Atomic Accessibility Radii for Molecular Dynamics Analysis
- Supplementary Material -

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Atom Type Radii

The following table shows the atom type radii of the MD trajectories 1, 2, 4, and 5 of Table 1. In addition, the plot in Figure 1 shows the maximal differences between the radii of the data sets.

	Atom	Atom Type Tree	Ligand	RNA	Mem. 1	Mem. 2	max Δ
0	C	C(N(H,H,H),C(O,N),H,C(H,C,H))	1.64	1.57	-	1.75	0.19
1	C	C(C(N,H,C),H,C(H,H,C),H)	1.61	1.54	1.63	1.61	0.08
2	C	C(C(H,C,H),H,H,C(H,H,C))	1.60	1.58	1.47	1.46	0.13
3	C	C(C(H,H,C),H,H,C(H,N,H))	1.48	1.50	1.62	1.62	0.15
4	C	C(C(H,H,C),H,N(H,H,H),H)	1.52	1.51	1.58	1.65	0.14
5	C	C(C(N,H,C),O,N(H,C))	1.42	1.44	1.45	1.41	0.04
6	C	C(N(H,C),H,C(N,O),C(H,H,C))	1.57	1.64	1.63	1.57	0.08
7	C	C(C(H,H,C),C(O,O),H,H)	1.56	1.62	1.49	1.49	0.13
8	C	C(C(C,H,H),O,O)	1.30	1.37	1.47	1.43	0.16
9	C	C(C(N,H,C),N(C,C),O)	1.44	1.52	1.49	1.48	0.07
10	C	C(N(C,C),H,H,C(H,H,C))	1.41	1.48	1.37	1.39	0.11
11	C	C(N(C,C),C(H,H,C),H,C(O,N))	1.54	1.52	1.79	1.68	0.27
12	C	C(C(H,H,C),H,H,C(N,O))	1.66	1.66	1.69	1.57	0.11
13	C	C(C(H,H,C),N(H,H),O)	1.42	1.51	1.53	1.47	0.11
14	C	C(C(N,H,C),C(C,C,H),H,H)	1.69	1.68	1.62	1.60	0.09
15	C	C(C(C,H,H),C(H,H,H),C(H,H,H),H)	1.66	1.72	1.68	1.69	0.06
16	C	C(C(C,C,H),H,H,H)	1.50	1.46	1.51	1.49	0.06
17	C	C(C(H,H,C),H,N(H,C),H)	1.61	1.57	1.59	1.57	0.05
18	C	C(N(H,C),N(H,H),N(H,H))	1.52	1.48	1.65	1.54	0.16
19	C	C(C(N,C,H),H,H,C(C,C))	1.59	1.63	1.63	1.66	0.07
20	C	C(C(H,H,C),C(C,H),C(H,C))	1.46	1.43	1.50	1.56	0.13
21	C	C(C(C,C),H,C(H,C))	1.41	1.38	1.47	1.44	0.09
22	C	C(C(H,C),H,C(H,C))	1.45	1.42	1.48	1.49	0.08
23	C	C(N(C,H),H,C(N,O),C(C,H,C))	1.73	1.64	1.67	1.64	0.09
24	C	C(C(N,H,C),C(C,H,H),H,C(H,H,H))	1.80	1.81	1.76	1.75	0.06
25	C	C(C(C,H,C),C(H,H,H),H,H)	1.61	1.55	1.63	1.57	0.08
