Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Representative structures from Hierarchical clustering result

Deciphering the Shape Selective Conformational Equilibrium of *E*- and *Z*-Locked Azobenzene-Tetraethyl Ammonium Ion in Regulating Photo-switchable K^+-ion Channel Blocking

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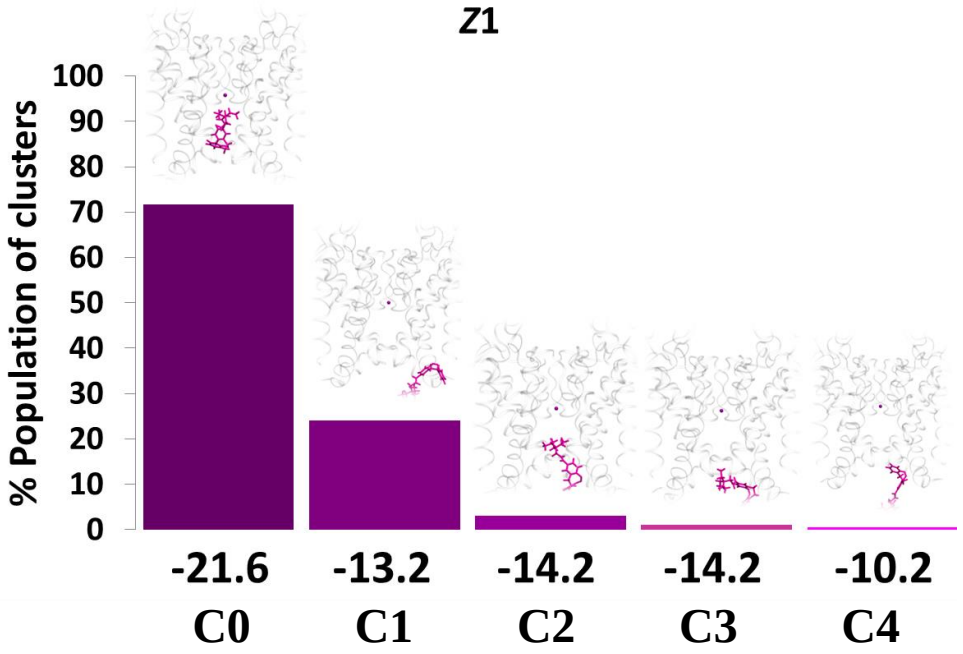
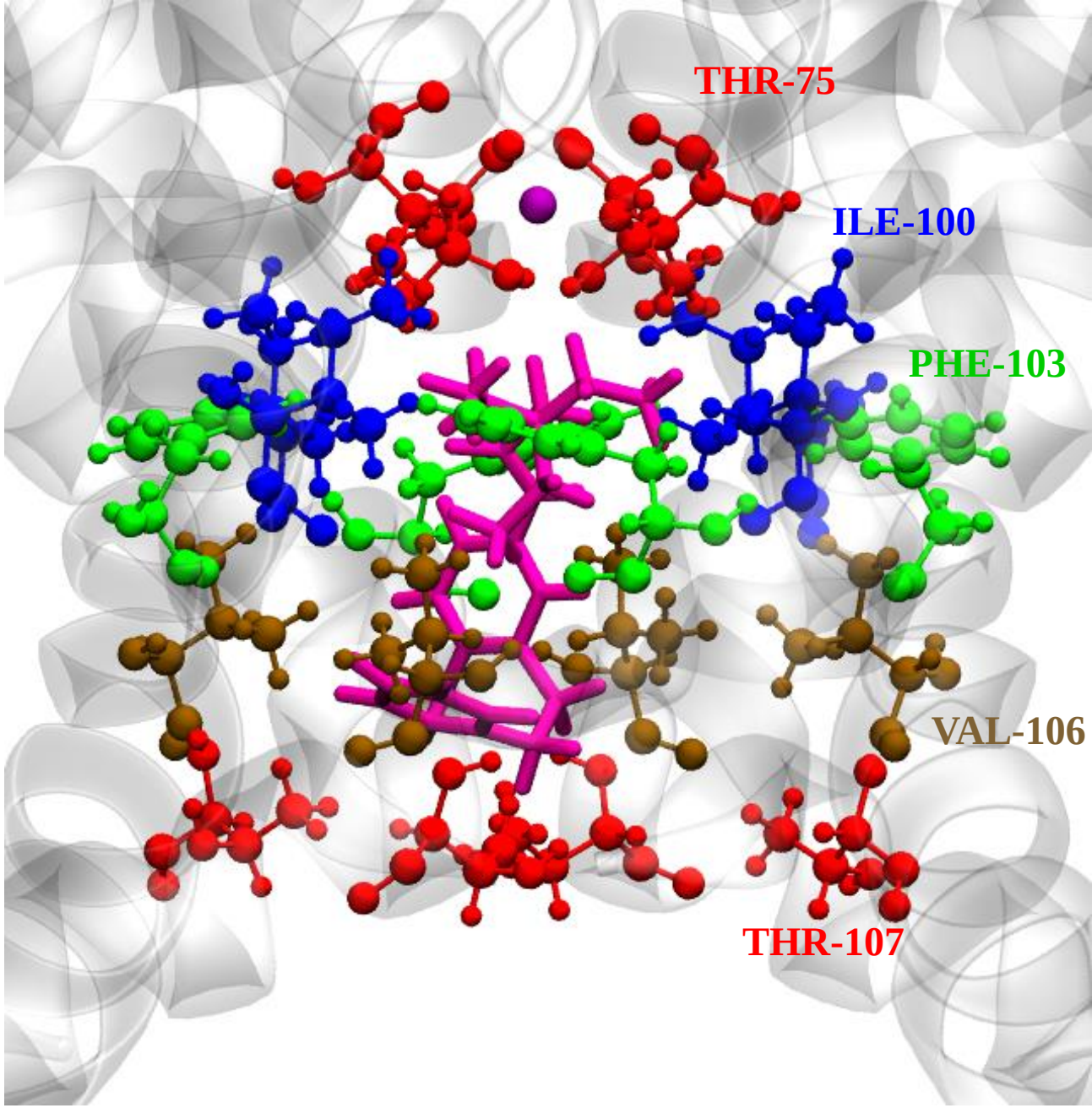
[b]Department of Chemistry, University of Calicut, Calicut University P. O., Malappuram, Kerala, India - 673 635. E-mail: susmita@uoc.ac.in

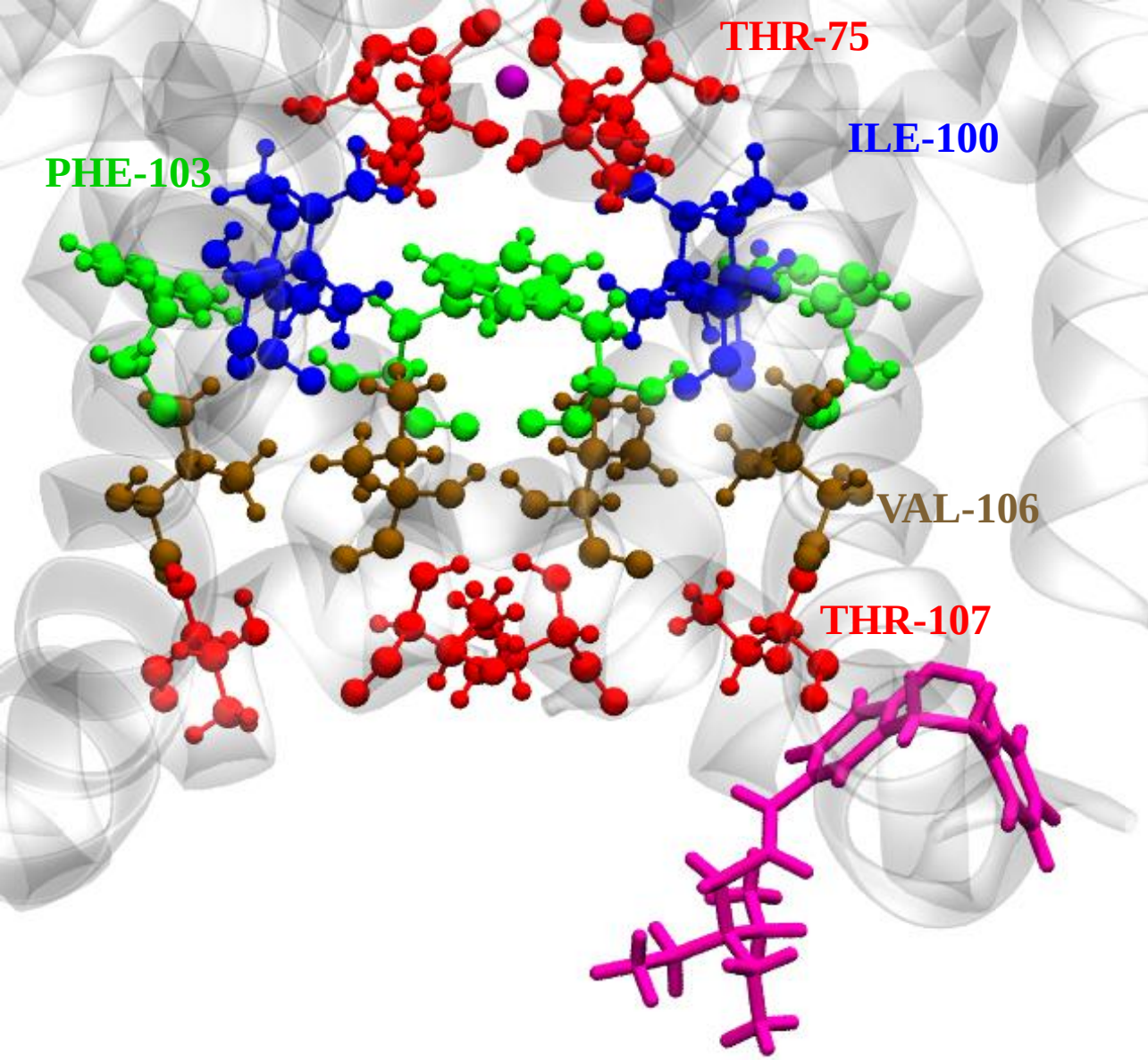


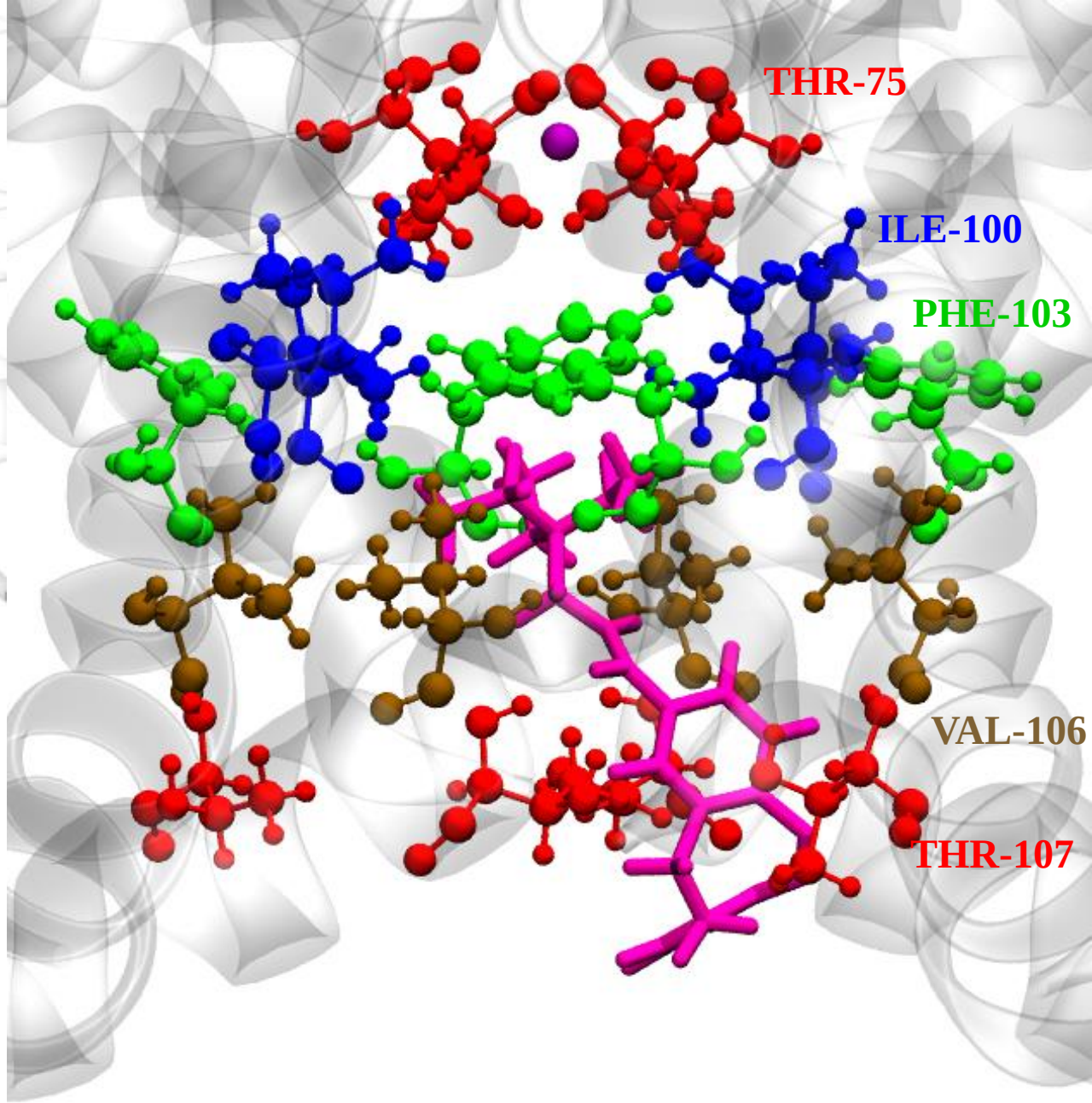
Cn (n = 0 – 1) indicate different clusters. The percentage population of clusters is given on the Y-axis. Corresponding binding energy (B.E.) is given in kcal/mol on the X-axis. Protein is represented in new cartoon model with K^+-ion (purple ball), and *Z*-LAB-TEA is shown in stick model (magenta colour).



***Z*1(C0)**

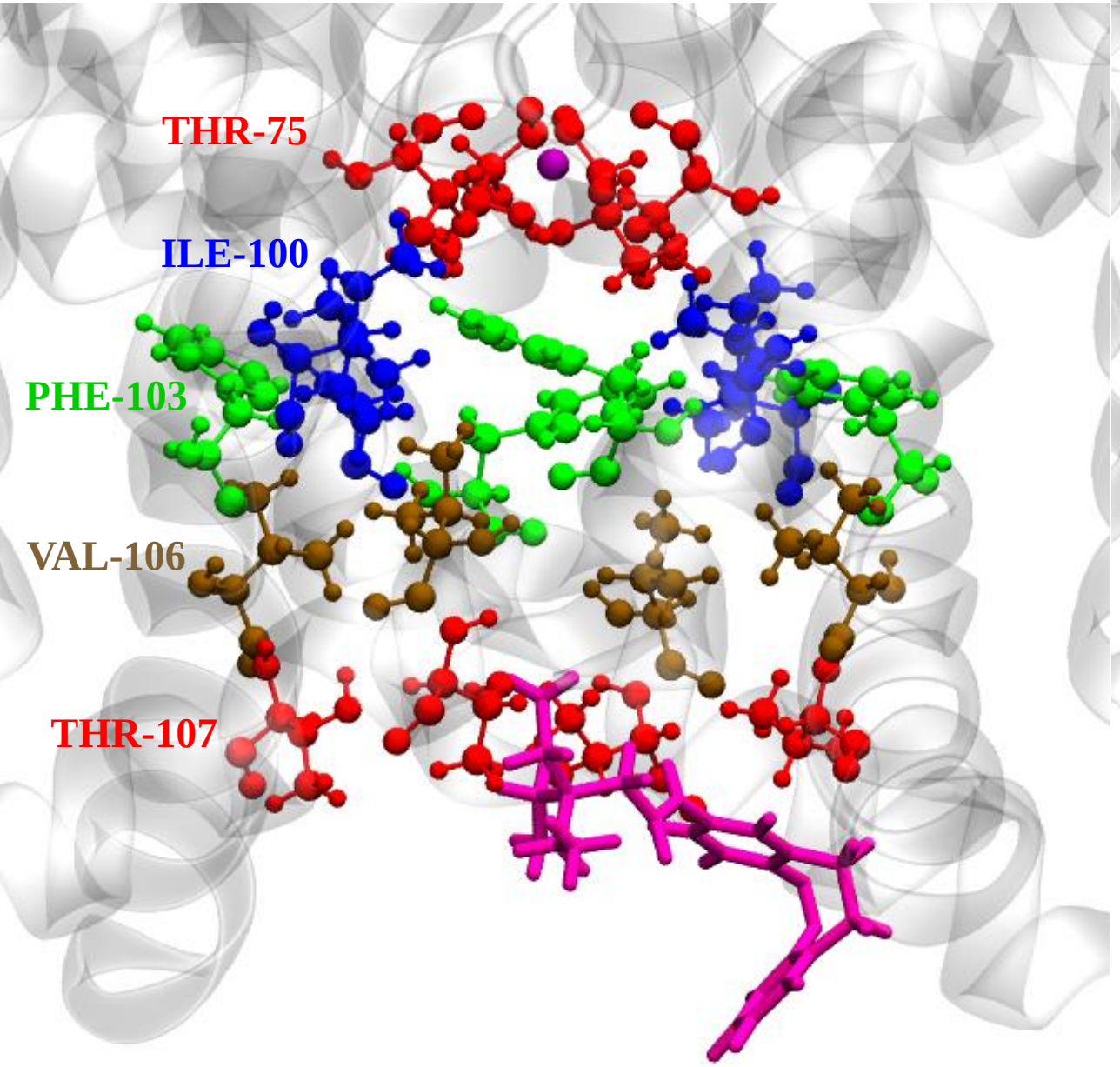
MM/PBSA Binding energy = -21.6 kcal/mol

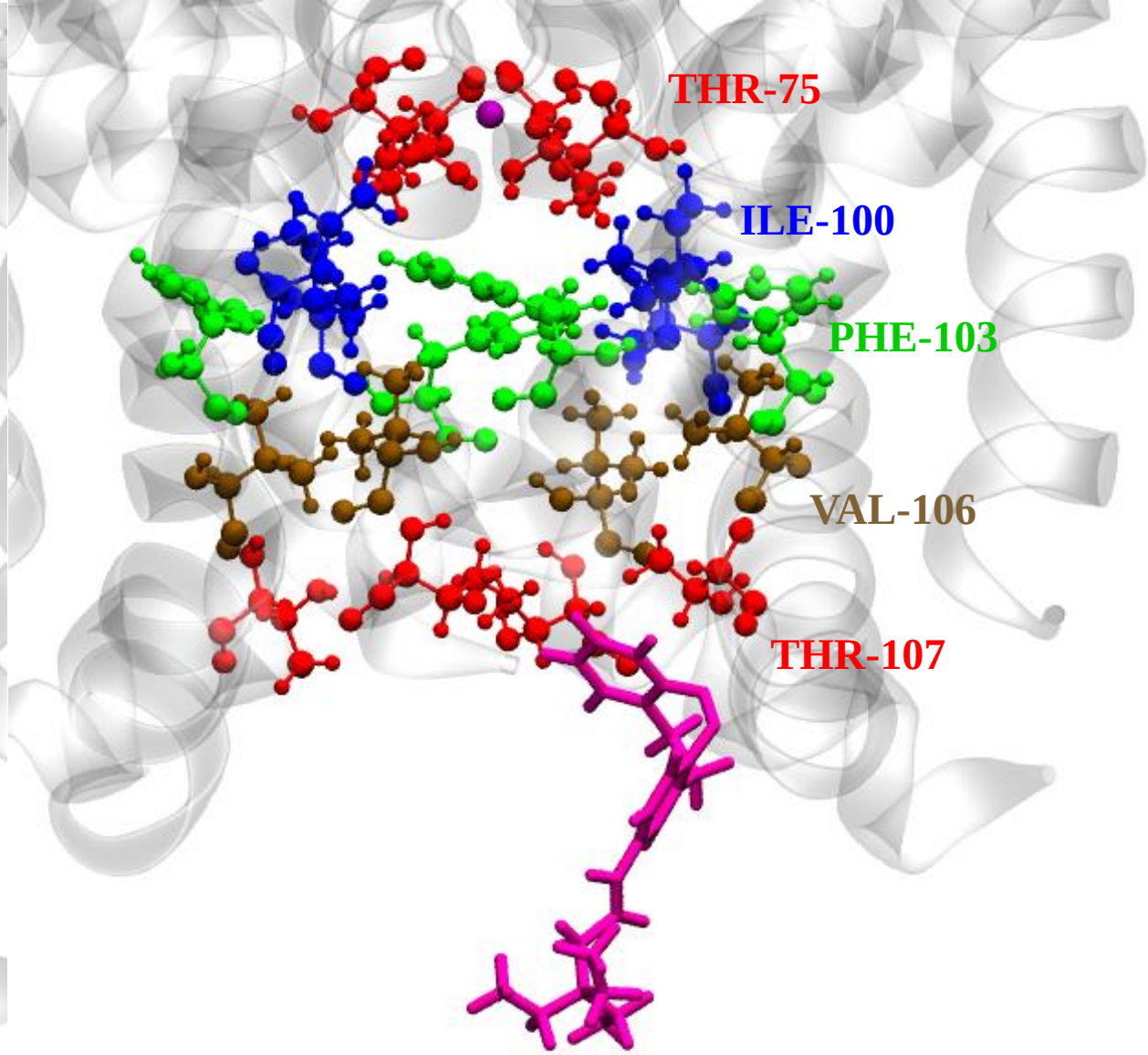




Z1 (C1)
MM/PBSA Binding energy = -13.2 kcal/mol

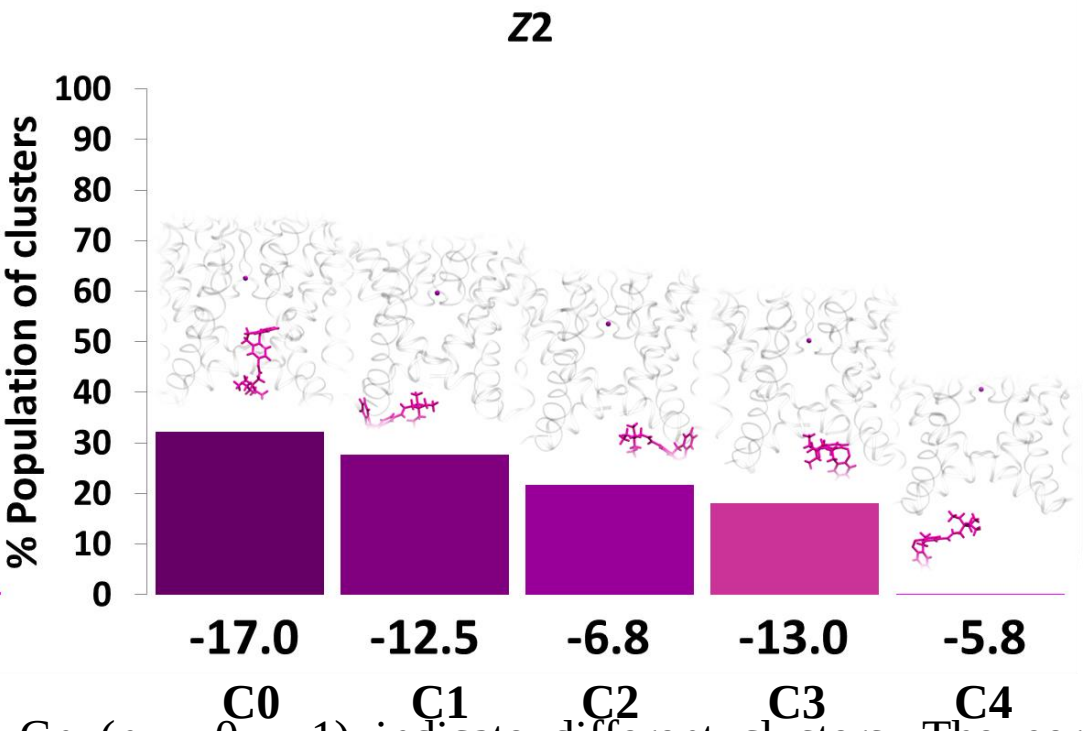
Z1 (C2)
MM/PBSA Binding energy = -14.2 kcal/mol





***Z*1 (C3)**
MM/PBSA Binding energy = -14.2 kcal/mol

***Z*1 (C4)**
MM/PBSA Binding energy = -10.2 kcal/mol



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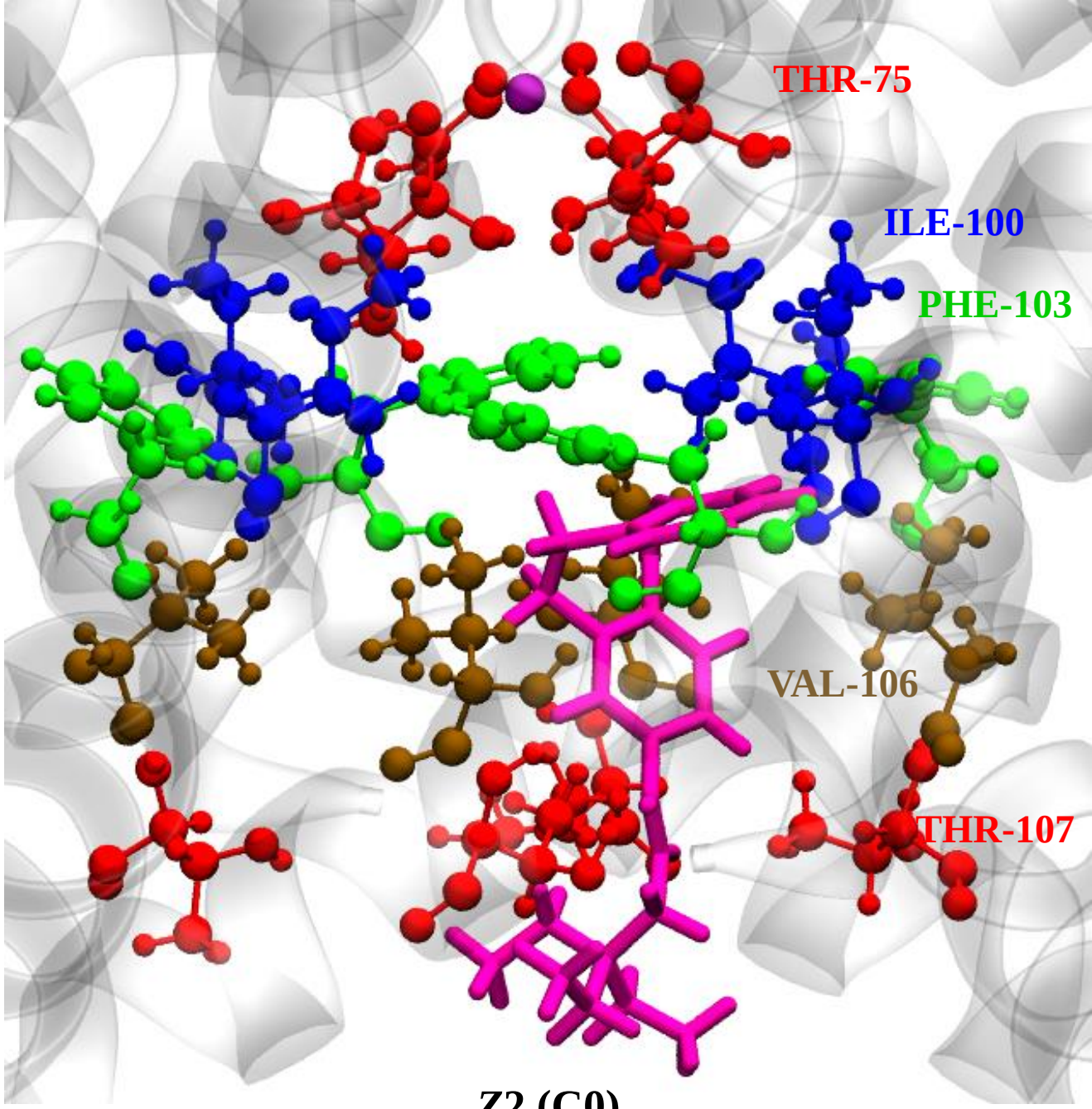
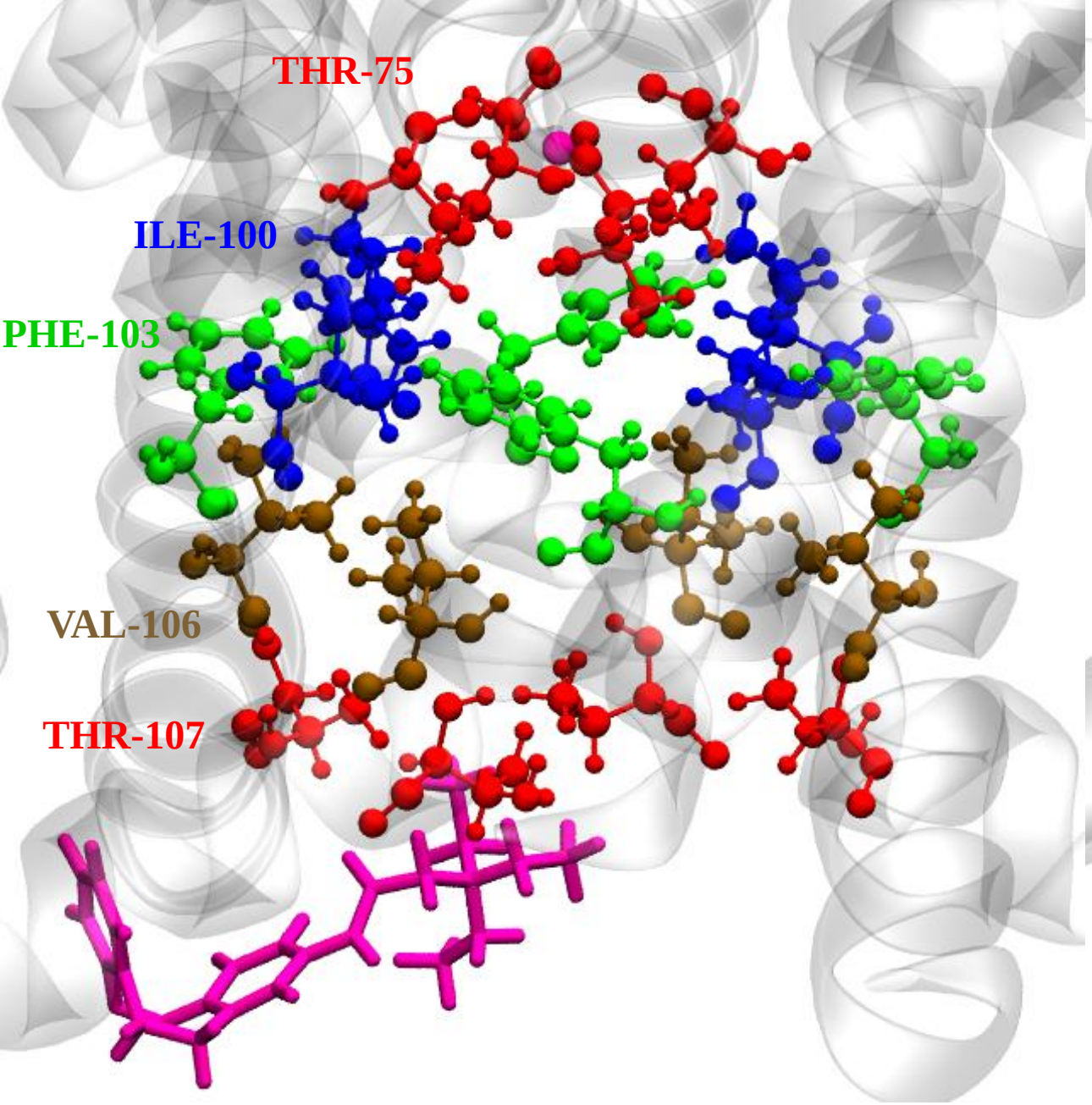
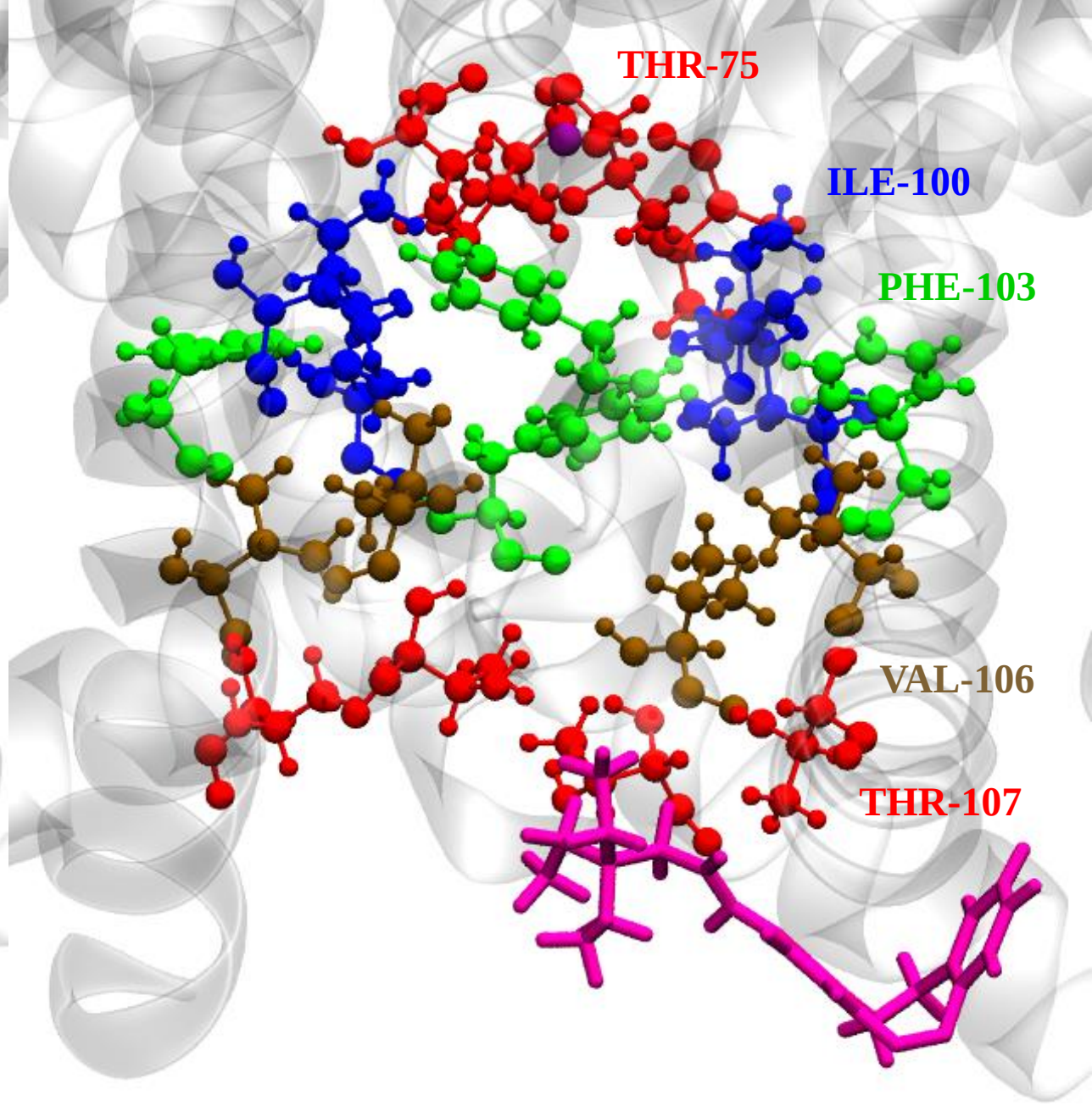


