

ELECTRONIC SUPPLEMENTARY INFORMATION

Exploration of the Forbidden Regions of the Ramachandran Plot (ϕ - ψ) with QTAIM

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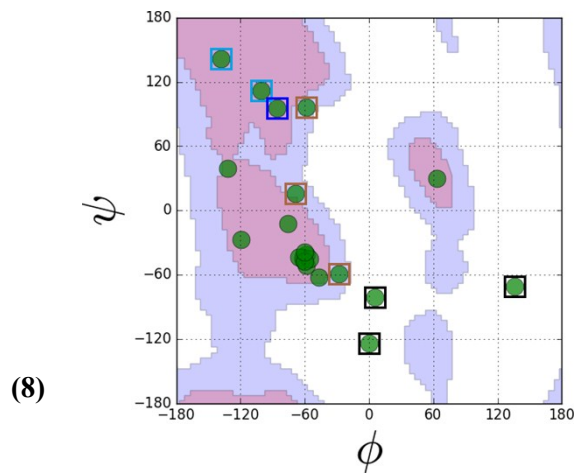
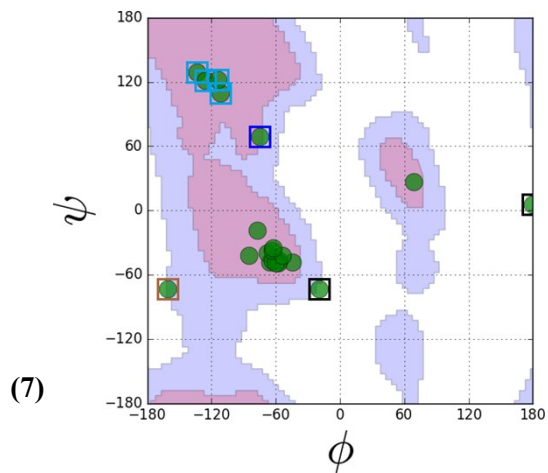
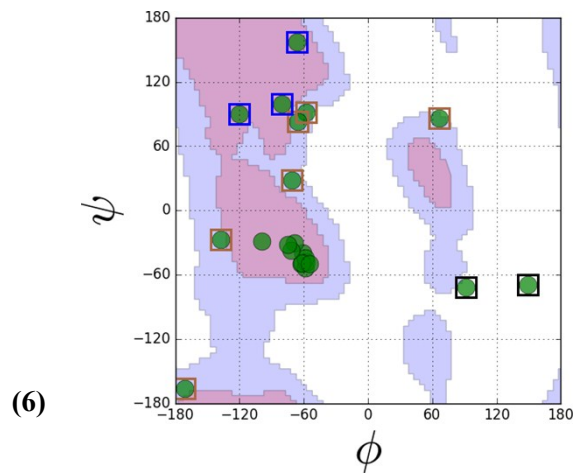
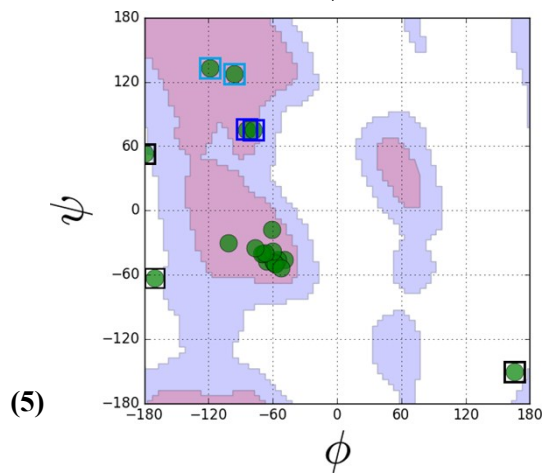
