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Supporting Information

Two Perturbations for Geometry Optimization of Off-Lattice Bead Protein Models

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Supporting Information

Table S1. The global-minimum geometries of the SHH and IPS model proteins.

Figure S1. Stereographic views of the global-minimum configurations of the SHH model proteins.

Figure S2. Stereographic views of the global-minimum configurations of the IPS model proteins.

Figure S3. The principle moments of inertia of 200 low-lying configurations of S13, S20.1 – S20.6, S21, and S34. The I_A , I_B , and I_C values are shown in colors of black, red, and blue, respectively. For the S13 SHH model, only 93 low-lying configurations were obtained.

Figure S4. The bond angles of 200 low-lying configurations of S13, S20.1 – S20.6, S21, and S34. For the S13 SHH model, only 93 low-lying configurations were obtained.

Figure S5. The torsional angles of 200 low-lying configurations of S13, S20.1 – S20.6, S21, and S34. For the S13 SHH model, only 93 low-lying configurations were obtained.

Table S1. The global-minimum geometries of the SHH and IPP model proteins.

SHH model				IPS model		
S13						
bead	x	y	z	x	y	z
1A	0.12183	0.64539	-0.62949	0.65562	0.15123	-0.22764
2B	0.12183	1.64539	-0.62949	0.65562	1.15123	-0.22764
3B	0.12183	1.70989	0.36843	0.65562	0.73400	0.68116
4A	0.13111	0.72059	0.51400	-0.23165	0.74355	0.2200
5B	0.27856	0.17367	1.33810	-0.28926	0.56635	1.20250
6B	0.74768	-0.57706	0.87299	-0.86435	-0.03083	0.64335
7A	0.65030	-0.14443	-0.02330	0.11043	-0.25396	0.64430
8B	0.57231	-1.08480	-0.35439	-0.46380	-1.00703	0.32314
9A	0.08011	-0.43903	-0.93811	0.40870	-0.92980	-0.15933
10B	-0.61206	-1.15833	-0.99734	-0.35994	-1.15970	-0.75628
11B	-1.18184	-0.74129	-0.28922	0.22261	-0.41929	-1.09156
12A	-0.49545	-0.06929	-0.01122	-0.41388	-0.16536	-0.36327
13B	-0.53622	-0.68070	0.77904	-0.08573	0.61962	-0.88875
S20.1						
bead	x	y	z	x	y	z
1B	-0.05424	-2.15972	-0.04369	-0.77583	-1.46430	-0.61807
2A	-0.05424	-1.15972	-0.04369	-0.77583	-0.46430	-0.61807
3A	-0.05424	-0.16169	0.01909	-0.77583	-0.85804	0.30115
4A	0.14395	0.30739	0.87972	-1.08213	0.09358	0.27660
5A	-0.81947	0.36380	0.61773	-0.10548	-0.05936	0.12571
6A	-0.92345	0.40286	-0.37608	-0.46515	0.63728	-0.49504
7A	-0.07253	0.42884	-0.90073	0.22101	0.01799	-0.87669
8B	0.58623	0.13969	-1.59530	0.40044	0.99206	-1.01448
9A	0.33507	-0.59025	-0.95960	0.65651	0.66279	-0.10563
10A	-0.65503	-0.57272	-0.82036	0.12680	1.51093	-0.09682
11A	-1.06348	-0.60410	0.09188	0.53603	1.27420	0.78437
12A	-0.50471	-0.65535	0.91962	-0.35863	0.85836	0.62107
13B	0.08284	-1.11597	1.58492	-0.03425	0.75707	1.56156
14A	0.56957	-0.72152	0.80549	-0.36208	-0.09983	1.16376
15A	0.98807	-0.54848	-0.08609	0.57234	0.15748	0.91747
16B	1.63460	0.14970	-0.39358	0.35243	-0.80130	0.73751
17A	0.76374	0.53515	-0.08857	0.90834	-0.41197	0.00308
18A	-0.10465	1.00962	0.05557	0.16817	-1.00809	-0.30803
19B	-0.30082	1.98734	0.13033	0.86372	-0.84798	-1.00845
20B	-0.49719	2.96515	0.20331	-0.07059	-0.94660	-1.35100
S20.2						
bead	x	y	z	x	y	z
1B	0.54766	-2.00509	0.17050	0.53567	-1.34748	-0.46629
2A	0.54766	-1.00509	0.17050	0.53567	-0.34748	-0.46629
3A	0.54766	-0.33021	0.90843	0.53567	-0.77045	0.43985
4B	0.79435	0.30711	1.63848	1.42748	-0.49032	0.08458
5A	0.49069	0.76072	0.80061	0.90907	0.26189	0.49130
6A	0.99788	0.95557	-0.03891	1.25743	0.47542	-0.42141
7A	0.71863	0.54865	-0.90864	0.34558	0.84776	-0.24851
8A	-0.20214	0.19517	-1.07366	0.46102	0.52223	-1.18697
9B	-1.19018	0.32014	-1.16394	-0.36630	1.05915	-1.02186

10A	-0.89466	0.10881	-0.23228	-0.43980	0.09655	-0.76112
11B	-1.40024	0.62296	0.46057	-1.32411	0.56335	-0.77048
12A	-0.50088	0.31067	0.76658	-1.17962	-0.00713	0.03803
13A	-0.45970	-0.65333	0.50388	-0.74325	0.89242	0.05786
14B	-0.84129	-1.41461	-0.02038	-0.82516	0.46561	0.95848
15A	-0.27685	-0.79843	-0.56968	0.05568	0.92387	0.83968
16A	0.65161	-0.54751	-0.84356	0.12277	0.00906	1.23796
17A	1.18628	-0.13821	-0.10423	-0.12965	0.04294	0.27093
18A	0.20674	0.05376	-0.04388	-0.57888	-0.70212	0.76395
19A	-0.12452	0.98563	-0.19184	-0.43396	-0.86477	-0.21203
20B	-0.79871	1.72328	-0.22856	-0.16532	-1.63048	0.37236

