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NH···O and OH···O interactions of glycine derivatives with squaric acid
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Table S2. Bond lengths (Å), bond and torsion angles (°) optimized by the B3LYP/6-311G(d,p) approach for the complexes of squaric acid with glycine (**1a**), sarcosine (**2a**), dimethylglycine (**3a**) and betaine (**4a**).

Parameters	**1a**		**2a**	**3a**		**4a**	
	A[a]	B[b]		A[a]	B[b]	A[a]	B[b]
Bond lengths							
C(1)-C(2)	1.544		1.531	1.533	1.530	1.516	1.516
C(2)-C(3)	1.491		1.489	1.490	1.480	1.462	1.462
C(3)-C(4)	1.392		1.392	1.398	1.399	1.410	1.411
C(4)-C(1)	1.478		1.467	1.465	1.481	1.490	1.490
O(1)-C(1)	1.215		1.208	1.219	1.212	1.210	1.217
O(2)-C(2)	1.201		1.219	1.201	1.220	1.227	1.227
O(3)-C(3)	1.305		1.296	1.309	1.302	1.303	1.302
O(4)-C(4)	1.322		1.323	1.317	1.305	1.285	1.285
C(5)-C(6)	1.532	1.523	1.555	1.556	1.559	1.554	1.554
C(6)-N(1)	1.469	1.465	1.500	1.510	1.506	1.528	1.528
O(5)-C(5)	1.215	1.217	1.247	1.229	1.242	1.262	1.262
O(6)-C(5)	1.320	1.324	1.251	1.267	1.255	1.233	1.233
N(1)-C(7)			1.482	1.491	1.489	1.497	1.497
N(1)-C(8)				1.489	1.482	1.503	1.503
N(1)-C(9)						1.512	1.512
Bond angles							
C(1)-C(2)-C(3)	86.67		88.01	86.56	87.91	88.33	88.37
C(2)-C(3)-C(4)	92.86		91.00	92.50	92.10	92.74	92.73
C(3)-C(4)-C(1)	93.02		94.42	92.74	92.97	91.39	91.38
C(4)-C(1)-C(2)	87.45		86.55	88.16	87.01	87.54	87.55
O(1)-C(1)-C(2)	136.60		138.32	136.92	136.47	135.29	135.29
O(1)-C(1)-C(4)	135.94		135.13	143.90	136.52	137.17	137.16
O(2)-C(2)-C(1)	136.77		135.51	137.03	135.69	134.23	134.23
O(2)-C(2)-C(3)	136.55		136.47	136.40	136.39	137.45	137.43

O(3)-C(3)-C(2)	130.72		137.44	129.09	136.69	136.38	136.39
O(3)-C(3)-C(4)	136.42		131.55	138.38	131.19	130.88	130.88
O(4)-C(4)-C(1)	136.02		132.87	128.72	135.56	137.11	137.12
O(4)-C(4)-C(3)	130.93		132.68	138.51	131.44	131.50	131.50
N(1)-C(6)-C(5)	110.16	108.41	104.17	106.34	104.47	116.03	116.03
O(5)-C(5)-C(6)	123.29	123.37	116.28	116.62	115.89	109.58	109.58
O(6)-C(5)-C(6)	114.27	114.13	113.35	113.02	113.57	120.18	120.17
O(5)-C(5)-O(6)	122.43	122.48	130.31	130.35	130.52	130.23	130.23
C(6)-N(1)-C(7)			117.83	113.09	113.98	108.18	108.18
C(6)-N(1)-C(8)				114.29	114.00	110.26	110.26
C(7)-N(1)-C(8)				113.06	113.42	109.68	109.68
C(6)-N(1)-C(9)						110.23	110.23
C(7)-N(1)-C(9)						108.80	108.80
C(8)-N(1)-C(9)						109.67	109.67
Torsion angles							
C(1)-C(2)-C(3)-C(4)	0.16		-0.15	0.42	-0.31	0.19	0.19
C(2)-C(3)-C(4)-C(1)	-0.17		0.16	-0.43	0.32	-0.19	0.19
C(3)-C(4)-C(1)-C(2)	0.16		-0.15	0.42	-0.30	0.19	-0.19
C(4)-C(1)-C(2)-C(3)	-0.15		0.14	-0.39	0.28	-0.18	0.18
O(1)-C(1)-C(2)-C(3)	178.76		179.88	-179.25	-179.43	-179.55	179.55
O(1)-C(1)-C(4)-C(3)	-178.77		-179.90	179.38	179.41	179.54	-179.53
O(1)-C(1)-C(2)-O(2)	-0.22		-0.56	-0.73	0.17	0.06	-0.07
O(1)-C(1)-C(4)-O(4)	-1.03		-1.01	-0.70	0.19	0.38	-0.32
O(2)-C(2)-C(1)-C(4)	-179.14		179.68	179.12	179.89	179.43	-179.44
O(2)-C(2)-C(3)-C(4)	179.15		-179.67	-178.11	-179.90	-179.40	179.40
O(2)-C(2)-C(3)-O(3)	0.05		0.35	1.55	-0.47	0.20	-0.19
O(3)-C(3)-C(2)-C(1)	-178.95		179.90	-179.91	179.11	179.79	-179.78
O(3)-C(3)-C(4)-C(1)	178.85		-179.88	179.94	-179.15	-179.83	179.82
O(3)-C(3)-C(4)-O(4)	0.93		1.24	0.00	0.11	-0.54	0.54
O(4)-C(4)-C(1)-C(2)	177.90		178.78	-179.61	-179.52	-179.03	179.03

O(4)-C(4)-C(3)-C(2)	-178.09		-178.71	179.60	179.59	179.09	-179.09
O(5)-C(5)-C(6)-N(1)	-176.42	-160.34	143.51	-176.36	-174.04	170.91	-170.90
O(6)-C(5)-C(6)-N(1)	4.05	20.24	34.03	4.18	4.54	-8.03	8.04
C(5)-C(6)-N(1)-C(7)			162.19	105.52	114.01	-175.63	175.62
C(5)-C(6)-N(1)-C(8)				-123.20	113.59	64.45	-64.45
C(5)-C(6)-N(1)-C(9)						-56.78	56.78

[a] Part A - the positions denoted by the unprimed atomic labels.
[b] Part B - the positions denoted by the primed atomic labels.