

Photophysical Pathways of Cytosine in Aqueous Solution

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 Supplemental Data

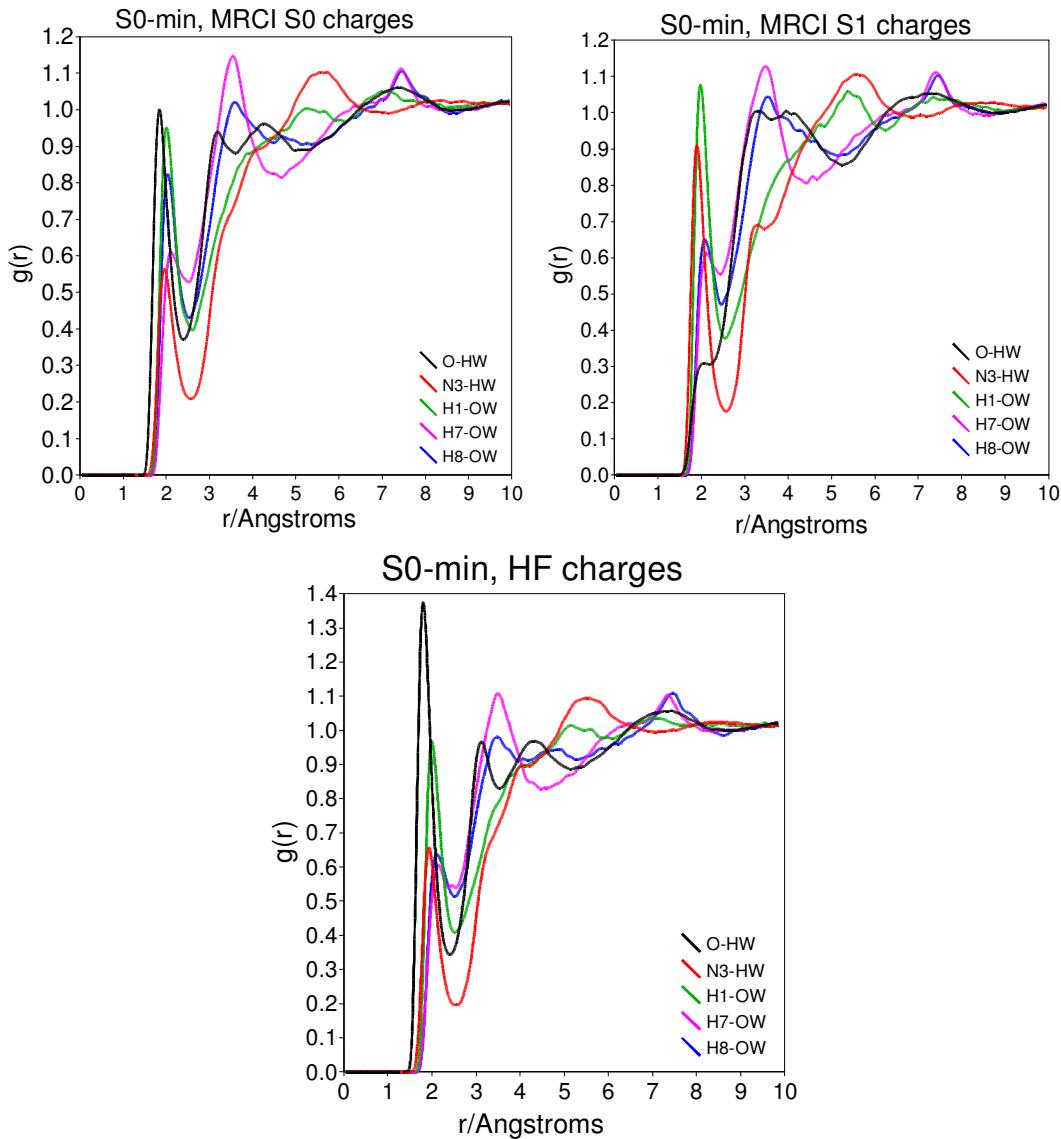


Figure SD-1. Select radial distribution function plots. The radial distribution, $g(r)$, is plotted with respect to r , the radial distance from the selected cytosine atom, in Angstroms, for each cytosine geometry and state-specific partial atomic charge set, as described in the text. Particular cytosine geometry and charge set are given at the top of each plot. Line colors correspond to the different cytosine-water atom pairs: black = O-HW, red = N3-HW, green = H1-OW, magenta = H7-OW, blue = H8-OW, where HW and OW are water hydrogen and oxygen, respectively, and O, N3, H1, H7 and H8 are cytosine atoms, as defined in the text. GS HF charges are the CHELPG charges derived from the HF density of the S_0 -min geometry. MRCI S_0 and S_1 charges are the CHELPG charges derived from the MRCI S_0 and S_1 densities, respectively, for the specific geometry given in the plot.