***Z*2 (C0)**

MM/PBSA Binding energy = -17.0 kcal/mol



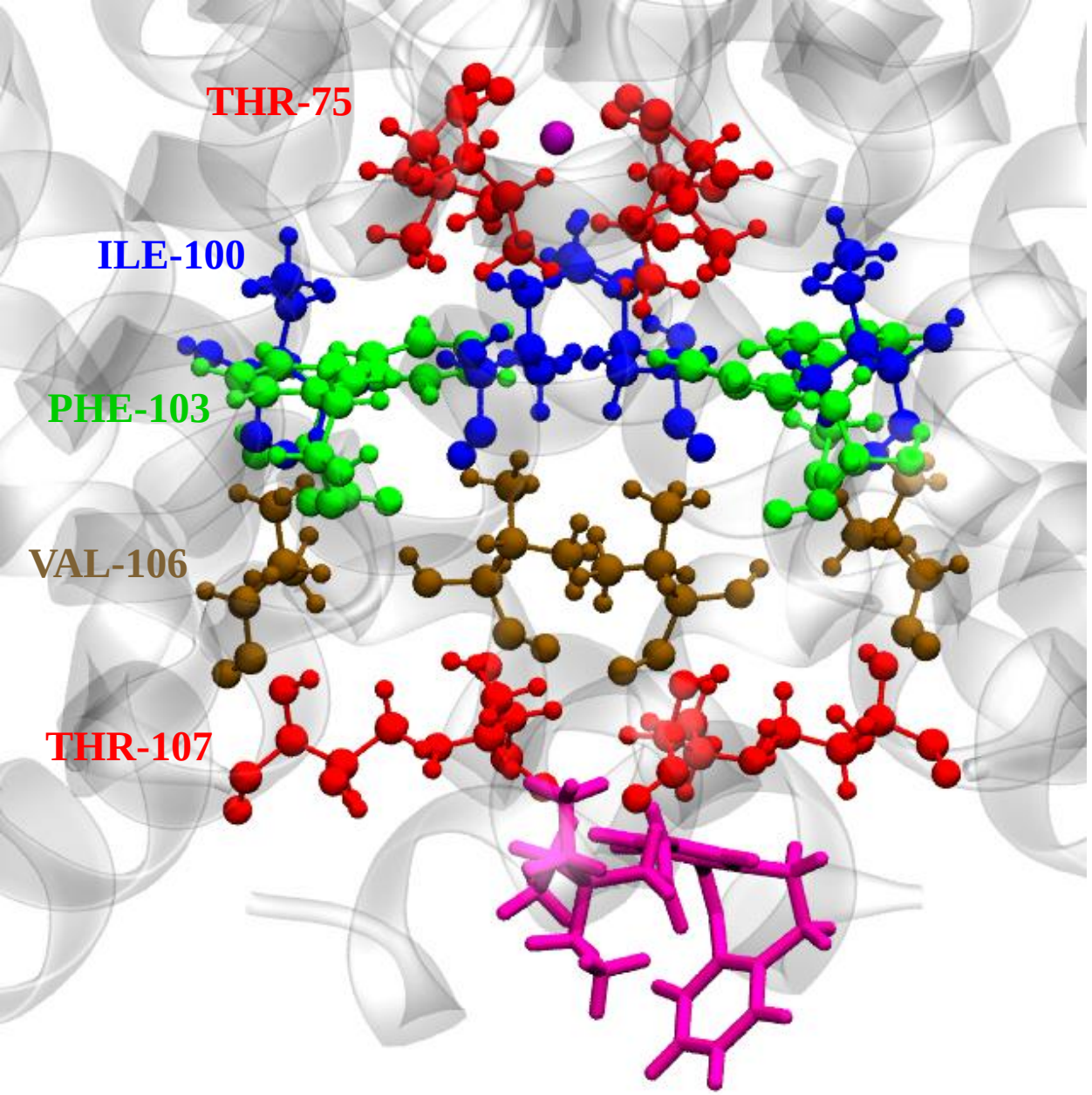


***Z*2 (C1)**

MM/PBSA Binding energy = -12.5 kcal/mol

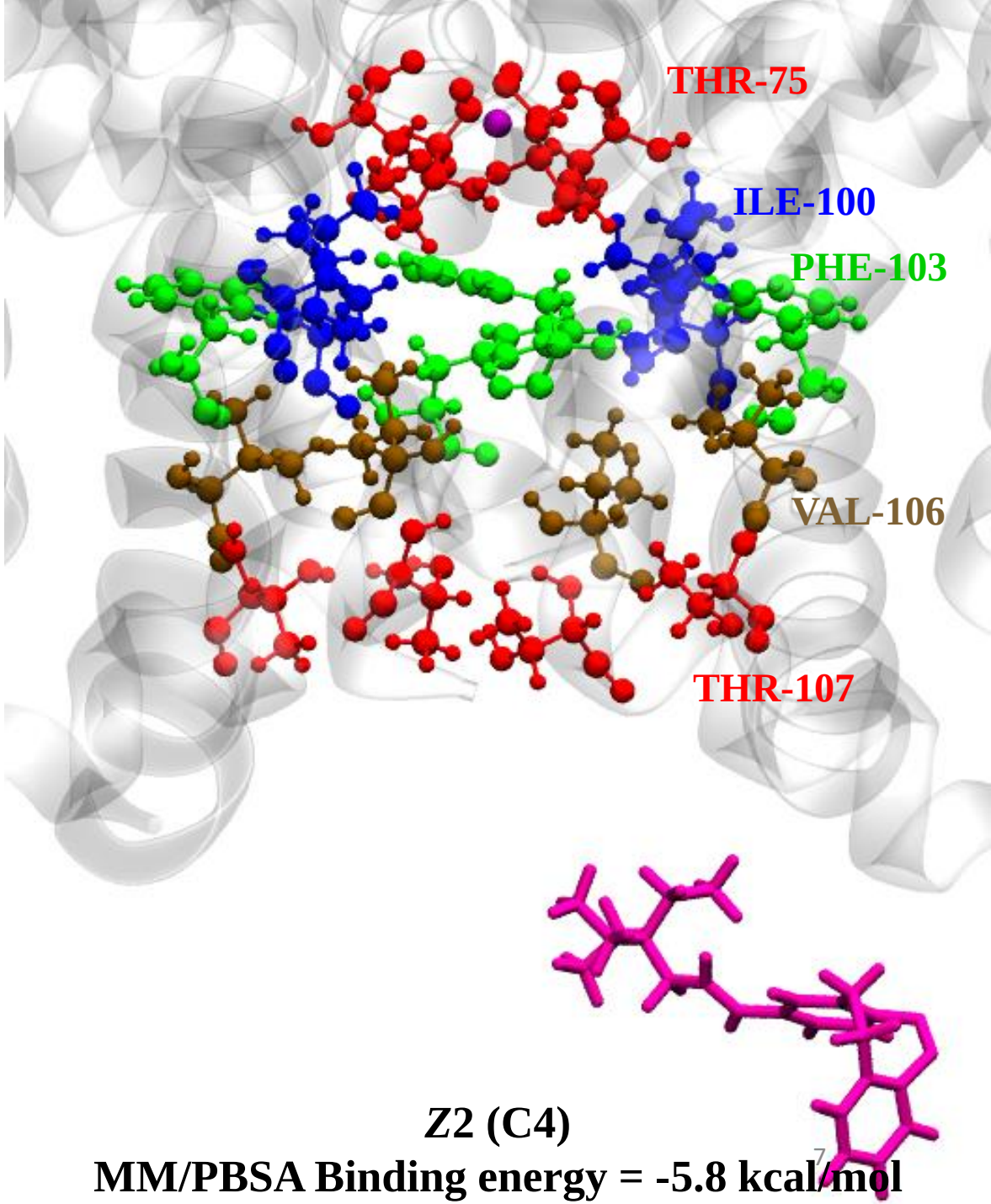
***Z*2 (C2)**

MM/PBSA Binding energy = -6.8 kcal/mol



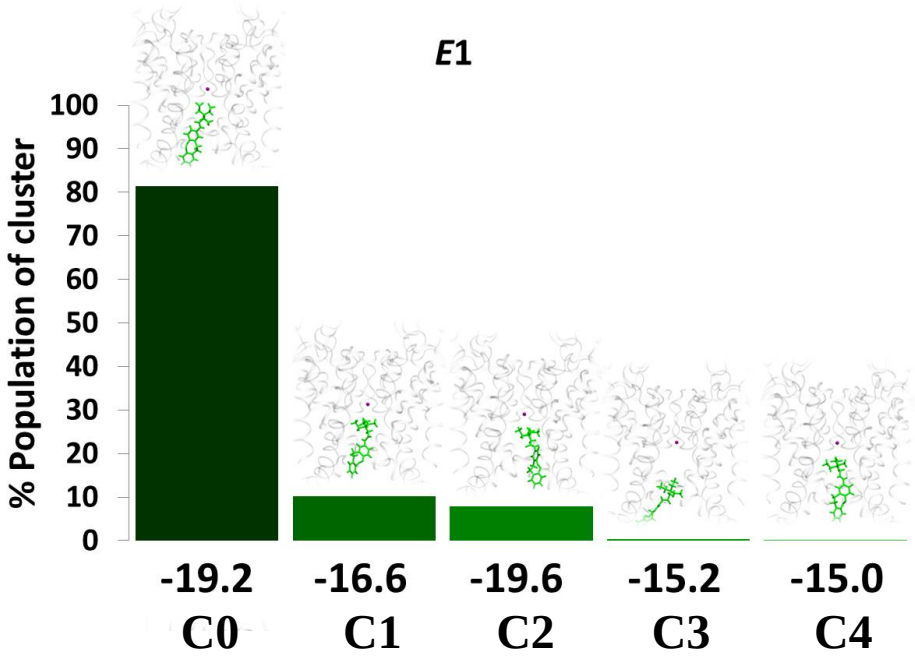
*Z*2 (C3)

MM/PBSA Binding energy = -13.0 kcal/mol



*Z*2 (C4)

MM/PBSA Binding energy = -5.8 kcal/mol



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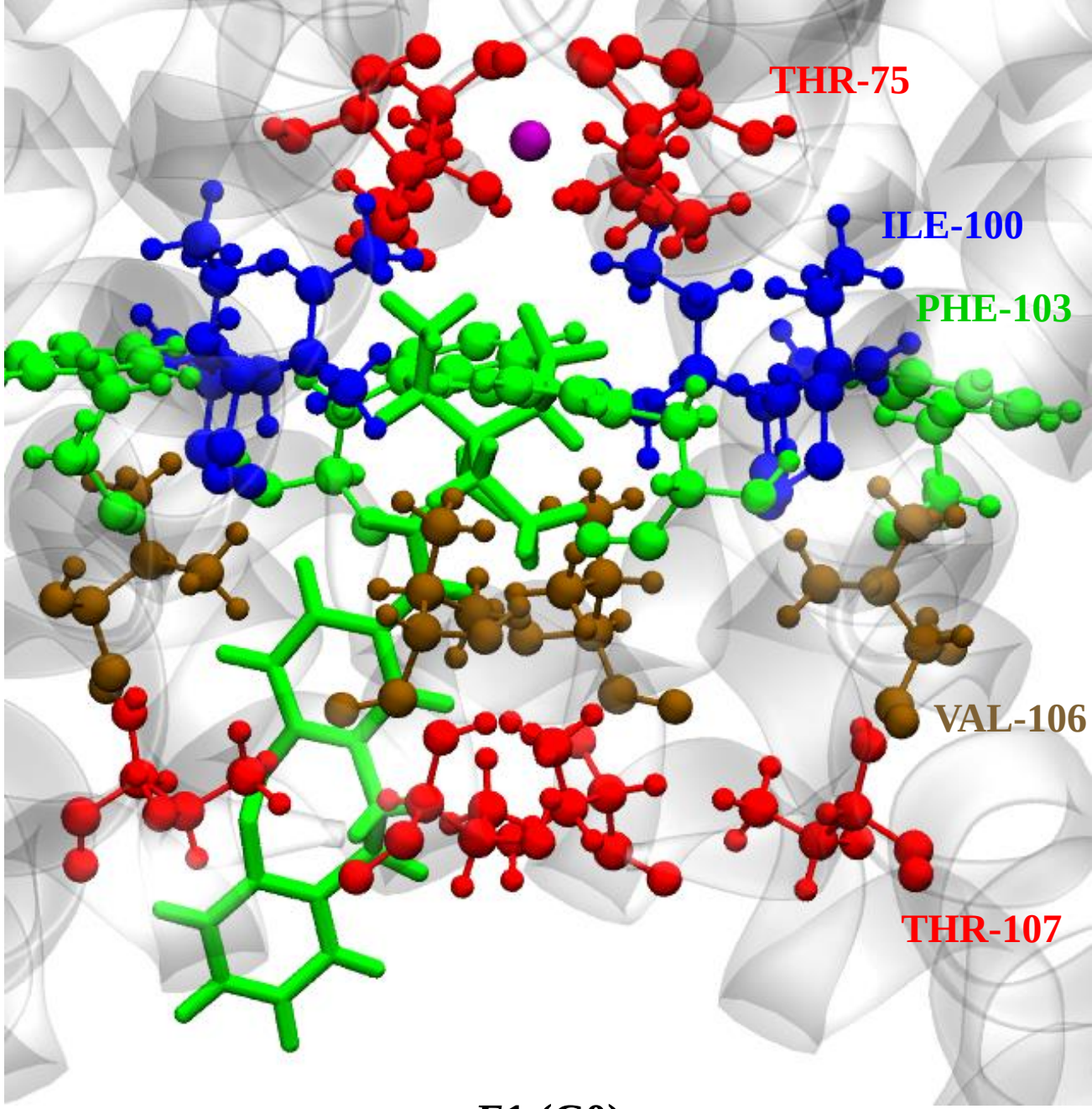
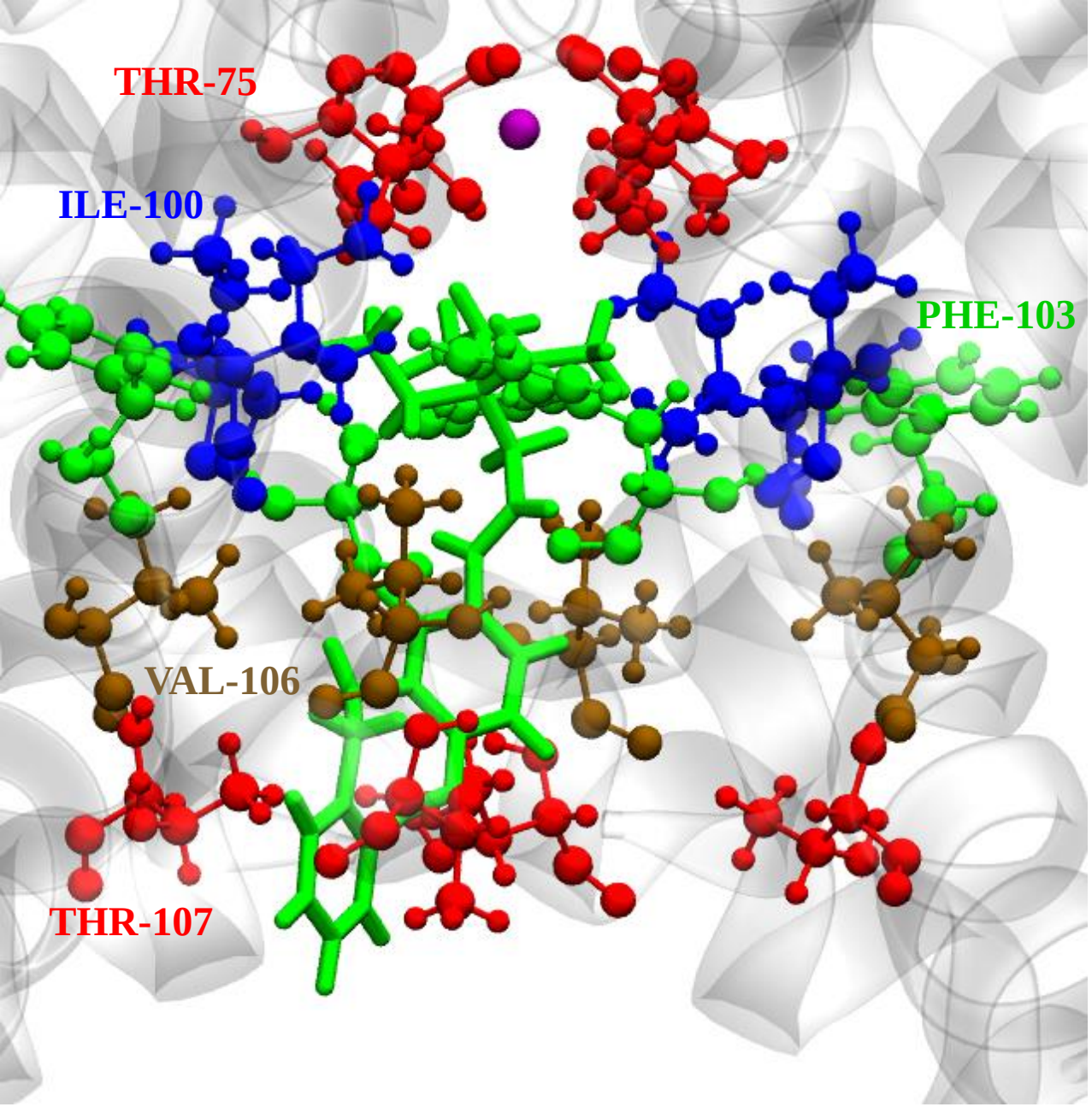
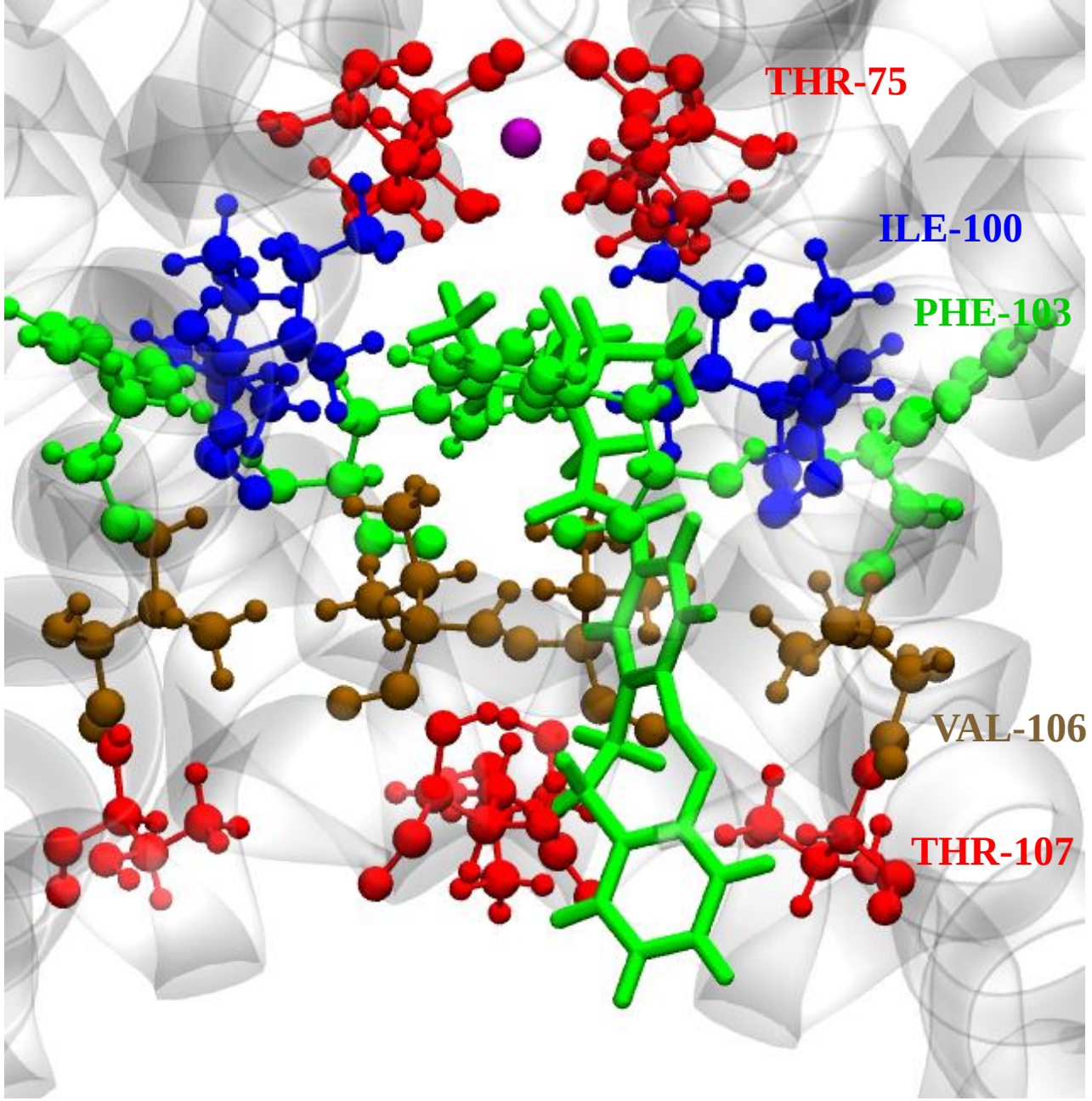


***E*1 (C0)**

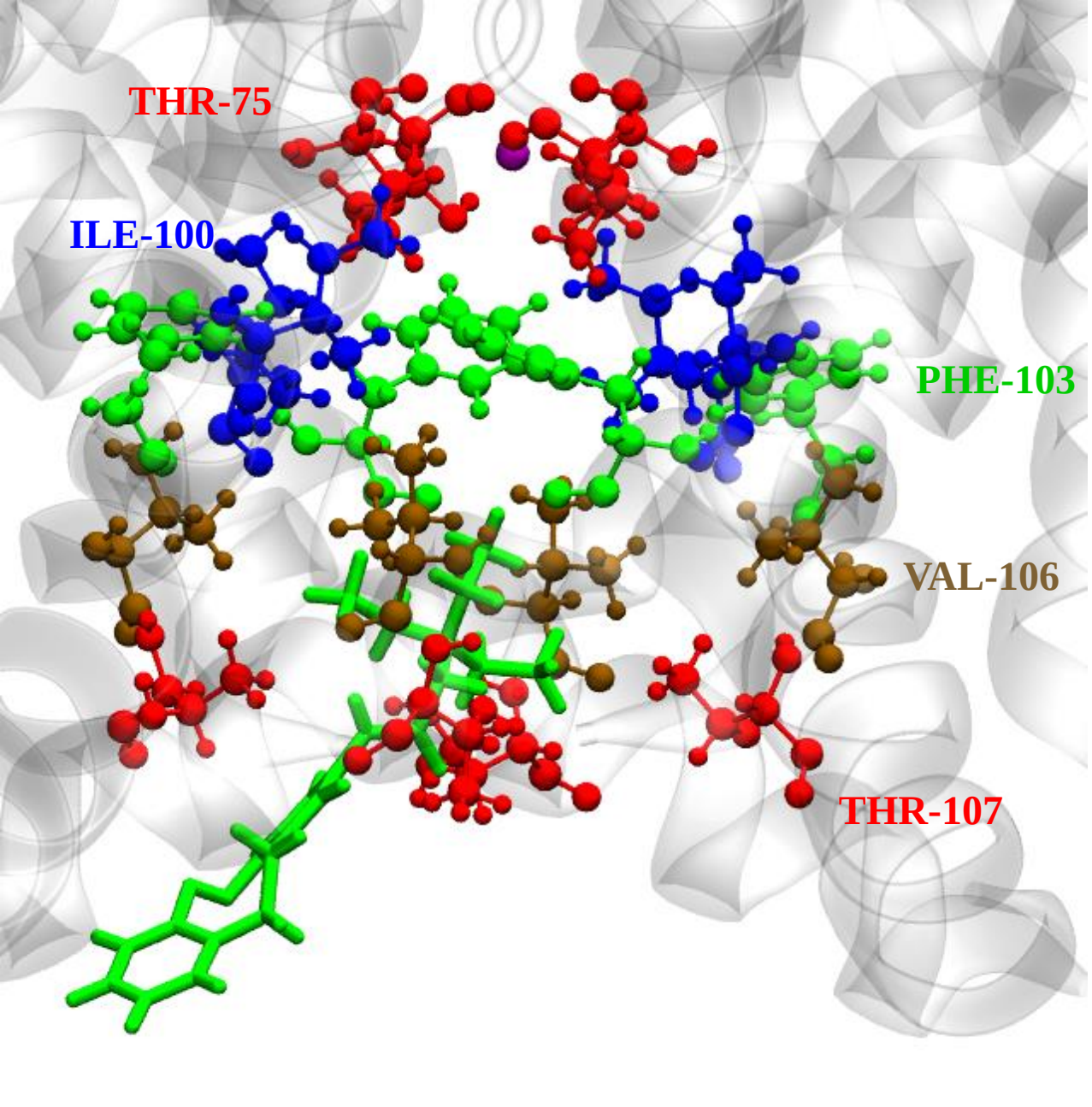
MM/PBSA Binding energy = -19.2 kcal/mol

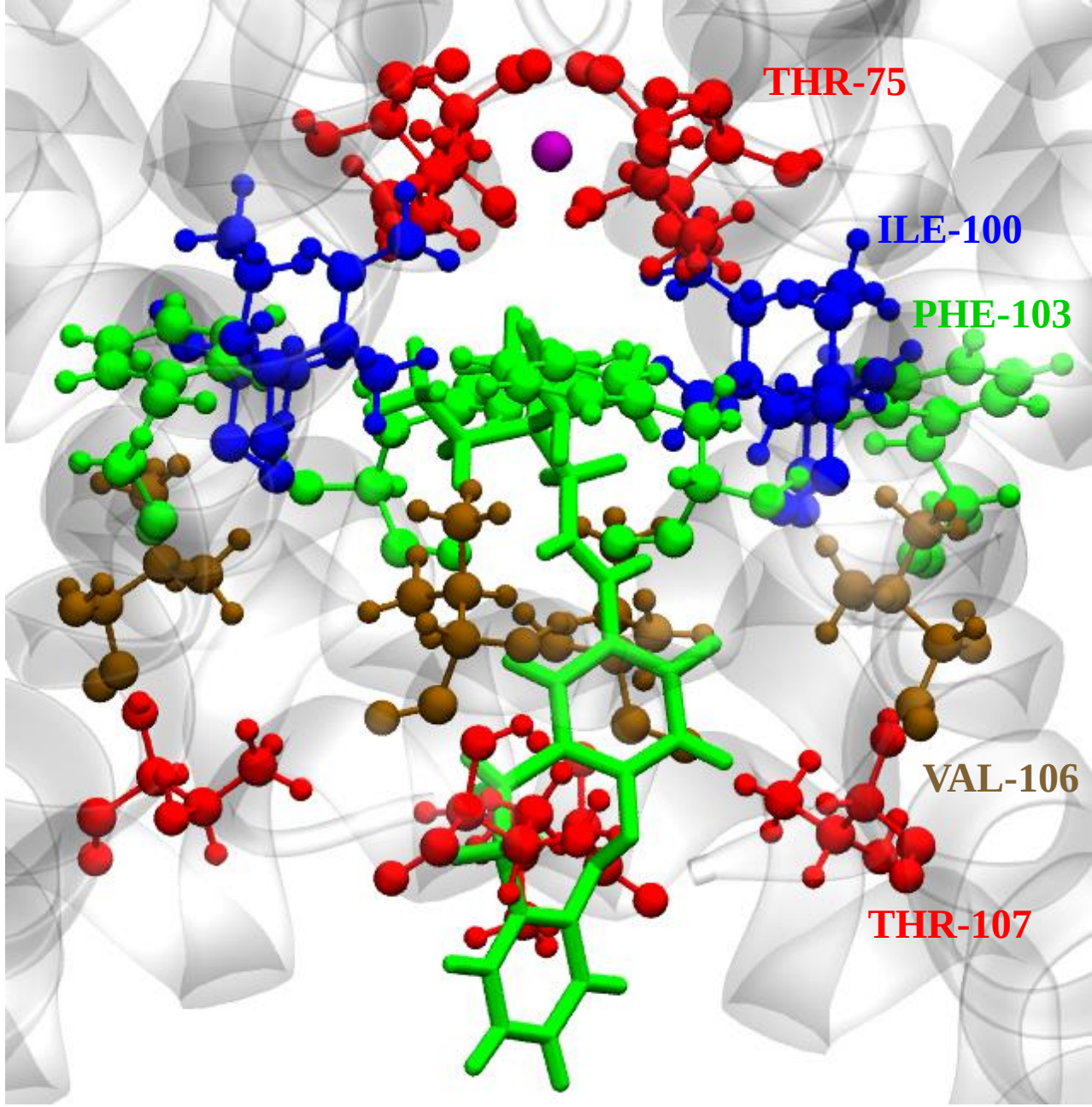




***E*1 (C1)**
MM/PBSA Binding energy = -16.6 kcal/mol

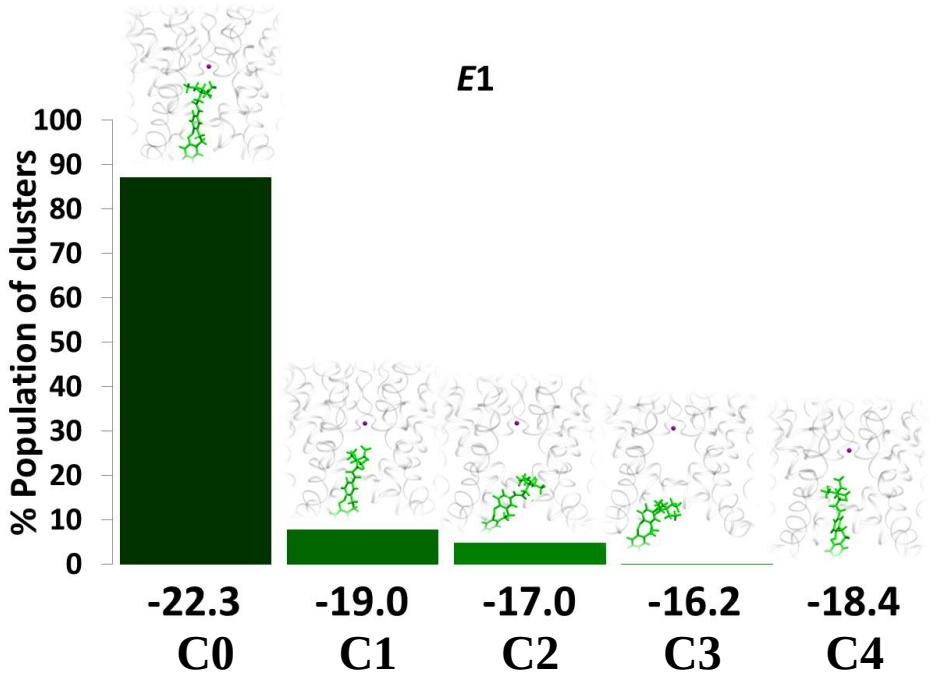
***E*1 (C2)**
MM/PBSA Binding energy = -19.6 kcal/mol





***E*1 (C3)**
MM/PBSA Binding energy = -15.2 kcal/mol

***E*1 (C4)**
MM/PBSA Binding energy = -15.0 kcal/mol



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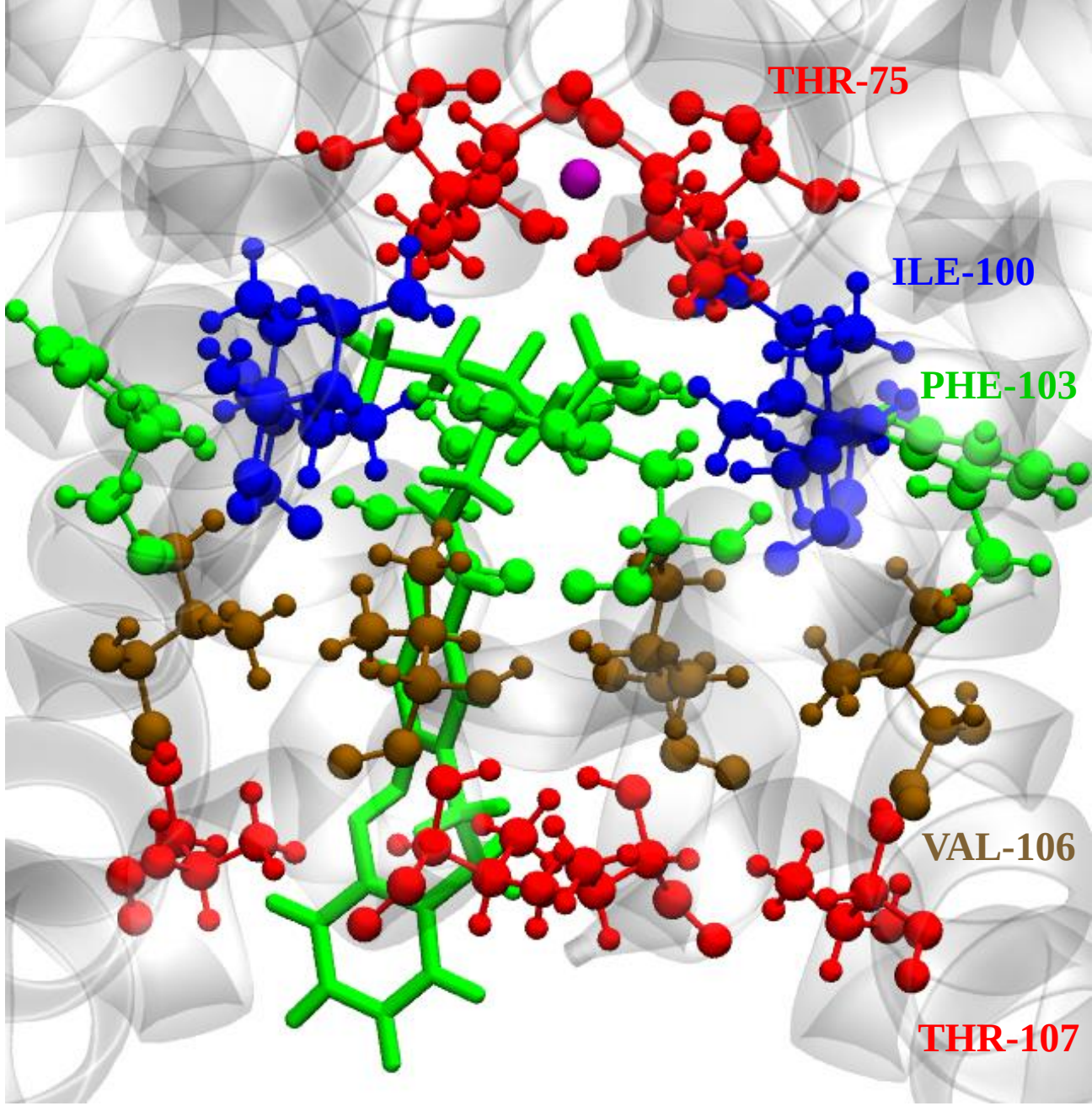
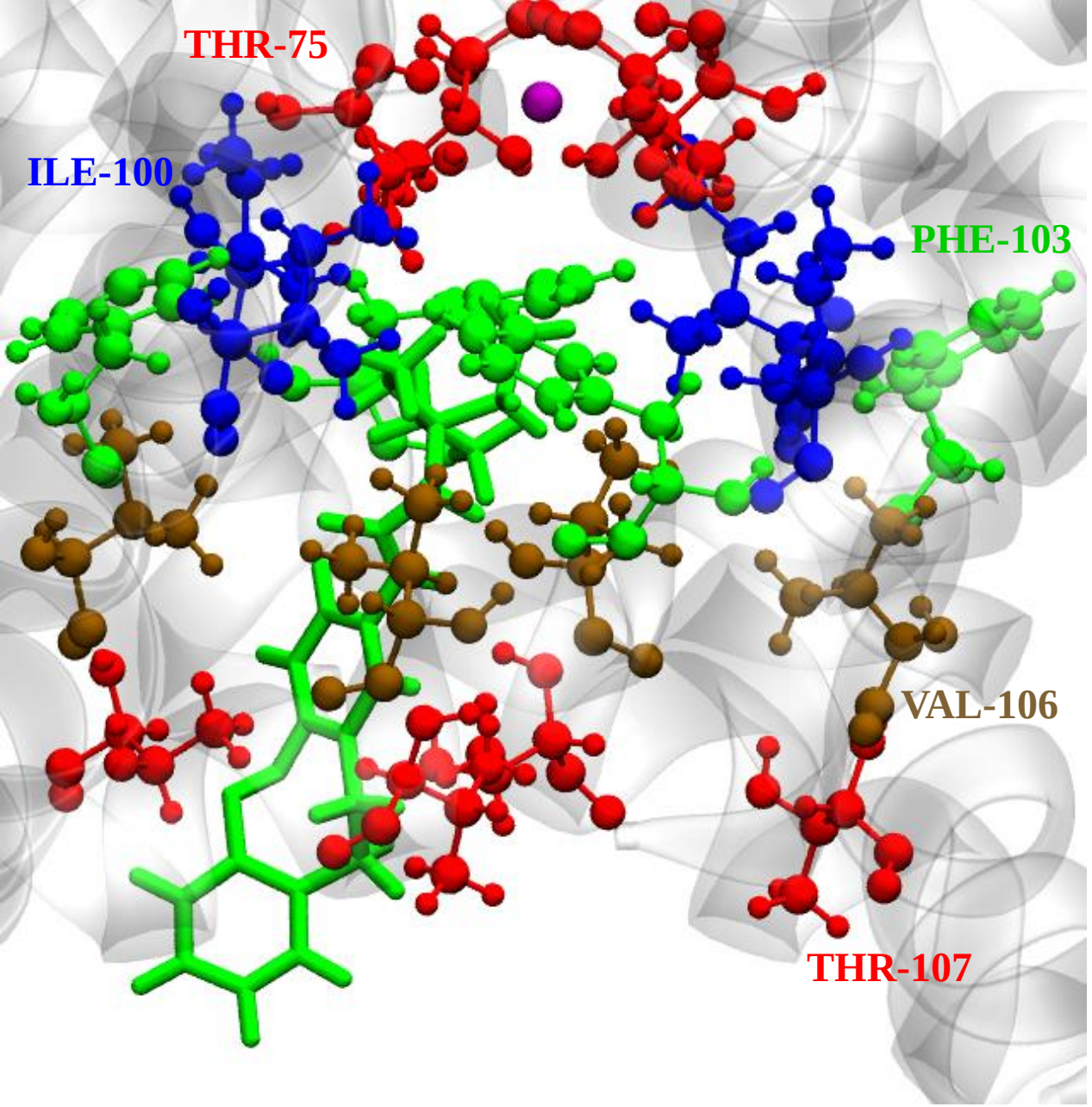
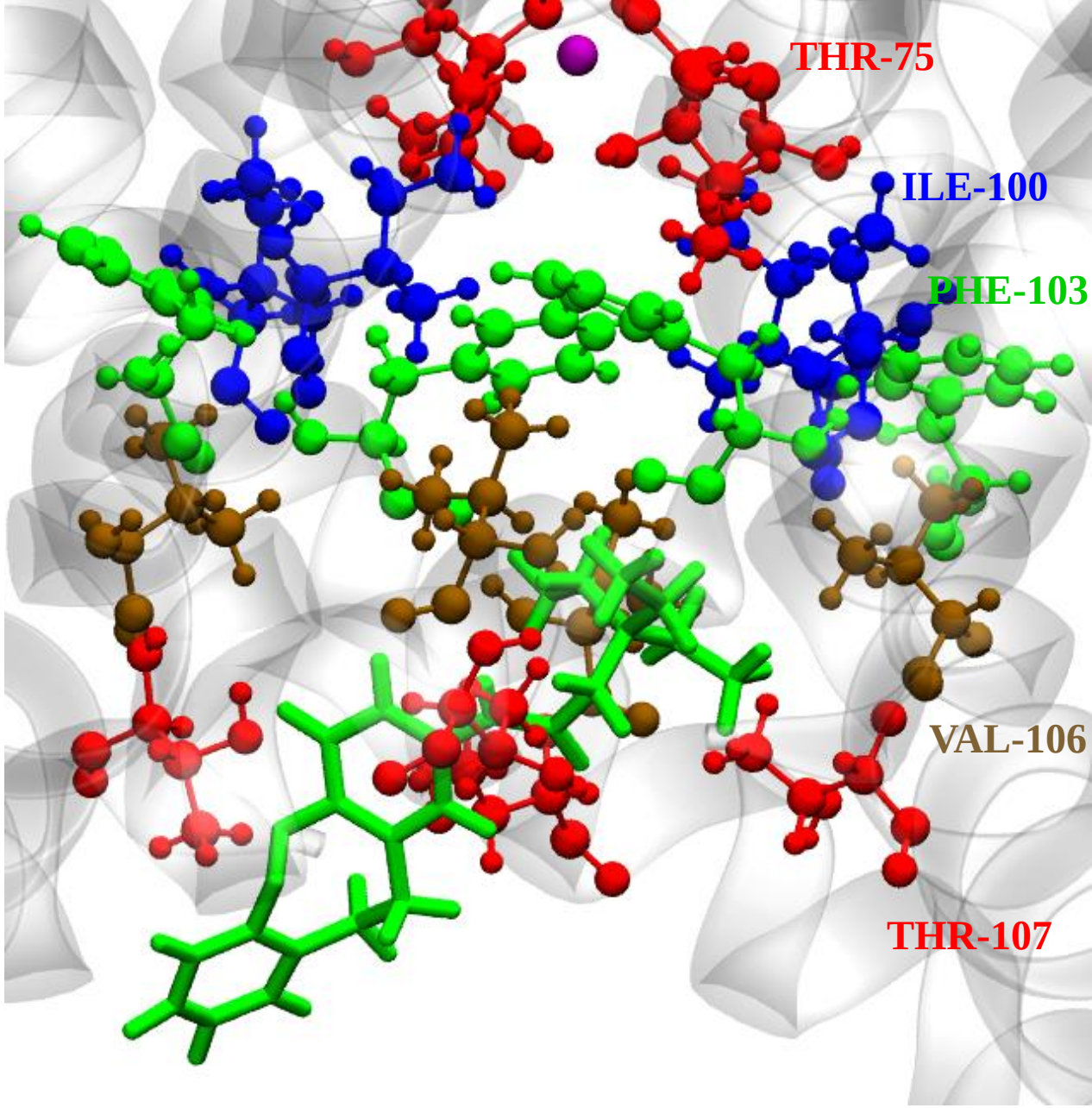


