Deciphering Deamidation and Isomerization in Therapeutic Proteins: Effect of Neighboring Residue

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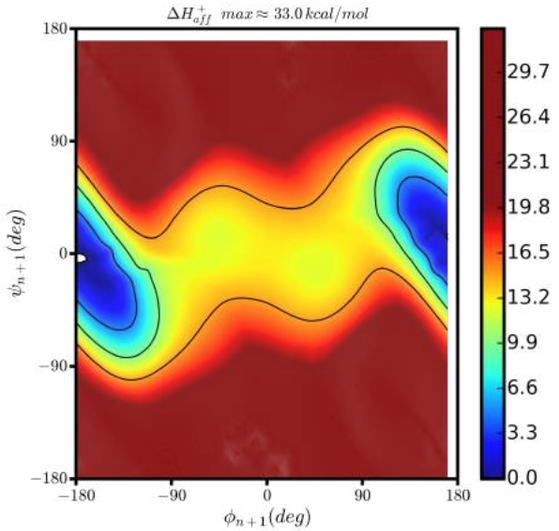
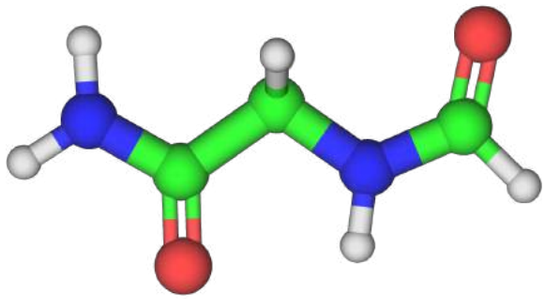
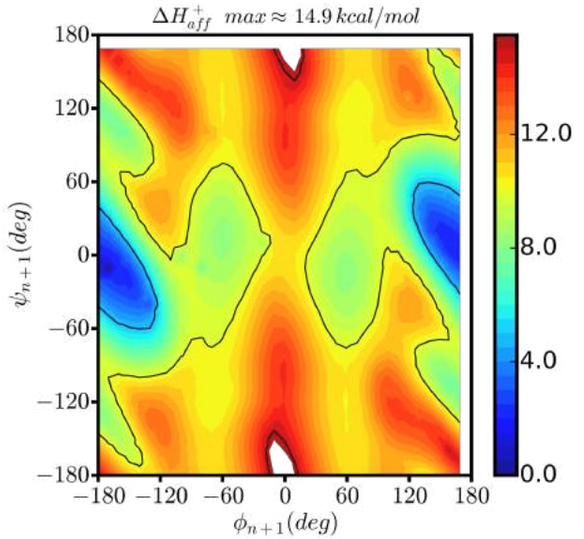
Figure S1: Backbone amide proton affinity (kcal/mol) surface as a function of the backbone dihedral angles for N-formyl-glycinamide calculated using different QM models.



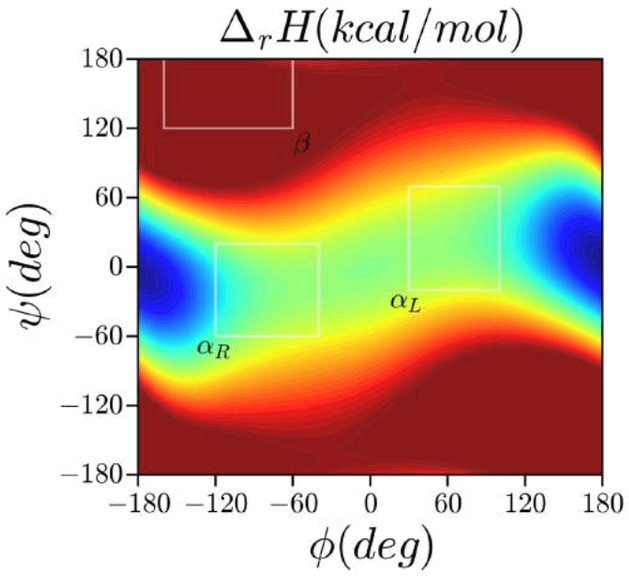
M062X/6-311++G(d,p)

2-acetamido-N-methylacetamide

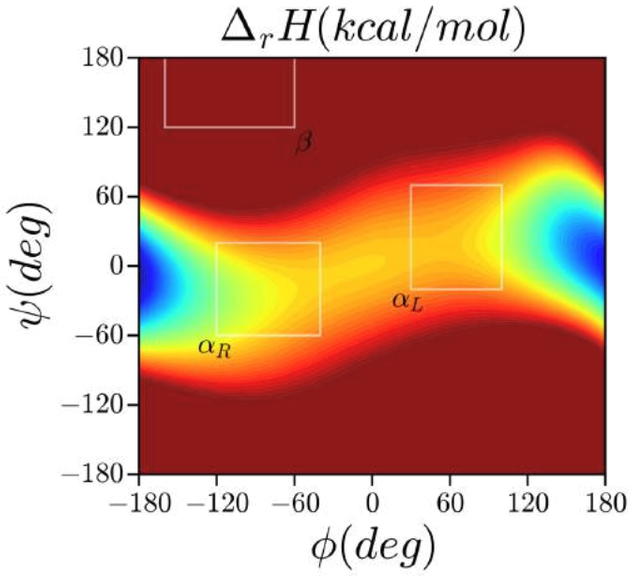




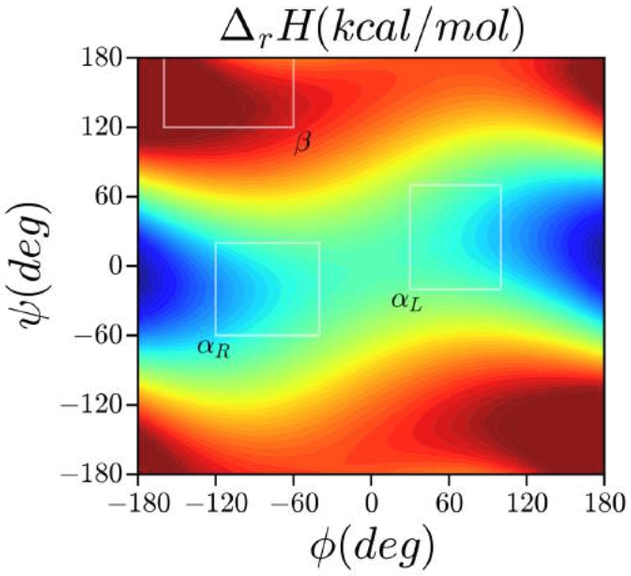
M062X/6-311++G(d,p)
SCRF=SMD



PM6-D3H4



PM7

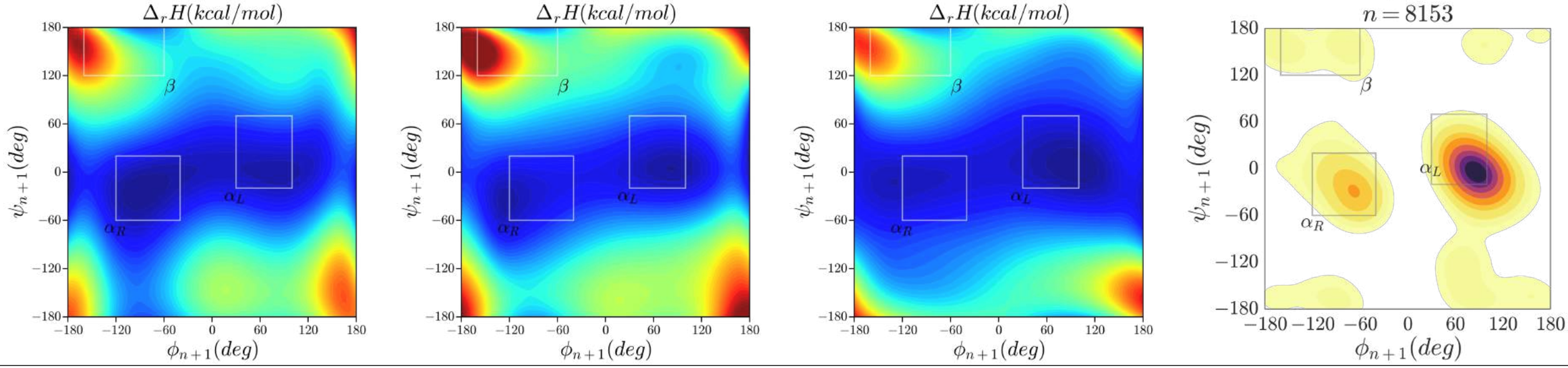


RM1

Figure S2: ASP-GLY and ASN-GLY dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

PM6 PM7 RM1 Rama

ASP-GLY



ASN-GLY

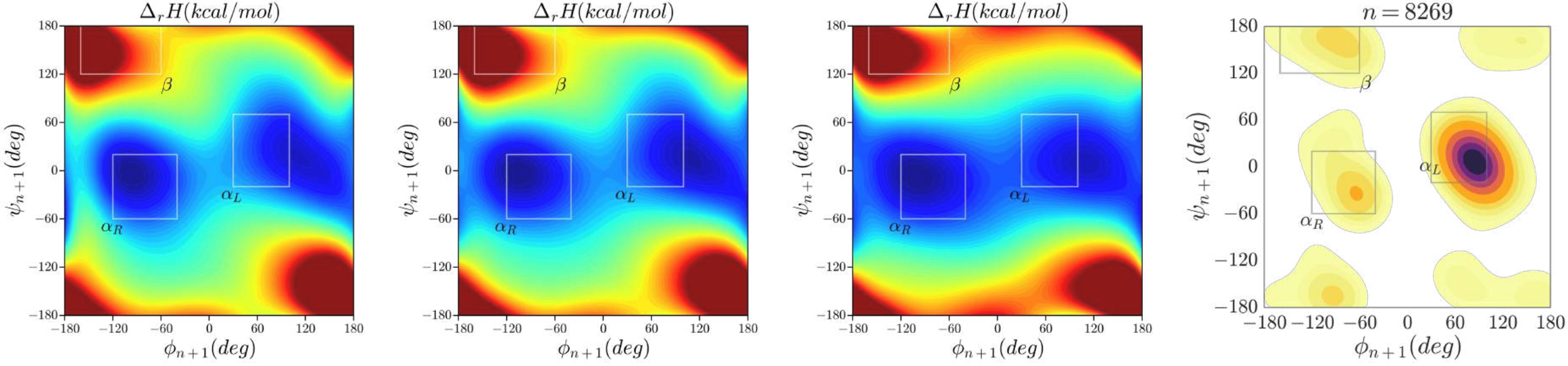


Figure S3: ASP-ALA and ASN-ALA dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

