JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 49 (2016)

Supporting information for article:

Accurate optimization of amino acid form factors for computing small-angle X-ray scattering intensity of atomistic protein structures

Dudu Tong, Sichun Yang and Lanyuan Lu

Supporting Information

Accurate optimization of amino acid form factors for computing small-angle X-ray scattering intensity of atomistic protein structures

Dudu Tong[a], Sichun Yang[b] and Lanyuan Lu[a*]

[a] School of Biological Sciences, Nanyang Technological University,

60 Nanyang Drive, Singapore, 637551

[b] Center for Proteomics and Department of Nutrition, Case Western Reserve University,

10900 Euclid Ave, BRB 929, Cleveland, OH 44106-4988

* Corresponding author: LYLU@ntu.edu.sg

Table S1. Coarse-grained form factors for the two-bead COE scheme obtained by our EDM method, corresponding to Fig 1(b).

q	BB	ALA	CYS	ASP	GLU	PHE	GLY	HIS	ILE	LYS	LEU	MET	ASN	PRO	GLN	ARG	SER	THR	VAL	TRP	TYR
0.000	10.563	-1.532	8.191	9.614	8.656	-1.395	-0.578	10.808	-4.351	0.422	-4.335	5.964	9.405	-1.922	8.470	12.755	3.450	2.521	-3.421	5.134	3.586
0.010	10.556	-1.523	8.200	9.621	8.660	-1.385	-0.570	10.816	-4.343	0.430	-4.327	5.973	9.414	-1.916	8.478	12.764	3.456	2.531	-3.412	5.144	3.594
0.020	10.536	-1.501	8.223	9.638	8.667	-1.358	-0.552	10.834	-4.322	0.453	-4.306	5.998	9.439	-1.901	8.498	12.789	3.473	2.557	-3.389	5.170	3.612
0.030	10.503	-1.464	8.261	9.665	8.680	-1.315	-0.521	10.865	-4.289	0.491	-4.274	6.036	9.479	-1.875	8.530	12.830	3.502	2.597	-3.354	5.212	3.642
0.040	10.460	-1.414	8.311	9.703	8.701	-1.260	-0.478	10.907	-4.245	0.545	-4.233	6.085	9.530	-1.836	8.574	12.885	3.543	2.651	-3.309	5.265	3.684
0.050	10.407	-1.353	8.369	9.748	8.730	-1.197	-0.423	10.962	-4.194	0.617	-4.185	6.140	9.590	-1.784	8.629	12.953	3.596	2.714	-3.256	5.328	3.735
0.060	10.346	-1.283	8.432	9.801	8.770	-1.130	-0.357	11.028	-4.138	0.705	-4.133	6.198	9.658	-1.718	8.694	13.033	3.660	2.784	-3.198	5.395	3.794
0.070	10.278	-1.207	8.498	9.861	8.823	-1.063	-0.283	11.105	-4.077	0.811	-4.079	6.258	9.732	-1.637	8.769	13.123	3.734	2.859	-3.135	5.466	3.860
0.080	10.204	-1.125	8.567	9.928	8.889	-0.995	-0.200	11.192	-4.013	0.931	-4.020	6.320	9.813	-1.544	8.853	13.223	3.814	2.938	-3.066	5.540	3.930
0.090	10.126	-1.041	8.637	10.002	8.970	-0.926	-0.111	11.291	-3.944	1.066	-3.957	6.386	9.900	-1.440	8.948	13.332	3.898	3.020	-2.991	5.616	4.006
0.100	10.044	-0.956	8.711	10.082	9.064	-0.855	-0.017	11.402	-3.870	1.213	-3.887	6.460	9.991	-1.327	9.053	13.451	3.985	3.106	-2.908	5.696	4.086
0.110	9.958	-0.870	8.789	10.168	9.168	-0.779	0.081	11.524	-3.793	1.371	-3.810	6.540	10.085	-1.206	9.165	13.580	4.073	3.194	-2.820	5.780	4.171
0.120	9.871	-0.784	8.870	10.258	9.277	-0.698	0.183	11.656	-3.713	1.536	-3.727	6.627	10.181	-1.080	9.283	13.719	4.164	3.286	-2.727	5.867	4.262
0.130	9.784	-0.697	8.952	10.352	9.386	-0.612	0.288	11.795	-3.632	1.706	-3.638	6.715	10.277	-0.949	9.403	13.867	4.257	3.379	-2.632	5.958	4.358
0.140	9.699	-0.611	9.036	10.447	9.492	-0.520	0.395	11.938	-3.549	1.879	-3.545	6.802	10.376	-0.816	9.524	14.019	4.353	3.474	-2.535	6.054	4.458
0.150	9.615	-0.525	9.119	10.544	9.593	-0.421	0.504	12.082	-3.465	2.051	-3.448	6.885	10.479	-0.681	9.645	14.174	4.452	3.571	-2.439	6.155	4.564
0.160	9.535	-0.439	9.200	10.640	9.689	-0.317	0.612	12.225	-3.378	2.220	-3.348	6.963	10.584	-0.547	9.764	14.328	4.552	3.668	-2.344	6.260	4.674
0.170	9.459	-0.354	9.279	10.735	9.781	-0.208	0.719	12.367	-3.288	2.385	-3.246	7.036	10.693	-0.412	9.880	14.477	4.654	3.764	-2.251	6.369	4.785
0.180	9.389	-0.272	9.354	10.825	9.870	-0.093	0.823	12.506	-3.196	2.543	-3.144	7.107	10.804	-0.279	9.990	14.620	4.755	3.858	-2.159	6.480	4.895
0.190	9.326	-0.193	9.427	10.909	9.956	0.026	0.924	12.641	-3.104	2.692	-3.042	7.179	10.914	-0.147	10.093	14.753	4.853	3.948	-2.069	6.592	5.002
0.200	9.270	-0.120	9.495	10.986	10.040	0.146	1.021	12.772	-3.013	2.831	-2.944	7.254	11.020	-0.019	10.188	14.874	4.947	4.034	-1.981	6.703	5.104
0.210	9.224	-0.051	9.559	11.055	10.121	0.267	1.114	12.896	-2.924	2.958	-2.850	7.332	11.121	0.105	10.275	14.983	5.034	4.115	-1.896	6.812	5.199
0.220	9.187	0.011	9.619	11.118	10.198	0.385	1.202	13.012	-2.838	3.072	-2.761	7.412	11.213	0.221	10.353	15.078	5.113	4.191	-1.815	6.916	5.287
0.230	9.158	0.068	9.674	11.175	10.270	0.499	1.283	13.118	-2.754	3.175	-2.679	7.492	11.296	0.328	10.425	15.161	5.183	4.265	-1.737	7.016	5.366
0.240	9.139	0.120	9.726	11.228	10.336	0.607	1.359	13.214	-2.671	3.268	-2.601	7.573	11.367	0.426	10.491	15.234	5.244	4.335	-1.662	7.112	5.437

0.250	9.127	0.170	9.776	11.277	10.395	0.709	1.427	13.298	-2.590	3.352	-2.529	7.652	11.427	0.515	10.553	15.298	5.297	4.403	-1.592	7.203	5.501
0.260	9.123	0.216	9.824	11.324	10.449	0.805	1.488	13.370	-2.511	3.428	-2.460	7.730	11.475	0.596	10.611	15.354	5.344	4.469	-1.524	7.291	5.559
0.270	9.127	0.260	9.870	11.367	10.495	0.893	1.538	13.429	-2.434	3.498	-2.395	7.805	11.513	0.670	10.664	15.401	5.386	4.530	-1.461	7.375	5.612
0.280	9.139	0.299	9.914	11.405	10.535	0.974	1.578	13.476	-2.361	3.561	-2.333	7.876	11.542	0.737	10.710	15.440	5.424	4.586	-1.401	7.454	5.662
0.290	9.159	0.333	9.954	11.439	10.568	1.048	1.606	13.509	-2.292	3.619	-2.275	7.942	11.562	0.796	10.749	15.470	5.457	4.636	-1.345	7.530	5.710
0.300	9.187	0.362	9.991	11.466	10.595	1.119	1.622	13.533	-2.225	3.671	-2.220	8.003	11.576	0.849	10.782	15.492	5.487	4.680	-1.291	7.601	5.756
0.310	9.222	0.385	10.023	11.486	10.618	1.188	1.627	13.549	-2.161	3.719	-2.166	8.058	11.584	0.896	10.809	15.506	5.512	4.718	-1.240	7.670	5.802
0.320	9.264	0.403	10.050	11.501	10.636	1.258	1.624	13.560	-2.096	3.764	-2.112	8.108	11.588	0.938	10.832	15.514	5.532	4.753	-1.188	7.739	5.847
0.330	9.310	0.417	10.073	11.510	10.651	1.331	1.614	13.569	-2.030	3.806	-2.057	8.154	11.590	0.978	10.851	15.516	5.548	4.784	-1.135	7.807	5.894
0.340	9.360	0.431	10.094	11.514	10.663	1.409	1.601	13.577	-1.959	3.844	-1.999	8.199	11.590	1.016	10.868	15.515	5.561	4.815	-1.081	7.875	5.943
0.350	9.412	0.444	10.112	11.514	10.672	1.490	1.586	13.585	-1.885	3.879	-1.939	8.242	11.589	1.054	10.881	15.511	5.572	4.845	-1.023	7.944	5.993
0.360	9.466	0.459	10.128	11.510	10.679	1.574	1.571	13.593	-1.807	3.910	-1.876	8.286	11.586	1.091	10.890	15.505	5.580	4.876	-0.963	8.013	6.045
0.370	9.522	0.475	10.141	11.503	10.686	1.660	1.556	13.600	-1.725	3.937	-1.810	8.333	11.583	1.129	10.895	15.498	5.587	4.906	-0.899	8.081	6.095
0.380	9.579	0.493	10.151	11.494	10.693	1.744	1.542	13.606	-1.642	3.960	-1.744	8.383	11.579	1.166	10.896	15.491	5.592	4.935	-0.835	8.146	6.144
0.390	9.639	0.510	10.158	11.483	10.701	1.827	1.527	13.610	-1.559	3.979	-1.676	8.436	11.574	1.201	10.894	15.481	5.594	4.962	-0.770	8.209	6.188
0.400	9.700	0.524	10.164	11.473	10.710	1.907	1.512	13.612	-1.476	3.995	-1.609	8.491	11.567	1.234	10.890	15.467	5.595	4.985	-0.708	8.268	6.228
0.410	9.764	0.534	10.169	11.462	10.719	1.984	1.493	13.612	-1.396	4.010	-1.543	8.545	11.556	1.264	10.885	15.448	5.593	5.004	-0.650	8.325	6.264
0.420	9.831	0.539	10.175	11.451	10.728	2.058	1.471	13.611	-1.320	4.023	-1.479	8.595	11.540	1.291	10.879	15.423	5.589	5.019	-0.597	8.379	6.294
0.430	9.901	0.538	10.181	11.440	10.735	2.131	1.445	13.608	-1.248	4.038	-1.416	8.641	11.520	1.316	10.871	15.392	5.582	5.029	-0.550	8.433	6.320
0.440	9.974	0.531	10.186	11.426	10.742	2.204	1.415	13.603	-1.180	4.055	-1.356	8.681	11.495	1.340	10.862	15.355	5.571	5.036	-0.508	8.489	6.342
0.450	10.050	0.519	10.191	11.412	10.747	2.280	1.382	13.597	-1.116	4.074	-1.297	8.716	11.466	1.365	10.852	15.312	5.556	5.040	-0.471	8.548	6.361
0.460	10.128	0.505	10.193	11.396	10.749	2.360	1.345	13.590	-1.054	4.095	-1.239	8.748	11.435	1.390	10.843	15.266	5.537	5.043	-0.436	8.613	6.379
0.470	10.210	0.489	10.191	11.379	10.750	2.445	1.304	13.583	-0.994	4.118	-1.182	8.779	11.402	1.415	10.835	15.218	5.513	5.044	-0.402	8.685	6.399
0.480	10.295	0.473	10.185	11.361	10.747	2.536	1.260	13.576	-0.933	4.141	-1.124	8.809	11.367	1.438	10.830	15.169	5.487	5.044	-0.366	8.763	6.421
0.490	10.382	0.457	10.176	11.342	10.740	2.631	1.212	13.570	-0.871	4.165	-1.066	8.840	11.331	1.459	10.824	15.120	5.460	5.044	-0.329	8.845	6.447
0.500	10.472	0.442	10.164	11.321	10.729	2.731	1.159	13.563	-0.809	4.187	-1.007	8.872	11.293	1.478	10.819	15.070	5.432	5.043	-0.288	8.931	6.477

