Supporting Information

Indicator of the Stacking Interaction in the DNA Double-Helical Structure: ChiraSac Study

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Table S1. Coordinates (in Å) of the X-ray model (ΔR = ±0.0 Å).

Number	Atom	X	Y	Z
1	O	-1.432282	3.062011	-3.450226
2	C	-1.138262	3.490870	-2.161283
3	C	-1.915137	2.528261	-1.219174
4	O	-1.320891	1.323154	-1.375799
5	C	-1.621770	2.901323	0.265451
6	C	-1.628809	1.605828	1.037130
7	C	-1.266929	0.590283	-0.084329
8	H	-0.974033	3.638239	-4.074116
9	H	-1.444211	4.528044	-1.957733
10	H	-0.073154	3.378197	-1.913239
11	H	-2.997050	2.543000	-1.425223
12	H	-0.625882	3.348168	0.309203
13	H	-2.366970	3.605291	0.572057
14	H	-0.906520	1.580956	1.851807
15	H	-2.630750	1.405642	1.426690
16	H	-1.998429	-0.226477	-0.121334
17	N	0.000000	0.000000	0.000000
18	C	0.239568	-1.340766	-0.062023
19	N	1.539695	-1.611381	-0.011031
20	C	2.148276	-0.389995	-0.058155
21	C	3.532836	0.000000	0.000000
22	O	4.502321	-0.808603	-0.026452
23	N	3.779739	1.309969	-0.013485
24	C	2.803696	2.266223	-0.046150
25	N	3.118214	3.496942	-0.094761
26	N	1.499384	1.988189	0.000000
27	C	1.245867	0.653004	-0.005153
28	H	-0.562239	-2.065763	-0.063037
29	H	4.784831	1.591405	-0.055666
30	H	4.089711	3.819805	-0.156257
31	H	2.367052	4.165956	-0.141998
32	C	-1.595288	5.985599	3.664306
33	C	-0.142795	6.492148	3.934044
34	O	0.658077	5.342355	4.420207

35	C	0.589455	7.031564	2.681000
36	O	1.465878	8.076670	3.177415
37	C	1.600657	5.953497	2.353511
38	C	1.872978	5.303173	3.707615
39	H	-1.531128	5.321048	2.828149
40	H	-1.971340	5.434864	4.533398
41	H	-2.277598	6.810190	3.436497
42	H	-0.149108	7.254029	4.723933
43	H	-0.059358	7.318627	1.848420
44	H	0.921239	8.849000	3.382774
45	H	2.495112	6.375228	1.893731
46	H	1.147011	5.219127	1.683709
47	H	2.712731	5.734848	4.252991
48	N	2.155898	3.818258	3.584928
49	C	3.491331	3.476523	3.527805
50	O	4.397289	4.305401	3.574793
51	N	3.767504	2.117041	3.457195
52	C	2.778628	1.192373	3.448611
53	N	3.187495	-0.108864	3.345742
54	C	1.450109	1.590299	3.534293
55	C	1.168995	2.876426	3.617265
56	H	4.195893	-0.313362	3.240795
57	H	2.516375	-0.820974	3.105038
58	H	0.650781	0.857718	3.552181
59	H	0.166739	3.281517	3.674881
60	O	11.767668	3.465081	6.589134
61	C	11.462624	3.826726	5.223108
62	C	12.249438	2.931988	4.271812
63	O	11.842007	1.550491	4.529691
64	C	11.978992	3.215769	2.838008
65	C	11.893135	1.869904	2.152480
66	C	11.686715	0.790622	3.388851
67	H	11.370272	4.151229	7.139010
68	H	10.395148	3.675684	5.014789
69	H	11.726805	4.867956	4.995251
70	H	13.324149	3.016309	4.471772

