Table S2: Parameters of the U_{rot} potentials for the 19 natural amino-acid residues with side chains [eqs. (3 – 7)].

Parameter[a]	Cys	Met	Phe	Ile	Leu	Val	Trp	Tyr	Ala
$a_{\circ}^{(11)}$	2.51605	0.24238	2.90528	2.54701	1.68074	2.85342	2.92162	2.84839	29.58180
$a_{1}^{(11)}$	1.51929	-3.86782	1.56340	-0.48056	2.20626	2.37246	0.68492	1.22045	5.30240
$a_{2}^{(11)}$	-0.54971	-2.51944	0.26070	-0.21517	-1.02049	0.34731	-0.59915	0.16459	-8.74785
$a_{3}^{(11)}$	-1.03116	-1.84006	-1.43661	0.83732	-4.44200	-1.68786	-1.78615	-1.41606	6.25203
$b_{11}^{(11)}$	1.14397	0.34635	1.03599	0.72954	1.74090	1.16716	1.27231	0.86491	53.43450
$b_{12}^{(11)}$	-0.75560	2.56072	1.07811	0.38901	-0.55626	1.45065	-1.44288	1.09154	0.06659
$b_{13}^{(11)}$	2.23496	-0.45695	0.32429	0.04543	0.35981	1.57411	0.99100	0.34693	15.72600
$b_{22}^{(11)}$	2.48856	0.10413	1.02414	0.04329	1.50504	2.01749	1.20764	0.95936	11.09290
$b_{23}^{(11)}$	1.28945	-1.20550	1.58252	-0.84954	1.45281	0.96613	0.17445	1.44025	68.83980
$b_{33}^{(11)}$	-1.09211	-0.23211	0.84045	1.77407	-1.44737	-0.32158	0.44667	1.02076	26.12760
$a_{\circ}^{(12}$	-2.97612	0.37399	-0.98359	-1.45127	-4.57678	-3.24356	-1.46551	-0.95541	-30.97710
$a_{1}^{(12)}$	-2.50713	0.80783	0.28431	1.33736	-4.97452	-1.33795	-0.60316	0.35288	-4.64674
$a_{2}^{(12)}$	1.07203	0.70786	-0.31229	0.61389	1.65854	1.40769	-0.22843	-0.37406	8.80411
$a_{3}^{(12)}$	-0.95678	-0.99396	-1.07451	-1.30001	2.95523	-0.43921	-0.70119	-0.93948	-27.39160
$b_{11}^{(12)}$	-2.53337	-1.43290	-0.65970	-1.11554	-3.05383	-0.48251	-1.34335	-0.77477	-15.91100
$b_{12}^{(12)}$	1.51301	4.67210	0.42843	0.05134	1.90392	1.50076	3.35213	0.83683	8.86996
$b_{13}^{(12)}$	-0.87081	-2.67538	-3.52701	0.18282	4.28999	-3.71279	-3.30484	-3.08056	-12.06390
$b_{22}^{(12)}$	-1.69125	2.58128	-0.82814	0.27950	-0.61735	-2.71987	-0.43142	-0.53621	-5.66423
$b_{23}^{(12)}$	2.24227	2.11275	-0.14242	0.10872	1.49912	0.80043	0.89213	-0.50661	-1.83919
$b_{33}^{(12)}$	1.26610	-0.79436	0.50052	-0.61536	-0.81608	-0.03510	0.31278	0.35279	-12.90520
$c_{111}^{(12)}$	-1.57099	0.40142	-0.77139	0.49608	-2.08039	-0.59011	-0.80766	-0.77676	-3.40765
$c_{112}^{(12)}$	0.65497	1.69693	0.23025	-0.15955	0.23693	0.01793	0.37317	0.37771	-8.09089
$c_{113}^{(12)}$	1.06364	-0.72304	-0.78212	0.46186	2.23788	0.06958	-0.56830	-0.47843	5.99944
$c_{122}^{(12)}$	0.99927	-1.08367	-0.22990	0.75453	-0.77260	-0.75257	-0.42677	-0.17175	3.45665
$c_{123}^{(12)}$	-0.77130	-0.74886	-0.81246	0.00510	-1.40331	-0.74686	-0.87304	-1.33337	3.76587
$c_{133}^{(12)}$	-1.95198	1.49514	1.28514	0.08683	-2.20789	0.00024	0.63318	1.30068	-4.69626
$c_{222}^{(12)}$	0.96461	-1.22510	-0.09761	0.57628	0.49668	0.50307	-0.14932	-0.21144	12.81400