Table S2. Coarse-grained form factors for the two-bead per-residue scheme obtained by the IBA method, corresponding to Fig 1(c).

q	BB	ALA	CYS	ASP	GLU	PHE	GLY	HIS	ILE	LYS	LEU	MET	ASN	PRO	GLN	ARG	SER	THR	VAL	TRP	TYR
0.000	10.726	-1.652	7.918	9.479	8.548	-1.477	-0.720	10.729	-4.445	0.278	-4.445	5.852	9.252	-2.793	8.320	12.605	3.299	2.368	-3.514	4.984	3.473
0.010	10.726	-1.641	7.919	9.480	8.549	-1.474	-0.720	10.730	-4.414	0.287	-4.409	5.854	9.252	-2.778	8.321	12.607	3.300	2.369	-3.494	4.987	3.476
0.020	10.726	-1.631	7.921	9.481	8.552	-1.466	-0.720	10.733	-4.382	0.312	-4.372	5.859	9.254	-2.761	8.325	12.611	3.301	2.373	-3.473	4.995	3.484
0.030	10.727	-1.620	7.924	9.484	8.557	-1.454	-0.720	10.738	-4.348	0.349	-4.335	5.867	9.256	-2.743	8.330	12.619	3.304	2.378	-3.452	5.010	3.497
0.040	10.727	-1.609	7.929	9.488	8.564	-1.438	-0.720	10.745	-4.314	0.395	-4.297	5.878	9.260	-2.725	8.337	12.630	3.307	2.386	-3.429	5.030	3.516
0.050	10.728	-1.598	7.935	9.492	8.573	-1.418	-0.719	10.754	-4.277	0.447	-4.259	5.893	9.265	-2.704	8.346	12.644	3.311	2.395	-3.405	5.055	3.539
0.060	10.729	-1.586	7.942	9.498	8.585	-1.394	-0.719	10.765	-4.240	0.504	-4.219	5.911	9.271	-2.683	8.357	12.661	3.316	2.407	-3.380	5.086	3.568
0.070	10.730	-1.575	7.951	9.505	8.598	-1.366	-0.719	10.778	-4.201	0.564	-4.179	5.932	9.278	-2.660	8.371	12.681	3.322	2.421	-3.353	5.123	3.602
0.080	10.732	-1.563	7.961	9.513	8.613	-1.333	-0.718	10.794	-4.160	0.626	-4.137	5.956	9.286	-2.637	8.386	12.704	3.329	2.437	-3.325	5.165	3.641
0.090	10.733	-1.550	7.972	9.522	8.630	-1.297	-0.718	10.811	-4.118	0.690	-4.095	5.983	9.295	-2.611	8.403	12.730	3.337	2.456	-3.296	5.212	3.684
0.100	10.735	-1.537	7.985	9.532	8.649	-1.256	-0.717	10.830	-4.074	0.755	-4.051	6.014	9.305	-2.585	8.422	12.758	3.346	2.476	-3.266	5.265	3.731
0.110	10.737	-1.524	7.999	9.543	8.670	-1.211	-0.716	10.851	-4.028	0.822	-4.006	6.047	9.316	-2.557	8.443	12.790	3.356	2.498	-3.234	5.323	3.783
0.120	10.739	-1.511	8.014	9.555	8.693	-1.162	-0.716	10.874	-3.980	0.889	-3.959	6.083	9.328	-2.527	8.466	12.823	3.366	2.521	-3.201	5.385	3.839
0.130	10.741	-1.497	8.031	9.568	8.717	-1.109	-0.715	10.898	-3.931	0.958	-3.911	6.123	9.341	-2.497	8.491	12.860	3.378	2.547	-3.166	5.453	3.900
0.140	10.744	-1.483	8.049	9.582	8.743	-1.052	-0.714	10.925	-3.880	1.027	-3.862	6.165	9.355	-2.465	8.517	12.899	3.390	2.575	-3.130	5.525	3.963
0.150	10.746	-1.469	8.068	9.596	8.771	-0.991	-0.713	10.953	-3.827	1.096	-3.811	6.210	9.370	-2.431	8.545	12.940	3.403	2.604	-3.092	5.602	4.031
0.160	10.749	-1.454	8.088	9.612	8.801	-0.926	-0.712	10.983	-3.773	1.167	-3.758	6.258	9.386	-2.396	8.575	12.983	3.418	2.635	-3.053	5.683	4.102
0.170	10.751	-1.439	8.110	9.629	8.833	-0.857	-0.711	11.015	-3.716	1.238	-3.704	6.309	9.403	-2.359	8.607	13.029	3.433	2.667	-3.013	5.769	4.176
0.180	10.754	-1.423	8.133	9.646	8.865	-0.785	-0.710	11.048	-3.658	1.309	-3.648	6.362	9.421	-2.321	8.640	13.076	3.448	2.701	-2.971	5.858	4.253
0.190	10.757	-1.407	8.157	9.665	8.900	-0.709	-0.709	11.083	-3.598	1.381	-3.591	6.418	9.440	-2.282	8.674	13.125	3.465	2.737	-2.927	5.952	4.333
0.200	10.761	-1.391	8.182	9.684	8.936	-0.629	-0.708	11.120	-3.535	1.453	-3.531	6.476	9.459	-2.241	8.711	13.176	3.482	2.774	-2.882	6.049	4.415
0.210	10.764	-1.374	8.208	9.704	8.973	-0.545	-0.707	11.158	-3.471	1.526	-3.470	6.537	9.480	-2.198	8.748	13.229	3.500	2.812	-2.836	6.151	4.500
0.220	10.767	-1.357	8.235	9.725	9.012	-0.458	-0.705	11.198	-3.406	1.600	-3.408	6.600	9.501	-2.154	8.787	13.283	3.519	2.852	-2.788	6.255	4.588
0.230	10.771	-1.339	8.264	9.747	9.052	-0.368	-0.704	11.239	-3.338	1.674	-3.343	6.666	9.523	-2.109	8.827	13.338	3.539	2.893	-2.738	6.363	4.678
0.240	10.774	-1.321	8.294	9.770	9.093	-0.274	-0.703	11.281	-3.268	1.748	-3.277	6.734	9.546	-2.062	8.869	13.395	3.560	2.936	-2.687	6.475	4.769
0.250	10.778	-1.303	8.324	9.793	9.136	-0.177	-0.701	11.325	-3.197	1.823	-3.209	6.804	9.569	-2.014	8.912	13.453	3.581	2.979	-2.635	6.589	4.863

0.260	10.782	-1.284	8.356	9.817	9.179	-0.077	-0.700	11.370	-3.124	1.898	-3.139	6.876	9.593	-1.964	8.956	13.511	3.603	3.024	-2.581	6.706	4.958
0.270	10.785	-1.265	8.389	9.841	9.224	0.027	-0.698	11.417	-3.049	1.973	-3.067	6.950	9.618	-1.913	9.001	13.571	3.626	3.069	-2.526	6.826	5.055
0.280	10.789	-1.245	8.422	9.867	9.270	0.133	-0.696	11.464	-2.972	2.049	-2.994	7.027	9.644	-1.860	9.047	13.631	3.649	3.116	-2.469	6.949	5.154
0.290	10.793	-1.225	8.457	9.893	9.316	0.242	-0.695	11.513	-2.893	2.126	-2.919	7.105	9.670	-1.806	9.094	13.691	3.673	3.164	-2.411	7.073	5.254
0.300	10.797	-1.205	8.493	9.919	9.364	0.354	-0.693	11.562	-2.813	2.203	-2.842	7.185	9.697	-1.751	9.142	13.752	3.698	3.212	-2.351	7.200	5.355
0.310	10.801	-1.184	8.529	9.946	9.412	0.469	-0.691	11.613	-2.731	2.280	-2.763	7.266	9.724	-1.694	9.190	13.814	3.723	3.262	-2.290	7.329	5.457
0.320	10.805	-1.163	8.567	9.974	9.461	0.586	-0.689	11.665	-2.647	2.357	-2.682	7.350	9.752	-1.636	9.240	13.875	3.749	3.312	-2.227	7.460	5.561
0.330	10.809	-1.141	8.605	10.002	9.511	0.706	-0.687	11.717	-2.562	2.435	-2.600	7.434	9.781	-1.577	9.290	13.936	3.775	3.363	-2.163	7.593	5.665
0.340	10.813	-1.119	8.644	10.031	9.562	0.828	-0.685	11.770	-2.475	2.513	-2.516	7.521	9.810	-1.516	9.341	13.998	3.803	3.415	-2.098	7.727	5.770
0.350	10.817	-1.097	8.684	10.060	9.613	0.953	-0.683	11.824	-2.386	2.591	-2.430	7.609	9.839	-1.454	9.392	14.059	3.830	3.467	-2.032	7.862	5.876
0.360	10.821	-1.074	8.725	10.090	9.664	1.079	-0.681	11.879	-2.296	2.670	-2.343	7.698	9.869	-1.391	9.444	14.120	3.859	3.521	-1.964	7.998	5.982
0.370	10.825	-1.050	8.767	10.120	9.716	1.208	-0.679	11.934	-2.204	2.749	-2.254	7.789	9.899	-1.326	9.496	14.180	3.888	3.575	-1.895	8.136	6.089
0.380	10.829	-1.027	8.809	10.150	9.769	1.339	-0.677	11.990	-2.111	2.828	-2.164	7.880	9.930	-1.260	9.549	14.239	3.917	3.629	-1.824	8.274	6.197
0.390	10.833	-1.003	8.852	10.181	9.822	1.471	-0.675	12.046	-2.016	2.907	-2.071	7.973	9.961	-1.193	9.602	14.298	3.947	3.684	-1.753	8.414	6.304
0.400	10.837	-0.978	8.896	10.212	9.875	1.605	-0.672	12.103	-1.921	2.986	-1.978	8.067	9.992	-1.125	9.656	14.356	3.977	3.740	-1.680	8.553	6.412
0.410	10.840	-0.953	8.940	10.244	9.928	1.741	-0.670	12.160	-1.823	3.066	-1.883	8.162	10.024	-1.056	9.709	14.413	4.008	3.796	-1.606	8.693	6.520
0.420	10.844	-0.928	8.985	10.275	9.981	1.878	-0.668	12.217	-1.725	3.146	-1.786	8.258	10.056	-0.985	9.763	14.469	4.040	3.852	-1.531	8.833	6.629
0.430	10.848	-0.902	9.031	10.307	10.035	2.017	-0.665	12.275	-1.625	3.225	-1.688	8.354	10.088	-0.914	9.817	14.524	4.071	3.909	-1.455	8.973	6.737
0.440	10.851	-0.876	9.077	10.339	10.088	2.157	-0.663	12.333	-1.524	3.305	-1.588	8.452	10.120	-0.841	9.871	14.578	4.104	3.967	-1.378	9.113	6.845
0.450	10.854	-0.849	9.124	10.371	10.142	2.298	-0.660	12.391	-1.422	3.385	-1.488	8.550	10.152	-0.767	9.925	14.631	4.136	4.024	-1.300	9.253	6.953
0.460	10.858	-0.823	9.171	10.404	10.195	2.440	-0.658	12.449	-1.319	3.465	-1.386	8.649	10.185	-0.693	9.978	14.682	4.169	4.082	-1.220	9.392	7.060
0.470	10.861	-0.795	9.219	10.436	10.248	2.583	-0.655	12.507	-1.214	3.545	-1.282	8.748	10.217	-0.617	10.032	14.731	4.203	4.141	-1.140	9.531	7.168
0.480	10.864	-0.768	9.267	10.468	10.302	2.726	-0.652	12.564	-1.109	3.625	-1.178	8.848	10.250	-0.541	10.086	14.779	4.236	4.199	-1.059	9.669	7.275
0.490	10.866	-0.740	9.315	10.501	10.354	2.871	-0.649	12.622	-1.003	3.704	-1.072	8.948	10.282	-0.464	10.139	14.825	4.271	4.258	-0.977	9.806	7.381
0.500	10.869	-0.711	9.364	10.533	10.407	3.016	-0.647	12.680	-0.896	3.784	-0.965	9.048	10.315	-0.386	10.192	14.870	4.305	4.317	-0.894	9.941	7.487