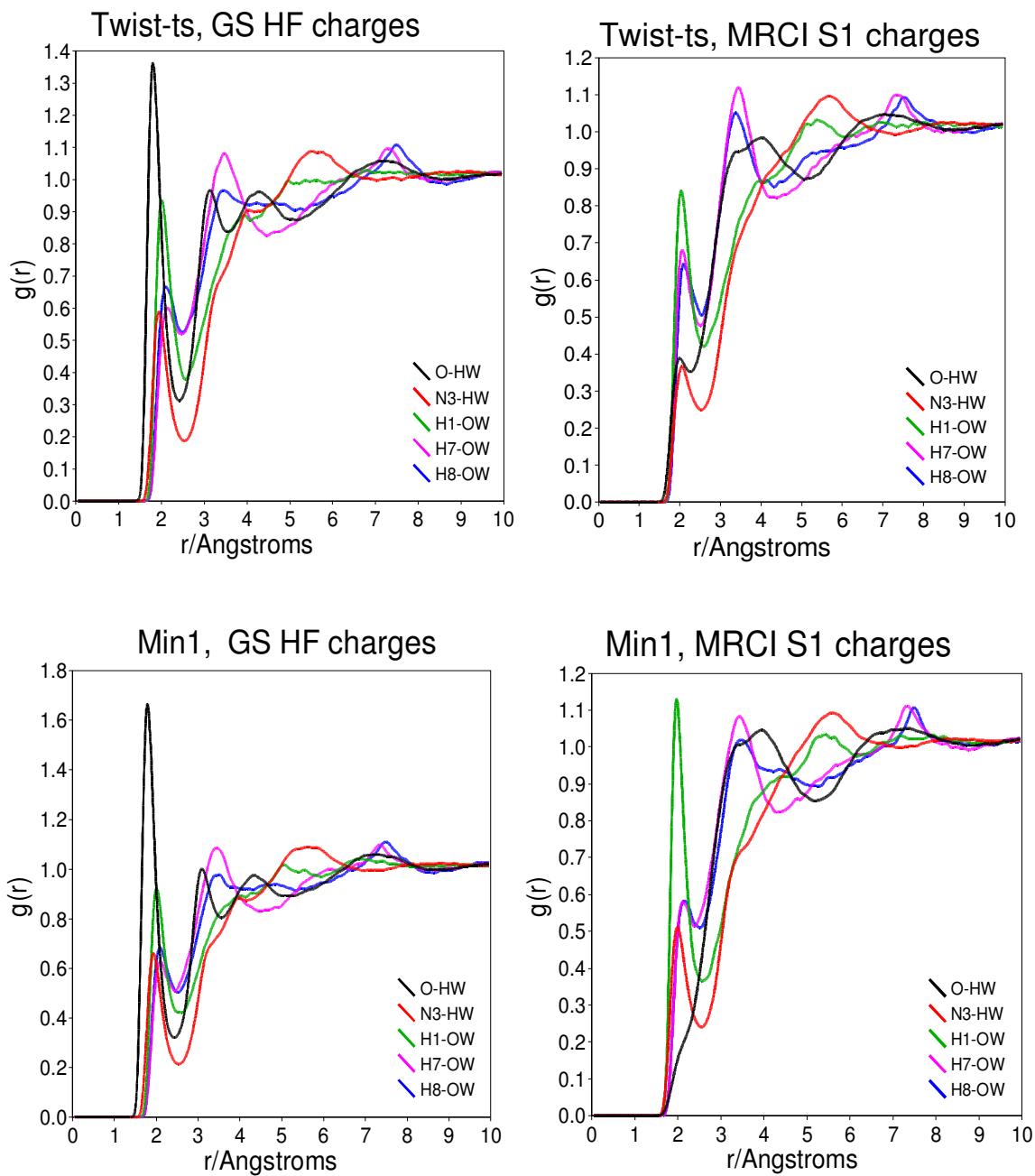


Figure SD-1 continued.