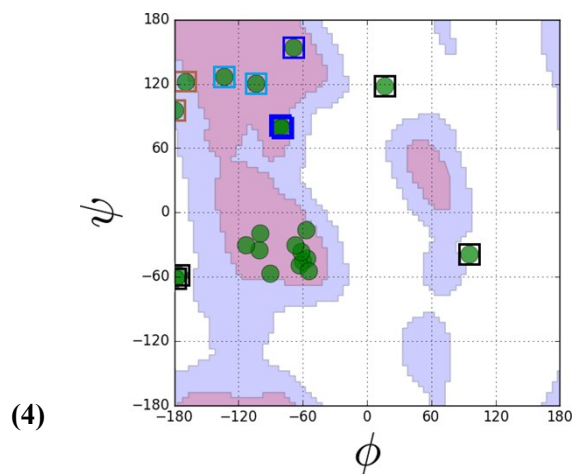
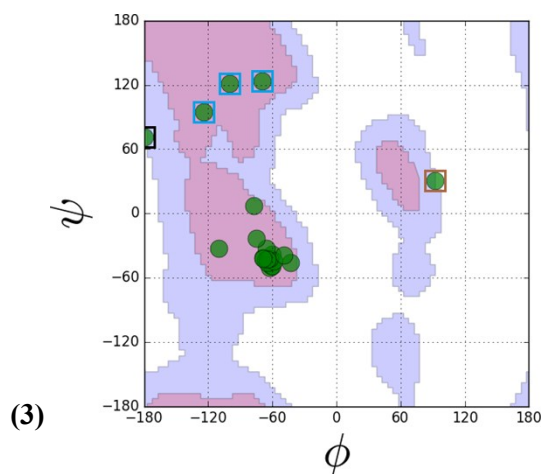
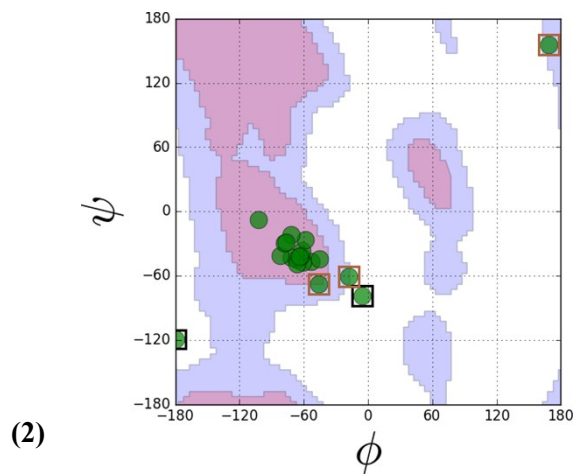
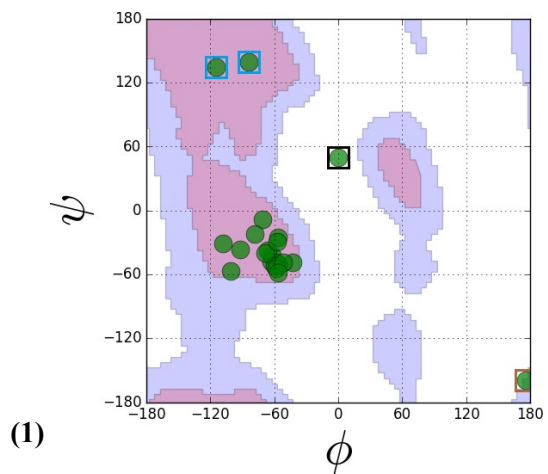
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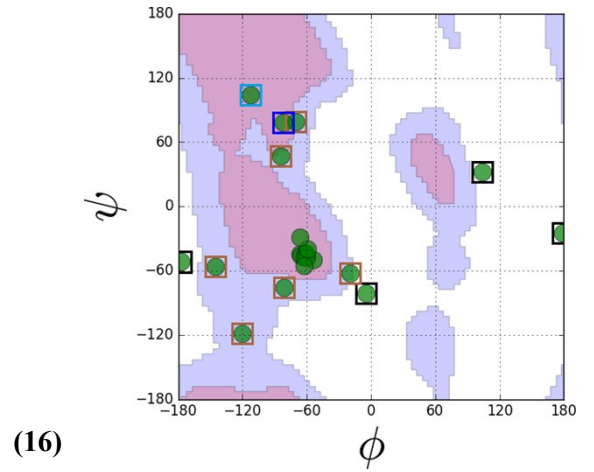
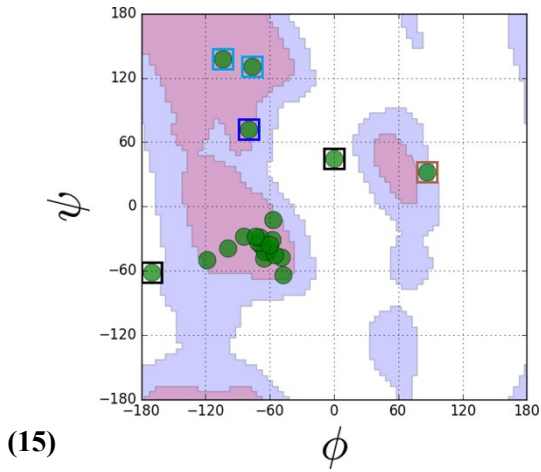
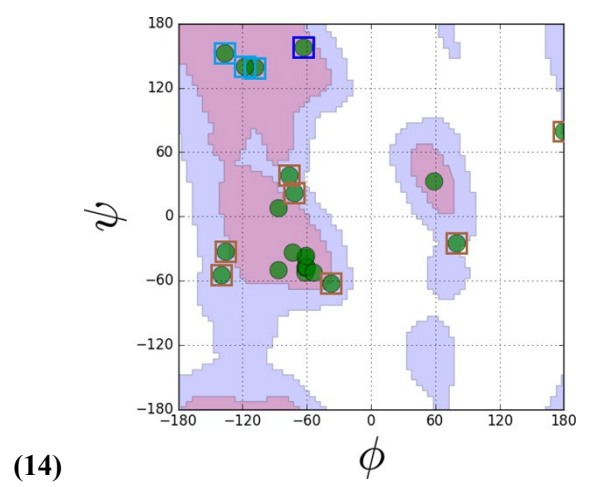
