Electronic supplementary materials *Mendeleev Commun.*, 2026, **36**, 142–144

Efficiency of green-to-red chromophore conversion for AzamiGreen-derived fluorescent proteins

Vladimir B. Krapivin, Roman A. Stepanyuk and Maria G. Khrenova

Table of Contents

Classical molecular dynamic simulations of proteins

The structures of AzamiGreen (AG) and mutant protein AzamiRed1.0 (AR1.0) were taken from the Protein Data Bank (PDB ID 8I4J and 8I4K, respectively) and used for molecular dynamics (MD) simulations. The structures of intermediate mutant proteins were obtained from AR1.0 by replacing the corresponding residues in the molecular editor. MD simulations were performed using the NAMD3[S1] computational package. The CHARMM36, CGenFF and TIP3P force field parameters were used. Protein molecules were placed into a water box with 10 Å minimal distance between solute and boundary. The productive 500 ns phase of MD was preceded by 5000 steps minimization and 5 ps relaxation at 300 K. An isobaric-isothermal ensemble with a Nosé-Hoover barostat and a Langevin thermostat was used. For obtain the most abundant conformation of the chromophore environment, similar to crystal structures of AG and AR1.0, the trajectories were clustering using TTClust[S2] program and Ward's algorithm[S3].

Computational protocol

The initial full-atom structures of the considered proteins were obtained from classical MD simulation trajectories using the clustering method as described above. Conformations of the chromophore environment similar to the crystal structures of AG and AR1.0 and most abundant along 500 ns trajectories were selected. Protein structures in the water box were optimized using QM/MM potentials, and further single-point energy calculations were performed in the presence of water molecules only at distances less than 10 Å from the chromophore. For the AG protein, the initial structure of the red form was obtained by removing hydrogen atoms and changing the conformation of the corresponding peptide bond in a molecular editor, followed by 1000-step MM optimization. In contrast, for the AR0.6, AR1.0, AR1.6 proteins, the green form was obtained by adding hydrogen atoms and editing the structure from the red form of the chromophore. For the AR0.1 protein, two different conformations were considered for both the green and red forms. The QM part of the system included the chromophore (residues 62–64), the nearest residues 65 and 66, the polar residues of the surrounding side chains of Arg91, Lys159, His193 and Glu211, and two to three nearest water molecules.

The QM/MM optimization was performed in the ChemShell program[S4] using the CHARMM36[S5] force field parameters for standard protein residues, CGenFF[S6] for the chromophore, and TIP3P[S7] for water. The QM subsystem was modeled using the hybrid PBE0[S8] functional with empirical corrections for dispersion interactions D3[S9] and the 6-31G** valence-split basis set. Single-point energy calculations were performed using the ORCA program[S10] at the same level of theory. The analysis of electronic structure descriptors was performed based on the ORCA program output using the Multiwfn service.[S11] The contribution of chromophore resonance forms was calculated using the NRT method in the NBO6 program,[S12] taking into account P- and I-forms explicitly specified in the input file using the NRTSTR option.

Table S1 Calculated potential energies (a.u.) of green and red states of considered proteins

	[a]Etot	[b]Eqm	[b]Eqm/mm	[c]Eqm_only
AG green	-3006.579550	-2768.836484	-2771.024222	-2768.318178
AG red	-3004.608611	-2767.584262	-2769.748247	-2767.065023
AR0.1 green (conf 1)	-2736.578002	-2642.901443	-2644.187858	-2642.262407
AR0.1 red (conf 1)	-2734.565065	-2641.648855	-2642.948277	-2641.011362
AR0.1 green (conf 2)	-2736.820882	-2642.886301	-2644.226964	-2642.217979
AR0.1 red (conf 2)	-2735.347380	-2641.647009	-2642.986101	-2640.973434
AR0.6 green	-2756.757763	-2662.834803	-2664.355418	-2661.910744
AR0.6 red	-2754.846557	-2661.595610	-2663.139666	-2660.665906
AR1.0 green	-2833.285579	-2739.212052	-2740.927443	-2738.267906
AR1.0 red	-2831.413730	-2737.975147	-2739.689372	-2737.016085
AR1.6 green	-2756.722962	-2662.816281	-2664.487600	-2661.917940
AR1.6 red	-2754.646504	-2661.581691	-2663.215562	-2660.675913
[d]Chromophore green				-1099.463795
Chromophore red				-1098.244104

[a] Results of QM/MM optimization in water box using ChemShell program. The initial full-atom structures were obtained from the classical MD simulation trajectories by the clusterisation.

[b] Results of QM/MM single point calculations of optimized structures containing all protein residues and water molecules only at a distance less than 10 Å from the chromophore with use of the ORCA program. Eqm is the energy of QM-subsystem taking into account electrostatic interactions with MM part. Eqm/mm is the total energy Eqm plus potential energy of MM-part

[c] Results of single point calculations of only QM-part optimized structures using the ORCA program.

[d] Total electronic energies of green and red states of chromophore optimized in gas phase.