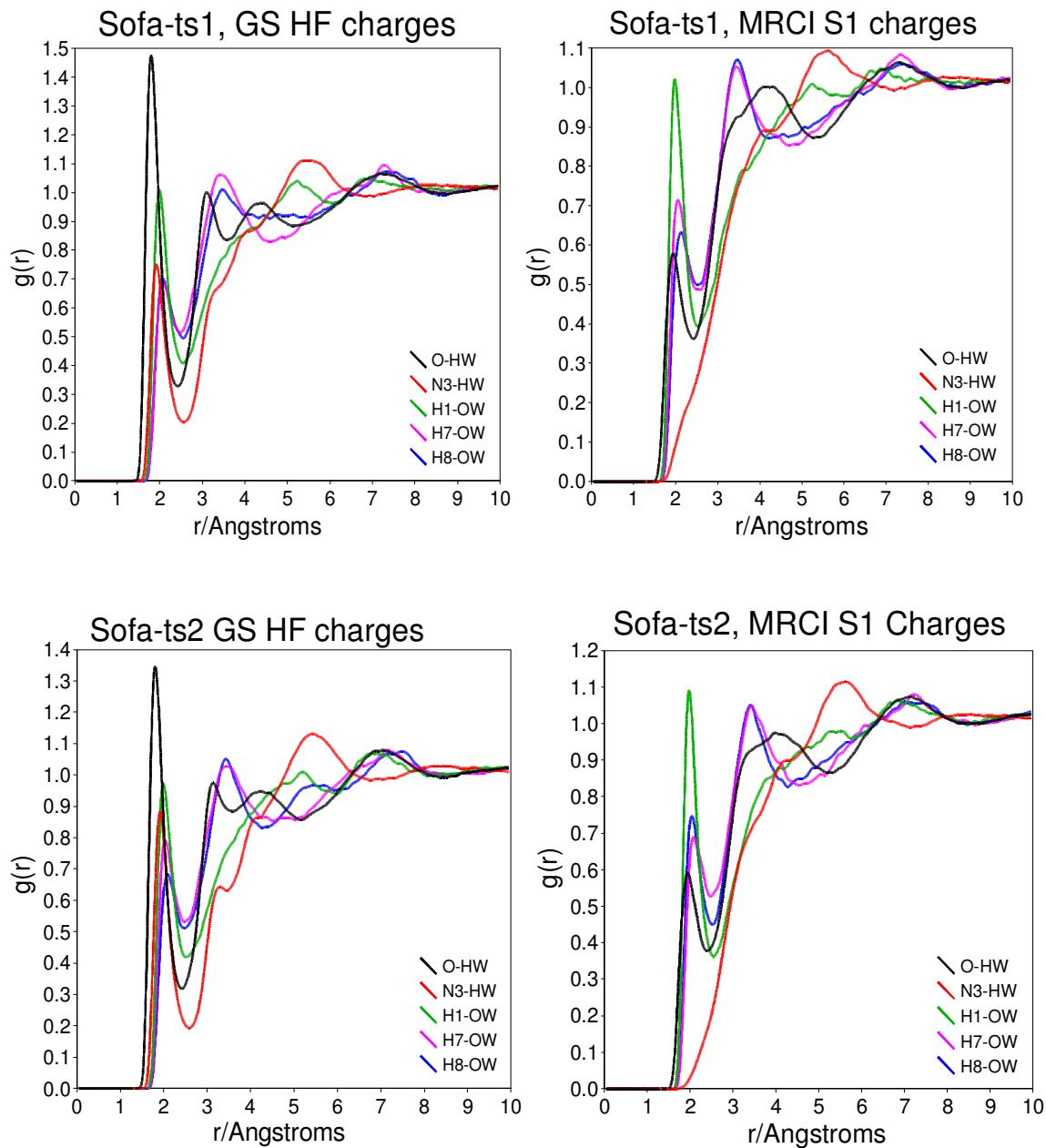


Figure SD-1 continued.

