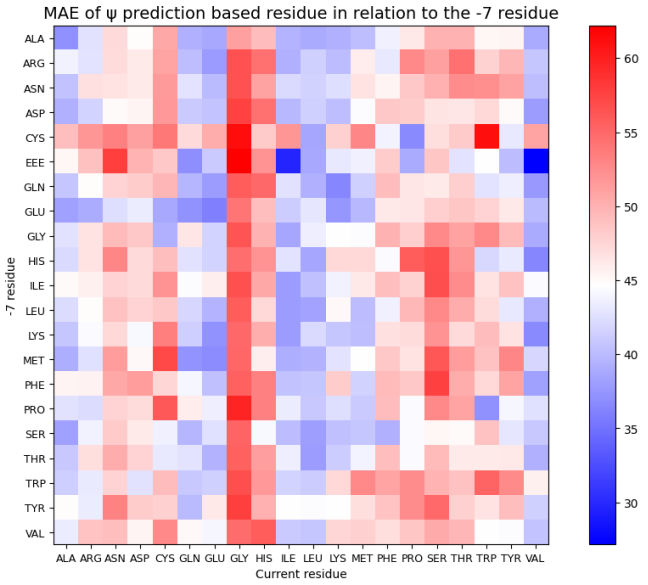
MAE of ψ prediction based residue in relation to the -7 residue
-7 residue
Current residue
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60
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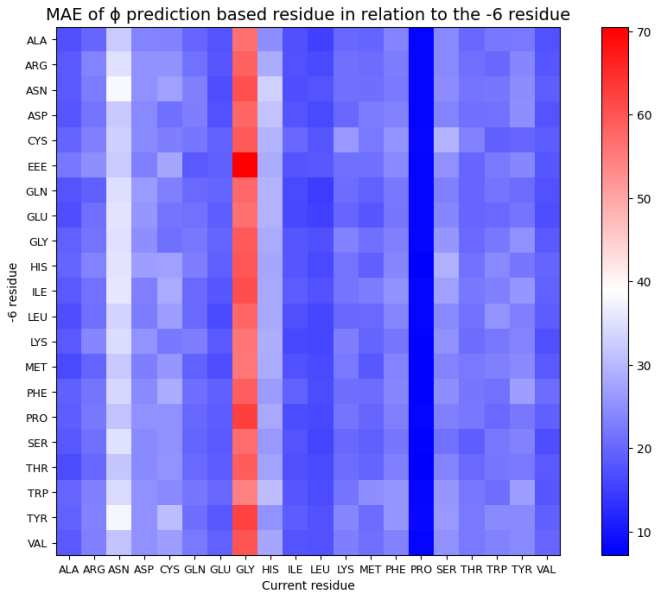
MAE of ϕ prediction based residue in relation to the -6 residue
-6 residue
Current residue
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70
60
50
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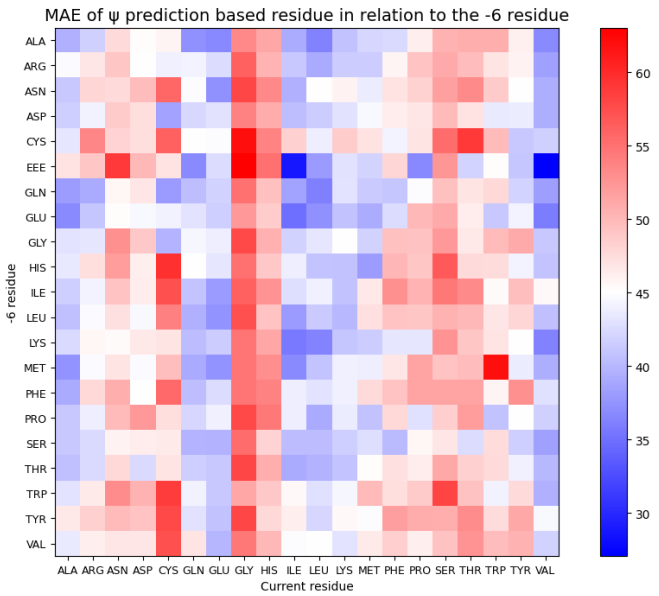
MAE of ψ prediction based residue in relation to the -6 residue
-6 residue
Current residue
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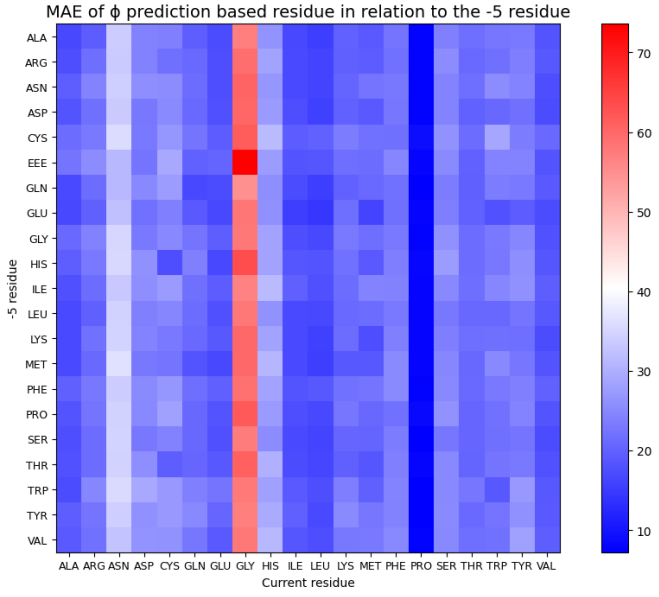
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-5 residue
Current residue
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70
60
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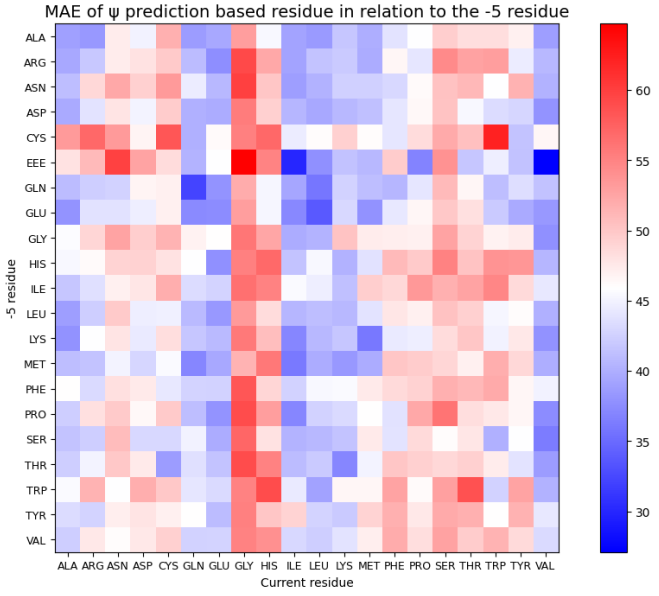
MAE of ψ prediction based residue in relation to the -5 residue
-5 residue
Current residue
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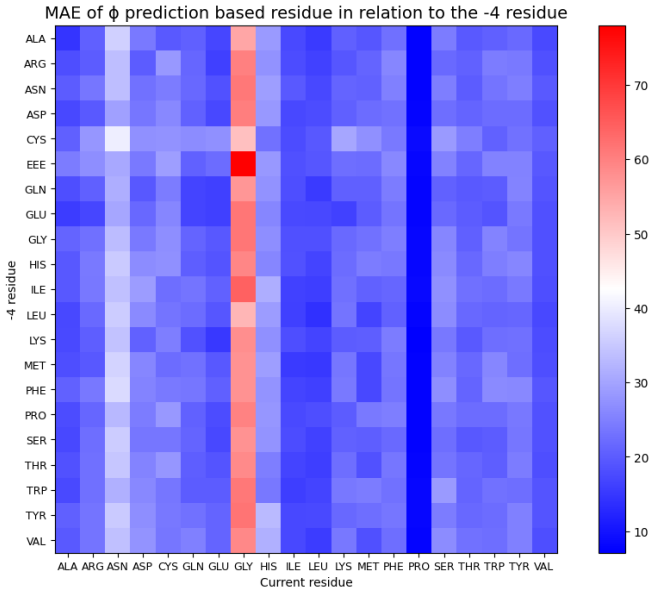
MAE of ϕ prediction based residue in relation to the -4 residue
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Current residue
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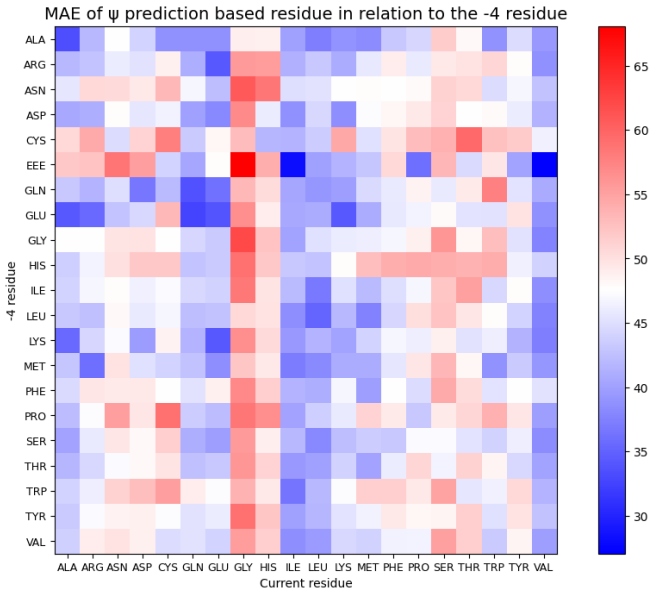
10 20 30 40 50 60 70


MAE of ψ prediction based residue in relation to the -4 residue
-4 residue
Current residue
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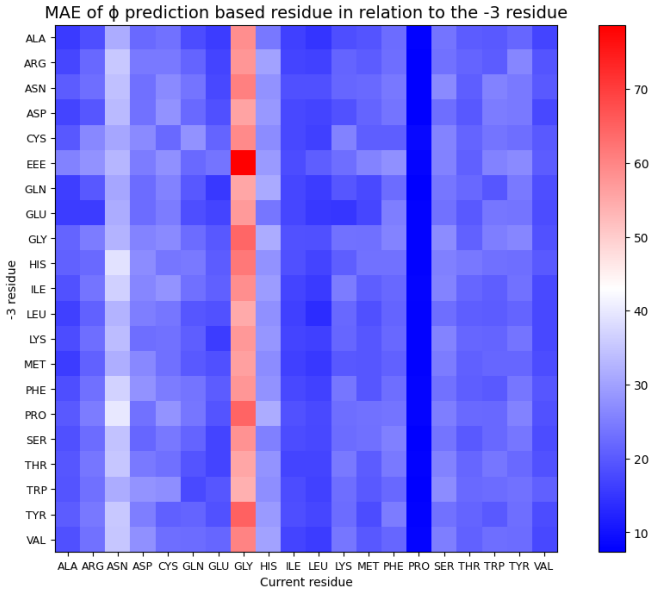
30 35 40 45 50 55 60 65