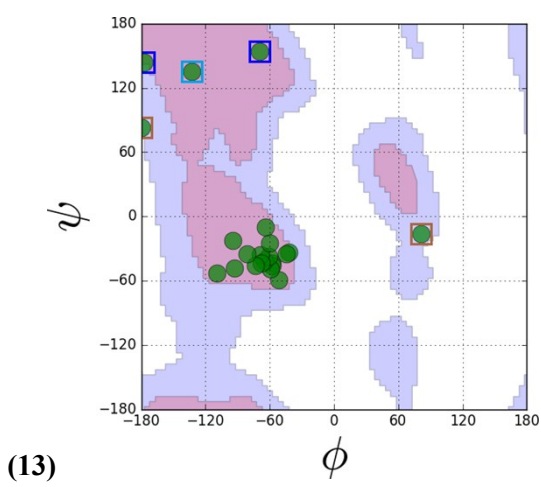
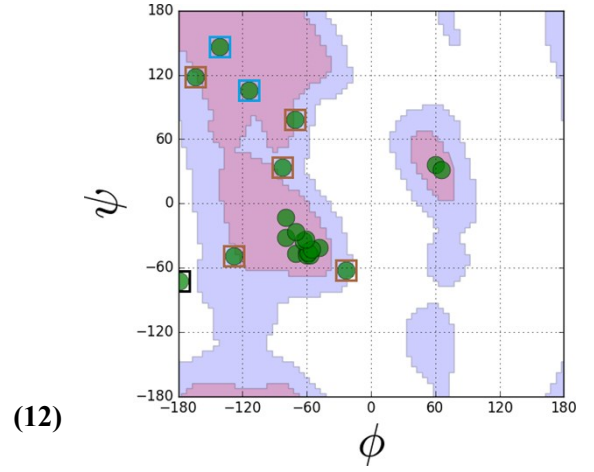
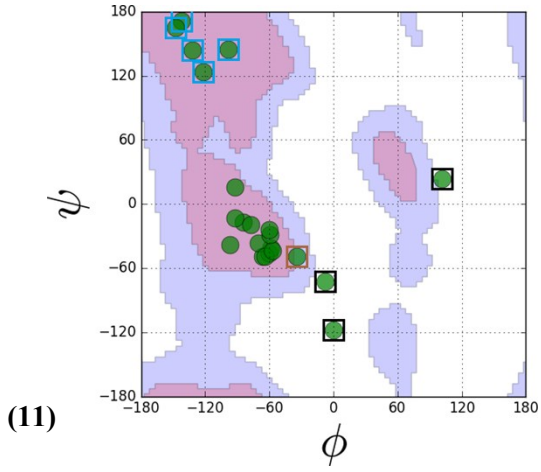
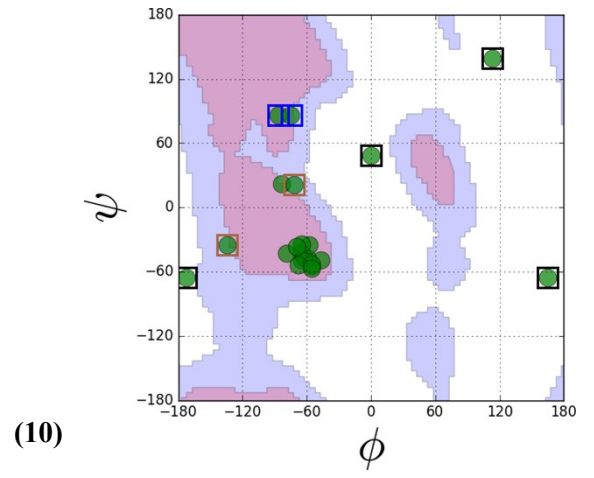
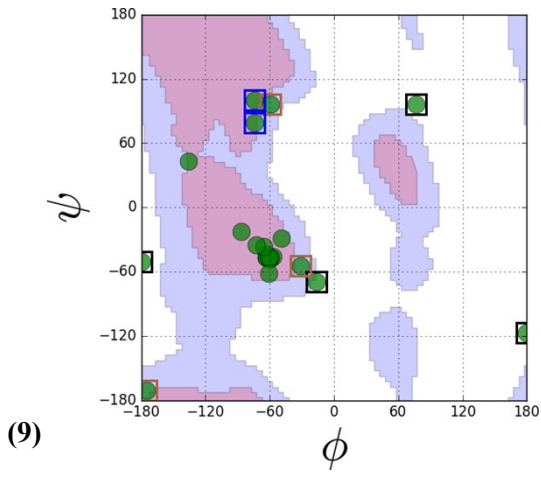
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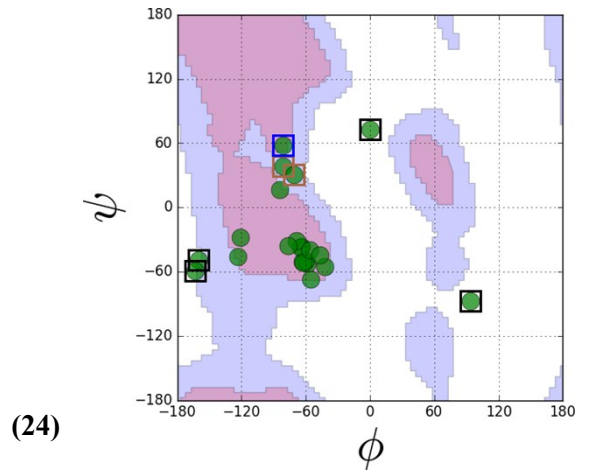
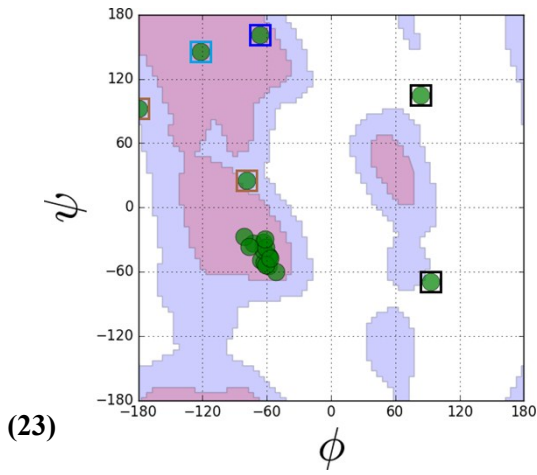