26	C	C(C(C,H,H),H,H,H)	1.49	1.51	1.53	1.49	0.04
27	C	C(N(H,C),H,H,C(O,N))	1.58	1.54	1.55	1.61	0.07
28	C	C(C(N,H,H),O,N(H,C))	1.51	1.50	1.50	1.49	0.02
29	C	C(N(H,C),H,C(H,O,H),C(O,N))	1.75	1.58	1.78	1.71	0.20
30	C	C(C(N,H,C),H,O(H),H)	1.53	1.61	1.64	1.55	0.11
31	C	C(N(C,H),C(C,H,O),H,C(N,O))	1.71	1.69	1.76	1.78	0.09
32	C	C(C(N,H,C),C(H,H,H),H,O(H))	1.64	1.68	1.68	1.66	0.04
33	C	C(C(C,H,O),H,H,H)	1.52	1.57	1.55	1.56	0.05
34	C	C(C(N,H,C),C(O,O),H,H)	1.66	1.59	1.59	1.62	0.07
35	C	C(C(N,H,C),C(C,N),H,H)	1.56	1.61	-	1.64	0.08
36	C	C(C(C,H,H),C(N,H),N(C))	1.45	1.59	-	1.42	0.16

	Atom	Atom Type Tree	Ligand	RNA	Mem. 1	Mem. 2	max Δ
37	C	C(N(C),H,N(H,C))	1.45	1.48	-	1.24	0.24
38	C	C(C(C,N),N(H,C),H)	1.49	1.46	-	1.37	0.12
39	C	C(C(C,H,H),C(H,N),C(C,C))	1.57	1.64	1.42	1.57	0.22
40	C	C(C(C,C),H,N(H,C))	1.47	1.63	1.24	1.52	0.39
41	C	C(N(H,C),C(C,C),C(H,C))	1.55	1.50	1.47	1.49	0.08
42	C	C(C(N,C),H,C(H,C))	1.56	1.44	1.50	1.49	0.12
43	C	C(C(C,C),C(N,C),C(C,H))	1.66	1.72	1.49	1.49	0.23
44	C	C(N(C,H),H,C(H,S,H),C(N,O))	1.85	1.72	-	-	0.13
45	C	C(C(N,H,C),H,S(H),H)	1.60	1.72	-	-	0.12
46	C	C(C(N,C,H),H,C(H,H,H),C(H,H,H))	1.79	1.83	1.75	1.68	0.15
47	C	C(C(N,H,C),H,H,C(S,H,H))	1.60	1.69	1.63	1.63	0.09
48	C	C(C(H,H,C),S(C),H,H)	1.59	1.56	1.63	1.68	0.11
49	C	C(S(C),H,H,H)	1.57	1.50	1.52	1.56	0.07
50	C	C(C(N,C,H),H,H,C(N,O))	1.73	1.68	1.66	1.66	0.07
51	C	C(C(H,C),H,C(O,C))	1.47	1.47	1.49	1.47	0.02
52	C	C(C(H,C),O(H),C(C,H))	1.53	1.51	1.53	1.53	0.02
53	C	C(N(C,H),H,C(O,N),C(H,H,H))	1.66	1.74	1.75	1.60	0.15
54	C	C(C(N,H,C),H,H,H)	1.56	1.56	1.53	1.54	0.04
55	C	C(C(H,C),N(H,C),C(N,H))	1.49	1.40	-	-	0.09
56	C	C(C(N,C),N(C),H)	1.43	1.39	-	-	0.04
57	C	C(N(C,H),C(O,H,H),H,C(O,O))	1.91	1.91	-	-	0.00
58	C	C(C(N,H,C),O,O)	1.68	1.55	-	1.57	0.13
59	C	C(C(O,N),C(O,H,H),C(C,C))	1.59	-	-	-	0.00
60	C	C(C(C,C),C(C,H),C(C,O,C))	1.69	-	-	-	0.00