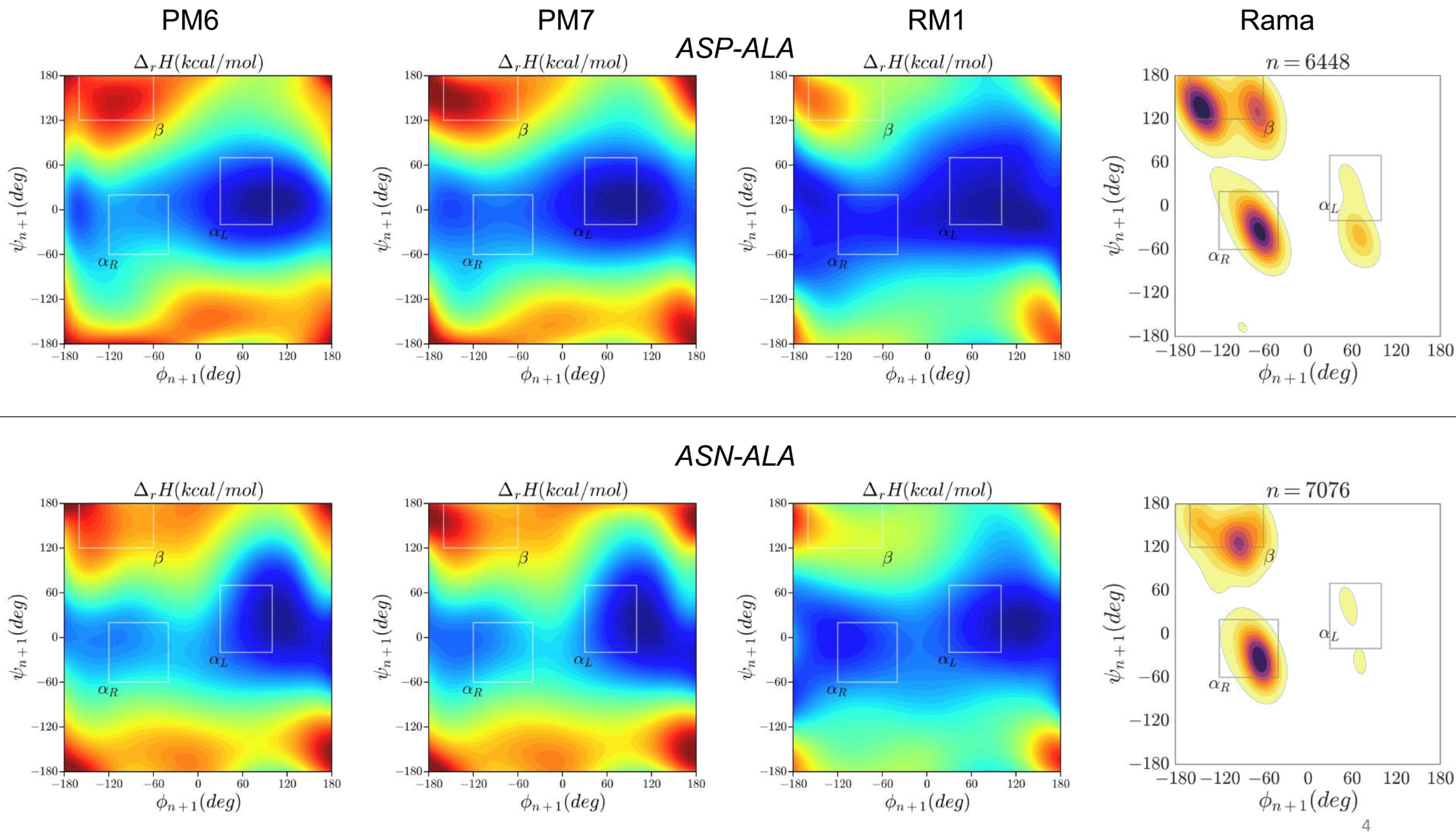


Figure S4: ASP-SER and ASN-SER dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

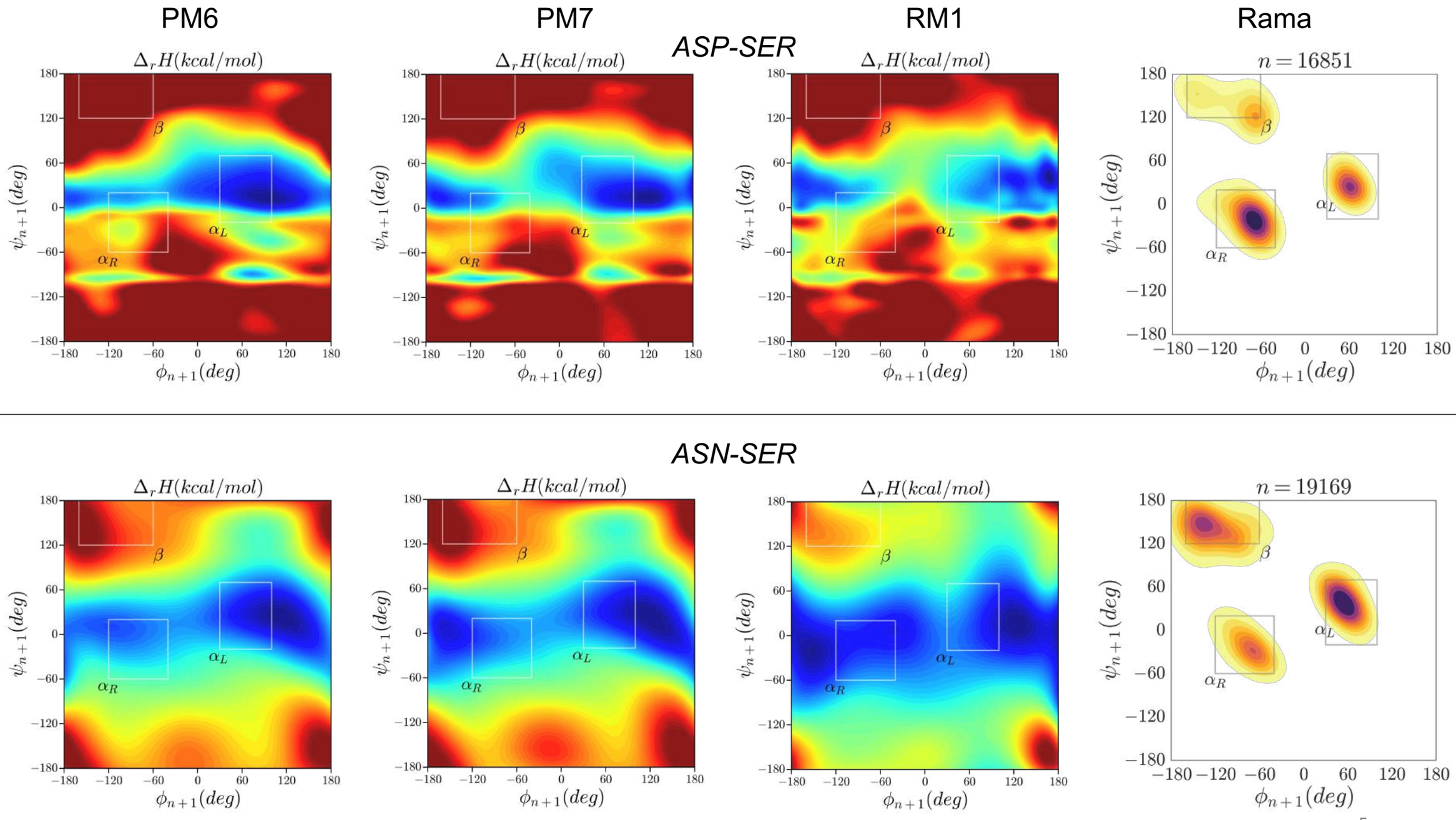


Figure S5: ASP-THR and ASN-THR dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