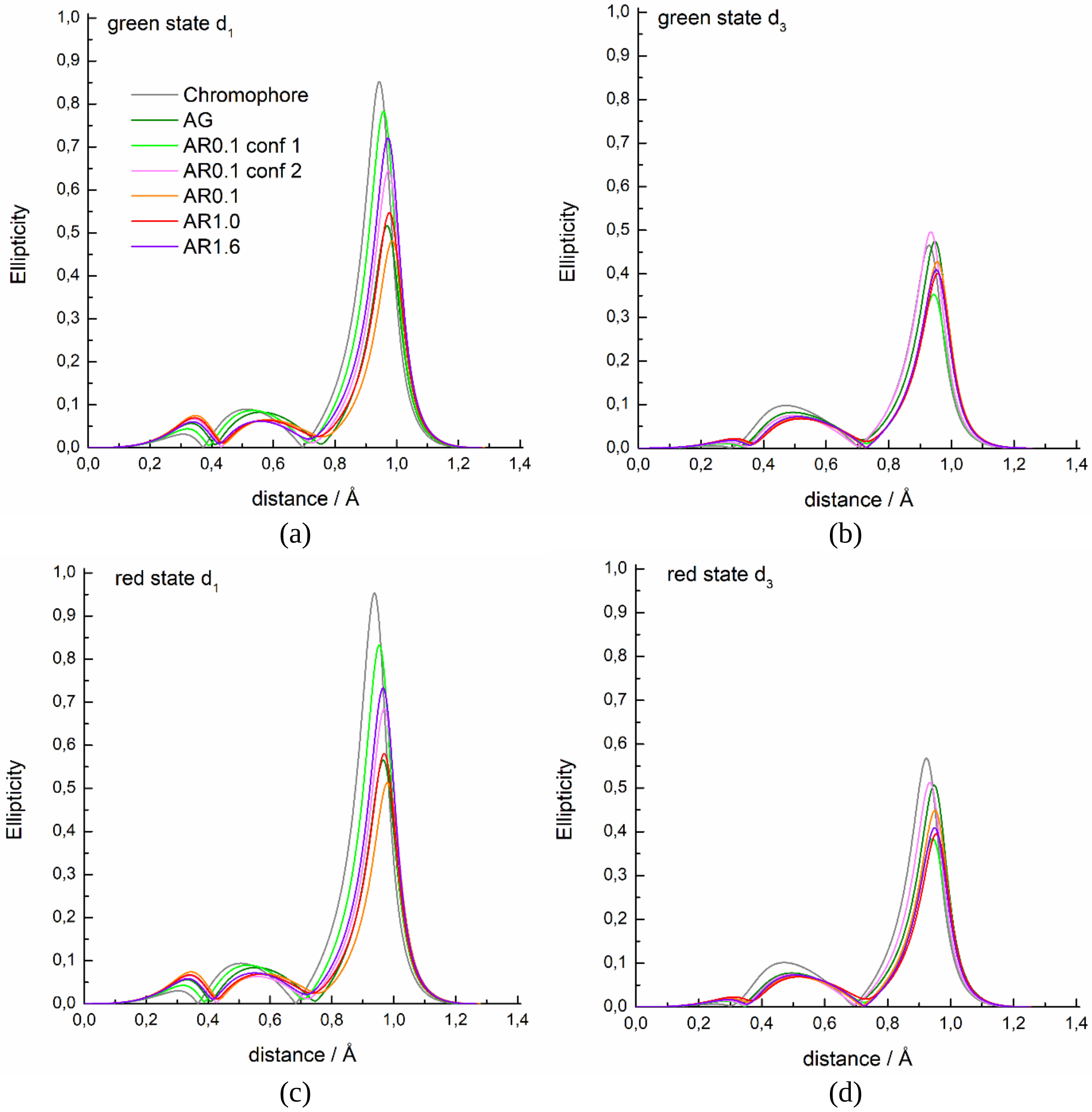

Figure S1 Ellipticity of the electron density along the C-O bonds of chromophore in green (a-b) and red (c-d) states

