

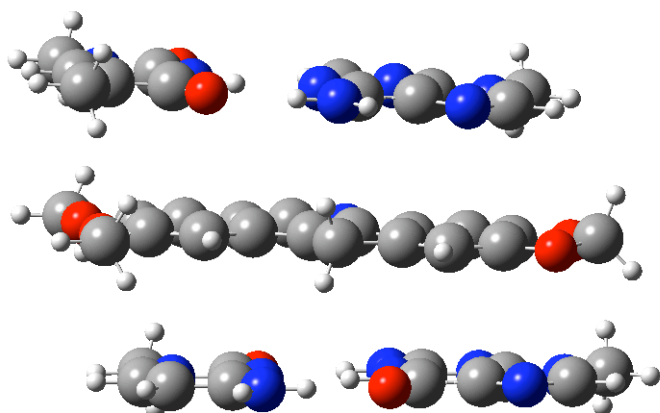
Supporting Information

The Binding Orientation of a Norindenoisoquinoline in the Topoisomerase I-DNA Cleavage Complex is Governed by π - π Stacking Interactions

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Model A (Crystal structure)

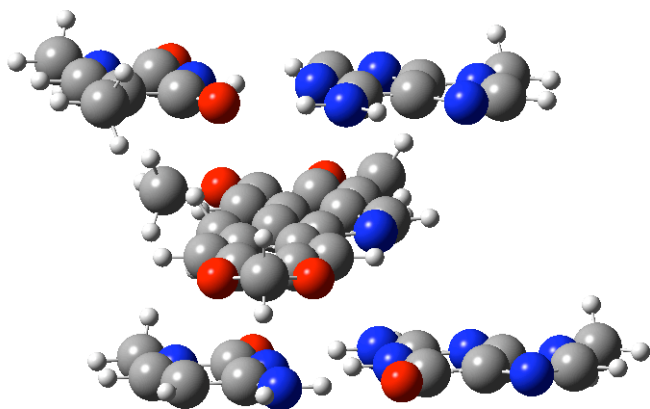


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C	-0.68966535	1.16806725	-0.00026547
C	3.52138916	1.21780043	0.00014952
N	4.25120675	0.14277737	0.00015558
C	3.58929035	-1.02313955	0.00000780
C	2.22458666	-1.15677221	0.00016873
C	1.84248448	-2.61825285	0.00022484
C	3.19515378	-3.30225777	-0.00015368
C	4.20936858	-2.35513324	-0.00051657
C	5.56262229	-2.70596076	0.00124230
C	5.81436781	-4.04837572	0.00414130
C	4.80543611	-4.99823503	0.00506088
C	3.47673739	-4.66848096	0.00265979
O	5.36393295	-6.23637948	-0.00872523
C	6.74571204	-6.04988120	0.18681436
O	7.01638035	-4.68506936	-0.01220721
O	-2.02186246	1.27824563	-0.00035999
C	-2.81230967	0.12255291	-0.00059727
O	-0.78744076	3.50974944	-0.00054547
C	-0.21072456	4.78378298	-0.00177816
H	-0.51661817	-0.93922779	0.00003645
H	1.90272620	3.37226035	-0.00018294
H	4.04678790	2.15977620	0.00014976
H	1.25664169	-2.88765521	-0.87585116
H	1.25696117	-2.88740898	0.87658034
H	6.34297893	-1.96945024	-0.00157984
H	2.71146666	-5.42273263	0.00115562
H	7.29622554	-6.63890862	-0.53140043
H	7.01051353	-6.33178751	1.20106756
H	-3.83770706	0.46059830	-0.00078766
H	-2.63295618	-0.47852550	0.88514486
H	-2.63253622	-0.47854477	-0.88628723
H	-1.03062357	5.48639111	-0.00229662
H	0.39721072	4.94265958	-0.88750367
H	0.39742460	4.94442633	0.88361156