MAE of ϕ prediction based residue in relation to the -3 residue
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Current residue
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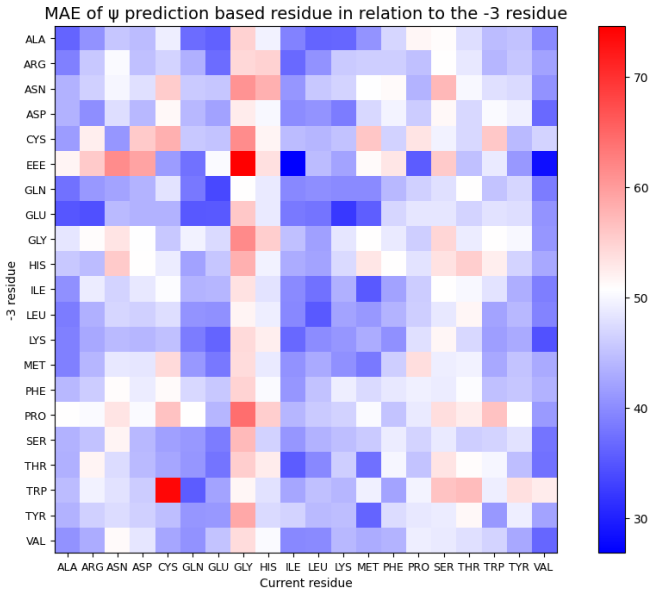
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-3 residue
Current residue
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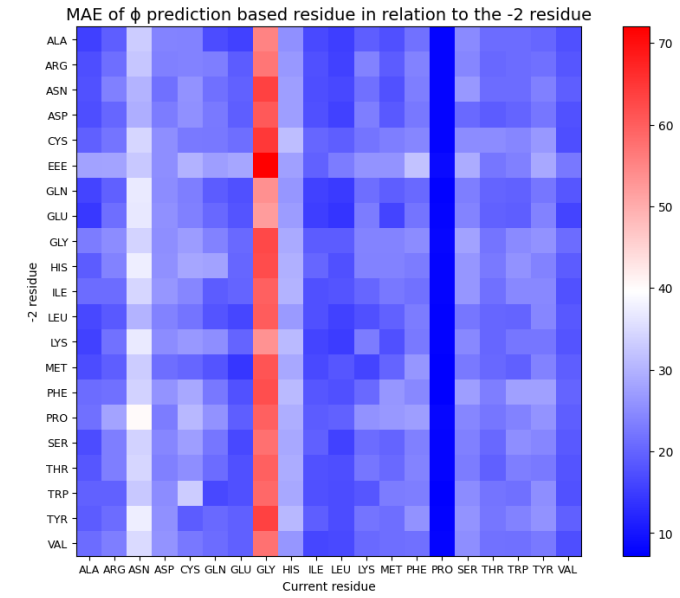
30 40 50 60 70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Current residue
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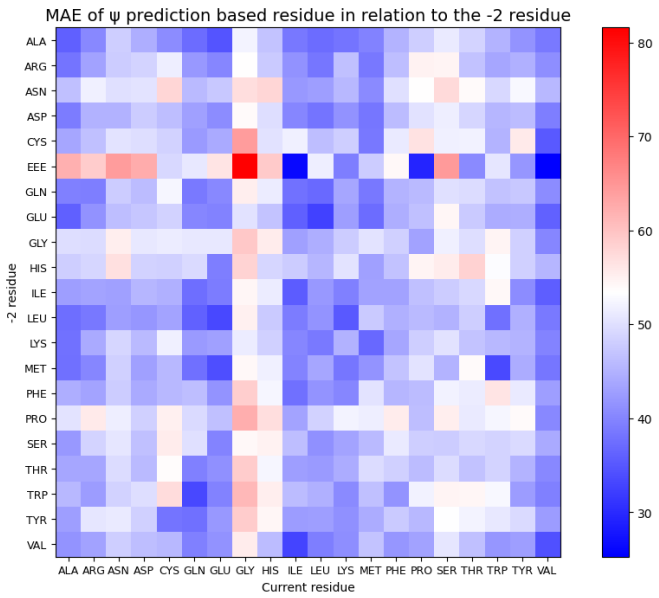
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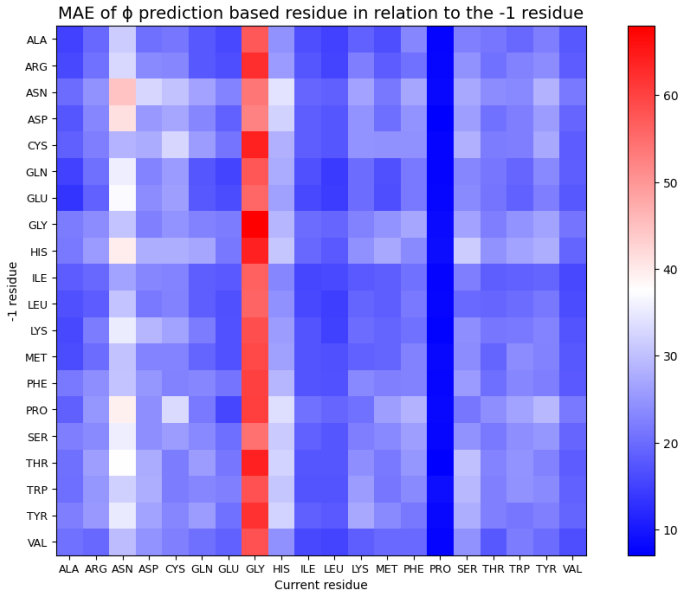
MAE of ϕ prediction based residue in relation to the -1 residue
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Current residue
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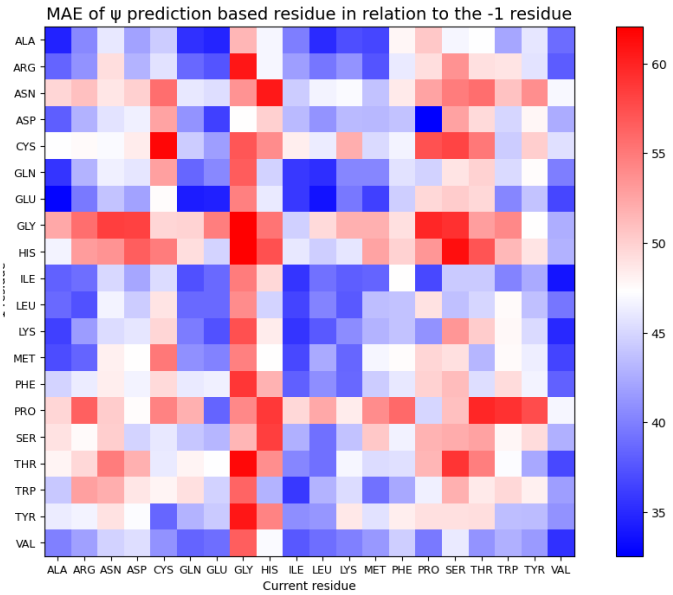
MAE of ψ prediction based residue in relation to the -1 residue
Current residue
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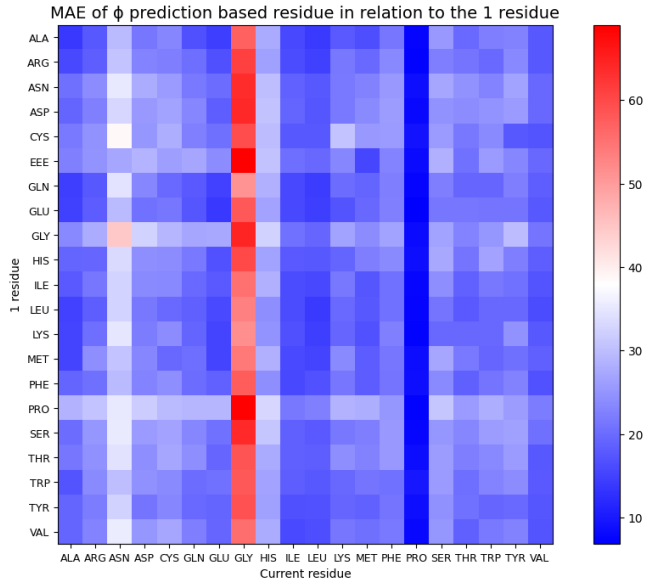
MAE of ϕ prediction based residue in relation to the 1 residue
1 residue
Current residue
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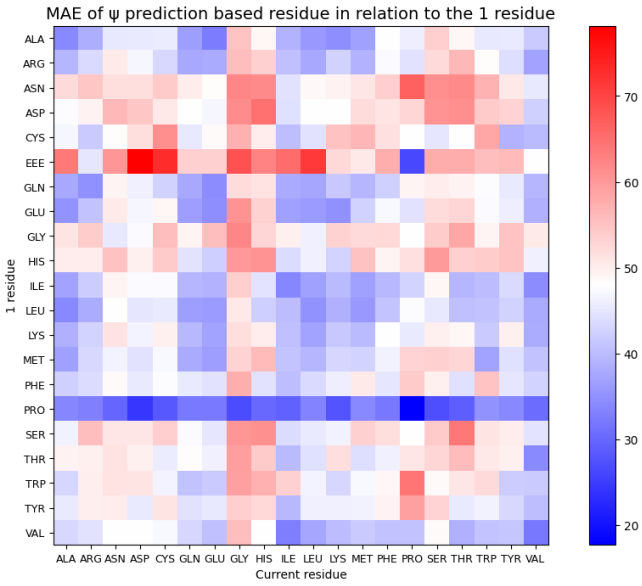
10 20 30 40 50 60