Table S2 Cartesian coordinates (Å) of QM-part optimized structure for AG protein in green state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	10.242	9.040	-18.629	57	1	12.974	17.229	-17.741
2	8	11.307	8.901	-18.030	58	6	13.912	18.662	-19.097
3	7	10.062	9.923	-19.632	59	1	13.042	18.972	-19.679
4	1	9.195	9.894	-20.153	60	1	14.532	19.559	-19.003
5	6	11.140	10.740	-20.193	61	7	14.714	17.721	-19.869
6	1	12.038	10.513	-19.607	62	1	15.715	17.926	-19.920
7	6	9.062	16.339	-25.067	63	6	14.338	16.505	-20.290
8	6	8.637	17.201	-23.996	64	7	13.080	16.066	-20.164
9	1	8.188	18.152	-24.262	65	1	12.816	15.304	-20.799
10	6	9.650	15.089	-24.677	66	1	12.335	16.681	-19.834
11	1	9.971	14.450	-25.489	67	7	15.237	15.699	-20.843
12	6	9.832	14.735	-23.369	68	1	14.954	14.733	-21.097
13	1	10.320	13.804	-23.104	69	1	16.226	15.912	-20.810
14	6	8.824	16.844	-22.689	70	6	3.840	16.312	-17.940
15	1	8.517	17.525	-21.896	71	1	3.614	15.280	-17.657
16	6	9.422	15.604	-22.317	72	1	3.555	16.436	-18.990
17	6	9.624	15.329	-20.952	73	7	5.249	16.591	-17.745
18	1	9.314	16.109	-20.257	74	1	5.496	17.544	-17.461
19	6	10.157	14.215	-20.335	75	6	6.266	15.789	-18.042
20	8	8.973	16.674	-26.288	76	7	6.027	14.566	-18.514
21	6	10.269	14.076	-18.900	77	1	6.806	13.990	-18.833
22	8	10.014	14.841	-17.946	78	1	5.134	14.379	-18.994
23	7	10.721	12.772	-18.735	79	7	7.516	16.216	-17.836
24	6	10.810	12.192	-19.992	80	1	7.653	17.109	-17.388
25	7	10.511	13.014	-20.945	81	1	8.339	15.613	-17.926
26	6	11.342	10.490	-21.685	82	6	12.086	17.016	-26.058
27	1	12.173	11.116	-22.020	83	1	11.134	17.178	-26.576
28	1	10.457	10.858	-22.210	84	1	12.163	15.939	-25.880
29	6	10.729	12.138	-17.447	85	6	11.633	18.970	-24.384
30	1	10.968	11.077	-17.550	86	1	11.415	19.835	-24.989
31	1	9.745	12.235	-16.984	87	6	12.011	17.702	-24.743
32	6	11.733	12.723	-16.480	88	7	11.543	18.979	-23.015
33	8	11.417	12.898	-15.295	89	1	11.192	19.697	-22.348
34	7	12.953	12.959	-16.974	90	7	12.147	16.993	-23.570
35	1	13.181	12.679	-17.938	91	1	12.393	15.991	-23.455
36	6	14.030	13.421	-16.125	92	6	11.833	17.774	-22.547
37	1	13.575	13.887	-15.251	93	1	11.757	17.487	-21.515
38	6	14.915	12.273	-15.662	94	6	13.925	12.875	-24.054
39	1	15.350	11.772	-16.532	95	1	14.755	13.427	-24.507
40	1	14.288	11.535	-15.153	96	1	13.061	13.042	-24.700
41	6	16.018	12.741	-14.728	97	6	13.734	13.579	-22.714
42	8	16.095	13.899	-14.325	98	8	14.488	13.233	-21.740
43	7	16.911	11.791	-14.392	99	8	12.933	14.540	-22.633
44	1	16.783	10.836	-14.718	100	8	14.256	12.073	-19.296
45	1	17.664	12.014	-13.760	101	1	14.166	12.385	-20.221
46	6	14.874	14.426	-16.896	102	1	14.890	12.708	-18.913
47	8	15.515	14.110	-17.906	103	8	9.356	15.379	-28.705
48	7	14.903	15.659	-16.372	104	1	9.246	15.737	-27.802
49	1	14.455	15.792	-15.464	105	1	8.651	15.779	-29.236
50	6	15.548	16.789	-16.975	106	1	9.350	8.439	-18.340
51	1	15.660	16.555	-18.034	107	1	11.493	9.460	-22.015
52	6	14.724	18.063	-16.761	108	1	16.596	16.906	-16.638
53	1	15.327	18.967	-16.890	109	1	3.264	16.976	-17.298
54	1	14.378	18.077	-15.722	110	1	12.915	17.351	-26.696
55	6	13.522	18.177	-17.699	111	1	14.173	11.801	-24.017
56	1	12.821	18.910	-17.285					