H	0.30233285	5.38308447	4.42355442
H	8.47412630	-0.82540399	3.89246878
H	-1.25683852	5.44469473	3.60015430
H	0.24256269	5.45063504	2.67056789
H	8.41062746	-0.76069517	2.13459489
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N	5.71302069	0.29966178	3.15182602
C	5.75808103	-1.03126704	3.10161119
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H	-2.95519811	0.17761013	4.33951863
H	-2.37182383	3.54895375	3.57274056
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H	2.33604004	-2.99989125	3.15297581
H	1.39804809	-1.55369136	3.24004840
H	4.34631365	1.80542982	3.25635769
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H	9.00809661	-3.54341549	-2.28167776
H	0.23978604	4.17178420	-3.60914513
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N	0.39568556	-1.77855420	-3.40151199
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C	1.18164363	3.64146836	-3.57899174
C	8.70395452	-4.05856091	-3.18400577
N	7.27109675	-4.24433537	-3.20888949
C	6.57211426	-5.43047490	-3.17298659
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N	4.25048954	-1.75883126	-3.35040944
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H	-1.59423389	0.01503463	-3.48884967
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H	3.45903488	-1.13618803	-3.38640567
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Model B (NORIND_R90)

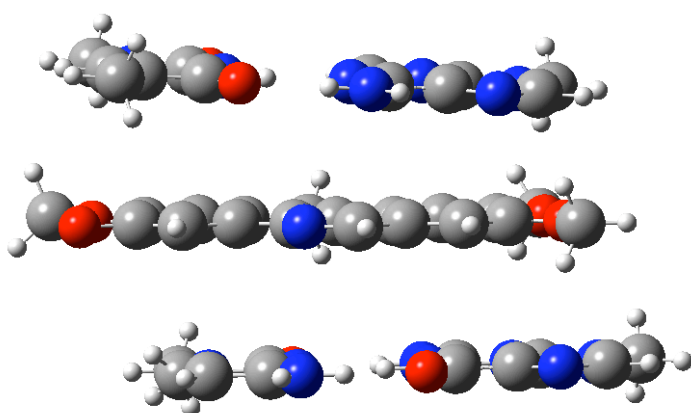


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C	0.01114868	2.43011260	-0.00036225
C	-0.68966535	1.16806725	-0.00026547
C	3.52138916	1.21780043	0.00014952
N	4.25120675	0.14277737	0.00015558
C	3.58929035	-1.02313955	0.00000780
C	2.22458666	-1.15677221	0.00016873
C	1.84248448	-2.61825285	0.00022484
C	3.19515378	-3.30225777	-0.00015368
C	4.20936858	-2.35513324	-0.00051657
C	5.56262229	-2.70596076	0.00124230
C	5.81436781	-4.04837572	0.00414130
C	4.80543611	-4.99823503	0.00506088
C	3.47673739	-4.66848096	0.00265979
O	5.36393295	-6.23637948	-0.00872523
C	6.74571204	-6.04988120	0.18681436
O	7.01638035	-4.68506936	-0.01220721
O	-2.02186246	1.27824563	-0.00035999
C	-2.81230967	0.12255291	-0.00059727
O	-0.78744076	3.50974944	-0.00054547
C	-0.21072456	4.78378298	-0.00177816
H	-0.51661817	-0.93922779	0.00003645
H	1.90272620	3.37226035	-0.00018294
H	4.04678790	2.15977620	0.00014976
H	1.25664169	-2.88765521	-0.87585116
H	1.25696117	-2.88740898	0.87658034
H	6.34297893	-1.96945024	-0.00157984

H	2.71146666	-5.42273263	0.00115562
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H	-2.63253622	-0.47854477	-0.88628723
H	-1.03062357	5.48639111	-0.00229662
H	0.39721072	4.94265958	-0.88750367
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H	4.35185497	-3.68833649	-3.35792713
H	2.16018072	-4.77133220	-3.41665159
H	8.54737335	3.91320638	-3.23879899
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Model C (NORIND_R180)