Table S3. Coarse-grained form factors for the two-bead Cα+COM scheme obtained by our EDM method, corresponding to Fig S2(c).

q	BB	ALA	CYS	ASP	GLU	PHE	GLY	HIS	ILE	LYS	LEU	MET	ASN	PRO	GLN	ARG	SER	THR	VAL	TRP	TYR
0.000	13.271	-4.240	5.483	6.906	5.948	-4.103	-3.286	8.100	-7.059	-2.286	-7.043	3.256	6.697	-4.630	5.762	10.047	0.742	-0.187	-6.129	2.426	0.878
0.010	13.258	-4.225	5.497	6.915	5.953	-4.087	-3.274	8.113	-7.045	-2.271	-7.028	3.272	6.713	-4.620	5.775	10.065	0.753	-0.172	-6.114	2.444	0.891
0.020	13.201	-4.162	5.558	6.959	5.986	-4.021	-3.221	8.168	-6.986	-2.208	-6.969	3.337	6.778	-4.574	5.830	10.138	0.803	-0.110	-6.052	2.517	0.946
0.030	13.109	-4.062	5.655	7.028	6.040	-3.917	-3.137	8.257	-6.893	-2.104	-6.874	3.438	6.879	-4.498	5.918	10.254	0.884	-0.012	-5.955	2.632	1.036
0.040	12.989	-3.930	5.782	7.119	6.112	-3.781	-3.023	8.375	-6.770	-1.962	-6.751	3.567	7.009	-4.394	6.035	10.407	0.994	0.114	-5.829	2.781	1.156
0.050	12.845	-3.772	5.932	7.226	6.201	-3.623	-2.884	8.519	-6.626	-1.785	-6.606	3.713	7.160	-4.263	6.174	10.592	1.128	0.262	-5.682	2.954	1.300
0.060	12.683	-3.594	6.098	7.347	6.308	-3.450	-2.724	8.683	-6.465	-1.574	-6.447	3.870	7.325	-4.108	6.335	10.802	1.281	0.424	-5.517	3.143	1.464
0.070	12.507	-3.402	6.275	7.478	6.435	-3.268	-2.548	8.866	-6.290	-1.332	-6.277	4.034	7.501	-3.932	6.514	11.032	1.449	0.596	-5.338	3.341	1.643
0.080	12.319	-3.201	6.460	7.620	6.585	-3.082	-2.358	9.066	-6.102	-1.065	-6.097	4.204	7.686	-3.739	6.711	11.277	1.626	0.776	-5.146	3.543	1.832
0.090	12.124	-2.996	6.651	7.773	6.757	-2.892	-2.159	9.282	-5.905	-0.774	-5.908	4.381	7.877	-3.533	6.925	11.534	1.808	0.961	-4.945	3.745	2.028
0.100	11.924	-2.791	6.844	7.934	6.951	-2.701	-1.954	9.513	-5.701	-0.467	-5.712	4.566	8.072	-3.317	7.153	11.801	1.991	1.150	-4.737	3.941	2.227
0.110	11.724	-2.590	7.035	8.101	7.158	-2.511	-1.746	9.757	-5.497	-0.149	-5.510	4.754	8.268	-3.096	7.390	12.076	2.173	1.341	-4.528	4.130	2.426
0.120	11.529	-2.396	7.222	8.272	7.369	-2.324	-1.538	10.008	-5.298	0.174	-5.307	4.943	8.463	-2.870	7.630	12.357	2.353	1.530	-4.323	4.310	2.623
0.130	11.340	-2.208	7.400	8.445	7.576	-2.139	-1.333	10.262	-5.109	0.495	-5.105	5.127	8.656	-2.643	7.868	12.642	2.532	1.717	-4.125	4.482	2.818
0.140	11.161	-2.026	7.569	8.617	7.773	-1.957	-1.132	10.515	-4.929	0.809	-4.906	5.301	8.849	-2.415	8.102	12.928	2.711	1.902	-3.935	4.650	3.012
0.150	10.991	-1.850	7.729	8.788	7.957	-1.776	-0.934	10.763	-4.758	1.113	-4.711	5.466	9.044	-2.189	8.331	13.210	2.891	2.082	-3.755	4.818	3.206
0.160	10.831	-1.678	7.880	8.957	8.131	-1.592	-0.741	11.005	-4.592	1.402	-4.519	5.622	9.241	-1.966	8.553	13.484	3.071	2.259	-3.583	4.988	3.400
0.170	10.683	-1.512	8.023	9.121	8.294	-1.405	-0.553	11.239	-4.431	1.674	-4.331	5.772	9.439	-1.746	8.766	13.747	3.251	2.431	-3.419	5.162	3.593
0.180	10.547	-1.352	8.158	9.278	8.450	-1.215	-0.370	11.466	-4.273	1.927	-4.148	5.921	9.636	-1.532	8.967	13.993	3.428	2.596	-3.263	5.338	3.783
0.190	10.425	-1.201	8.287	9.423	8.599	-1.021	-0.193	11.684	-4.120	2.158	-3.971	6.071	9.830	-1.325	9.153	14.219	3.602	2.754	-3.112	5.515	3.968
0.200	10.317	-1.059	8.409	9.555	8.741	-0.827	-0.021	11.891	-3.972	2.366	-3.802	6.224	10.015	-1.128	9.321	14.423	3.767	2.904	-2.968	5.691	4.147
0.210	10.225	-0.930	8.524	9.672	8.876	-0.635	0.144	12.087	-3.829	2.550	-3.643	6.379	10.188	-0.944	9.471	14.604	3.921	3.044	-2.831	5.862	4.314
0.220	10.148	-0.811	8.633	9.775	9.001	-0.450	0.302	12.268	-3.694	2.709	-3.495	6.533	10.344	-0.775	9.604	14.761	4.061	3.176	-2.701	6.027	4.469
0.230	10.088	-0.705	8.735	9.866	9.115	-0.273	0.450	12.433	-3.565	2.847	-3.360	6.683	10.481	-0.624	9.722	14.897	4.185	3.300	-2.579	6.183	4.607
0.240	10.044	-0.610	8.830	9.945	9.217	-0.110	0.587	12.580	-3.443	2.965	-3.237	6.826	10.597	-0.492	9.826	15.014	4.293	3.416	-2.466	6.329	4.728
0.250	10.014	-0.525	8.919	10.016	9.306	0.039	0.710	12.708	-3.329	3.067	-3.127	6.960	10.693	-0.377	9.918	15.112	4.386	3.523	-2.361	6.465	4.831