***E*1 (C0)**

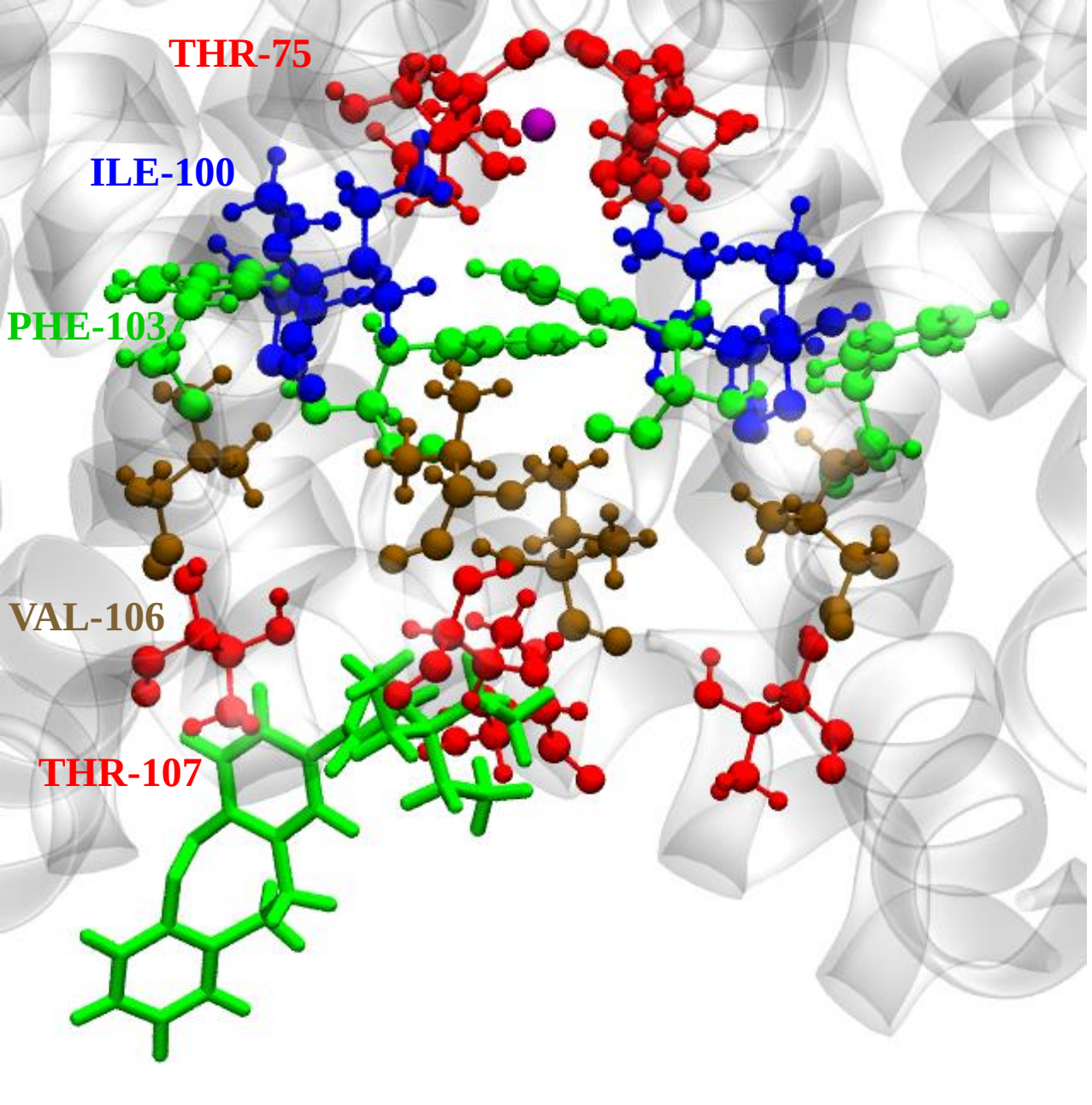
MM/PBSA Binding energy = -22.3 kcal/mol

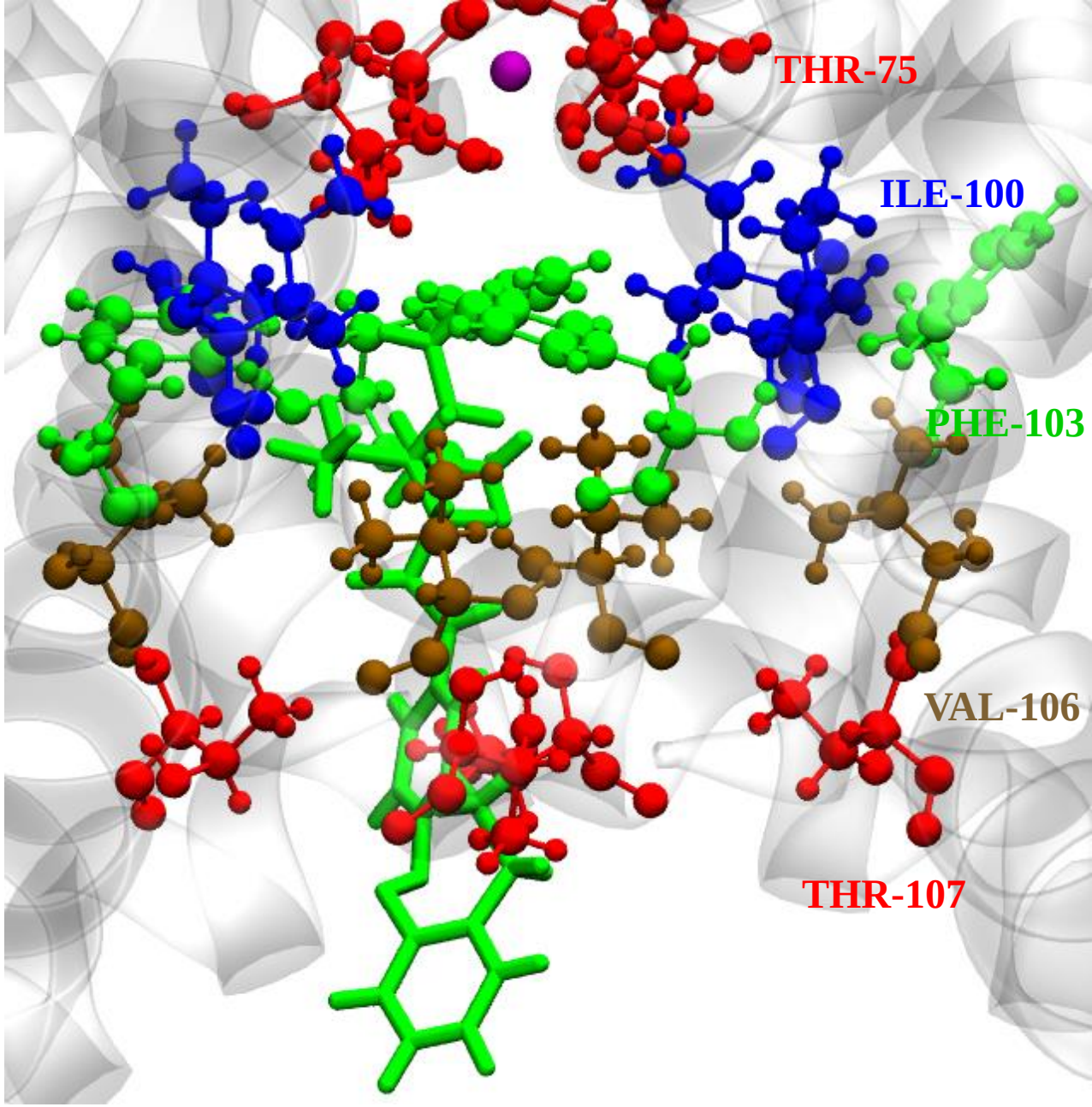




***E*1 (C1)**
MM/PBSA Binding energy = -19.0 kcal/mol

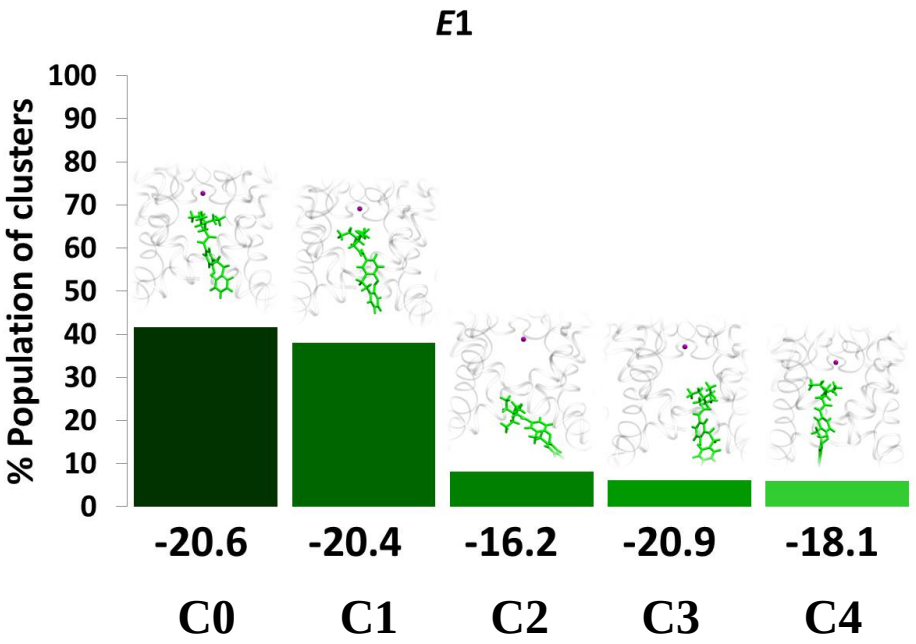
***E*1 (C2)**
MM/PBSA Binding energy = -17.0 kcal/mol





***E*1 (C3)**
MM/PBSA Binding energy = -16.2 kcal/mol

***E*1 (C4)**
MM/PBSA Binding energy = -18.4 kcal/mol



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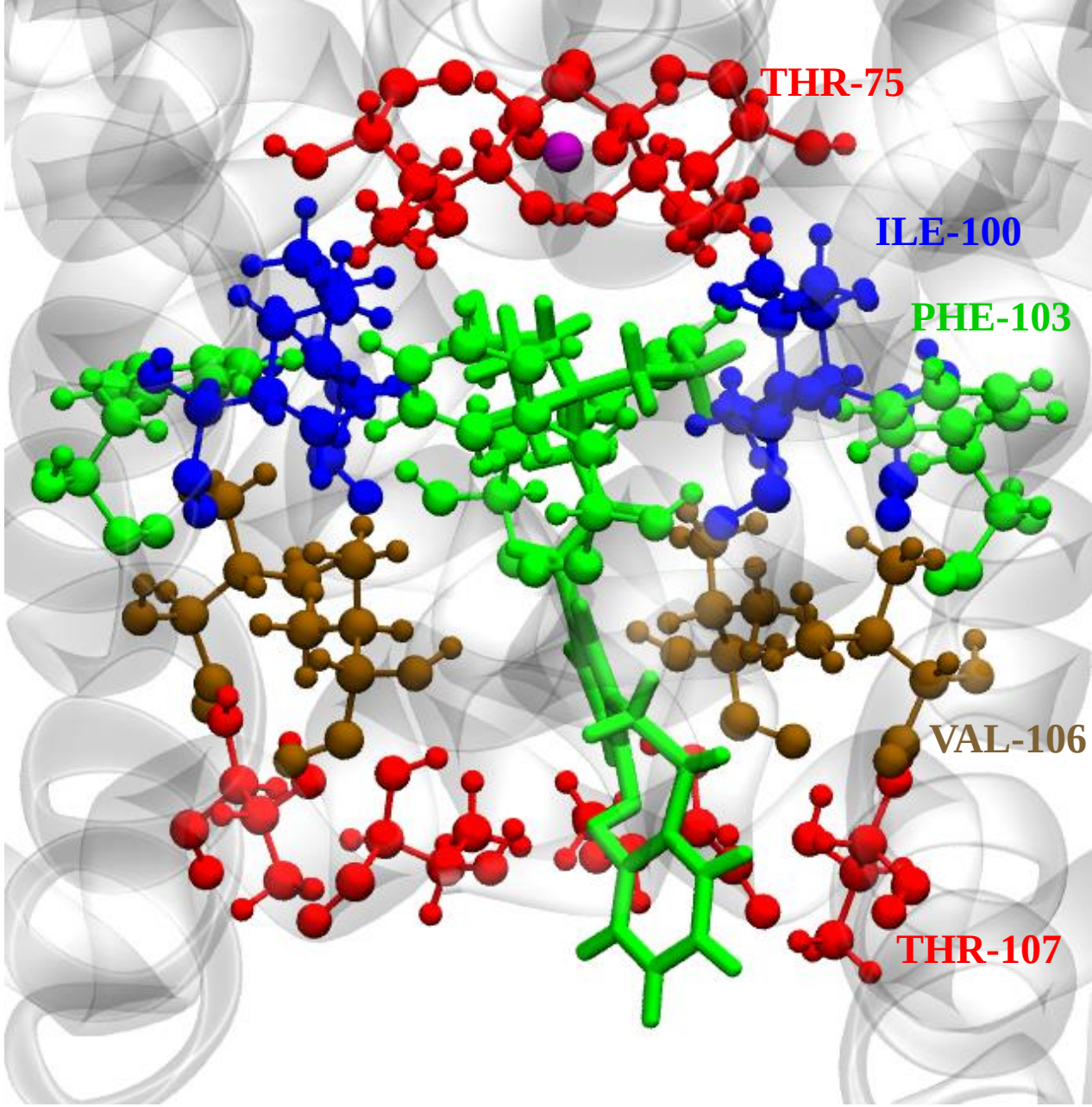
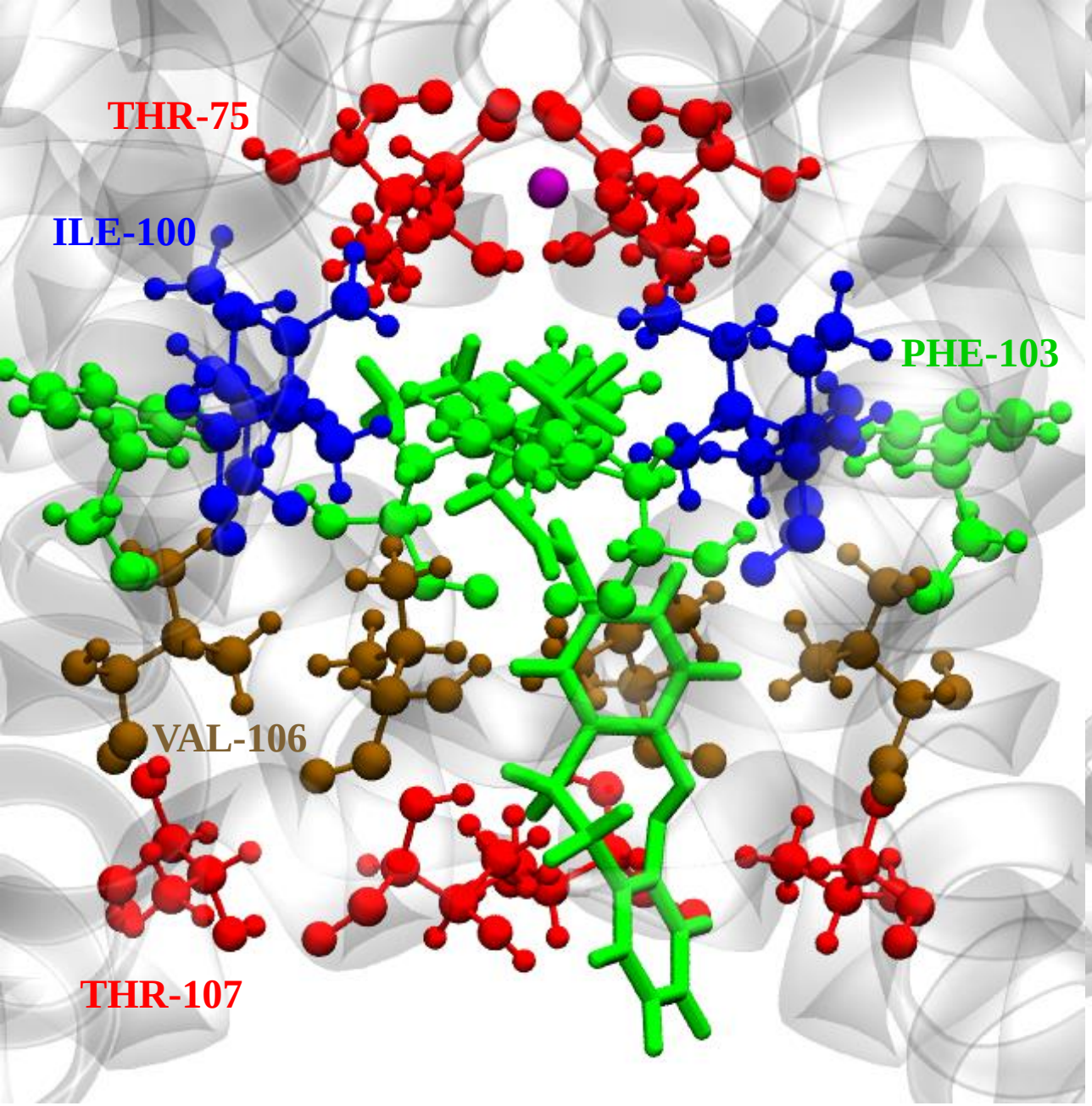
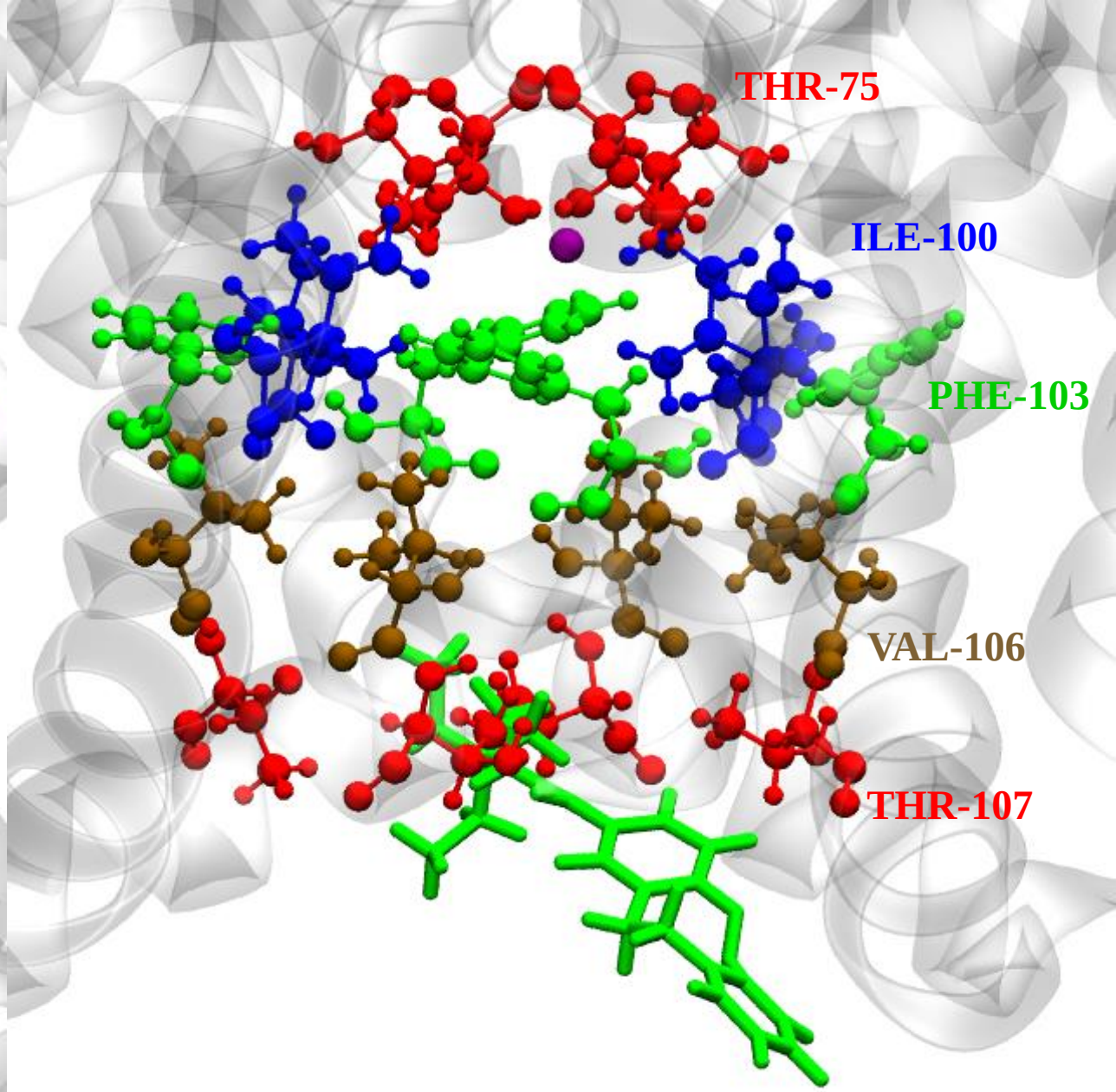


***E*1 (C0)**

MM/PBSA Binding energy = -20.6 kcal/mol



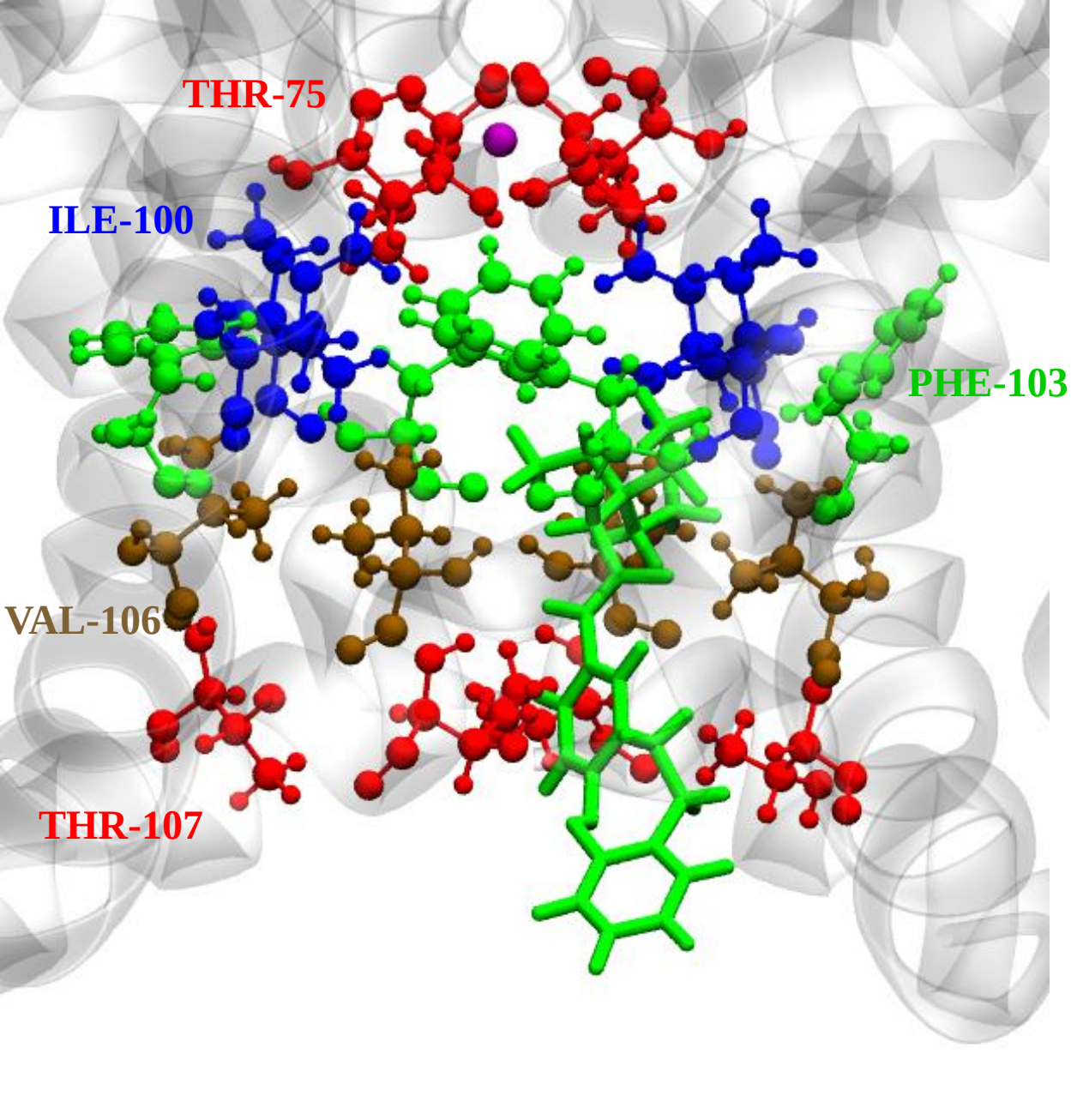


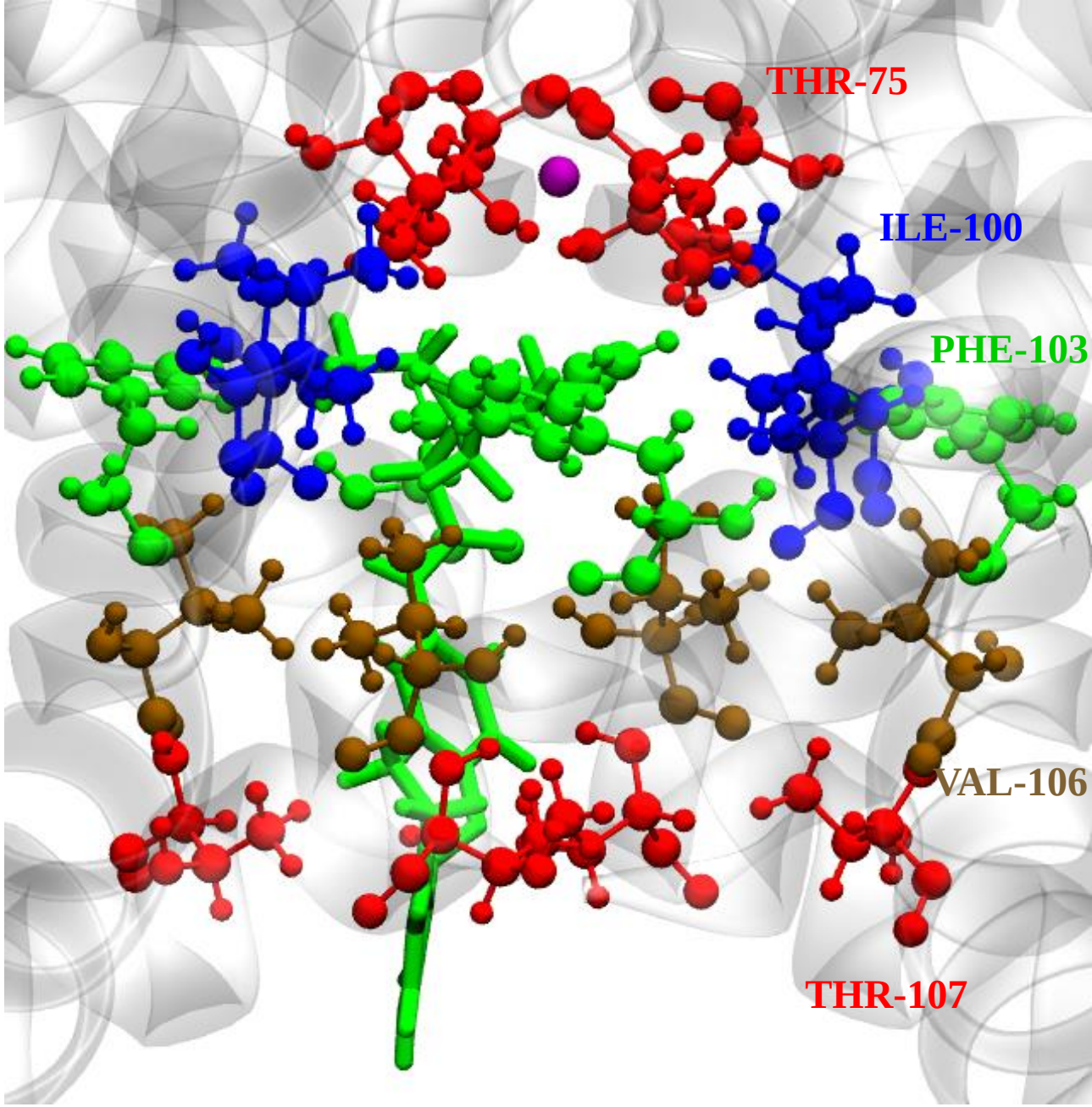
***E*1 (C1)**

MM/PBSA Binding energy = -20.4 kcal/mol

***E*1 (C2)**

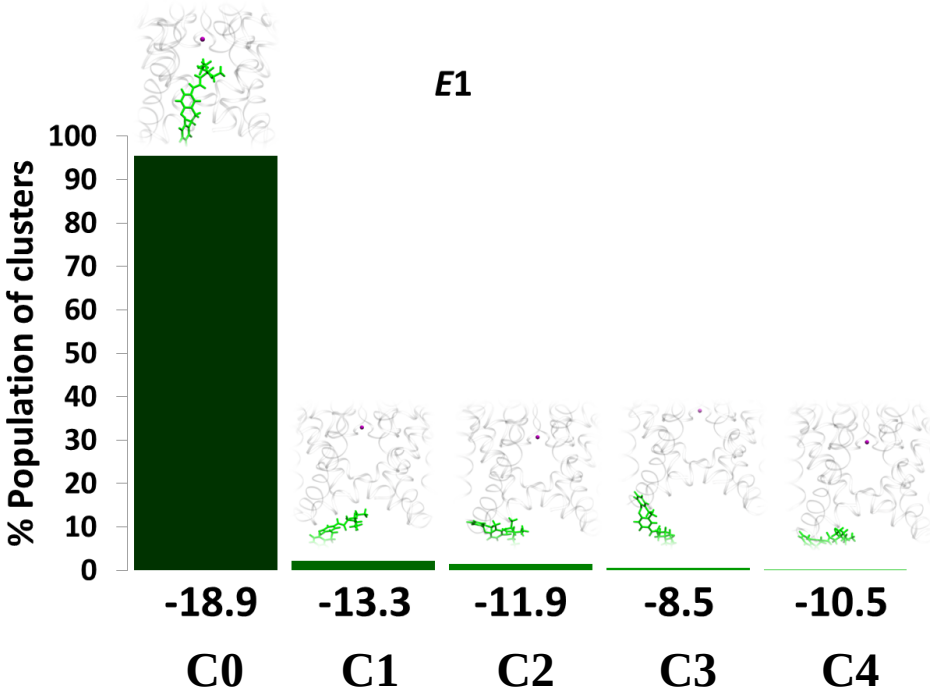
MM/PBSA Binding energy = -16.2 kcal/mol





***E*1 (C3)**
MM/PBSA Binding energy = -20.9 kcal/mol

***E*1 (C4)**
MM/PBSA Binding energy = -18.1 kcal/mol



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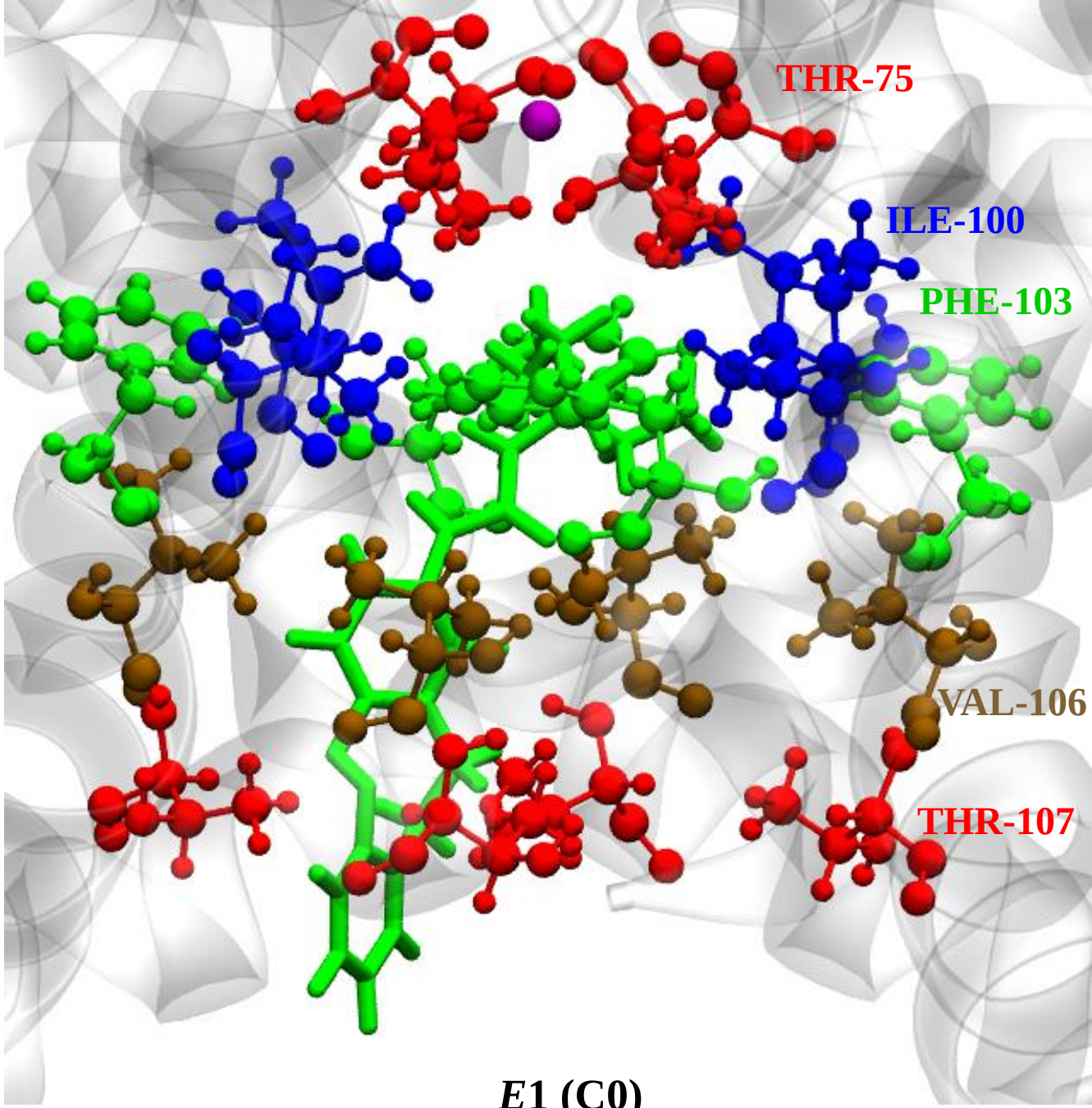
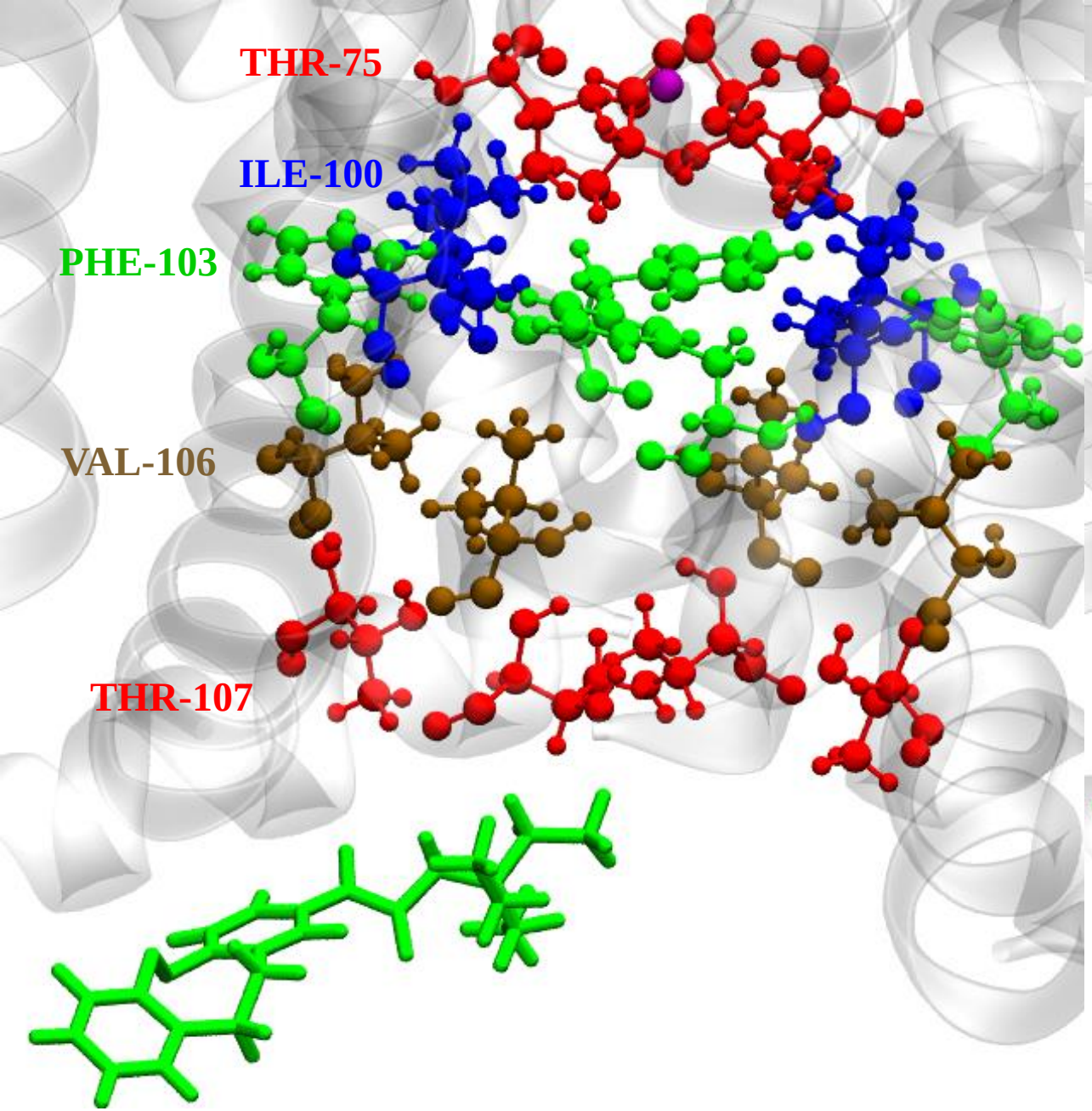
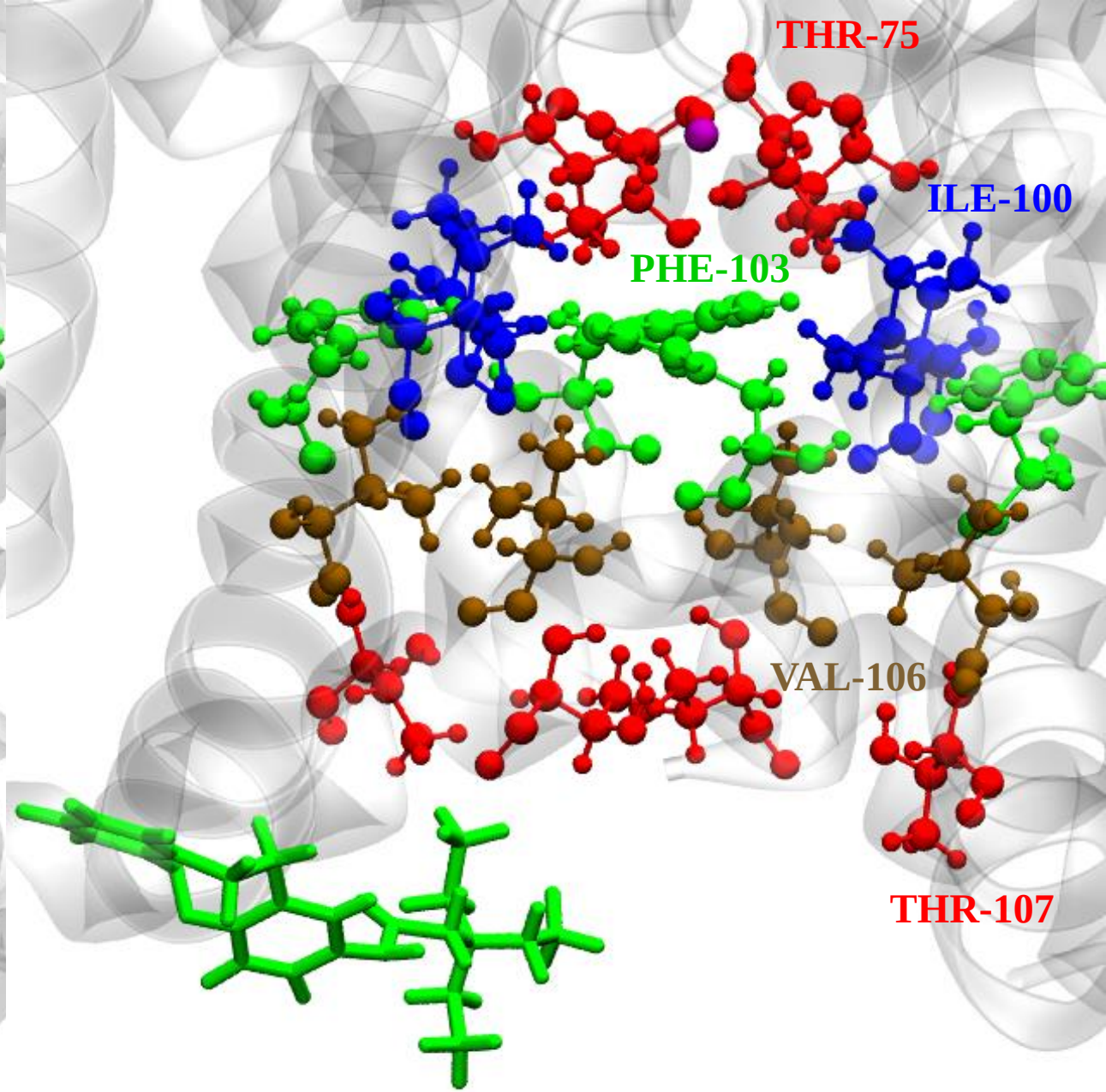