71	H	11.017200	3.724168	2.736783
72	H	12.763750	3.875249	2.531187
73	H	11.068348	1.795571	1.448424
74	H	12.830764	1.651193	1.630959
75	H	12.424012	-0.022061	3.323560
76	N	10.430564	0.238922	3.347352
77	C	10.162752	-1.086467	3.359825
78	N	8.854222	-1.406888	3.316898
79	C	8.272190	-0.185519	3.256082
80	C	6.892350	0.155934	3.258679
81	O	5.940080	-0.690050	3.273046
82	N	6.606862	1.455005	3.260562
83	C	7.562721	2.411095	3.292590
84	N	7.169116	3.656024	3.270234
85	N	8.876229	2.215632	3.283624
86	C	9.177225	0.864394	3.293863
87	H	10.964862	-1.810932	3.414121
88	H	5.595704	1.716507	3.299906
89	H	6.182769	3.924877	3.346712
90	H	7.884948	4.359211	3.347881
91	C	11.803903	6.139047	-0.502085
92	C	10.422262	6.536388	-0.876999
93	O	9.677583	5.353904	-1.308229
94	C	9.604187	7.140304	0.270295
95	O	8.845213	8.149657	-0.251691
96	C	8.618092	5.930092	0.675843
97	C	8.433852	5.253712	-0.650891
98	H	11.831775	5.450020	0.316062
99	H	12.398478	7.038001	-0.285907
100	H	12.278911	5.664921	-1.376239
101	H	10.447045	7.250564	-1.710634
102	H	10.231062	7.435272	1.122199
103	H	8.309348	8.534504	0.452831
104	H	9.126914	5.262210	1.373293
105	H	7.688938	6.297337	1.117495
106	H	7.597930	5.621935	-1.246418

107	N	8.187536	3.738677	-0.479289
108	C	6.843268	3.397524	-0.341511
109	O	5.953047	4.240051	-0.388594
110	N	6.578001	2.063087	-0.218126
111	C	7.591774	1.147791	-0.176089
112	N	7.258652	-0.176096	-0.019082
113	C	8.943163	1.520806	-0.227195
114	C	9.208374	2.816171	-0.396312
115	H	6.263635	-0.431907	0.083096
116	H	7.966018	-0.821394	0.293683
117	H	9.734782	0.784484	-0.176784
118	H	10.199858	3.249121	-0.465088

Table S2. Coordinates (in Å) of the rotational model at ΔR = ±0.0 Å (ΔA = 30°).

Number	Atom	X	Y	Z
1	O	-6.611152	1.375483	-3.334420
2	C	-6.317132	1.804342	-2.045478
3	C	-7.094007	0.841733	-1.103368
4	O	-6.499761	-0.363374	-1.259993
5	C	-6.800640	1.214795	0.381256
6	C	-6.807679	-0.080700	1.152936
7	C	-6.445799	-1.096245	0.031476
8	H	-6.152903	1.951711	-3.958311
9	H	-6.623081	2.841516	-1.841927
10	H	-5.252024	1.691669	-1.797433
11	H	-8.175920	0.856472	-1.309417
12	H	-5.804752	1.661640	0.425009
13	H	-7.545840	1.918763	0.687863
14	H	-6.085390	-0.105572	1.967612
15	H	-7.809620	-0.280886	1.542496
16	H	-7.177299	-1.913005	-0.005529
17	N	-5.178870	-1.686528	0.115805
18	C	-4.939302	-3.027294	0.053782
19	N	-3.639175	-3.297909	0.104774
20	C	-3.030594	-2.076523	0.057650
21	C	-1.646034	-1.686528	0.115805