$c_{223}^{(12)}$	-2.49265	-0.60438	-0.58735	-0.51684	-0.60065	-1.25613	-0.55909	-0.65089	-23.92370
$c_{233}^{(12)}$	-0.53516	0.23525	-0.44342	0.19720	0.92525	0.88722	-0.45376	-0.53901	4.08151
$c_{333}^{(12)}$	0.48288	0.32317	0.28904	-1.24512	1.35444	0.74959	0.43279	0.18420	-9.46834

Table S2 (continued)

Parameter[a]	Cys	Met	Phe	Ile	Leu	Val	Trp	Tyr	Ala
$a_{\circ}^{(21)}$	1.85391	2.22233	0.76666	1.30316	2.98901	2.34369	0.74505	0.51572	12.85830
$a_{1}^{(21)}$	4.00197	3.33934	2.29069	-0.11612	4.11687	1.16380	3.22668	1.82590	8.45145
$a_{2}^{(21)}$	-0.08291	4.42027	-0.13522	0.03627	0.11266	-0.91008	0.57315	0.32891	-3.33216
$a_{3}^{(21)}$	0.82622	0.22970	-1.64952	-0.29714	-0.15936	-0.26674	-0.37484	-1.27062	6.67105
$b_{11}^{(21)}$	1.63209	-0.05991	0.53475	0.13112	0.67354	-0.56330	0.58434	0.34630	-15.86380
$b_{12}^{(21)}$	1.66771	2.34128	-0.35950	-0.42590	0.06041	-2.12425	0.67411	-0.22214	3.57087
$b_{13}^{(21)}$	-1.17122	-0.05072	-1.82356	0.19600	-3.33410	0.94504	-1.03151	-1.59346	8.87391
$b_{22}^{(21)}$	0.59394	2.54336	0.16334	1.05762	0.58645	1.76547	0.37478	0.32713	1.45649
$b_{23}^{(21)}$	-1.59910	-0.04292	-1.49499	0.18953	-2.00441	-3.05306	-0.39062	-1.40575	-17.55400
$b_{33}^{(21)}$	-0.36420	-0.29365	0.06328	0.11423	1.86576	1.15000	-0.20799	-0.16174	-0.41096
$a_{\circ}^{(22)}$	-2.29314	-0.53638	-0.80558	-1.07133	0.90740	-1.30236	-0.98651	-0.96498	-3.64673
$a_{1}^{(22)}$	-2.33545	1.07886	0.38410	1.01727	2.73626	-0.13382	0.62130	0.29009	-6.89021
$a_{2}^{(22)}$	-0.85889	-2.00329	-0.63636	-0.71490	-0.04225	-0.07089	-1.48210	-0.84620	-3.78829
$a_{3}^{(22)}$	-0.11627	-0.71328	-0.32117	-0.95675	-2.76198	-1.01247	-0.08079	-0.29735	-15.39710
$b_{11}^{(22)}$	-1.42793	0.49897	0.53480	-0.56566	2.25406	-0.25572	1.28514	0.40053	-7.14512
$b_{12}^{(22)}$	-1.44750	-3.53547	-0.80036	0.10767	-0.36860	0.26602	-0.97289	-0.61502	-11.87840
$b_{13}^{(22)}$	-0.41698	-1.84322	-2.04254	0.41614	-6.67784	-2.40662	-2.51630	-1.62189	-4.67815
$b_{22}^{(22)}$	-1.83497	-2.26615	-1.27849	-0.09355	-2.65542	-1.58579	-1.99115	-1.36734	7.97568
$b_{23}^{(22)}$	0.12752	1.42433	-0.24445	-0.57723	0.29198	1.52721	0.72171	-0.52979	-9.34330
$b_{33}^{(22)}$	0.97526	1.21319	-0.06493	-0.41220	1.39461	0.54573	-0.27678	-0.00013	-4.48287
$c_{111}^{(22)}$	-0.66321	-0.12624	-0.00275	0.15054	0.69796	-0.05921	0.47016	-0.06604	-2.33245
$c_{112}^{(22)}$	-0.06051	-0.49249	-0.47087	0.58543	-0.21442	0.25242	-1.38931	-0.38697	-3.22406
$c_{113}^{(22)}$	0.18036	-0.68689	-0.69215	0.39512	-3.29798	1.11247	-1.26028	-0.33307	8.45463
$c_{122}^{(22)}$	-1.10955	0.54346	-0.10285	0.36485	-0.68506	-0.29992	0.33546	0.01666	4.18947