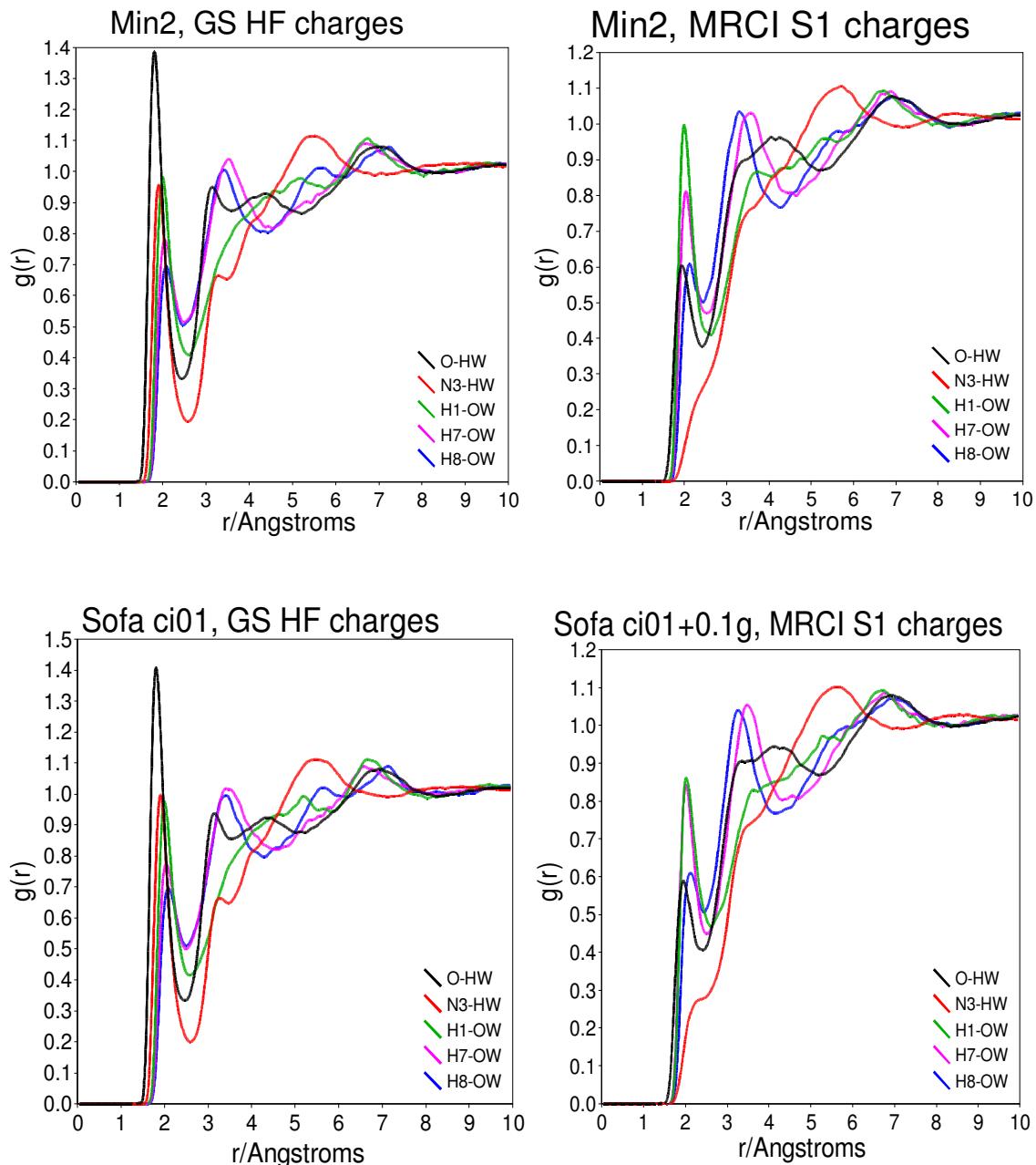


Figure SD-1 continued.