MAE of ψ prediction based residue in relation to the 1 residue
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Current residue
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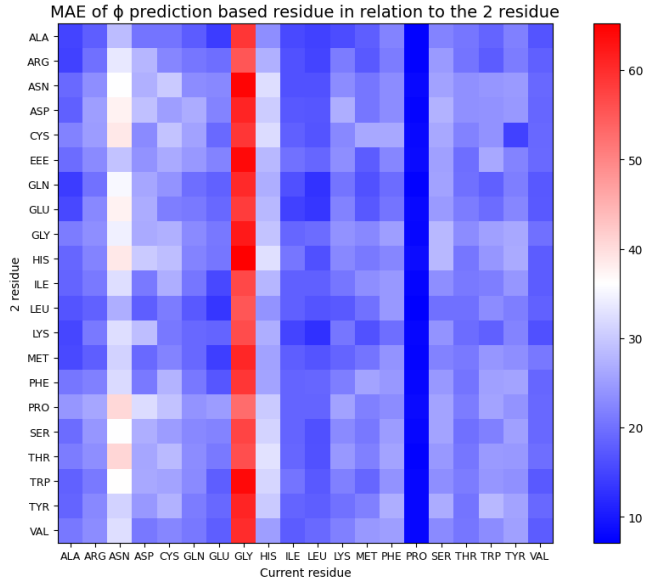
20 30 40 50 60 70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Current residue
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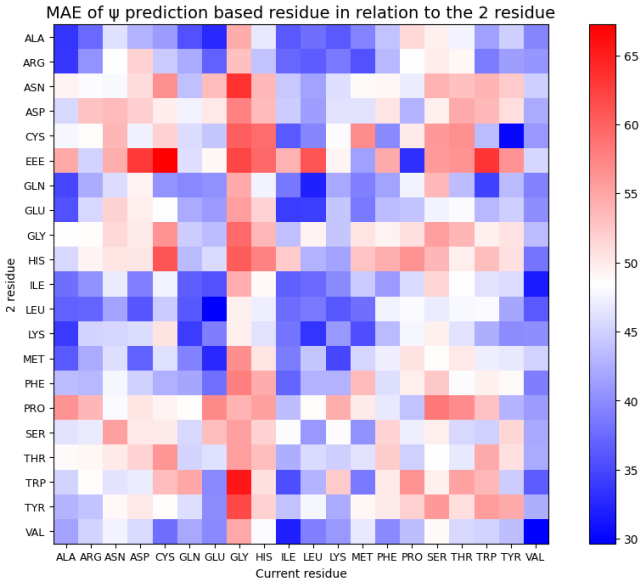
MAE of ψ prediction based residue in relation to the 2 residue
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Current residue
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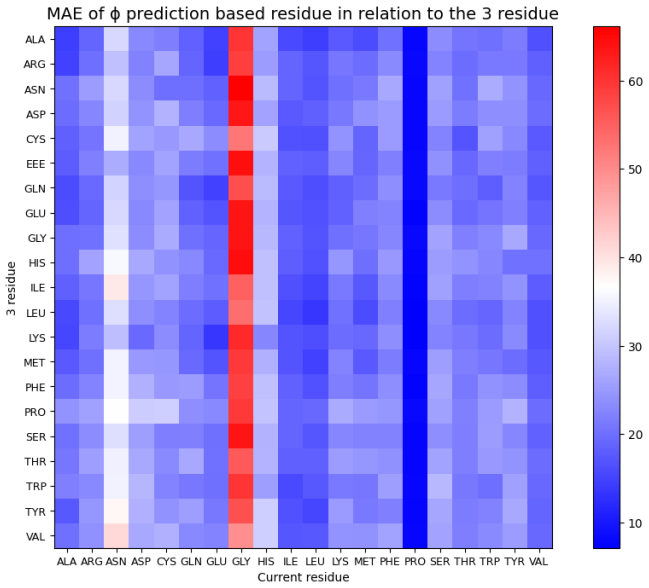
MAE of ϕ prediction based residue in relation to the 3 residue
3 residue
Current residue
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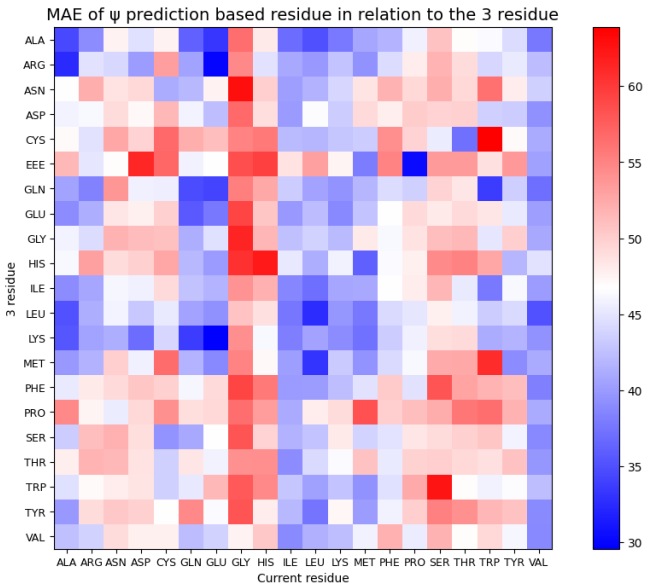
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Current residue
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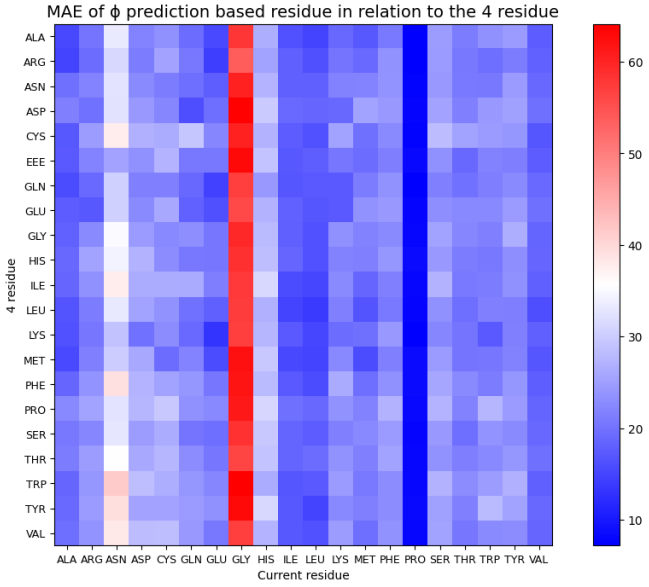
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4 residue
Current residue
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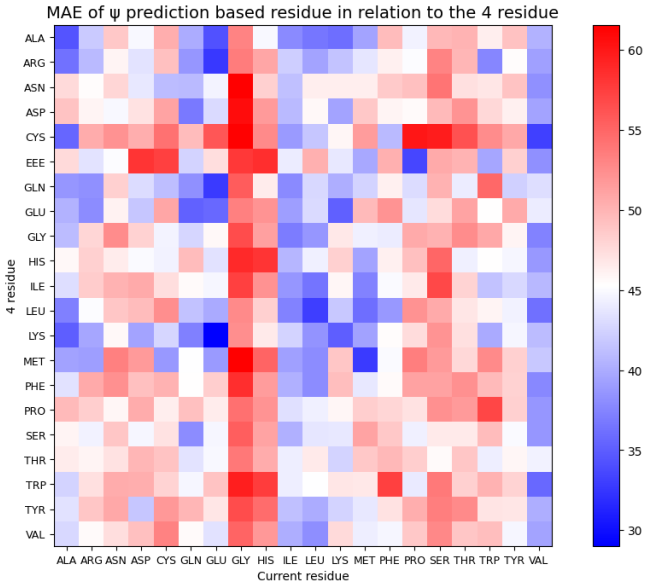
MAE of ψ prediction based residue in relation to the 4 residue
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Current residue
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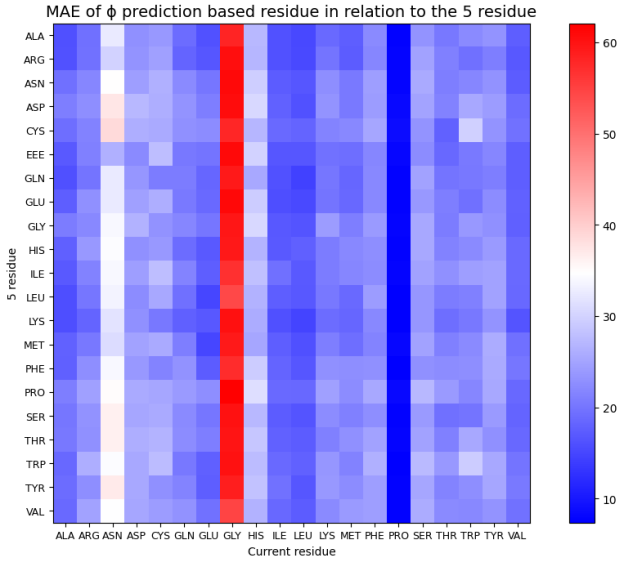
MAE of ϕ prediction based residue in relation to the 5 residue
5 residue
Current residue
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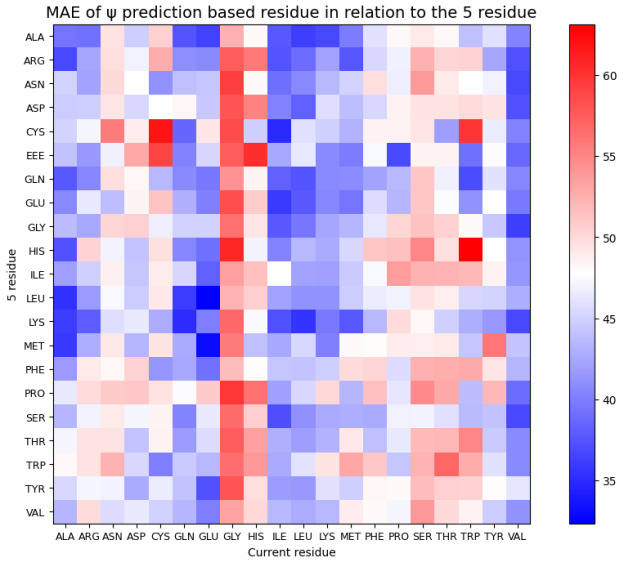
MAE of ψ prediction based residue in relation to the 5 residue
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Current residue
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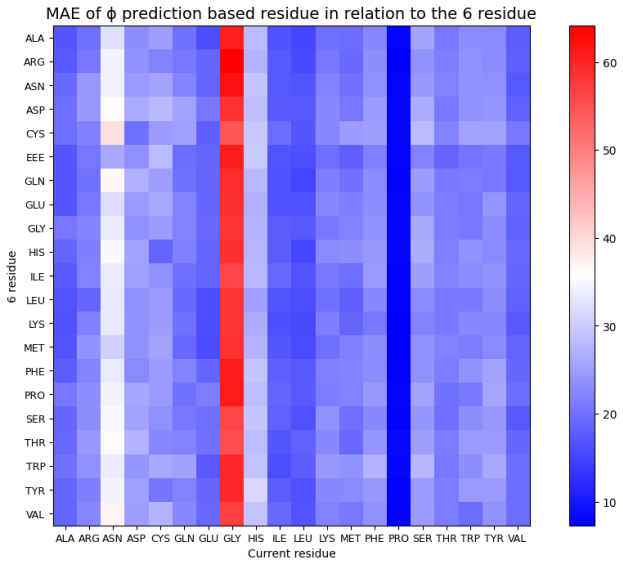
MAE of ϕ prediction based residue in relation to the 6 residue
6 residue
Current residue
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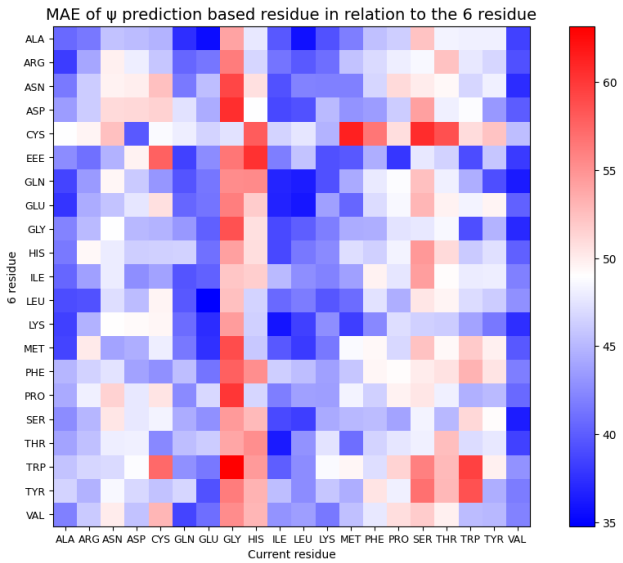
MAE of ψ prediction based residue in relation to the 6 residue
6 residue
Current residue
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60
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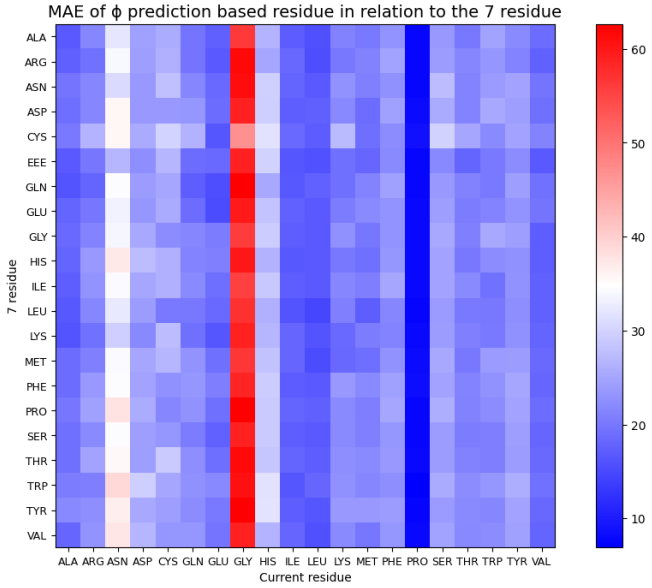
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7 residue
Current residue
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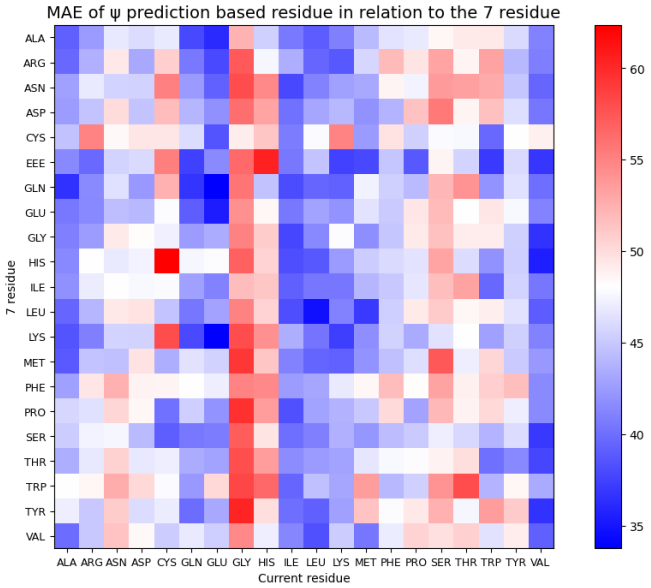
MAE of ψ prediction based residue in relation to the 7 residue
7 residue
Current residue
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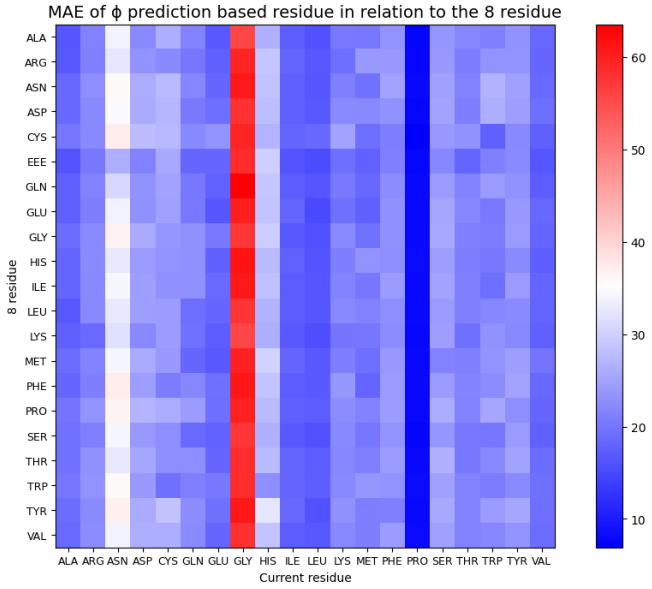
MAE of ϕ prediction based residue in relation to the 8 residue
8 residue
Current residue
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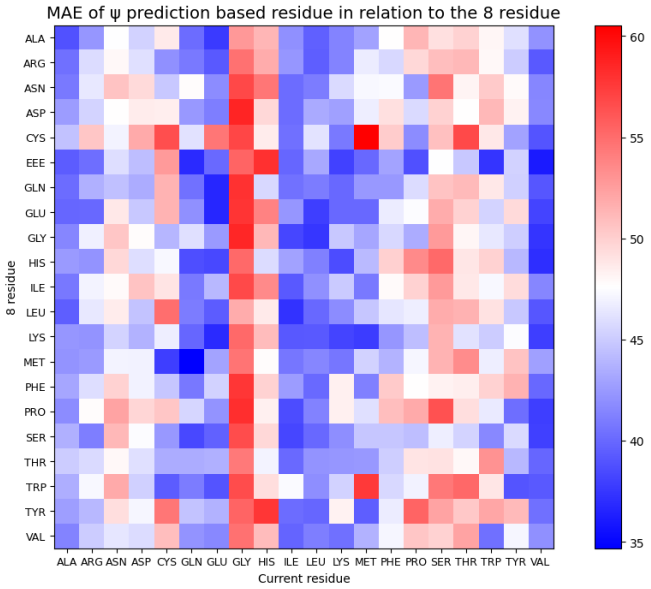
MAE of ψ prediction based residue in relation to the 8 residue
8 residue
Current residue
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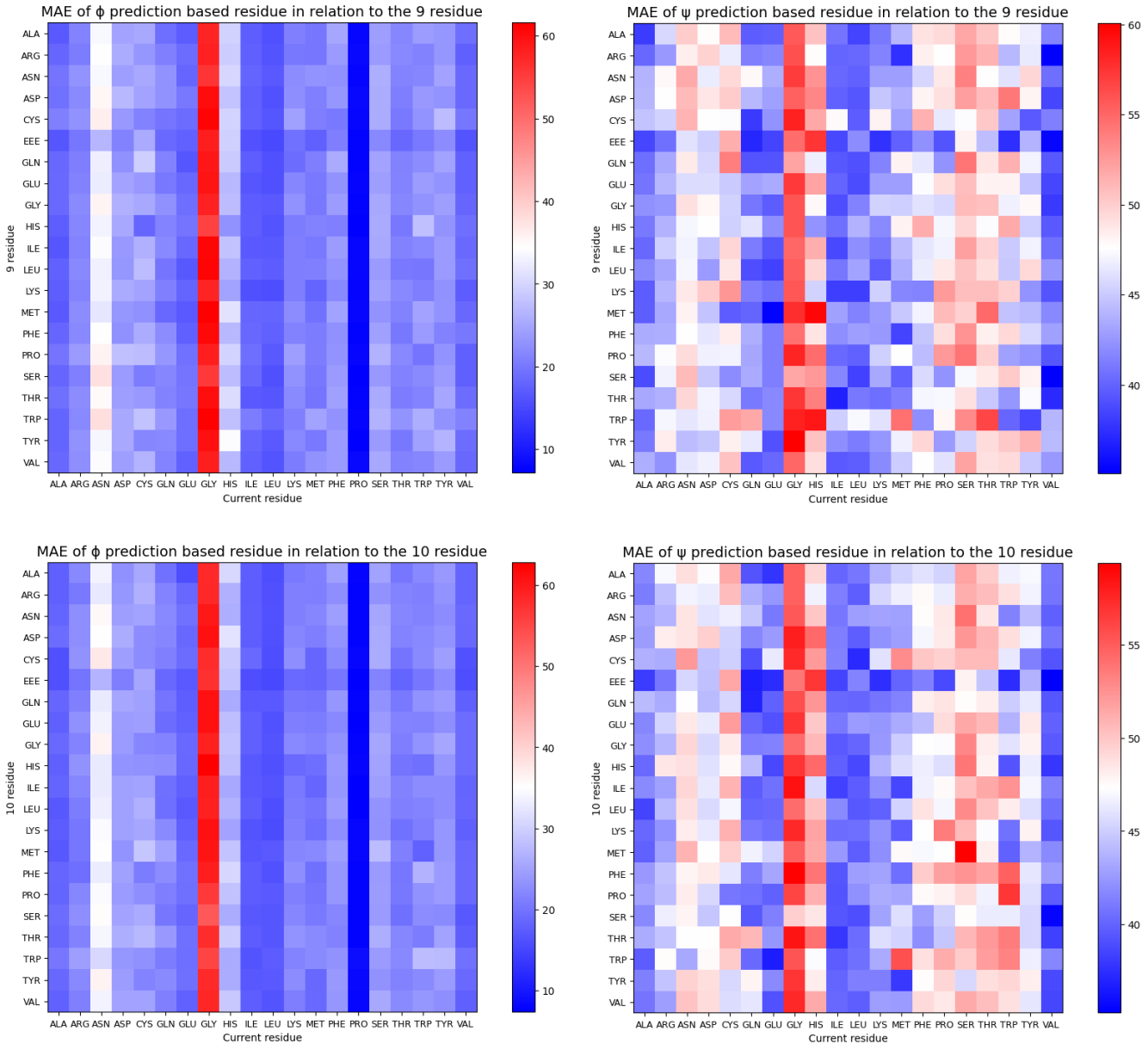