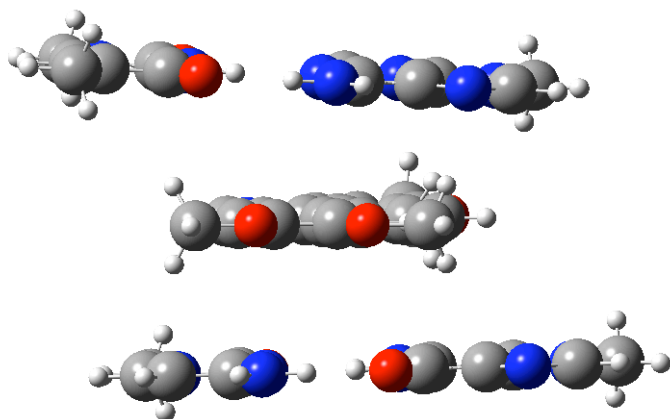


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C	0.01114868	2.43011260	-0.00036225
C	-0.68966535	1.16806725	-0.00026547
C	3.52138916	1.21780043	0.00014952
N	4.25120675	0.14277737	0.00015558
C	3.58929035	-1.02313955	0.00000780
C	2.22458666	-1.15677221	0.00016873
C	1.84248448	-2.61825285	0.00022484
C	3.19515378	-3.30225777	-0.00015368
C	4.20936858	-2.35513324	-0.00051657
C	5.56262229	-2.70596076	0.00124230
C	5.81436781	-4.04837572	0.00414130
C	4.80543611	-4.99823503	0.00506088
C	3.47673739	-4.66848096	0.00265979
O	5.36393295	-6.23637948	-0.00872523
C	6.74571204	-6.04988120	0.18681436
O	7.01638035	-4.68506936	-0.01220721
O	-2.02186246	1.27824563	-0.00035999
C	-2.81230967	0.12255291	-0.00059727

O	-0.78744076	3.50974944	-0.00054547
C	-0.21072456	4.78378298	-0.00177816
H	-0.51661817	-0.93922779	0.00003645
H	1.90272620	3.37226035	-0.00018294
H	4.04678790	2.15977620	0.00014976
H	1.25664169	-2.88765521	-0.87585116
H	1.25696117	-2.88740898	0.87658034
H	6.34297893	-1.96945024	-0.00157984
H	2.71146666	-5.42273263	0.00115562
H	7.29622554	-6.63890862	-0.53140043
H	7.01051353	-6.33178751	1.20106756
H	-3.83770706	0.46059830	-0.00078766
H	-2.63295618	-0.47852550	0.88514486
H	-2.63253622	-0.47854477	-0.88628723
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H	0.39721072	4.94265958	-0.88750367
H	0.39742460	4.94442633	0.88361156
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N	3.00321560	1.15854586	3.15915708
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N	-0.42434630	-1.15207401	3.13851370
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N	4.95660612	0.77792292	-3.40835453
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C	4.17181045	-4.64481366	-3.47078410
C	-3.35313570	3.06135393	-3.32304744
N	-1.92008354	3.24667596	-3.33821247
C	-1.22135292	4.43340129	-3.32236928
N	0.04691574	4.28118846	-3.33210883
C	0.22823037	2.91415292	-3.35455185
C	1.41252335	2.11907794	-3.37441833
O	2.57176834	2.46745710	-3.37575389
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H	5.86453822	1.17551056	-3.40553223
H	6.94708191	-1.01696513	-3.43576164
H	-1.73616326	5.37341461	-3.30510461
H	1.89318242	0.13572862	-3.40833405
H	-1.13721232	-1.50389383	-3.41343092
H	0.57808891	-1.69664897	-3.42524822

Model D (NORIND_R270)

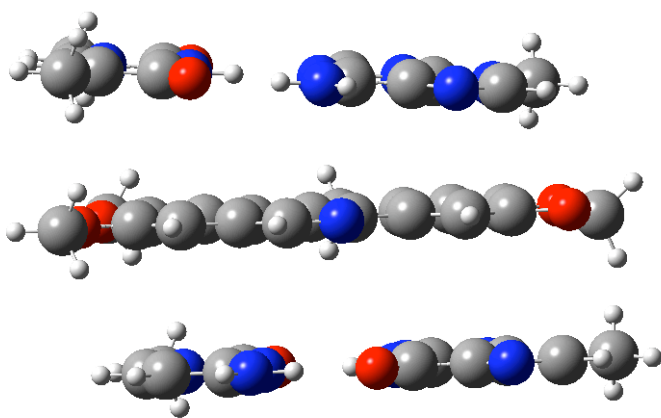


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C	0.01114868	2.43011260	-0.00036225
C	-0.68966535	1.16806725	-0.00026547
C	3.52138916	1.21780043	0.00014952
N	4.25120675	0.14277737	0.00015558
C	3.58929035	-1.02313955	0.00000780
C	2.22458666	-1.15677221	0.00016873
C	1.84248448	-2.61825285	0.00022484
C	3.19515378	-3.30225777	-0.00015368
C	4.20936858	-2.35513324	-0.00051657
C	5.56262229	-2.70596076	0.00124230
C	5.81436781	-4.04837572	0.00414130
C	4.80543611	-4.99823503	0.00506088