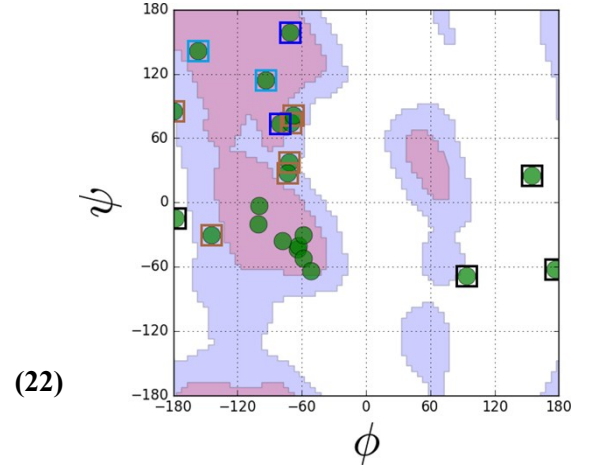
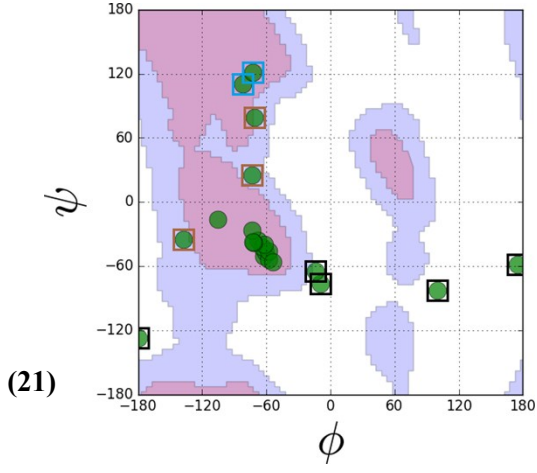
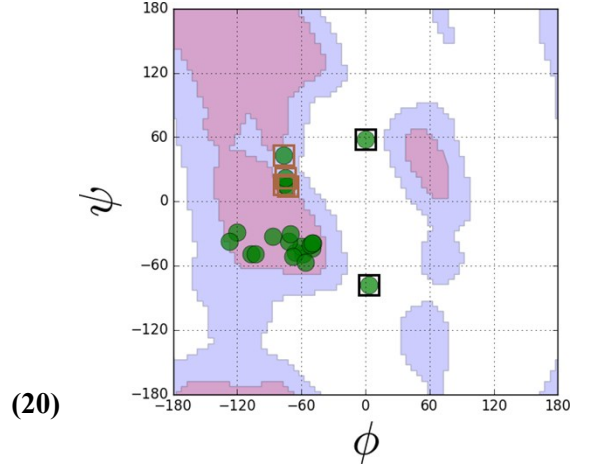
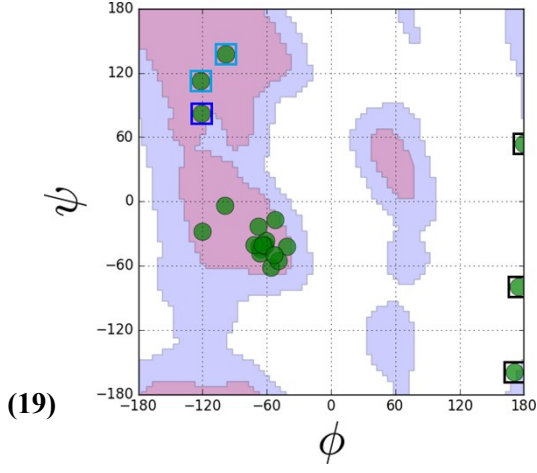
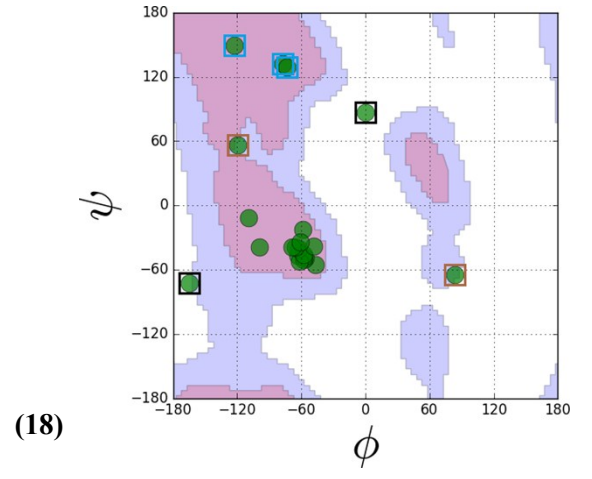
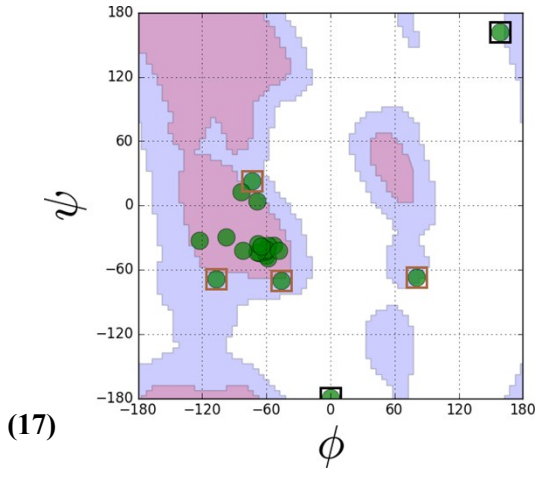
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1. Supplementary Materials S1.