S20.3

bead	x	y	z	x	y	z
1A	0.54756	-0.47608	-1.14737	-0.03989	-1.15688	0.04127
2A	0.54756	0.52392	-1.14737	-0.03989	-0.15688	0.04127
3A	0.54756	1.01314	-0.27521	-0.03989	-0.54102	0.96454
4A	0.53166	0.52085	0.59508	-0.55099	0.31042	0.84698
5B	0.23716	0.83906	1.49620	-1.05093	-0.40669	1.33259
6B	-0.70201	1.00947	1.19802	-1.57968	0.10934	0.65870
7A	-0.46489	0.82489	0.24423	-0.99023	-0.60346	0.27861
8A	-0.45202	0.87574	-0.75439	-0.99065	0.24818	-0.24553
9A	-0.45264	0.01419	-1.26206	-0.62129	-0.51188	-0.78022
10A	-0.45147	-0.83723	-0.73758	-0.10591	0.33454	-0.91422
11B	-0.14619	-1.73540	-0.42118	0.03798	-0.32374	-1.65311
12A	0.45148	-0.98516	-0.13846	0.87536	0.10978	-1.32017
13A	0.86051	-0.52490	0.64948	0.51222	-0.63253	-0.75705
14B	1.78882	-0.30842	0.34721	1.47839	-0.43709	-0.58877
15A	1.08404	0.01329	-0.28508	0.93809	-0.53377	0.24713
16A	0.08422	0.02883	-0.29626	0.85848	0.34824	-0.21734
17A	-0.26214	-0.34500	0.56414	0.58115	0.38038	0.74290
18B	-1.04321	-0.32467	1.18825	0.82924	1.27021	0.35995
19B	-1.69208	-0.13182	0.45219	0.01867	1.26834	0.94558
20A	-1.01394	0.00532	-0.26983	-0.12024	0.92451	0.01688

S20.4

bead	x	y	z	x	y	z
1A	0.40243	-0.40865	-1.02260	-0.81594	-0.26123	-0.40253
2A	0.40243	0.59135	-1.02260	-0.81594	0.73877	-0.40253
3A	0.40243	1.09770	-0.16027	-0.81594	0.37718	0.52981
4A	0.73228	0.81506	0.74046	-0.22161	1.17365	0.41839
5B	1.07104	0.18962	1.44335	-0.45327	0.94404	1.36370
6A	0.38973	-0.20365	0.82597	0.28826	0.38695	0.98982
7A	-0.52464	-0.54276	0.60478	-0.41371	-0.13880	1.47026
8B	-1.51771	-0.45611	0.68416	0.40494	-0.65936	1.22770
9A	-1.14339	-0.00456	-0.12577	-0.27921	-0.59491	0.50121
10B	-1.50097	-0.85491	-0.51183	0.40195	-1.29408	0.28399
11A	-0.50121	-0.84112	-0.49509	-0.40767	-1.30899	-0.30278
12A	0.37876	-0.92244	-0.02708	0.30217	-0.66061	-0.57799
13B	1.29033	-1.31393	0.09857	-0.39018	-0.79725	-1.28650
14B	1.79127	-0.45442	-0.00294	0.47631	-0.40325	-1.59305
15A	0.96678	0.09402	-0.14230	-0.13730	0.23809	-1.13243
16A	-0.03314	0.08404	-0.15044	0.81315	0.32437	-0.83378
17A	-0.40044	0.66335	0.57722	0.25593	1.12533	-0.61475
18B	-0.98063	1.42480	0.28813	0.86335	0.83588	0.12502
19A	-0.63435	0.92381	-0.50503	0.07831	0.24266	-0.05333
20A	-0.59099	0.11880	-1.09669	0.86640	-0.26843	0.28976

S20.5

bead	x	y	z	x	y	z
1B	-0.17056	-1.53652	0.65312	-0.81066	-1.05436	-0.15833
2A	-0.17056	-0.53652	0.65312	-0.81066	-0.05436	-0.15833
3A	-0.17056	0.33555	1.14250	-0.81066	-0.45279	0.75887
4B	0.34377	0.90501	1.78373	-1.15641	0.48512	0.73087
5B	0.59629	1.59921	1.10969	-0.53935	0.28335	1.49148
6A	0.06674	1.16563	0.38059	-0.12190	0.40556	0.59103
7A	-0.44888	0.36639	0.07181	0.29566	-0.33665	1.11522
8A	-0.93172	-0.47096	-0.18452	0.09862	-0.56771	0.16244
9B	-0.97296	-1.45098	-0.37911	0.99880	-0.97808	0.30827
10B	-0.29815	-2.18525	-0.45320	0.42125	-1.39568	-0.39319
11B	0.33488	-1.41344	-0.51301	0.82584	-0.52979	-0.68739
12A	0.17231	-0.43059	-0.42599	-0.14541	-0.60503	-0.91328
13B	-0.04630	-0.61087	-1.38500	0.29351	0.09261	-1.47953
14A	-0.53187	0.18733	-1.02848	-0.61596	0.36077	-1.16178
15B	-1.07518	0.96259	-1.35063	0.04097	1.11341	-1.11741
16A	-0.43061	1.22441	-0.63231	-0.47903	1.01437	-0.26900
17A	0.40126	0.67168	-0.58248	0.22395	0.32486	-0.44339
18B	1.33593	0.52182	-0.26007	0.58711	1.05849	0.13098
19A	0.64365	0.19392	0.38277	0.94227	0.14647	0.33612
20B	1.35252	0.50159	1.01748	0.76208	0.68943	1.15632

S20.6

bead	x	y	z	x	y	z
1A	-0.57451	-1.16656	0.01054	0.14482	-0.36869	-0.84044
2A	-0.57451	-0.16656	0.01054	0.14482	0.63131	-0.84044
3A	-0.57451	0.29654	0.89685	0.14482	0.19897	0.06127
4B	-0.47836	0.18768	1.88624	0.68423	1.04060	0.03492
5B	0.05184	-0.65564	1.79857	1.09063	0.26226	0.51350
6A	0.06080	-0.65025	0.79862	1.08535	0.14868	-0.48002
7B	0.96141	-1.04447	0.98161	1.69981	-0.49651	-0.02597
8B	1.27316	-0.98229	0.03348	1.11817	-0.90590	-0.72887
9A	0.37986	-0.66702	-0.28685	0.68381	-0.73534	0.15557
10B	0.92807	-0.25126	-1.01253	0.12848	-1.34631	-0.40863
11A	0.11559	0.28666	-0.78776	-0.39919	-0.73248	0.17855
12B	0.86186	0.94850	-0.85879	-0.87155	-0.92398	-0.68180
13B	1.29258	0.56579	-0.04146	-1.42426	-0.44958	0.00336
14A	0.38979	0.31856	0.31047	-0.78457	0.12743	-0.50443
15B	0.37662	1.31846	0.30641	-1.43940	0.68811	0.00236
16A	-0.47669	0.93365	-0.04542	-0.50977	1.05655	-0.00495
17B	-1.24694	1.29233	-0.57273	-0.96869	1.14715	0.87889
18A	-1.00590	0.36685	-0.86495	-0.74993	0.19497	0.66561
19B	-1.24300	-0.29232	-1.57857	0.03729	0.72498	0.98086
20A	-0.51718	-0.63869	-0.98425	0.18512	-0.26222	1.04067