C	3.47673739	-4.66848096	0.00265979
O	5.36393295	-6.23637948	-0.00872523
C	6.74571204	-6.04988120	0.18681436
O	7.01638035	-4.68506936	-0.01220721
O	-2.02186246	1.27824563	-0.00035999
C	-2.81230967	0.12255291	-0.00059727
O	-0.78744076	3.50974944	-0.00054547
C	-0.21072456	4.78378298	-0.00177816
H	-0.51661817	-0.93922779	0.00003645
H	1.90272620	3.37226035	-0.00018294
H	4.04678790	2.15977620	0.00014976
H	1.25664169	-2.88765521	-0.87585116
H	1.25696117	-2.88740898	0.87658034
H	6.34297893	-1.96945024	-0.00157984
H	2.71146666	-5.42273263	0.00115562
H	7.29622554	-6.63890862	-0.53140043
H	7.01051353	-6.33178751	1.20106756
H	-3.83770706	0.46059830	-0.00078766
H	-2.63295618	-0.47852550	0.88514486
H	-2.63253622	-0.47854477	-0.88628723
H	-1.03062357	5.48639111	-0.00229662
H	0.39721072	4.94265958	-0.88750367
H	0.39742460	4.94442633	0.88361156
H	8.43218966	1.92488552	4.50204779
H	2.23322474	-6.25120831	3.92338605
H	8.50706038	3.47868996	3.66965061
H	8.52805570	1.97329015	2.75003067
H	2.32635581	-6.19900367	2.16641673
H	0.81791170	-6.66145421	2.95435332
C	8.12344484	2.46970036	3.62081701
N	6.66962262	2.52654404	3.54253199
C	5.99914576	1.33060644	3.46872545
O	6.57211935	0.27716118	3.46742804
N	4.63788628	1.43120120	3.39739342
C	3.89214983	2.58293066	3.39294132
O	2.68917344	2.54308490	3.32606603
C	4.66154589	3.82609621	3.47389224
C	3.91415585	5.12955007	3.47421427
C	5.98779281	3.72175167	3.54299714
C	1.68574720	-6.01922100	3.01952809
N	1.24484633	-4.64149191	3.03710987
C	-0.03971306	-4.16650978	2.98337856
N	-0.12926750	-2.88853339	3.01670086
C	1.18180633	-2.46621888	3.09842209
C	1.77085923	-1.19370741	3.16737291
N	1.05970064	-0.06703300	3.16352061
N	3.10107216	-1.13281280	3.23934404
C	3.80825302	-2.26218807	3.24316802
N	3.37005710	-3.49477756	3.18329782
C	2.04011563	-3.54032982	3.11185426
H	4.13428037	0.55379533	3.34288859
H	3.32350821	5.23572903	2.57098506
H	4.59936526	5.96752849	3.53774510
H	3.22867671	5.18113528	4.31277650
H	6.61198382	4.59323087	3.60437446
H	-0.87125582	-4.84038327	2.91953832
H	0.07083692	-0.11828082	3.10936708
H	1.51541703	0.82043625	3.21378554
H	4.87390501	-2.12723442	3.30337946
H	7.10869105	0.44098565	-2.63919374
H	-0.38455661	-6.82520756	-2.29035210
H	7.35084267	1.93516164	-3.54941204

