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Comp Bio HW7

Part 1: Information on PHE30 residue

Atom#	AtomName	ResidueName	FoldedASA	UnfoldedASA	ASADifference
216	N	PHE	0.0	0.4	0.4
217	CA	PHE	0.0	3.3	3.3
218	C	PHE	0.0	0.22	0.22
219	O	PHE	0.0	14.25	14.25
220	CB	PHE	0.38	22.89	22.51
221	CG	PHE	0.0	1.76	1.76
222	CD1	PHE	2.97	24.99	22.02
223	CD2	PHE	0.0	19.49	19.49
224	CE1	PHE	4.18	31.93	27.75
225	CE2	PHE	0.0	29.17	29.17
226	CZ	PHE	0.0	31.59	31.59

Part 2: calculated free energy change due to
hydrophobic burial in kcal/mol for the entire protein.

ASA Sum for folded: 1981.8 A²

ASA Sum for unfolded: 4814 A²

Burial is $0.023 \text{ kcal/mol/A}^2 * (\text{folded} - \text{unfolded}) = 0.023 * (1981.8 - 4814) \text{ kcal/mol} = -65 \text{ kcal/mol}$