Table S3 Cartesian coordinates (Å) of QM-part optimized structure for AG protein in red state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	10.422	8.830	-18.643	56	6	13.960	18.642	-19.112
2	8	11.454	8.284	-18.267	57	1	13.090	18.970	-19.684
3	7	10.405	10.070	-19.168	58	1	14.591	19.530	-19.014
4	6	10.780	10.778	-20.160	59	7	14.746	17.701	-19.900
5	6	9.162	16.365	-25.216	60	1	15.748	17.903	-19.964
6	6	8.743	17.238	-24.148	61	6	14.367	16.482	-20.307
7	1	8.305	18.194	-24.412	62	7	13.111	16.040	-20.163
8	6	9.725	15.099	-24.824	63	1	12.842	15.276	-20.791
9	1	10.033	14.453	-25.637	64	1	12.371	16.657	-19.827
10	6	9.899	14.746	-23.517	65	7	15.260	15.673	-20.868
11	1	10.367	13.806	-23.245	66	1	14.976	14.703	-21.109
12	6	8.921	16.881	-22.844	67	1	16.249	15.884	-20.841
13	1	8.623	17.566	-22.052	68	6	3.842	16.292	-17.919
14	6	9.505	15.631	-22.468	69	1	3.622	15.257	-17.639
15	6	9.712	15.381	-21.110	70	1	3.546	16.422	-18.965
16	1	9.415	16.177	-20.428	71	7	5.251	16.575	-17.737
17	6	10.227	14.272	-20.451	72	1	5.496	17.525	-17.440
18	8	9.095	16.703	-26.434	73	6	6.269	15.794	-18.077
19	6	10.300	14.202	-19.008	74	7	6.034	14.582	-18.578
20	8	10.094	15.042	-18.106	75	1	6.810	14.015	-18.919
21	7	10.627	12.881	-18.757	76	1	5.138	14.400	-19.055
22	6	10.712	12.229	-19.982	77	7	7.516	16.234	-17.876
23	7	10.520	13.039	-20.990	78	1	7.647	17.122	-17.417
24	6	11.107	10.365	-21.572	79	1	8.353	15.666	-18.021
25	1	11.918	11.000	-21.939	80	6	12.238	16.974	-26.028
26	1	10.233	10.658	-22.164	81	1	11.266	17.095	-26.521
27	6	10.560	12.375	-17.416	82	1	12.363	15.903	-25.836
28	1	10.511	11.287	-17.446	83	6	11.830	18.965	-24.381
29	1	9.646	12.752	-16.952	84	1	11.675	19.841	-24.990
30	6	11.685	12.800	-16.501	85	6	12.171	17.682	-24.723
31	8	11.424	12.971	-15.300	86	7	11.699	18.984	-23.015
32	7	12.908	12.936	-17.023	87	1	11.362	19.717	-22.357
33	1	13.112	12.635	-17.987	88	7	12.247	16.975	-23.544
34	6	14.018	13.356	-16.191	89	1	12.465	15.965	-23.419
35	1	13.590	13.822	-15.304	90	6	11.933	17.772	-22.533
36	6	14.892	12.192	-15.746	91	1	11.818	17.497	-21.502
37	1	15.325	11.695	-16.618	92	6	13.901	12.830	-24.054
38	1	14.263	11.454	-15.240	93	1	14.711	13.389	-24.534
39	6	15.998	12.654	-14.809	94	1	13.019	12.983	-24.678
40	8	16.075	13.811	-14.403	95	6	13.737	13.542	-22.715
41	7	16.892	11.705	-14.474	96	8	14.504	13.203	-21.751
42	1	16.764	10.748	-14.794	97	8	12.934	14.504	-22.626
43	1	17.639	11.931	-13.837	98	8	14.230	12.003	-19.302
44	6	14.875	14.359	-16.959	99	1	14.142	12.293	-20.231
45	8	15.516	14.045	-17.968	100	1	14.867	12.648	-18.941
46	7	14.916	15.590	-16.429	101	8	9.231	15.305	-28.856
47	1	14.477	15.722	-15.516	102	1	9.221	15.729	-27.978
48	6	15.580	16.714	-17.024	103	1	8.575	15.770	-29.396
49	1	15.683	16.489	-18.086	104	1	9.451	8.335	-18.410
50	6	14.781	18.001	-16.791	105	1	11.299	9.318	-21.817
51	1	15.399	18.896	-16.915	106	1	16.633	16.813	-16.694
52	1	14.443	18.010	-15.750	107	1	3.277	16.955	-17.266
53	6	13.574	18.150	-17.716	108	1	13.030	17.324	-26.702
54	1	12.893	18.893	-17.288	109	1	14.163	11.760	-24.018
55	1	13.005	17.214	-17.761					