S21

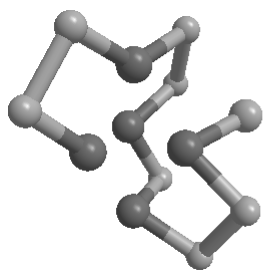
bead	x	y	z	x	y	z
1B	0.44609	-1.53606	0.59202	0.10510	-1.27159	0.05084
2A	0.44609	-0.53606	0.59202	0.10510	-0.27159	0.05084
3B	0.44609	-0.67019	1.58298	0.10510	-0.65646	0.97381
4A	-0.15556	0.08359	1.31870	-0.31568	0.24616	0.88316
5B	-0.37815	1.04187	1.49797	-0.85326	-0.50233	0.49487
6B	-0.28446	1.36117	0.55495	-1.35902	0.35318	0.60581

7A	0.03060	0.45787	0.26376	-0.75416	0.34957	-0.19051
8B	0.89830	0.93430	0.40551	-0.63450	1.15515	0.38977
9A	0.98896	0.11994	-0.16772	0.20952	0.81244	-0.02277
10B	1.43752	-0.37167	-0.91412	0.35210	1.16138	0.90346
11B	0.59972	-0.84953	-1.17822	1.18398	1.02100	0.36656
12A	0.03701	-0.45137	-0.45376	0.79064	0.18809	0.75583
13B	-0.28171	-1.39807	-0.50043	1.71919	0.06133	0.40692
14B	-0.83506	-1.38658	0.33244	1.08902	-0.68038	0.17727
15A	-0.67161	-0.40592	0.44013	1.01251	0.14094	-0.38805
16B	-1.50750	-0.38441	-0.10834	0.58526	-0.65718	-0.81288
17A	-0.83313	0.27720	-0.43619	0.05455	0.18065	-0.94090
18B	-1.06871	1.24742	-0.49262	-0.21576	-0.56562	-1.54919
19B	-0.15623	1.53190	-0.78665	-0.97273	-0.00183	-1.21883
20A	0.18676	0.59458	-0.84813	-0.65019	-0.70611	-0.58641
21B	0.65496	0.34006	-1.69430	-1.55678	-0.35680	-0.34960

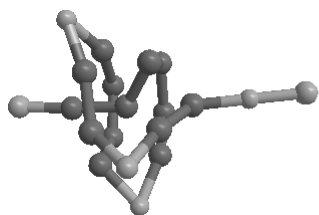
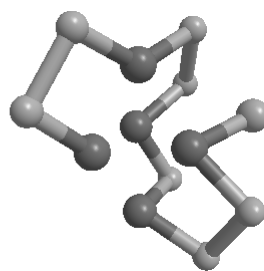
S34

bead	x	y	z	x	y	z
1A	0.25777	0.45073	-0.17745	0.31306	0.57255	0.02924
2B	0.25777	1.45073	-0.17745	0.31306	1.57255	0.02924
3B	0.25777	1.59281	0.81241	0.31306	1.13725	0.92953
4A	0.22863	0.60310	0.95245	-0.55809	1.09071	0.44071
5B	0.69210	0.49632	1.83211	-0.51877	0.57551	1.29688
6B	0.07843	-0.22066	2.16279	-1.35376	0.45789	0.75932
7A	-0.52138	-0.14714	1.36604	-0.53420	-0.00842	0.42631
8B	-1.32229	0.40000	1.12273	-1.03786	-0.45635	1.16502
9A	-0.69787	0.27323	0.35200	-0.17386	-0.89397	0.91604
10B	-0.94004	1.24327	0.33263	-0.15950	-0.38008	1.77377
11B	-0.95425	1.40956	-0.65335	0.70959	-0.78124	1.48438
12A	-0.68926	0.45230	-0.76926	0.42768	0.03829	0.98548
13B	-1.00841	0.47709	-1.71664	1.27578	-0.38939	0.67272
14B	-0.09283	0.33976	-2.09460	1.24750	0.60488	0.56965
15A	0.29963	0.06410	-1.21711	1.25306	0.08940	-0.28723
16B	-0.29257	-0.71261	-1.43163	1.19745	1.08122	-0.40214
17A	-0.25555	-0.52982	-0.44917	0.59357	0.58356	-1.02477
18B	-0.15285	-1.51798	-0.56309	0.50035	1.57884	-1.05169
19B	0.84203	-1.48341	-0.46807	-0.13442	1.08722	-1.64781
20A	0.86355	-0.48745	-0.38089	-0.37787	1.06983	-0.67806
21B	1.71830	-0.38948	-0.89061	-0.98403	0.54359	-1.27441
22A	1.24700	0.47985	-0.74176	-1.19900	0.45339	-0.30197
23B	1.50672	1.41239	-0.49093	-1.26238	-0.40578	-0.80972
24B	1.50466	1.21695	0.48979	-1.46654	-0.51391	0.16323
25A	1.17866	0.27604	0.39805	-0.61160	-0.94948	-0.11848
26B	1.62997	-0.11604	1.19966	-0.34672	-1.78751	0.35854
27B	0.85882	-0.74542	1.29564	0.28419	-1.52172	-0.37037
28A	0.25604	-0.43071	0.56242	0.69772	-1.42798	0.53528
29B	0.03777	-1.40062	0.67025	1.22460	-1.02201	-0.21143
30A	-0.77482	-0.83858	0.51599	0.39093	-0.52383	0.02692
31B	-1.13962	-1.71910	0.21331	0.62791	-0.52569	-0.94459
32B	-1.54659	-1.30371	-0.60022	-0.27594	-0.91616	-1.11949
33A	-1.35560	-0.35759	-0.33875	-0.27120	-0.02431	-0.66718
34B	-1.97168	-0.23793	-1.11729	-0.10376	-0.00884	-1.65294

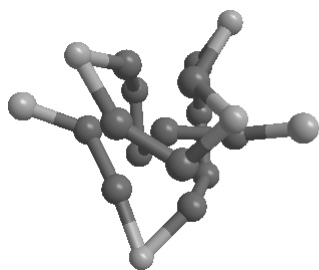
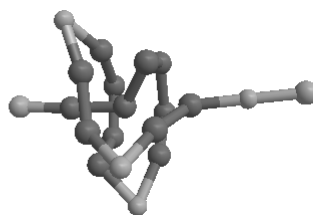
Figure S1. Stereographic views of the global-minimum configurations of the SHH model proteins.