$c_{123}^{(22)}$	-1.49843	1.44878	-0.39010	0.44526	-0.64285	-0.75652	-0.21826	-0.89689	-12.60820
$c_{133}^{(22)}$	-0.57131	0.66636	0.49036	0.50192	2.65406	0.22056	-0.18350	0.33950	-8.74235
$c_{222}^{(22)}$	-1.10140	-0.88704	-0.44502	-1.24249	-0.30655	0.07843	-0.42059	-0.79789	0.68796
$c_{223}^{(22)}$	-0.45620	0.23718	-0.11008	-0.65370	0.58505	-1.66867	0.72953	-0.42948	-19.72450
$c_{233}^{(22)}$	0.31459	-0.61965	0.28001	-0.05777	0.47625	-0.40138	0.32703	0.33894	-1.24989
$c_{333}^{(22)}$	0.16230	-0.27415	0.47784	-0.69824	0.00251	-0.45302	0.45498	0.46230	-4.13017
δ_{SC}	-0.19556	-0.00162	-0.41176	-0.36268	-0.22455	-0.41107	-0.36494	-0.39024	0.64333
$\delta_{p/2}$	-1.68224	-1.65596	-1.54820	-1.51860	-1.77870	-1.56962	-1.52335	-1.52480	-1.81715
μ_1	0.76713	5.11995	2.44359	2.52545	1.64352	1.49311	2.59134	2.79377	-2.05943
ϵ_1	6.28606	3.85081	3.91767	0.37440	8.32135	5.92220	3.99292	3.08775	10.86680
μ_2	4.99908	6.77231	3.42588	0.68294	8.66213	4.60954	3.50082	2.54354	1.83275
ϵ_2	4.99908	6.77231	3.42588	0.68294	8.66213	4.60954	3.50082	2.54354	1.83275

Table S2 (continued)

Parameter[a]	Thr	Ser	Glu	Asn	Glu	Asp	His	Arg	Lys	Pro
$a_{\circ}^{(11)}$	2.55287	3.26126	0.07053	2.88716	0.07053	3.39310	2.77184	15.63500	3.62920	4.18167
$a_{1}^{(11)}$	0.90868	2.37232	0.91388	1.50551	0.91388	1.53049	1.87142	15.48010	8.35476	0.81843
$a_{2}^{(11)}$	0.01369	-0.44189	0.97020	-0.88066	0.97020	-0.05620	0.64267	6.64887	-5.31665	1.55799
$a_{3}^{(11)}$	-1.91202	-7.14453	-1.41886	-1.80205	-1.41886	-1.82937	-1.62198	-18.86740	-6.44225	-2.59002
$b_{11}^{(11)}$	0.37403	1.44098	1.51923	1.31805	1.51923	0.14130	1.04056	8.11272	3.02912	3.17138
$b_{12}^{(11)}$	-0.00240	-0.94414	3.40886	0.40659	3.40886	1.94797	1.25505	0.56312	-1.23219	-3.04270
$b_{13}^{(11)}$	1.31457	-0.88391	-1.14177	-0.45076	-1.14177	-2.25684	0.15679	-5.93336	-4.59845	2.33064
$b_{22}^{(11)}$	2.53485	0.89289	2.36347	0.85385	2.36347	0.77178	0.85806	1.09187	-0.25350	2.03620
$b_{23}^{(11)}$	-0.33966	3.26712	-1.99853	1.91844	-1.99853	2.41802	2.11391	-1.13515	-0.18886	3.50246
$b_{33}^{(11)}$	-0.35824	0.96724	1.08195	0.72865	1.08195	2.51779	0.86464	6.42884	1.09574	-0.97218
$a_{\circ}^{(12}$	-2.46803	-4.50080	-5.89011	-1.49598	-5.89011	-2.16585	-0.94982	-11.55860	-4.35997	-2.66321
$a_{1}^{(12)}$	-0.62824	-4.68083	-3.46734	-1.30591	-3.46734	-2.02103	0.20262	-9.16484	-5.66128	0.06148
$a_{2}^{(12)}$	1.98221	1.27161	3.12824	-0.00677	3.12824	0.46515	-0.10823	0.61553	2.92707	0.33887
$a_{3}^{(12)}$	0.35334	4.06269	1.89145	-1.01811	1.89145	0.84916	-1.11941	6.20954	3.79064	-1.11172
$b_{11}^{(12)}$	-0.37257	-2.10063	-0.75110	-1.19671	-0.75110	-1.40864	-0.29454	-4.68229	-4.59566	0.40780
$b_{12}^{(12)}$	4.08459	2.31885	3.94559	1.71815	3.94559	0.95065	0.55860	1.52429	2.53264	4.21901