Figure S2. Mean absolute error of the current amino-acid residue in relation to the amino-acid residues at different positions of the sliding window for the ϕ (left) and ψ (right) dihedral angles.

Table S2. Real and predicted amino acid conformational propensites of the test dataset.

	Real			Predicted		
	Alpha	**Beta**	**Coil**	**Alpha**	**Beta**	**Coil**
Ala	4.48	2.97	0.90	4.71	2.75	0.90
Arg	2.21	2.02	0.65	2.25	1.96	0.67
Asn	1.44	1.93	0.98	1.05	2.11	1.18
Asp	2.15	2.51	1.18	1.98	2.28	1.57
Cys	0.40	0.78	0.17	0.35	0.85	0.16
Gln	1.72	1.44	0.50	1.70	1.40	0.56
Glu	3.45	2.14	0.85	3.60	1.95	0.89
Gly	1.34	1.54	4.70	1.20	1.21	5.17
His	0.78	1.14	0.39	0.68	1.17	0.46
Ile	2.24	3.09	0.30	2.02	3.40	0.20

Leu	4.24	3.80	0.97	4.24	3.77	1.00
Lys	2.65	2.24	0.81	2.66	2.16	0.88
Met	0.94	0.88	0.23	0.93	0.89	0.22
Phe	1.39	2.14	0.47	1.33	2.25	0.42
Pro	1.25	2.72	0.65	0.97	2.98	0.66
Ser	1.91	3.14	1.21	1.85	3.15	1.26
Thr	1.55	3.15	0.96	1.45	3.41	0.79
Trp	0.59	0.77	0.18	0.56	0.81	0.16
Tyr	1.21	1.95	0.44	1.09	2.10	0.41
Val	2.39	4.40	0.42	2.14	4.79	0.28

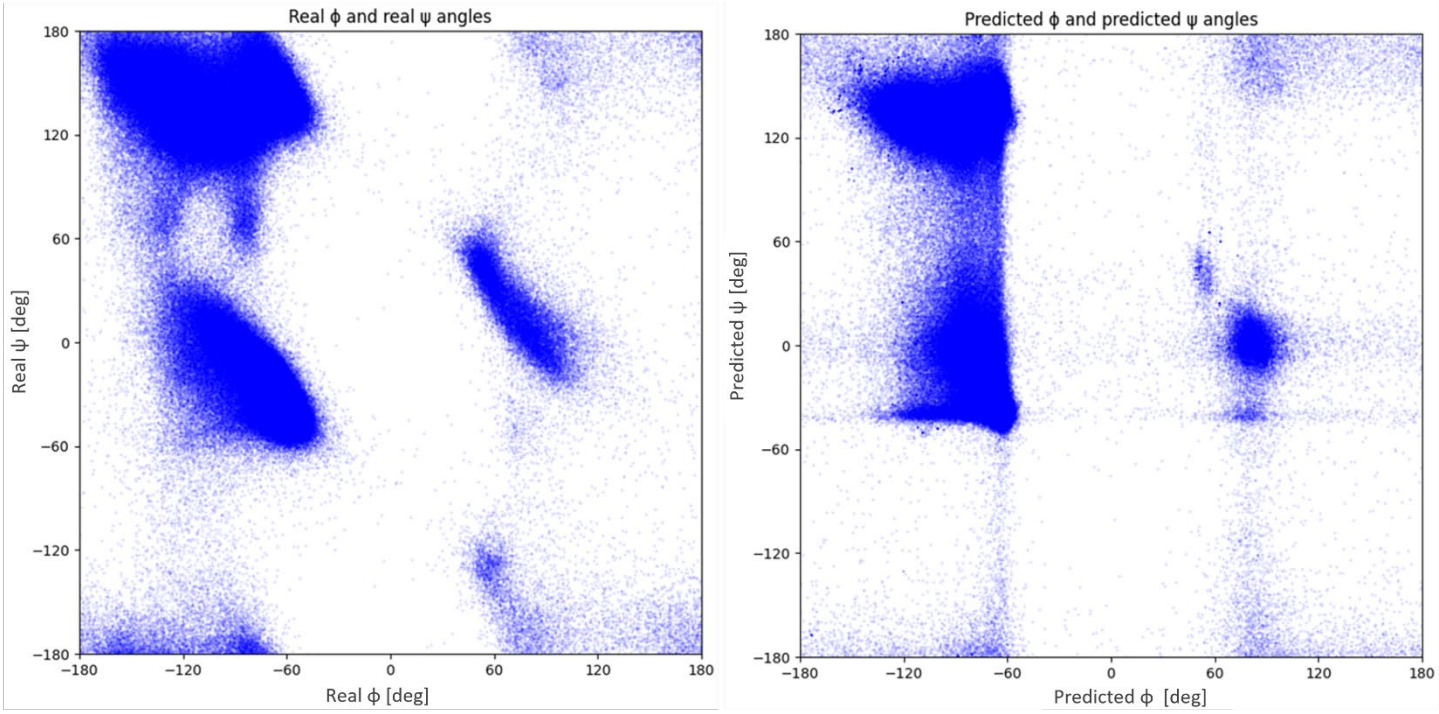

Figure 3. Ramachandran plots of actual and predicted dihedral angles.

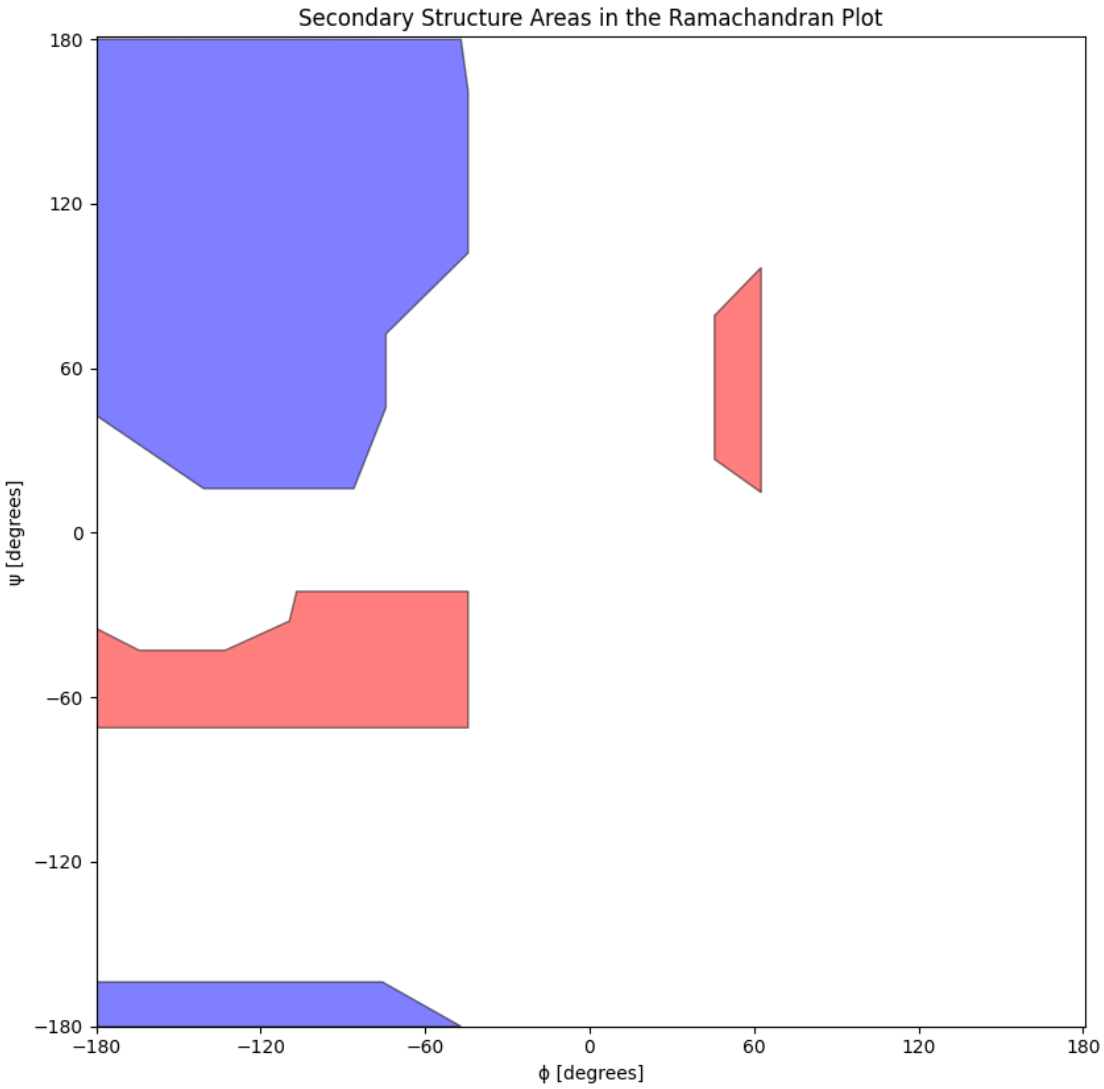

Figure S4. Secondary structure areas in the Ramachandran plot. The areas represent secondary structure elements: helices (red), sheets (purple), and undesignated (white). The areas are enclosed by the following points: helix = [(-180.0, -34.9), (-164.3, -42.9), (-133.0, -42.9), (-109.5, -32.2), (-106.9, -21.4), (-44.3, -21.4), (-44.3, -71.1), (-180.0, -71.1)] AND [(62.6, 14.7), (62.6, 96.7), (45.6, 79.2), (45.6, 26.8), (62.6, 14.7)]; sheet = [(-180.2, 42.9), (-140.8, 16.1), (-86.0, 16.1), (-74.3, 45.6), (-74.3, 72.5), (-44.3, 102.0), (-44.3, 161.1), (-46.9, 179.9), (-180, 180)] AND [(-180.0, -163.8), (-75.6, -163.8), (-46.9, -180.0), (-180.0, -180.0)].