Table S4 Cartesian coordinates (Å) of QM-part optimized structure for AR0.1 protein (conformation 1) in green state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	54.794	-27.885	20.080	56	1	56.876	-27.947	12.569
2	8	55.796	-28.512	19.711	57	1	57.575	-27.663	10.946
3	7	53.767	-27.537	19.293	58	6	56.656	-25.945	11.79
4	1	52.976	-27.084	19.741	59	1	55.836	-26.148	11.101
5	6	53.539	-28.068	17.940	60	1	57.286	-25.15	11.393
6	1	54.463	-28.586	17.652	61	7	56.028	-25.467	13.05
7	6	47.731	-24.074	13.593	62	1	55.399	-26.18	13.451
8	6	48.121	-25.255	14.314	63	1	55.443	-24.613	12.842
9	1	47.341	-25.976	14.535	64	1	56.702	-25.245	13.789
10	6	48.760	-23.118	13.321	65	6	56.169	-19.04	17.776
11	1	48.476	-22.216	12.791	66	1	55.132	-18.683	17.776
12	6	50.056	-23.358	13.689	67	1	56.359	-19.51	18.746
13	1	50.826	-22.627	13.451	68	7	56.395	-19.972	16.691
14	6	49.416	-25.476	14.695	69	1	56.991	-19.676	15.914
15	1	49.666	-26.385	15.229	70	6	55.754	-21.127	16.505
16	6	50.440	-24.542	14.381	71	7	54.943	-21.61	17.445
17	6	51.798	-24.669	14.722	72	1	54.853	-21.169	18.362
18	1	52.432	-23.867	14.339	73	1	54.44	-22.479	17.309
19	6	52.565	-25.521	15.492	74	7	55.928	-21.788	15.365
20	8	46.535	-23.914	13.182	75	1	56.476	-21.393	14.613
21	6	53.911	-25.107	15.776	76	1	55.477	-22.691	15.227
22	8	54.592	-24.164	15.359	77	6	49.324	-29.105	11.076
23	7	54.349	-25.994	16.748	78	1	50.244	-29.613	10.784
24	6	53.352	-26.918	16.972	79	1	49.071	-29.494	12.069
25	7	52.287	-26.669	16.246	80	6	50.906	-27.139	11.102
26	6	52.357	-29.039	17.990	81	1	51.887	-27.604	11.119
27	1	52.082	-29.322	16.977	82	6	49.645	-27.653	11.098
28	1	51.495	-28.526	18.429	83	7	50.784	-25.776	11.121
29	6	55.636	-25.777	17.357	84	1	51.619	-25.175	11.257
30	1	55.598	-26.027	18.415	85	7	48.783	-26.572	11.116
31	1	55.852	-24.711	17.256	86	1	47.735	-26.536	11.269
32	6	56.746	-26.534	16.641	87	6	49.495	-25.448	11.124
33	8	57.244	-26.175	15.582	88	1	49.065	-24.456	11.118
34	7	57.129	-27.640	17.303	89	6	50.366	-30.689	14.523
35	1	56.622	-27.904	18.142	90	1	49.325	-30.402	14.354
36	6	58.152	-28.523	16.834	91	1	50.733	-31.273	13.677
37	1	59.118	-28.021	16.907	92	6	51.222	-29.463	14.687
38	6	58.151	-29.767	17.738	93	8	52.404	-29.433	14.348
39	1	58.816	-30.525	17.315	94	8	50.618	-28.467	15.286
40	1	58.560	-29.493	18.718	95	1	51.269	-27.718	15.408
41	8	56.864	-30.312	17.851	96	8	53.888	-27.297	11.504
42	1	56.410	-29.882	18.588	97	1	53.639	-26.345	11.587
43	6	57.953	-28.948	15.387	98	1	54.099	-27.572	12.41
44	8	56.839	-29.135	14.891	99	8	54.596	-27.706	14.216
45	7	59.108	-29.194	14.735	100	1	55.327	-28.277	14.513
46	1	59.978	-28.993	15.238	101	1	53.767	-28.191	14.384
47	6	59.147	-29.492	13.315	102	8	46.238	-26.081	11.72
48	1	58.122	-29.675	12.992	103	1	46.274	-25.242	12.249
49	6	59.709	-28.317	12.489	104	1	45.776	-26.726	12.294
50	1	60.740	-28.094	12.829	105	1	54.725	-27.548	21.133
51	1	59.772	-28.629	11.424	106	1	52.550	-29.971	18.545
52	6	58.866	-27.036	12.546	107	1	59.674	-30.454	13.115
53	1	58.799	-26.657	13.590	108	1	56.855	-18.204	17.664
54	1	59.387	-26.254	11.943	109	1	48.592	-29.408	10.308
55	6	57.463	-27.228	11.963	110	1	50.402	-31.296	15.433

Table S5 Cartesian coordinates (Å) of QM-part optimized structure for AR0.1 protein (conformation 1) in red state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	55.116	-28.203	20.001	55	1	57.621	-27.686	10.809
2	8	55.984	-29.083	19.995	56	6	56.717	-25.965	11.675
3	7	54.636	-27.647	18.868	57	1	55.887	-26.125	10.984
4	6	53.546	-27.676	18.188	58	1	57.353	-25.172	11.282
5	6	47.721	-24.085	13.683	59	7	56.108	-25.513	12.948
6	6	48.129	-25.266	14.402	60	1	55.385	-26.202	13.225
7	1	47.357	-25.995	14.627	61	1	55.582	-24.615	12.781
8	6	48.737	-23.112	13.408	62	1	56.771	-25.387	13.723
9	1	48.436	-22.211	12.887	63	6	56.123	-19.094	17.802
10	6	50.037	-23.346	13.750	64	1	55.085	-18.741	17.810
11	1	50.800	-22.611	13.502	65	1	56.322	-19.570	18.768
12	6	49.428	-25.475	14.771	66	7	56.346	-20.017	16.709
13	1	49.699	-26.385	15.296	67	1	56.945	-19.716	15.937
14	6	50.442	-24.532	14.437	68	6	55.694	-21.163	16.504
15	6	51.807	-24.658	14.719	69	7	54.878	-21.655	17.438
16	1	52.431	-23.886	14.265	70	1	54.808	-21.239	18.369
17	6	52.607	-25.488	15.491	71	1	54.352	-22.506	17.291
18	8	46.528	-23.939	13.272	72	7	55.859	-21.798	15.349
19	6	53.985	-25.092	15.647	73	1	56.440	-21.399	14.623
20	8	54.649	-24.222	15.074	74	1	55.437	-22.715	15.189
21	7	54.465	-25.886	16.670	75	6	49.376	-29.092	11.193
22	6	53.450	-26.738	17.062	76	1	50.304	-29.590	10.912
23	7	52.347	-26.530	16.363	77	1	49.119	-29.479	12.185
24	6	52.343	-28.494	18.569	78	6	50.922	-27.089	11.226
25	1	51.540	-28.354	17.847	79	1	51.899	-27.546	11.286
26	1	51.978	-28.091	19.522	80	6	49.673	-27.635	11.208
27	6	55.782	-25.595	17.190	81	7	50.771	-25.730	11.208
28	1	55.793	-25.729	18.268	82	1	51.593	-25.111	11.346
29	1	55.994	-24.554	16.941	83	7	48.789	-26.572	11.190
30	6	56.875	-26.426	16.526	84	1	47.736	-26.552	11.334
31	8	57.483	-26.056	15.527	85	6	49.476	-25.432	11.185
32	7	57.147	-27.572	17.176	86	1	49.026	-24.449	11.156
33	1	56.430	-27.931	17.797	87	6	50.377	-30.598	14.662
34	6	58.171	-28.470	16.734	88	1	49.322	-30.312	14.592
35	1	59.134	-27.963	16.824	89	1	50.660	-31.148	13.764
36	6	58.146	-29.712	17.639	90	6	51.213	-29.348	14.754
37	1	58.838	-30.462	17.242	91	8	52.227	-29.174	14.080
38	1	58.511	-29.431	18.634	92	8	50.750	-28.471	15.614
39	8	56.853	-30.240	17.695	93	1	51.350	-27.671	15.618
40	1	56.443	-29.939	18.527	94	8	53.852	-27.058	12.733
41	6	57.996	-28.897	15.287	95	1	53.483	-26.184	12.451
42	8	56.887	-29.043	14.767	96	1	53.239	-27.439	13.377
43	7	59.154	-29.174	14.651	97	8	54.403	-29.068	16.055
44	1	60.021	-28.992	15.163	98	1	55.334	-29.108	15.776
45	6	59.187	-29.501	13.239	99	1	53.906	-29.165	15.235
46	1	58.159	-29.684	12.926	100	8	46.251	-26.109	11.786
47	6	59.752	-28.354	12.378	101	1	46.272	-25.275	12.321
48	1	60.787	-28.129	12.706	102	1	45.792	-26.764	12.353
49	1	59.804	-28.694	11.321	103	1	54.855	-27.771	20.992
50	6	58.919	-27.066	12.410	104	1	52.502	-29.576	18.693
51	1	58.854	-26.673	13.449	105	1	59.701	-30.472	13.065
52	1	59.449	-26.296	11.799	106	1	56.804	-18.253	17.688
53	6	57.514	-27.255	11.828	107	1	48.652	-29.405	10.419
54	1	56.926	-27.970	12.440	108	1	50.477	-31.238	15.543