0.260	9.999	-0.449	9.000	10.079	9.382	0.171	0.818	12.816	-3.221	3.155	-3.028	7.084	10.769	-0.278	10.000	15.194	4.466	3.621	-2.266	6.590	4.919
0.270	9.998	-0.382	9.075	10.135	9.444	0.287	0.909	12.904	-3.122	3.231	-2.941	7.197	10.827	-0.193	10.070	15.260	4.535	3.707	-2.179	6.703	4.993
0.280	10.010	-0.324	9.142	10.184	9.493	0.387	0.982	12.972	-3.031	3.295	-2.863	7.298	10.870	-0.123	10.130	15.311	4.593	3.783	-2.100	6.803	5.057
0.290	10.035	-0.275	9.203	10.225	9.532	0.475	1.035	13.021	-2.947	3.350	-2.794	7.386	10.899	-0.066	10.179	15.347	4.643	3.848	-2.029	6.892	5.112
0.300	10.072	-0.235	9.257	10.257	9.562	0.552	1.070	13.055	-2.870	3.397	-2.731	7.461	10.918	-0.021	10.217	15.370	4.684	3.904	-1.963	6.969	5.162
0.310	10.120	-0.204	9.303	10.279	9.586	0.624	1.090	13.076	-2.798	3.439	-2.674	7.526	10.928	0.013	10.248	15.383	4.716	3.951	-1.902	7.039	5.208
0.320	10.176	-0.179	9.343	10.291	9.605	0.694	1.096	13.089	-2.728	3.476	-2.620	7.582	10.932	0.039	10.273	15.387	4.740	3.992	-1.845	7.103	5.251
0.330	10.240	-0.159	9.375	10.295	9.620	0.765	1.092	13.097	-2.659	3.511	-2.566	7.629	10.930	0.059	10.293	15.384	4.756	4.027	-1.789	7.165	5.293
0.340	10.310	-0.142	9.402	10.292	9.630	0.838	1.082	13.102	-2.588	3.542	-2.513	7.671	10.923	0.074	10.308	15.375	4.765	4.057	-1.734	7.225	5.334
0.350	10.385	-0.128	9.423	10.282	9.636	0.912	1.066	13.106	-2.515	3.569	-2.458	7.710	10.913	0.087	10.319	15.363	4.769	4.084	-1.680	7.285	5.376
0.360	10.463	-0.115	9.438	10.266	9.639	0.986	1.047	13.108	-2.440	3.590	-2.404	7.748	10.899	0.099	10.324	15.349	4.767	4.107	-1.625	7.343	5.418
0.370	10.543	-0.102	9.447	10.245	9.640	1.058	1.027	13.107	-2.365	3.605	-2.349	7.789	10.881	0.107	10.323	15.334	4.761	4.125	-1.569	7.400	5.458
0.380	10.627	-0.092	9.448	10.221	9.639	1.127	1.005	13.103	-2.289	3.611	-2.295	7.833	10.860	0.113	10.314	15.318	4.751	4.139	-1.513	7.453	5.494
0.390	10.713	-0.085	9.443	10.194	9.636	1.190	0.983	13.094	-2.216	3.609	-2.243	7.880	10.837	0.113	10.301	15.299	4.737	4.146	-1.459	7.500	5.525
0.400	10.801	-0.082	9.433	10.165	9.632	1.247	0.959	13.079	-2.144	3.599	-2.194	7.929	10.810	0.108	10.283	15.276	4.719	4.149	-1.408	7.541	5.549
0.410	10.893	-0.086	9.422	10.134	9.628	1.297	0.935	13.059	-2.077	3.584	-2.149	7.975	10.778	0.096	10.261	15.245	4.697	4.147	-1.364	7.574	5.565
0.420	10.987	-0.098	9.411	10.102	9.621	1.342	0.907	13.033	-2.017	3.565	-2.110	8.015	10.740	0.079	10.236	15.206	4.673	4.140	-1.328	7.598	5.572
0.430	11.084	-0.117	9.401	10.067	9.612	1.382	0.876	13.003	-1.964	3.545	-2.077	8.046	10.695	0.059	10.207	15.156	4.645	4.130	-1.300	7.616	5.570
0.440	11.184	-0.143	9.393	10.029	9.602	1.419	0.840	12.969	-1.919	3.526	-2.052	8.066	10.643	0.037	10.177	15.098	4.614	4.118	-1.281	7.627	5.559
0.450	11.286	-0.173	9.384	9.988	9.590	1.454	0.801	12.931	-1.884	3.510	-2.032	8.074	10.586	0.015	10.145	15.033	4.577	4.105	-1.270	7.637	5.540
0.460	11.393	-0.208	9.373	9.946	9.576	1.490	0.756	12.891	-1.856	3.497	-2.018	8.074	10.524	-0.008	10.114	14.962	4.535	4.091	-1.264	7.647	5.516
0.470	11.503	-0.244	9.357	9.902	9.561	1.527	0.707	12.848	-1.834	3.486	-2.009	8.066	10.459	-0.032	10.084	14.887	4.487	4.074	-1.263	7.660	5.488
0.480	11.618	-0.283	9.335	9.858	9.543	1.566	0.652	12.803	-1.816	3.477	-2.004	8.053	10.391	-0.060	10.053	14.810	4.434	4.055	-1.264	7.675	5.460
0.490	11.739	-0.322	9.306	9.815	9.520	1.606	0.590	12.756	-1.801	3.469	-2.003	8.037	10.319	-0.094	10.021	14.732	4.377	4.031	-1.266	7.694	5.433
0.500	11.864	-0.361	9.272	9.771	9.493	1.646	0.520	12.709	-1.787	3.460	-2.007	8.018	10.245	-0.135	9.988	14.655	4.317	4.004	-1.269	7.716	5.408

Table S4. Coarse-grained form factors for the one-bead COE scheme obtained by the our EDM method, corresponding to Fig S1(b).

q	ALA	CYS	ASP	GLU	PHE	GLY	HIS	ILE	LYS	LEU	MET	ASN	PRO	GLN	ARG	SER	THR	VAL	TRP	TYR
0.000	9.032	18.754	20.177	19.220	9.168	9.986	21.372	6.212	10.985	6.229	16.527	19.968	8.642	19.033	23.318	14.013	13.084	7.143	15.697	14.150
0.010	9.034	18.758	20.166	19.206	9.172	9.983	21.368	6.219	10.995	6.232	16.525	19.970	8.635	19.029	23.325	14.011	13.086	7.149	15.698	14.150
0.020	9.039	18.772	20.136	19.164	9.184	9.975	21.359	6.239	11.024	6.242	16.518	19.974	8.615	19.018	23.344	14.005	13.091	7.166	15.703	14.152
0.030	9.048	18.794	20.087	19.100	9.201	9.964	21.345	6.270	11.074	6.257	16.505	19.979	8.585	19.002	23.372	13.996	13.098	7.191	15.708	14.154
0.040	9.061	18.822	20.023	19.019	9.220	9.952	21.328	6.309	11.148	6.273	16.483	19.981	8.552	18.987	23.408	13.986	13.105	7.217	15.710	14.153
0.050	9.076	18.852	19.948	18.929	9.235	9.942	21.309	6.349	11.246	6.288	16.450	19.980	8.520	18.975	23.449	13.976	13.111	7.241	15.706	14.147
0.060	9.092	18.880	19.866	18.841	9.241	9.936	21.293	6.385	11.369	6.297	16.406	19.976	8.497	18.969	23.491	13.967	13.116	7.258	15.689	14.133
0.070	9.109	18.901	19.786	18.764	9.232	9.937	21.280	6.411	11.515	6.297	16.352	19.973	8.487	18.971	23.534	13.958	13.120	7.267	15.654	14.109
0.080	9.126	18.911	19.713	18.707	9.207	9.946	21.274	6.421	11.678	6.286	16.293	19.974	8.494	18.984	23.578	13.948	13.122	7.266	15.599	14.075
0.090	9.143	18.907	19.656	18.675	9.165	9.962	21.276	6.416	11.849	6.263	16.234	19.981	8.520	19.006	23.624	13.937	13.125	7.258	15.522	14.030
0.100	9.159	18.889	19.618	18.668	9.109	9.986	21.289	6.392	12.021	6.228	16.181	19.994	8.567	19.039	23.675	13.924	13.128	7.242	15.429	13.976
0.110	9.174	18.860	19.601	18.679	9.042	10.019	21.314	6.352	12.187	6.185	16.138	20.011	8.635	19.078	23.734	13.914	13.133	7.222	15.325	13.918
0.120	9.190	18.824	19.605	18.703	8.968	10.060	21.350	6.298	12.339	6.137	16.105	20.034	8.725	19.121	23.800	13.911	13.141	7.200	15.219	13.858
0.130	9.207	18.784	19.626	18.729	8.893	10.113	21.396	6.234	12.475	6.088	16.080	20.062	8.833	19.166	23.871	13.918	13.152	7.175	15.121	13.802
0.140	9.225	18.745	19.662	18.753	8.821	10.176	21.449	6.164	12.593	6.042	16.056	20.099	8.954	19.212	23.942	13.940	13.169	7.149	15.039	13.753
0.150	9.244	18.709	19.709	18.772	8.757	10.249	21.509	6.095	12.692	6.002	16.030	20.145	9.083	19.256	24.008	13.977	13.192	7.121	14.978	13.714
0.160	9.266	18.680	19.763	18.786	8.703	10.328	21.574	6.031	12.772	5.971	16.001	20.201	9.215	19.299	24.062	14.029	13.225	7.094	14.939	13.687
0.170	9.290	18.658	19.822	18.797	8.665	10.413	21.644	5.975	12.835	5.949	15.970	20.266	9.344	19.338	24.103	14.096	13.265	7.069	14.923	13.671
0.180	9.317	18.646	19.882	18.807	8.644	10.501	21.722	5.930	12.881	5.937	15.941	20.337	9.469	19.373	24.126	14.175	13.314	7.050	14.926	13.665
0.190	9.347	18.644	19.940	18.820	8.641	10.592	21.806	5.896	12.913	5.933	15.918	20.413	9.587	19.402	24.132	14.261	13.368	7.040	14.945	13.666
0.200	9.381	18.652	19.996	18.836	8.657	10.687	21.898	5.874	12.934	5.937	15.904	20.490	9.697	19.424	24.120	14.352	13.427	7.042	14.974	13.671
0.210	9.420	18.669	20.047	18.856	8.690	10.785	21.995	5.863	12.948	5.946	15.900	20.566	9.799	19.442	24.092	14.443	13.490	7.056	15.011	13.675
0.220	9.464	18.693	20.093	18.878	8.735	10.889	22.096	5.863	12.959	5.959	15.907	20.641	9.894	19.457	24.052	14.532	13.559	7.082	15.053	13.675
0.230	9.515	18.723	20.133	18.900	8.790	10.996	22.197	5.874	12.973	5.977	15.924	20.712	9.981	19.473	24.003	14.617	13.633	7.117	15.098	13.668
0.240	9.575	18.757	20.169	18.920	8.849	11.106	22.294	5.896	12.993	5.999	15.952	20.777	10.062	19.491	23.950	14.698	13.715	7.160	15.145	13.653
0.250	9.644	18.796	20.201	18.939	8.910	11.217	22.382	5.928	13.019	6.025	15.988	20.838	10.137	19.514	23.895	14.777	13.805	7.210	15.195	13.634

