

Supplementary Material (ESI) for Organic and Biomolecular Chemistry  
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Nonbonded valence shell charge concentrations in L-Ala-L-Tyr-L-Ala with

...Water (1)						
Atom X	$\rho(\mathbf{r})$	$\nabla(\mathbf{r})$	$r_{X-CP}$	X'---X---CP	Angle	CP---X-CP <sub>2</sub>
O(1)	6.41	-126	0.341	C(2)---O(1)---CP	100	128
O(1)	6.54	-141	0.338	C(2)---O(1)---CP	119	
O(2)	6.61	-141	0.339	C(4)---O(2)---CP	102	155
O(2)	6.42	-133	0.340	C(4)---O(2)---CP	102	
O(3)	6.63	-127	0.343	C(6)---O(3)---CP	103	134
O(3)	6.79	-145	0.335	C(6)---O(3)---CP	123	
O(4)	6.93	-157	0.335	C(6)---O(4)---CP	97	157
O(4)	7.38	-188	0.332	C(6)---O(4)---CP	106	
O(5)	7.22	-185	0.333	C(24)---O(5)---CP	103	157
O(5)	6.41	-130	0.341	C(24)---O(5)---CP	96	
...EtOH (2)						
O(1)	5.49	-104	0.352	C(2)---O(1)---CP	109	98
O(1)	5.96	-123	0.346	C(2)---O(1)---CP	112	
O(2)	6.06	-125	0.345	C(4)---O(2)---CP	99	158
O(2)	6.24	-129	0.345	C(4)---O(2)---CP	95	
O(3)	6.38	-148	0.343	C(6)---O(3)---CP	125	107
O(3)	5.92	-122	0.346	C(6)---O(3)---CP	124	
O(4)	6.20	-127	0.344	C(6)---O(4)---CP	75	175
O(4)	6.75	-170	0.339	C(6)---O(4)---CP	104	
O(5)	6.44	-153	0.341	C(24)---O(5)---CP	109	166
O(5)	6.56	-159	0.341	C(24)---O(5)---CP	84	

Units: eÅ<sup>-3</sup>, eÅ<sup>-5</sup>, Å, deg