Table S6 Cartesian coordinates (Å) of QM-part optimized structure for AR0.1 protein (conformation 2) in green state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	40.253	8.529	21.695	56	1	41.972	10.697	28.763
2	8	40.503	9.712	21.963	57	1	43.227	10.490	30.049
3	7	39.597	7.684	22.502	58	6	43.296	9.072	28.433
4	1	39.418	6.741	22.170	59	1	44.300	8.733	28.669
5	6	38.969	8.082	23.766	60	1	43.147	9.015	27.359
6	1	39.191	9.148	23.875	61	7	42.335	8.152	29.077
7	6	37.910	1.959	29.136	62	1	41.341	8.307	28.769
8	6	39.221	2.279	29.643	63	1	42.347	8.287	30.109
9	1	39.578	1.717	30.501	64	1	42.583	7.156	28.938
10	6	37.480	2.705	27.972	65	6	46.707	2.507	25.710
11	1	36.517	2.435	27.555	66	1	46.193	1.550	25.842
12	6	38.228	3.710	27.437	67	1	46.705	2.751	24.644
13	1	37.857	4.262	26.581	68	7	46.096	3.560	26.489
14	6	39.978	3.258	29.073	69	1	46.564	3.852	27.349
15	1	40.963	3.485	29.475	70	6	44.957	4.193	26.212
16	6	39.512	4.039	27.967	71	7	44.310	3.955	25.069
17	6	40.358	5.035	27.475	72	1	44.815	3.620	24.247
18	1	41.341	5.059	27.942	73	1	43.434	4.437	24.869
19	6	40.266	6.018	26.494	74	7	44.459	5.030	27.108
20	8	37.169	1.098	29.677	75	1	44.859	5.069	28.033
21	6	41.416	6.814	26.181	76	1	43.682	5.670	26.894
22	8	42.571	6.860	26.642	77	6	36.869	4.597	30.821
23	7	40.998	7.640	25.151	78	1	36.672	4.746	29.755
24	6	39.673	7.369	24.893	79	1	36.961	3.524	31.000
25	7	39.215	6.411	25.660	80	6	39.182	4.798	31.965
26	6	37.460	7.869	23.724	81	1	39.258	3.876	32.521
27	1	37.041	8.110	24.701	82	6	38.152	5.250	31.190
28	1	37.237	6.814	23.534	83	7	40.174	5.748	31.910
29	6	41.793	8.767	24.755	84	1	41.152	5.687	32.249
30	1	41.847	8.870	23.671	85	7	38.560	6.470	30.690
31	1	42.797	8.565	25.143	86	1	38.069	7.027	29.988
32	6	41.242	10.025	25.422	87	6	39.781	6.751	31.132
33	8	40.659	9.971	26.495	88	1	40.348	7.642	30.921
34	7	41.397	11.194	24.753	89	6	34.869	7.538	27.393
35	1	41.817	11.179	23.834	90	1	34.303	6.708	27.828
36	6	40.512	12.305	25.074	91	1	34.819	8.367	28.100
37	1	40.854	13.138	24.460	92	6	36.319	7.104	27.349
38	6	39.069	11.960	24.699	93	8	37.101	7.352	28.262
39	1	38.762	11.069	25.258	94	8	36.662	6.411	26.286
40	1	38.406	12.771	25.005	95	1	37.623	6.145	26.367
41	8	38.917	11.800	23.302	96	8	39.647	8.444	28.805
42	1	39.477	11.070	22.986	97	1	39.186	7.849	28.199
43	6	40.596	12.764	26.530	98	1	39.220	9.327	28.627
44	8	39.583	12.892	27.222	99	8	35.773	-0.570	28.073
45	7	41.814	13.115	26.988	100	1	36.188	0.170	28.559
46	1	42.586	13.120	26.325	101	1	35.771	-1.280	28.731
47	6	42.062	13.320	28.404	102	8	38.349	10.686	28.379
48	1	41.380	12.677	28.964	103	1	38.855	11.435	28.026
49	6	43.508	12.938	28.766	104	1	37.661	10.551	27.700
50	1	44.207	13.681	28.350	105	1	40.594	8.083	20.736
51	1	43.607	12.982	29.873	106	1	36.951	8.489	22.975
52	6	43.919	11.539	28.303	107	1	41.785	14.334	28.776
53	1	43.853	11.454	27.194	108	1	47.741	2.426	26.018
54	1	44.983	11.361	28.583	109	1	36.033	4.970	31.428
55	6	43.044	10.470	28.951	110	1	34.395	7.804	26.435