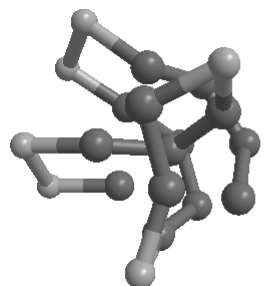
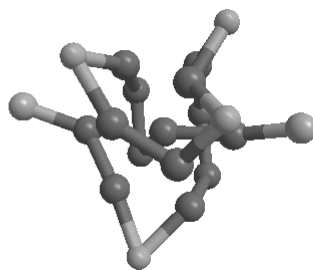
S13



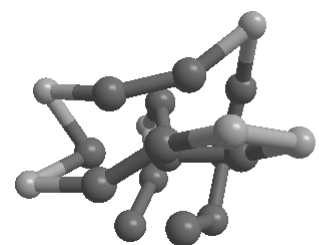
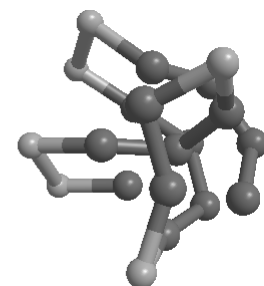
S20.1



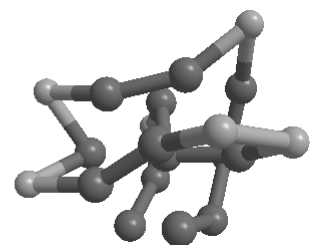
S20.2

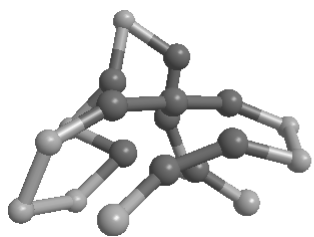


S20.3

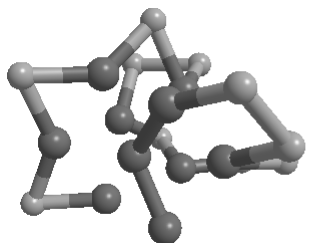
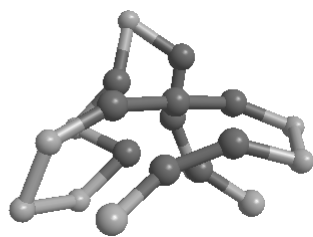


S20.4

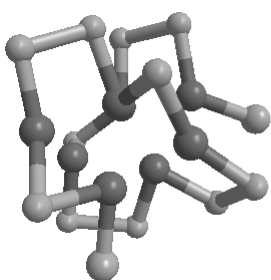
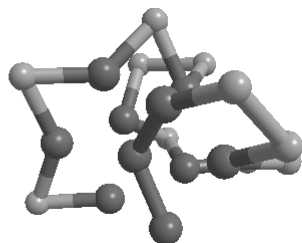




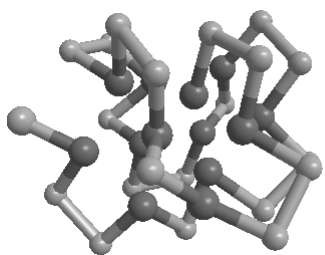
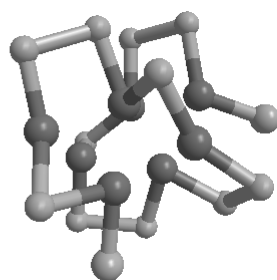
S20.5



S20.6



S21



S34

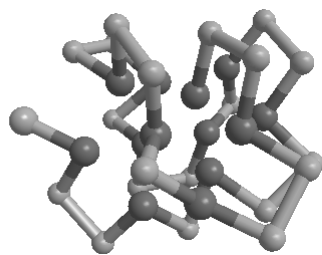
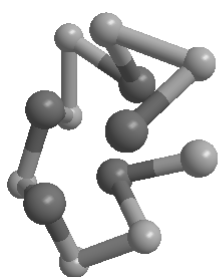
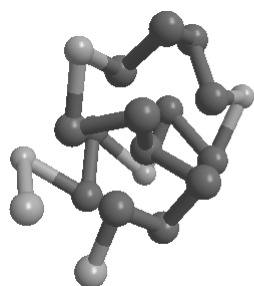
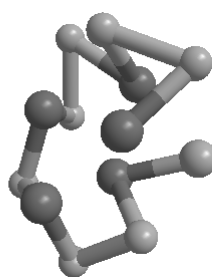


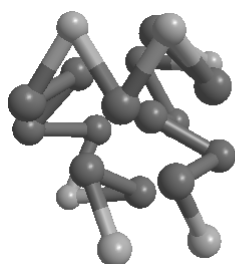
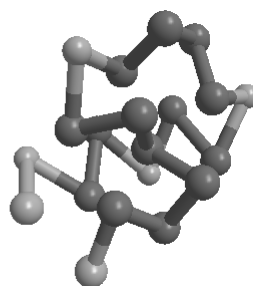
Figure S2. Stereographic views of the global-minimum configurations of the IPS model proteins.



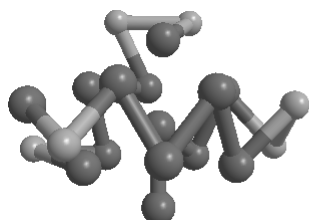
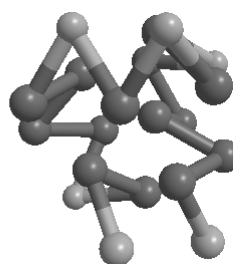
S13



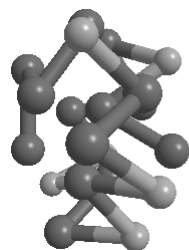
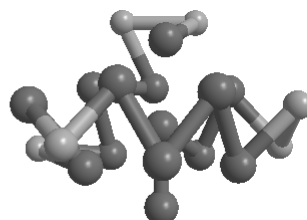
S20.1



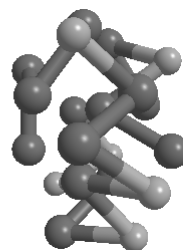
S20.2

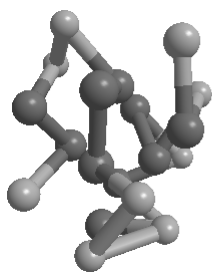


S20.3

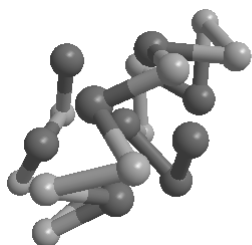
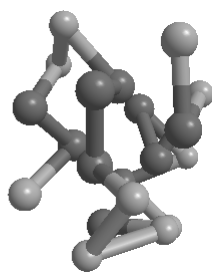


S20.4

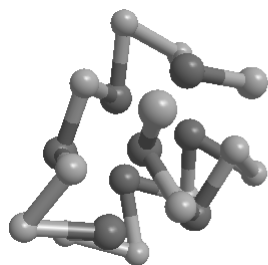
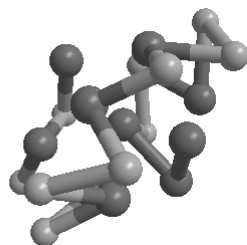




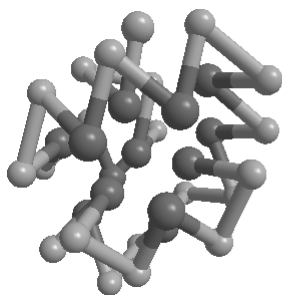
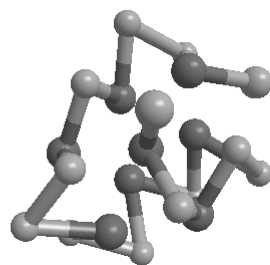
S20.5