61	C	C(C(C,C),C(O,O),O(H),C(C,H,H))	1.87	-	-	-	0.00
62	C	C(C(C,O,C),O,O(C))	1.66	-	-	-	0.00
63	C	C(C(C,C),O(C),H,H)	1.65	-	-	-	0.00
64	C	C(N(C,C),C(C,N),C(C,H))	1.61	-	-	-	0.00
65	C	C(C(C,C),C(N,C),H)	1.69	-	-	-	0.00
66	C	C(C(C,C),O,N(C,C))	1.60	-	-	-	0.00
67	C	C(H,H,C(C,C),N(C,C))	1.60	-	-	-	0.00
68	C	C(C(N,C),C(C,C),N(C))	1.59	-	-	-	0.00
69	C	C(H,C(C,C),C(C,C))	1.42	-	-	-	0.00
70	C	C(C(C,C),N(C),C(C,H))	1.46	-	-	-	0.00
71	C	C(C(H,H,N),C(C,N),C(H,C))	1.42	-	-	-	0.00
72	C	C(C(H,C),C(N,C),C(H,C))	1.42	-	-	-	0.00
73	C	C(C(C,O,C),C(H,H,H),H,H)	1.42	-	-	-	0.00
74	C	C(O(H),C(O,C,H),H,H)	-	1.50	-	-	0.00
75	C	C(C(O,H,H),O(C),C(C,O,H),H)	-	1.67	-	-	0.00
76	C	C(O(C),H,C(C,H,H),N(C,C))	-	1.64	-	-	0.00
77	C	C(N(C,C),C(C,C),H)	-	1.53	-	-	0.00
78	C	C(C(N,H),C(N,O),C(H,H,H))	-	1.44	-	-	0.00
79	C	C(C(C,C),H,H,H)	-	1.61	1.41	-	0.20
80	C	C(C(C,C),N(H,C),O)	-	1.59	-	-	0.00
81	C	C(N(C,C),N(H,C),O)	-	1.61	-	-	0.00
82	C	C(C(O,C,H),C(C,H,H),O(P),H)	-	1.87	-	-	0.00
83	C	C(C(O,H,N),C(C,O,H),H,H)	-	1.60	-	-	0.00
84	C	C(O(P),H,C(O,C,H),H)	-	1.51	1.38	1.42	0.13
85	C	C(N(C,C),N(C),H)	-	1.42	-	-	0.00
86	C	C(N(C),C(N,N),C(N,N))	-	1.45	-	-	0.00
87	C	C(C(N,C),N(H,H),N(C))	-	1.56	-	-	0.00
88	C	C(N(C),H,N(C))	-	1.54	-	-	0.00
89	C	C(N(C,C),C(N,C),N(C))	-	1.55	-	-	0.00
90	C	C(N(C),C(O,N),C(N,N))	-	1.58	-	-	0.00
91	C	C(C(N,C),O,N(H,C))	-	1.54	-	-	0.00
92	C	C(N(H,C),N(H,H),N(C))	-	1.48	-	-	0.00

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93	C	C(C(H,O,C),C(C,H,H),H,O(H))	-	1.78	-	-	0.00
94	C	C(N(H,H,H),C(H,O,C),C(O,N),H)	-	-	1.75	-	0.00
95	C	C(C(H,C,H),O(H),O)	-	-	1.58	-	0.00
96	C	C(N(H,C),H,C(H,C))	-	-	1.53	-	0.00
97	C	C(C(N,H),H,C(C,C))	-	-	1.69	-	0.00
98	C	C(C(H,C),C(H,C),C(H,H,H))	-	-	1.74	-	0.00
99	C	C(C(C,H),C(C,C,C),C(C,C))	-	-	1.75	-	0.00
100	C	C(C(C,C),C(C,H,H),C(H,H,H))	-	-	1.58	-	0.00