***E*1 (C0)**

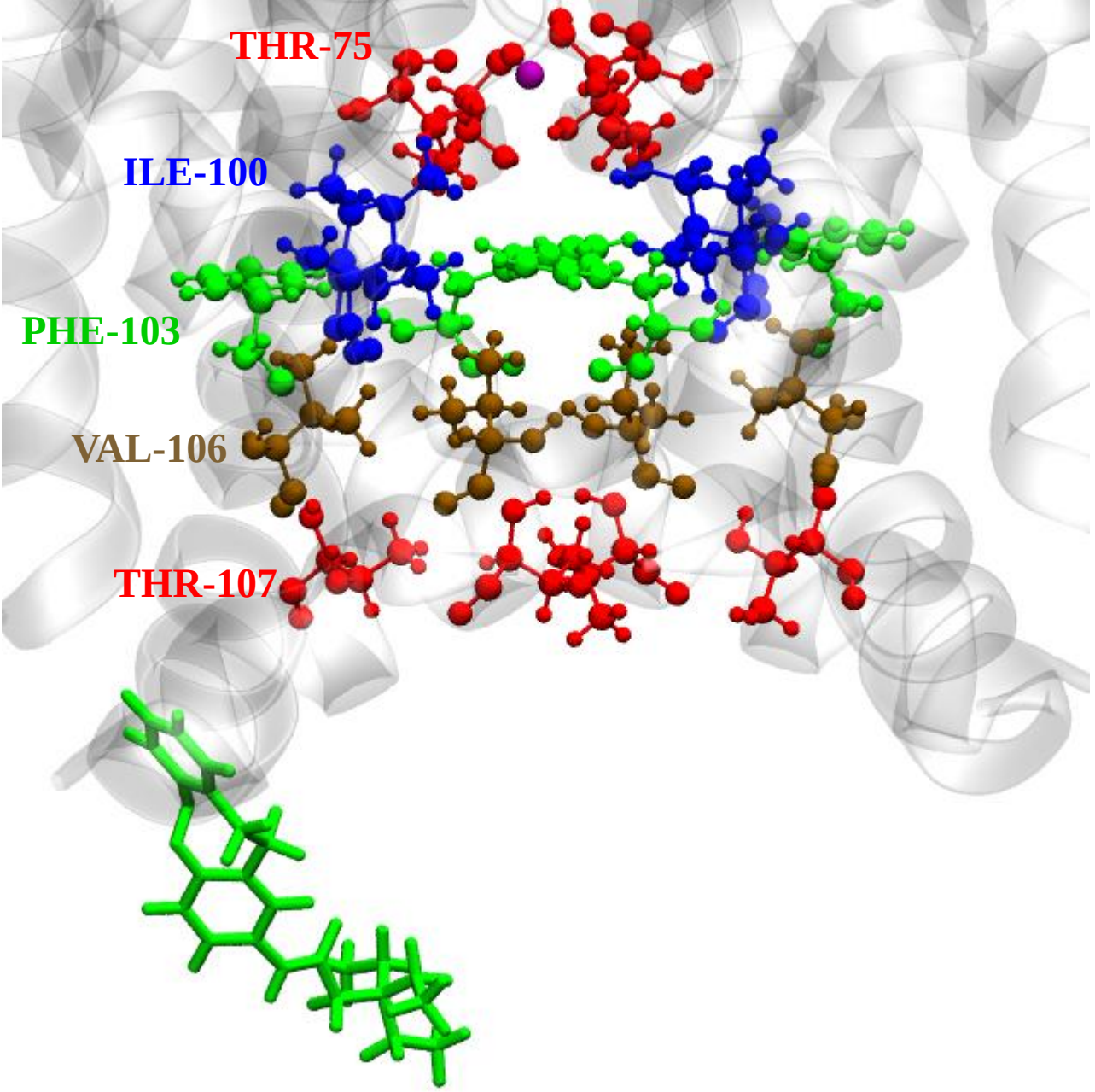
MM/PBSA Binding energy = -18.9 kcal/mol

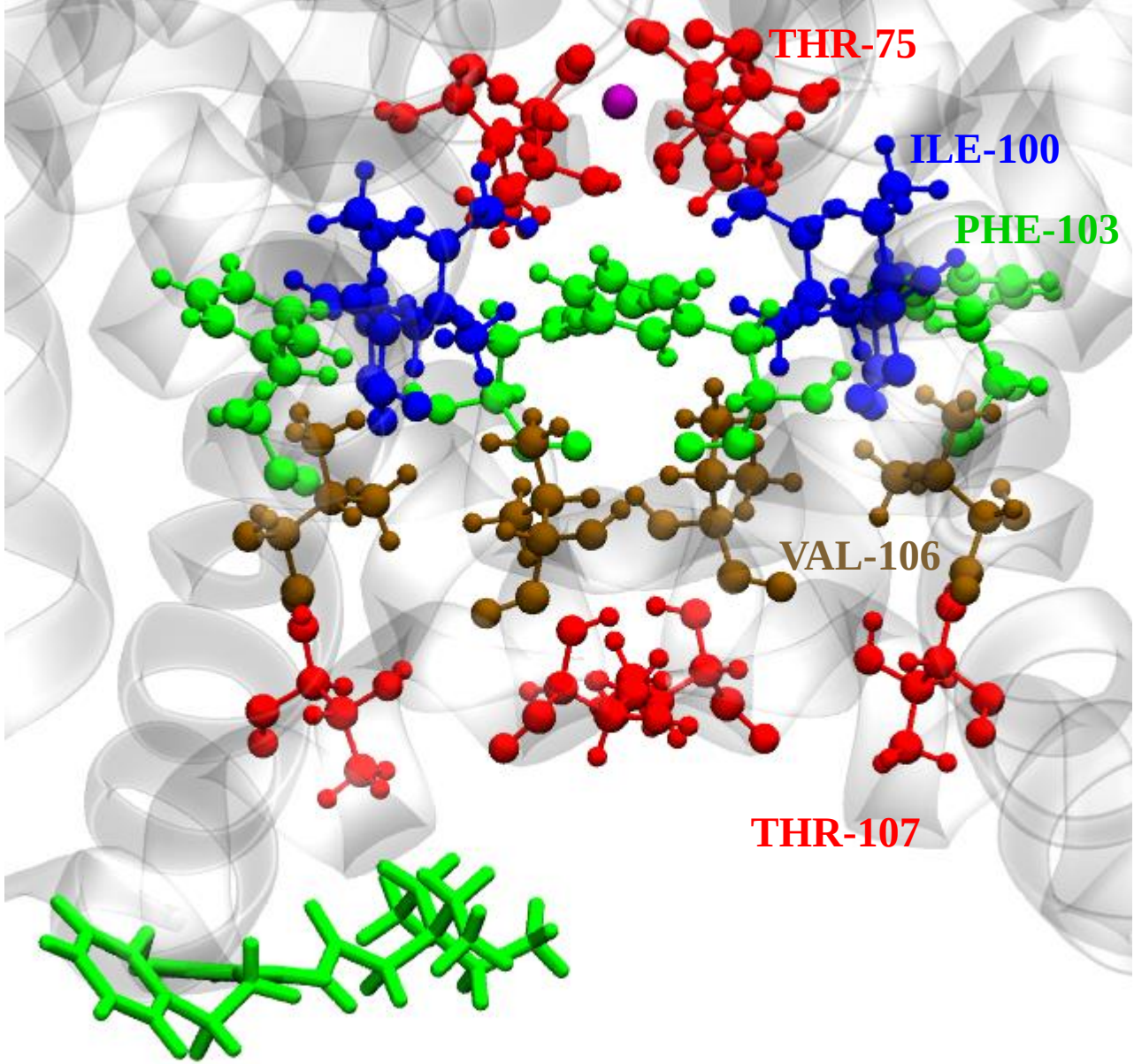




***E*1 (C1)**
MM/PBSA Binding energy = -13.3 kcal/mol

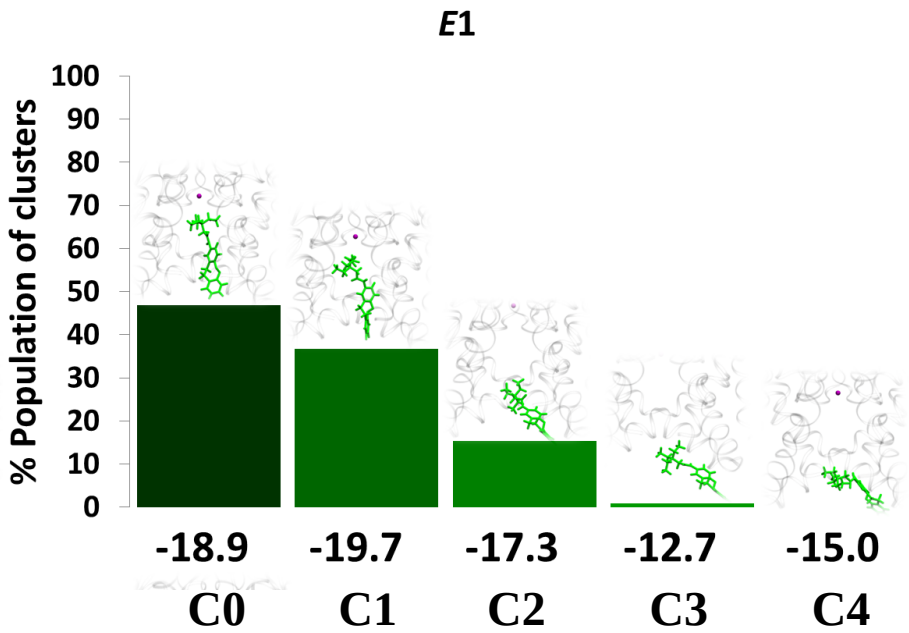
***E*1 (C2)**
MM/PBSA Binding energy = -11.9 kcal/mol





***E*1 (C3)**
MM/PBSA Binding energy = -8.5 kcal/mol

***E*1 (C4)**
MM/PBSA Binding energy = -10.5 kcal/mol



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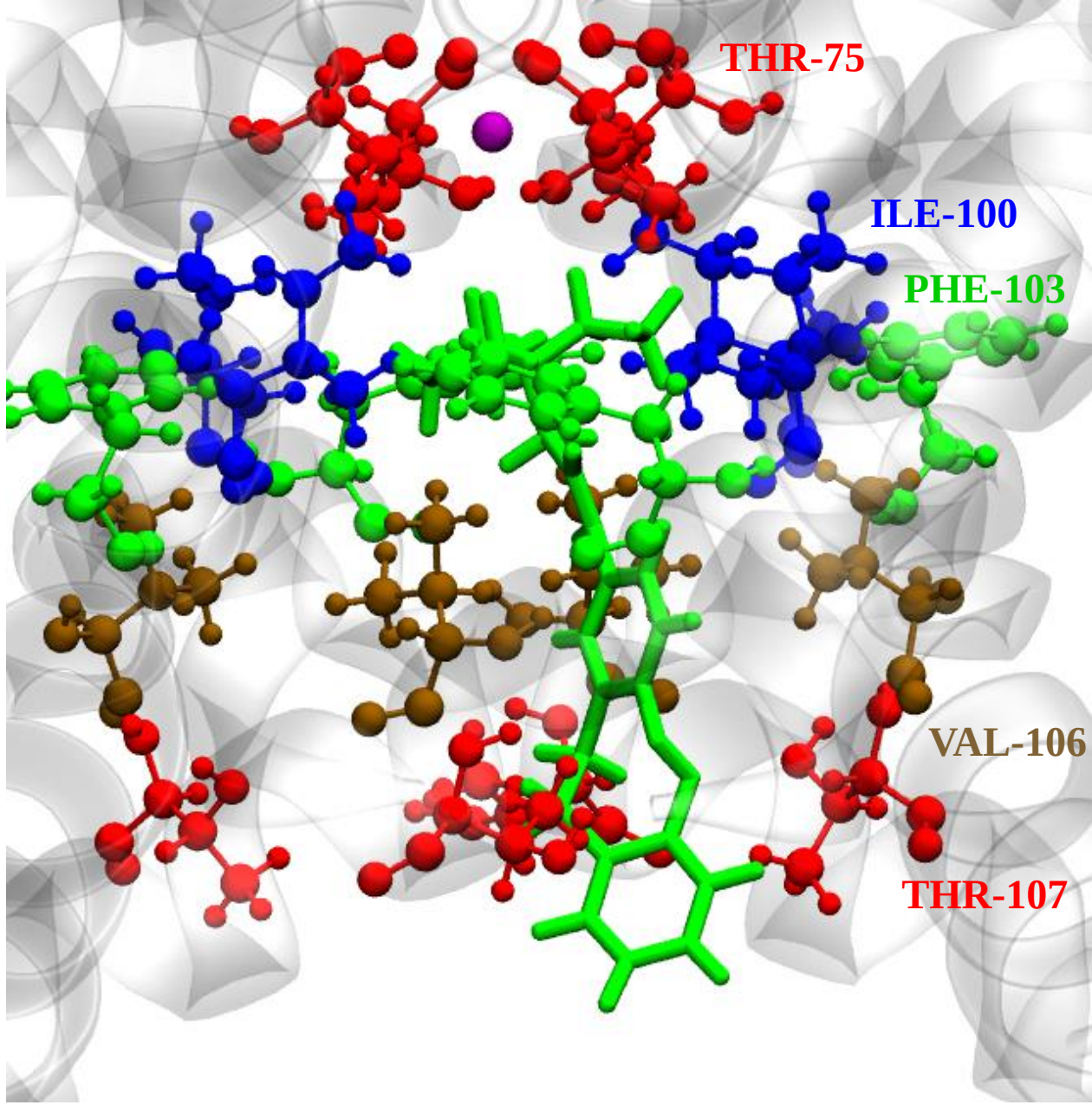
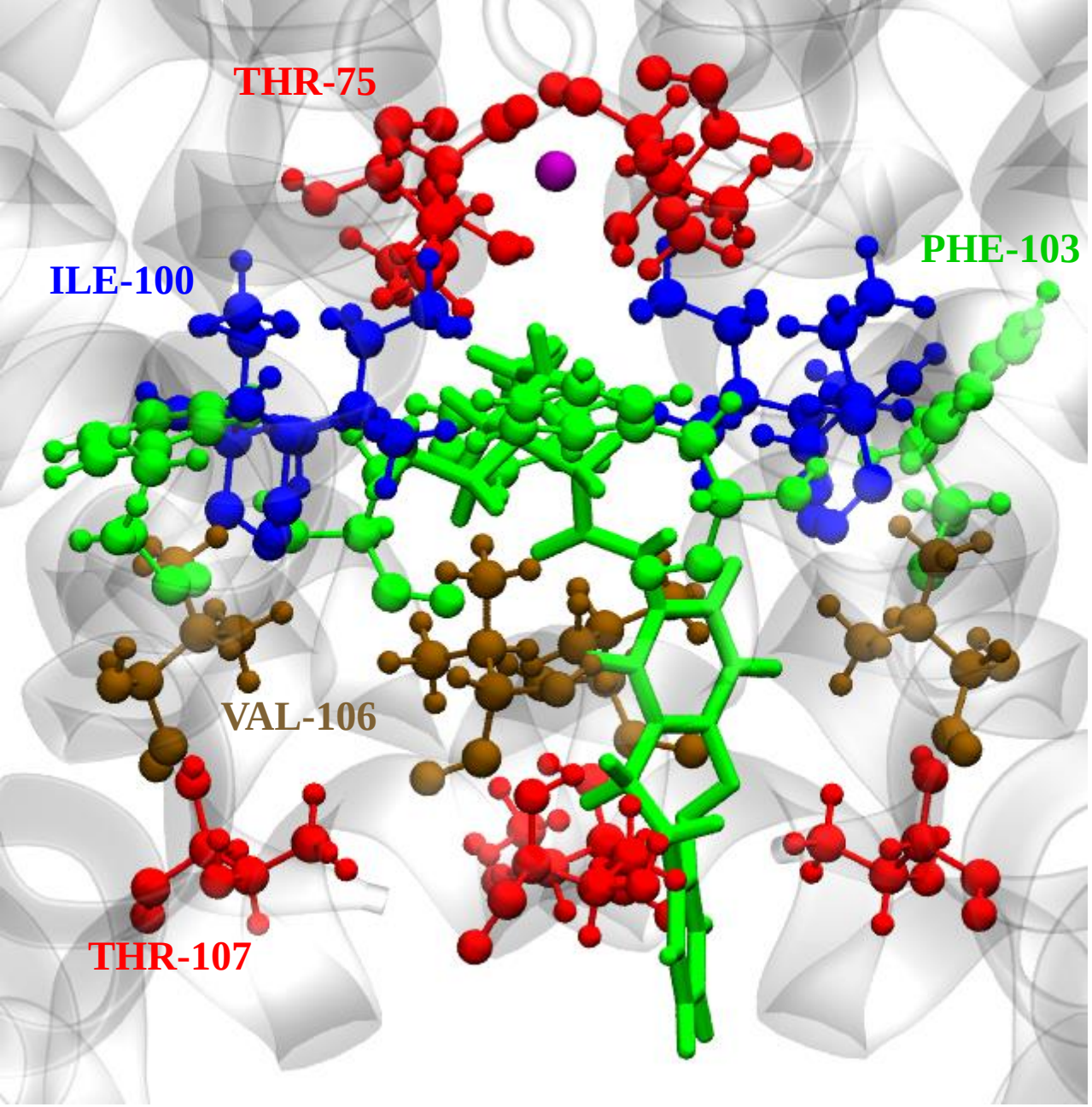
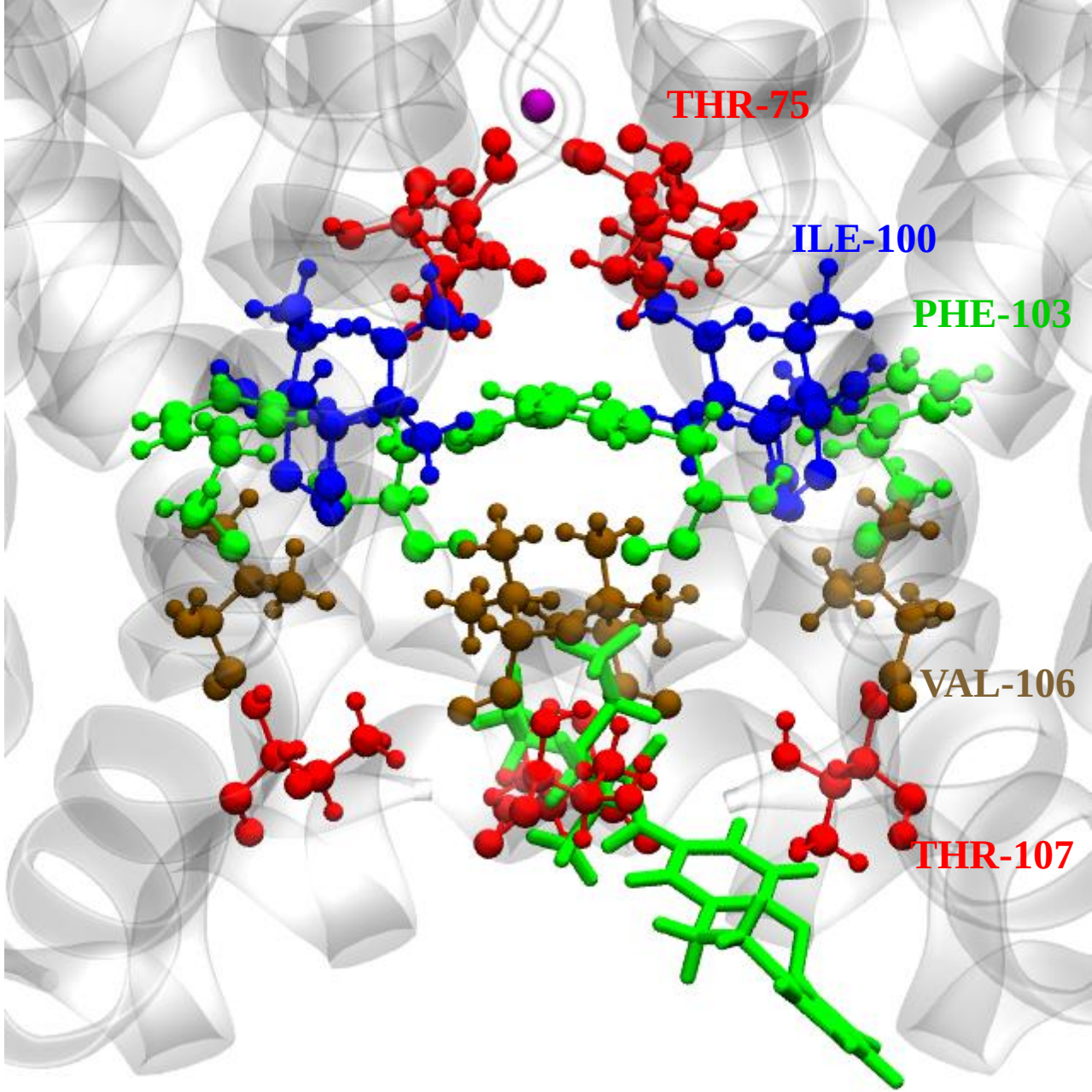


***E*1 (C0)**

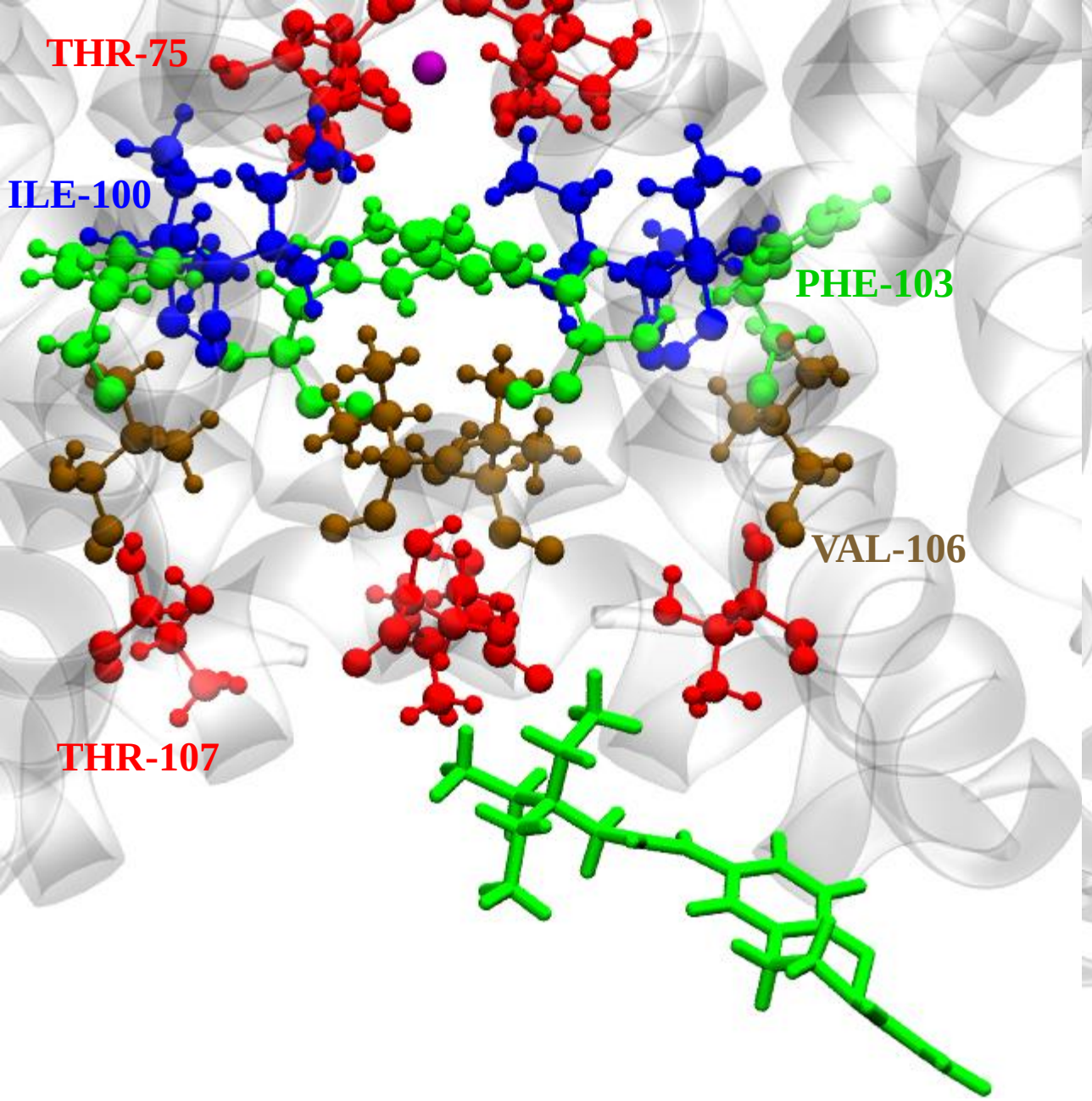
MM/PBSA Binding energy = -18.9 kcal/mol



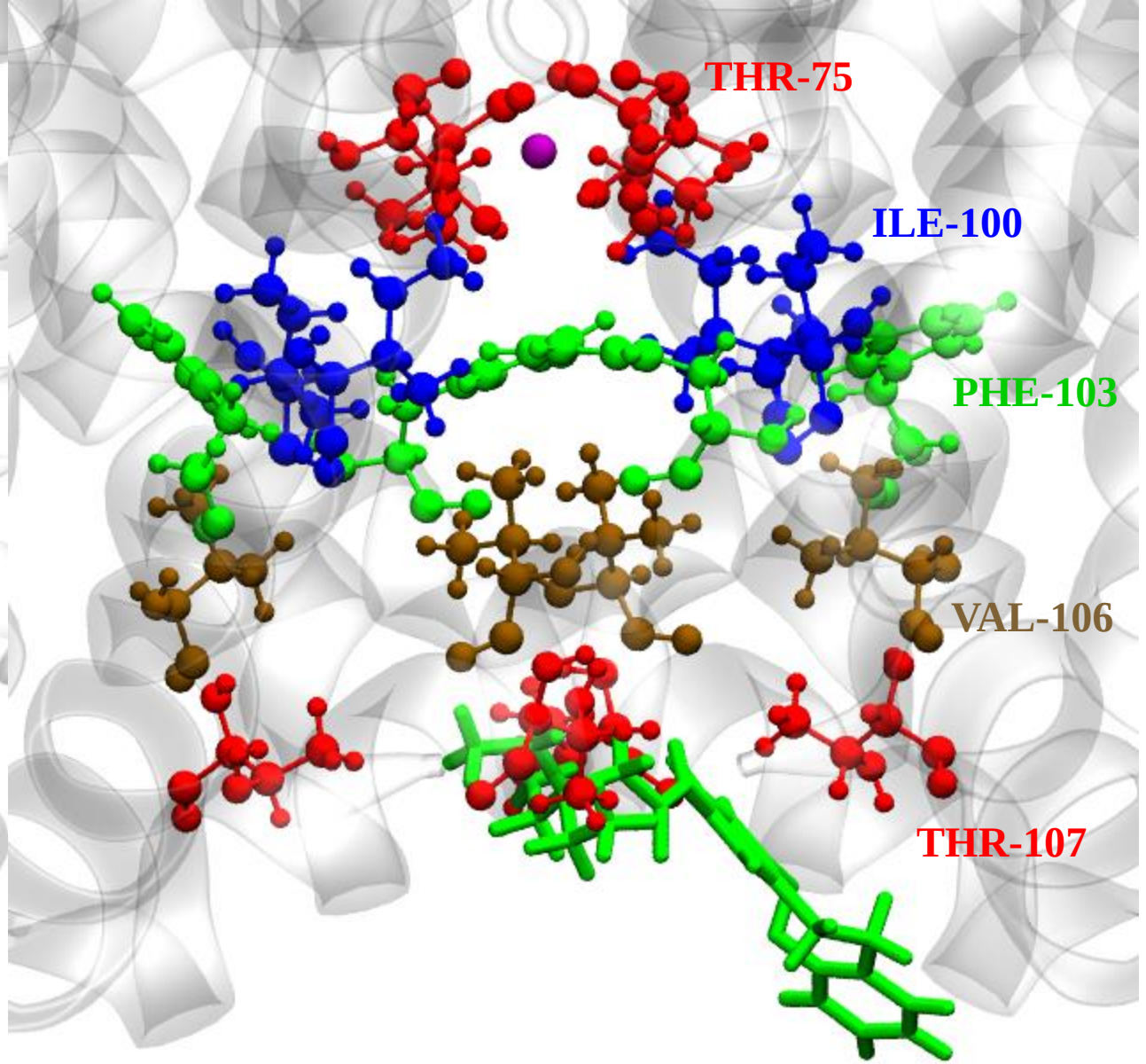


***E*1 (C1)**
MM/PBSA Binding energy = -19.7 kcal/mol

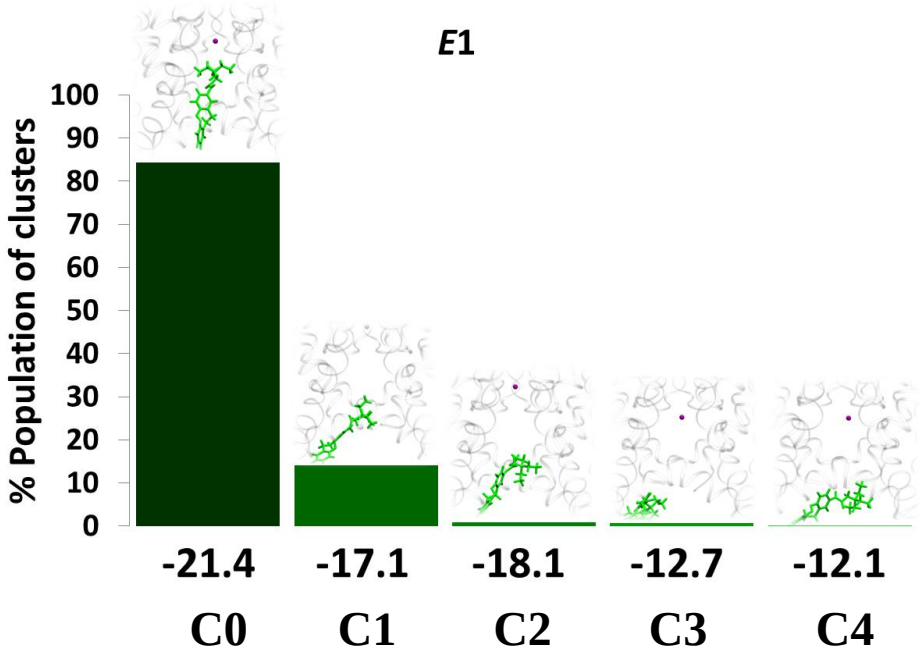
***E*1 (C2)**
MM/PBSA Binding energy = -17.3 kcal/mol



***E*1 (C3)**
MM/PBSA Binding energy = -12.7 kcal/mol



***E*1 (C4)**
MM/PBSA Binding energy = -15.0 kcal/mol



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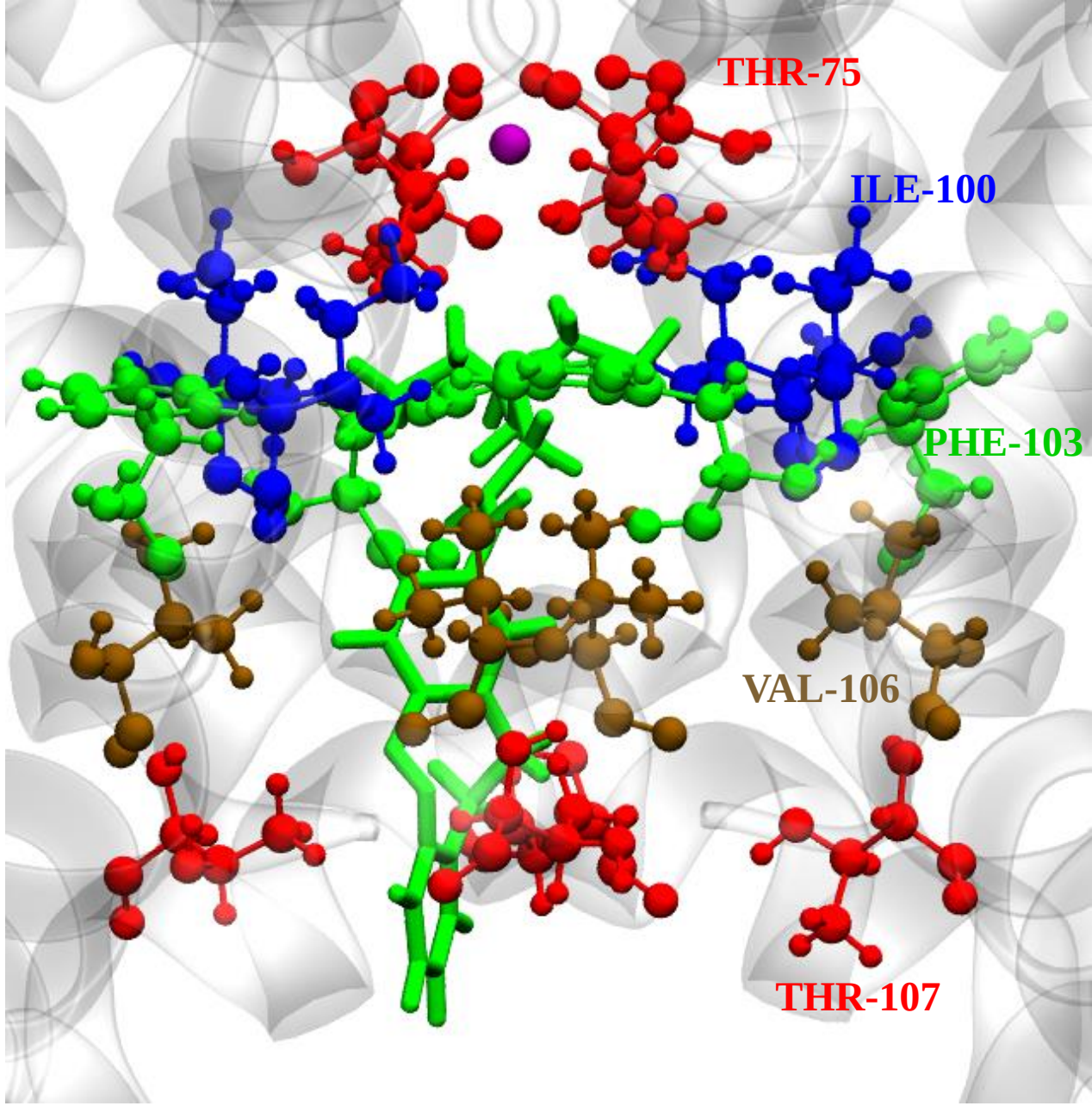

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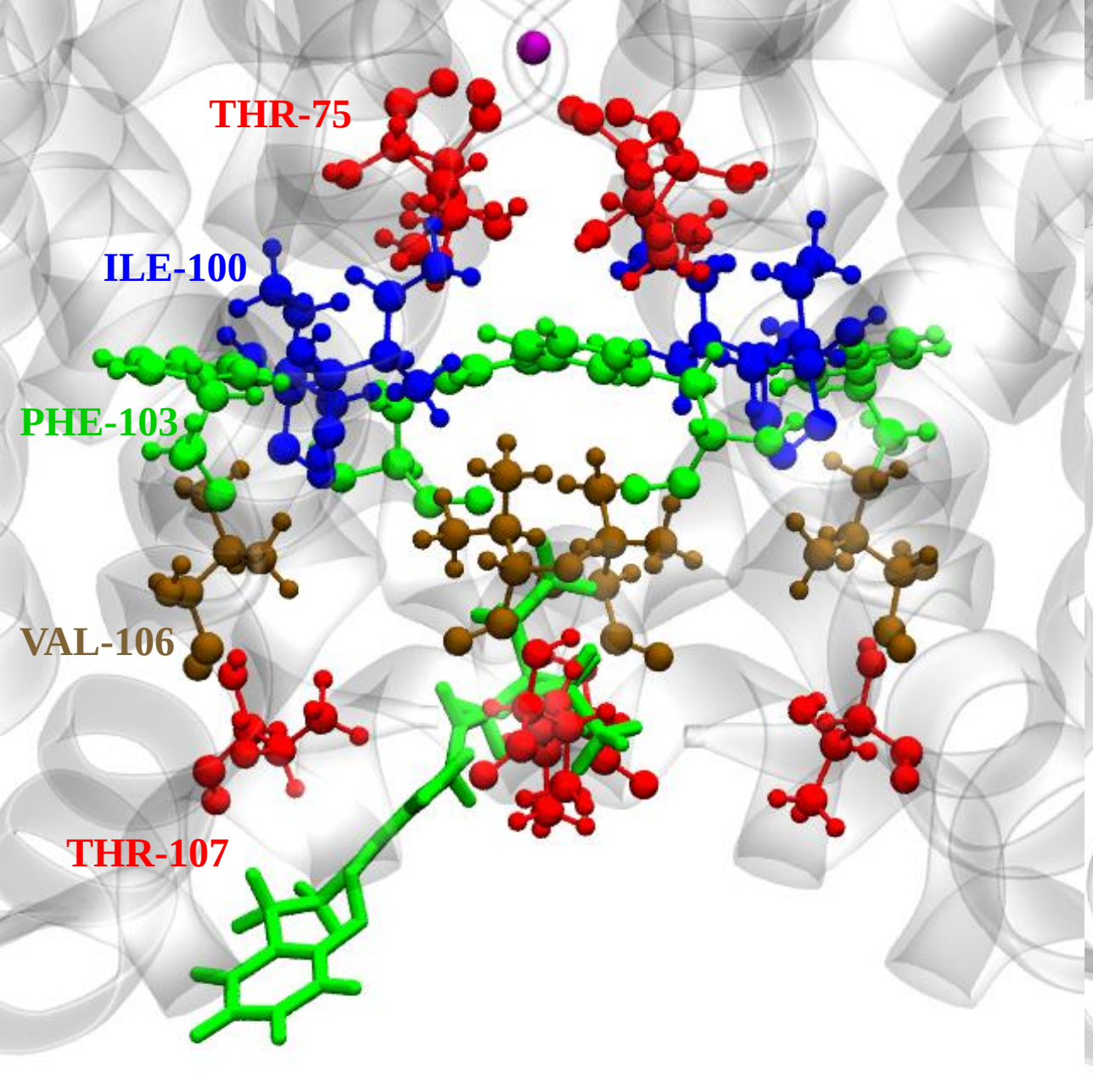