$b_{13}^{(12)}$	-2.59886	5.04789	0.94398	-2.75109	0.94398	0.20363	-3.53876	4.97614	4.92293	-1.23265
$b_{22}^{(12)}$	-1.19146	-0.62060	-2.94859	-0.15280	-2.94859	-0.39684	-1.02980	-5.90920	2.10474	-2.28572
$b_{23}^{(12)}$	0.79401	0.77214	-0.88537	0.78440	-0.88537	-1.75878	0.03928	3.75096	0.44858	0.59509
$b_{33}^{(12)}$	-0.90882	-1.75134	1.29956	-0.13532	1.29956	-0.33277	0.36798	-0.91317	-1.68990	-0.74839
$c_{111}^{(12)}$	-0.44769	-1.67604	-1.28646	-0.58219	-1.28646	-1.00296	-0.56938	-2.57727	-2.29753	3.79494
$c_{112}^{(12)}$	0.70640	0.48164	2.27490	0.32072	2.27490	0.66581	0.28859	0.11315	1.92750	2.04775
$c_{113}^{(12)}$	0.57096	1.90555	1.06656	-0.91559	1.06656	-0.03615	-1.03814	0.84095	1.40007	-2.32625
$c_{122}^{(12)}$	-0.35977	-1.05550	-4.81025	-0.71562	-4.81025	-0.82336	-0.43962	-5.17365	-1.44721	-1.78620
$c_{123}^{(12)}$	-0.39156	-0.88415	-0.13345	0.14400	-0.13345	0.18751	-0.82740	0.25605	-1.51484	-0.41458
$c_{133}^{(12)}$	0.18149	-1.97281	-0.81524	-0.01391	-0.81524	-0.21213	1.21229	-1.25096	-1.96904	-1.95941
$c_{222}^{(12)}$	-0.55837	0.54882	1.37992	-0.09276	1.37992	0.17417	-0.03773	1.53839	0.33237	-1.49282
$c_{223}^{(12)}$	-0.90860	0.34776	2.48768	-0.78605	2.48768	0.31436	-0.66097	3.72847	0.98455	0.26237
$c_{233}^{(12)}$	1.82731	0.26330	0.82556	-0.23028	0.82556	-0.37133	-0.35719	-1.05335	0.61891	-0.22548
$c_{333}^{(12)}$	0.68690	1.82858	0.83578	0.68966	0.83578	0.58700	0.57198	1.62187	1.57661	0.98520

Table S2 (continued)

Parameter[a]	Thr	Ser	Glu	Asn	Glu	Asp	His	Arg	Lys	Pro
$a_{\circ}^{(21)}$	1.18283	2.45418	2.03556	1.06731	2.03556	0.64177	0.96761	-3.09179	3.90223	3.10880
$a_{1}^{(21)}$	0.57114	5.86142	2.80228	3.57589	2.80228	3.38578	2.53596	0.25389	1.63827	0.72726
$a_{2}^{(21)}$	-2.28123	-1.77056	1.98615	0.26015	1.98615	-1.08596	-0.25597	-13.73370	5.39342	1.38087
$a_{3}^{(21)}$	-0.36287	0.28207	-1.29632	-0.52327	-1.29632	-1.75134	-1.68776	7.57893	-0.49815	0.38206
$b_{11}^{(21)}$	-0.51317	1.15369	1.86006	1.16675	1.86006	1.66685	0.74041	0.67034	1.25533	1.95345
$b_{12}^{(21)}$	-3.80774	-1.03712	0.03090	-0.84489	0.03090	-1.95688	-0.57688	-5.31761	-1.55655	-2.86474
$b_{13}^{(21)}$	0.83421	-5.38116	-0.04977	-0.88700	-0.04977	-0.95367	-2.17105	-3.28938	-2.35832	0.67255
$b_{22}^{(21)}$	-0.30925	0.32411	2.80632	0.11518	2.80632	0.08257	0.09704	-1.72308	3.18032	0.24888
$b_{23}^{(21)}$	-1.65137	-3.28773	-0.31975	-1.51085	-0.31975	-0.13096	-2.28168	6.42583	0.51629	-4.20944
$b_{33}^{(21)}$	2.00847	1.00011	0.93087	-0.20298	0.93087	-1.06729	0.12051	-1.99999	-0.26797	0.96227
$a_{\circ}^{(22)}$	-1.07983	-0.71722	-1.84705	-0.09531	-1.84705	0.27987	-0.63784	-4.81969	-3.39112	-2.54078