Table S7 Cartesian coordinates (Å) of QM-part optimized structure for AR0.1 protein (conformation 2) in red state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	39.879	8.942	21.596	55	1	43.275	10.527	30.075
2	8	39.640	10.137	21.397	56	6	43.299	9.082	28.481
3	7	39.909	8.407	22.826	57	1	44.309	8.742	28.688
4	6	39.136	7.732	23.595	58	1	43.117	9.018	27.414
5	6	37.902	1.934	29.080	59	7	42.354	8.171	29.159
6	6	39.197	2.263	29.630	60	1	41.357	8.313	28.855
7	1	39.527	1.706	30.500	61	1	42.378	8.321	30.188
8	6	37.507	2.658	27.886	62	1	42.601	7.173	29.028
9	1	36.567	2.365	27.432	63	6	46.660	2.566	25.605
10	6	38.260	3.667	27.372	64	1	46.137	1.610	25.708
11	1	37.920	4.205	26.494	65	1	46.652	2.845	24.546
12	6	39.959	3.247	29.084	66	7	46.063	3.597	26.424
13	1	40.927	3.489	29.516	67	1	46.554	3.877	27.275
14	6	39.519	4.020	27.957	68	6	44.904	4.214	26.197
15	6	40.361	5.028	27.509	69	7	44.238	4.005	25.059
16	1	41.314	5.089	28.030	70	1	44.737	3.744	24.207
17	6	40.289	5.999	26.504	71	1	43.327	4.436	24.906
18	8	37.150	1.083	29.611	72	7	44.405	4.997	27.140
19	6	41.435	6.827	26.229	73	1	44.827	5.009	28.055
20	8	42.559	6.892	26.758	74	1	43.644	5.663	26.959
21	7	41.058	7.615	25.165	75	6	36.918	4.624	30.782
22	6	39.757	7.274	24.827	76	1	36.738	4.792	29.717
23	7	39.292	6.321	25.617	77	1	37.013	3.549	30.949
24	6	37.733	7.331	23.227	78	6	39.210	4.809	31.971
25	1	37.309	6.664	23.974	79	1	39.279	3.878	32.512
26	1	37.789	6.782	22.280	80	6	38.191	5.275	31.188
27	6	41.852	8.765	24.811	81	7	40.199	5.764	31.953
28	1	42.000	8.825	23.735	82	1	41.173	5.697	32.302
29	1	42.818	8.606	25.303	83	7	38.604	6.507	30.722
30	6	41.203	10.015	25.401	84	1	38.131	7.082	30.025
31	8	40.609	9.969	26.469	85	6	39.817	6.783	31.191
32	7	41.325	11.168	24.701	86	1	40.386	7.679	31.013
33	1	41.735	11.148	23.779	87	6	34.942	7.522	27.303
34	6	40.464	12.295	25.031	88	1	34.378	6.693	27.743
35	1	40.827	13.129	24.428	89	1	34.902	8.350	28.011
36	6	39.004	12.027	24.641	90	6	36.386	7.079	27.247
37	1	38.699	11.055	25.048	91	8	37.172	7.288	28.165
38	1	38.371	12.780	25.114	92	8	36.724	6.404	26.166
39	8	38.801	12.124	23.250	93	1	37.680	6.120	26.245
40	1	39.137	11.335	22.783	94	8	39.665	8.429	28.835
41	6	40.574	12.741	26.493	95	1	39.225	7.845	28.204
42	8	39.578	12.868	27.209	96	1	39.246	9.319	28.650
43	7	41.801	13.091	26.937	97	8	35.798	-0.628	28.016
44	1	42.567	13.106	26.267	98	1	36.184	0.127	28.498
45	6	42.058	13.309	28.348	99	1	35.800	-1.331	28.682
46	1	41.382	12.668	28.918	100	8	38.390	10.668	28.408
47	6	43.509	12.946	28.711	101	1	38.902	11.403	28.032
48	1	44.197	13.682	28.267	102	1	37.699	10.528	27.733
49	1	43.618	13.023	29.816	103	1	40.244	8.319	20.746
50	6	43.925	11.538	28.288	104	1	37.040	8.172	23.092
51	1	43.845	11.421	27.184	105	1	41.782	14.321	28.727
52	1	44.995	11.375	28.559	106	1	47.694	2.463	25.907
53	6	43.066	10.487	28.982	107	1	36.069	4.980	31.382
54	1	41.991	10.710	28.814	108	1	34.460	7.788	26.351