0.260	9.725	18.842	20.234	18.955	8.974	11.328	22.460	5.969	13.053	6.058	16.033	20.894	10.210	19.541	23.840	14.857	13.904	7.268	15.246	13.615
0.270	9.817	18.896	20.268	18.972	9.040	11.437	22.525	6.019	13.094	6.100	16.086	20.946	10.282	19.575	23.785	14.942	14.013	7.335	15.301	13.602
0.280	9.920	18.960	20.307	18.994	9.111	11.544	22.578	6.080	13.141	6.154	16.147	20.995	10.355	19.614	23.731	15.035	14.131	7.414	15.358	13.599
0.290	10.033	19.035	20.353	19.022	9.193	11.649	22.624	6.155	13.193	6.225	16.216	21.044	10.433	19.659	23.676	15.139	14.257	7.509	15.419	13.610
0.300	10.155	19.123	20.408	19.060	9.290	11.753	22.666	6.250	13.249	6.318	16.294	21.094	10.517	19.711	23.623	15.253	14.393	7.623	15.485	13.639
0.310	10.285	19.225	20.469	19.108	9.409	11.857	22.710	6.369	13.308	6.436	16.381	21.148	10.609	19.770	23.571	15.375	14.536	7.759	15.559	13.685
0.320	10.422	19.341	20.537	19.164	9.554	11.960	22.759	6.517	13.371	6.582	16.479	21.208	10.710	19.838	23.521	15.501	14.688	7.917	15.642	13.747
0.330	10.565	19.470	20.608	19.225	9.726	12.065	22.813	6.697	13.438	6.757	16.588	21.275	10.819	19.914	23.471	15.628	14.847	8.097	15.733	13.825
0.340	10.714	19.612	20.678	19.288	9.922	12.170	22.870	6.910	13.508	6.959	16.708	21.348	10.936	19.994	23.421	15.754	15.014	8.299	15.833	13.916
0.350	10.870	19.763	20.746	19.350	10.137	12.277	22.925	7.154	13.581	7.184	16.839	21.427	11.058	20.077	23.368	15.878	15.187	8.521	15.940	14.016
0.360	11.034	19.921	20.810	19.410	10.366	12.386	22.974	7.425	13.655	7.430	16.981	21.509	11.184	20.158	23.312	16.000	15.363	8.759	16.052	14.121
0.370	11.207	20.080	20.869	19.469	10.601	12.497	23.013	7.716	13.729	7.691	17.133	21.594	11.315	20.237	23.252	16.120	15.539	9.013	16.167	14.225
0.380	11.390	20.240	20.925	19.527	10.837	12.611	23.043	8.023	13.800	7.964	17.294	21.682	11.451	20.313	23.189	16.241	15.715	9.280	16.284	14.324
0.390	11.583	20.398	20.982	19.587	11.071	12.729	23.065	8.340	13.868	8.248	17.461	21.770	11.590	20.387	23.119	16.364	15.888	9.556	16.402	14.417
0.400	11.784	20.555	21.043	19.648	11.302	12.850	23.083	8.665	13.931	8.539	17.628	21.861	11.732	20.463	23.043	16.491	16.060	9.839	16.520	14.502
0.410	11.992	20.715	21.110	19.713	11.531	12.975	23.100	8.995	13.990	8.837	17.790	21.952	11.876	20.539	22.956	16.624	16.230	10.125	16.639	14.579
0.420	12.206	20.879	21.185	19.781	11.760	13.104	23.120	9.329	14.046	9.140	17.944	22.043	12.022	20.614	22.858	16.766	16.400	10.413	16.757	14.651
0.430	12.425	21.049	21.266	19.851	11.993	13.238	23.144	9.666	14.101	9.449	18.089	22.133	12.170	20.686	22.748	16.917	16.572	10.704	16.878	14.718
0.440	12.650	21.225	21.354	19.924	12.231	13.379	23.172	10.007	14.158	9.764	18.226	22.221	12.323	20.756	22.624	17.076	16.748	10.997	17.001	14.779
0.450	12.883	21.406	21.447	19.998	12.475	13.526	23.204	10.353	14.218	10.084	18.361	22.308	12.482	20.825	22.489	17.244	16.930	11.297	17.129	14.837
0.460	13.125	21.590	21.545	20.075	12.727	13.681	23.240	10.707	14.279	10.410	18.501	22.396	12.646	20.895	22.343	17.420	17.120	11.607	17.262	14.892
0.470	13.379	21.775	21.650	20.153	12.983	13.843	23.280	11.070	14.340	10.744	18.652	22.486	12.816	20.966	22.187	17.602	17.322	11.931	17.396	14.947
0.480	13.648	21.961	21.762	20.231	13.243	14.010	23.324	11.444	14.398	11.086	18.816	22.575	12.989	21.040	22.023	17.788	17.534	12.269	17.531	15.003
0.490	13.934	22.146	21.879	20.307	13.503	14.180	23.371	11.829	14.450	11.436	18.996	22.663	13.163	21.113	21.854	17.976	17.758	12.620	17.664	15.061
0.500	14.237	22.331	22.000	20.378	13.759	14.352	23.420	12.224	14.492	11.795	19.189	22.745	13.335	21.183	21.679	18.165	17.989	12.982	17.793	15.119

Table S5. Coarse-grained form factors for the one-bead per-residue scheme obtained by the IBA method, corresponding to Fig S1(c).

q	ALA	CYS	ASP	GLU	PHE	GLY	HIS	ILE	LYS	LEU	MET	ASN	PRO	GLN	ARG	SER	THR	VAL	TRP	TYR
0.000	9.041	18.610	20.171	19.240	9.214	9.972	21.420	6.247	10.970	6.247	16.544	19.943	8.616	19.012	23.297	13.991	13.060	7.178	15.676	14.165
0.010	9.041	18.609	20.170	19.238	9.217	9.972	21.420	6.250	10.970	6.251	16.544	19.943	8.618	19.011	23.294	13.991	13.061	7.180	15.677	14.165
0.020	9.043	18.609	20.168	19.235	9.225	9.972	21.417	6.260	10.970	6.261	16.544	19.941	8.622	19.008	23.285	13.992	13.063	7.187	15.681	14.164
0.030	9.047	18.607	20.164	19.228	9.239	9.973	21.413	6.277	10.970	6.278	16.544	19.937	8.630	19.002	23.271	13.993	13.066	7.197	15.687	14.162
0.040	9.051	18.605	20.159	19.220	9.257	9.974	21.407	6.299	10.970	6.302	16.544	19.933	8.640	18.994	23.251	13.994	13.071	7.212	15.696	14.159
0.050	9.057	18.603	20.153	19.208	9.281	9.976	21.400	6.329	10.970	6.333	16.544	19.927	8.654	18.984	23.225	13.995	13.078	7.231	15.707	14.156
0.060	9.064	18.600	20.145	19.195	9.310	9.978	21.391	6.364	10.970	6.370	16.544	19.919	8.670	18.971	23.193	13.997	13.085	7.254	15.720	14.153
0.070	9.073	18.596	20.135	19.179	9.344	9.980	21.380	6.405	10.969	6.414	16.544	19.911	8.689	18.956	23.156	13.999	13.095	7.281	15.736	14.148
0.080	9.083	18.592	20.125	19.160	9.383	9.982	21.367	6.453	10.969	6.464	16.544	19.901	8.712	18.939	23.114	14.001	13.105	7.312	15.754	14.143
0.090	9.094	18.587	20.112	19.139	9.426	9.985	21.353	6.506	10.969	6.519	16.543	19.890	8.737	18.919	23.065	14.003	13.117	7.347	15.774	14.137
0.100	9.106	18.582	20.099	19.115	9.474	9.988	21.337	6.564	10.969	6.580	16.543	19.877	8.764	18.898	23.012	14.006	13.130	7.386	15.796	14.131
0.110	9.120	18.576	20.083	19.089	9.526	9.991	21.320	6.628	10.968	6.647	16.543	19.863	8.795	18.874	22.953	14.009	13.144	7.428	15.820	14.124
0.120	9.135	18.570	20.067	19.061	9.582	9.995	21.301	6.696	10.968	6.719	16.542	19.848	8.828	18.848	22.889	14.013	13.160	7.474	15.845	14.117
0.130	9.151	18.563	20.049	19.030	9.642	9.999	21.280	6.770	10.968	6.795	16.541	19.831	8.864	18.819	22.819	14.016	13.177	7.524	15.873	14.109
0.140	9.168	18.555	20.029	18.997	9.706	10.003	21.258	6.847	10.967	6.876	16.540	19.813	8.902	18.789	22.745	14.020	13.195	7.576	15.901	14.100
0.150	9.186	18.547	20.008	18.962	9.772	10.007	21.234	6.929	10.967	6.961	16.539	19.794	8.943	18.756	22.666	14.024	13.214	7.632	15.931	14.091
0.160	9.206	18.538	19.986	18.924	9.842	10.012	21.208	7.015	10.966	7.050	16.537	19.773	8.986	18.721	22.582	14.028	13.234	7.691	15.962	14.081
0.170	9.226	18.528	19.962	18.884	9.915	10.017	21.181	7.104	10.966	7.142	16.535	19.751	9.031	18.685	22.493	14.032	13.255	7.752	15.993	14.071
0.180	9.248	18.518	19.937	18.842	9.990	10.022	21.152	7.197	10.965	7.238	16.533	19.727	9.079	18.646	22.400	14.037	13.277	7.817	16.026	14.061
0.190	9.271	18.508	19.910	18.798	10.067	10.028	21.121	7.292	10.965	7.337	16.530	19.703	9.128	18.604	22.303	14.041	13.300	7.884	16.059	14.050
0.200	9.294	18.496	19.882	18.751	10.147	10.034	21.089	7.391	10.965	7.438	16.527	19.677	9.180	18.561	22.201	14.046	13.324	7.953	16.092	14.039
0.210	9.319	18.484	19.853	18.703	10.228	10.040	21.055	7.492	10.964	7.541	16.523	19.649	9.233	18.516	22.096	14.051	13.349	8.025	16.126	14.028
0.220	9.344	18.471	19.822	18.652	10.310	10.046	21.019	7.595	10.964	7.647	16.519	19.620	9.289	18.469	21.986	14.056	13.375	8.098	16.160	14.016
0.230	9.371	18.458	19.790	18.599	10.394	10.052	20.982	7.700	10.964	7.754	16.515	19.590	9.346	18.420	21.873	14.061	13.401	8.174	16.193	14.004
0.240	9.398	18.443	19.756	18.544	10.479	10.059	20.943	7.807	10.963	7.863	16.509	19.559	9.405	18.369	21.757	14.066	13.428	8.251	16.226	13.992

0.250	9.426	18.429	19.721	18.487	10.564	10.066	20.902	7.916	10.963	7.973	16.504	19.526	9.465	18.316	21.638	14.071	13.456	8.331	16.259	13.979
0.260	9.455	18.413	19.684	18.429	10.650	10.073	20.860	8.025	10.963	8.085	16.497	19.492	9.527	18.262	21.515	14.076	13.484	8.411	16.291	13.967
0.270	9.485	18.396	19.646	18.368	10.737	10.080	20.816	8.136	10.963	8.196	16.490	19.456	9.591	18.205	21.390	14.081	13.513	8.493	16.322	13.955
0.280	9.515	18.379	19.607	18.306	10.823	10.088	20.771	8.248	10.964	8.309	16.482	19.419	9.655	18.147	21.262	14.086	13.542	8.576	16.352	13.942
0.290	9.546	18.361	19.566	18.242	10.909	10.096	20.724	8.360	10.964	8.421	16.473	19.381	9.721	18.087	21.132	14.090	13.571	8.661	16.382	13.930
0.300	9.577	18.343	19.524	18.176	10.995	10.103	20.675	8.473	10.965	8.534	16.464	19.342	9.788	18.026	21.001	14.095	13.601	8.746	16.409	13.917
0.310	9.609	18.323	19.480	18.108	11.080	10.111	20.625	8.586	10.966	8.647	16.454	19.301	9.855	17.963	20.867	14.100	13.631	8.832	16.436	13.905
0.320	9.642	18.303	19.435	18.039	11.164	10.119	20.574	8.699	10.967	8.759	16.442	19.258	9.924	17.898	20.732	14.104	13.661	8.918	16.460	13.893
0.330	9.675	18.282	19.389	17.969	11.248	10.127	20.520	8.812	10.968	8.871	16.430	19.215	9.993	17.832	20.596	14.108	13.691	9.005	16.484	13.882
0.340	9.709	18.260	19.342	17.897	11.330	10.136	20.466	8.924	10.970	8.982	16.417	19.170	10.064	17.764	20.458	14.112	13.721	9.093	16.505	13.870
0.350	9.743	18.237	19.293	17.824	11.411	10.144	20.410	9.036	10.972	9.092	16.404	19.124	10.134	17.695	20.321	14.116	13.751	9.181	16.524	13.859
0.360	9.777	18.214	19.242	17.749	11.490	10.153	20.352	9.148	10.975	9.201	16.389	19.076	10.205	17.625	20.183	14.120	13.781	9.269	16.542	13.849
0.370	9.812	18.190	19.191	17.674	11.568	10.161	20.293	9.259	10.978	9.309	16.373	19.027	10.277	17.554	20.045	14.123	13.811	9.357	16.557	13.839
0.380	9.847	18.164	19.138	17.597	11.644	10.170	20.233	9.368	10.981	9.416	16.357	18.977	10.349	17.481	19.907	14.126	13.841	9.444	16.570	13.830
0.390	9.882	18.138	19.084	17.519	11.718	10.178	20.171	9.477	10.985	9.521	16.339	18.926	10.421	17.408	19.770	14.128	13.870	9.532	16.581	13.821
0.400	9.917	18.111	19.028	17.440	11.790	10.187	20.108	9.585	10.990	9.624	16.320	18.873	10.493	17.333	19.633	14.131	13.899	9.619	16.590	13.812
0.410	9.953	18.083	18.972	17.361	11.860	10.196	20.044	9.691	10.995	9.726	16.301	18.819	10.566	17.258	19.498	14.132	13.928	9.706	16.596	13.805
0.420	9.988	18.055	18.914	17.280	11.928	10.205	19.978	9.796	11.001	9.826	16.280	18.764	10.638	17.181	19.364	14.134	13.956	9.792	16.600	13.798
0.430	10.024	18.025	18.855	17.199	11.994	10.213	19.912	9.899	11.008	9.924	16.259	18.707	10.710	17.104	19.233	14.134	13.984	9.878	16.602	13.792
0.440	10.060	17.995	18.794	17.117	12.058	10.222	19.844	10.001	11.015	10.020	16.236	18.650	10.782	17.026	19.103	14.135	14.011	9.963	16.601	13.787
0.450	10.095	17.963	18.733	17.035	12.119	10.231	19.775	10.101	11.023	10.114	16.213	18.591	10.854	16.948	18.976	14.135	14.037	10.047	16.598	13.783
0.460	10.131	17.931	18.670	16.953	12.177	10.239	19.705	10.199	11.032	10.205	16.189	18.531	10.925	16.869	18.851	14.134	14.063	10.130	16.592	13.780
0.470	10.167	17.898	18.606	16.870	12.233	10.248	19.634	10.295	11.042	10.295	16.164	18.469	10.996	16.790	18.729	14.133	14.087	10.212	16.585	13.778
0.480	10.202	17.864	18.542	16.787	12.287	10.257	19.562	10.389	11.053	10.381	16.138	18.407	11.066	16.710	18.611	14.131	14.111	10.293	16.575	13.777
0.490	10.237	17.829	18.476	16.704	12.338	10.265	19.489	10.481	11.064	10.466	16.111	18.343	11.136	16.630	18.496	14.129	14.135	10.373	16.563	13.777
0.500	10.272	17.793	18.409	16.621	12.387	10.274	19.415	10.571	11.077	10.548	16.084	18.279	11.205	16.550	18.385	14.126	14.157	10.452	16.548	13.778

