Deriving quantitative information on polarization of electron density from multipolar model – possible?

(Supplementary Materials)

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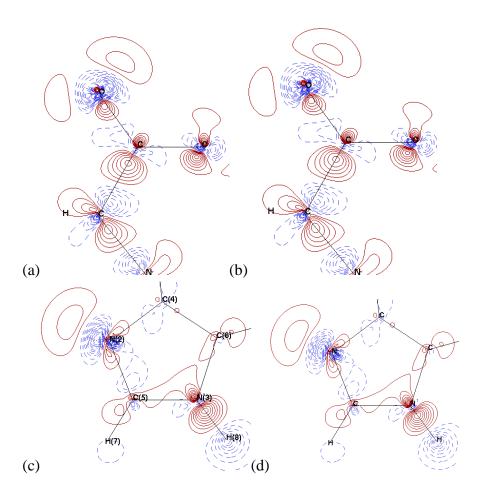[1] Department of Chemistry, University of Warsaw, ul. Pasteura 1, 02-093 Warszawa, Poland

Figure S1 Interaction density maps of HIS generated with different grid used : (a) and (c) grid points are distributed every 0.05 Å in each direction, (b) and (d) grid points are distributed every 0.025 Å in each direction. Contour interval is equal $0.025e\text{Å}^{-3}$, positive values are in red and negative values are in blue.

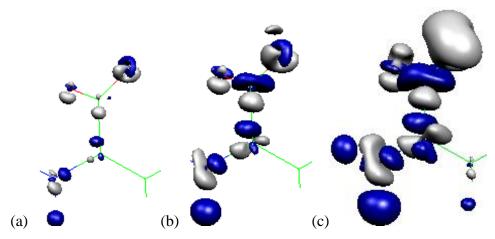(a)   (b)   (c)

Figure S2. 3D interaction density maps (Molekel 4.3; Portmann) for ALA obtained by subtracting DZPisol from DZPperturb models. Positive white and negative blue isosurfaces are shown, the isosurface values are equal to: (a) 0.1 e$Å^{-3}$, (b) 0.05 e$Å^{-3}$, (c) 0.025 e$Å^{-3}$.

Table S1. Coulombic energies of interactions [kJ/mol] of HIS and ALA dimers calculated from the given models. Results were arranged according to the Ecs values obtained from SAPT(DFT), from the lowest to the highest ones. The symmetry cards are presented below.

	13	14	10	8	12	15	9	16	17	15
SAPT$_{Ecs}$	-318	-237	-215	-196	-153	-77	-66	-55	-20	-16
SAPT$_{Ees}$	-217	-122	-152	-131	-101	-60	-29	-37	-9	-4
DZP$_{perturb}$	-305	-206	-234	-227	-185	-118	-28	-84	-5	-5
cc-pVDZ$_{perturb}$	-274	-180	-202	-194	-159	-100	-24	-73	-4	-6
MM_DZP$_{perturb}$	-180	-118	-140	-138	-110	-45	-32	-41	-6	-13
MM_cc-pVDZ$_{perturb}$	-195	-122	-157	-153	-109	-46	-36	-45	-8	-8
CR	-170	-113	-138	-134	-106	-45	-30	-38	-5	-15

	symmetry	
HA - HA	1-x, 1/2+y, -z	1
HA - HA	2-x, 1/2 +y, -z	2
HA -HA	1 +x, y, z	3
HA- HA	1 +x, y, 1+ z	4
HA H$_2$O	2-x, 1/2 +y, 1-z	5
HA H$_2$O	1 +x, 1+y, -1+z	6
HA H$_2$O	1 +x, 1+y, z	7
LALA -LALA	x, y, 1+z	8
LALA - LALA	3/2-x, -y, 1/2+z	9
LALA -LALA	-1/2+x, 1/2-y, 1-z	10
HIS-HIS	1+x, y, z	11
HIS-HIS	-x, 1-y, -z	12
HIS-HIS	x, 1/2-y, ½+z	13
HIS-HIS	-x, 1/2+y, 1/2-z	14
HIS-HIS	1-x, -1/2+y, ½-z	15
HIS-HIS	1-x, 1-y, 1-z	16
HIS-HIS	-1+x, 1/2-y, -1/2+z	17
GH-GH	-1+x, y, z	18
GH-GH	1+x, 1+y, z	19
GH -GH	1-x, ½+y, 1-z	20
GH 1H$_2$O	x, y, z	21
GH 1H$_2$O	2-x, ½+y, 2-z	22
GH 2H$_2$O	x, y, z	23
GH 2H$_2$O	2-x, ½+y, 2-z	24

Table S2. Coulombic energies of interactions [kJ/mol] of GH and HA dimers calculated from the given models. The symmetry cards are presented above.

	18	19	20	1	2	3	4
SAPT$_{Ecs}$	-236	-125	-250	-226	-173	-118	-10
SAPT$_{Ees}$	-149	-100	-154	-160	-119	-27	-1
DZP$_{perturb}$	-281	-114	-313	-190	-123	-84	-14
MM_DZP$_{perturb}$	-172	-62	-177	-151	-103	-36	-2
CR	-154	-61	-134	-159	-105	-20	1