S20.6



S21



S34

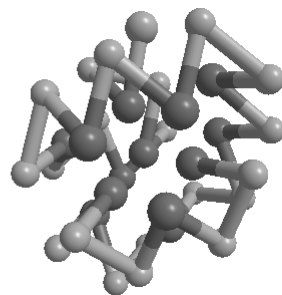
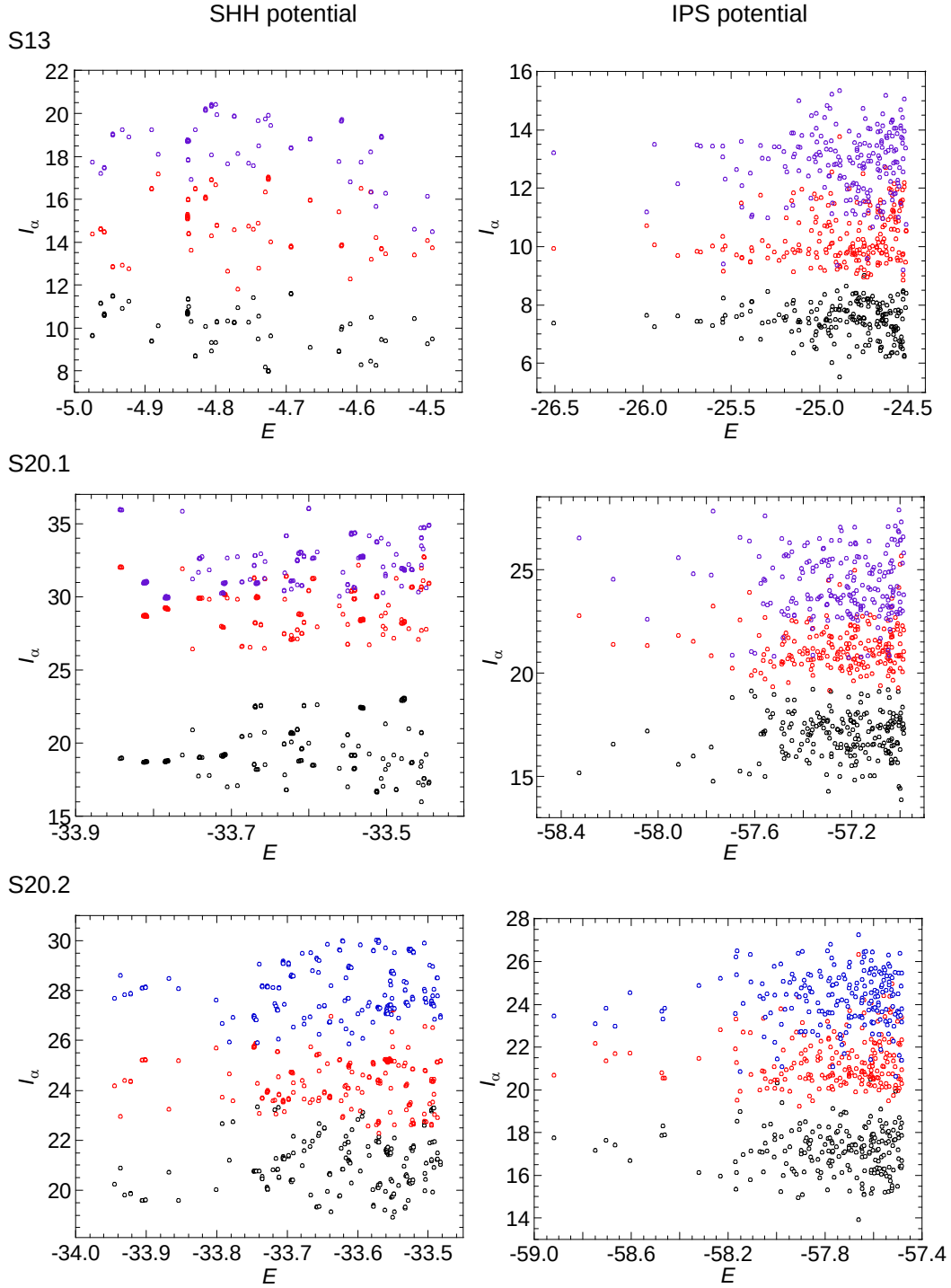
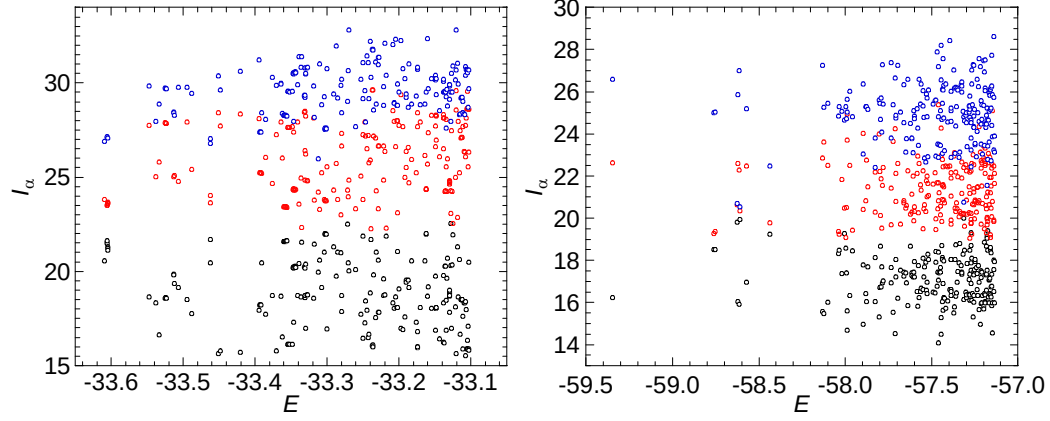


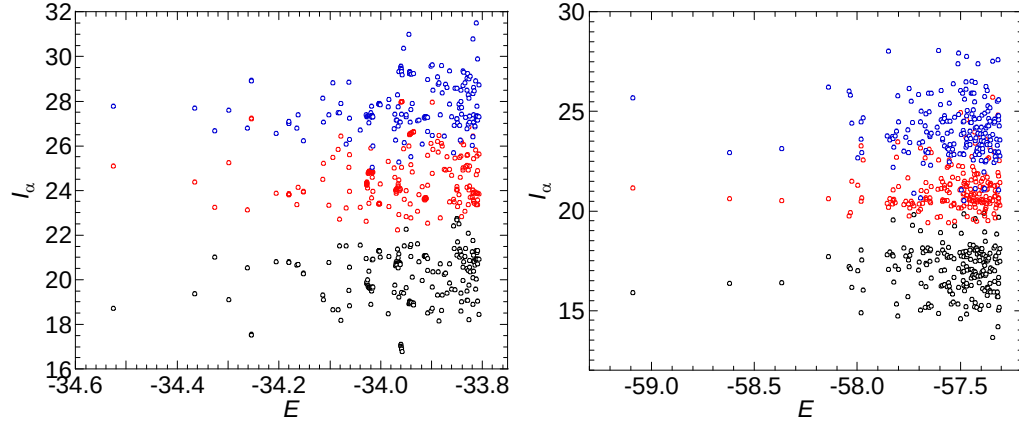
Figure S3. The principle moments of inertia of 200 low-lying configurations of S13, S20.1 – S20.6, S21, and S34. The I_A , I_B , and I_C values are shown in colors of black, red, and blue, respectively. For the S13 SHH model, only 93 low-lying configurations were obtained.