Table S6. Coarse-grained form factors for the one-bead Cα scheme obtained by our EDM method, corresponding to Fig S2(d).

q	ALA	CYS	ASP	GLU	PHE	GLY	HIS	ILE	LYS	LEU	MET	ASN	PRO	GLN	ARG	SER	THR	VAL	TRP	TYR
0.000	9.032	18.754	20.177	19.220	9.168	9.986	21.372	6.212	10.985	6.229	16.527	19.968	8.642	19.033	23.318	14.013	13.084	7.143	15.697	14.150
0.010	9.033	18.758	20.176	19.209	9.170	9.986	21.366	6.210	10.986	6.227	16.529	19.970	8.637	19.031	23.315	14.009	13.087	7.141	15.703	14.144
0.020	9.037	18.770	20.173	19.179	9.173	9.988	21.351	6.204	10.988	6.221	16.534	19.976	8.625	19.023	23.305	13.997	13.096	7.136	15.721	14.127
0.030	9.044	18.789	20.169	19.134	9.177	9.991	21.328	6.190	10.992	6.208	16.540	19.982	8.609	19.011	23.288	13.981	13.108	7.124	15.746	14.099
0.040	9.054	18.809	20.167	19.081	9.174	9.998	21.301	6.166	11.001	6.187	16.540	19.988	8.596	18.995	23.261	13.964	13.122	7.101	15.772	14.062
0.050	9.067	18.827	20.168	19.028	9.159	10.010	21.272	6.126	11.015	6.151	16.530	19.991	8.590	18.976	23.224	13.951	13.136	7.063	15.792	14.016
0.060	9.082	18.838	20.175	18.983	9.125	10.026	21.246	6.069	11.033	6.099	16.507	19.992	8.596	18.957	23.177	13.945	13.146	7.008	15.800	13.960
0.070	9.097	18.836	20.193	18.953	9.067	10.047	21.225	5.994	11.054	6.029	16.471	19.990	8.618	18.937	23.119	13.948	13.154	6.938	15.789	13.893
0.080	9.109	18.821	20.222	18.941	8.982	10.071	21.212	5.903	11.072	5.942	16.425	19.989	8.652	18.917	23.051	13.960	13.160	6.857	15.757	13.816
0.090	9.114	18.795	20.264	18.947	8.872	10.095	21.207	5.798	11.085	5.841	16.371	19.988	8.697	18.895	22.971	13.979	13.163	6.768	15.702	13.727
0.100	9.108	18.761	20.317	18.966	8.741	10.120	21.209	5.682	11.091	5.732	16.313	19.985	8.750	18.871	22.881	14.004	13.164	6.677	15.626	13.629
0.110	9.091	18.724	20.379	18.991	8.593	10.144	21.218	5.556	11.092	5.616	16.249	19.978	8.808	18.841	22.782	14.032	13.165	6.587	15.527	13.522
0.120	9.060	18.686	20.445	19.014	8.433	10.169	21.228	5.419	11.092	5.496	16.171	19.966	8.871	18.803	22.676	14.061	13.164	6.498	15.406	13.410
0.130	9.017	18.645	20.512	19.028	8.265	10.192	21.235	5.272	11.095	5.373	16.070	19.950	8.935	18.760	22.564	14.090	13.161	6.411	15.266	13.294
0.140	8.965	18.598	20.579	19.028	8.093	10.213	21.235	5.115	11.106	5.246	15.935	19.931	8.999	18.713	22.443	14.116	13.157	6.322	15.107	13.176
0.150	8.905	18.540	20.642	19.015	7.918	10.227	21.222	4.951	11.127	5.116	15.756	19.914	9.062	18.666	22.313	14.136	13.150	6.226	14.932	13.055
0.160	8.841	18.464	20.703	18.990	7.746	10.232	21.196	4.781	11.161	4.983	15.534	19.899	9.122	18.623	22.172	14.149	13.140	6.120	14.745	12.930
0.170	8.773	18.368	20.761	18.958	7.579	10.229	21.156	4.606	11.209	4.848	15.273	19.888	9.182	18.587	22.016	14.153	13.124	6.000	14.549	12.799
0.180	8.703	18.250	20.812	18.925	7.423	10.221	21.104	4.427	11.269	4.712	14.988	19.883	9.245	18.555	21.845	14.152	13.101	5.867	14.348	12.659
0.190	8.632	18.112	20.853	18.893	7.283	10.211	21.044	4.247	11.339	4.576	14.694	19.885	9.312	18.523	21.656	14.148	13.069	5.723	14.144	12.509
0.200	8.558	17.960	20.881	18.865	7.162	10.206	20.978	4.066	11.413	4.443	14.407	19.895	9.384	18.484	21.450	14.146	13.031	5.574	13.943	12.350
0.210	8.485	17.801	20.894	18.839	7.062	10.211	20.909	3.887	11.486	4.313	14.138	19.913	9.458	18.432	21.226	14.148	12.989	5.424	13.745	12.182
0.220	8.413	17.643	20.891	18.814	6.980	10.228	20.841	3.717	11.553	4.191	13.896	19.936	9.528	18.362	20.986	14.155	12.951	5.278	13.552	12.007
0.230	8.345	17.493	20.872	18.784	6.915	10.259	20.776	3.560	11.610	4.078	13.682	19.961	9.587	18.276	20.734	14.163	12.922	5.141	13.365	11.828
0.240	8.286	17.360	20.842	18.745	6.865	10.303	20.715	3.422	11.655	3.977	13.497	19.983	9.631	18.174	20.472	14.171	12.907	5.015	13.185	11.646
0.250	8.239	17.248	20.803	18.694	6.829	10.356	20.658	3.309	11.687	3.893	13.343	19.993	9.658	18.062	20.202	14.177	12.910	4.905	13.014	11.465

0.260	8.207	17.163	20.759	18.625	6.808	10.412	20.602	3.227	11.707	3.828	13.223	19.986	9.669	17.944	19.926	14.181	12.930	4.814	12.856	11.291
0.270	8.188	17.106	20.713	18.539	6.802	10.464	20.541	3.179	11.718	3.788	13.142	19.958	9.667	17.825	19.642	14.187	12.965	4.748	12.718	11.131
0.280	8.184	17.074	20.666	18.434	6.815	10.505	20.468	3.168	11.724	3.777	13.100	19.907	9.658	17.708	19.354	14.195	13.010	4.709	12.603	10.992
0.290	8.192	17.061	20.617	18.312	6.851	10.533	20.379	3.198	11.726	3.799	13.092	19.837	9.645	17.595	19.062	14.207	13.060	4.700	12.517	10.879
0.300	8.212	17.058	20.564	18.177	6.917	10.547	20.269	3.271	11.726	3.859	13.110	19.752	9.633	17.485	18.768	14.225	13.111	4.724	12.461	10.793
0.310	8.244	17.057	20.504	18.033	7.018	10.549	20.138	3.386	11.726	3.958	13.145	19.659	9.627	17.376	18.476	14.247	13.161	4.783	12.432	10.727
0.320	8.286	17.053	20.432	17.881	7.157	10.543	19.988	3.544	11.725	4.098	13.188	19.562	9.626	17.269	18.186	14.272	13.212	4.877	12.426	10.676
0.330	8.336	17.045	20.344	17.722	7.333	10.531	19.823	3.741	11.723	4.279	13.232	19.465	9.630	17.163	17.900	14.300	13.266	5.006	12.434	10.634
0.340	8.393	17.036	20.238	17.557	7.541	10.516	19.646	3.974	11.717	4.495	13.276	19.370	9.633	17.057	17.618	14.327	13.323	5.167	12.452	10.599
0.350	8.456	17.027	20.112	17.387	7.773	10.502	19.462	4.237	11.707	4.743	13.321	19.272	9.633	16.949	17.337	14.352	13.383	5.359	12.471	10.568
0.360	8.524	17.020	19.966	17.211	8.019	10.487	19.272	4.524	11.690	5.013	13.371	19.171	9.629	16.833	17.054	14.376	13.445	5.575	12.487	10.541
0.370	8.596	17.015	19.802	17.029	8.268	10.474	19.077	4.826	11.664	5.296	13.430	19.062	9.622	16.707	16.767	14.396	13.504	5.810	12.497	10.517
0.380	8.673	17.010	19.620	16.840	8.512	10.461	18.878	5.134	11.628	5.584	13.499	18.944	9.615	16.571	16.473	14.414	13.559	6.056	12.499	10.494
0.390	8.753	17.005	19.424	16.643	8.743	10.449	18.675	5.442	11.580	5.869	13.576	18.819	9.612	16.428	16.173	14.426	13.608	6.306	12.495	10.470
0.400	8.835	17.002	19.218	16.438	8.958	10.436	18.470	5.744	11.523	6.147	13.653	18.688	9.615	16.283	15.864	14.430	13.648	6.550	12.489	10.446
0.410	8.916	17.006	19.008	16.227	9.157	10.422	18.265	6.039	11.457	6.414	13.720	18.552	9.626	16.139	15.547	14.427	13.677	6.783	12.484	10.419
0.420	8.994	17.019	18.798	16.014	9.341	10.406	18.061	6.322	11.389	6.672	13.769	18.410	9.646	15.999	15.221	14.416	13.697	7.000	12.485	10.391
0.430	9.067	17.043	18.590	15.801	9.516	10.387	17.856	6.593	11.323	6.922	13.796	18.265	9.676	15.862	14.887	14.400	13.709	7.197	12.492	10.362
0.440	9.132	17.076	18.386	15.592	9.684	10.368	17.651	6.851	11.264	7.165	13.801	18.118	9.717	15.731	14.547	14.382	13.714	7.378	12.507	10.331
0.450	9.192	17.111	18.187	15.392	9.847	10.350	17.446	7.094	11.213	7.402	13.788	17.973	9.767	15.602	14.203	14.361	13.716	7.543	12.526	10.299
0.460	9.249	17.141	17.995	15.201	10.007	10.336	17.241	7.322	11.174	7.634	13.763	17.834	9.827	15.477	13.861	14.337	13.715	7.697	12.548	10.268
0.470	9.306	17.159	17.810	15.020	10.163	10.328	17.038	7.536	11.144	7.860	13.734	17.704	9.892	15.356	13.523	14.309	13.712	7.846	12.567	10.241
0.480	9.367	17.161	17.632	14.847	10.317	10.328	16.840	7.739	11.123	8.079	13.707	17.581	9.959	15.238	13.196	14.277	13.707	7.992	12.578	10.221
0.490	9.434	17.147	17.463	14.681	10.467	10.336	16.647	7.933	11.109	8.292	13.684	17.465	10.024	15.126	12.883	14.243	13.702	8.139	12.579	10.212
0.500	9.507	17.118	17.302	14.519	10.613	10.351	16.463	8.122	11.098	8.499	13.668	17.351	10.081	15.020	12.588	14.207	13.698	8.289	12.566	10.214