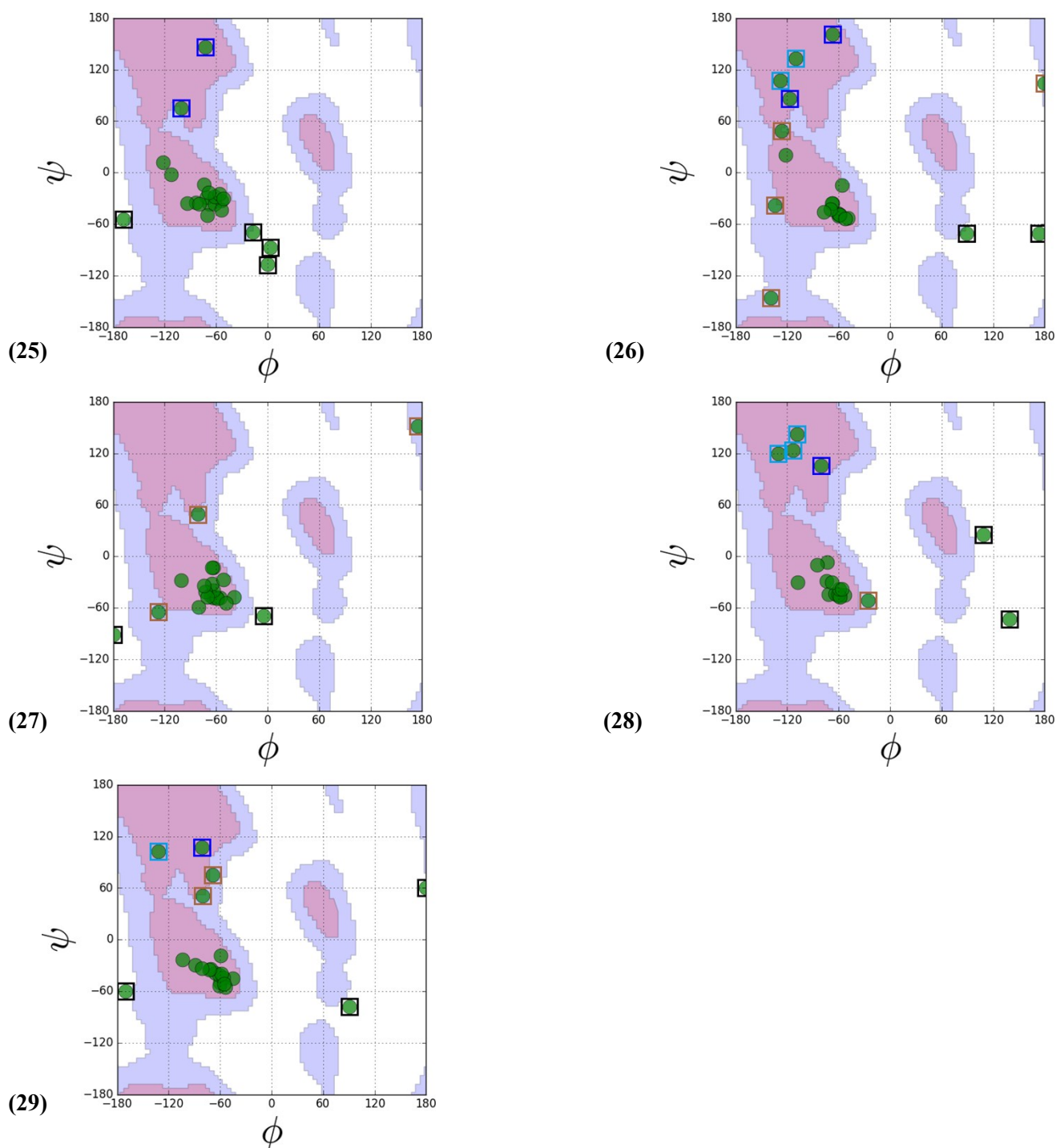
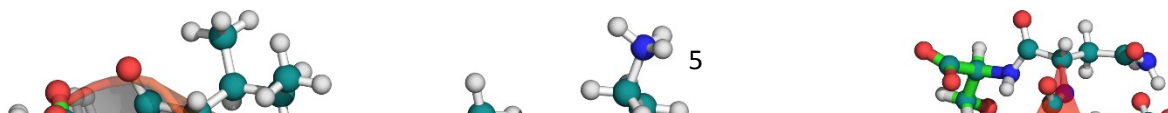