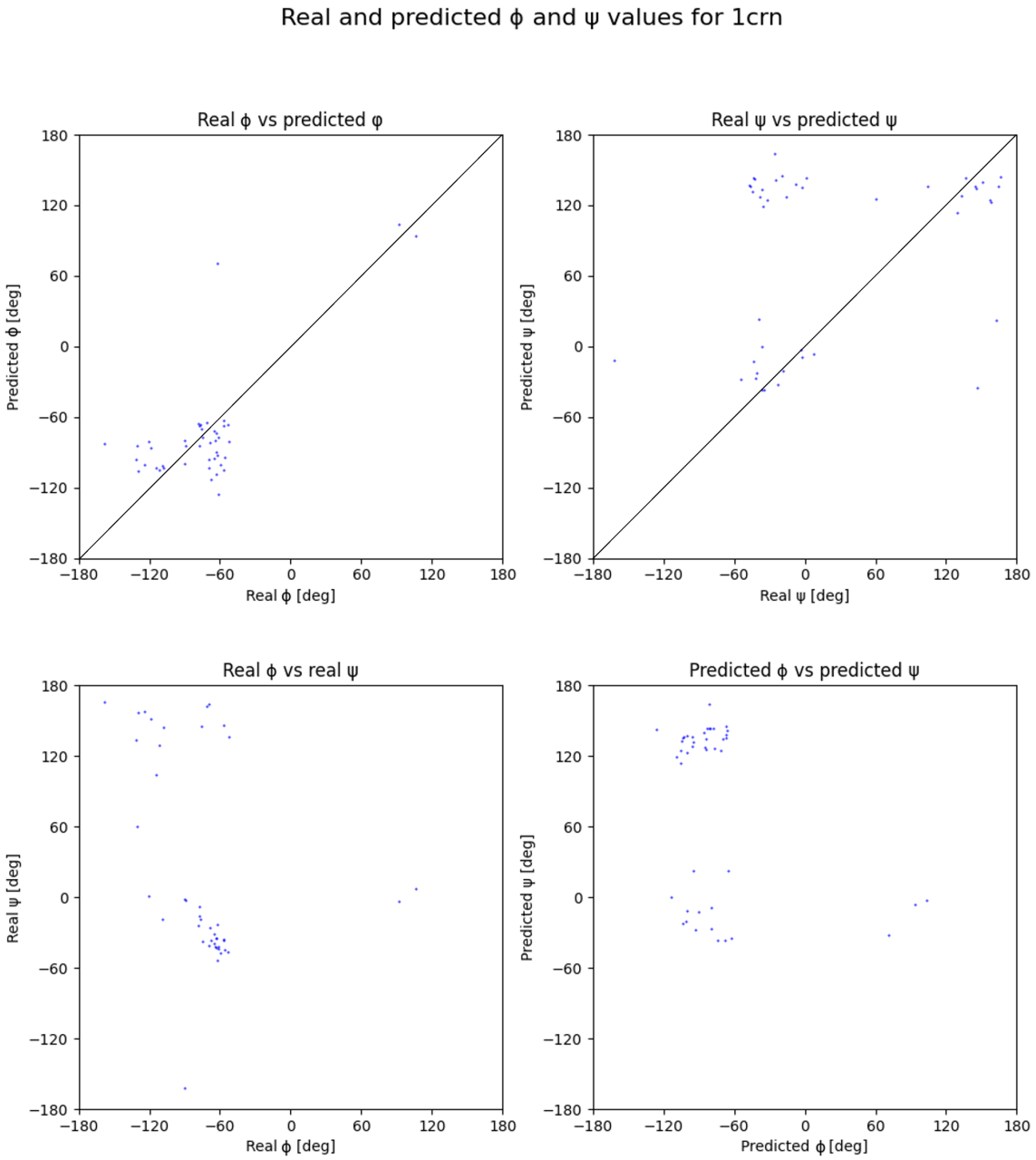

Figure S5. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 1CRN (ϕ error = 24.91°; ψ error = 80.86°).

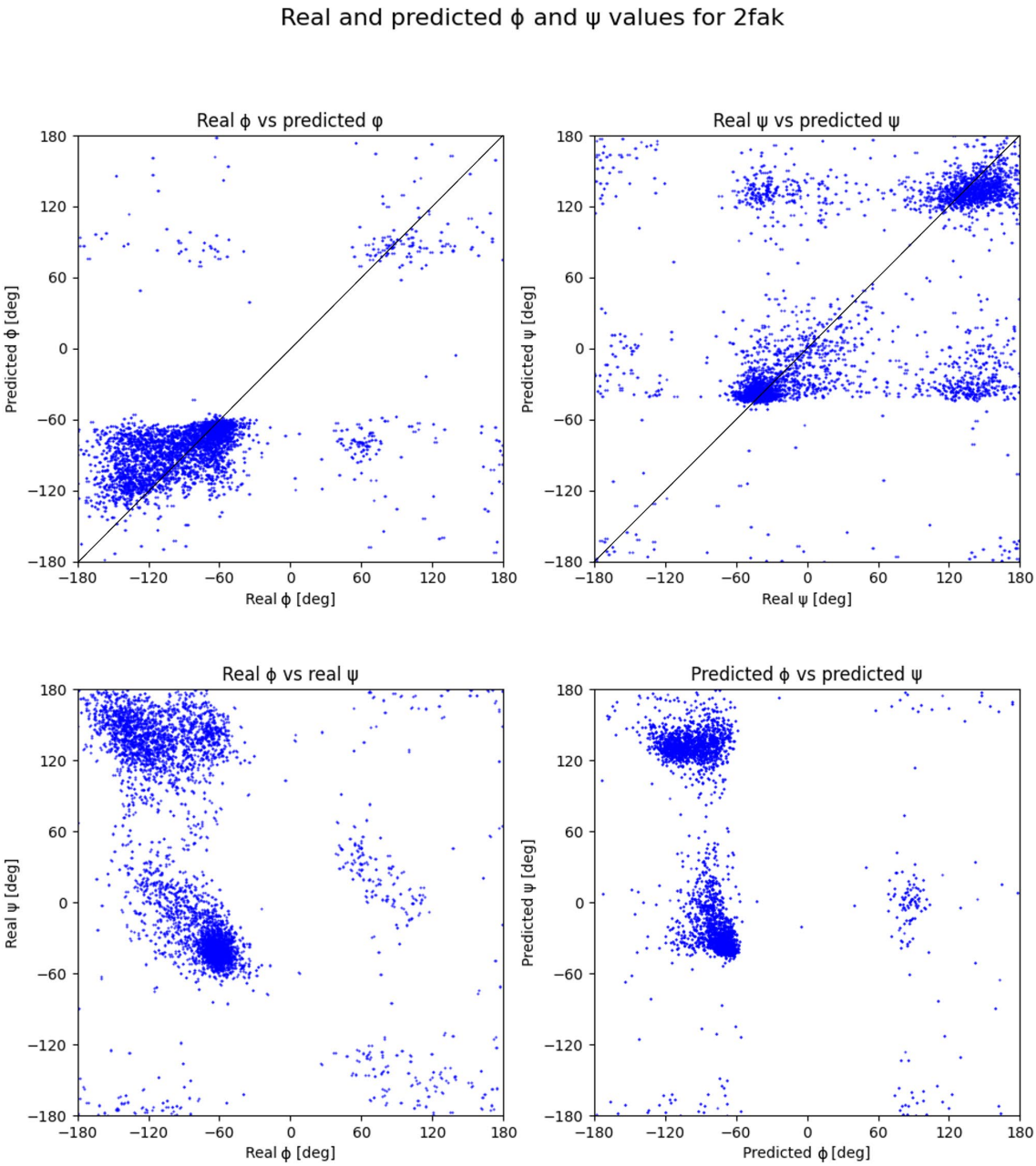

Figure S6. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 2FAK (ϕ error = 25.71°; ψ error = 41.96°).

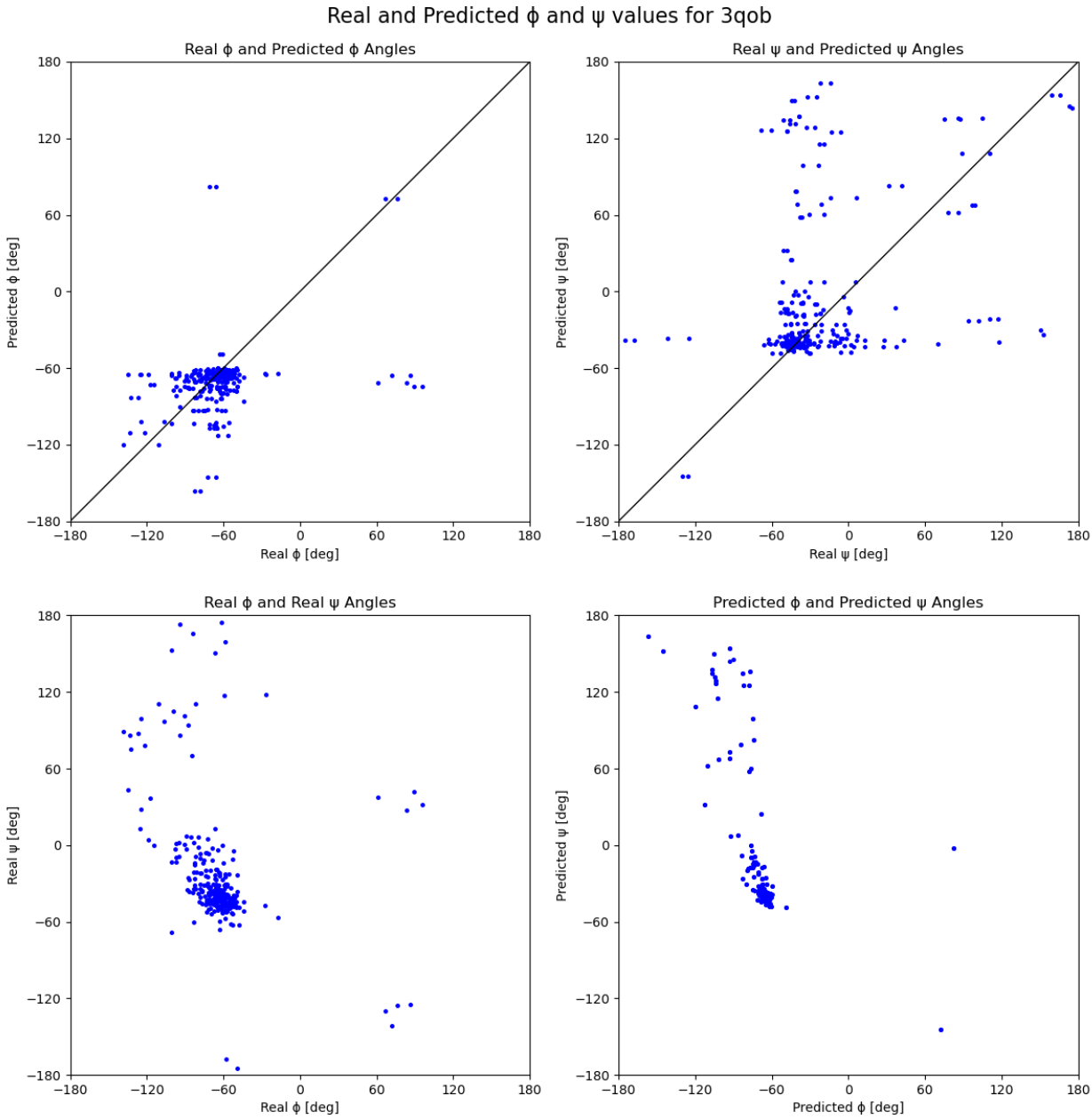

Figure S7. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 3QOB (ϕ error = 17.76°; ψ error = 36.43°).