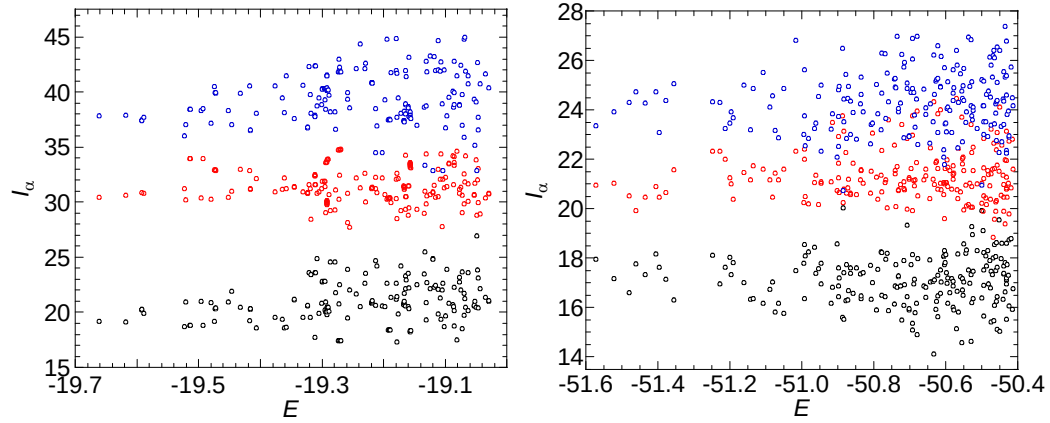
S20.3



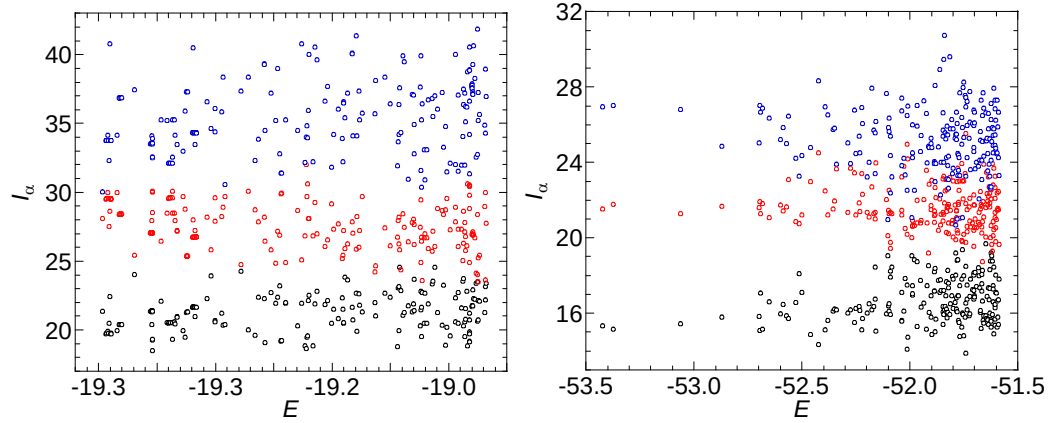
S20.4



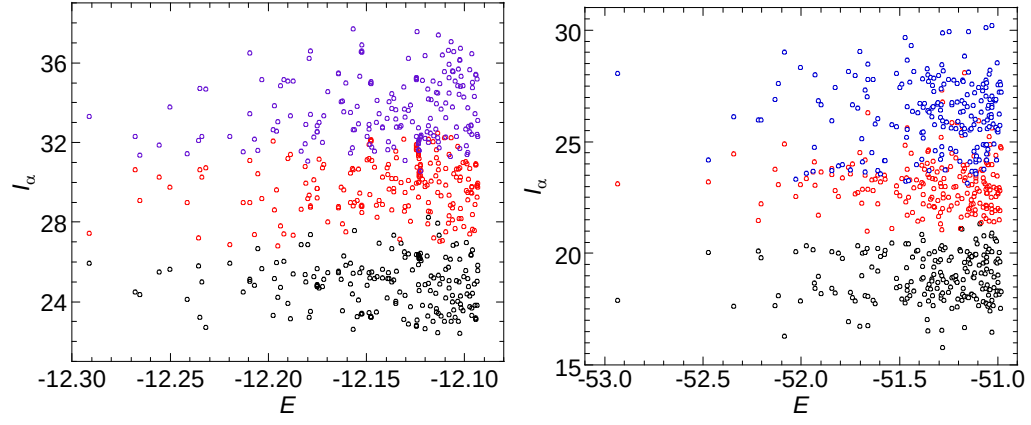
S20.5



S20.6



S21



S34

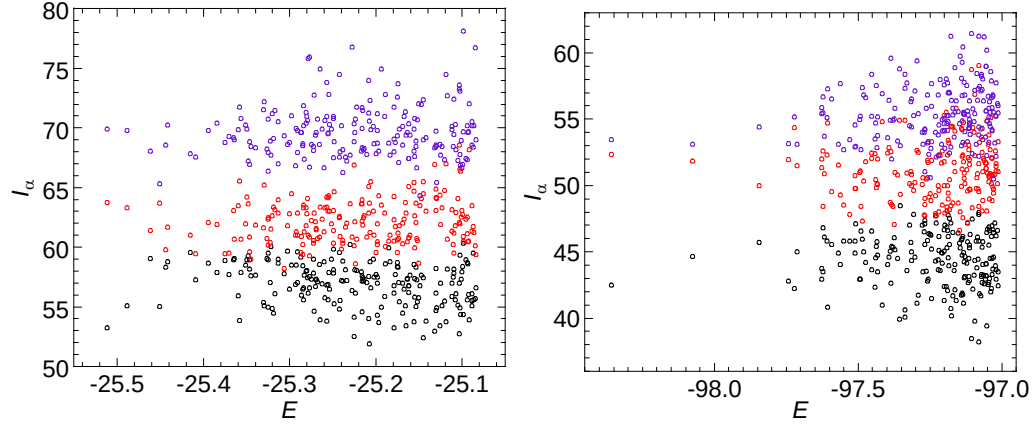