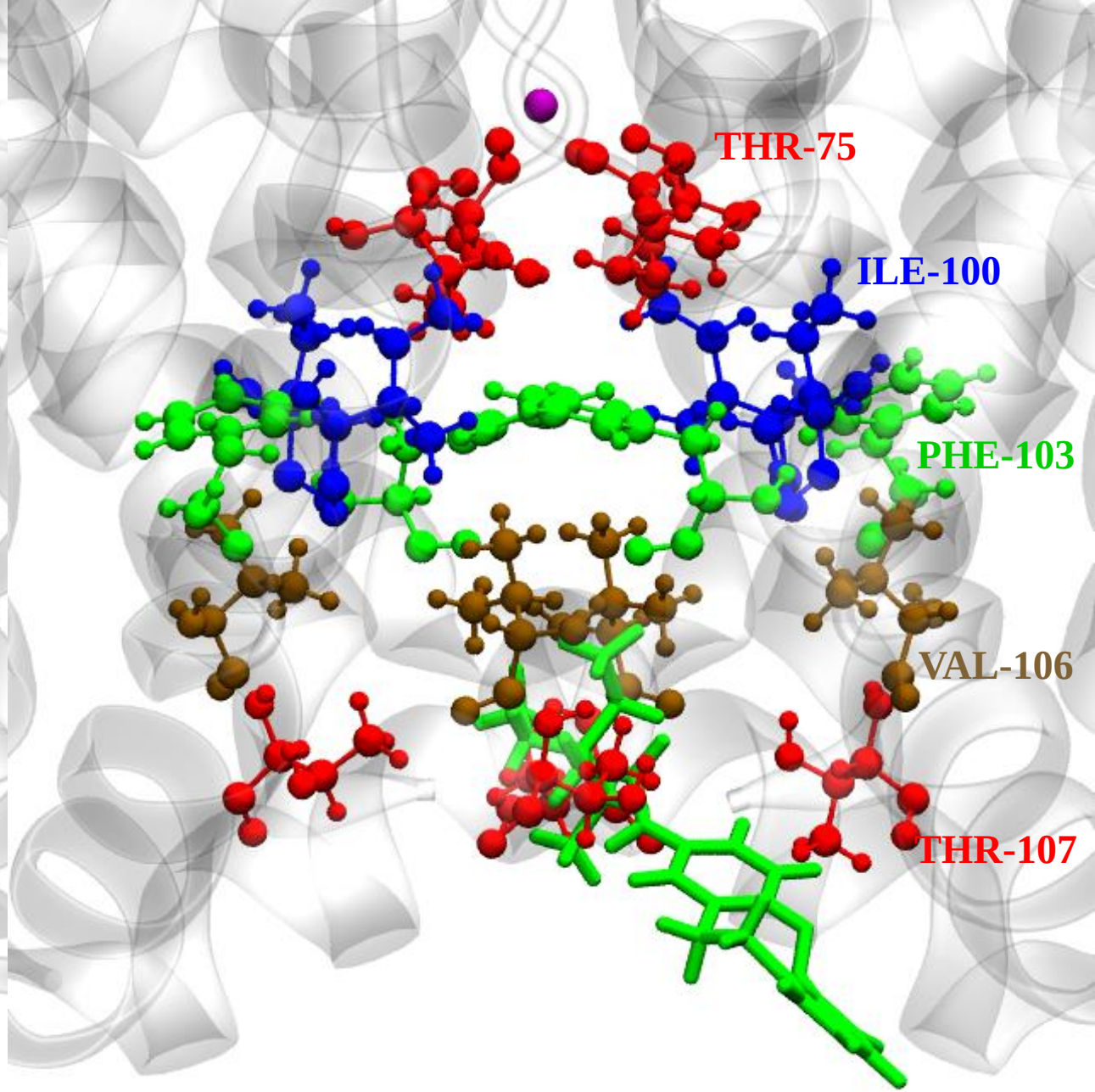

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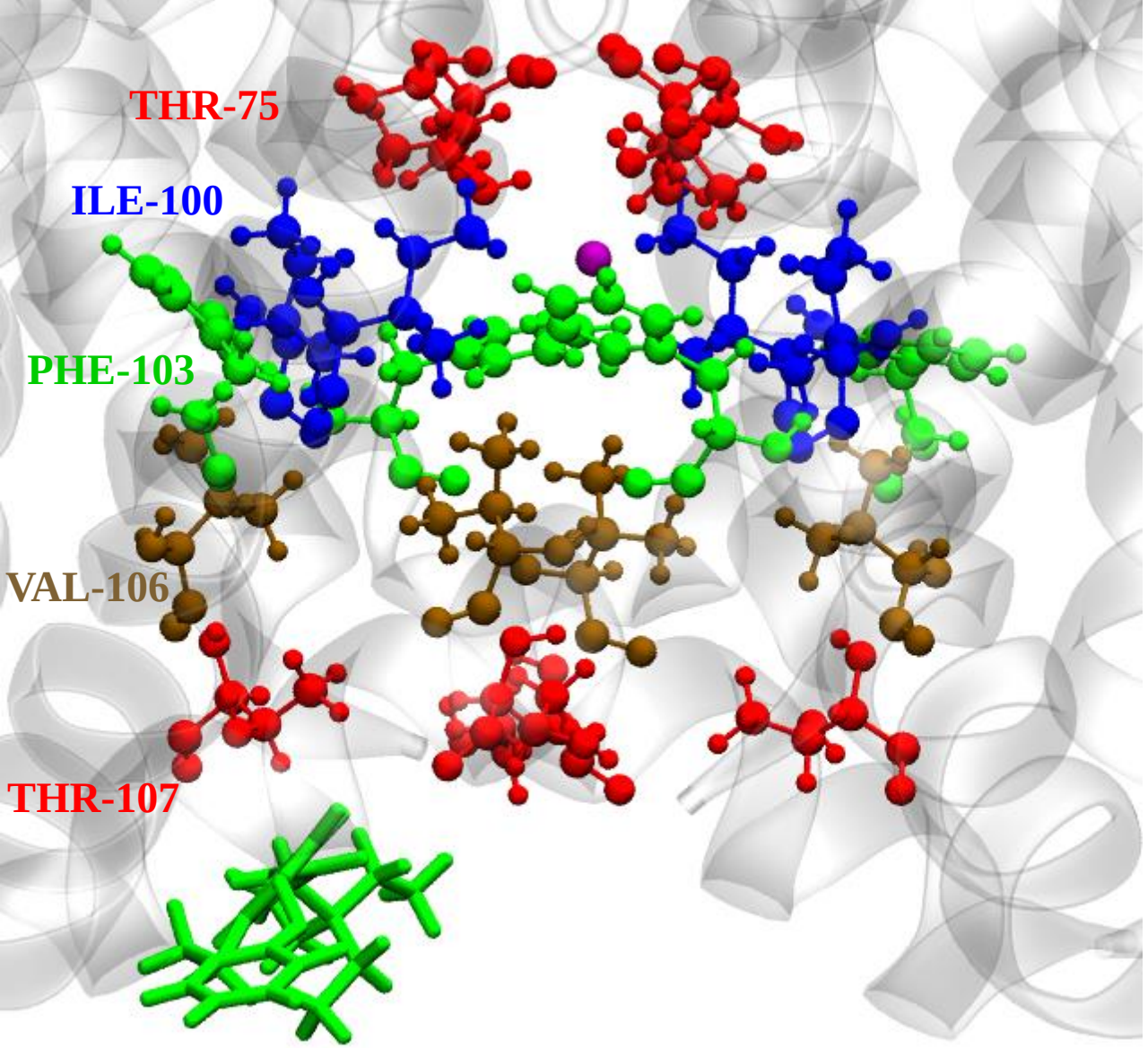
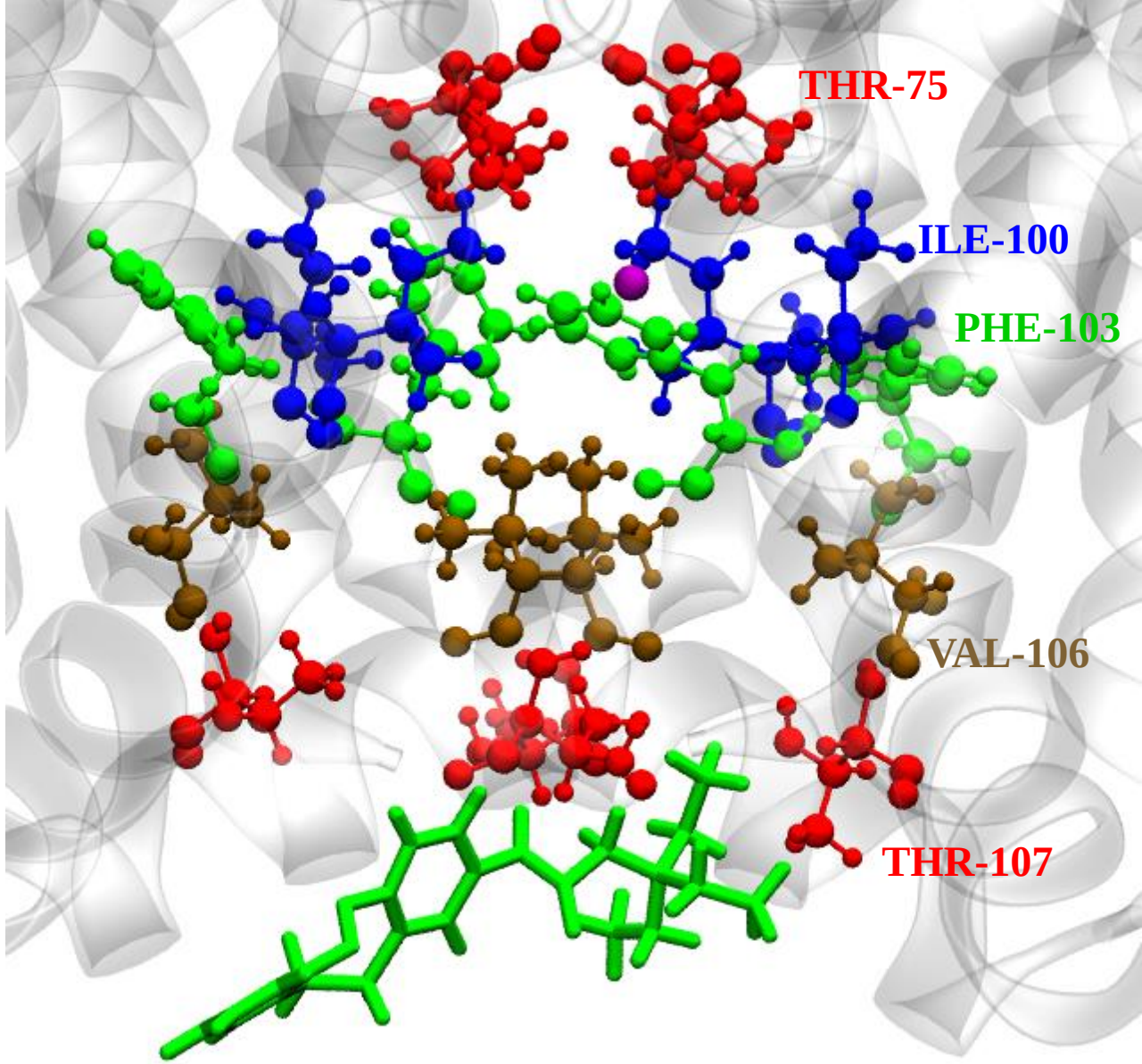
MM/PBSA Binding energy = -17.1 kcal/mol

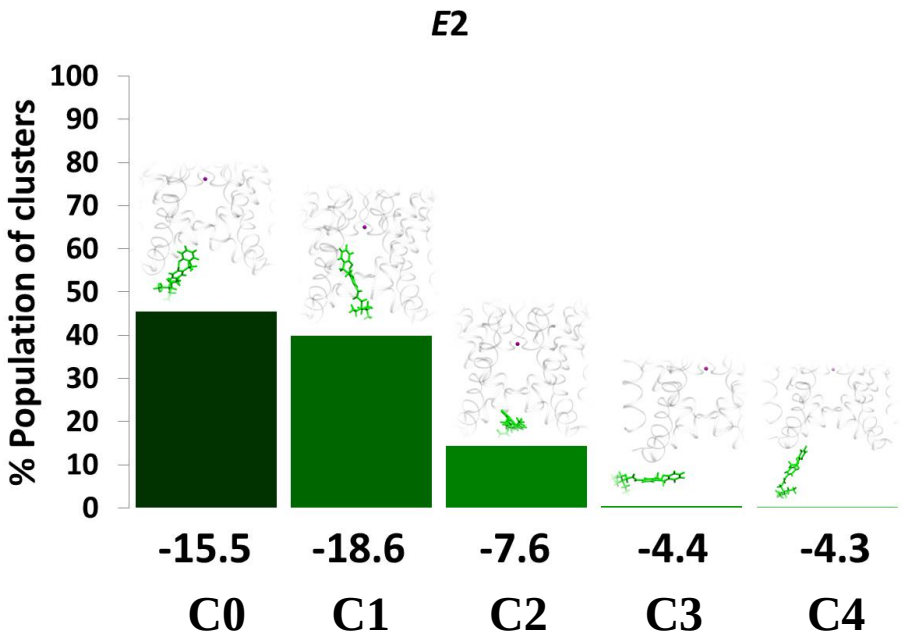
***E*1 (C2)**
MM/PBSA Binding energy = -18.1 kcal/mol





***E*1 (C3)**
MM/PBSA Binding energy = -12.7 kcal/mol

***E*1 (C4)**
MM/PBSA Binding energy = -12.1 kcal/mol



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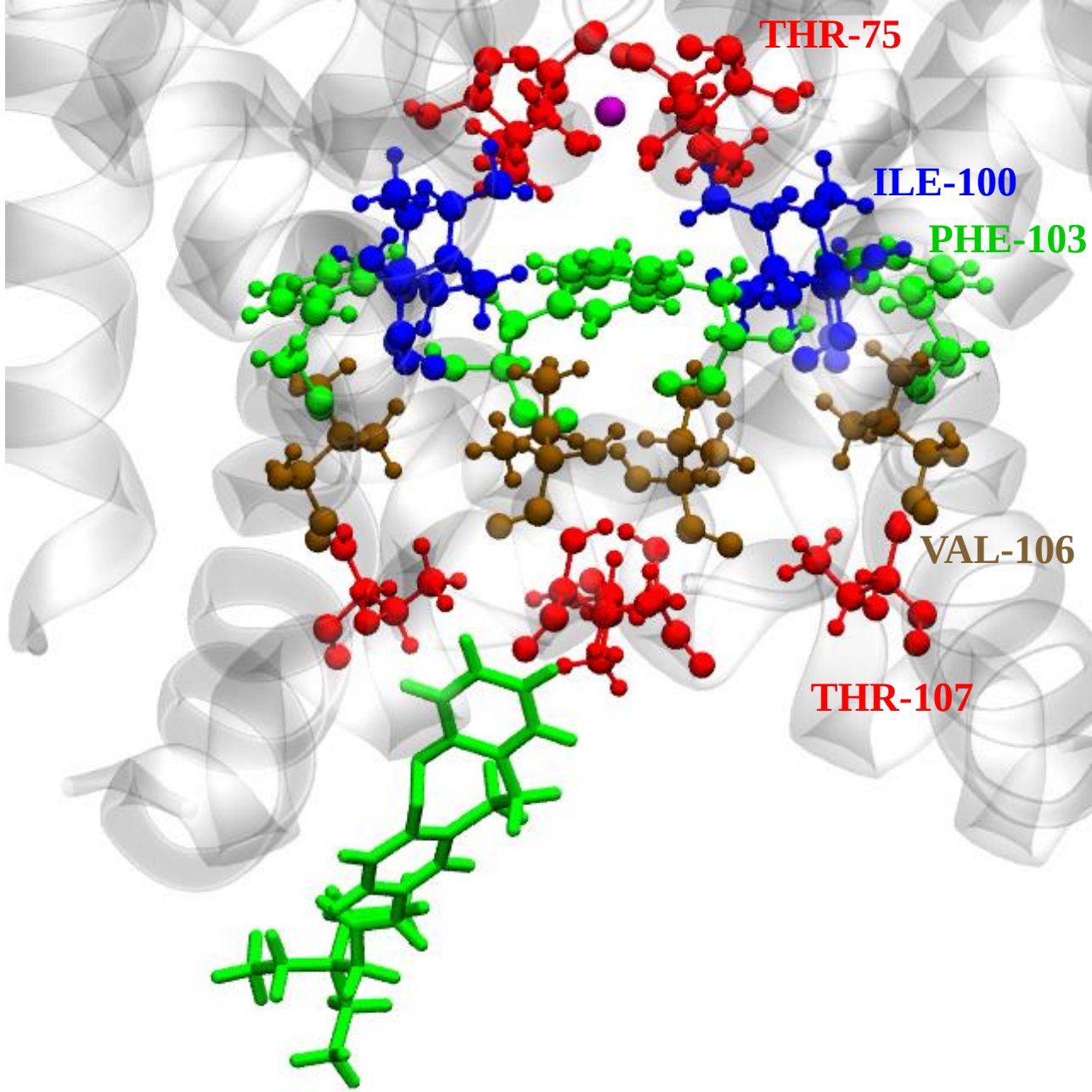
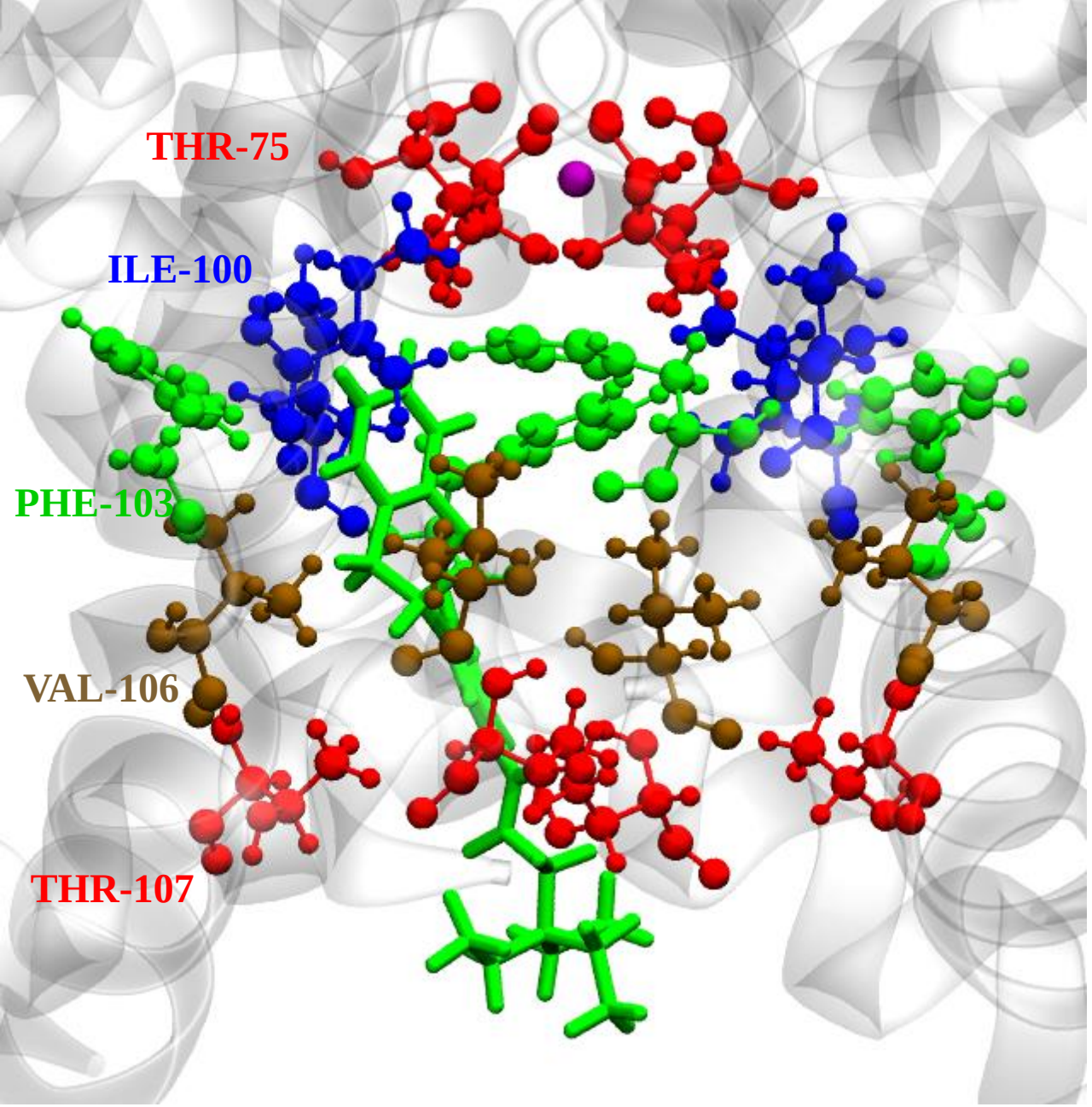
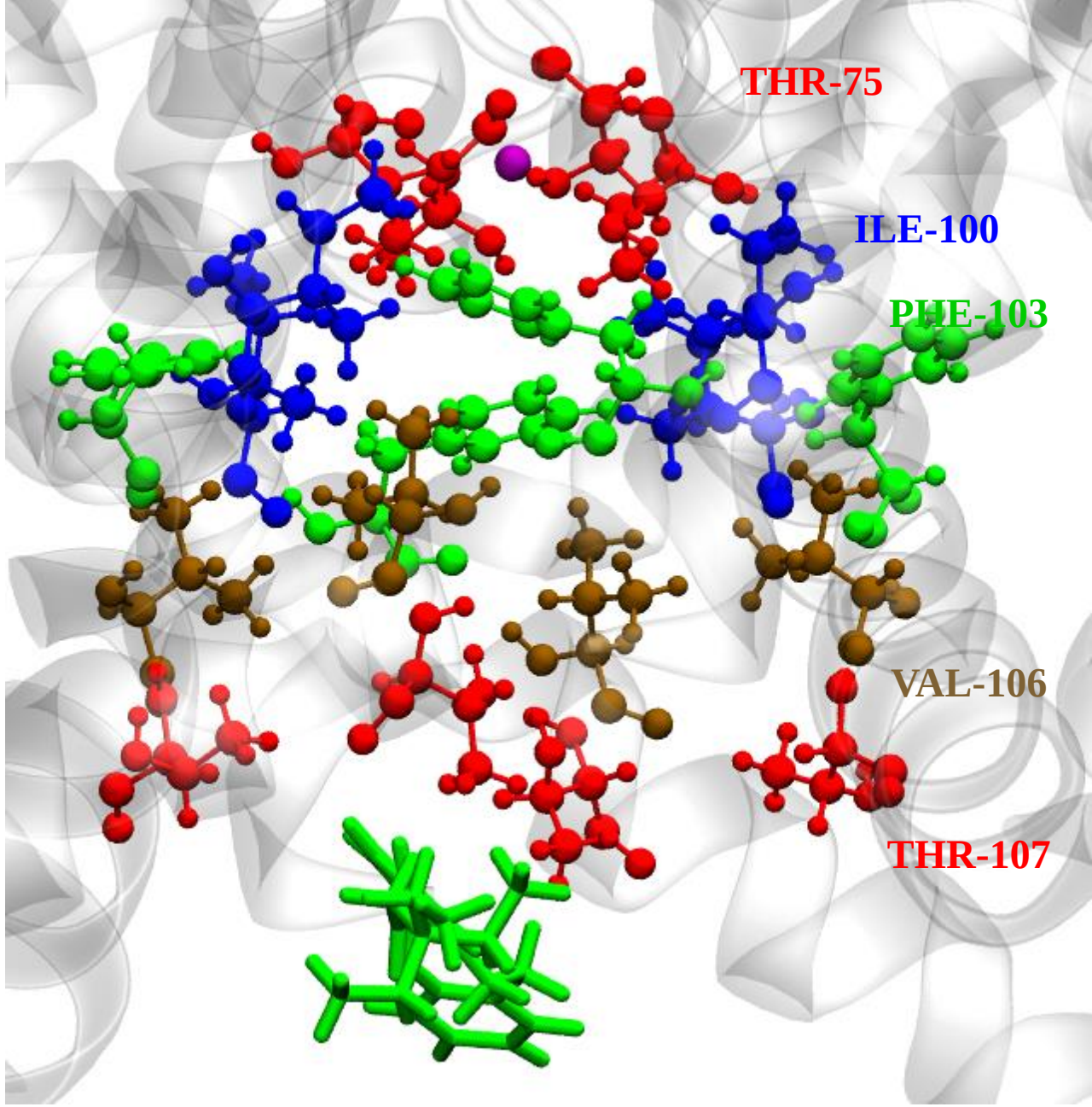


***E*2 (C0)**

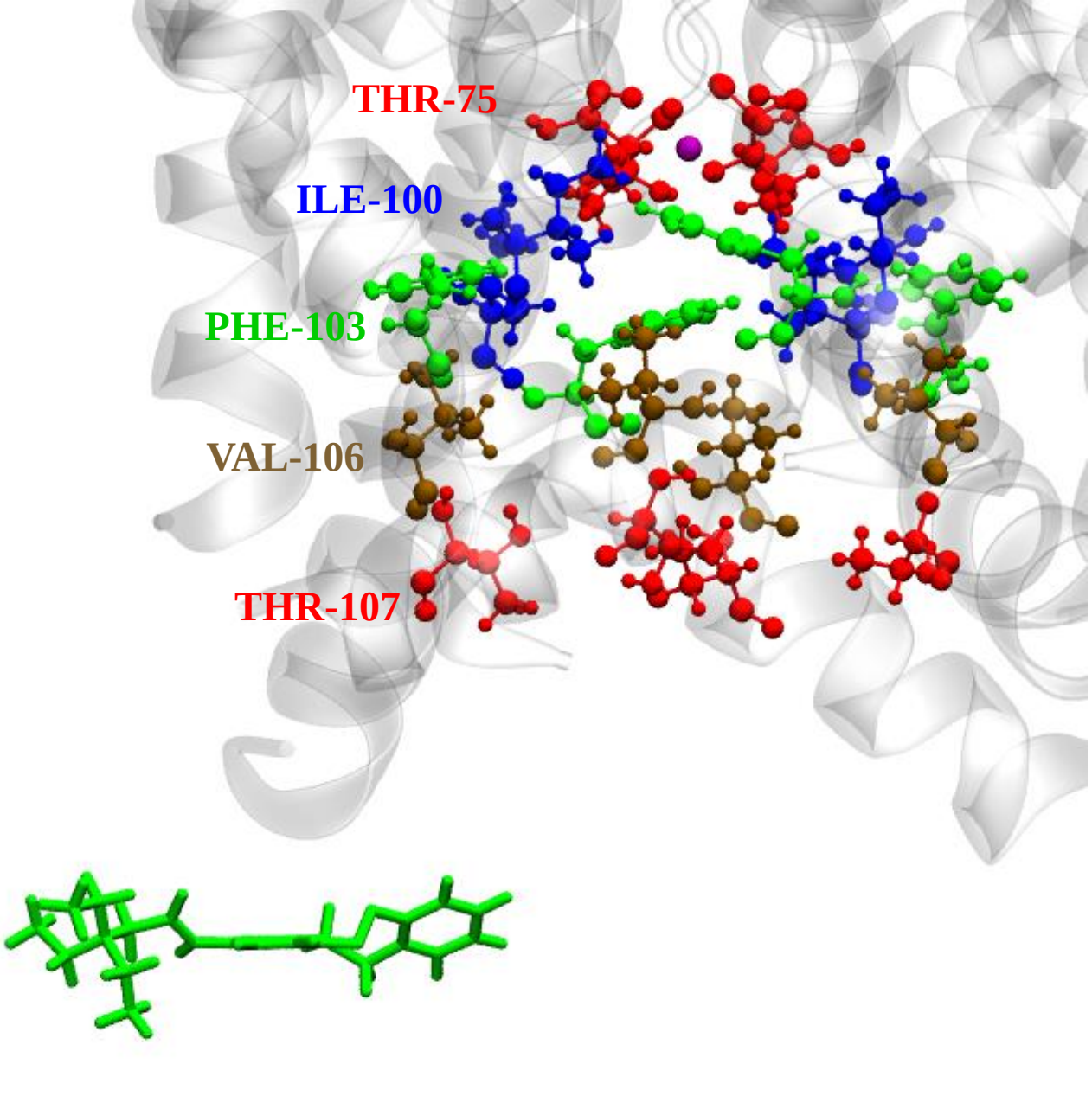
MM/PBSA Binding energy = -15.5 kcal/mol

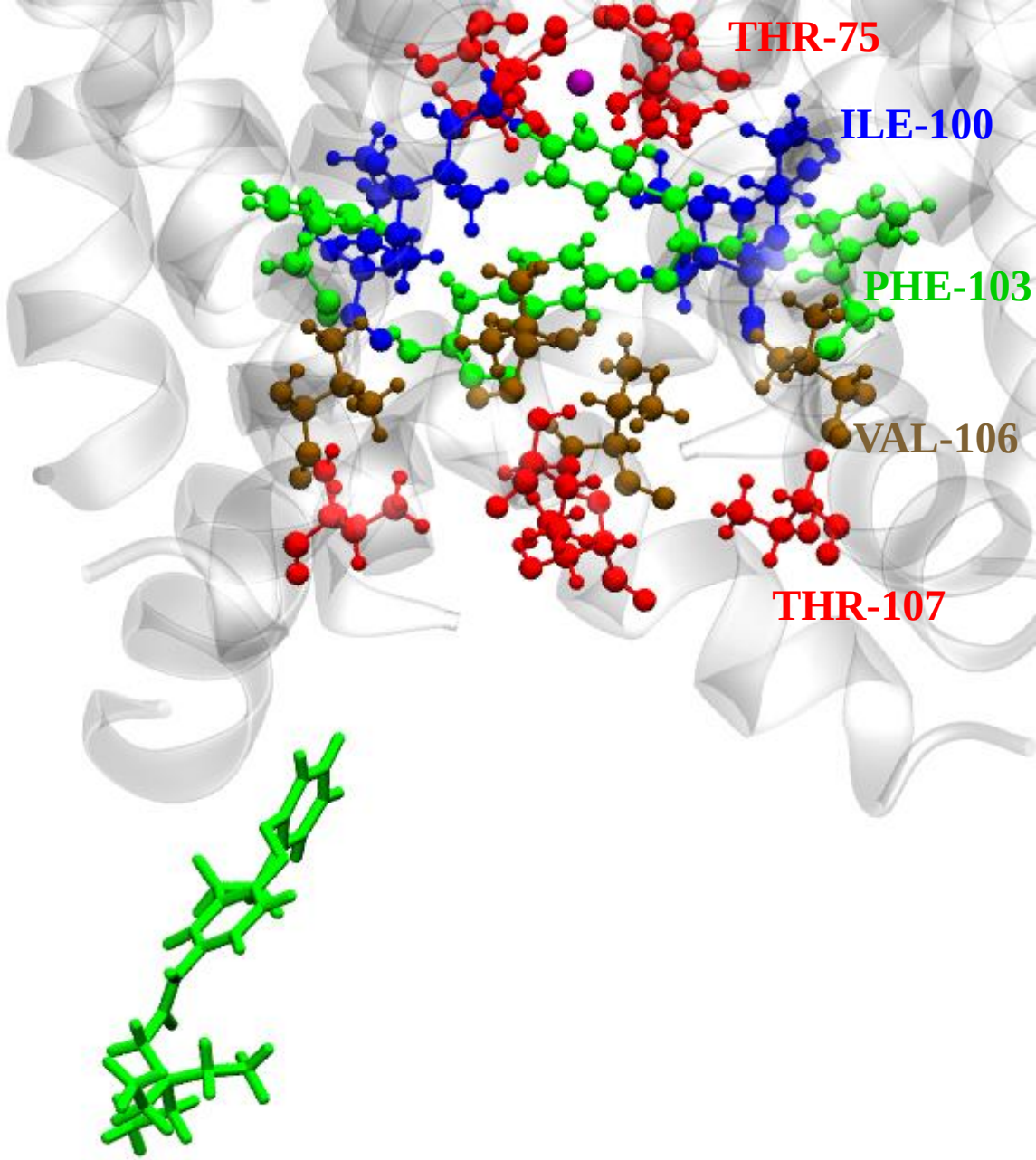




***E*2 (C1)**
MM/PBSA Binding energy = -18.6 kcal/mol

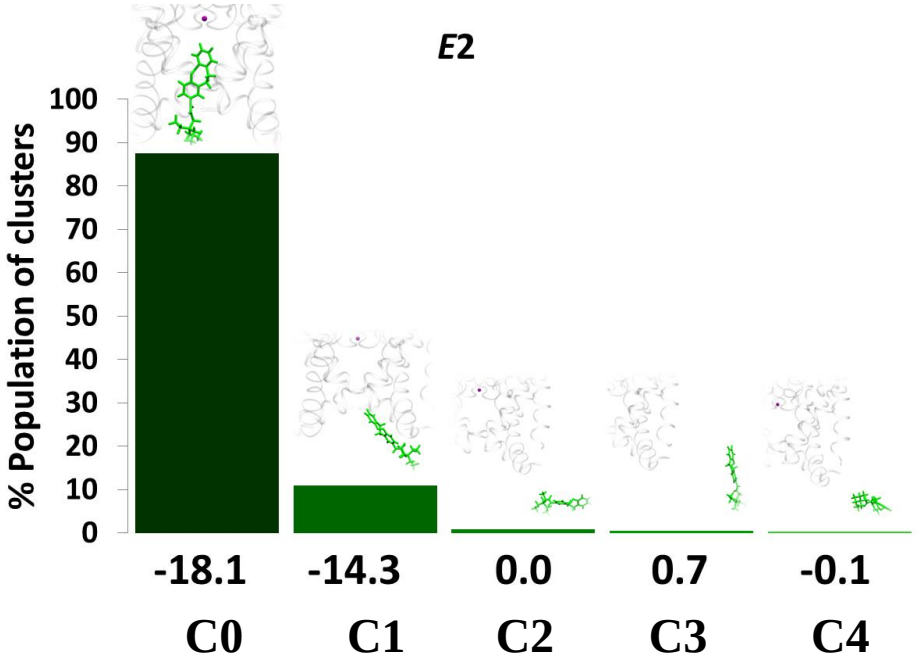
***E*2 (C2)**
MM/PBSA Binding energy = -7.6 kcal/mol