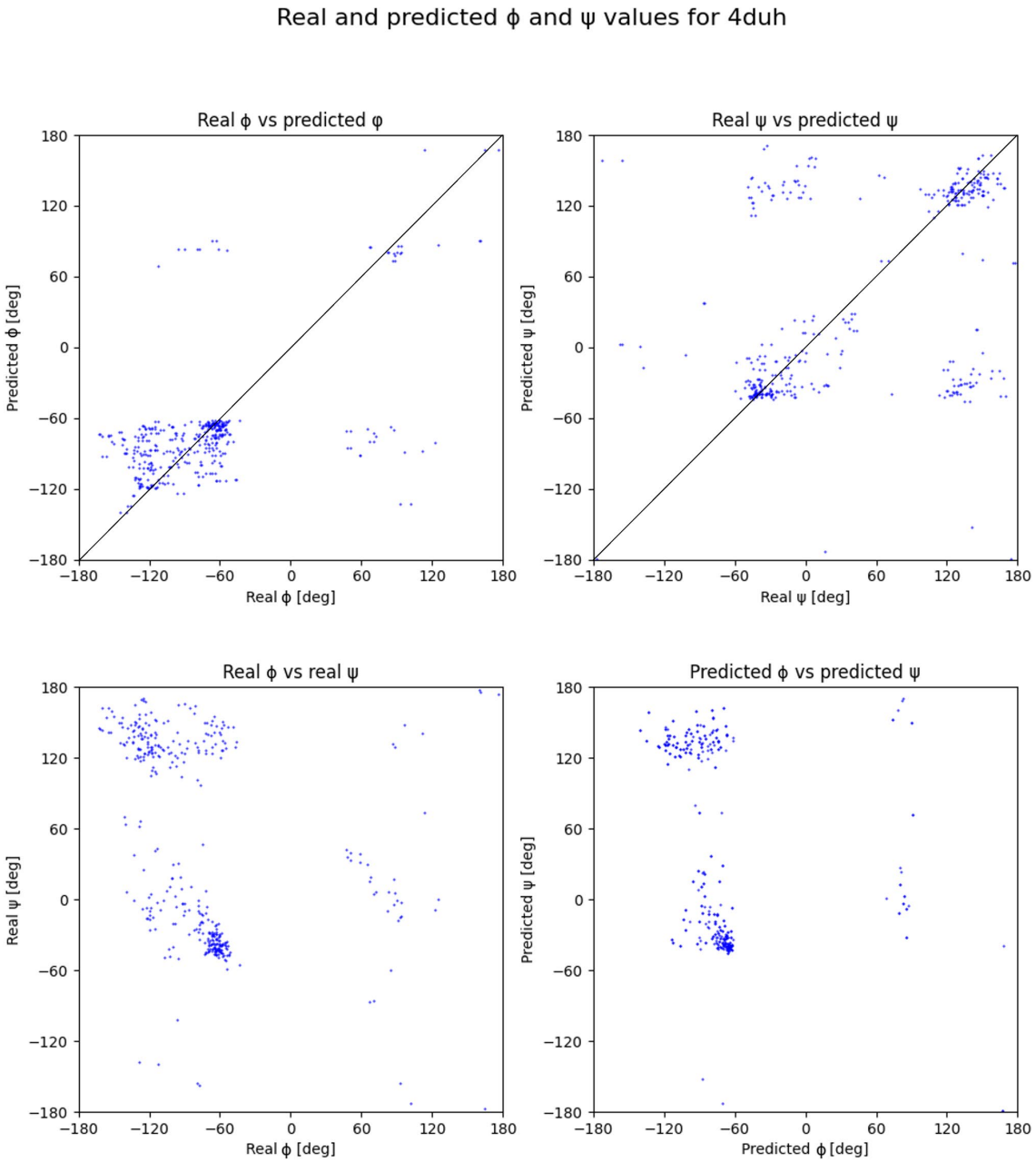

Figure S8. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 4DUH (ϕ error = 29.86°; ψ error = 48.16°).

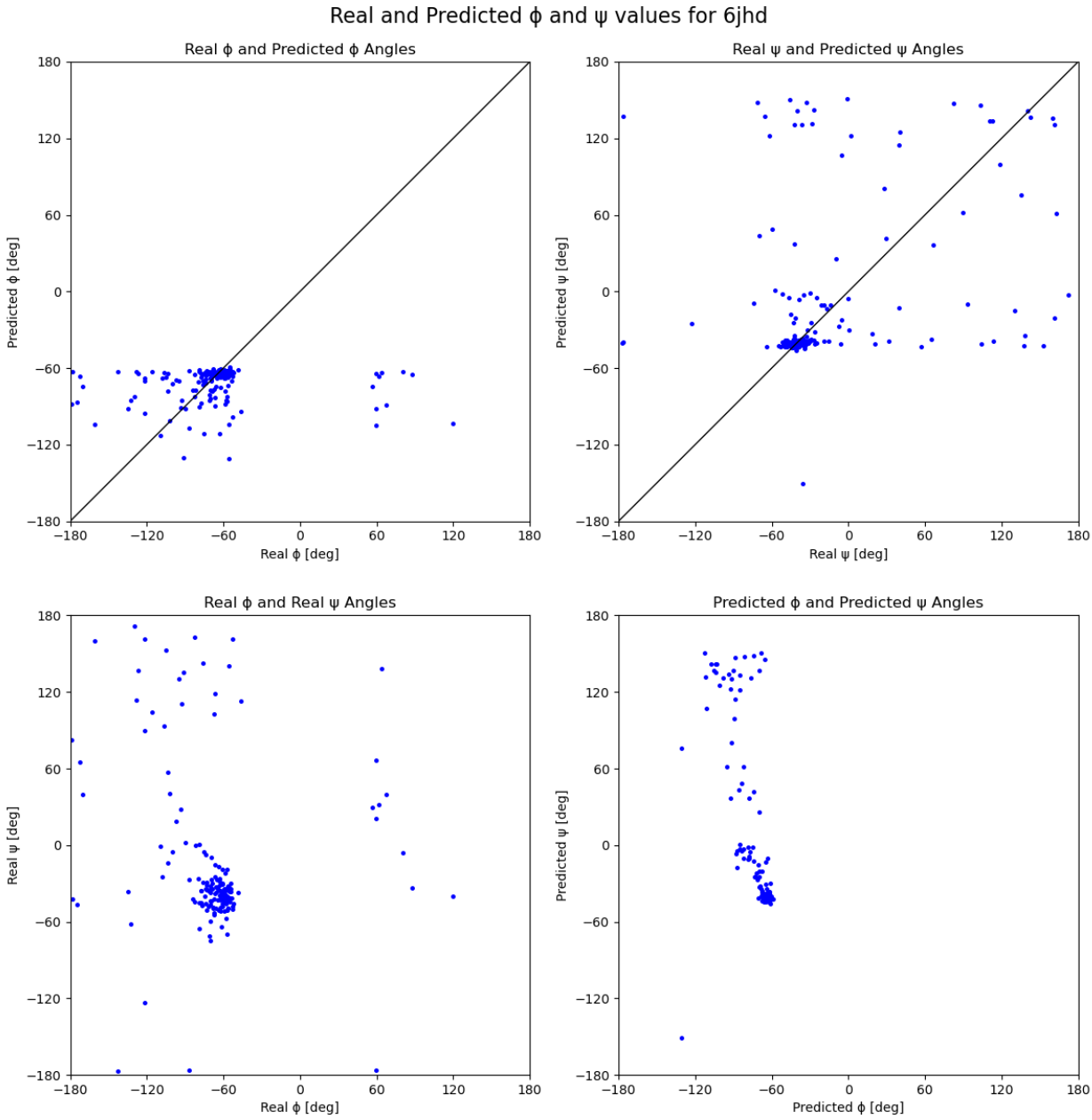

Figure S9. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 6JHD (ϕ error = 24.57°; ψ error = 39.91°).

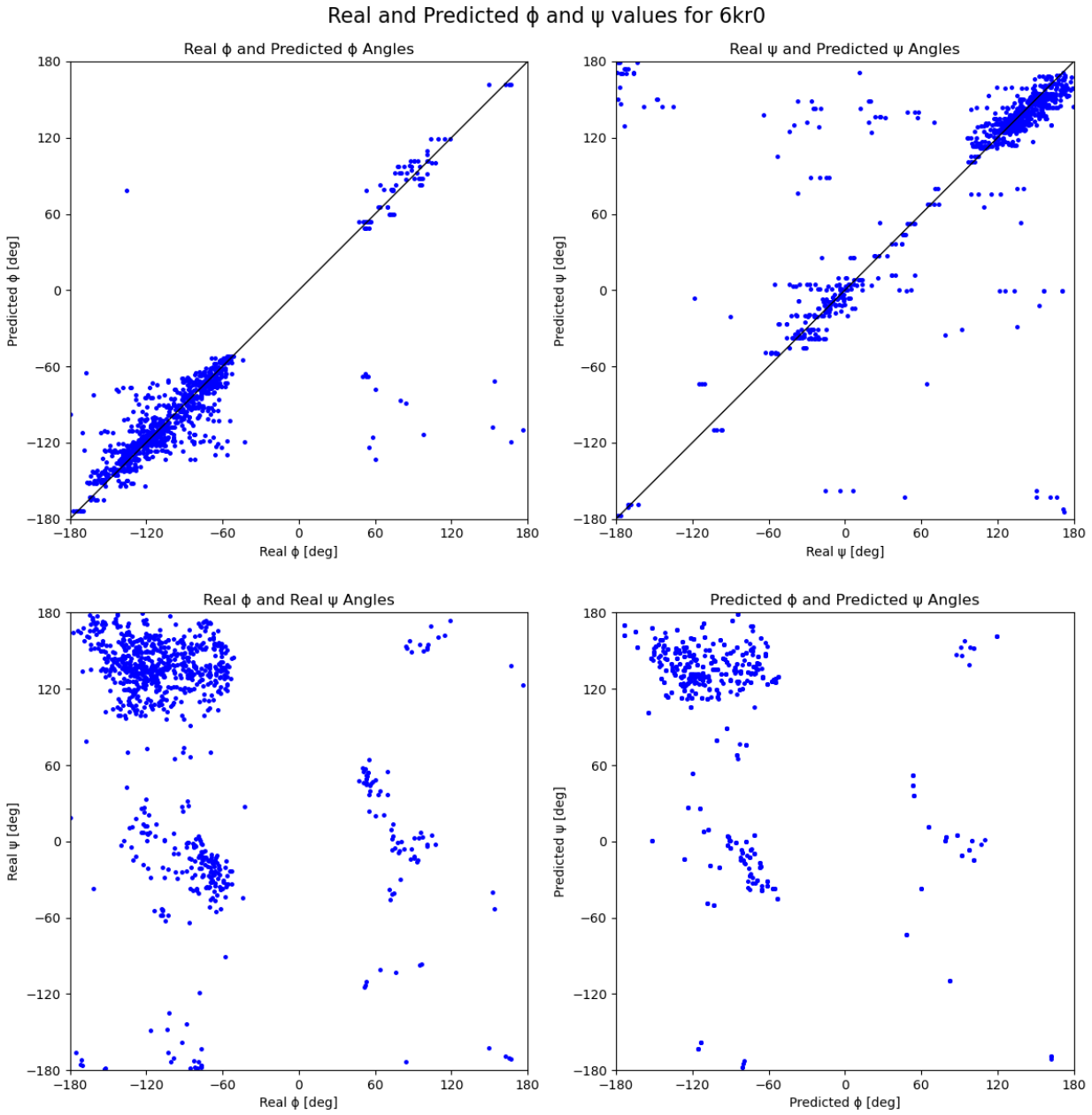

Figure S10. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 6KR0 (ϕ error = 12.27°; ψ error = 16.10°).