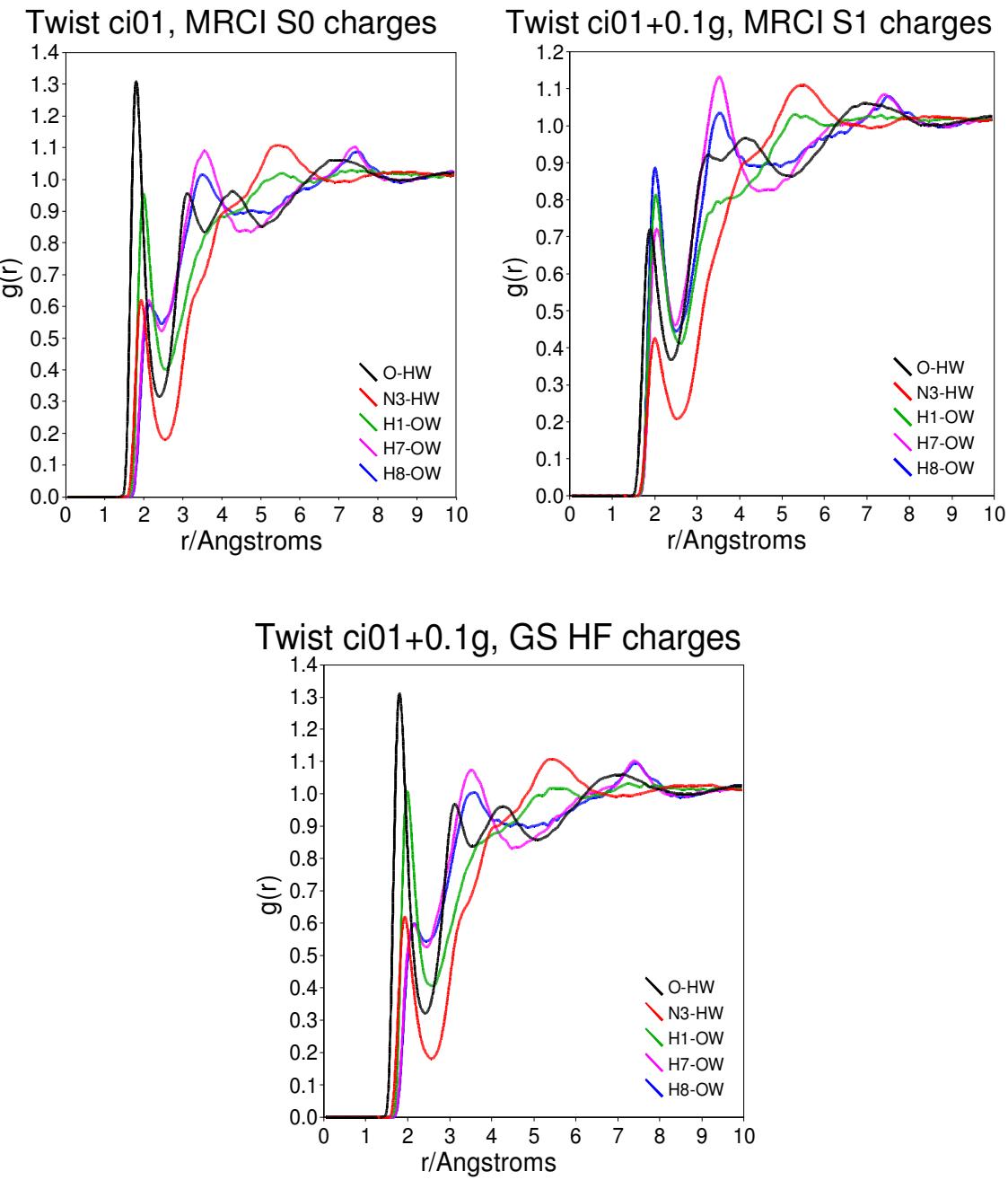


Figure SD-1 continued.

S₀-min, GS HF charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	1.32	1.85	0.35	2.45	0.96	3.15
N3-HW	0.65	1.95	0.20	2.55	1.09	5.55
H1-OW	0.93	2.05	0.41	2.55	1.02	5.15
H7-OW	0.61	2.15	0.54	2.55	1.10	3.55
H8-OW	0.63	2.15	0.52	2.55	0.98	3.45

S₀-min, MRCI S₀ charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	1.00	1.85	0.38	2.45	0.94	3.15
N3-HW	0.56	1.95	0.21	2.55	1.10	5.75
H1-OW	0.93	2.05	0.40	2.65	1.00	5.25
H7-OW	0.60	2.15	0.53	2.55	1.15	3.55
H8-OW	0.82	2.05	0.43	2.55	1.02	3.55

S₀-min, MRCI S₁ charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	0.31	2.05	0.31	2.15	1.00	3.35
N3-HW	0.87	1.95	0.18	2.55	1.10	5.45
H1-OW	1.06	1.95	0.38	2.55	1.06	5.35
H7-OW	0.61	2.15	0.55	2.45	1.13	3.45
H8-OW	0.64	2.05	0.47	2.45	1.04	3.55