***E*2 (C3)**
MM/PBSA Binding energy = -4.4 kcal/mol

***E*2 (C4)**
MM/PBSA Binding energy = -4.3 kcal/mol



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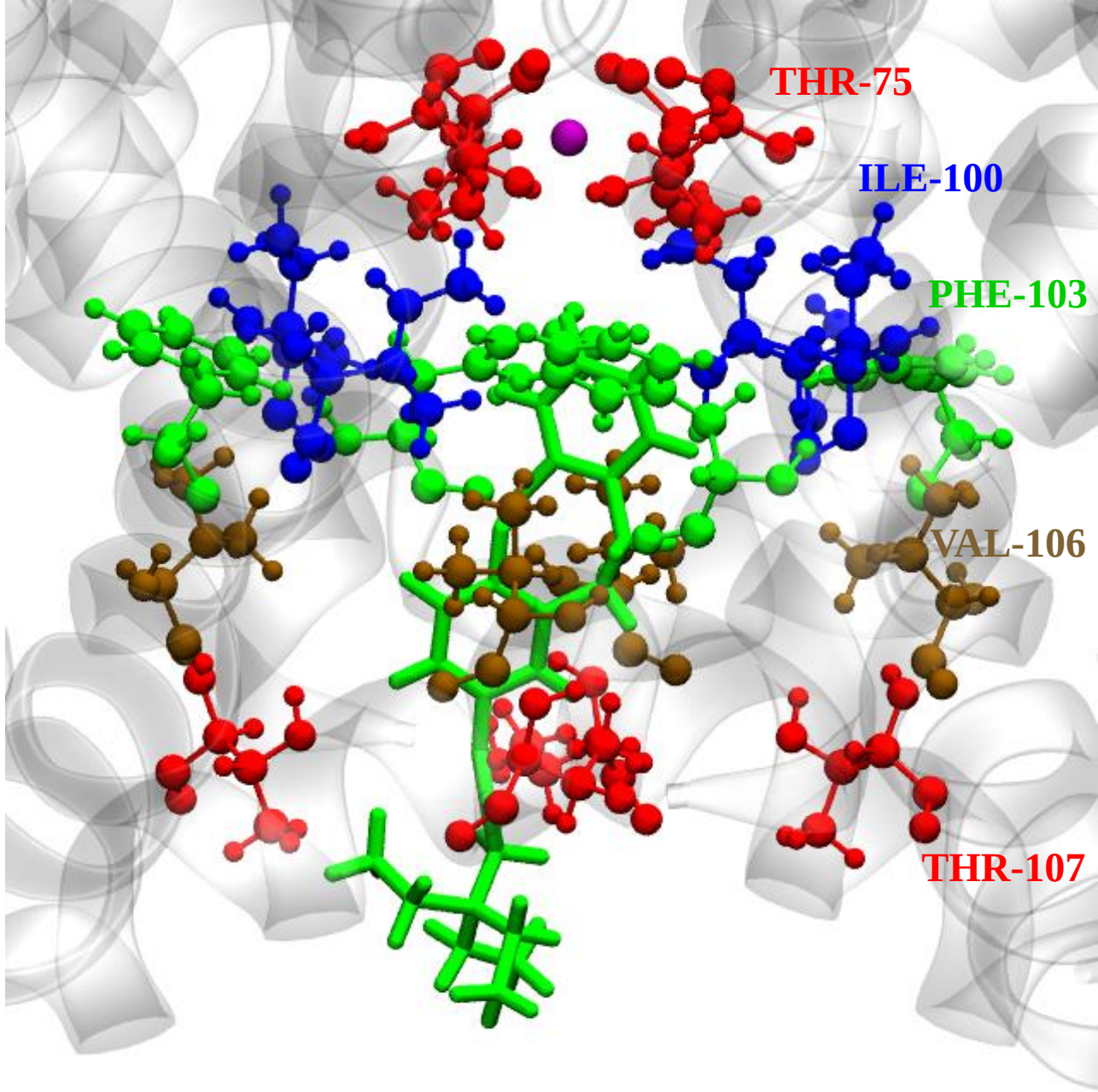
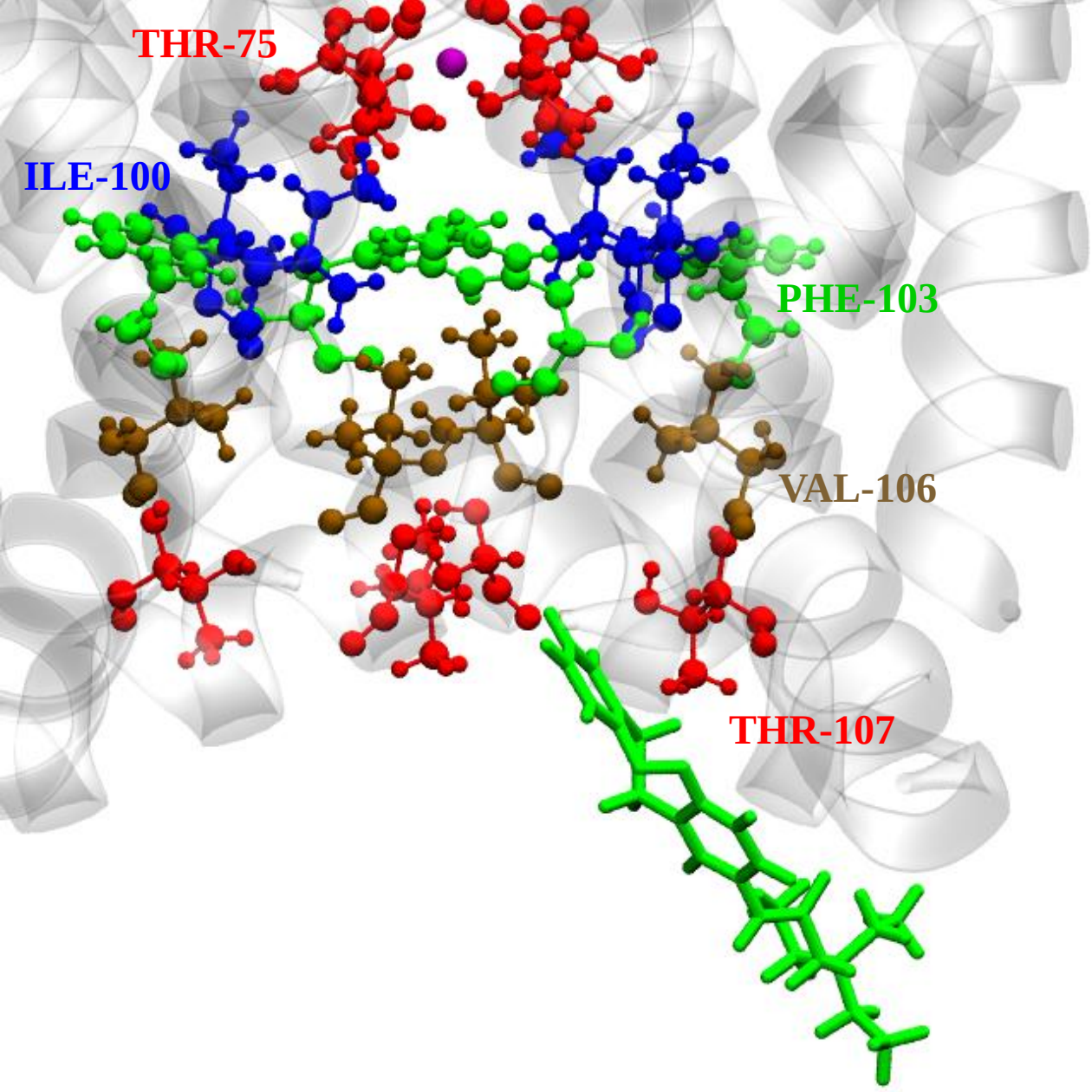
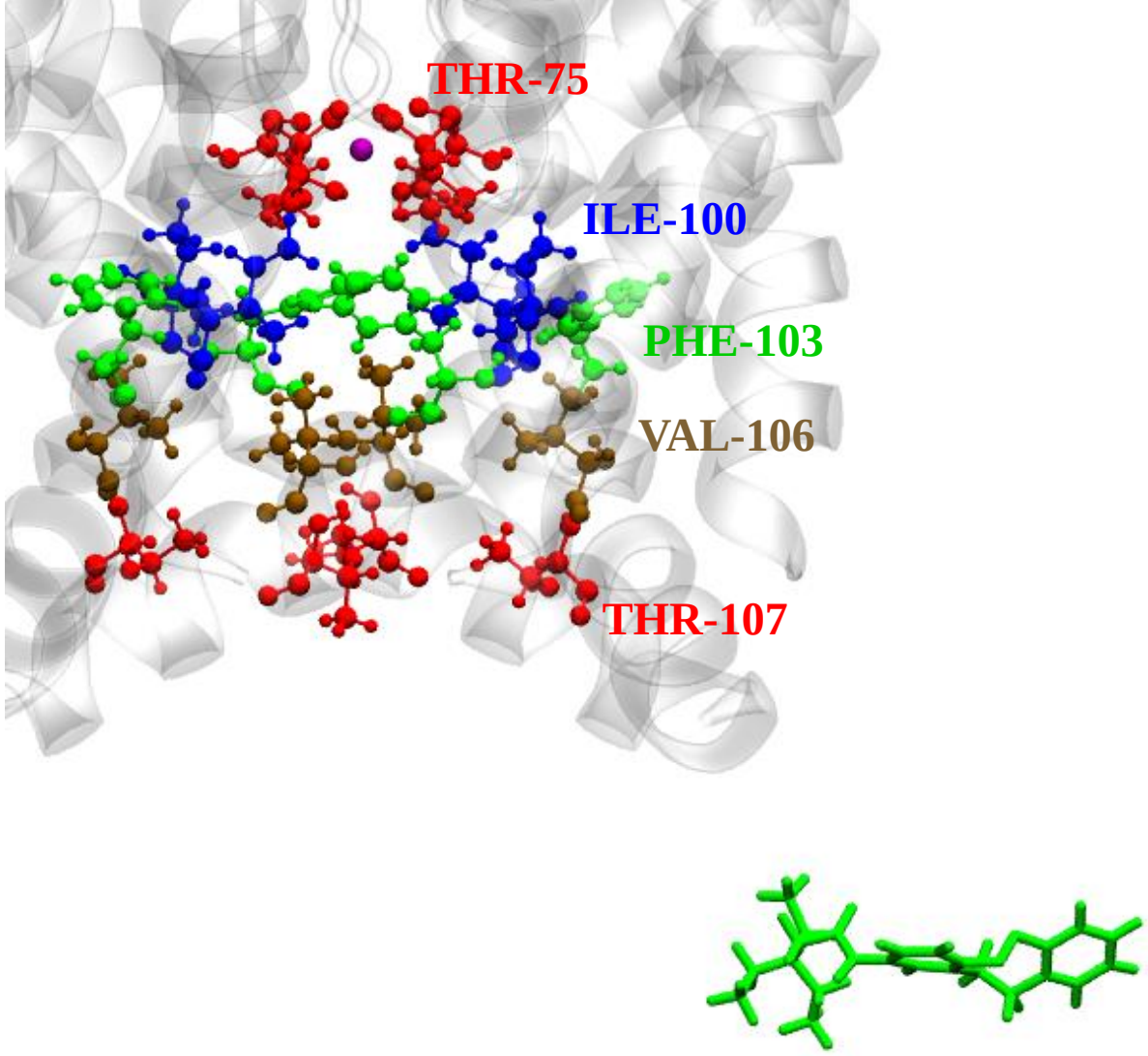


***E*2 (C0)**

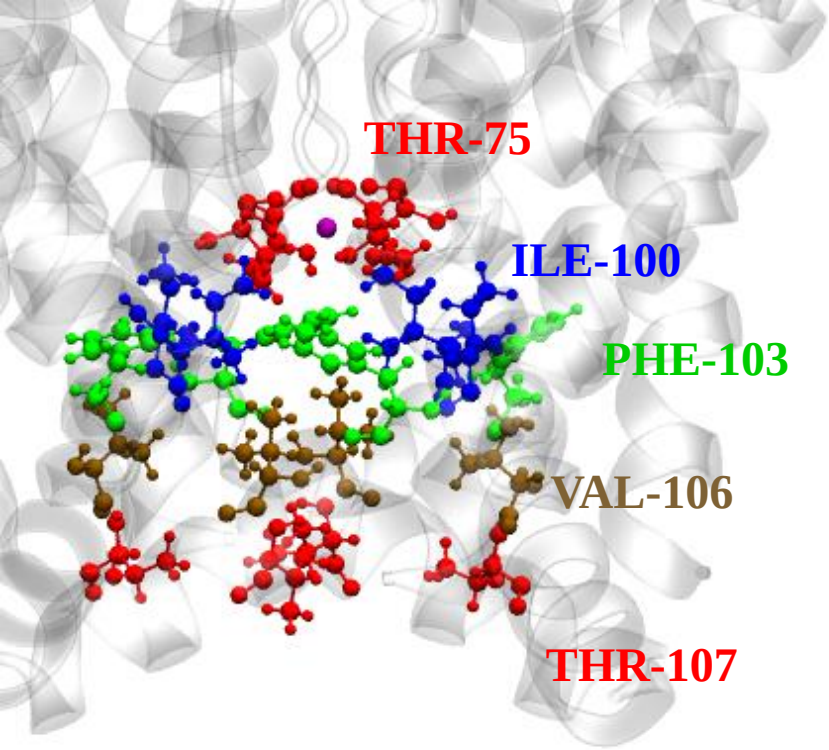
MM/PBSA Binding energy = -18.1 kcal/mol





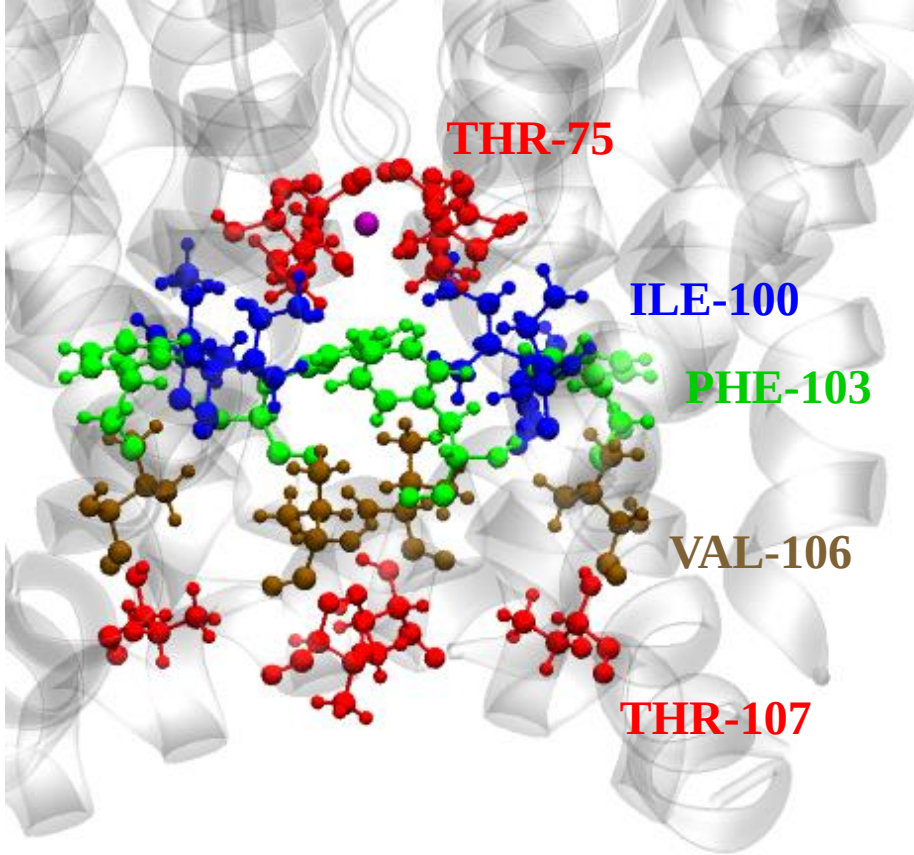
***E*2 (C1)**
MM/PBSA Binding energy = -14.3 kcal/mol

***E*2 (C2)**
MM/PBSA Binding energy = 0.0 kcal/mol



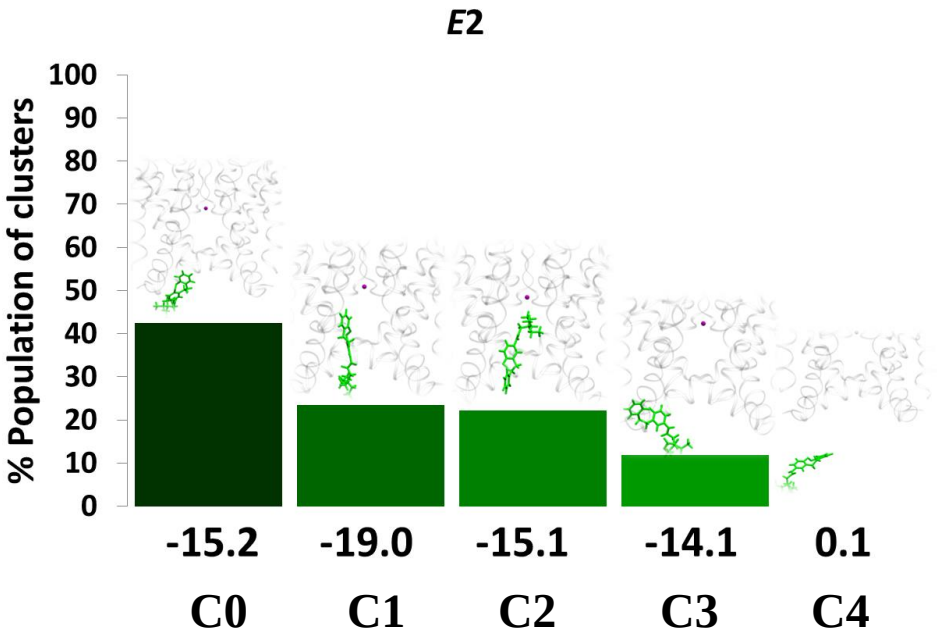
*E*2 (C3)

MM/PBSA Binding energy = 0.7 kcal/mol



*E*2 (C4)

MM/PBSA Binding energy = -0.1 kcal/mol



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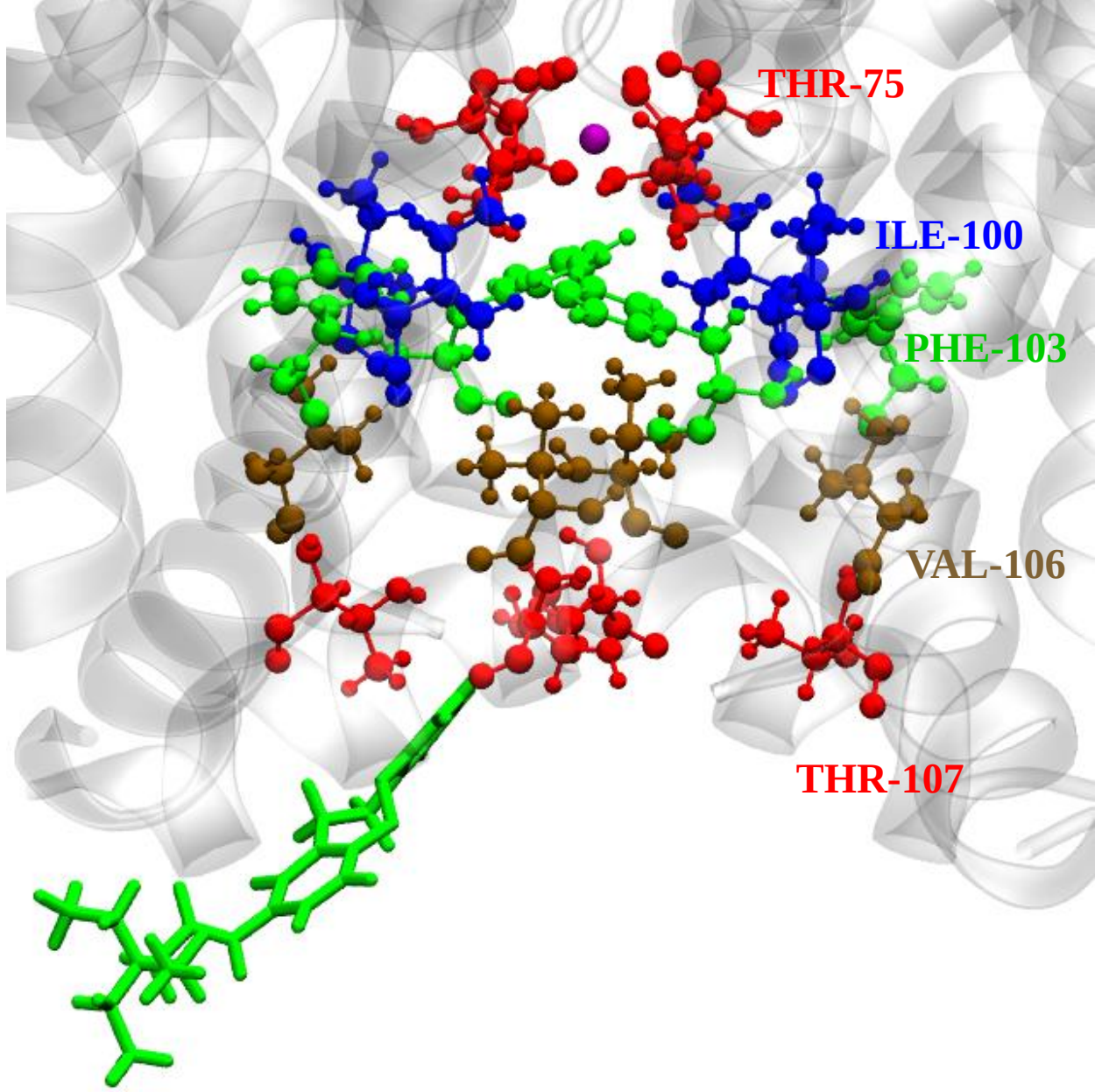
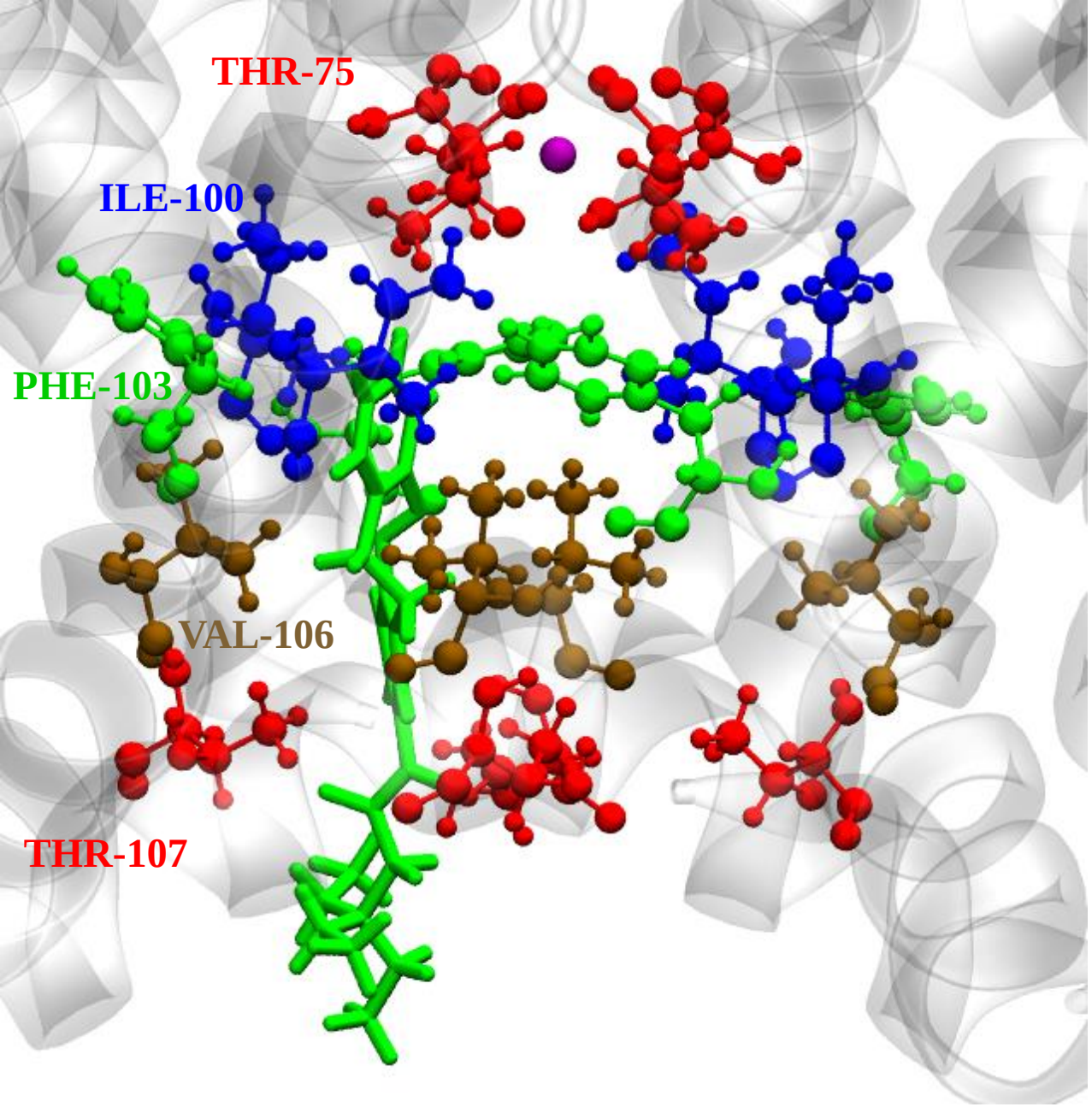
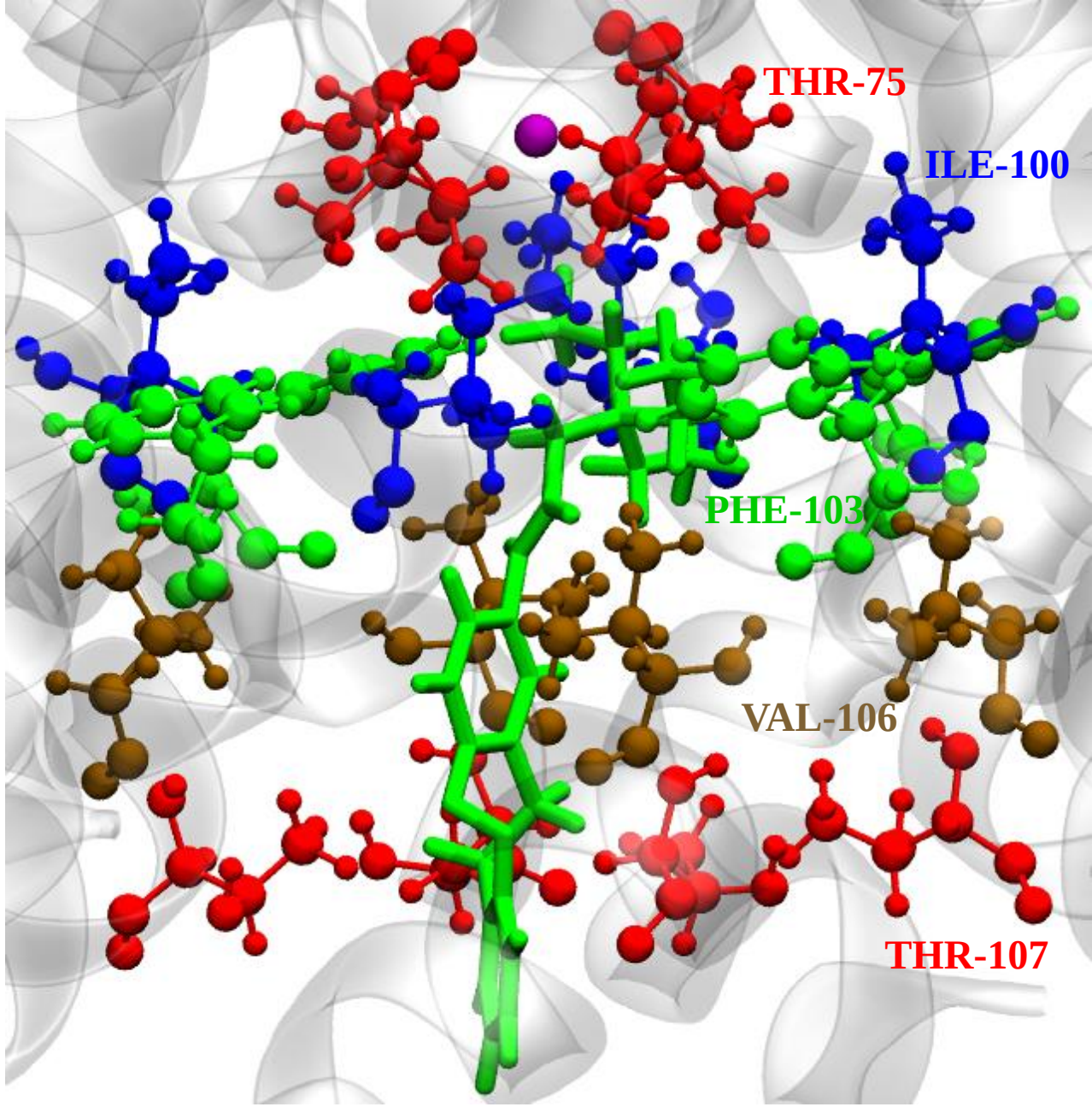


***E*2 (C0)**

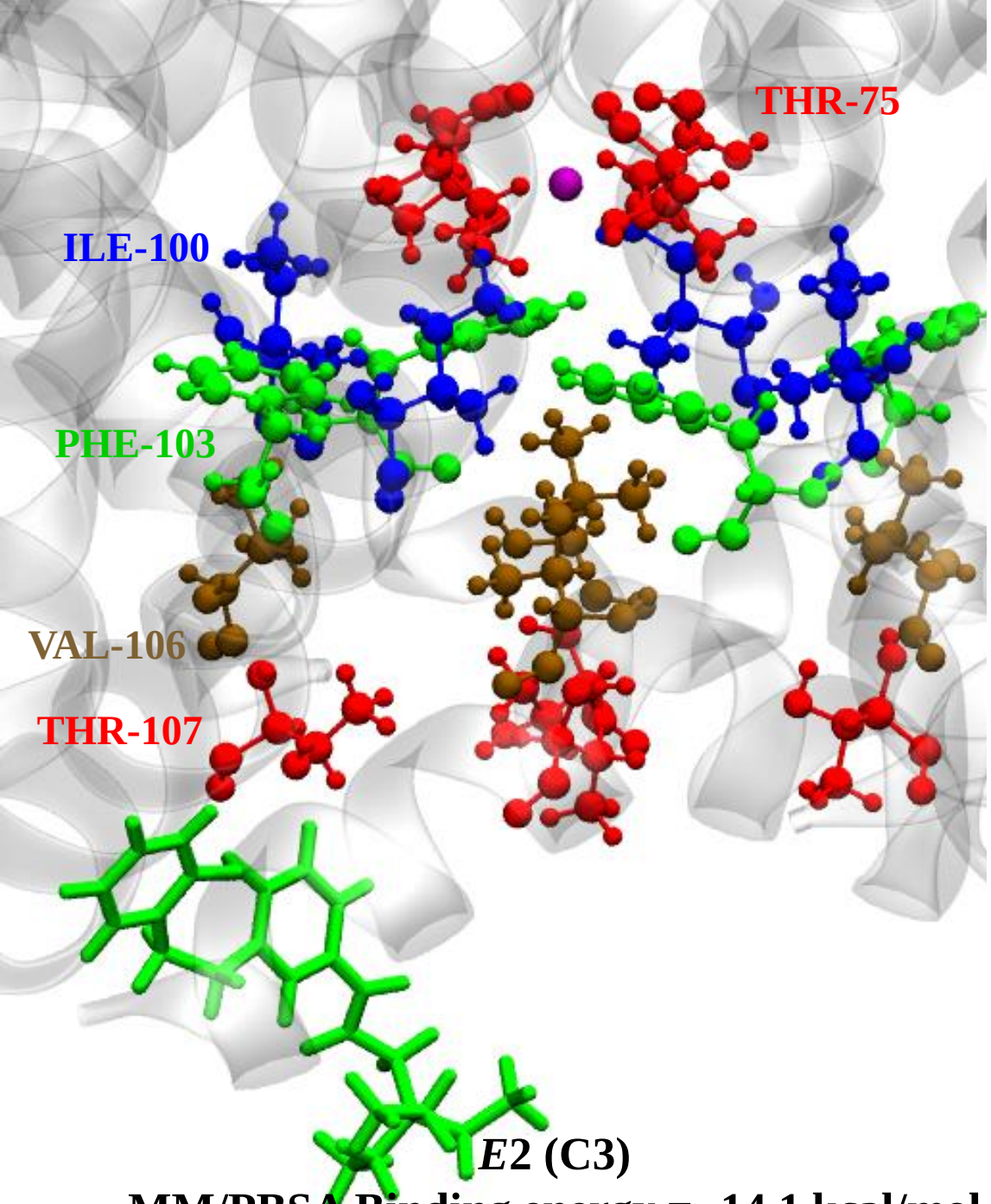
MM/PBSA Binding energy = -15.2 kcal/mol





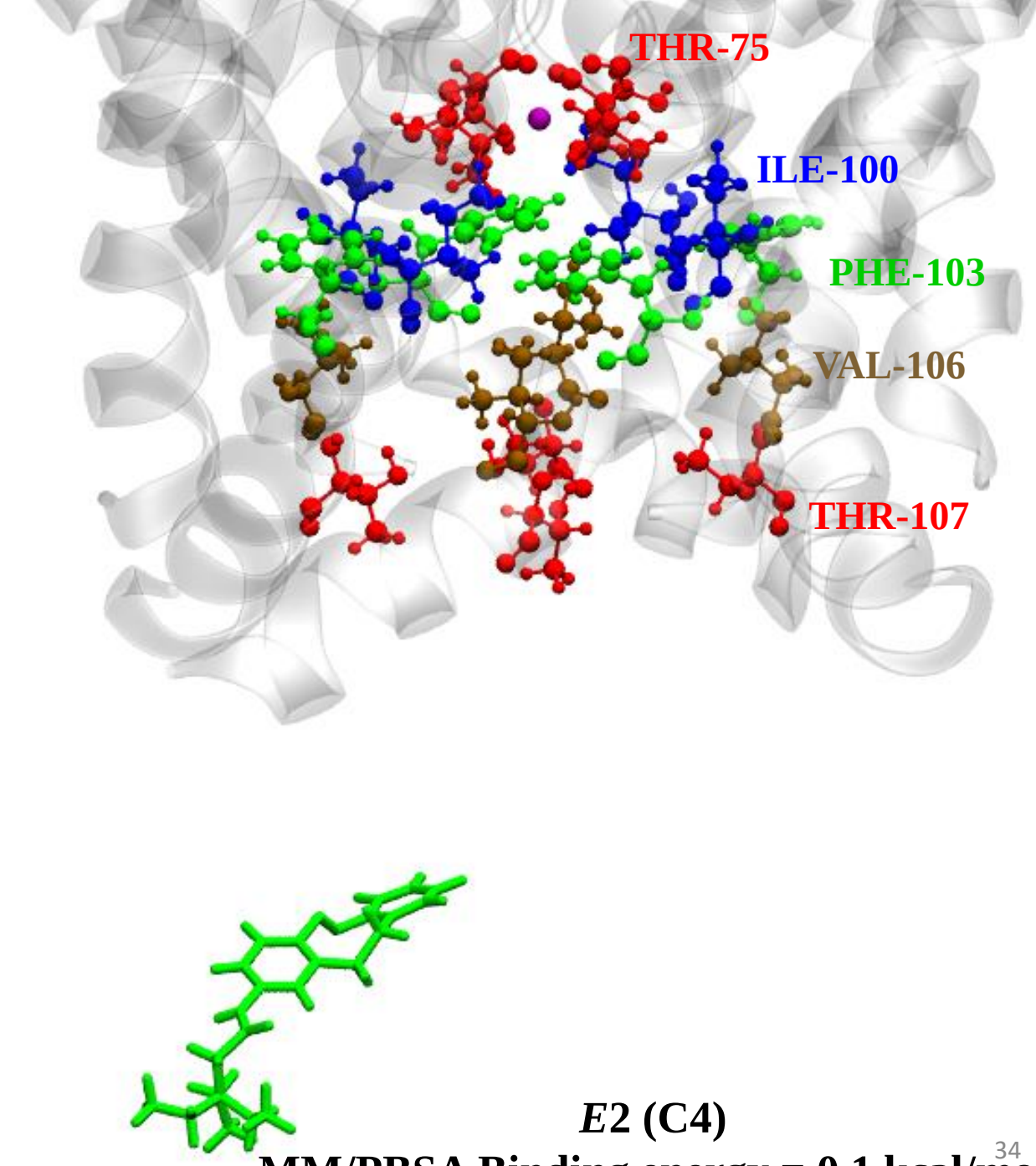
***E*2 (C1)**
MM/PBSA Binding energy = -19.0 kcal/mol

***E*2 (C2)**
MM/PBSA Binding energy = -15.1 kcal/mol



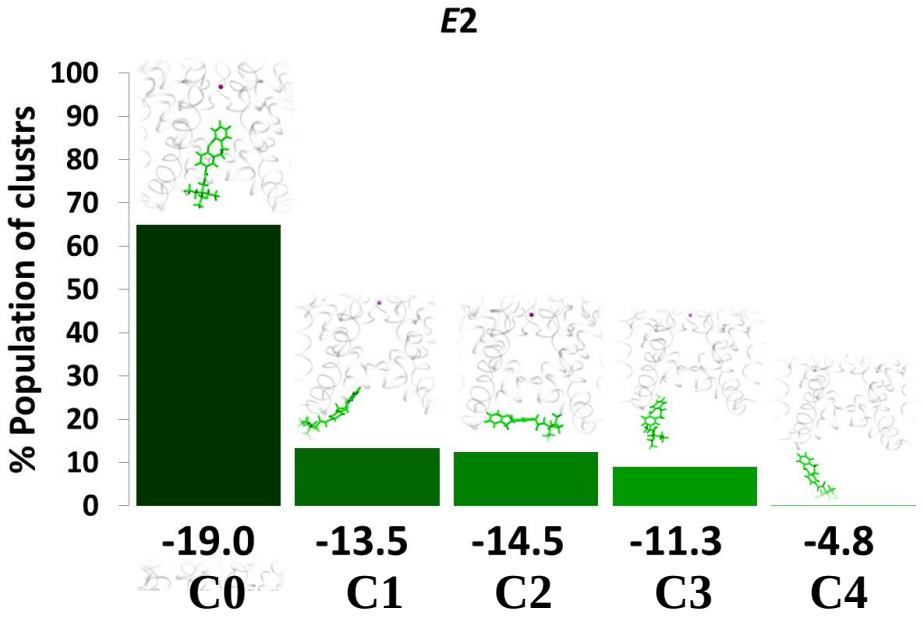
*E*2 (C3)

MM/PBSA Binding energy = -14.1 kcal/mol



*E*2 (C4)