Table S7. Comparison of the mean and standard deviation of R values for the six intrinsic disordered protein NMR structure ensembles, using our EDM method. Results from one and two bead COE models are shown.

PDB (No. of structures)	R (2-bead COE)	R (1-bead COE)
1A5R (10)	0.057 ± 0.022	0.115 ± 0.054
1R8U (20)	0.028 ± 0.010	0.425 ± 0.076
2FFT (20)	0.017 ± 0.007	0.090 ± 0.037
2L14 (20)	0.026 ± 0.013	0.183 ± 0.036
2LJL (20)	0.058 ± 0.018	0.174 ± 0.060
2LY4 (10)	0.049 ± 0.022	0.144 ± 0.047

Figure S1

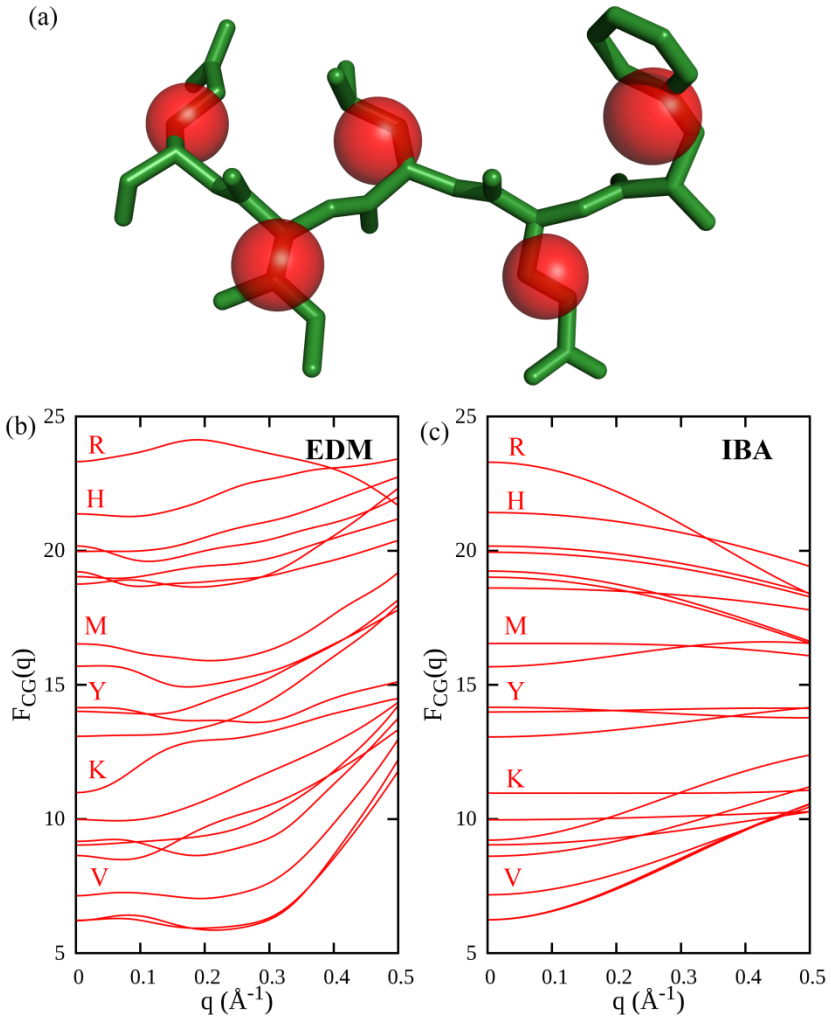

Figure S1 The CG form factors obtained by (b) EDM and (c) IBA, using the one-bead COE CG scheme illustrated in (a). The red curves show the CG form factors representing the 20 types of protein residues. The ordering of the residue form factors is the follows, based on their intensity at q = 0: Arg, His, Asp, Asn, Glu, Cys, Gln, Met, Trp, Tyr, Ser, Thr, Lys, Gly, Phe, Ala, Pro, Val, Leu and Ile.

Figure S2

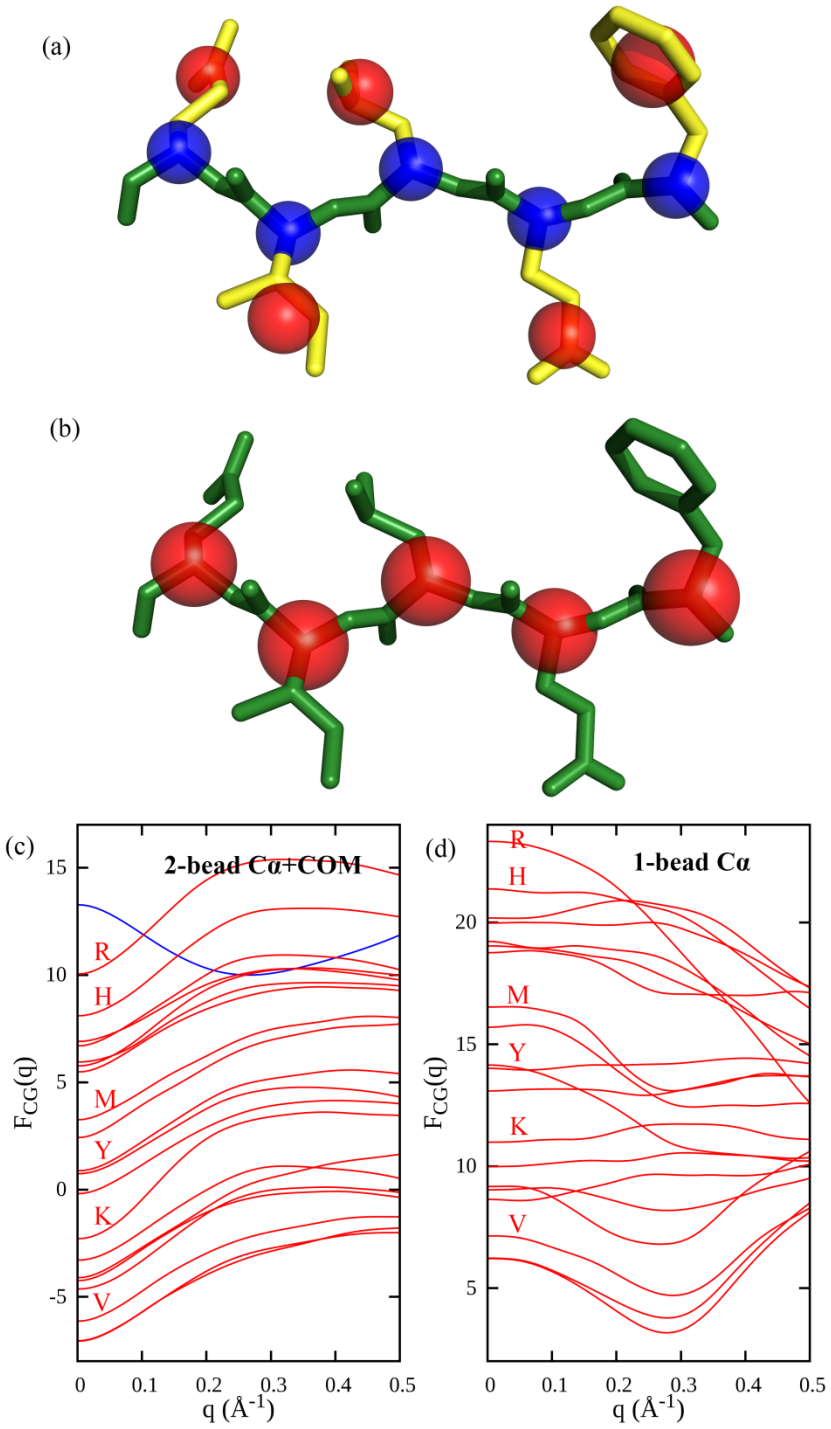

Figure S2 The CG form factors obtained by the EDM method using (a) the two-bead Cα + COM and (b) one-bead Cα CG schemes respectively. The blue curve in (c) shows the CG form factor of the residue backbone. The red curves in (c) represent the CG form factors of the 20 types of residue side-chains, while the red curves in (d) represent the CG form factors of the 20 types of protein residues. The ordering of the side-chain form factors in (c) and the residue form factors in (d) is the follows, based on their intensity at $q = 0$: Arg, His, Asp, Asn, Glu, Cys, Gln, Met, Trp, Tyr, Ser, Thr, Lys, Gly, Phe, Ala, Pro, Val, Leu and Ile.