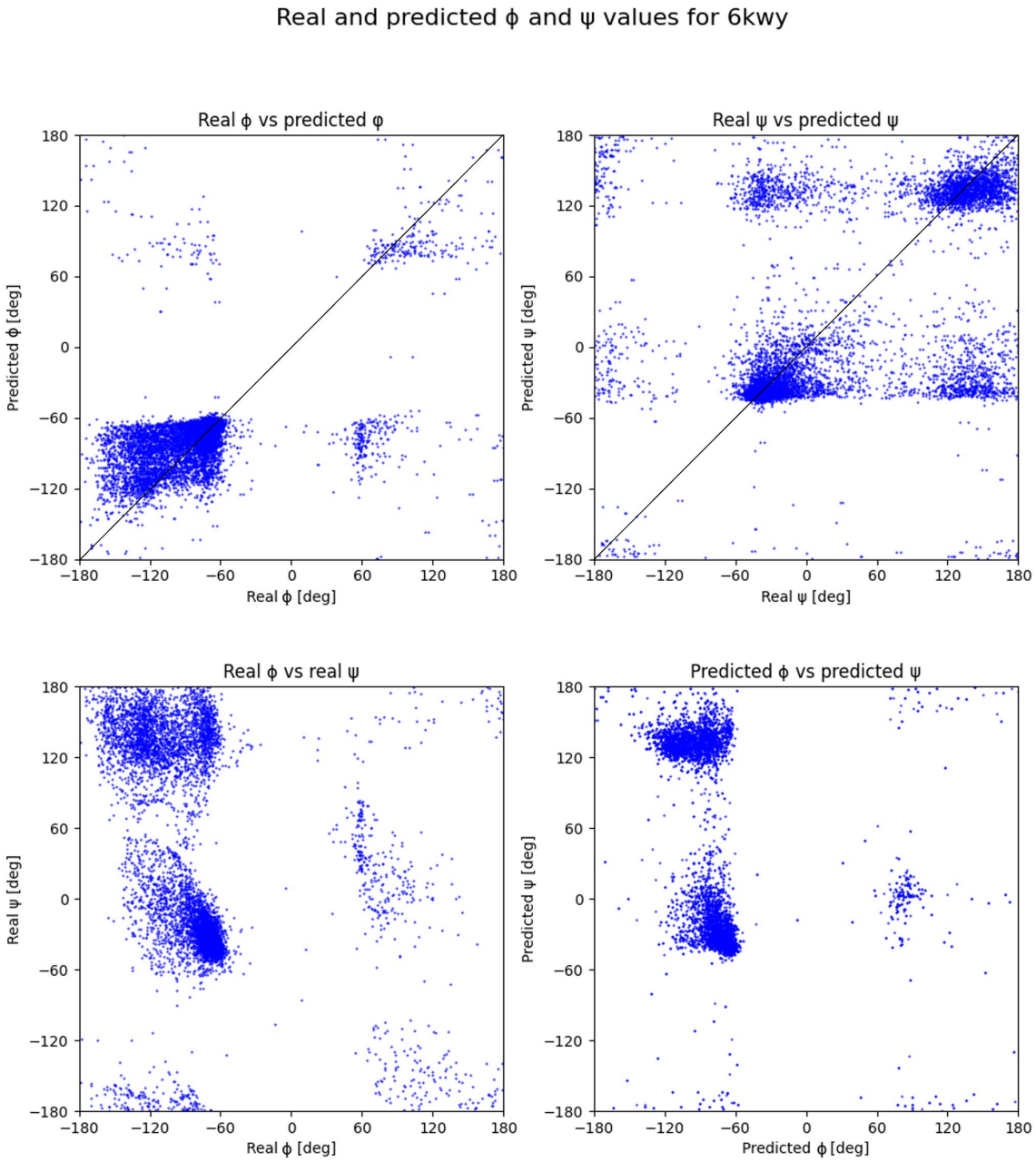

Figure S11. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 6KWY (ϕ error = 22.78°; ψ error = 42.43°).

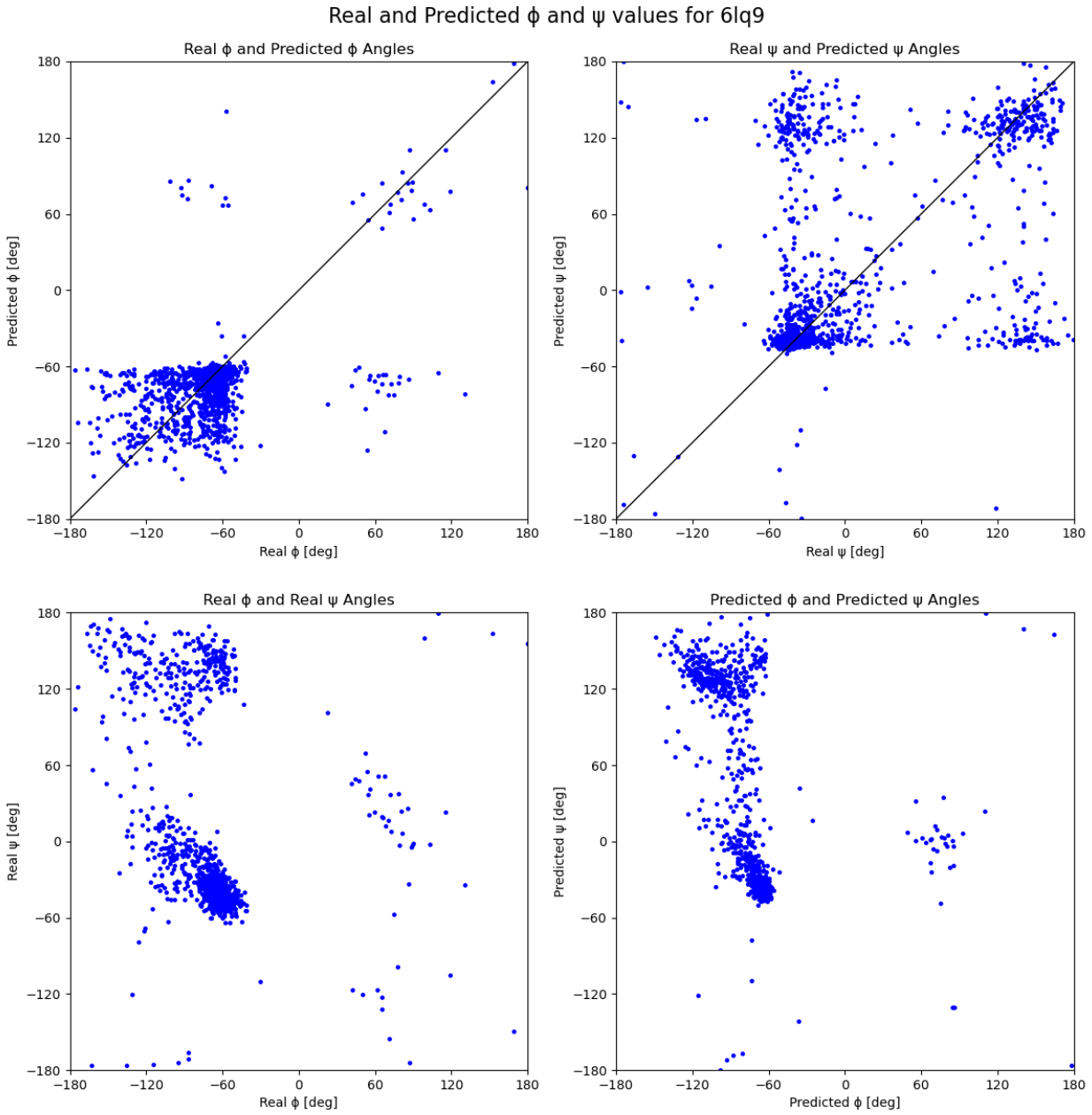

Figure S12. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 6LQ9 (ϕ error = 18.83°; ψ error = 40.67°).

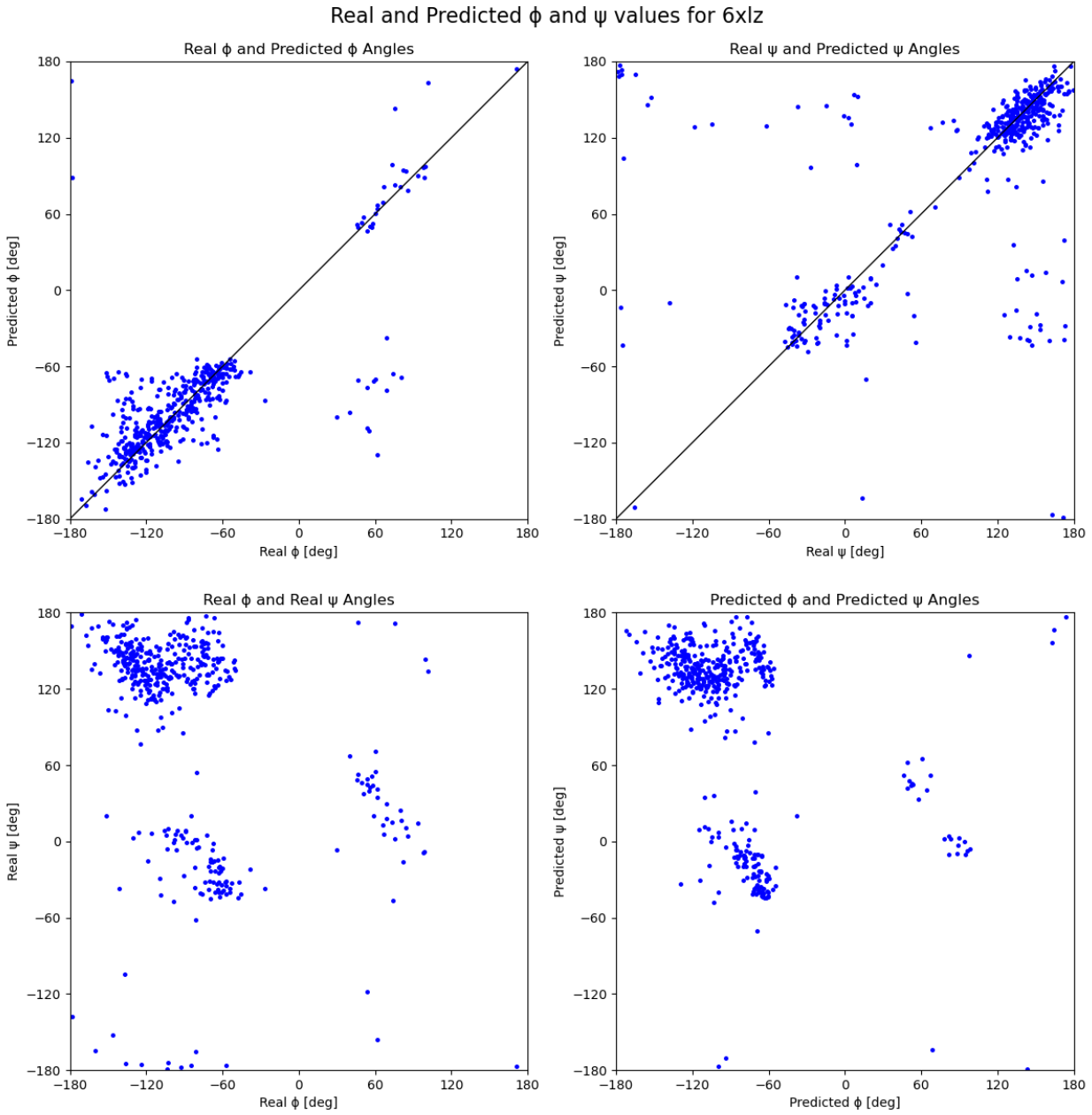

Figure S13. Real and predicted ϕ and ψ angles for the protein structure PDB ID: 6XLZ (ϕ error = 17.45°; ψ error = 23.29°).

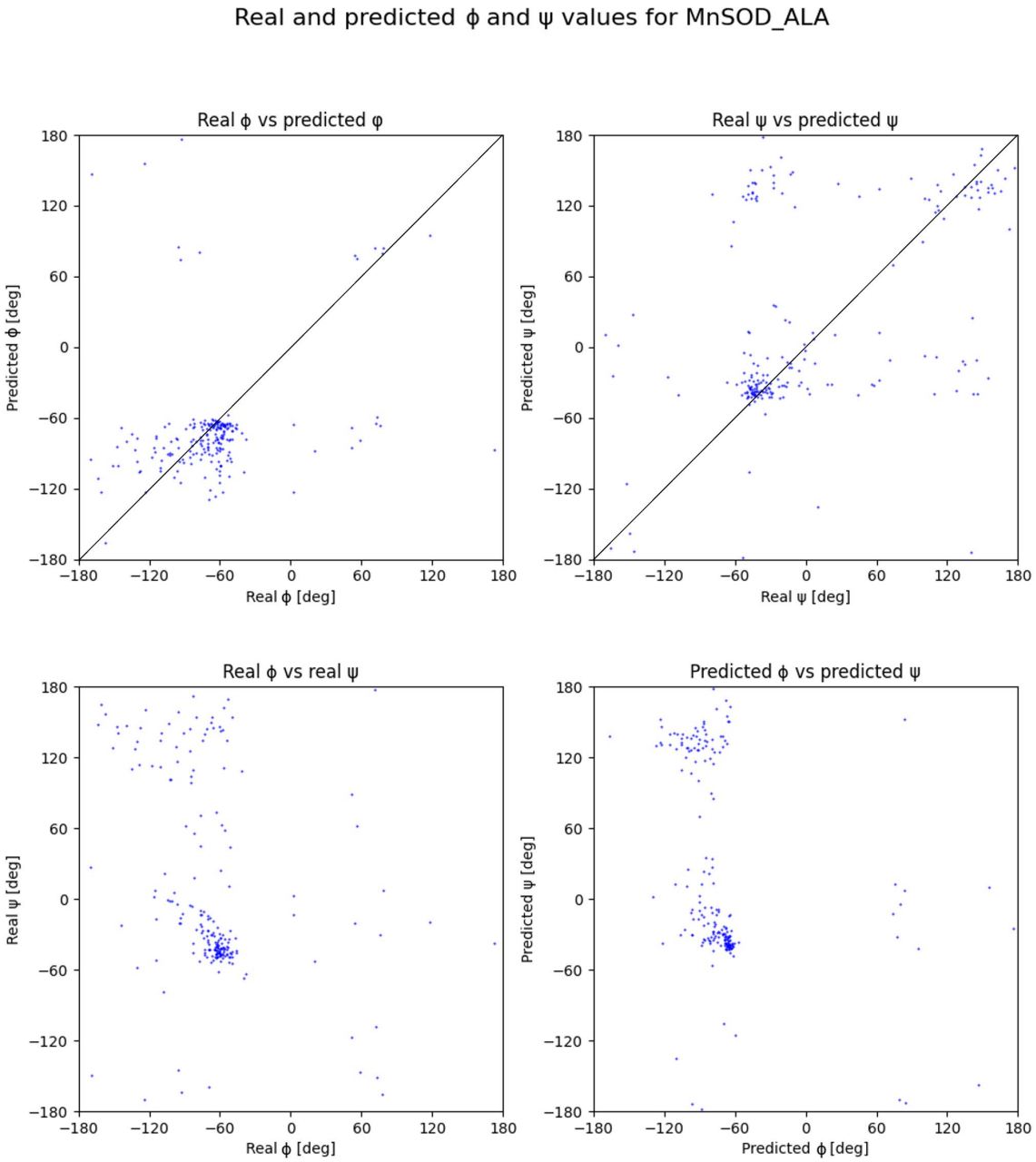

Figure S14. Real and predicted ϕ and ψ angles for the protein structure of MnSOD_ALA (ϕ error = 26.82°; ψ error = 51.12°).