22	O	-0.676549	-2.495131	0.089353
23	N	-1.399131	-0.376559	0.102320
24	C	-2.375174	0.579695	0.069655
25	N	-2.060656	1.810414	0.021044
26	N	-3.679486	0.301661	0.115805
27	C	-3.933003	-1.033524	0.110652
28	H	-5.741109	-3.752291	0.052768
29	H	-0.394039	-0.095123	0.060139
30	H	-1.089159	2.133277	-0.040452
31	H	-2.811818	2.479428	-0.026193
32	C	-8.016128	0.336026	3.780111
33	C	-7.011507	1.500957	4.049849
34	O	-5.743035	0.905643	4.536013
35	C	-6.647068	2.334229	2.796806
36	O	-6.410616	3.677529	3.293220
37	C	-5.232308	1.906197	2.469317
38	C	-4.671309	1.479160	3.823421
39	H	-7.628289	-0.207412	2.943954
40	H	-8.066432	-0.328951	4.649203
41	H	-9.019322	0.708987	3.552303
42	H	-7.397915	2.157608	4.839738
43	H	-7.352488	2.258427	1.964225
44	H	-7.268453	4.074067	3.498579
45	H	-4.668553	2.718654	2.009536
46	H	-5.257992	1.043391	1.799514
47	H	-4.159899	2.272878	4.368796
48	N	-3.683836	0.334646	3.700734
49	C	-2.356449	0.706412	3.643610
50	O	-1.986306	1.877220	3.690599
51	N	-1.437535	-0.332848	3.573001
52	C	-1.831593	-1.628072	3.564417
53	N	-0.826885	-2.550543	3.461547
54	C	-3.181087	-1.947717	3.650098
55	C	-4.067603	-0.974456	3.733071
56	H	0.148662	-2.223444	3.356600
57	H	-1.052037	-3.502808	3.220843

58	H	-3.507035	-2.981815	3.667987
59	H	-5.138127	-1.124765	3.790687
60	O	4.816790	4.834671	6.704939
61	C	4.371792	4.995343	5.338913
62	C	5.500562	4.613884	4.387617
63	O	5.838464	3.213757	4.645496
64	C	5.124458	4.724423	2.953813
65	C	5.723036	3.515941	2.268286
66	C	6.083912	2.478045	3.504656
67	H	4.129561	5.230195	7.254815
68	H	3.522851	4.330799	5.130594
69	H	4.079964	6.029165	5.111056
70	H	6.389128	5.224264	4.587577
71	H	4.037322	4.683813	2.852588
72	H	5.474338	5.687928	2.646993
73	H	5.045916	3.039173	1.564229
74	H	6.644402	3.795346	1.746765
75	H	7.128772	2.142890	3.439366
76	N	5.271903	1.372183	3.463157
77	C	5.702666	0.090457	3.475630
78	N	4.729656	-0.841301	3.432704
79	C	3.614917	-0.074580	3.371888
80	C	2.249214	-0.468793	3.374484
81	O	1.847516	-1.677572	3.388851
82	N	1.352439	0.513491	3.376368
83	C	1.702192	1.819419	3.408396
84	N	0.738856	2.700757	3.386039
85	N	2.937455	2.306897	3.399430
86	C	3.873744	1.287189	3.409668
87	H	6.759546	-0.135893	3.529927
88	H	0.345999	0.234380	3.415712
89	H	-0.249772	2.440417	3.462518
90	H	1.007191	3.667650	3.463687
91	C	6.625033	4.452519	-0.386279
92	C	5.243392	4.849860	-0.761193
93	O	4.498713	3.667376	-1.192424

94	C	4.425317	5.453776	0.386101
95	O	3.666343	6.463129	-0.135885
96	C	3.439222	4.243564	0.791648
97	C	3.254982	3.567184	-0.535085
98	H	6.652905	3.763492	0.431868
99	H	7.219608	5.351473	-0.170102
100	H	7.100041	3.978393	-1.260433
101	H	5.268175	5.564036	-1.594828
102	H	5.052192	5.748744	1.238004
103	H	3.130478	6.847976	0.568636
104	H	3.948044	3.575682	1.489099
105	H	2.510068	4.610809	1.233300
106	H	2.419060	3.935407	-1.130613
107	N	3.008666	2.052149	-0.363484
108	C	1.664398	1.710996	-0.225706
109	O	0.774177	2.553523	-0.272788
110	N	1.399131	0.376559	-0.102320
111	C	2.412904	-0.538737	-0.060284
112	N	2.079782	-1.862624	0.096723
113	C	3.764293	-0.165722	-0.111390
114	C	4.029504	1.129643	-0.280506
115	H	1.084765	-2.118435	0.198902
116	H	2.787148	-2.507922	0.409489
117	H	4.555912	-0.902044	-0.060979
118	H	5.020988	1.562593	-0.349282