Figure S3

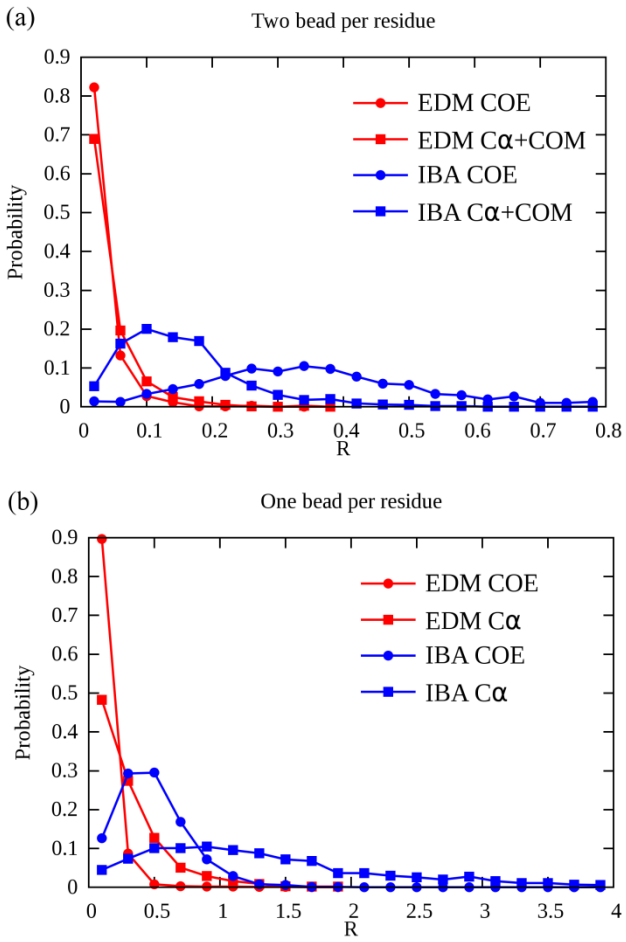

Figure S3 Distribution of R values describing the difference of SAXS profiles between CG and all-atom models. Two different CG schemes are shown: (a) two-bead-per-residue model and (b) one-bead-per-residue model. The results of EDM and IBA are presented in red and blue curves, respectively, where spherical circles represent that the position of each CG bead is placed at its corresponding COE and cubic points represent that the position of each bead is placed at its Cα atom (in the case of a one-bead-per-residue model) or at the Cα atom for its backbone and the centre of mass (COM) of its side-chain (in the case of a two-bead-per-residue model). The R values are computed for the range $q \leq 0.35$ Å^{-1}.

Figure S4

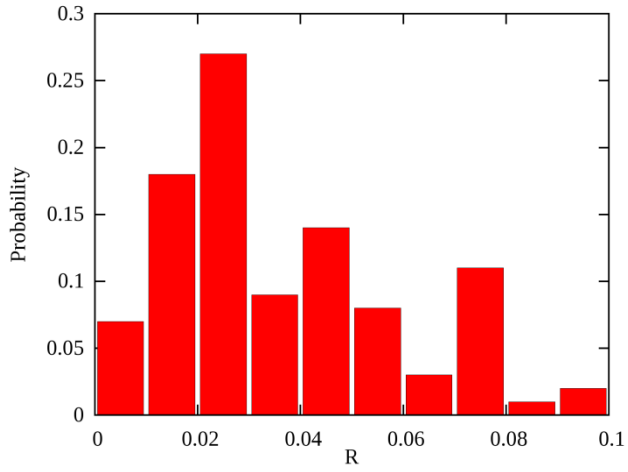

Figure S4 Distribution of R values describing the difference of SAXS profiles between CG and all-atom models for a dataset containing NMR structure ensembles of intrinsic disordered proteins. Six proteins (PDB entries: 1A5R, 1R8U, 2FFT, 2L14, 2LJL, and 2LY4) with total 100 structure models are contained in the dataset. The form factors obtained by our EDM method together with the two-bead COE CG scheme are used to compute the CG SAXS profiles.

Figure S5

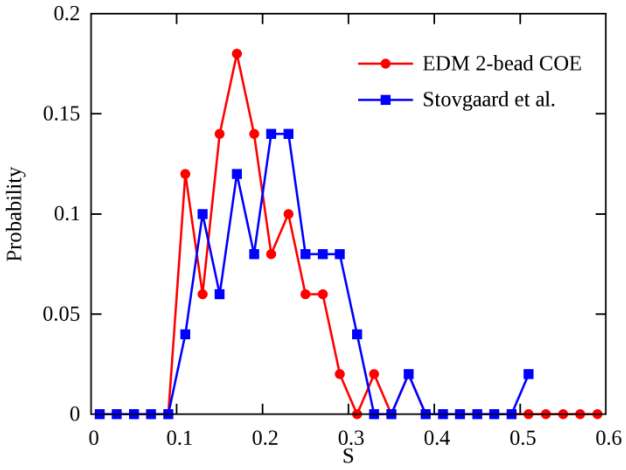

Figure S5 Comparison of the *S* value distribution of the EDM method with that reported by Stovgaard et al. (Stovgaard *et al.*, 2010) *S* is evaluated by $S = \sqrt{\frac{1}{N_q - 1}\sum_q \left[\frac{I_{CG}(q) - I_{AA}(q)}{\sigma(q)}\right]^2}$, where the empirical standard error $\sigma(q_i) = I(q_i)(q_i + \alpha)\beta$ with α=0.15 and β=0.3. We use the same protein dataset from Stovgaard et al. The red histogram shows the distribution of *S* values from our method, and the blue histogram shows the results reported by Stovgaard et al.

Figure S6

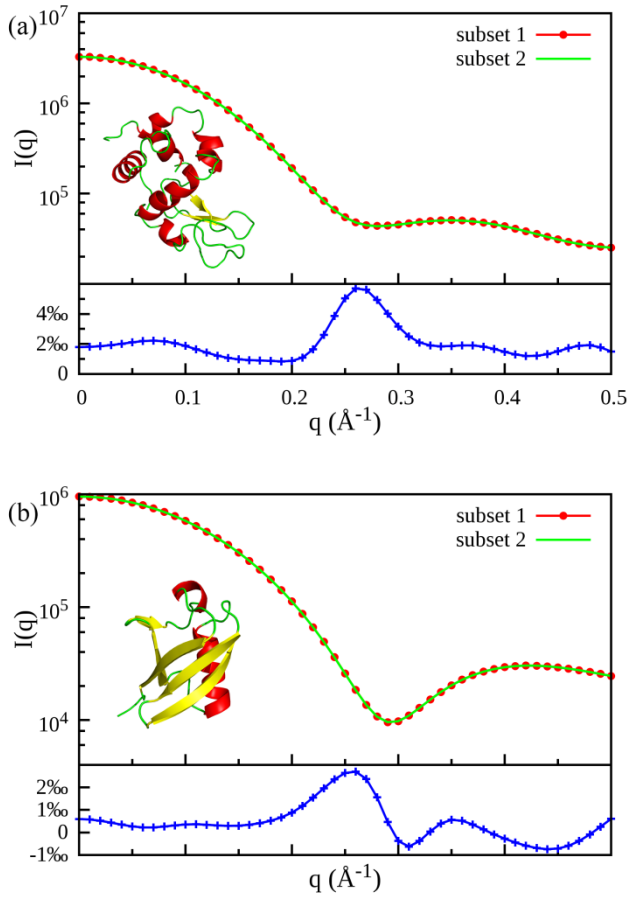

Figure S6 Comparison of CG SAXS profiles computed from different sets of CG form factors. The red line with spheres shows the CG SAXS profiles evaluated with the CG form factors obtained from protein set 1, while the green line shows the results when protein set 2 is used for parameterization. The definition of the two protein sets can be found in section 3.4 of the main text. The blues lines show the relative errors using the atomistic results as the standard. The two proteins are (a) Lysozyme (1LYZ) with 129 residues and (b) Ubiquitin (1UBQ) with 76 residues.

Figure S7

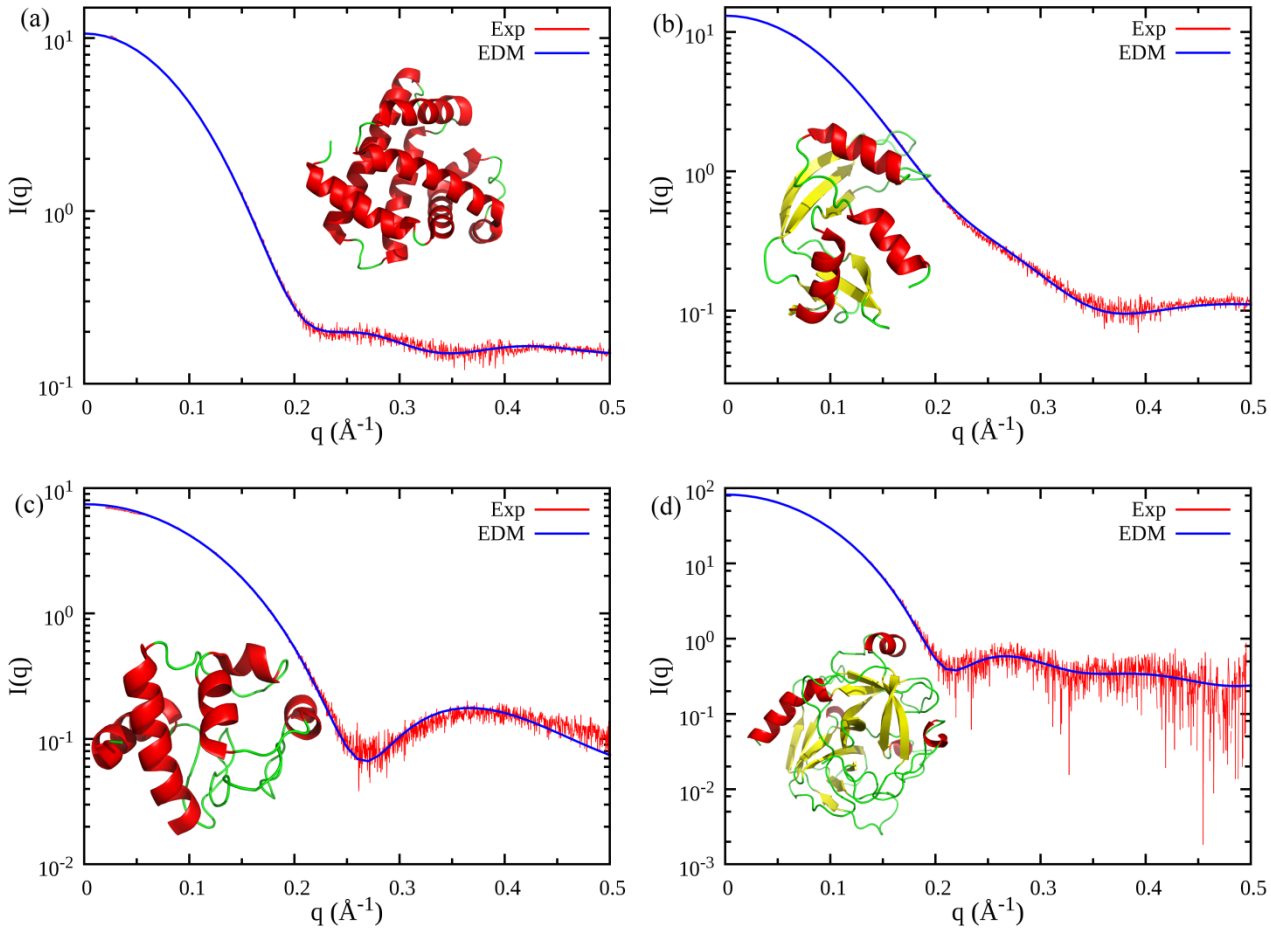

Figure S7 Comparison of EDM-based and experimental SAXS profiles for four additional example proteins, (a) Myoglobin, (b) RNase, (c) Cytochrome C and (d) Chymotrypsinogen A. The experimental SAXS profiles (in red) are obtained from the SASBDB database (http://www.sasbdb.org/). The EDM-based computed SAXS profiles are shown in blue. To achieve a best-fit between computed and experimental SAXS profiles, the scattering contributions from the surrounding hydration layer and from the protein excluded volume are optimized.

Reference

Stovgaard, K., Andreetta, C., Ferkinghoff-Borg, J. & Hamelryck, T. (2010). *Bmc Bioinformatics* **11**, 429.