101	C	C(C(C,C),C(H,H,C),H,H)	-	-	1.73	-	0.00
102	C	C(C(H,H,C),H,C(C,C,C),H)	-	-	1.62	-	0.00
103	C	C(C(C,C),C(H,C,H),C(H,H,H),C(H,H,H))	-	-	1.70	-	0.00
104	C	C(C(C,C,C),H,H,H)	-	-	1.49	-	0.00
105	C	C(N(H,C),H,H,C(O,O))	-	-	1.79	-	0.00
106	C	C(C(N,H,H),O,O)	-	-	1.59	-	0.00
107	C	C(N(C,C,C),H,H,C(H,O,H))	-	-	1.40	1.42	0.03
108	C	C(N(C,C,C),H,H,H)	-	-	1.41	1.42	0.01
109	C	C(C(N,H,H),H,O(P),H)	-	-	1.53	1.43	0.10
110	C	C(C(O,H,H),C(H,O,H),H,O(C))	-	-	1.59	1.56	0.03
111	C	C(O(C),O,C(C,H,H))	-	-	1.46	1.40	0.06
112	C	C(C(C,H,O),H,O(C),H)	-	-	1.52	1.47	0.04
113	C	C(C(H,C,H),C(C,H),H,H)	-	-	1.48	1.51	0.03
114	C	C(C(C,H,H),C(H,C),H)	-	-	1.46	1.50	0.04
115	C	C(C(C,H,H),H,C(H,H,H),H)	-	-	1.49	1.53	0.04
116	C	C(C(N,H,H),O,N(C,C))	-	-	-	1.51	0.00
117	C	C(C(O,O),N(H,C),H,C(H,C,H))	-	-	-	1.93	0.00
118	H	H(N(H,H,C))	0.42	0.42	0.29	0.27	0.15
119	H	H(C(N,C,C))	0.81	0.79	0.77	0.79	0.04
120	H	H(C(C,C,H))	0.86	0.87	0.81	0.80	0.07
121	H	H(C(C,N,H))	0.66	0.64	0.50	0.52	0.16
122	H	H(N(C,C))	0.42	0.42	0.37	0.34	0.08
123	H	H(N(C,H))	0.41	0.41	0.33	0.32	0.09
124	H	H(C(C,C,C))	0.90	0.91	0.82	0.82	0.09
125	H	H(C(C,H,H))	0.81	0.83	0.80	0.83	0.03
126	H	H(C(C,C))	0.84	0.88	0.77	0.81	0.11
127	H	H(C(C,O,H))	0.77	0.82	0.81	0.85	0.07
128	H	H(O(C))	0.32	0.30	0.30	0.31	0.02
129	H	H(C(C,C,O))	0.85	0.82	0.82	0.84	0.03
130	H	H(C(N,N))	0.82	0.88	-	0.68	0.20
131	H	H(C(C,N))	0.86	0.83	0.73	0.94	0.21
132	H	H(C(C,S,H))	0.79	0.84	0.81	0.91	0.12
133	H	H(S(C))	0.44	0.47	-	-	0.03
134	H	H(C(S,H,H))	0.85	0.83	0.78	0.85	0.07
135	H	H(O(H))	0.24	0.23	0.27	0.27	0.04
136	H	H(C(O,C,N))	-	0.87	-	-	0.00
137	H	H(C(N,H,H))	-	-	0.52	0.52	0.00
138	N	N(H,H,H,C(C,H,C))	1.40	1.39	1.34	1.37	0.06
139	N	N(C(C,H,H),H,H,H)	1.38	1.37	1.30	1.29	0.09
140	N	N(C(C,O),H,C(H,C,C))	1.36	1.34	1.34	1.35	0.03
141	N	N(C(C,O),C(H,H,C),C(C,H,C))	1.61	1.60	1.52	1.47	0.15