Figure S1. The Ramachandran plots (ϕ - ψ) for twenty nine conformers of the magainin-2 peptide with the amino acid sequence GIGKWLHS AKKFGKAFVGEIMNS. The data points corresponding to the backbone in the magainin-2 peptide backbone are represented by the green circles. The magenta, blue and white regions correspond to the 'favored', 'allowed' and 'forbidden' regions respectively. The black, brown, pale blue and dark blue squares are indicating the 'forbidden', 'allowed', 'beta-sheet' and regions close to beta-sheet character in the conventional Ramachandran plot (ϕ - ψ) respectively.

2. Supplementary Materials S2.



(1)

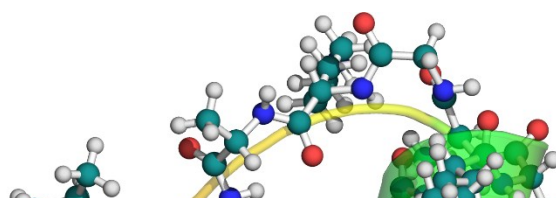
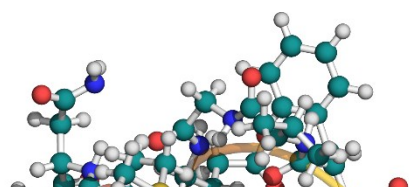
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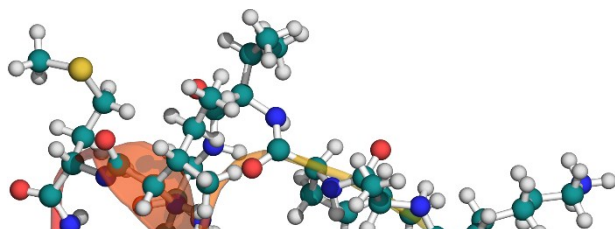
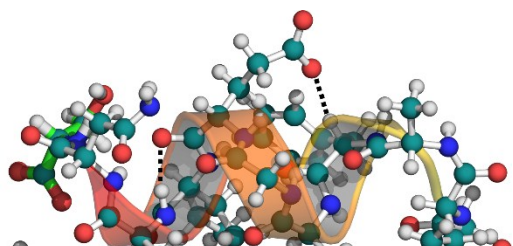
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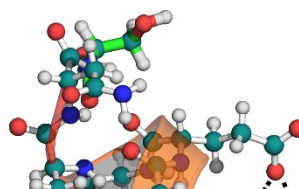
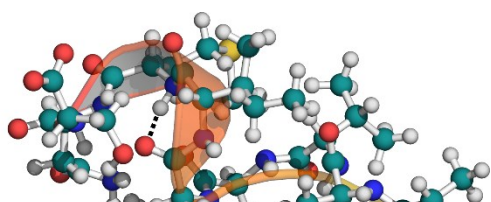
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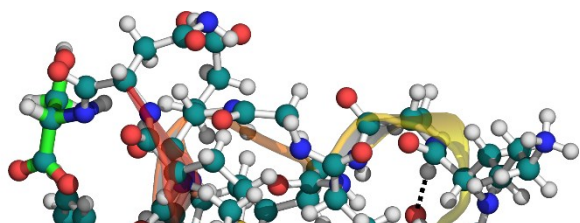
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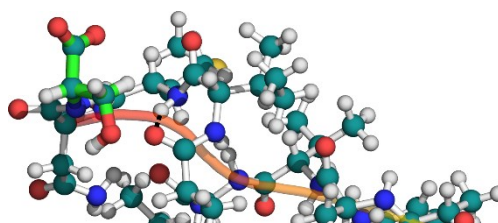
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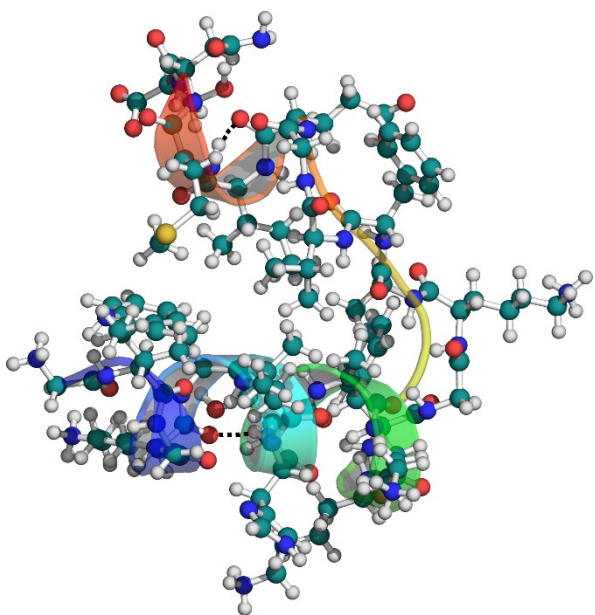