Twist ci01, MRCI S₀ charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	1.26	1.85	1.26	2.35	0.96	4.25
N3-HW	0.62	1.95	0.18	2.55	1.11	5.45
H1-OW	0.92	1.95	0.40	2.55	1.02	5.55
H7-OW	0.62	2.15	0.52	2.45	1.09	7.25
H8-OW	0.61	2.15	0.54	2.45	1.01	7.25

Twist ci01+0.1g, MRCI S₁ charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	0.70	1.85	0.37	2.35	0.97	4.15
N3-HW	0.41	2.05	0.21	2.55	1.11	5.45
H1-OW	0.81	2.05	0.42	2.55	1.03	5.55
H7-OW	0.72	2.05	0.46	2.45	1.13	3.55
H8-OW	0.87	2.05	0.45	2.55	1.03	3.55

Table SD-1. Select radial distribution function data. The first and second peaks of the radial distribution function $g(r)$, $g_{\text{max}1}$ and $g_{\text{max}2}$, respectively, and their respective radial distances from designated cytosine atoms, $r_{\text{max}1}$ and $r_{\text{max}2}$, as well as the minimum $g(r)$ between these two maxima, g_{min} , and its radial distance r_{min} , are given for select cytosine-water atom pairs, as defined in the text, for each cytosine geometry and state-specific partial atomic charge set. GS HF charges are the CHELPG charges derived from the HF density of the S₀-min geometry. MRCI S₀ and S₁ charges are the CHELPG charges derived from the MRCI S₀ and S₁ densities, respectively, for the specific geometry given.

Twist *ci*01+0.1g, GS HF charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	1.26	1.85	0.32	2.45	0.97	3.15
N3-HW	0.62	1.95	0.18	2.55	1.11	5.45
H1-OW	0.98	1.95	0.41	2.55	1.02	5.55
H7-OW	0.60	2.15	0.53	2.45	1.07	3.55
H8-OW	0.60	2.15	0.55	2.45	1.00	3.55

Twist-ts, GS HF charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	1.29	1.85	0.32	2.45	0.97	3.15
N3-HW	0.59	1.95	0.19	2.55	1.09	5.55
H1-OW	0.91	2.05	0.38	2.55	0.99	5.15
H7-OW	0.60	2.15	0.52	2.45	1.08	3.45
H8-OW	0.66	2.15	0.53	2.45	0.97	3.35

Twist-ts, MRCI S₁ charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	0.38	2.05	0.35	2.25	0.98	4.05
N3-HW	0.37	2.05	0.25	2.55	1.09	5.75
H1-OW	0.84	2.05	0.42	2.55	1.03	5.35
H7-OW	0.68	2.05	0.48	2.55	1.12	3.45
H8-OW	0.63	2.05	0.51	2.45	1.05	3.35

Min1, GS HF charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	1.61	1.75	0.32	2.45	0.99	3.05
N3-HW	0.66	1.95	0.22	2.55	1.09	5.65
H1-OW	0.90	2.05	0.42	2.65	1.02	5.05
H7-OW	0.62	2.15	0.51	2.45	1.09	3.45
H8-OW	0.67	2.05	0.51	2.55	0.98	3.45

Min1, MRCI S₁ charges

	<i>g</i> _{max1}	<i>r</i> _{max1}	<i>g</i> _{min1}	<i>r</i> _{min1}	<i>g</i> _{max2}	<i>r</i> _{max2}
O-HW	1.05	3.95	0.85	5.15	1.05	7.35
N3-HW	0.50	1.95	0.24	2.55	1.09	5.55
H1-OW	1.12	1.95	0.37	2.55	1.03	5.45
H7-OW	0.58	2.15	0.52	2.35	1.08	3.45
H8-OW	0.58	2.15	0.51	2.55	1.02	3.45

Table SD-1 continued.