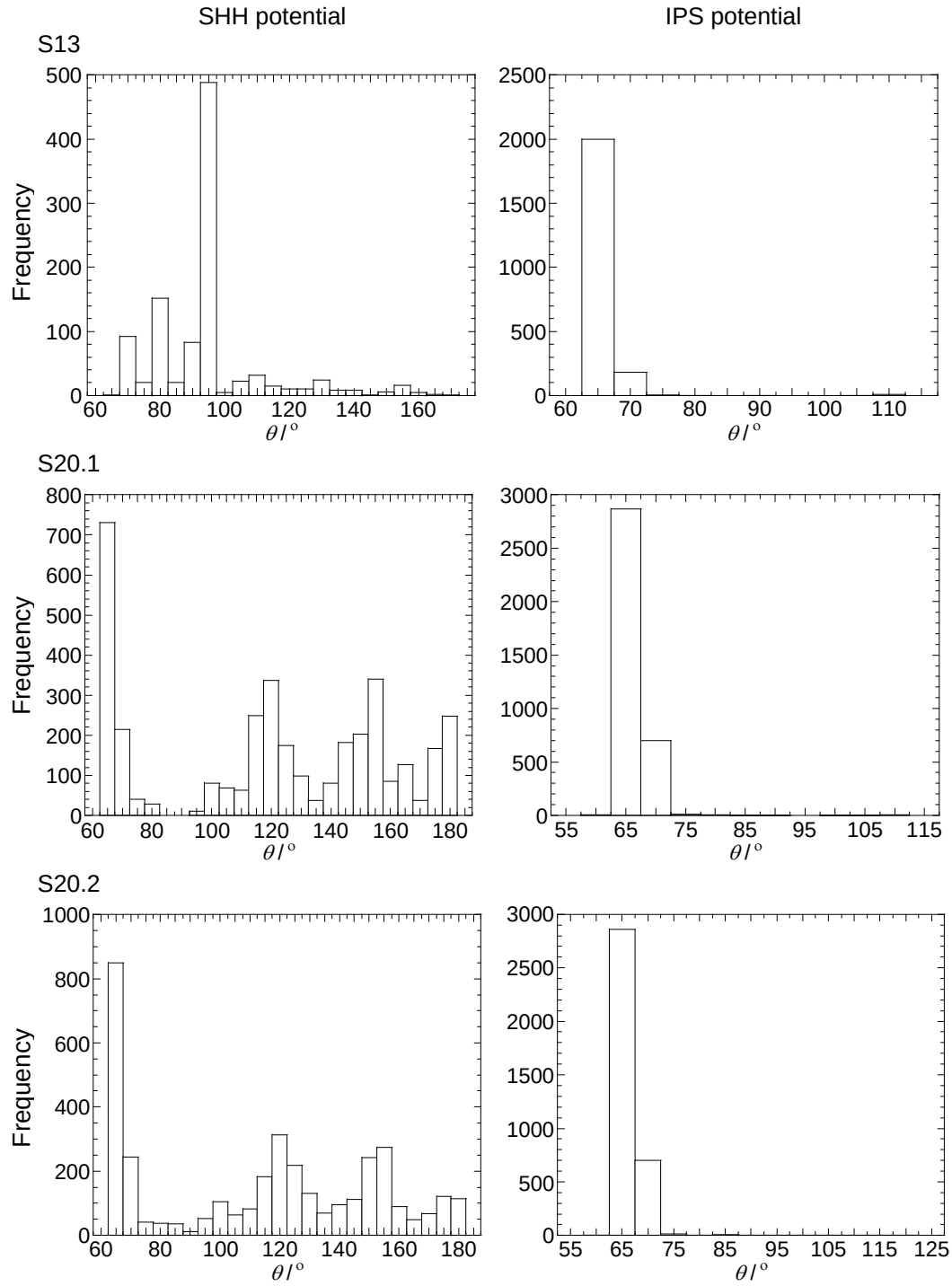
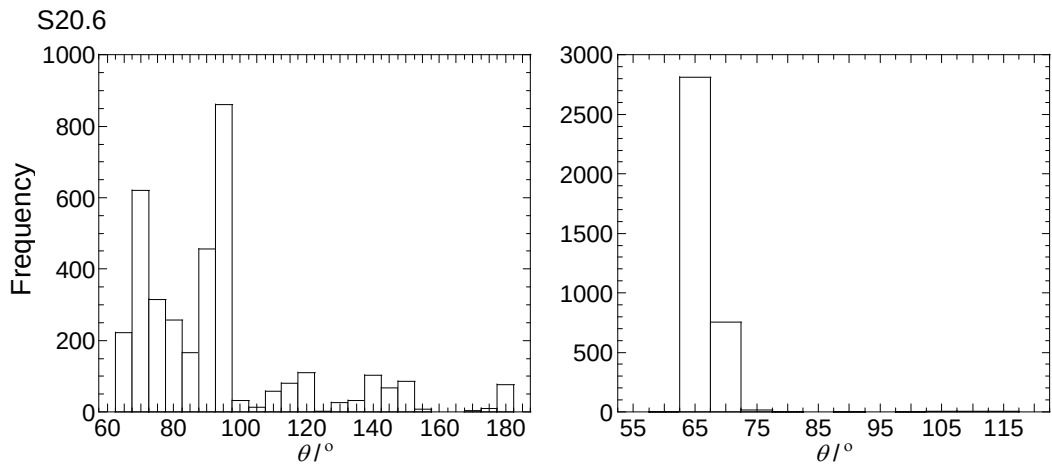
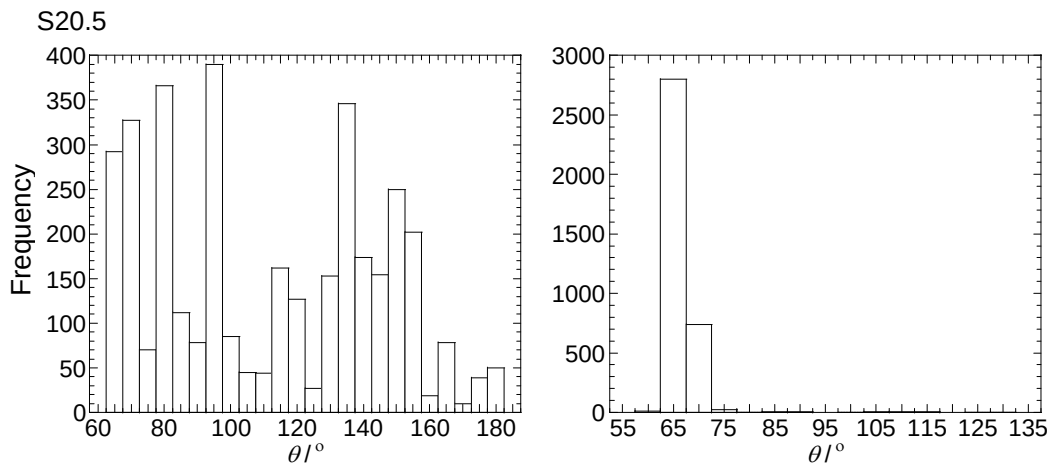
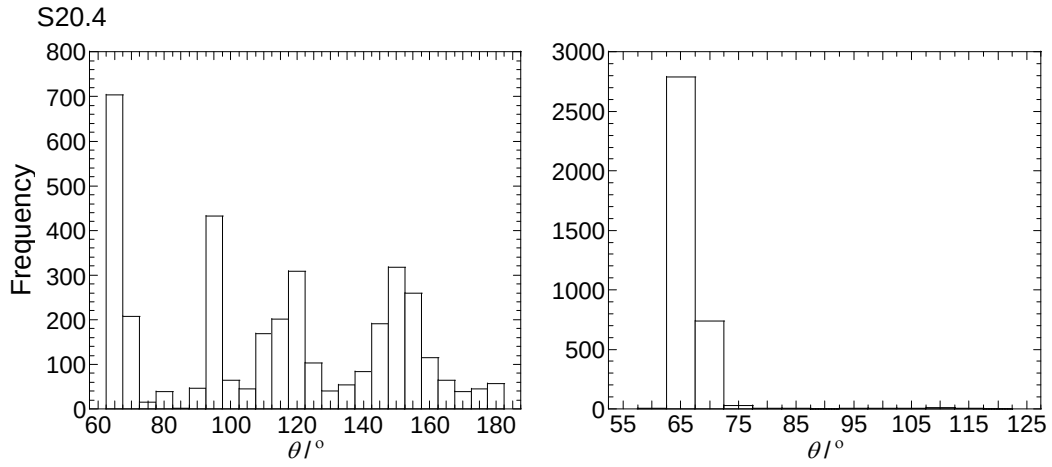
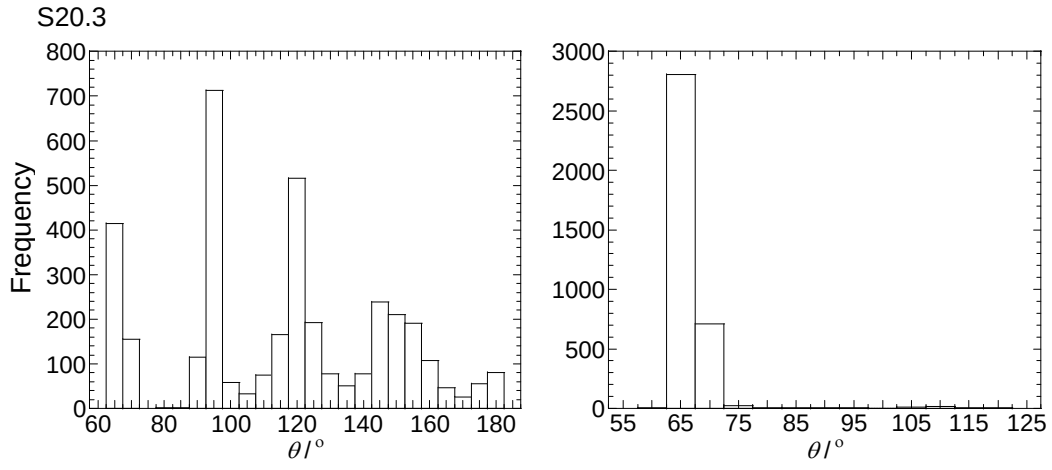