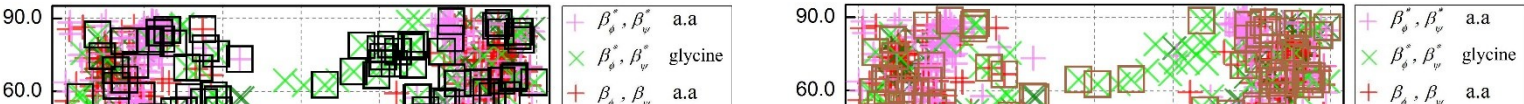
Figure S2. The ball and stick renderings of the magainin-01 to magainin-29 conformers are presented in sub-figures **(1-29)** respectively. The carbon, hydrogen, oxygen, nitrogen and sulphur atoms are indicated by the green, white, red, blue and yellow spheres respectively. The colored ribbon is superimposed on the structures to represent the α -helix with blue and red representing the start and termination of the GIGKWLHSAKKFGKAFVGEIMNS amino acid sequence. Hydrogen bond *BCP* bond-paths possessing a degree of covalent character, that is total local energy density $H(\mathbf{r}_b) < 0$ are indicated by the thick black dashed lines.

3. Supplementary Materials S3.

Table S3. The solution sets of the Poincaré-Hopf relation ($n = 361$), where b , r and c represent the numbers of $BCPs$, $RCPs$ and $CCPs$, see equation (1) of the main text, the topological complexity Σ_{brc} and relative energy ΔE for the molecular graphs of the twenty-nine conformers of magainin-2. The α -helix structure magainin-2 peptide with the twenty-three amino acid sequence GIGKWLHSAKKFGKAFVGEIMNS.

Molecular graph	b	r	c	Σ_{brc}	$\Delta E(\text{au})$
magainin-06	478	145	27	650	0.0000
magainin-18	474	145	31	650	0.0150
magainin-28	473	148	35	656	0.0206
magainin-03	473	149	36	658	0.0268
magainin-12	473	141	28	642	0.0371
magainin-07	462	136	34	632	0.0575
magainin-15	479	148	29	656	0.0580
magainin-16	477	155	38	670	0.0665
magainin-26	453	115	22	590	0.0920
magainin-23	476	149	33	658	0.1178
magainin-13	481	152	31	664	0.1264
magainin-09	480	153	33	666	0.1345
magainin-19	472	142	30	644	0.1459
magainin-08	459	122	23	604	0.1513
magainin-14	469	144	35	648	0.1594
magainin-24	467	133	26	626	0.1605
magainin-04	459	118	19	596	0.1644
magainin-20	451	111	20	582	0.1821
magainin-11	474	145	31	650	0.1859
magainin-27	470	141	31	642	0.1886
magainin-29	469	137	28	634	0.1960
magainin-10	466	138	32	636	0.1981
magainin-01	473	148	35	656	0.1987
magainin-21	465	133	28	626	0.2008
magainin-22	459	118	19	596	0.2134
magainin-17	469	140	31	640	0.2165
magainin-02	469	146	37	652	0.2251
magainin-25	463	123	20	606	0.2343
magainin-05	464	132	28	624	0.2807

4. Supplementary Materials S4.



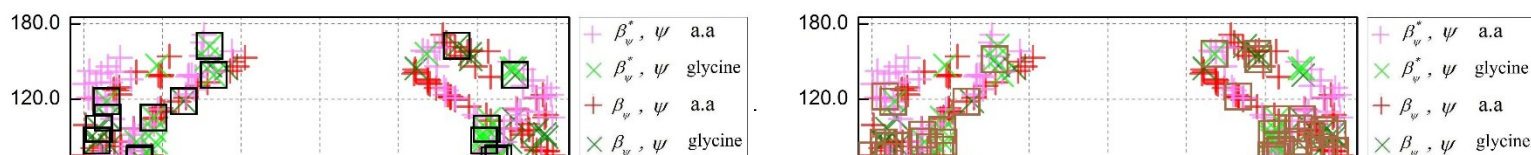
(a)