142	N	N(C(C,O),H,H)	1.33	1.40	1.37	1.37	0.06
143	N	N(C(C,H,H),H,C(N,N))	1.31	1.36	1.32	1.33	0.05
144	N	N(C(N,N),H,H)	1.36	1.35	1.29	1.31	0.07
145	N	N(C(C,O),H,C(H,H,C))	1.39	1.41	1.38	1.32	0.08
146	N	N(C(C,C),C(H,N))	1.32	1.30	-	1.31	0.02
147	N	N(C(H,N),H,C(C,H))	1.40	1.36	-	1.41	0.05
148	N	N(C(C,H),H,C(C,C))	1.36	1.39	1.35	1.37	0.05

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149	N	N(C(C,C),H,C(N,H))	1.35	1.35	-	-	0.00
150	N	N(C(N,H),C(C,H))	1.32	1.36	-	-	0.04
151	N	N(C(C,C),C(C,O),C(H,H,C))	1.68	-	-	-	0.00
152	N	N(C(C,C),C(C,C))	1.42	-	-	-	0.00
153	N	N(C(O,H,C),C(N,O),C(C,H))	-	1.56	-	-	0.00
154	N	N(C(C,O),H,C(N,O))	-	1.44	-	-	0.00
155	N	N(C(O,H,C),C(N,H),C(C,N))	-	1.55	-	-	0.00
156	N	N(C(C,N),H,H)	-	1.53	-	-	0.00
157	N	N(C(C,N),C(H,N))	-	1.33	-	-	0.00
158	N	N(C(C,O),H,C(N,N))	-	1.42	-	-	0.00
159	N	N(C(N,N),C(C,N))	-	1.37	-	-	0.00
160	N	N(C(C,H,H),H,C(H,C))	-	-	1.38	-	0.00
161	N	N(C(H,H,H),C(H,H,H),C(H,H,H),C(H,H,C))	-	-	1.77	1.78	0.01
162	O	O(C(C,N))	1.17	1.15	1.18	1.16	0.02
163	O	O(C(C,O))	1.15	1.15	1.13	1.14	0.02
164	O	O(C(C,H,H),H)	1.26	1.26	1.29	1.22	0.07
165	O	O(C(C,C,H),H)	1.20	1.24	1.24	1.26	0.06
166	O	O(C(C,C),H)	1.28	1.25	1.25	1.20	0.08
167	O	O(C(C,O),C(C,H,H))	1.28	-	1.31	1.21	0.09
168	O	O(C(C,C,C),H)	1.30	-	-	-	0.00
169	O	O(H,H)	1.18	1.19	1.20	1.20	0.02
170	O	O(C(C,C,H),C(H,C,N))	-	1.28	-	-	0.00
171	O	O(C(N,N))	-	1.19	-	-	0.00
172	O	O(C(C,C,H),P(O,O,O))	-	1.33	-	-	0.00
173	O	O(P(O,O,O))	-	1.17	1.15	1.14	0.03
174	O	O(P(O,O,O),C(H,C,H))	-	1.19	1.22	1.10	0.12
175	O	O(C(C,O),H)	-	-	1.26	-	0.00
176	O	O(C(C,C,H),C(O,C))	-	-	1.31	1.20	0.11
177	P	P(O(C),O,O(C),O)	-	1.68	1.78	1.76	0.09
178	S	S(C(C,H,H),H)	1.56	1.52	-	-	0.04
179	S	S(C(C,H,H),C(H,H,H))	1.49	1.56	1.57	1.62	0.13
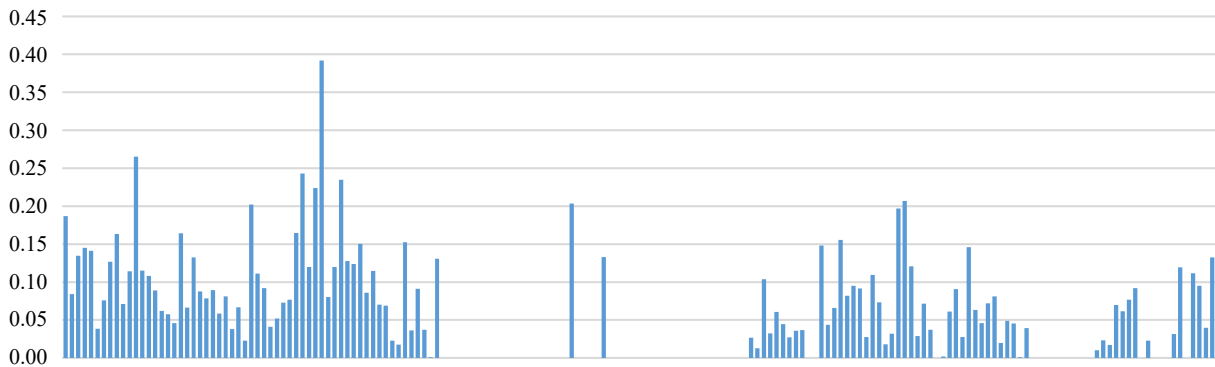
Figure 1: *Maximal difference of the atom type radii.*