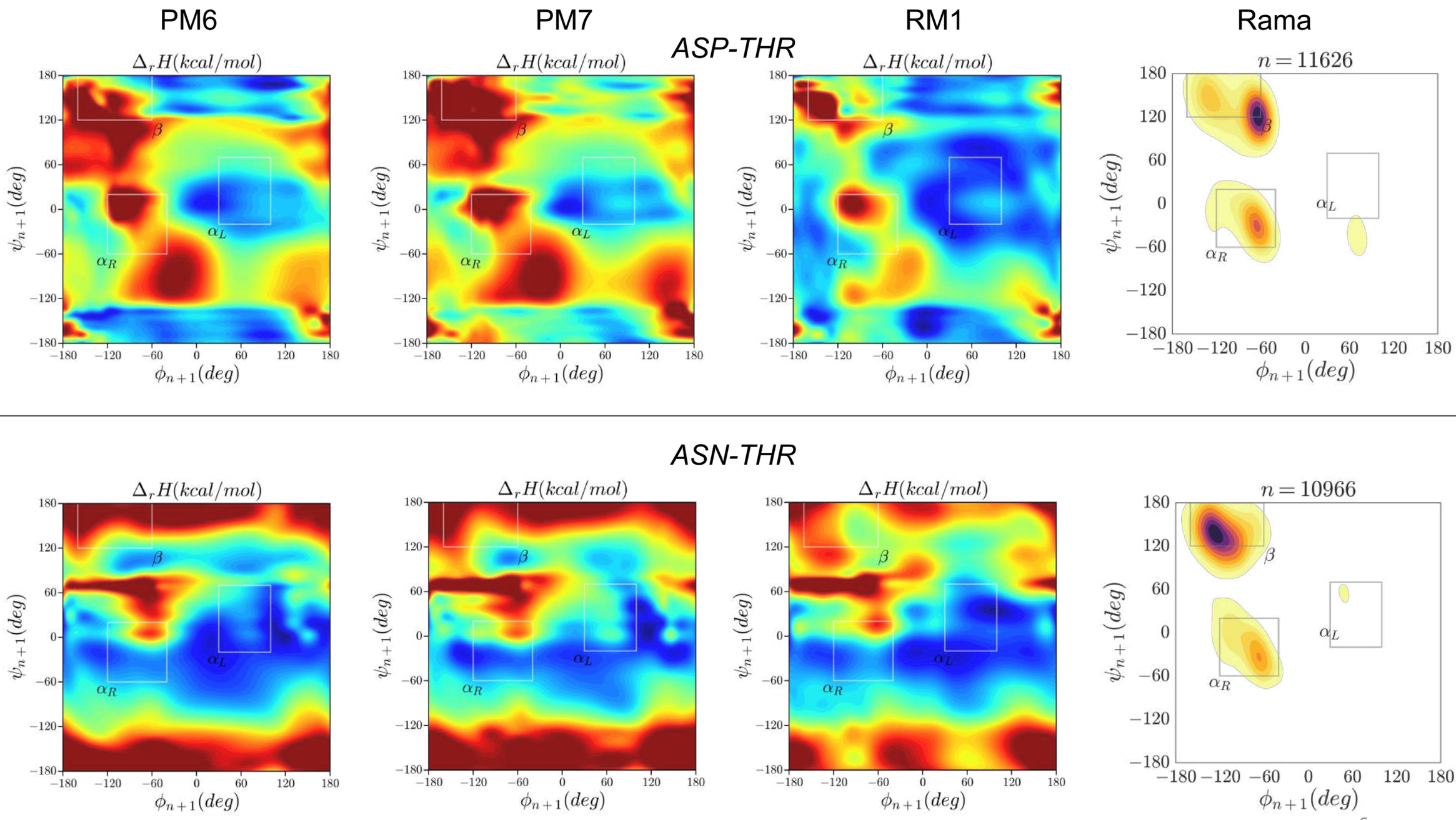


Figure S6: ASP-ASP and ASN-ASP dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

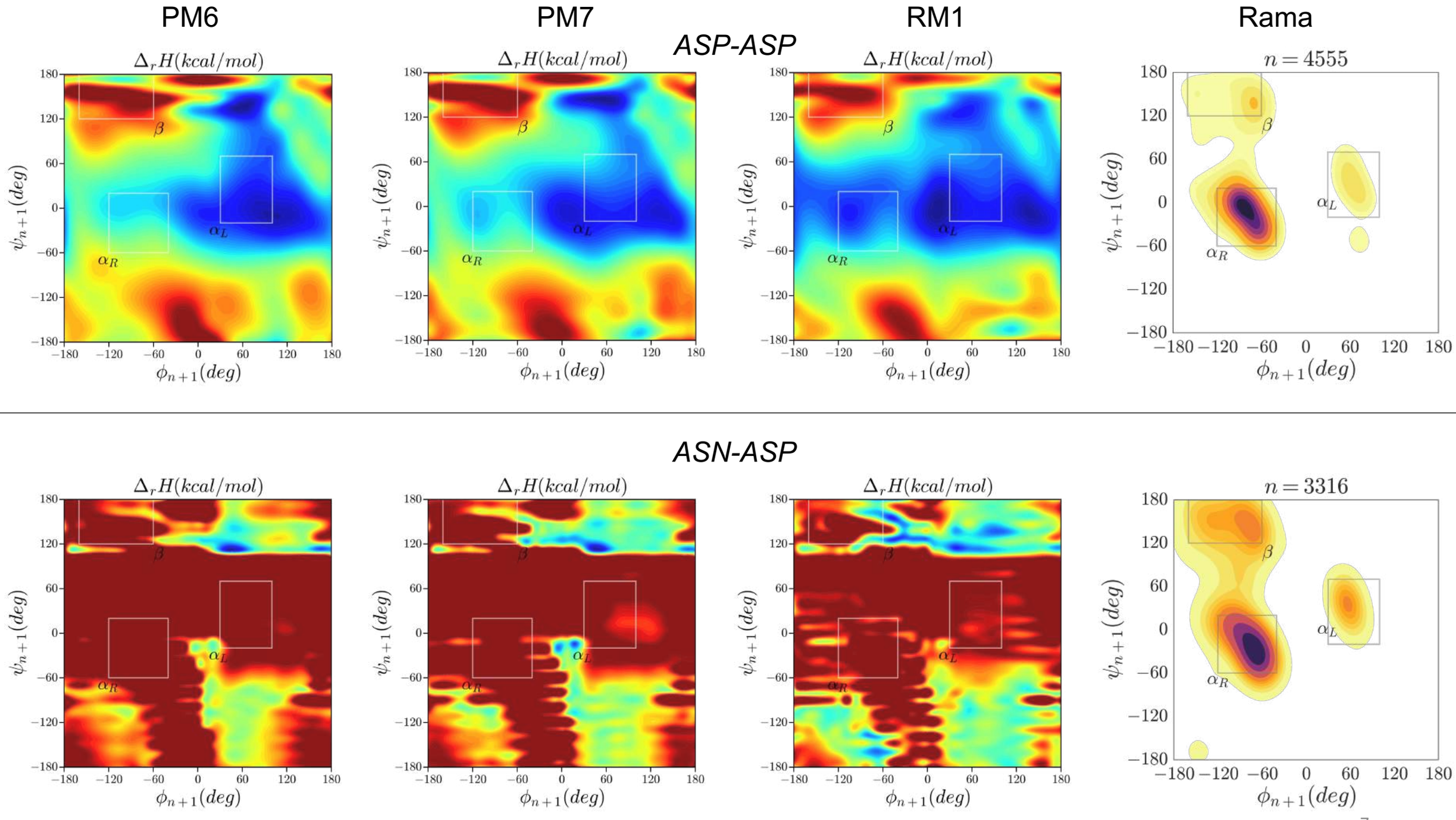


Figure S7: ASP-GLU and ASN-GLU dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