H	7.07646870	0.40758624	-4.39250439
H	-0.29247838	-6.85150092	-4.04773940
H	-1.85508999	-7.00329900	-3.24647677
N	5.38794855	1.26221605	-3.50038627
C	4.89337396	2.52203863	-3.51564789
C	4.52367270	0.16928107	-3.46358873
O	5.00701298	-0.94179435	-3.45096619
N	3.19450950	0.39780511	-3.44350727
C	2.71198106	1.61932188	-3.45798779
N	1.39794707	1.77986000	-3.43696249
C	3.57825966	2.76965266	-3.49611467
C	6.82014867	0.99346267	-3.52171362
C	-0.88504744	-6.52693851	-3.20283090
N	-1.07042914	-5.09429406	-3.23992894
C	-2.25701079	-4.39524673	-3.22771028
N	-2.10483360	-3.12732000	-3.25890147
C	-0.73796699	-2.94656635	-3.29308701
C	0.05699161	-1.76285016	-3.33719551
O	-0.29136114	-0.60373312	-3.35499470
N	1.41696711	-2.07434163	-3.36065039
C	1.94778144	-3.32713336	-3.34470358
N	3.28155550	-3.40587984	-3.37361706
N	1.22934497	-4.41309922	-3.30432730
C	-0.09292583	-4.15907480	-3.28093922
H	5.61869441	3.31333472	-3.54410126
H	0.78909441	0.97838406	-3.40922148
H	1.00040704	2.68776956	-3.44627694
H	3.19266667	3.76940126	-3.50820341
H	-3.19690547	-4.90959093	-3.19607425
H	2.04009231	-1.28305520	-3.39165984
H	3.67957515	-4.31334746	-3.35842025
H	3.87229111	-2.59848512	-3.39916597

Model E (NORIND_FLIP)

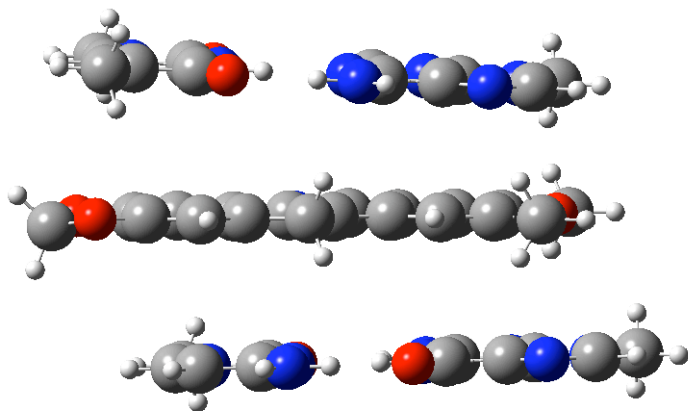


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C	1.36322937	2.44448399	-0.00018611
C	0.01114868	2.43011260	-0.00036225
C	-0.68966535	1.16806725	-0.00026547
C	3.52138916	1.21780043	0.00014952
N	4.25120675	0.14277737	0.00015558

C	3.58929035	-1.02313955	0.00000780
C	2.22458666	-1.15677221	0.00016873
C	1.84248448	-2.61825285	0.00022484
C	3.19515378	-3.30225777	-0.00015368
C	4.20936858	-2.35513324	-0.00051657
C	5.56262229	-2.70596076	0.00124230
C	5.81436781	-4.04837572	0.00414130
C	4.80543611	-4.99823503	0.00506088
C	3.47673739	-4.66848096	0.00265979
O	5.36393295	-6.23637948	-0.00872523
C	6.74571204	-6.04988120	0.18681436
O	7.01638035	-4.68506936	-0.01220721
O	-2.02186246	1.27824563	-0.00035999
C	-2.81230967	0.12255291	-0.00059727
O	-0.78744076	3.50974944	-0.00054547
C	-0.21072456	4.78378298	-0.00177816
H	-0.51661817	-0.93922779	0.00003645
H	1.90272620	3.37226035	-0.00018294
H	4.04678790	2.15977620	0.00014976
H	1.25664169	-2.88765521	-0.87585116
H	1.25696117	-2.88740898	0.87658034
H	6.34297893	-1.96945024	-0.00157984
H	2.71146666	-5.42273263	0.00115562
H	7.29622554	-6.63890862	-0.53140043
H	7.01051353	-6.33178751	1.20106756
H	-3.83770706	0.46059830	-0.00078766
H	-2.63295618	-0.47852550	0.88514486
H	-2.63253622	-0.47854477	-0.88628723
H	-1.03062357	5.48639111	-0.00229662
H	0.39721072	4.94265958	-0.88750367
H	0.39742460	4.94442633	0.88361156
H	-3.56136559	-0.27142466	-4.51500279
H	5.03193277	-5.85777139	-3.76920679
H	-4.15994939	1.18502539	-3.71923297
H	-3.67514360	-0.21687293	-2.76423840
H	4.91943549	-5.79866054	-2.01359004
H	6.49865474	-5.74302008	-2.79658357
C	-3.45835393	0.36629580	-3.64816054
N	-2.10945855	0.91256184	-3.57721388
C	-1.07482816	0.01537854	-3.47793922
O	-1.25841633	-1.16932764	-3.44940904
N	0.17219706	0.57139180	-3.41459649
C	0.48518610	1.90705455	-3.44040981
O	1.63066966	2.27736375	-3.37755545
C	-0.65847078	2.81510570	-3.54753573
C	-0.39514026	4.29398127	-3.58171184
C	-1.87128330	2.26743973	-3.60870727
C	5.46520055	-5.43328983	-2.87332542
N	5.41503822	-3.98842566	-2.92520384
C	6.46351887	-3.10644539	-2.88796065
N	6.11640034	-1.87445929	-2.95178088
C	4.74007763	-1.92172833	-3.03805920
C	3.75621043	-0.92487770	-3.13458448
N	4.04511710	0.37551925	-3.16022293
N	2.48387769	-1.31846319	-3.20251317
C	2.19962697	-2.62005768	-3.17679904
N	3.02805615	-3.63049883	-3.08967431
C	4.29495472	-3.22258083	-3.02263378
H	0.94227688	-0.08286974	-3.34145505
H	0.12124178	4.61467415	-2.68367660
H	-1.32280359	4.84960564	-3.66219938
H	0.23609397	4.55419084	-4.42406784