Figure S4. The bond angles of 200 low-lying configurations of S13, S20.1 – S20.6, S21, and S34.

For the S13 SHH model, only 93 low-lying configurations were obtained.





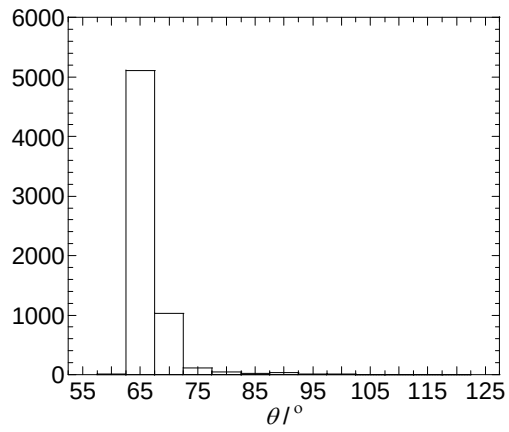
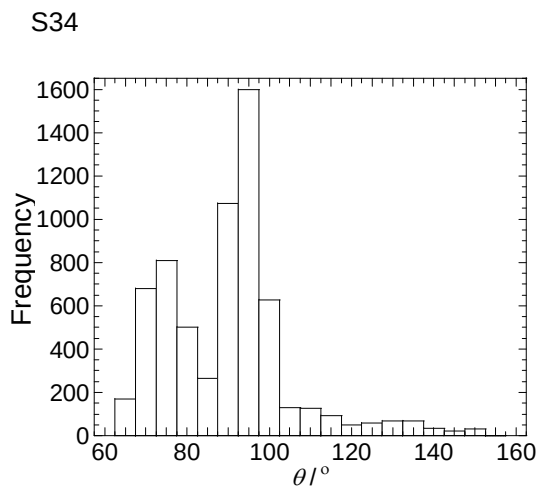
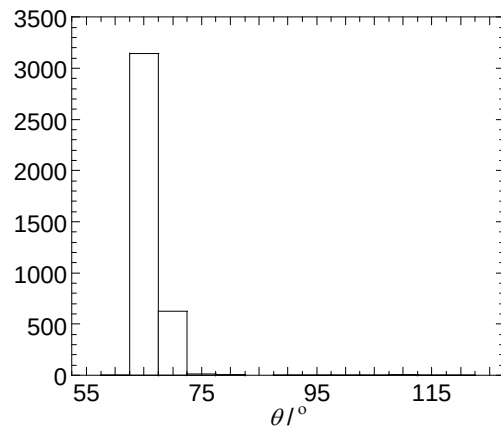
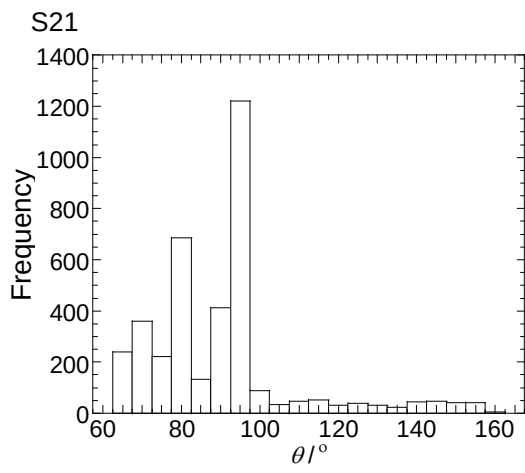


Figure S5. The torsional angles of 200 low-lying configurations of S13, S20.1 – S20.6, S21, and S34. For the S13 SHH model, only 93 low-lying configurations were obtained.