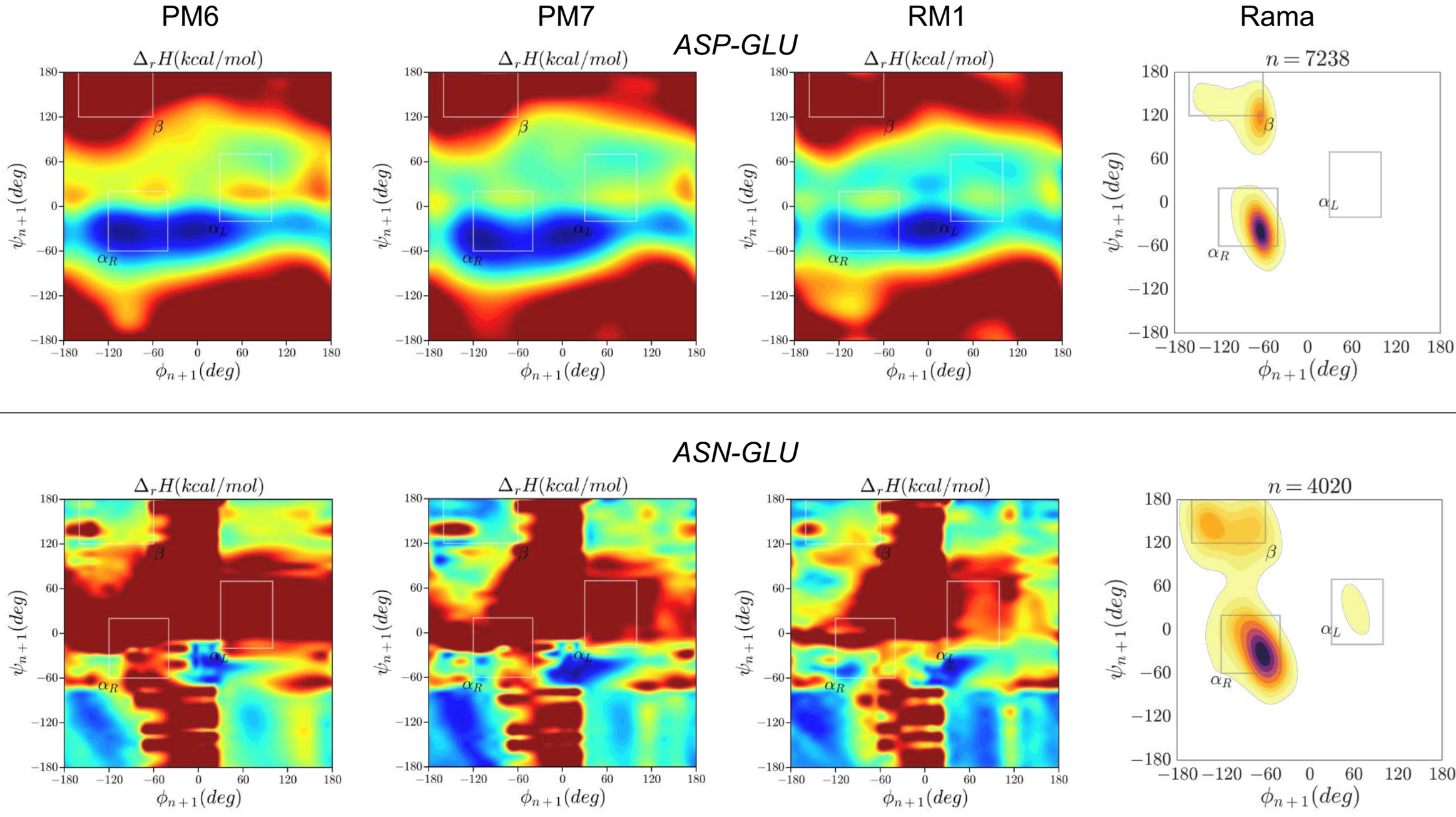
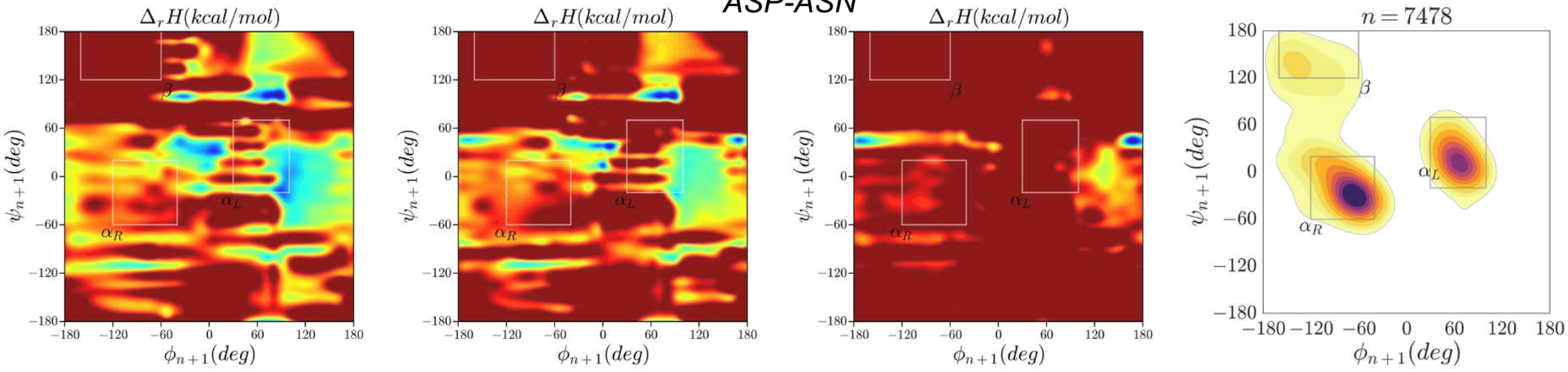


Figure S8: ASP-ASN and ASN-ASN dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

PM6 PM7 RM1 Rama

ASP-ASN



ASN-ASN

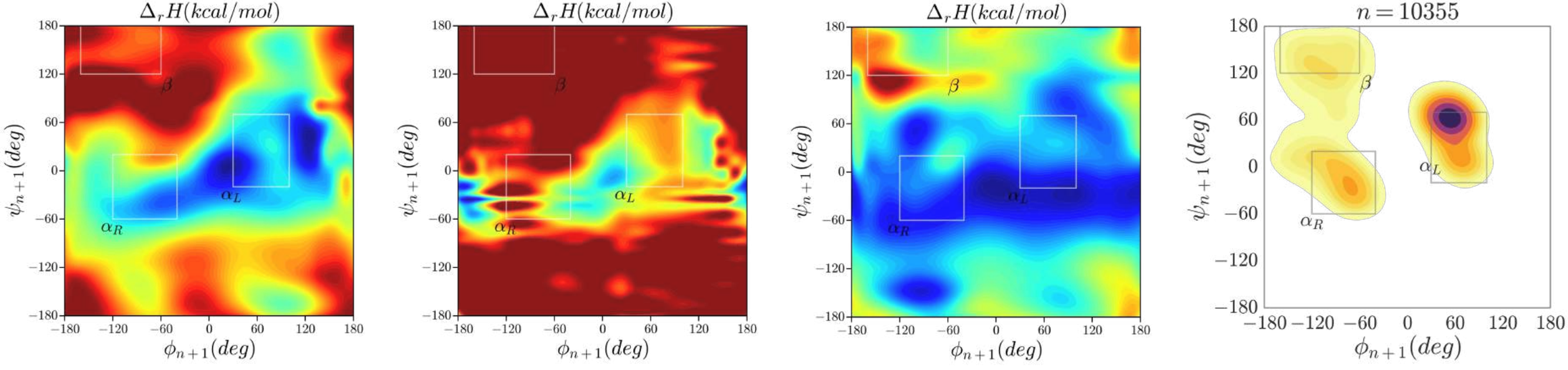


Figure S9: ASP-GLN and ASN-GLN dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

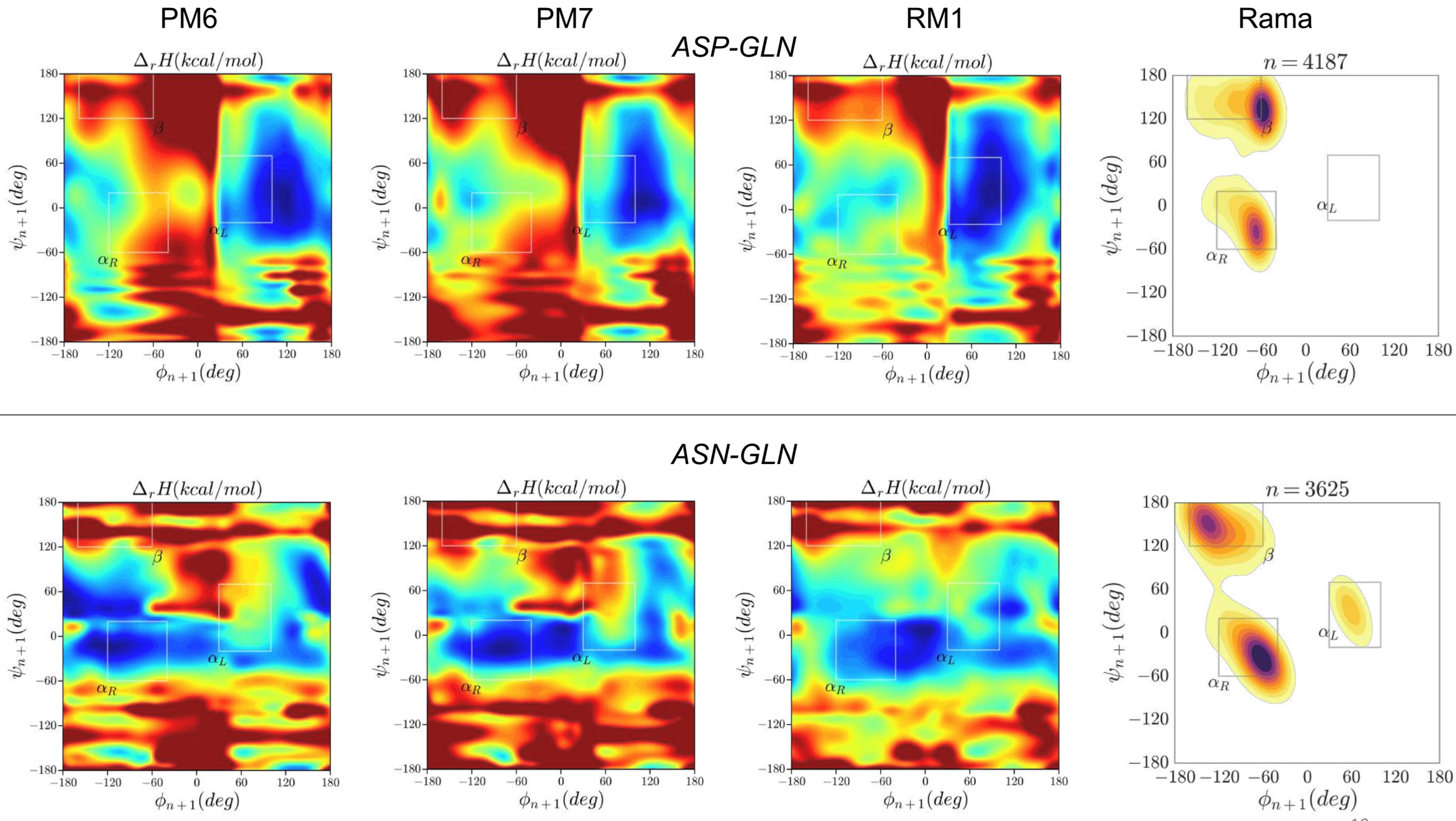


Figure S10: ASP-VAL and ASN-VAL dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