H	-2.75283443	2.87524279	-3.68808380
H	7.47350226	-3.45823486	-2.81165782
H	4.99296990	0.66249463	-3.10893368
H	3.31669793	1.0552452	-3.22953386
H	1.15125606	-2.85434162	-3.23580354
H	-1.84387632	-1.05214674	2.65379360
H	7.66425696	-5.36736325	2.44554706
H	-2.58009780	0.29354525	3.52945772
H	-1.80947254	-1.03128599	4.40725682
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H	9.10461395	-5.01582026	3.39956416
N	-0.50507813	0.32200353	3.48827376
C	-0.46504103	1.67482049	3.47174601
C	0.67763815	-0.41542772	3.47374726
O	0.59793530	-1.62442302	3.48935425
N	1.85162890	0.24796517	3.44281337
C	1.89326594	1.56065154	3.42645890
N	3.07597779	2.15494097	3.39624922
C	0.68927758	2.35144527	3.44096709
C	-1.76247292	-0.41400799	3.52182662
C	8.03088095	-4.89617611	3.34867639
N	7.72144256	-3.48463292	3.35121539
C	8.60230951	-2.42645574	3.31764513
N	8.03078956	-1.28403273	3.31954875
C	6.68304678	-1.57470870	3.35506992
C	5.53489110	-0.72827539	3.37451058
O	5.47129371	0.48046518	3.36353851
N	4.35990052	-1.48006288	3.41088510
C	4.28338022	-2.83851820	3.42666692
N	3.05443580	-3.36232432	3.46290186
N	5.32648558	-3.61872393	3.40896603
C	6.48539182	-2.93374151	3.37416831
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H	0.71457090	3.42266594	3.42785724
H	9.66080104	-2.59379706	3.29429209
H	3.50605318	-0.94517630	3.42578055
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Model F (NORIND_FLIP_R180)