(b)

(c)

Figure 4. QTAIM interpreted Ramachandran plots $\{(\beta_\phi, \beta_\phi^*), (\beta_\psi, \beta_\psi^*)\}$ of the backbone shared-shell *BCPs* for the complete set of magainin-2 peptide molecular graphs are presented in sub-figure (a-c). When the nomenclature (x-y) is used the ‘-’ is to be interpreted as a hyphen and not a subtraction sign, the ‘,’ is to be interpreted as indicating that the bracketed quantities are superimposed onto the same axes. The pale green crosses indicate the β_ϕ^* and β_ψ^* (the least preferred responses), the dark green crosses represent the β_ϕ and β_ψ (the most preferred responses) for the glycine amino acid *BCPs*. The corresponding quantities for the remaining amino acids are given by the pink (β_ϕ^* and β_ψ^*) and red (β_ϕ and β_ψ) pluses respectively in the magainin-2 peptide structure. In sub-figure (b) we superimpose on the $\{(\beta_\phi, \beta_\phi^*), (\beta_\psi, \beta_\psi^*)\}$ plot the black (sub-figure (a)), brown (sub-figure (b)), pale blue and dark blue squares (sub-figure (c)) that indicate the ‘forbidden’, ‘allowed’, ‘beta sheet’ inside of the ‘allowed’ region but close to beta-sheet region from the conventional Ramachandran plot (ϕ - ψ) respectively.

5. Supplementary Materials S5.



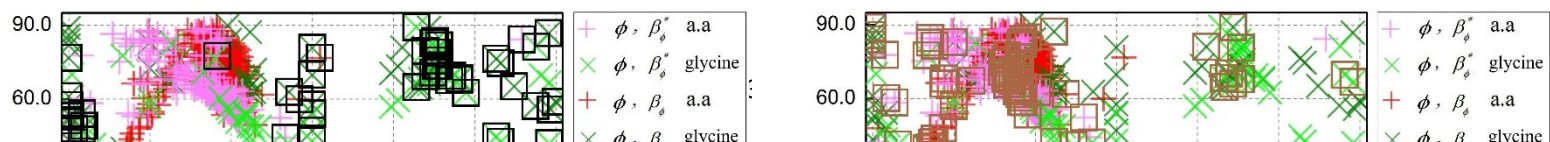
(a)

(b)

(c)

Figure S5. Plots of β_{ψ}^* , β_{ψ} versus ψ of the backbone shared-shell *BCPs* for the complete set of 29 magainin-2 peptide molecular graphs are presented in sub-figures (a-c). See the figure caption of **Figure S4** for further details.

6. Supplementary Materials S6.



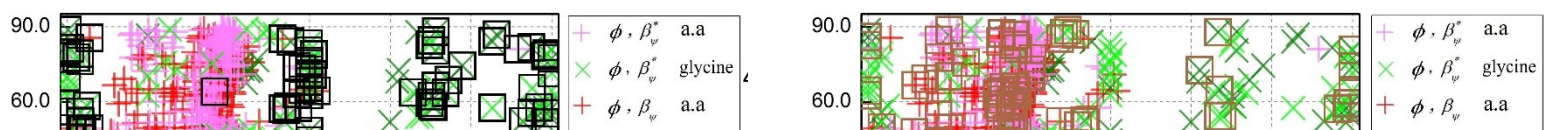
(a)

(b)

(c)

Figure S6. Plots of ϕ versus response β_ϕ^* , β_ϕ of the backbone shared-shell *BCPs* for the complete set of 29 magainin-2 peptide molecular graphs are presented in sub-figures (a-c). See the figure caption of **Figure S4** for further details.

7. Supplementary Materials S7



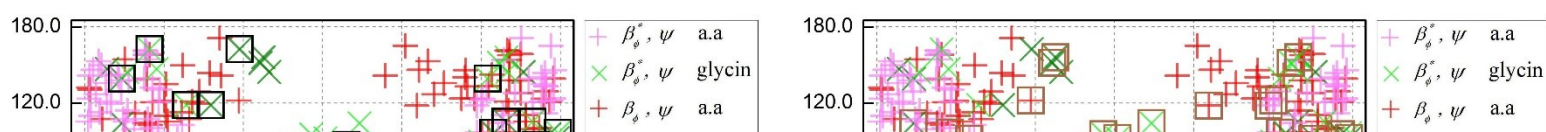
(a)

(b)

(c)

Figure S7. Plots of ϕ versus the response β^*_{ψ} , β_{ψ} of the backbone shared-shell *BCPs* for the complete set of 29 magainin-2 peptide molecular graphs are presented in sub-figures (a-c). See the figure caption of **Figure S4** for further details.

8. Supplementary Materials S8.



(a)

(b)

(c)

Figure S8. Plots of ψ versus the response β_ϕ^* , β_ϕ versus ψ of the backbone shared-shell *BCPs* for the complete set of 29 magainin-2 peptide molecular graphs are presented in sub-figures **(a-c)**. See the figure caption of **Figure S4** for further details.