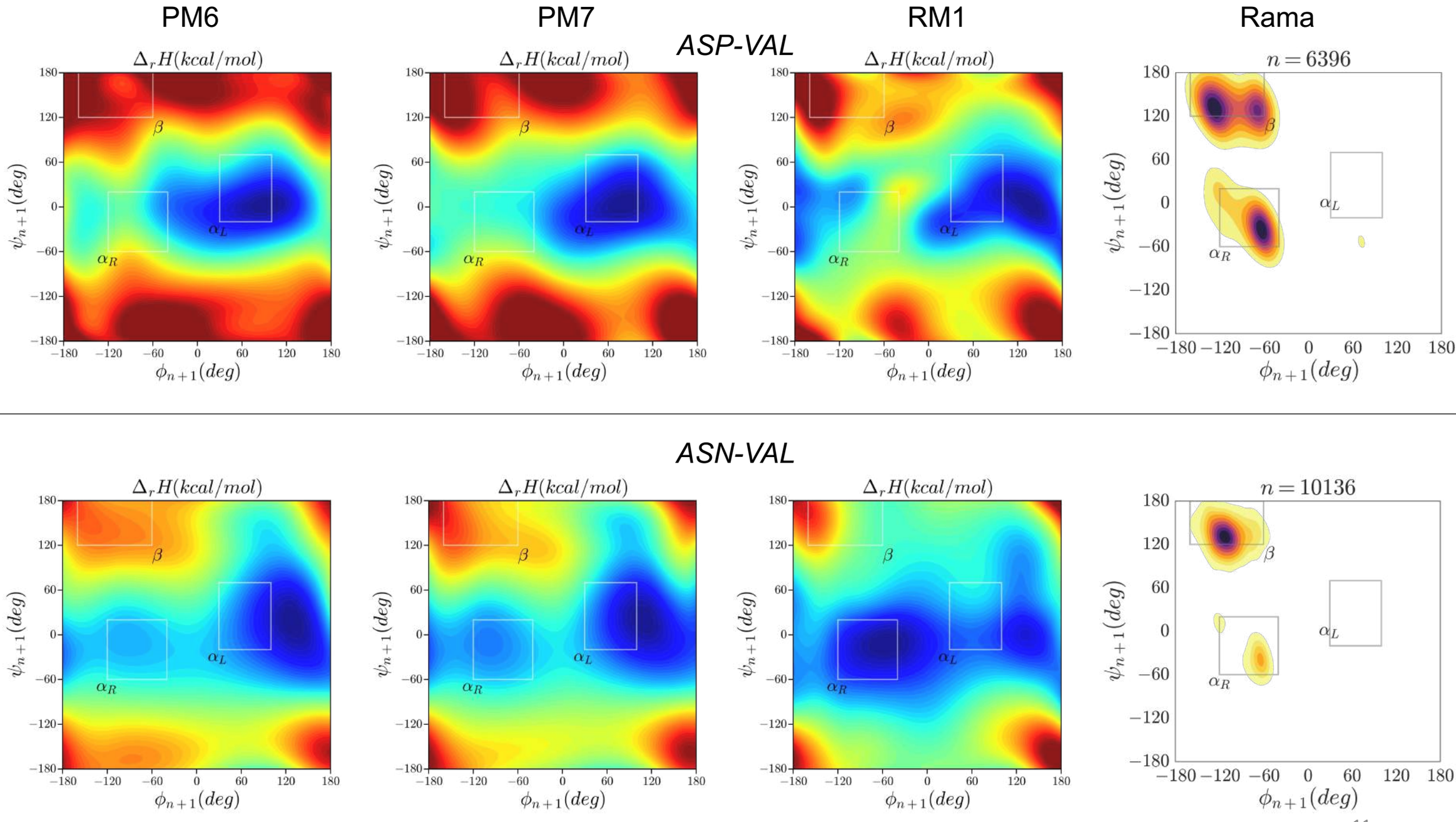


Figure S11: ASP-LEU and ASN-LEU dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

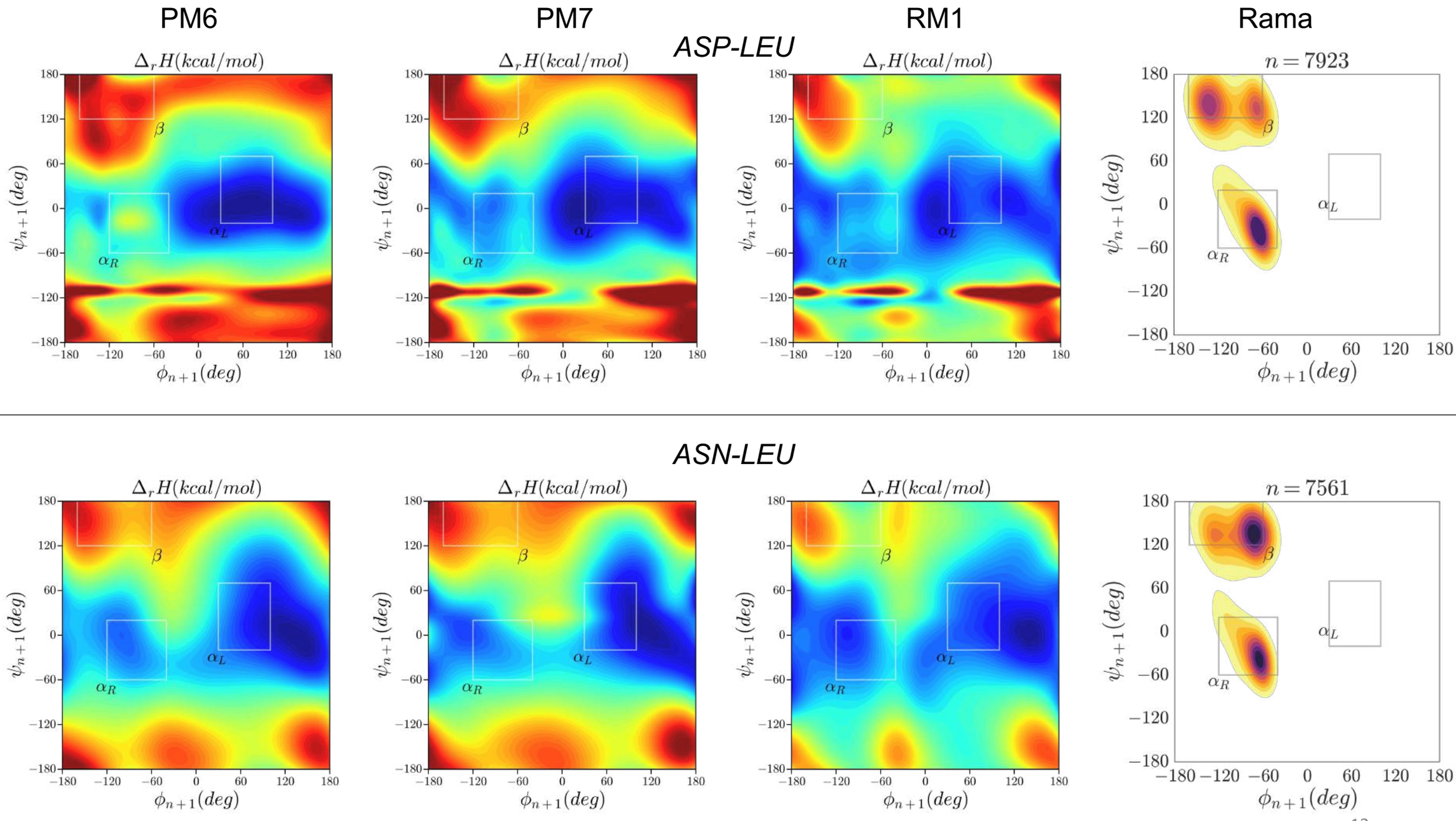


Figure S12: ASP-ILE and ASN-ILE dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