Element

X

Y

Z

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C	1.36322937	2.44448399	-0.00018611
C	0.01114868	2.43011260	-0.00036225
C	-0.68966535	1.16806725	-0.00026547
C	3.52138916	1.21780043	0.00014952
N	4.25120675	0.14277737	0.00015558
C	3.58929035	-1.02313955	0.00000780
C	2.22458666	-1.15677221	0.00016873
C	1.84248448	-2.61825285	0.00022484
C	3.19515378	-3.30225777	-0.00015368
C	4.20936858	-2.35513324	-0.00051657
C	5.56262229	-2.70596076	0.00124230
C	5.81436781	-4.04837572	0.00414130
C	4.80543611	-4.99823503	0.00506088
C	3.47673739	-4.66848096	0.00265979
O	5.36393295	-6.23637948	-0.00872523
C	6.74571204	-6.04988120	0.18681436
O	7.01638035	-4.68506936	-0.01220721
O	-2.02186246	1.27824563	-0.00035999
C	-2.81230967	0.12255291	-0.00059727
O	-0.78744076	3.50974944	-0.00054547
C	-0.21072456	4.78378298	-0.00177816
H	-0.51661817	-0.93922779	0.00003645
H	1.90272620	3.37226035	-0.00018294
H	4.04678790	2.15977620	0.00014976
H	1.25664169	-2.88765521	-0.87585116
H	1.25696117	-2.88740898	0.87658034
H	6.34297893	-1.96945024	-0.00157984
H	2.71146666	-5.42273263	0.00115562
H	7.29622554	-6.63890862	-0.53140043
H	7.01051353	-6.33178751	1.20106756
H	-3.83770706	0.46059830	-0.00078766
H	-2.63295618	-0.47852550	0.88514486
H	-2.63253622	-0.47854477	-0.88628723
H	-1.03062357	5.48639111	-0.00229662
H	0.39721072	4.94265958	-0.88750367
H	0.39742460	4.94442633	0.88361156
H	8.92411732	-0.75358086	-4.44898223
H	0.32458035	4.84728843	-3.91310458
H	9.51478453	-2.19158820	-3.61468848
H	9.02088246	-0.76849489	-2.69640945
H	0.42002270	4.82791738	-2.15559057
H	-1.15152707	4.75440554	-2.95241899
C	8.81262234	-1.37153691	-3.56897460
N	7.46304132	-1.91620548	-3.49878909
C	6.42759469	-1.01711892	-3.42989061
O	6.61102789	0.16794957	-3.42639041
N	5.17995181	-1.57169312	-3.36609695
C	4.86708079	-2.90763222	-3.36472230
O	3.72100001	-3.27654985	-3.30463238
C	6.01162382	-3.81774956	-3.44016503
C	5.74847439	-5.29704861	-3.44342819
C	7.22503362	-3.27147514	-3.50193154
C	-0.11741045	4.44313263	-3.01209890
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N	-0.76820695	0.88336620	-3.01635111
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C	1.59354254	-0.06984711	-3.15470745
N	1.30475622	-1.37052313	-3.15372763

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C	1.05398802	2.22974101	-3.09999501
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H	5.12542125	-5.57631903	-4.28577142
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H	-2.12643208	2.46975643	-2.92527016
H	0.35641881	-1.65636947	-3.10516405
H	2.03373959	-2.05184187	-3.20056442
H	4.19956768	1.85712087	-3.27425221
H	7.13726893	0.18900901	2.68320174
H	-2.36800496	4.49729389	2.28530525
H	7.86471458	-1.13650645	3.59629316
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H	-2.30007183	4.55145073	4.04315393
H	-3.81759390	4.16726195	3.23300256
N	5.79018956	-1.16611621	3.53561525
C	5.75016555	-2.51896519	3.54931138
C	4.60775150	-0.42933176	3.49292343
O	4.68743246	0.77971587	3.48194600
N	3.43404330	-1.09338314	3.46560777
C	3.39242218	-2.40610806	3.47855363
N	2.20999388	-3.00105823	3.45031378
C	4.59612560	-3.19623941	3.52264104
C	7.04728045	-0.42939642	3.56471602
C	-2.74343058	4.04661576	3.19526013
N	-2.43418572	2.63552532	3.23273161
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N	-2.74345128	0.43473778	3.24784934
C	-1.39608508	0.72629152	3.28986823
C	-0.24826476	-0.11935880	3.33959547
O	-0.18469599	-1.32803126	3.35658597
N	0.92639951	0.63318873	3.37035999
C	1.00291149	1.99166189	3.35615145
N	2.23150349	2.51628919	3.39245718
N	-0.03988758	2.77115252	3.31068133
C	-1.19847627	2.08543041	3.28013812
H	6.69997391	-3.01877057	3.58259065
H	1.36636285	-2.45233026	3.41839022
H	2.14245935	-3.98989613	3.45826947
H	4.57084256	-4.26748523	3.53352606
H	-4.37299758	1.74341586	3.17714951
H	1.78000354	0.09887014	3.40563910
H	2.29967182	3.50487858	3.37859528
H	3.06009415	1.95587348	3.42211030

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