Sofa-ts1, GS HF charges

	$g_{\max 1}$	$r_{\max 1}$	$g_{\min 1}$	$r_{\min 1}$	$g_{\max 2}$	$r_{\max 2}$
O-HW	1.40	1.85	0.33	2.45	0.99	3.15
N3-HW	0.74	1.95	0.20	2.55	1.11	5.55
H1-OW	0.96	2.05	0.41	2.55	1.04	5.25
H7-OW	0.68	2.05	0.52	2.45	1.06	3.45
H8-OW	0.70	2.05	0.50	2.55	1.01	3.45

Sofa-ts1, MRCI S₁ charges

	$g_{\max 1}$	$r_{\max 1}$	$g_{\min 1}$	$r_{\min 1}$	$g_{\max 2}$	$r_{\max 2}$
O-HW	0.58	1.95	0.36	2.45	1.00	4.15
N3-HW	1.09	5.65	0.99	7.15	1.03	8.75
H1-OW	1.00	1.95	0.39	2.55	1.01	5.25
H7-OW	0.71	2.05	0.49	2.55	1.05	3.45
H8-OW	0.63	2.15	0.50	2.55	1.07	3.45

Sofa-ts2, GS HF charges

	$g_{\max 1}$	$r_{\max 1}$	$g_{\min 1}$	$r_{\min 1}$	$g_{\max 2}$	$r_{\max 2}$
O-HW	1.30	1.85	0.32	2.45	0.97	3.15
N3-HW	0.87	1.95	0.20	2.55	1.13	5.45
H1-OW	0.94	1.95	0.42	2.55	1.01	5.15
H7-OW	0.79	2.05	0.53	2.45	1.03	3.45
H8-OW	0.67	2.05	0.51	2.45	1.05	3.45

Sofa-ts2, MRCI S₁ charges

	$g_{\max 1}$	$r_{\max 1}$	$g_{\min 1}$	$r_{\min 1}$	$g_{\max 2}$	$r_{\max 2}$
O-HW	0.59	1.95	0.38	2.35	0.97	3.95
N3-HW	1.11	5.65	0.99	7.15	1.03	8.55
H1-OW	1.07	1.95	0.36	2.55	0.98	5.55
H7-OW	0.68	2.05	0.53	2.45	1.05	3.45
H8-OW	0.74	2.05	0.45	2.55	1.05	3.45

Sofa-min, GS HF charges

	$g_{\max 1}$	$r_{\max 1}$	$g_{\min 1}$	$r_{\min 1}$	$g_{\max 2}$	$r_{\max 2}$
O-HW	1.34	1.85	0.33	2.45	0.93	4.35
N3-HW	0.92	1.95	0.20	2.55	1.11	5.55
H1-OW	0.94	1.95	0.41	2.55	0.98	5.15
H7-OW	0.78	2.05	0.52	2.45	1.04	3.55
H8-OW	0.69	2.05	0.51	2.45	1.00	3.45

Table SD-1 continued.

Sofa-min, MRCI S₁ charges

	$g_{\max 1}$	$r_{\max 1}$	$g_{\min 1}$	$r_{\min 1}$	$g_{\max 2}$	$r_{\max 2}$
O-HW	0.60	1.95	0.38	2.45	0.96	4.05
N3-HW	1.10	5.75	0.99	7.15	1.03	8.85
H1-OW	0.96	1.95	0.41	2.65	1.09	6.75
H7-OW	0.81	2.05	0.47	2.55	1.03	3.55
H8-OW	0.60	2.15	0.50	2.45	1.03	3.35

Sofa *ci01*, GS HF charges

	$g_{\max 1}$	$r_{\max 1}$	$g_{\min 1}$	$r_{\min 1}$	$g_{\max 2}$	$r_{\max 2}$
O-HW	1.36	1.85	0.33	2.45	0.94	3.15
N3-HW	0.97	1.95	0.20	2.55	1.11	5.45
H1-OW	0.94	1.95	0.42	2.55	0.99	5.15
H7-OW	0.77	2.05	0.50	2.45	1.02	3.45
H8-OW	0.69	2.05	0.52	2.45	0.99	3.45

Sofa *ci01+0.1g*, MRCI S₁ charges

	$g_{\max 1}$	$r_{\max 1}$	$g_{\min 1}$	$r_{\min 1}$	$g_{\max 2}$	$r_{\max 2}$
O-HW	0.59	1.95	0.41	2.45	0.94	4.15
N3-HW	1.10	5.65	0.99	7.15	1.03	8.75
H1-OW	0.85	2.05	0.47	2.65	0.97	5.25
H7-OW	0.83	2.05	0.45	2.55	1.05	3.45
H8-OW	0.61	2.15	0.51	2.45	1.04	3.25

Table SD-1 continued.