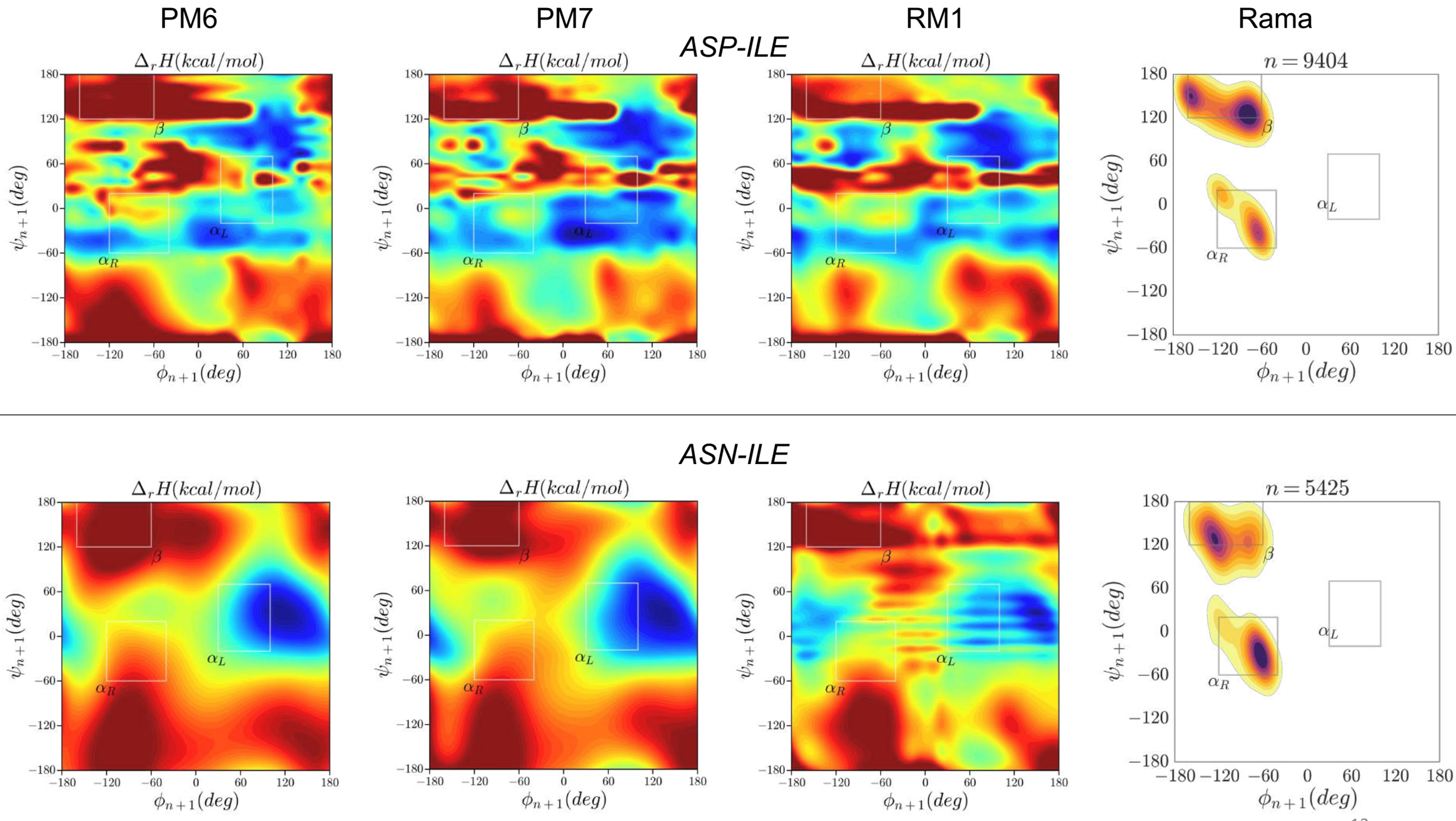


Figure S13: ASP-MET and ASN-MET dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

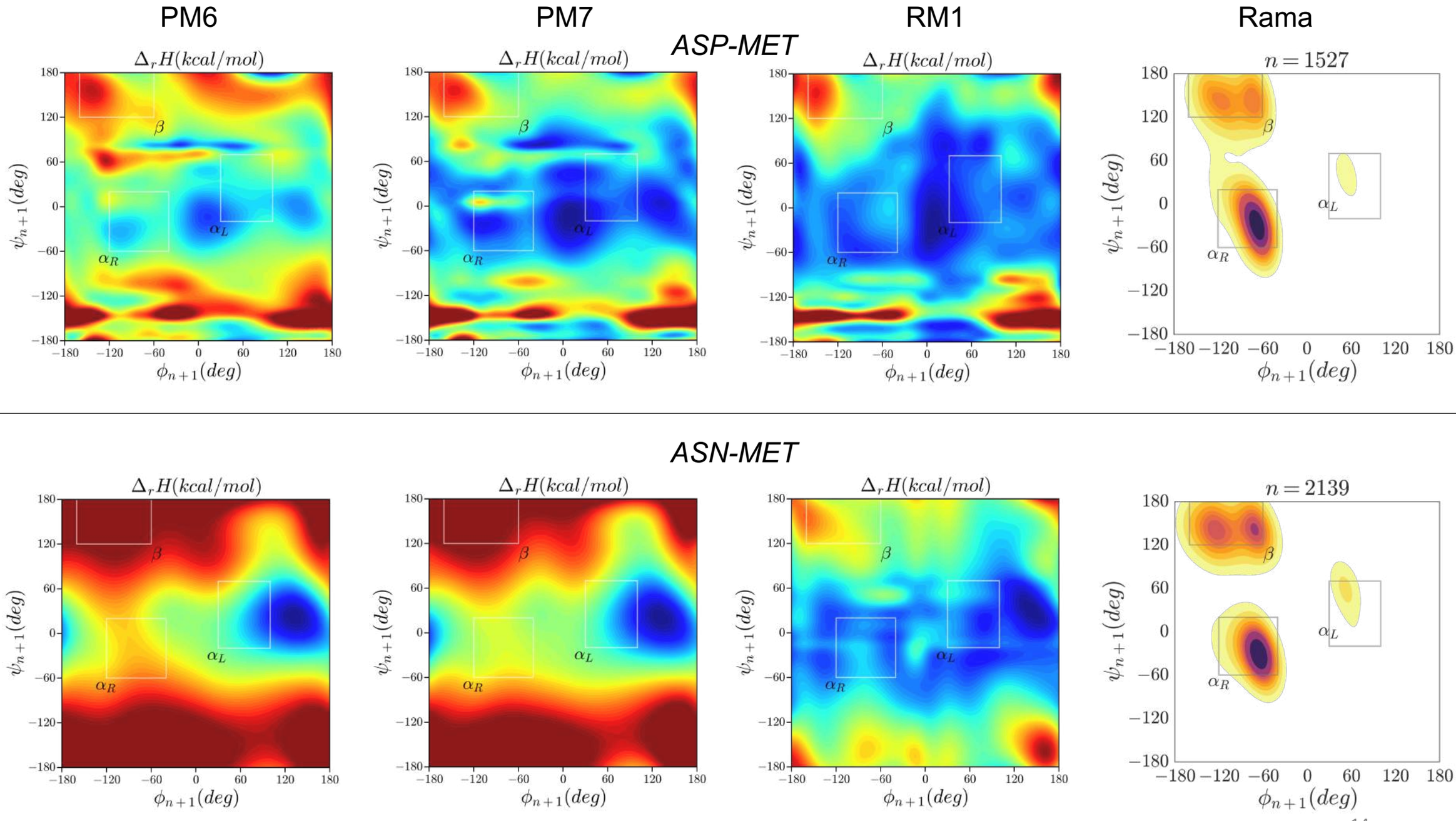


Figure S14: ASP-PHE and ASN-PHE dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

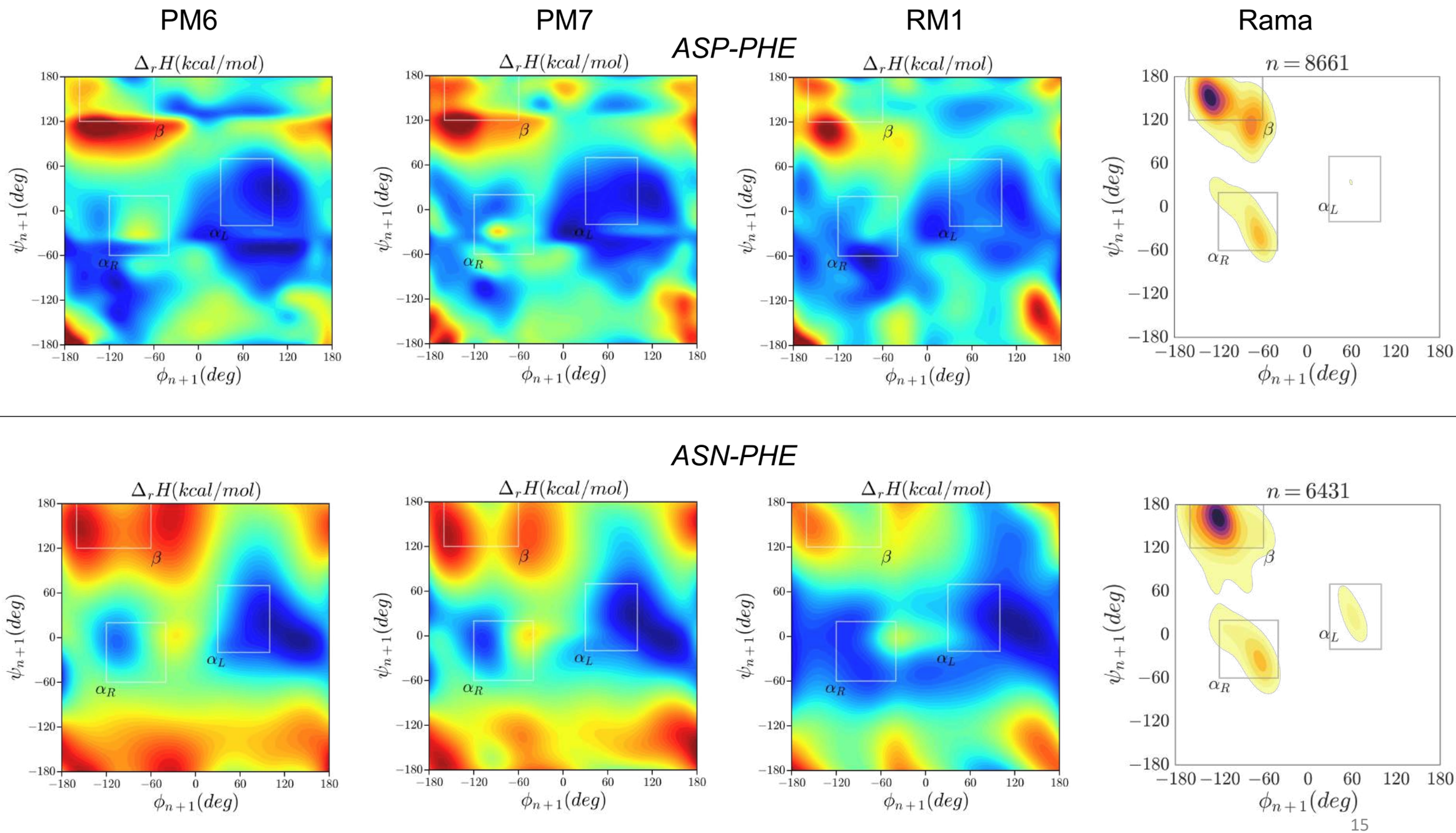


Figure S15: ASP-TYR and ASN-TYR dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