MM/PBSA Binding energy = 0.1 kcal/mol



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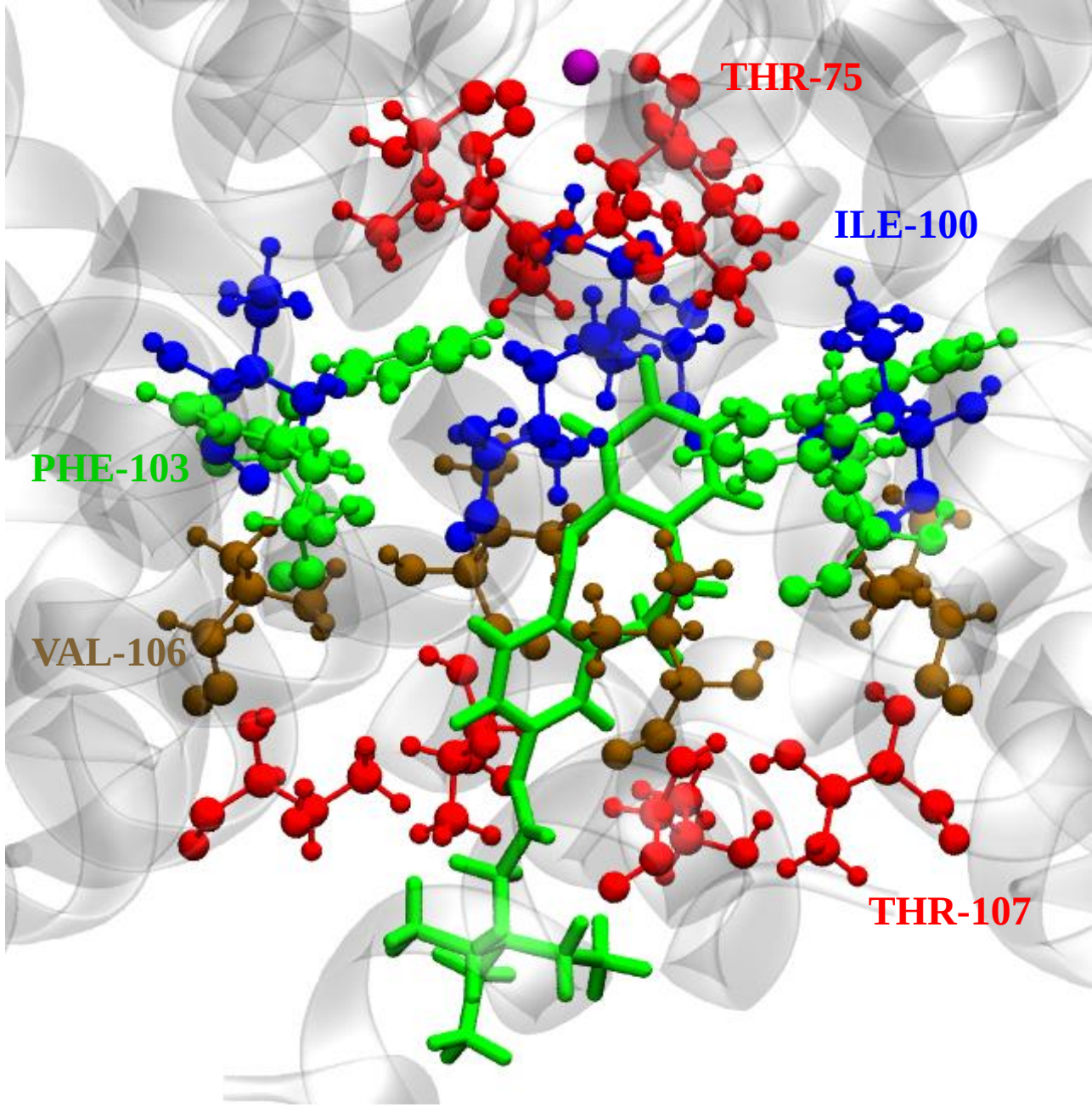
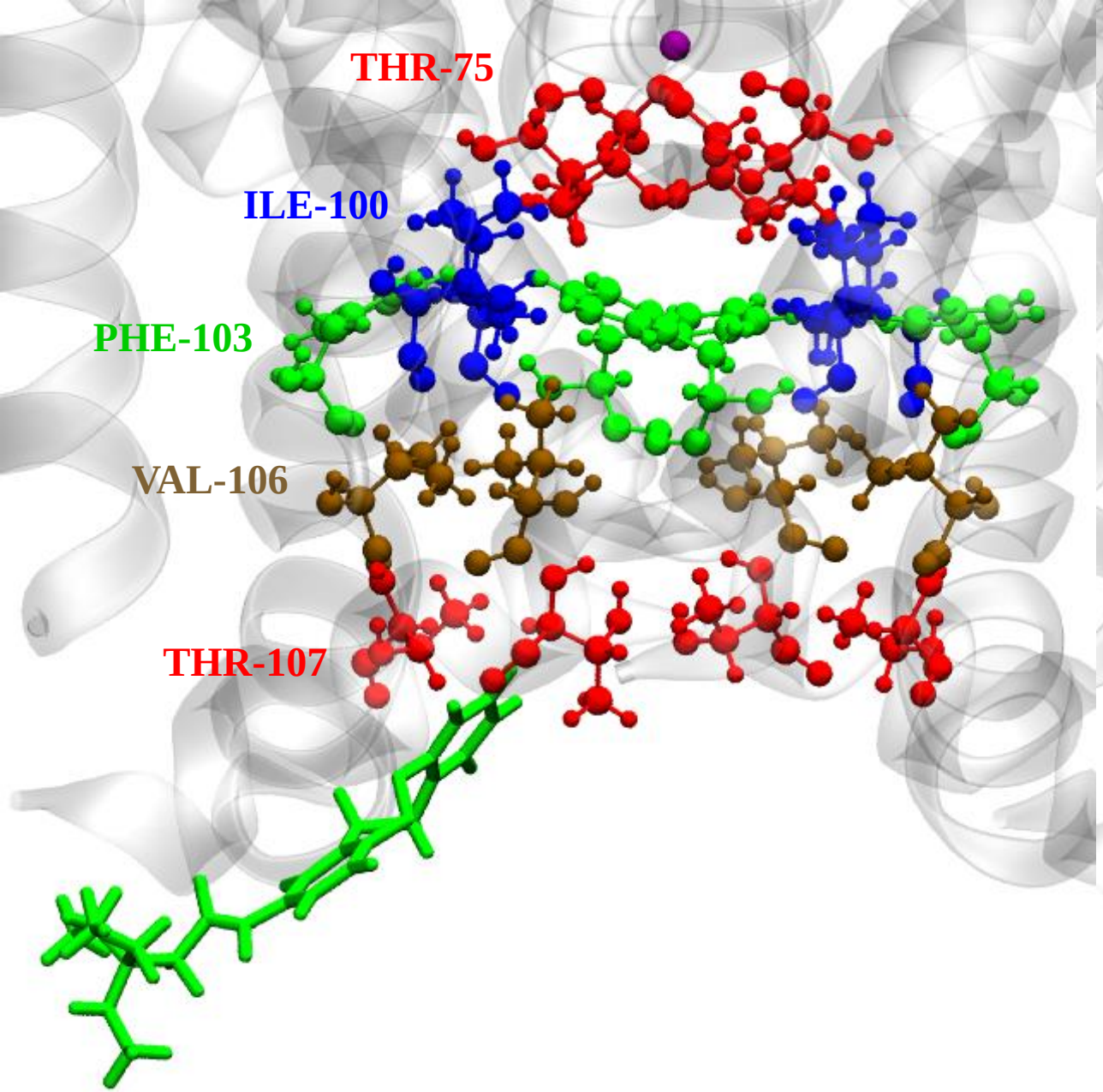
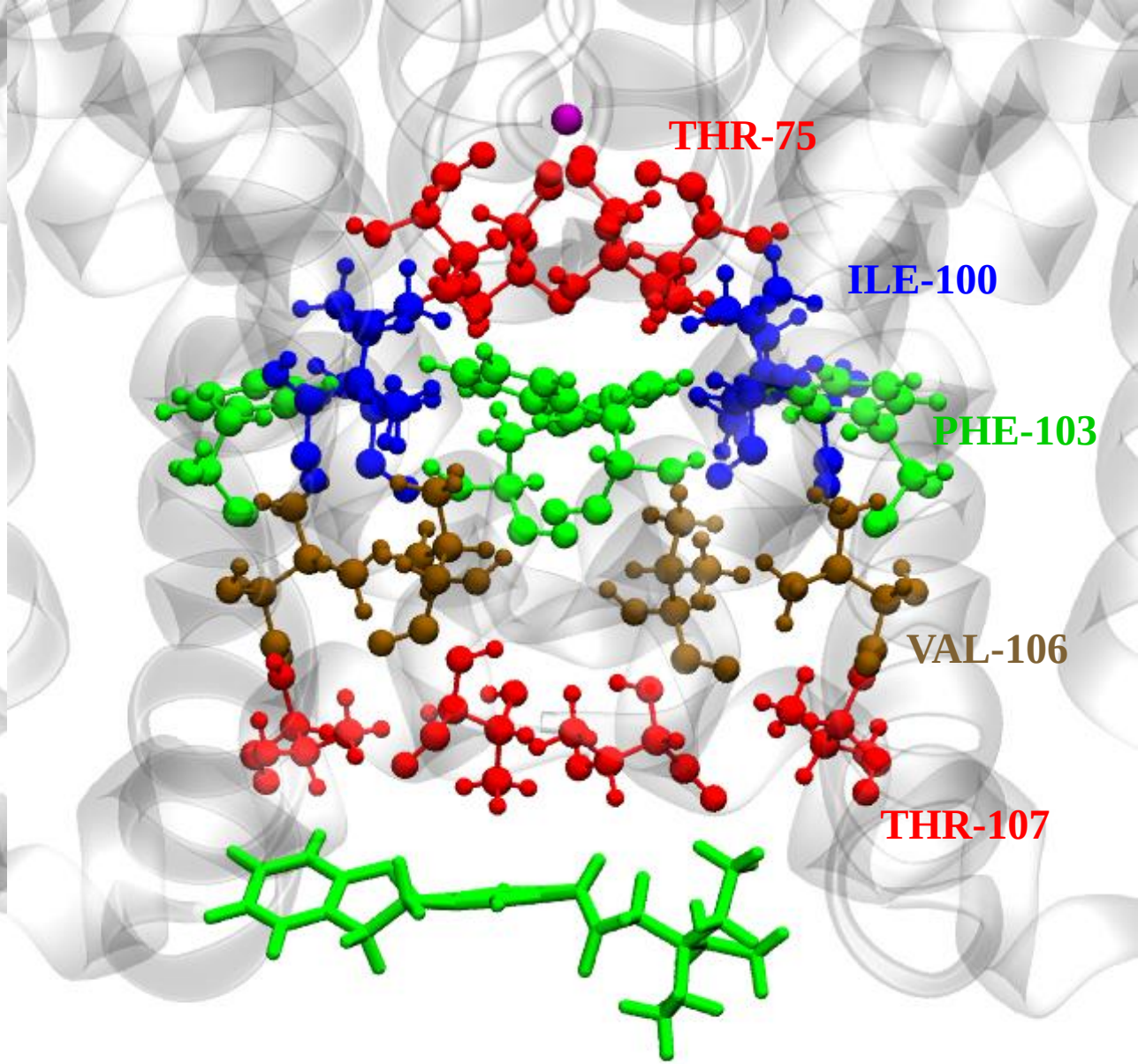


***E*2 (C0)**

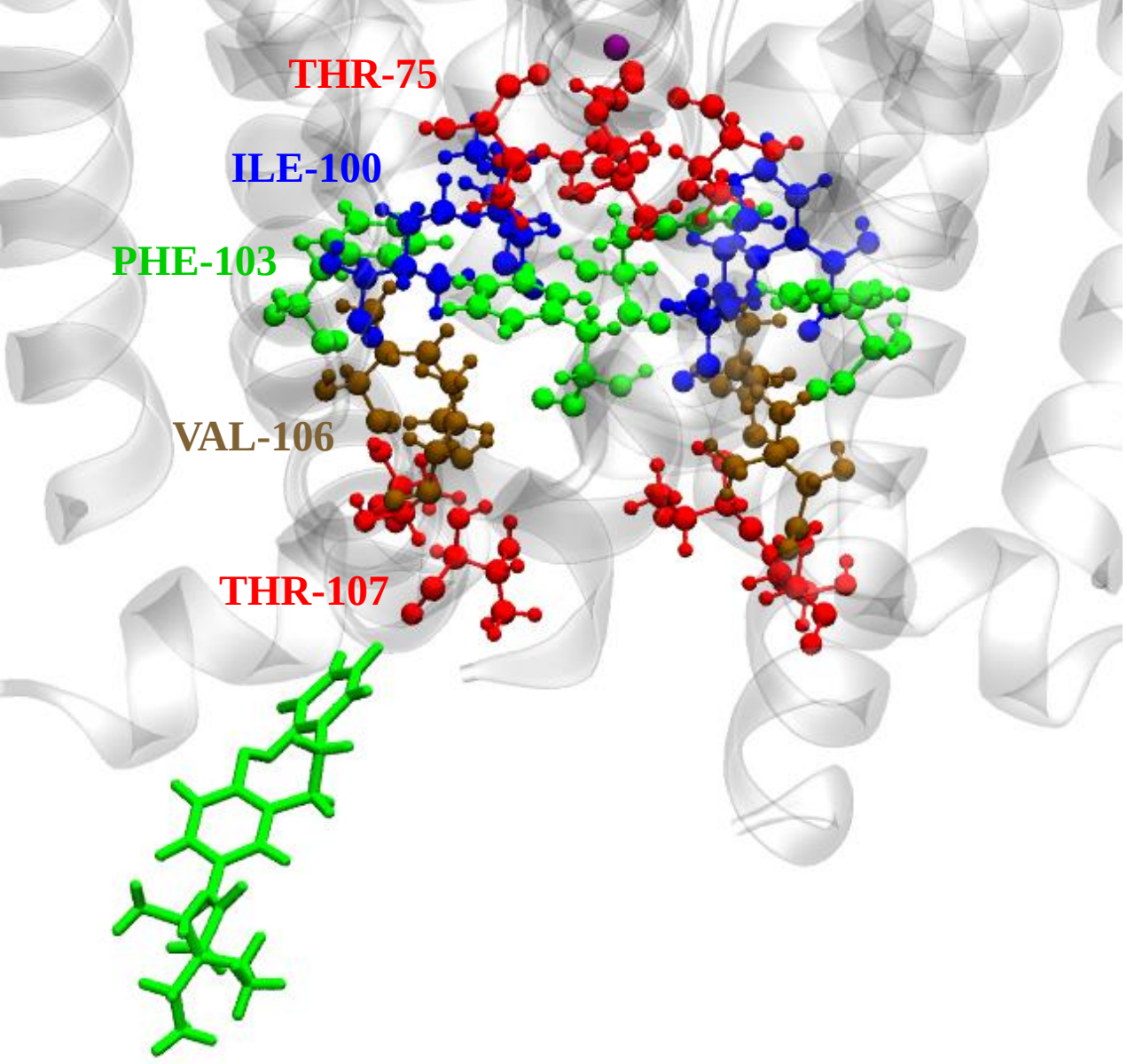
MM/PBSA Binding energy = -19.0 kcal/mol

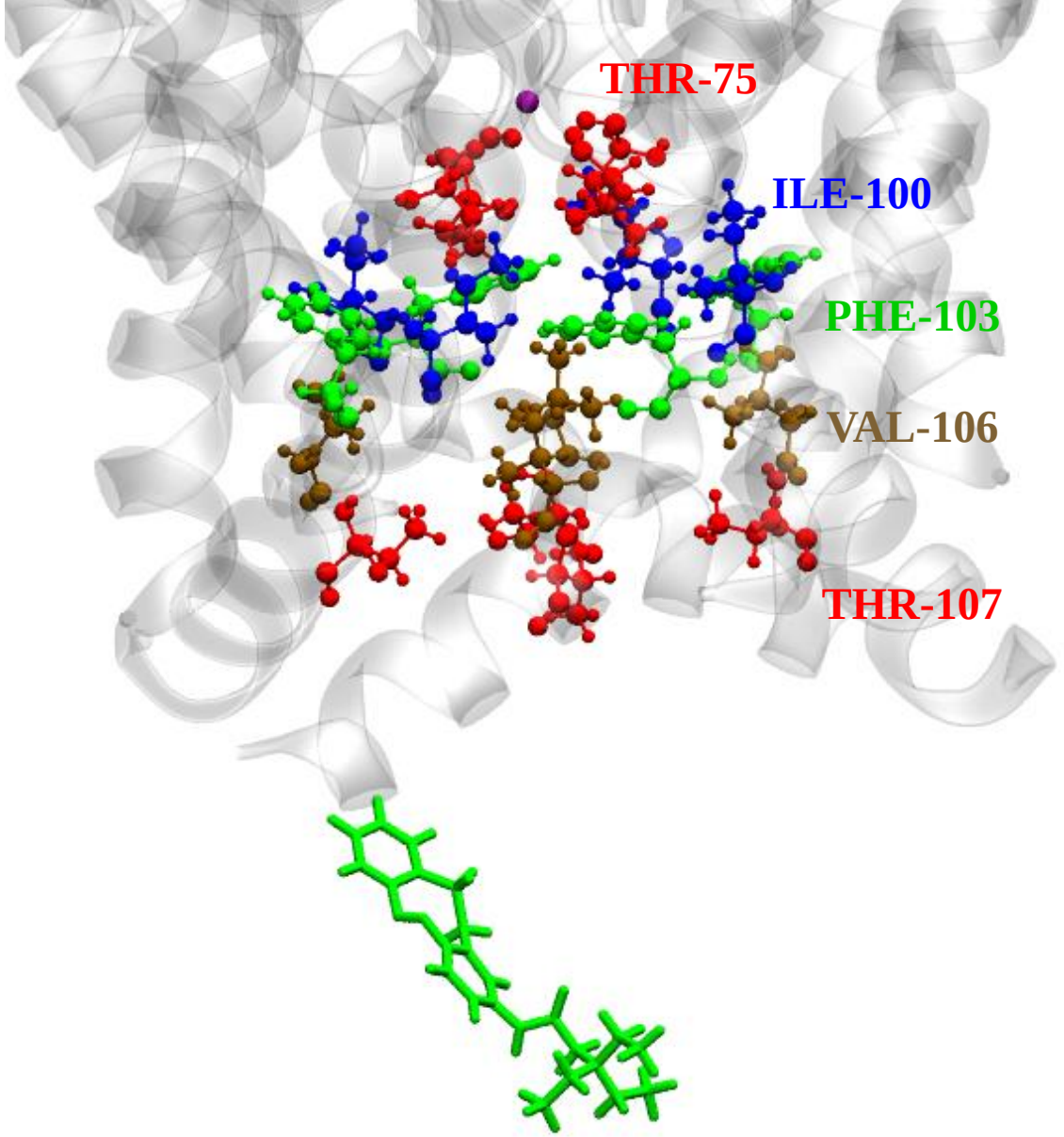




***E*2 (C1)**
MM/PBSA Binding energy = -13.5 kcal/mol

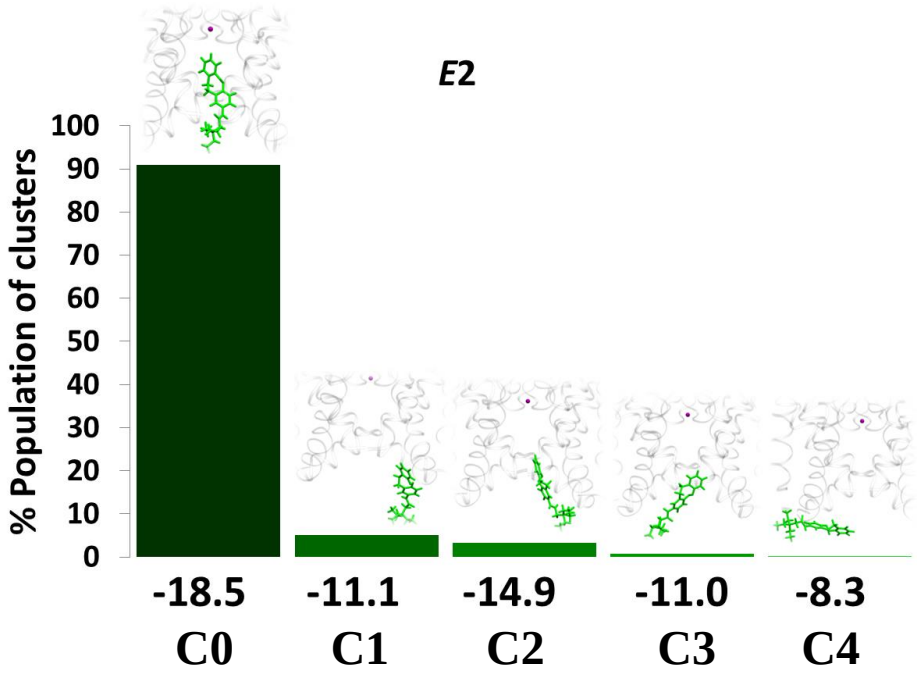
***E*2 (C2)**
MM/PBSA Binding energy = -14.5 kcal/mol





***E*2 (C3)**
MM/PBSA Binding energy = -11.3 kcal/mol

***E*2 (C4)**
MM/PBSA Binding energy = -4.8 kcal/mol



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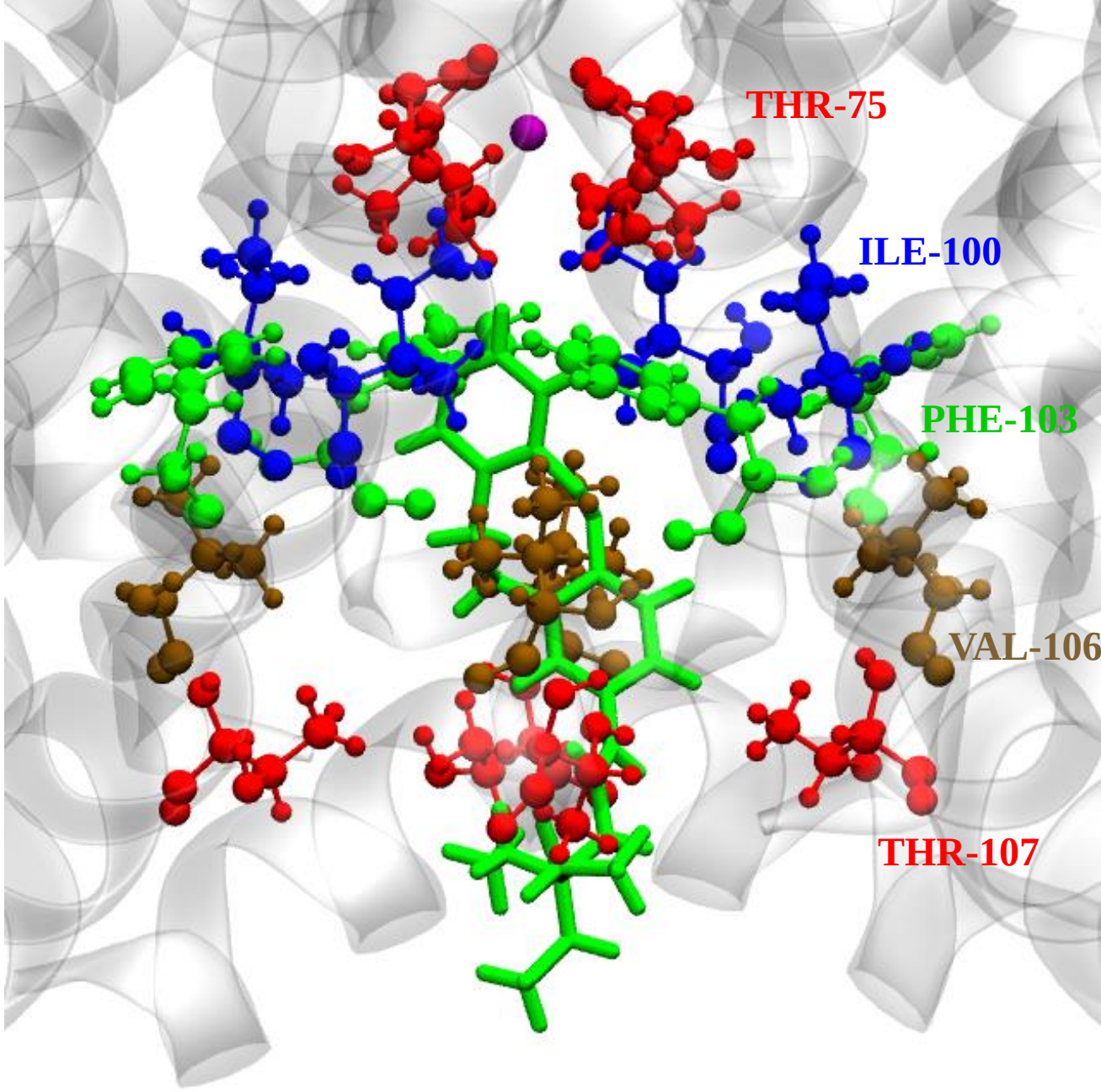
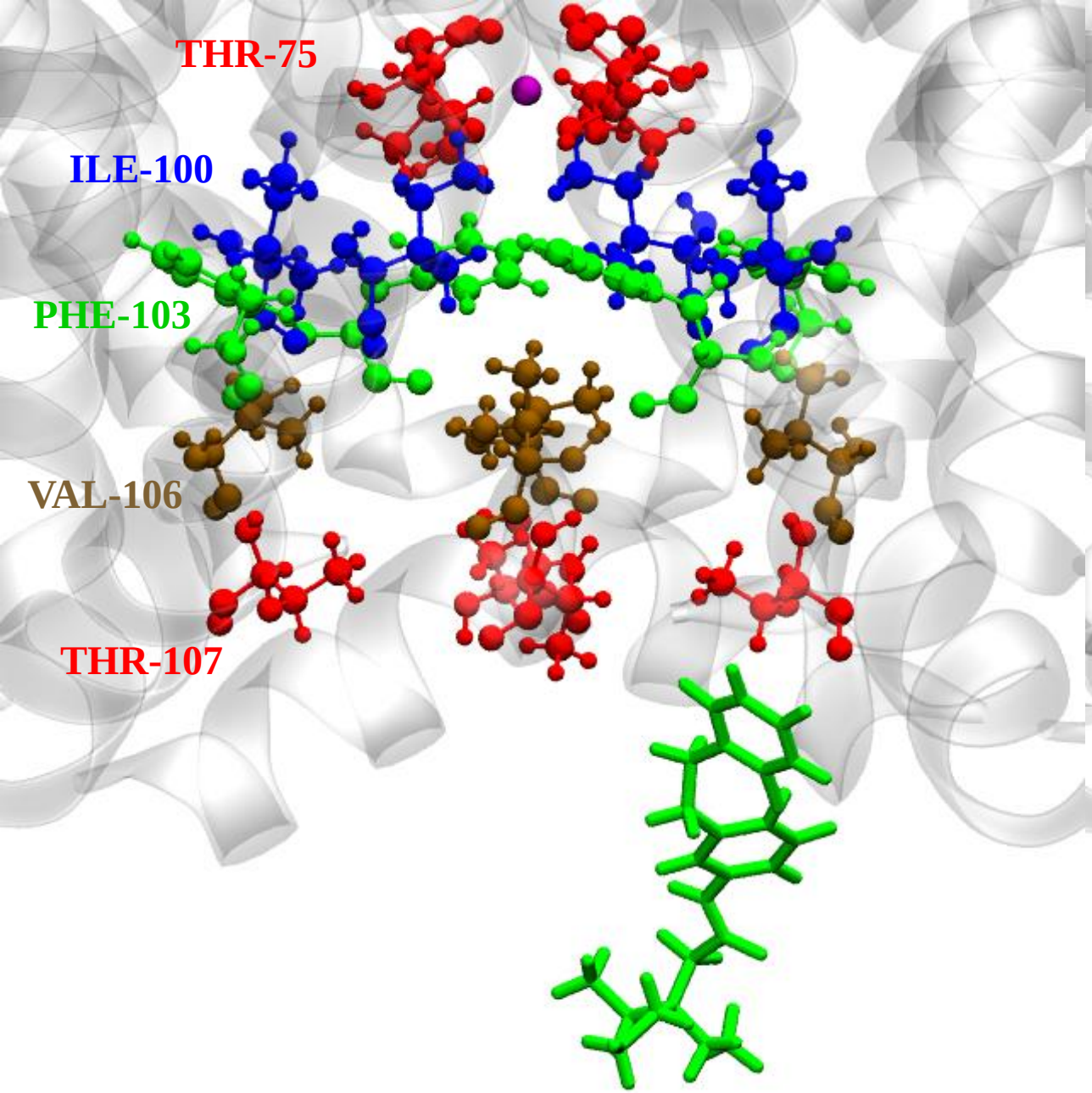
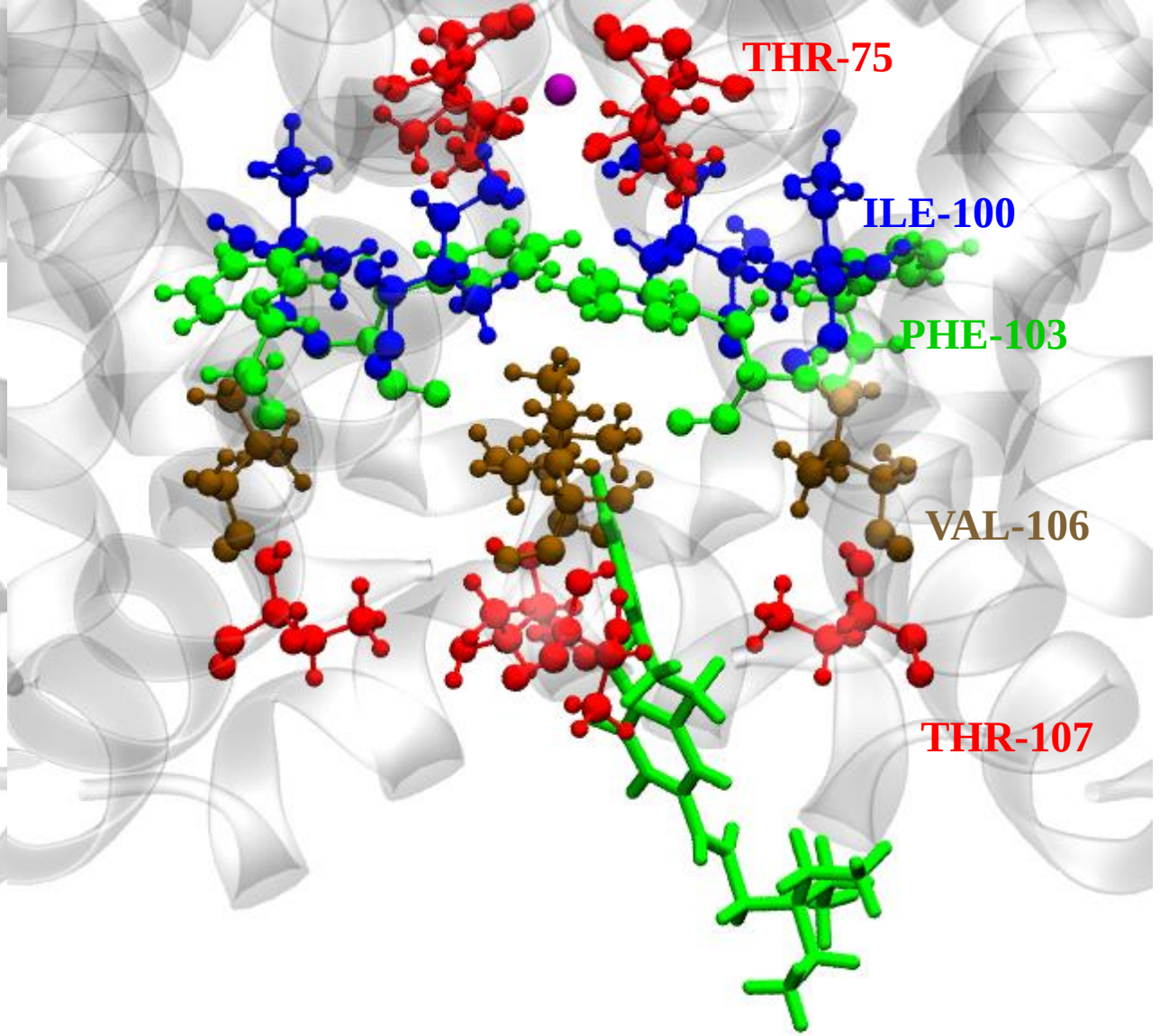


***E*2 (C0)**

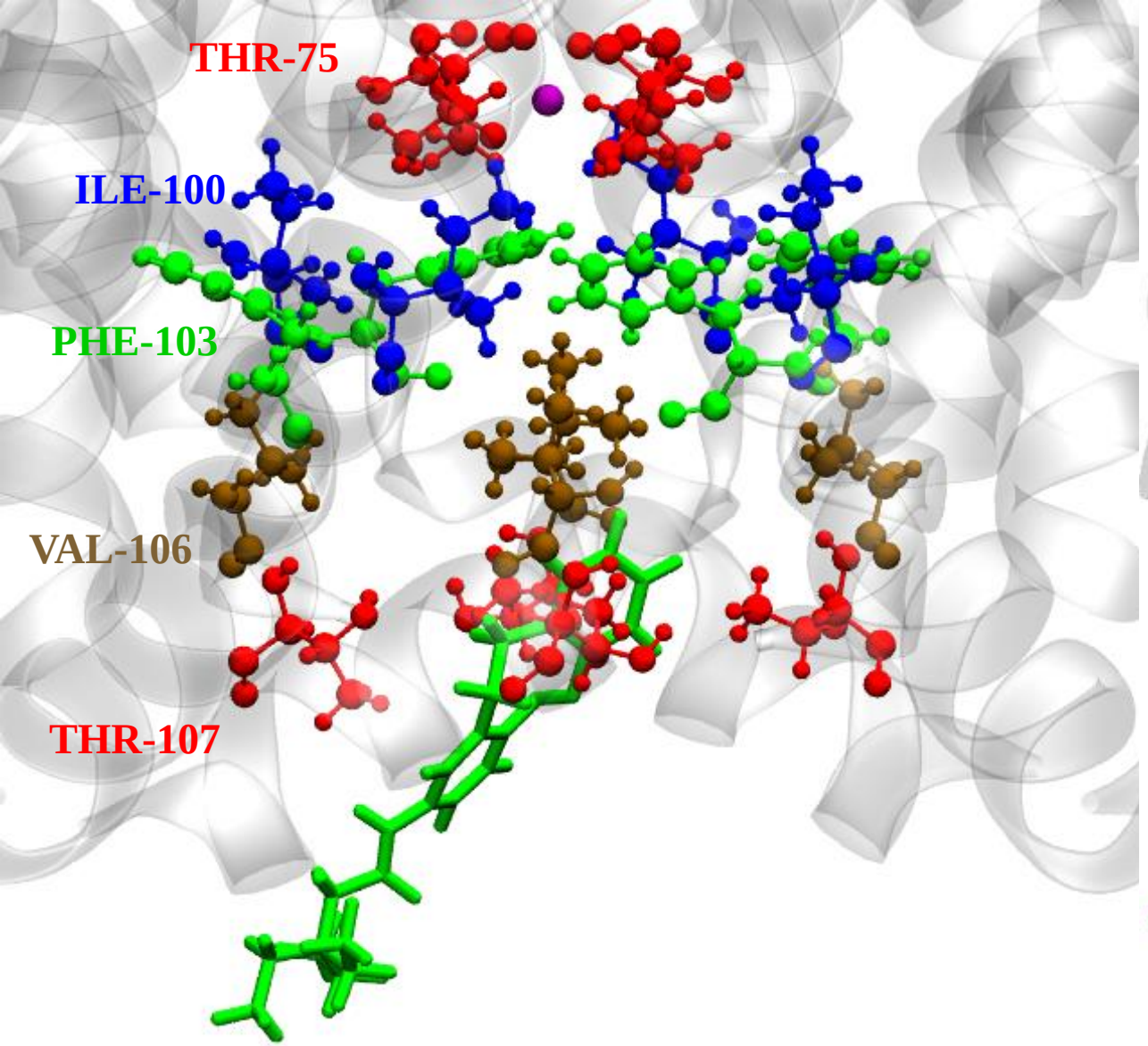
MM/PBSA Binding energy = -18.5 kcal/mol

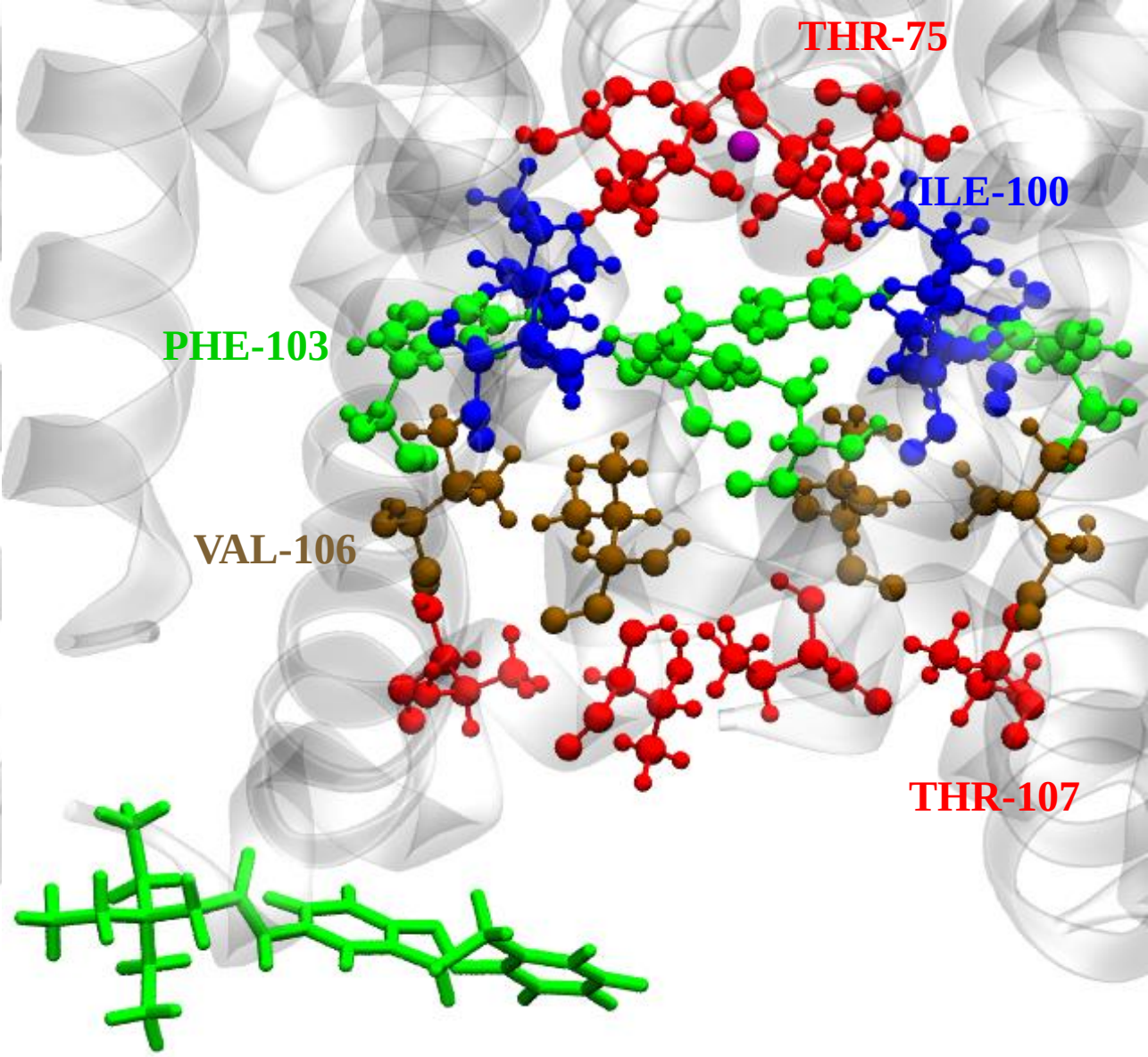




***E*2 (C1)**
MM/PBSA Binding energy = -11.1 kcal/mol

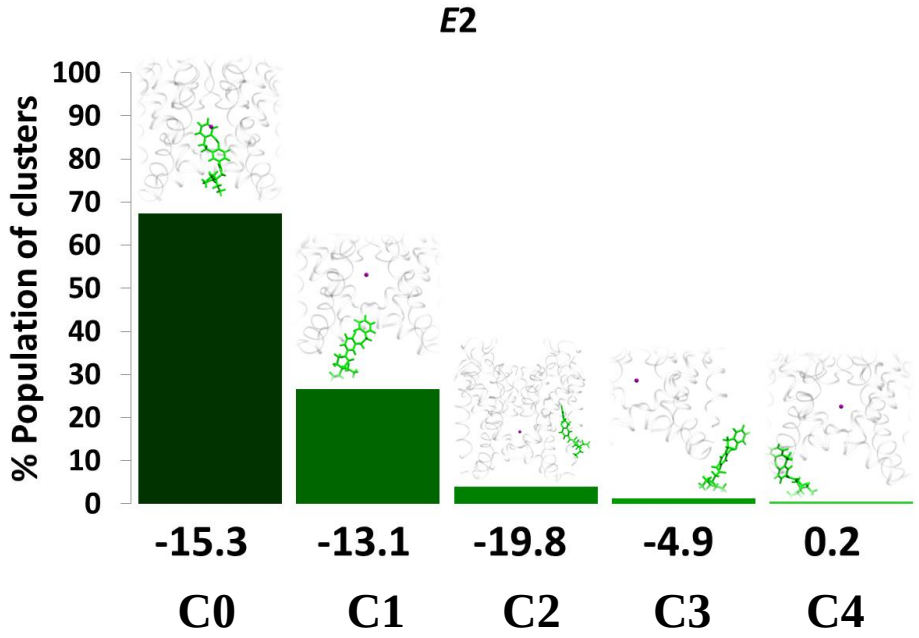
***E*2 (C2)**
MM/PBSA Binding energy = -14.9 kcal/mol