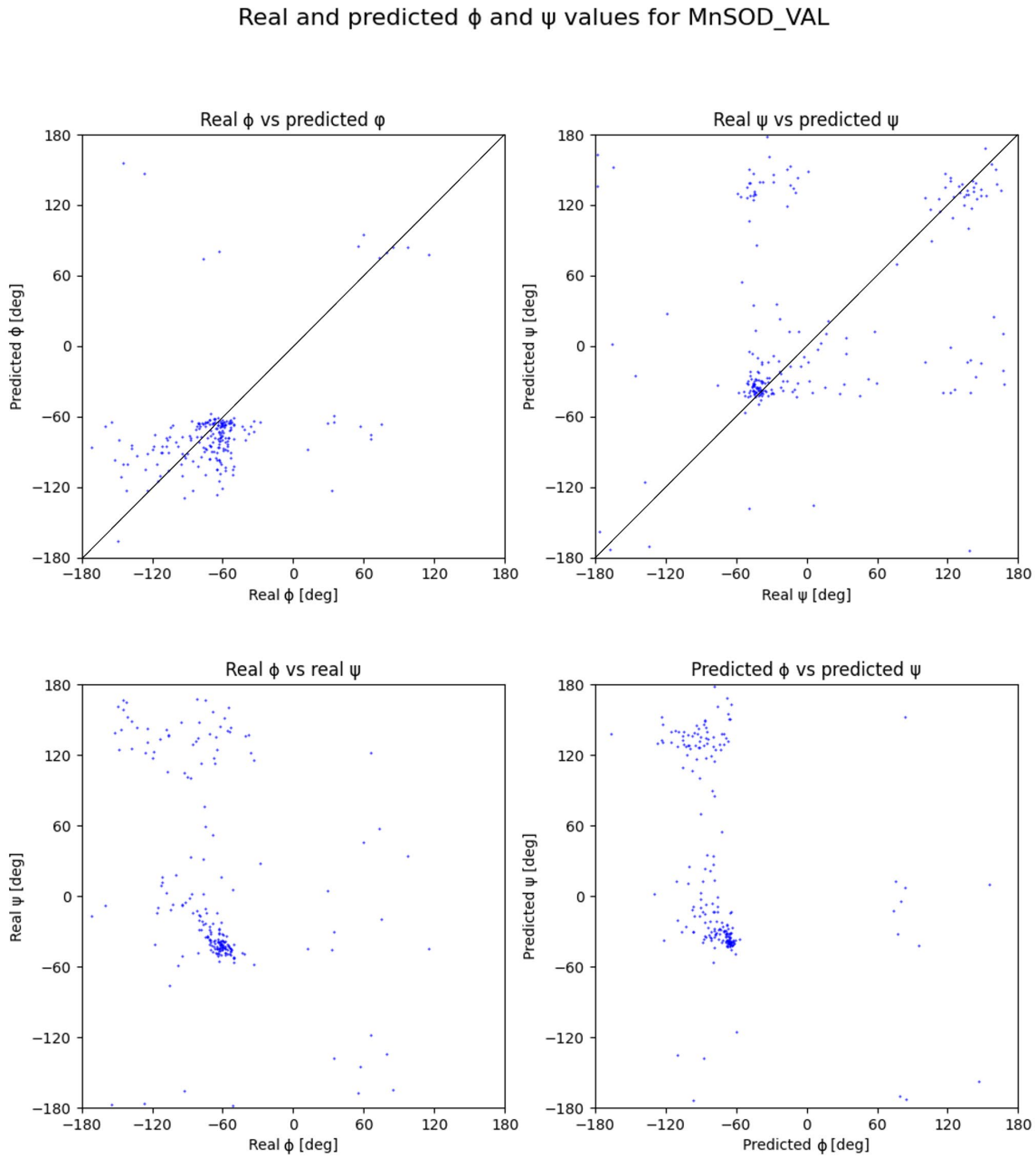

Figure S15. Real and predicted ϕ and ψ angles for the protein structure of MnSOD_VAL (ϕ error = 26.41°; ψ error = 50.44°).

Table S3. Per-model mean absolute errors of the predicted phi and psi dihedral angle of our model compared to an online tool DISSpred.

	Our model		DISSpred	
PDB ID	**Phi**	**Psi**	**Phi**	**Psi**
1CRN	22.63	77.65	32.70	49.86
2FAK	20.58	35.08	29.85	35.77
4DUH	28.65	54.18	42.60	85.49
6KWY	26.19	44.18	43.28	91.98
6JHD	24.57	39.90	25.76	34.35
6KR0	12.24	16.70	47.25	90.02
6LQ9	26.57	48.82	37.57	73.66
3QOB	18.12	37.80	19.94	32.03

6XLZ	16.59	27.03	43.40	81.24
MnSOD-ALA	26.69	50.94	31.06	60.28
MnSOD-VAL	27.65	50.16	31.99	58.17
Average	**22.77**	**43.86**	**35.03**	**62.99**

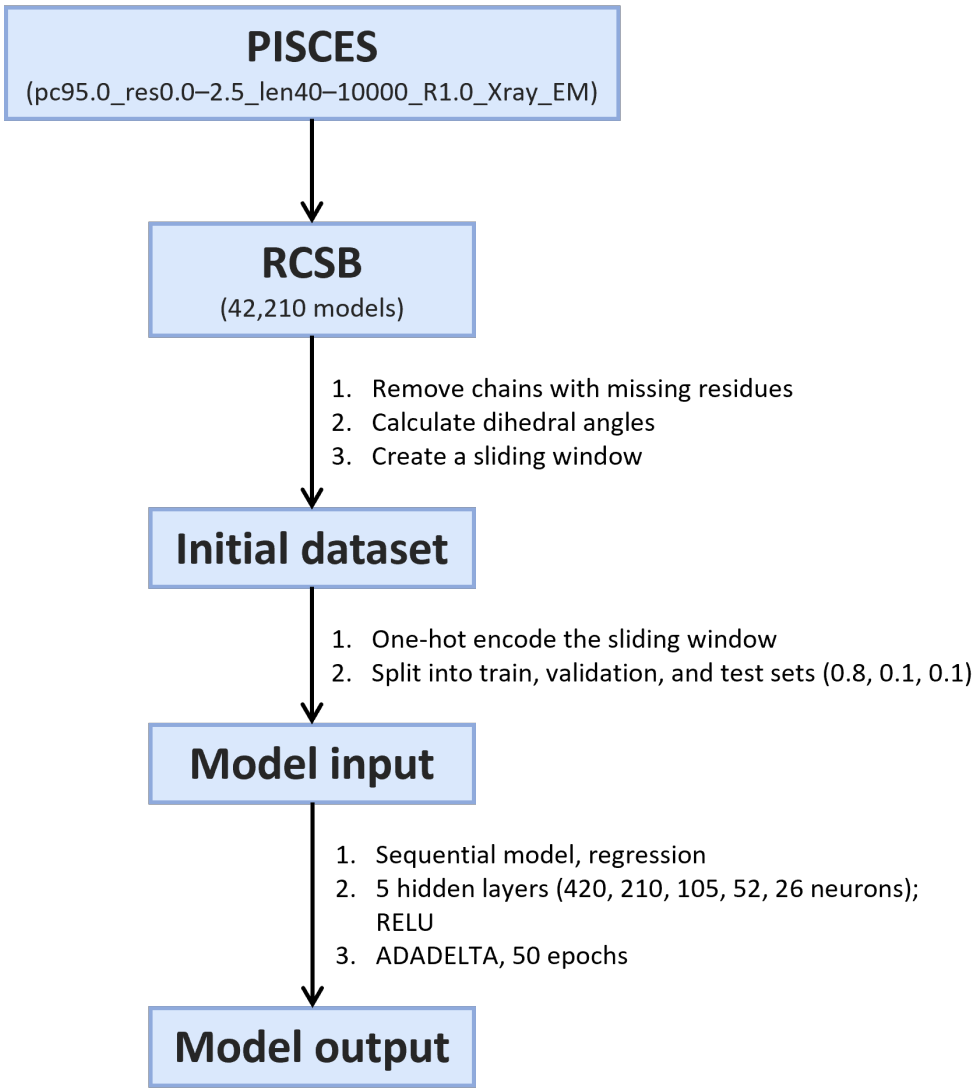

Figure S16. The process of generating output, which involves accessing the PISCES and RCSB datasets, converting the coordinates to dihedral angles, and transforming the sequence into a sliding window format.

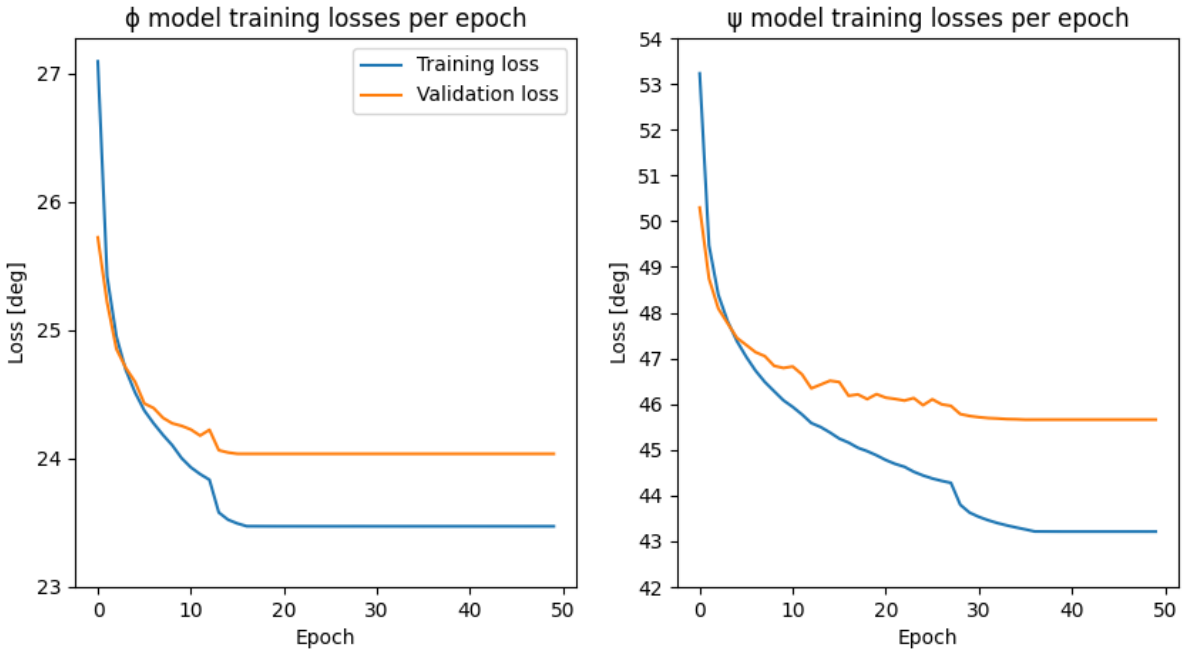

Figure S17. Training and validation loss function values during the ϕ and ψ model training.