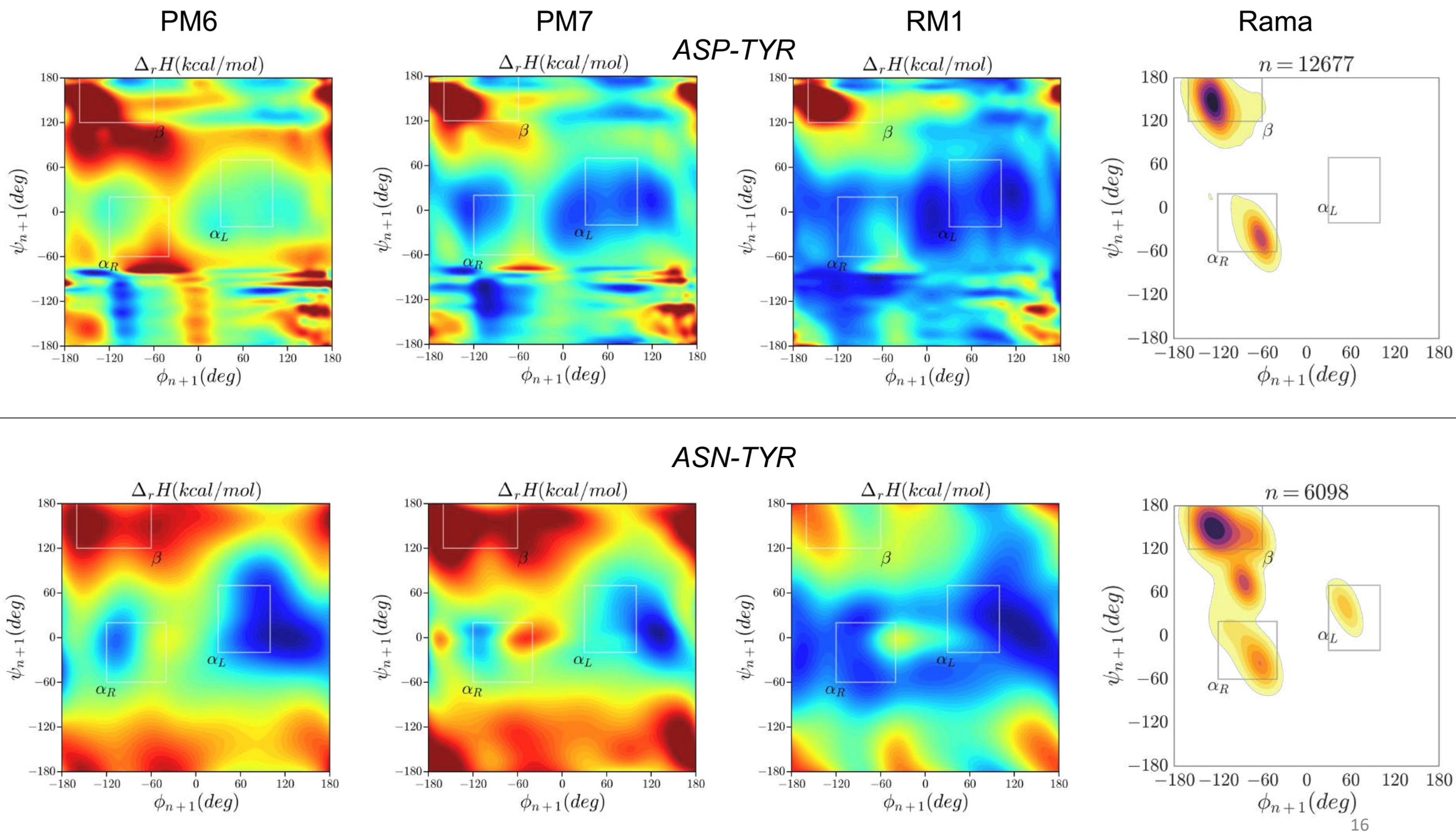


Figure S16: ASP-HIS and ASN-HIS dipeptide backbone amide proton affinity (kcal/mol) as a function of the backbone dihedral angles calculated using different QM models, and the respective Ramachandran energy (kcal/mol) surfaces calculated from the kernel density estimation of backbone conformations observed in the PDB database of crystallized antibodies (far right).

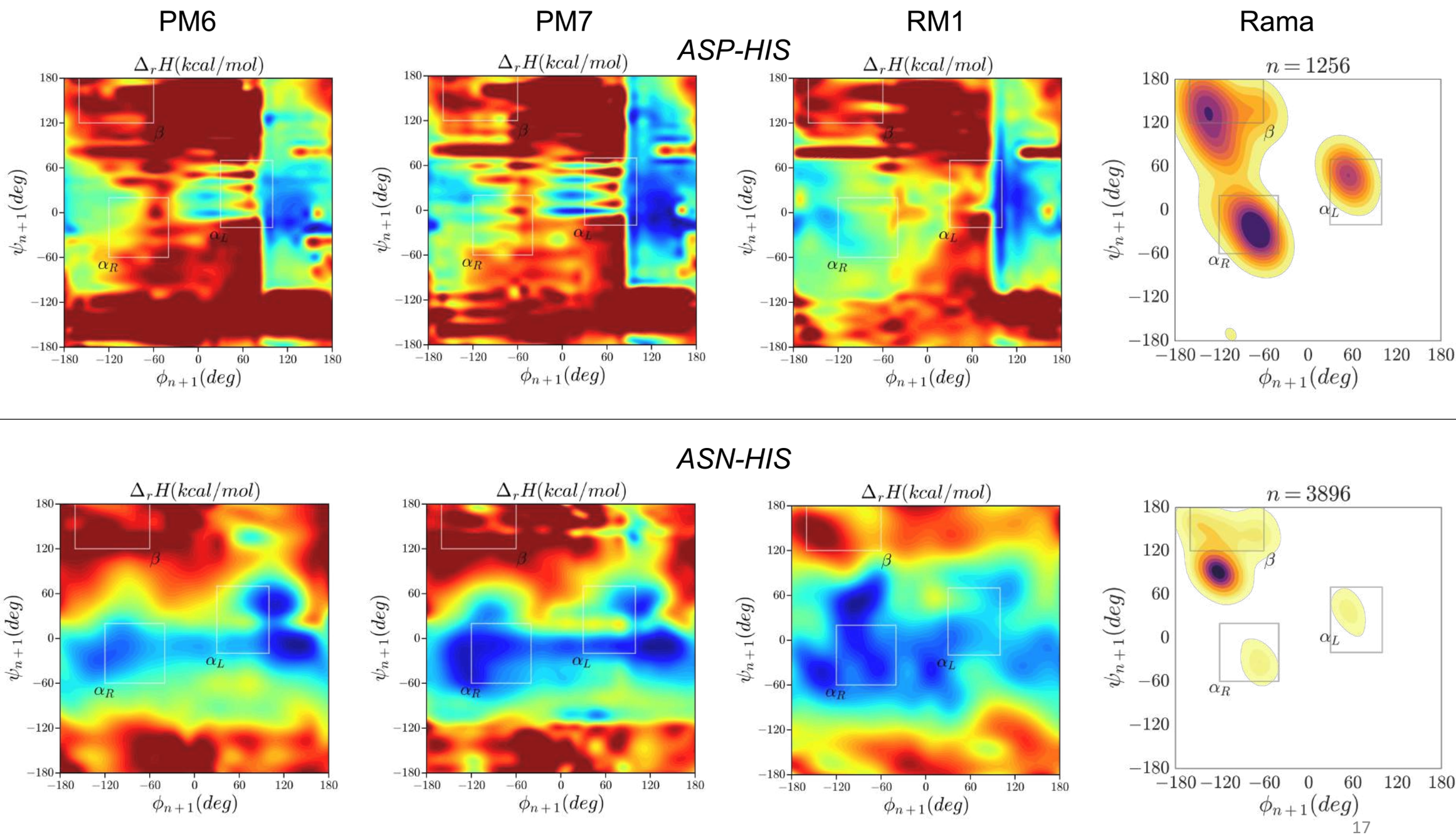


Figure S17: Plots of the normalized probability of finding NX dipeptides in the right-handed helix (top) and left-handed (bottom) helix conformation obtained from Ramachandran energy surfaces from the PDB of crystalized antibodies in the X-axis and the normalized minimum PM6 proton affinity of the backbone amide for the same secondary structure conformations in Y-axis.

