Component	β-α	β-α	γ-β	α-γ	α-β
Bond	0.1	0.4	0.0	0.6	0.5
Angle	0.3	0.4	0.4	1.2	0.0
Dihedral	1.0	1.9	0.0	1.2	1.1
Improper	0.0	0.0	0.1	0.0	0.1
Total Conformational[1]	0.9	2.2	0.0	2.6	1.4
Electrostatic	1.0	0.0	3.0	2.9	4.4
van Der Waals	0.7	0.5	1.6	0.0	0.5
Total Non-bonded[1]	1.2	0.0	4.2	2.4	4.4
Total[1]	**0.0**	**0.1**	**2.0**	**2.9**	**3.6**

1 The values in each row are offset so that the lowest energy interface (underlined) in the row has a value of 0, for consistency with Figures 6C and S4; consequently, the values in a given "Total" row may differ from the sum of the previous rows by a value that is constant across the interfaces.