***E*2 (C3)**
MM/PBSA Binding energy = -11.0 kcal/mol

***E*2 (C4)**
MM/PBSA Binding energy = -8.3 kcal/mol



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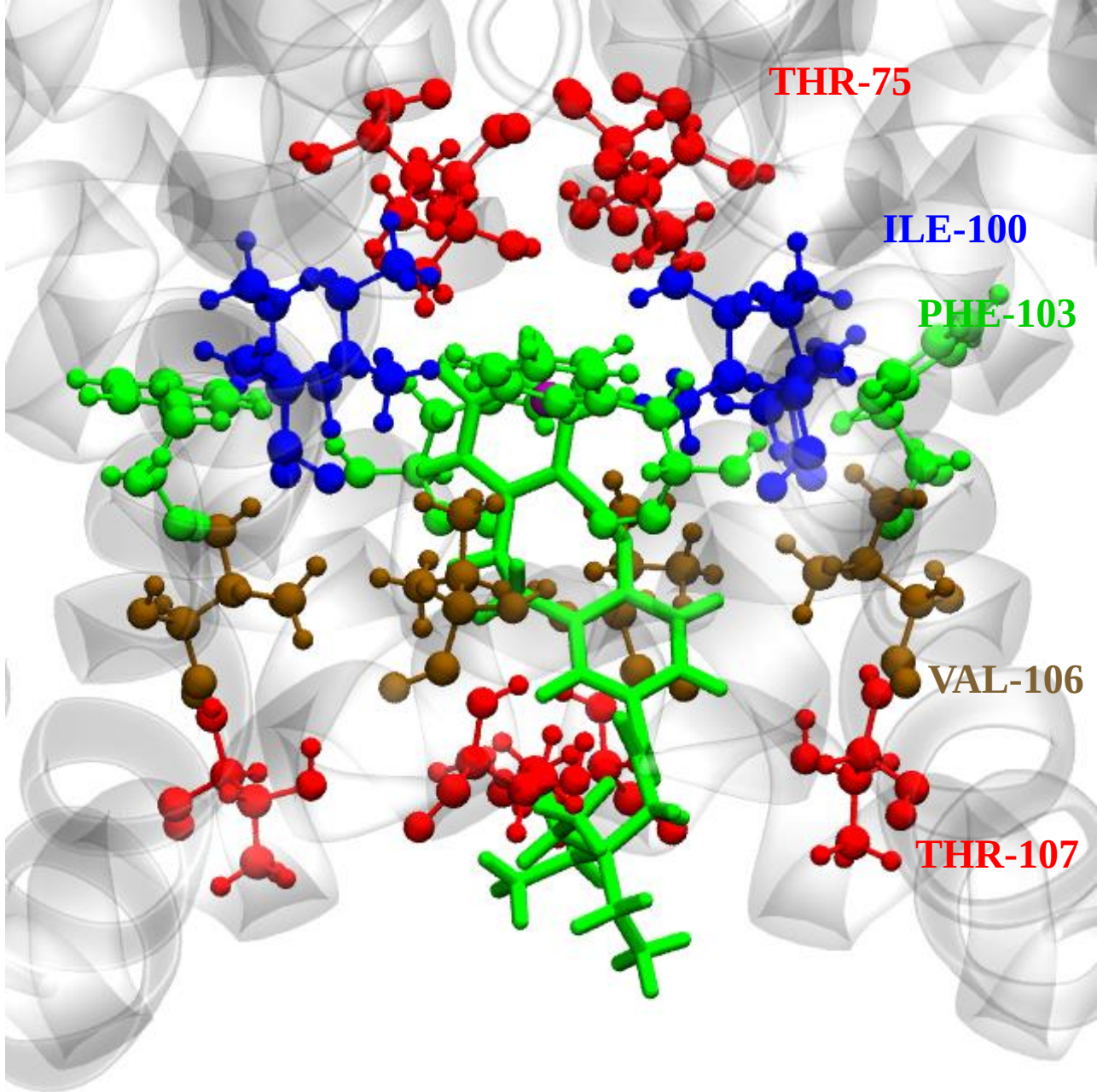
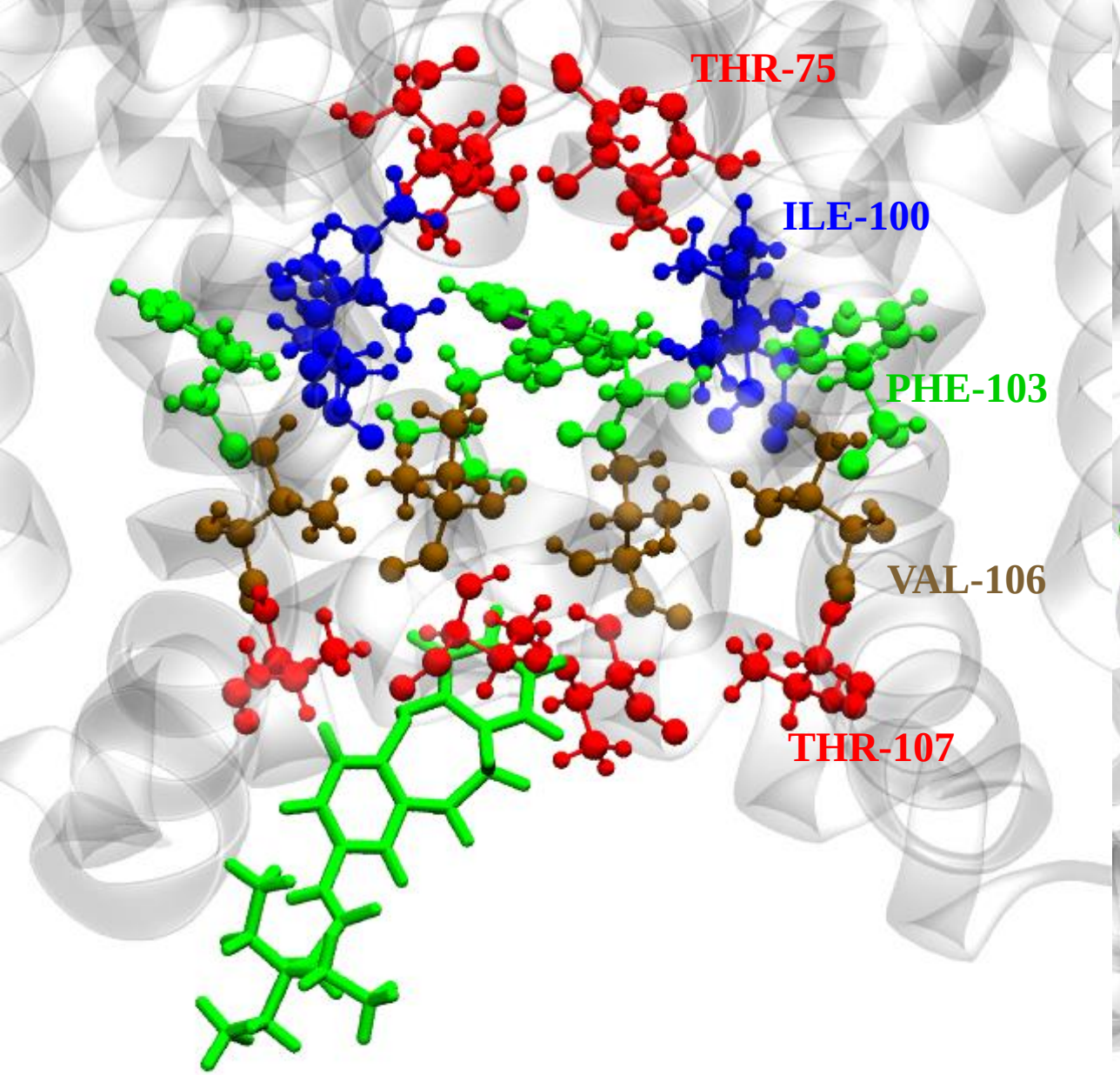
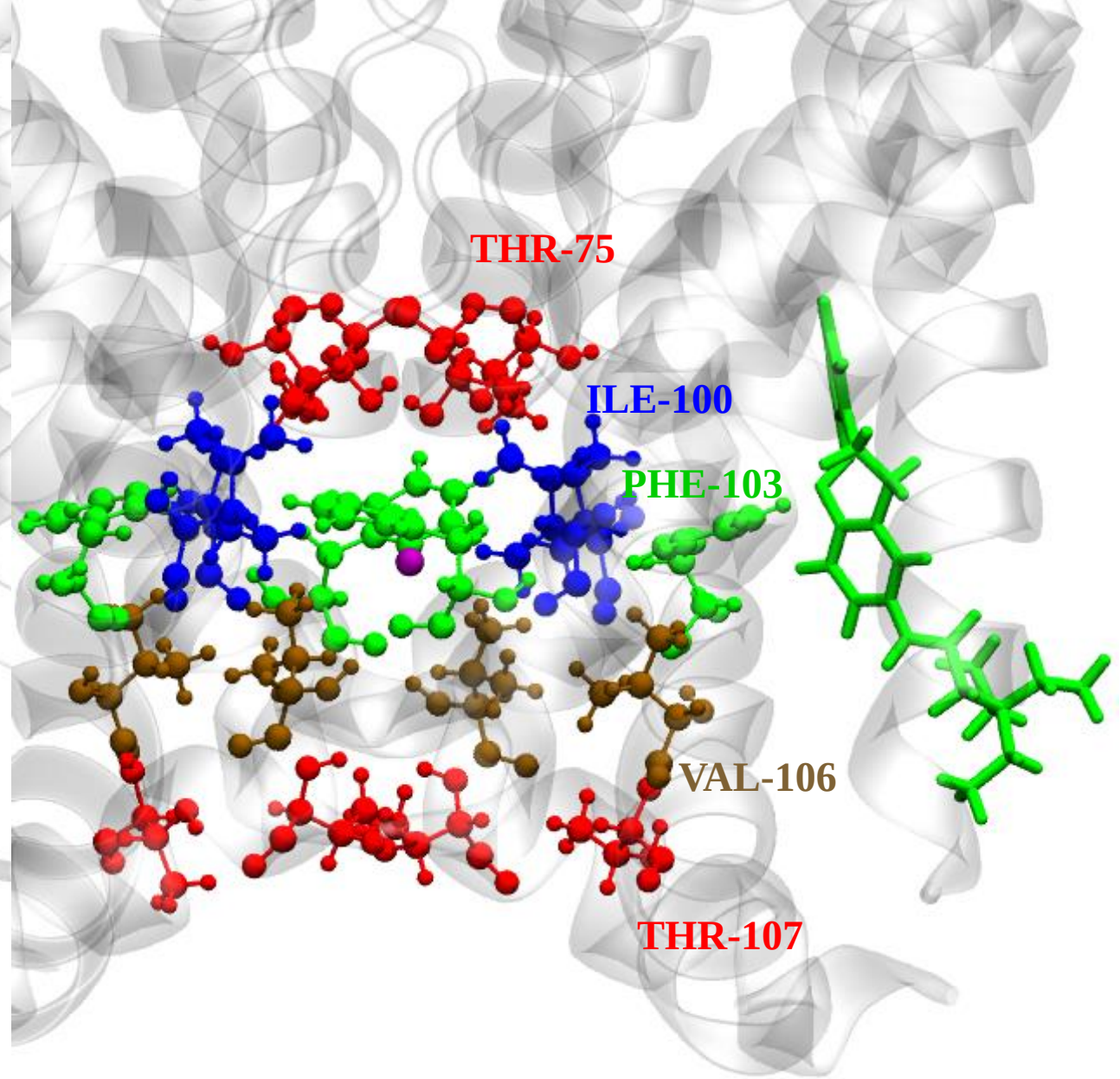


***E*2 (C0)**

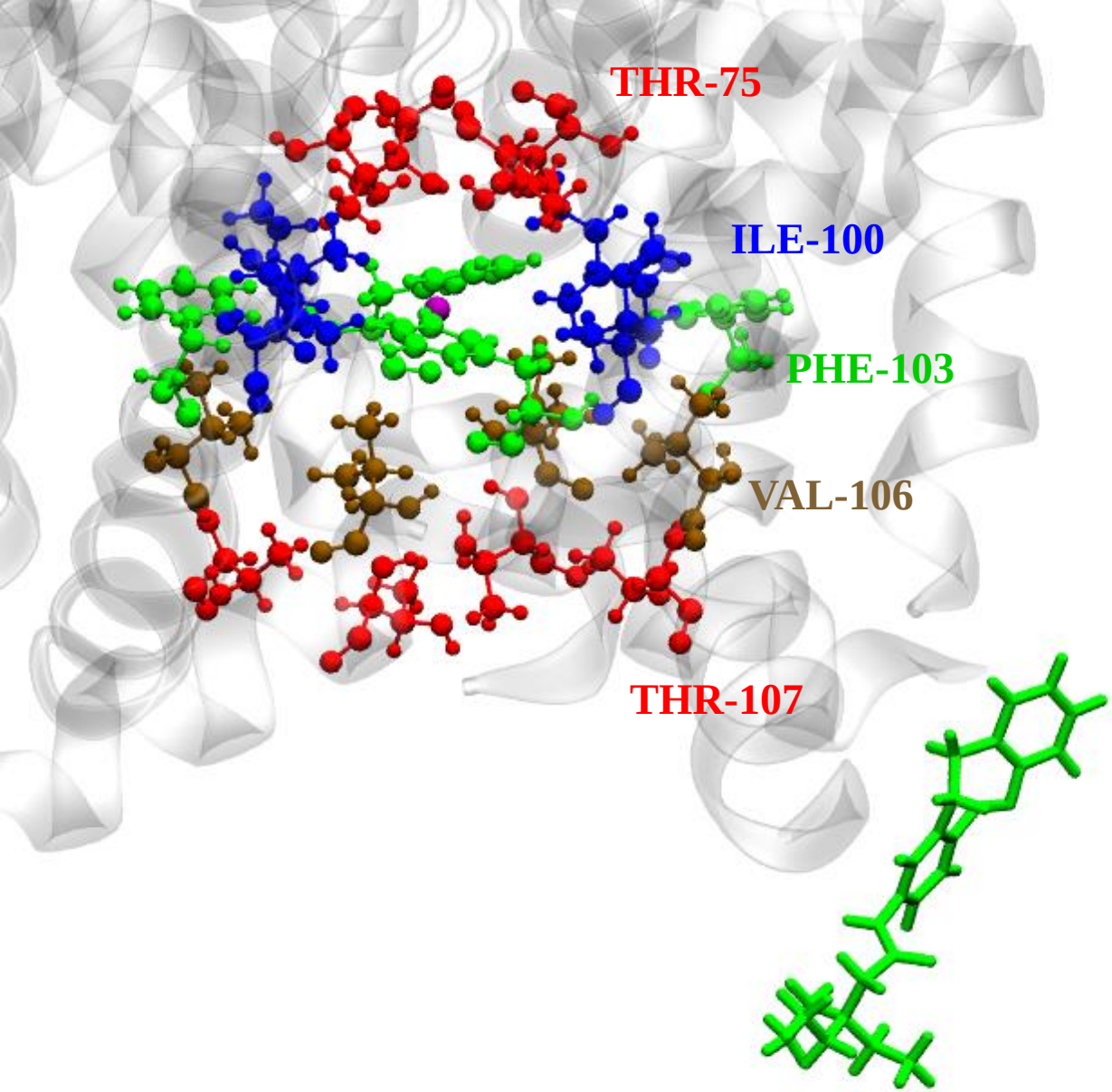
MM/PBSA Binding energy = -15.3 kcal/mol

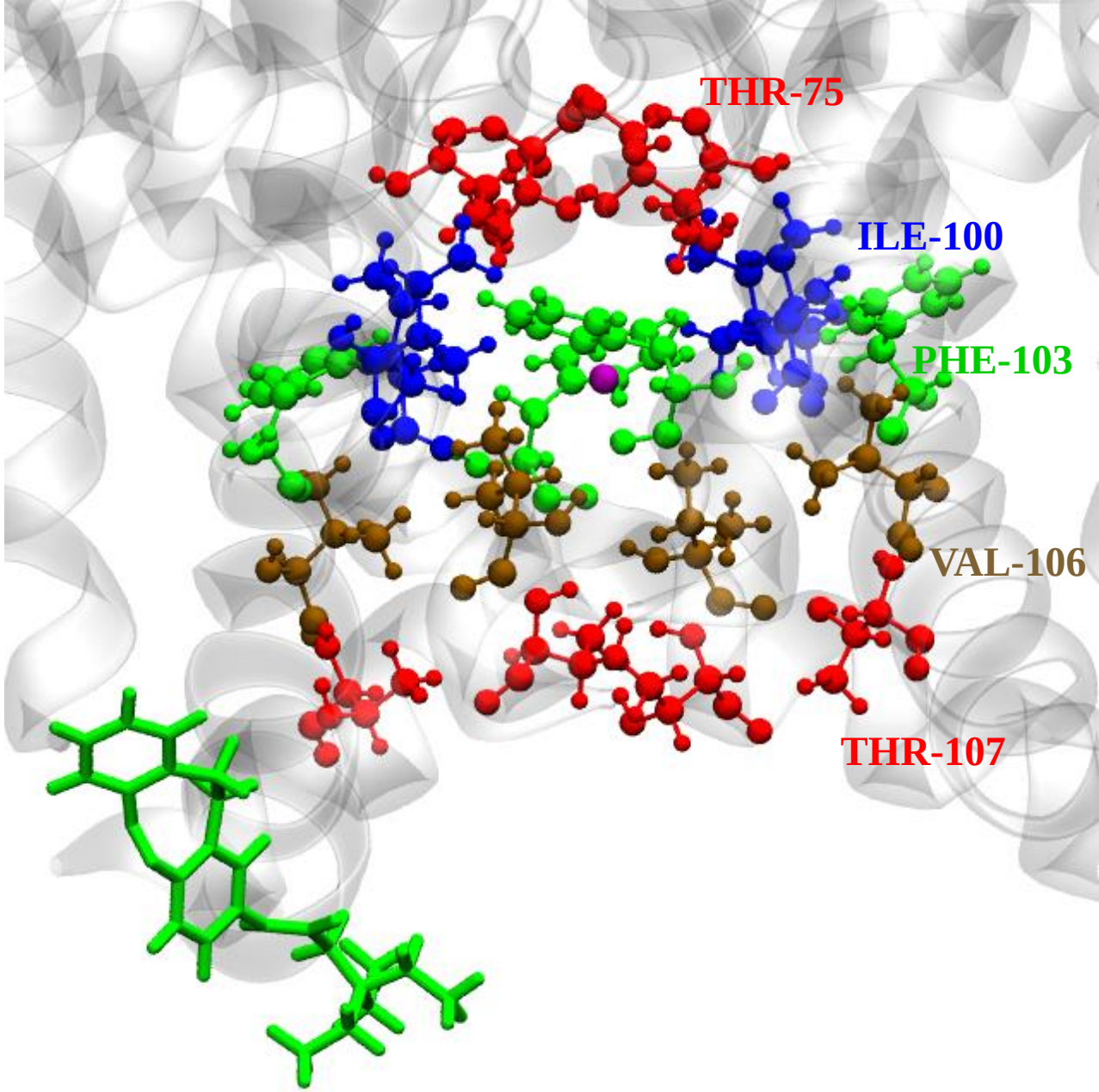




***E*2 (C1)**
MM/PBSA Binding energy = -13.1 kcal/mol

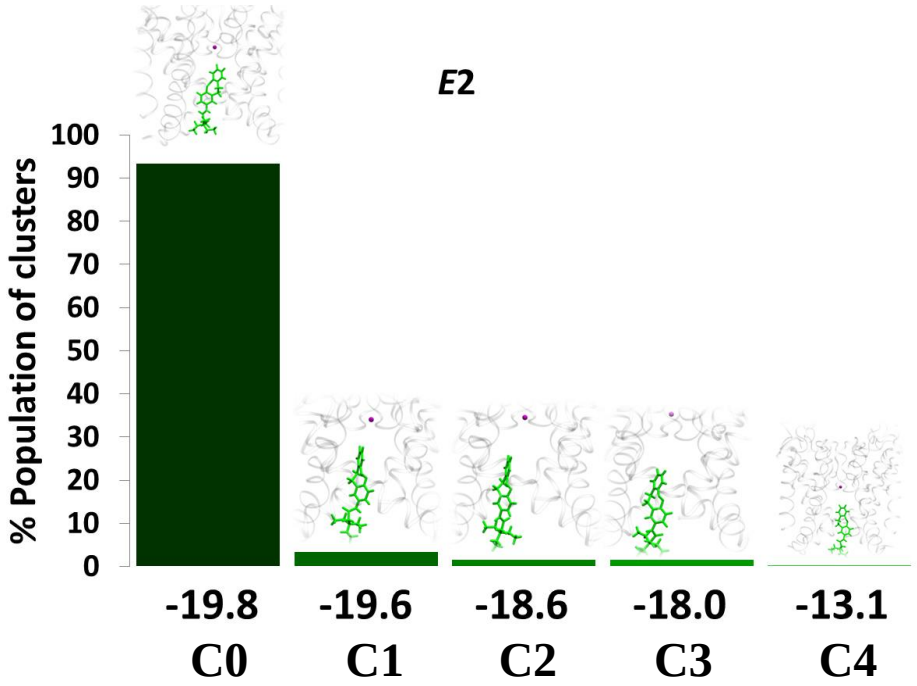
***E*2 (C2)**
MM/PBSA Binding energy = -19.8 kcal/mol





***E*2 (C3)**
MM/PBSA Binding energy = -4.9 kcal/mol

***E*2 (C4)**
MM/PBSA Binding energy = 0.2 kcal/mol



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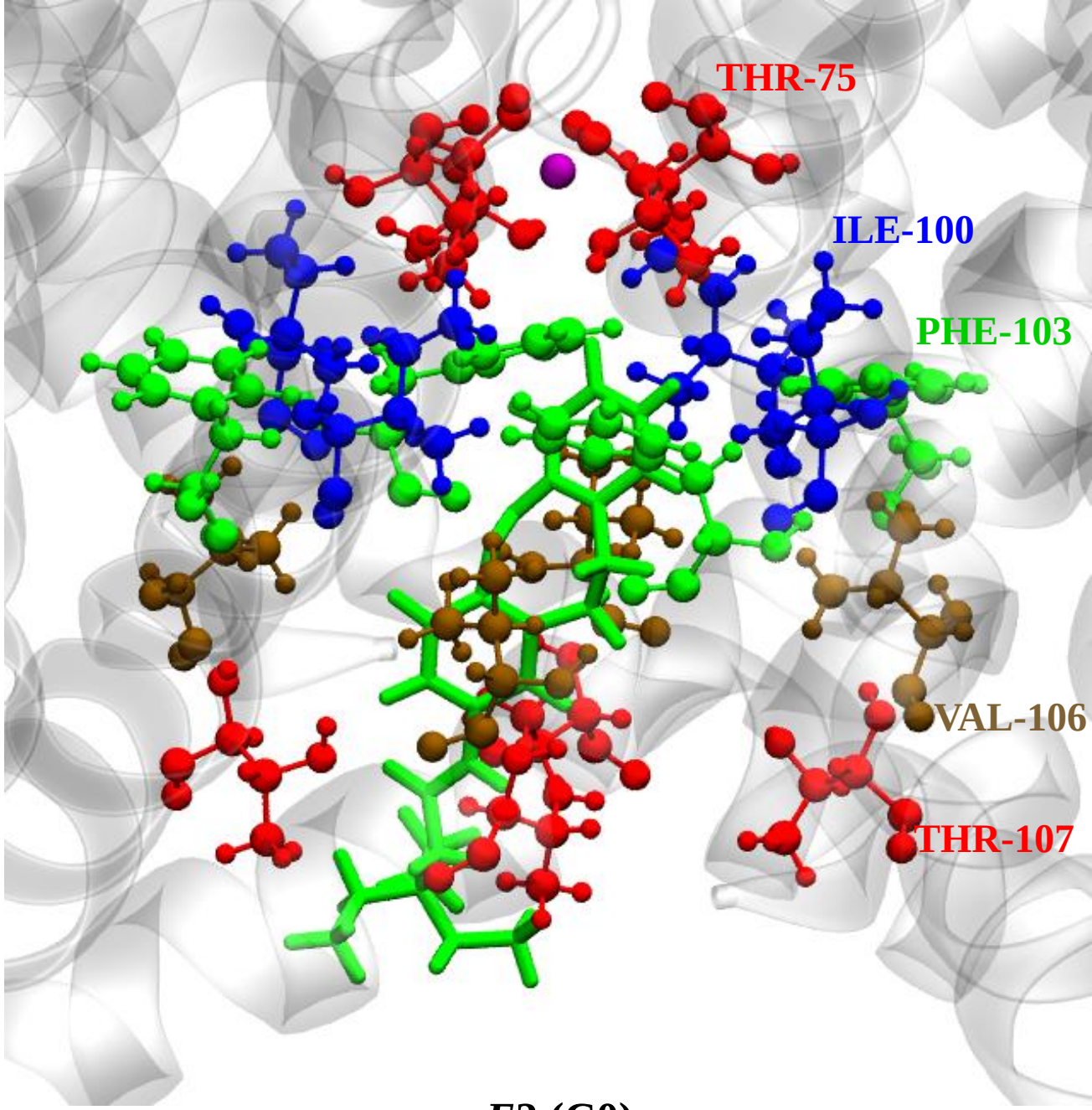
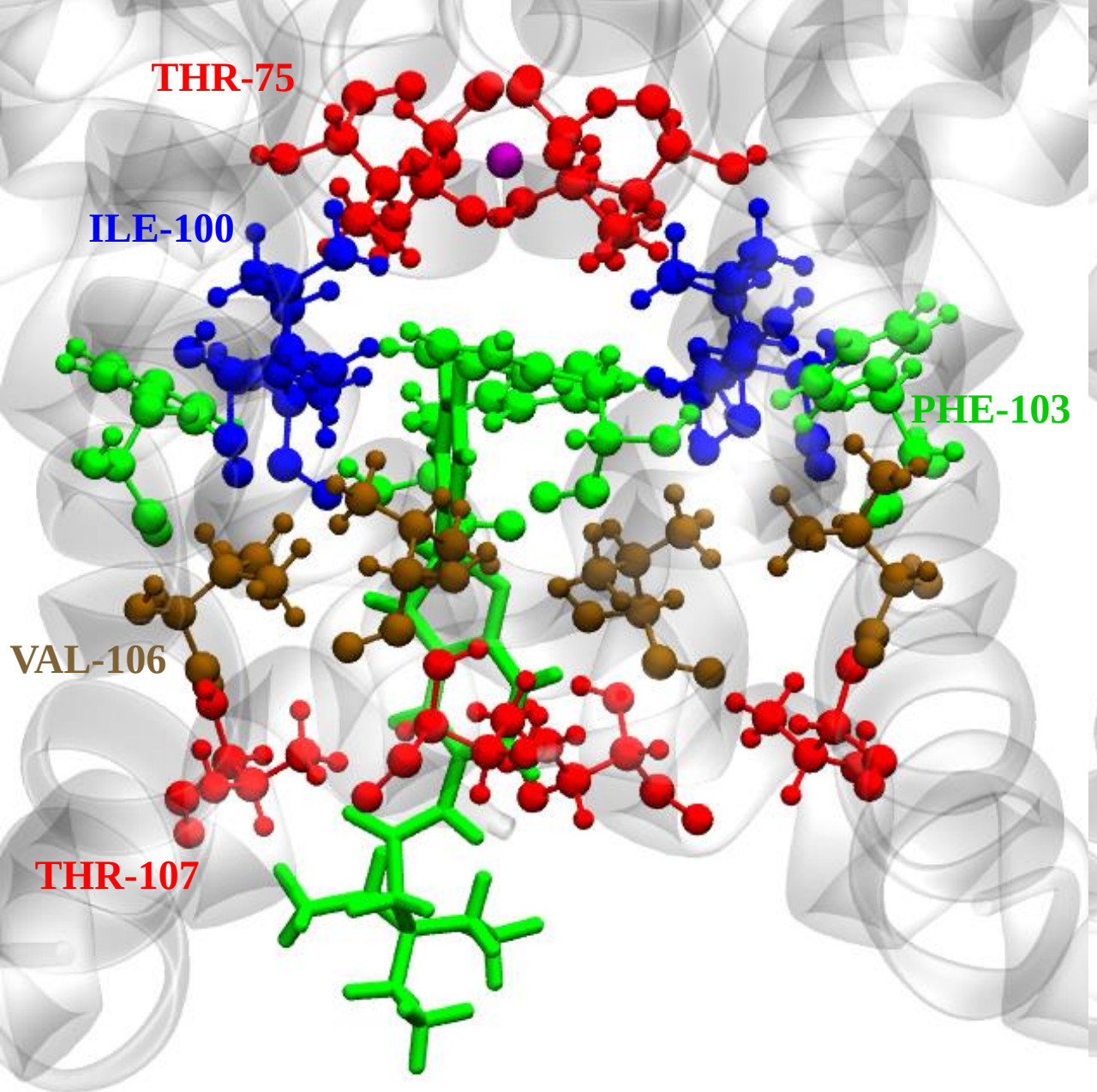
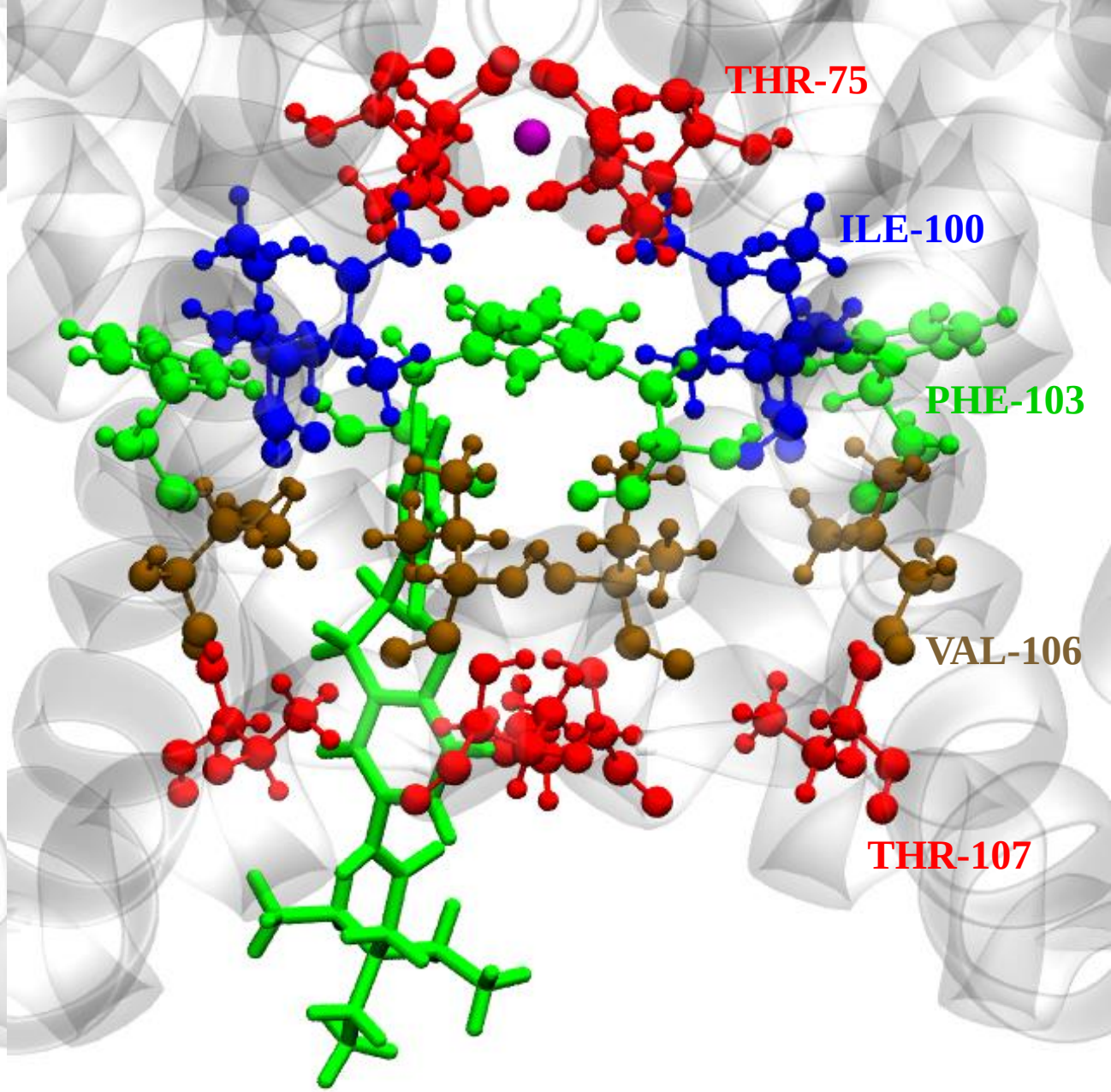


***E*2 (C0)**

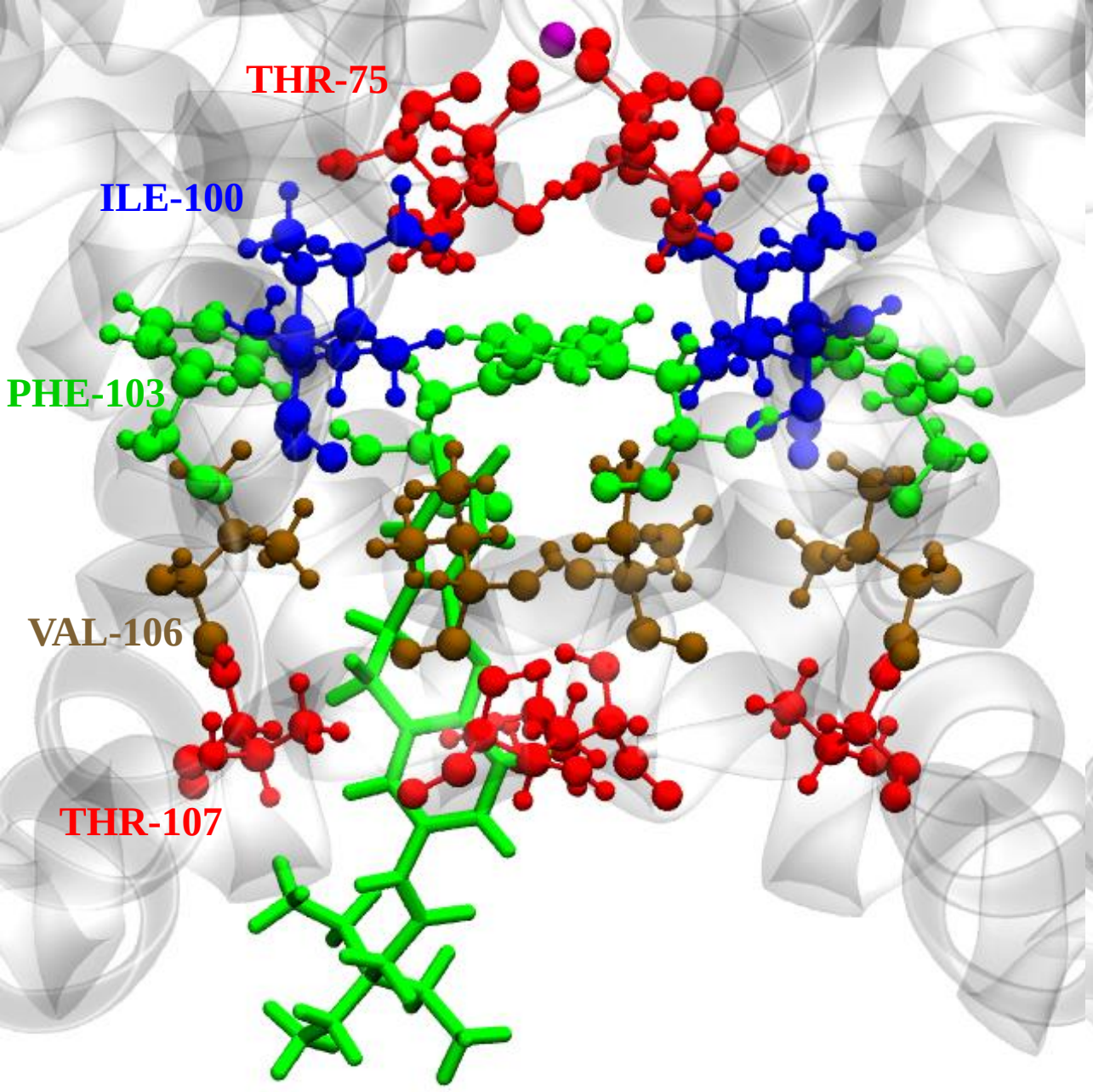
MM/PBSA Binding energy = -19.8 kcal/mol

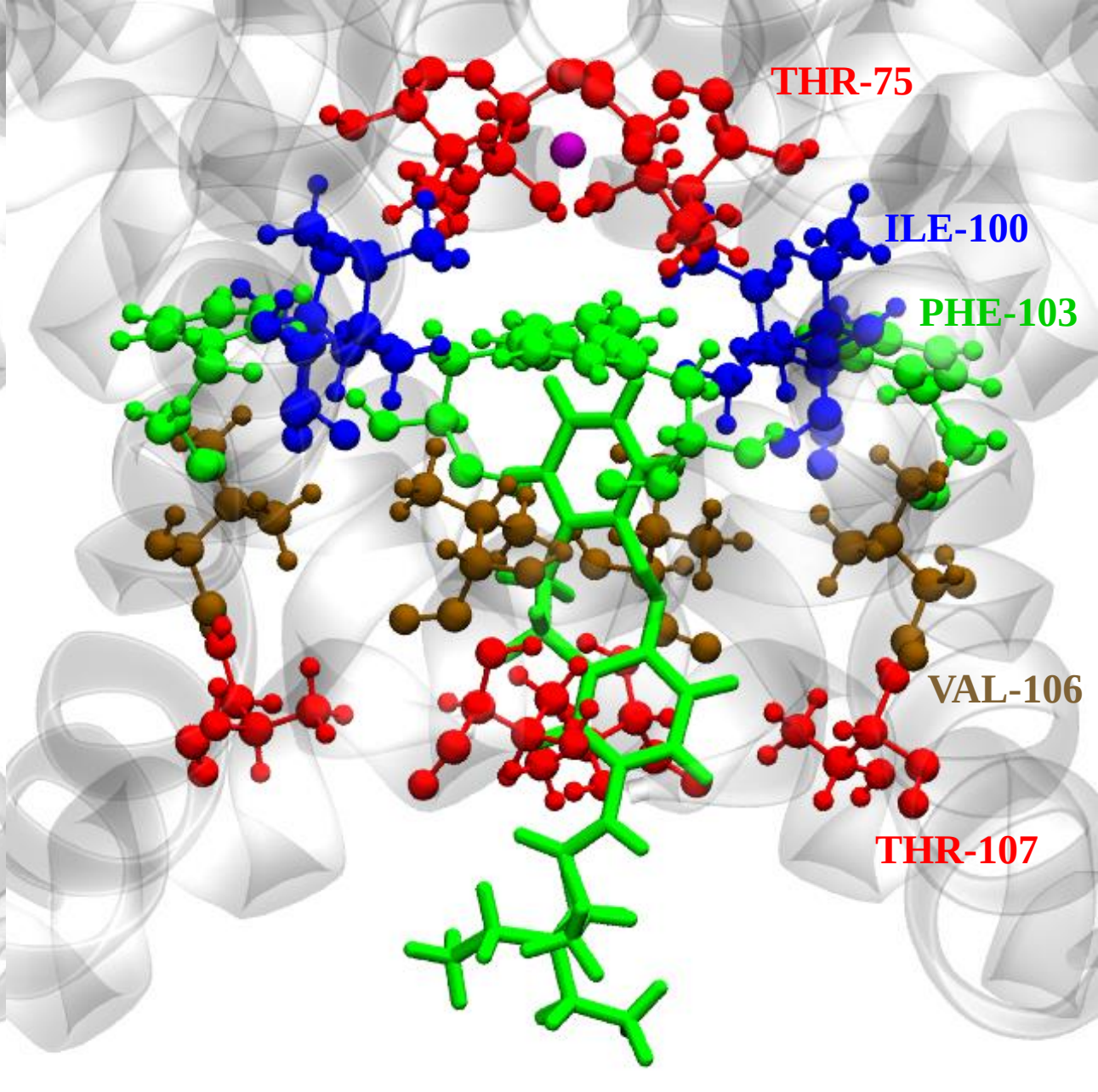




***E*2 (C1)**
MM/PBSA Binding energy = -19.6 kcal/mol

***E*2 (C2)**
MM/PBSA Binding energy = -18.6 kcal/mol





***E*2 (C3)**
MM/PBSA Binding energy = -18.0 kcal/mol

***E*2 (C4)**
MM/PBSA Binding energy = -13.1 kcal/mol