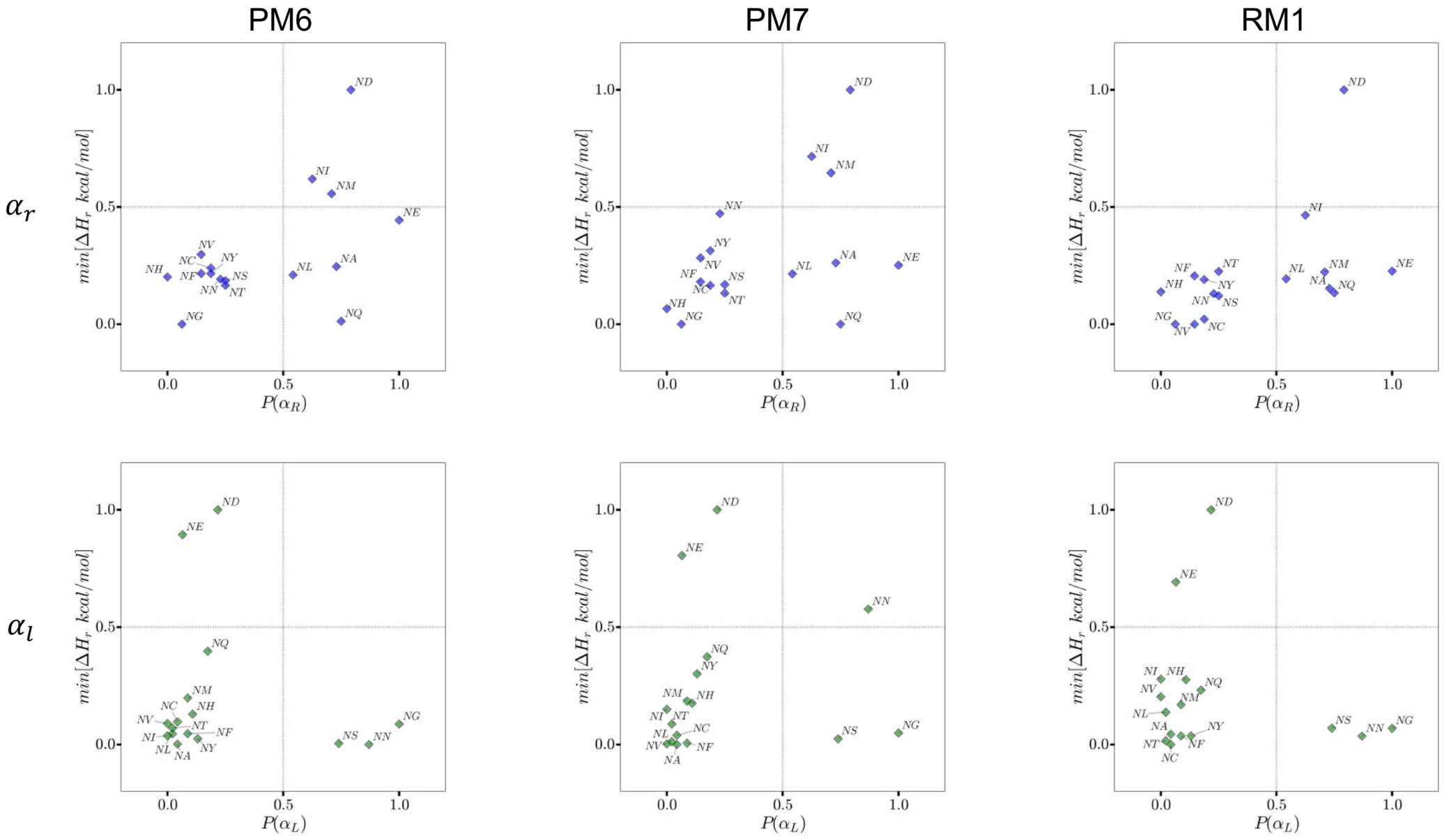


Figure S18: Plots of the normalized probability of finding NX dipeptides in the beta secondary conformation obtained from Ramachandran energy surfaces from the PDB of crystalized antibodies in the X-axis and the normalized minimum PM6 proton affinity of the backbone amide for the same secondary structure conformations in Y-axis.

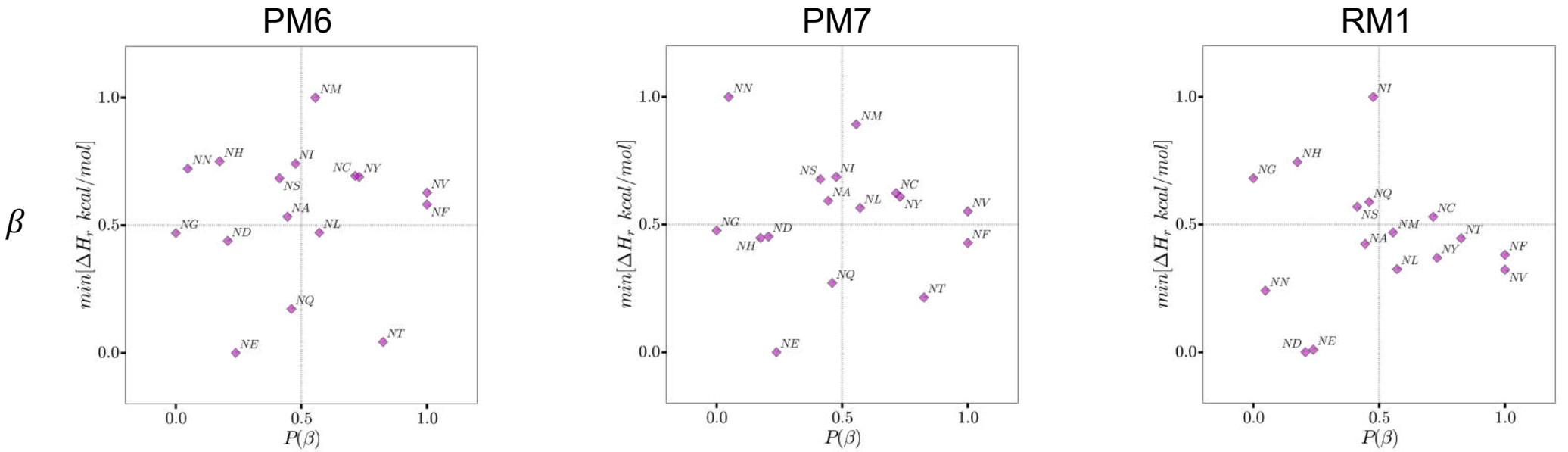


Figure S19: Plots of the normalized probability of finding DX dipeptides in the right-handed helix (top) and left-handed (bottom) helix conformation obtained from Ramachandran energy surfaces from the PDB of crystalized antibodies in the X-axis and the normalized minimum PM6 proton affinity of the backbone amide for the same secondary structure conformations in Y-axis.

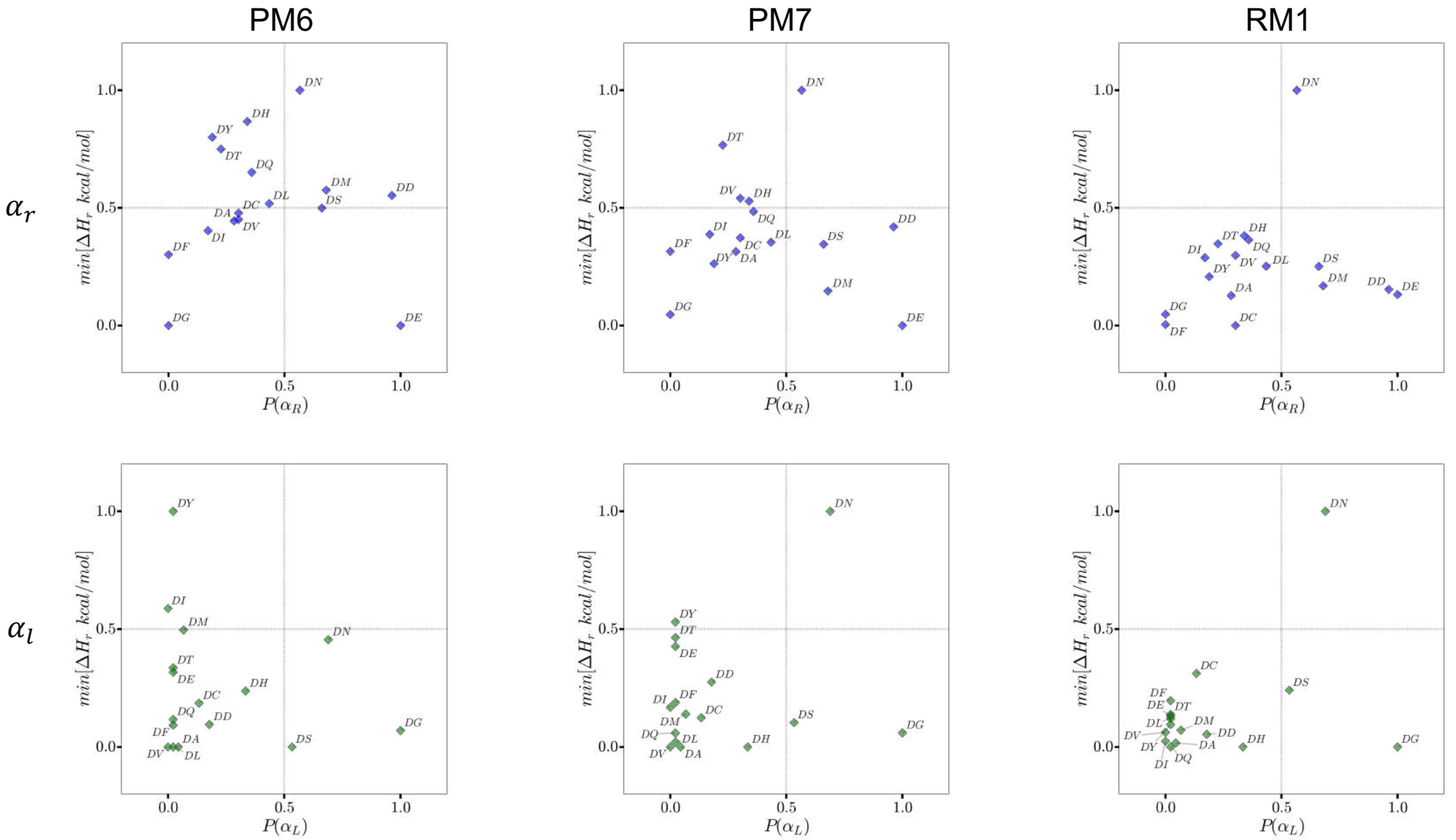


Figure S20: Plots of the normalized probability of finding NX dipeptides in the beta conformation obtained from Ramachandran energy surfaces from the PDB of crystalized antibodies in the X-axis and the normalized minimum PM6 proton affinity of the backbone amide for the same secondary structure conformations in Y-axis.