$a_{1}^{(22)}$	-0.14879	0.05863	0.64224	0.06653	0.64224	1.09148	-0.02765	-4.63146	-2.58127	0.60753
$a_{2}^{(22)}$	-0.23855	1.74885	-1.74023	0.32779	-1.74023	0.59705	-0.51097	0.26779	-2.37086	-2.70560
$a_{3}^{(22)}$	0.16830	-0.54907	-1.12783	-1.94687	-1.12783	-1.80929	-0.72192	3.15499	2.16189	-0.47233
$b_{11}^{(22)}$	0.44911	0.23395	1.30221	-0.96199	1.30221	0.56147	-0.31507	-2.48197	-1.26464	-0.26071
$b_{12}^{(22)}$	0.49441	2.58216	-1.16250	1.06916	-1.16250	0.66385	-0.42922	-3.99992	-2.24975	0.97797
$b_{13}^{(22)}$	-0.54404	-2.78644	-2.46571	-3.38919	-2.46571	-4.02824	-2.23032	3.12405	1.93211	-2.37238
$b_{22}^{(22)}$	-1.44560	-1.67587	-2.24561	-1.13909	-2.24561	-1.58277	-1.22222	-0.00579	-1.93422	-1.01987
$b_{23}^{(22)}$	2.77195	-1.61105	0.82103	-0.48021	0.82103	-1.13178	0.03856	-1.86804	2.81856	1.60970
$b_{33}^{(22)}$	-0.07806	0.74367	2.24622	2.01119	2.24622	1.32756	0.89348	-2.41691	-0.01696	-1.22064
$c_{111}^{(22)}$	0.66255	-0.41824	-0.61816	-0.90092	-0.61816	-0.09999	-0.66707	0.11227	-1.07566	-0.77697
$c_{112}^{(22)}$	-0.64122	0.65321	0.39804	0.14621	0.39804	0.29905	-0.38466	-2.24747	-2.52235	-2.49677
$c_{113}^{(22)}$	1.14290	-1.61491	-0.88037	-0.93095	-0.88037	-1.89548	-0.80518	0.41547	-0.16033	-1.36443
$c_{122}^{(22)}$	-0.50283	-1.12235	-2.03925	-0.77292	-2.03925	-0.92772	-0.58424	-3.66036	-0.72945	3.47331
$c_{123}^{(22)}$	0.46713	-2.09200	-1.65231	-0.93245	-1.65231	0.02649	-0.56838	3.54113	3.31827	-0.82091
$c_{133}^{(22)}$	-0.30993	1.58161	0.04404	1.73650	0.04404	2.10156	1.22564	-0.91846	-0.85573	-2.09985
$c_{222}^{(22)}$	0.58124	0.21464	-1.40075	0.02157	-1.40075	0.15569	-0.32201	1.34760	0.43378	0.53099
$c_{223}^{(22)}$	-0.25375	0.77935	1.38994	-0.25950	1.38994	0.43133	0.10432	0.89250	1.57209	-0.20975
$c_{233}^{(22)}$	-0.18210	0.90712	-0.50057	0.16249	-0.50057	0.14443	0.19677	1.15695	-0.30160	-0.74945
$c_{333}^{(22)}$	-0.71635	0.29981	0.04551	-0.75426	0.04551	-0.32917	-0.02633	1.78041	0.86334	1.13745
δ_{SC}	-0.43556	-0.31913	-0.44702	-0.43141	-0.44702	-0.46898	-0.40446	0.20926	-0.58555	-0.32748
$\delta_{p/2}$	-1.53686	-1.76088	-1.22419	-1.57343	-1.22419	-1.61967	-1.58591	0.05262	-1.11281	-1.71415
μ_1	0.65792	3.27728	9.87103	1.70268	9.87103	0.67495	2.50496	16.45130	6.15379	2.05306
ϵ_1	5.46858	10.25320	1.15581	4.38423	1.15581	5.38965	4.24201	29.57570	15.33200	6.34873
μ_2	4.34855	8.11291	5.54108	5.55750	5.54108	6.09192	4.34401	16.78170	10.15870	5.23230
ϵ_2	4.34855	8.11291	5.54108	5.55750	5.54108	6.09192	4.34401	16.78170	10.15870	5.23230

[a] $a_{\circ}^{(11)} - c_{333}^{(22)}$ are expressed in kcal/mol, δ_{SC} and $\delta_{p/2}$ in Å, μ_1 and μ_2 in kcal/(mol×Å), and ϵ_1 and ϵ_2 in kcal/(mol×Å^6).