Table S8 Cartesian coordinates (Å) of QM-part optimized structure for AR0.6 protein in green state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	17.839	-21.482	39.135	59	1	17.875	-13.084	36.037
2	8	18.924	-21.019	38.784	60	1	17.626	-12.736	37.746
3	7	16.659	-21.202	38.552	61	7	16.337	-14.187	36.950
4	1	15.826	-21.657	38.908	62	1	16.131	-14.670	37.846
5	6	16.530	-20.398	37.340	63	1	16.316	-14.917	36.219
6	1	17.557	-20.189	37.024	64	1	15.549	-13.517	36.783
7	6	9.459	-17.142	36.347	65	6	14.371	-14.991	44.763
8	6	9.857	-15.949	37.027	66	1	13.327	-15.320	44.711
9	1	9.142	-15.136	37.078	67	1	14.977	-15.870	45.002
10	6	10.439	-18.180	36.218	68	7	14.795	-14.402	43.505
11	1	10.139	-19.076	35.683	69	1	15.001	-13.402	43.477
12	6	11.707	-18.030	36.714	70	6	14.873	-15.058	42.344
13	1	12.449	-18.808	36.574	71	7	14.620	-16.363	42.286
14	6	11.124	-15.814	37.535	72	1	14.463	-16.922	43.128
15	1	11.413	-14.895	38.040	73	1	14.670	-16.879	41.417
16	6	12.095	-16.843	37.398	74	7	15.166	-14.391	41.229
17	6	13.391	-16.623	37.910	75	1	15.289	-13.391	41.242
18	1	13.554	-15.658	38.397	76	1	15.386	-14.893	40.369
19	6	14.512	-17.429	37.906	77	6	7.064	-18.124	38.932
20	8	8.276	-17.276	35.861	78	1	6.348	-18.722	39.488
21	6	15.740	-17.016	38.538	79	1	7.878	-18.789	38.636
22	8	16.097	-15.938	39.076	80	7	6.419	-17.666	37.678
23	7	16.575	-18.102	38.404	81	1	5.708	-16.928	37.784
24	6	15.886	-19.077	37.679	82	1	7.146	-17.336	36.980
25	7	14.676	-18.716	37.387	83	1	5.989	-18.494	37.215
26	6	15.784	-21.168	36.249	84	6	10.329	-16.475	33.307
27	1	15.573	-20.494	35.417	85	1	10.479	-17.540	33.509
28	1	14.821	-21.511	36.635	86	1	9.371	-16.185	33.742
29	6	17.974	-18.025	38.712	87	6	11.600	-14.383	34.229
30	1	18.307	-18.868	39.321	88	1	10.919	-13.552	34.137
31	1	18.115	-17.101	39.283	89	6	11.445	-15.701	33.902
32	6	18.777	-17.979	37.423	90	7	12.883	-14.247	34.702
33	8	18.215	-17.822	36.331	91	1	13.313	-13.438	35.183
34	7	20.095	-18.163	37.498	92	7	12.639	-16.311	34.201
35	1	20.544	-18.271	38.415	93	1	12.831	-17.325	34.156
36	6	20.842	-18.464	36.287	94	6	13.491	-15.428	34.698
37	1	21.889	-18.588	36.582	95	1	14.488	-15.660	35.042
38	6	20.322	-19.773	35.700	96	6	14.125	-19.876	32.006
39	1	20.224	-20.488	36.531	97	1	13.083	-19.742	31.713
40	1	19.319	-19.589	35.305	98	1	14.785	-19.379	31.291
41	8	21.195	-20.227	34.698	99	6	14.278	-19.176	33.315
42	1	20.708	-20.877	34.157	100	8	13.334	-18.907	34.048
43	6	20.765	-17.305	35.281	101	8	15.517	-18.787	33.586
44	8	20.365	-17.458	34.128	102	1	15.516	-18.271	34.443
45	7	21.196	-16.110	35.753	103	8	16.277	-16.530	35.157
46	1	21.539	-16.080	36.716	104	1	16.849	-17.058	35.760
47	6	20.881	-14.851	35.091	105	1	16.861	-16.435	34.363
48	1	19.913	-14.944	34.590	106	8	8.379	-19.378	34.017
49	6	20.825	-13.695	36.112	107	1	8.236	-18.647	34.646
50	1	21.861	-13.370	36.338	108	1	7.686	-20.033	34.199
51	1	20.316	-12.837	35.623	109	1	17.760	-22.175	39.994
52	6	20.149	-13.989	37.460	110	1	16.352	-22.026	35.861
53	1	20.770	-14.706	38.040	111	1	21.610	-14.613	34.274
54	1	20.134	-13.045	38.050	112	1	14.508	-14.280	45.577
55	6	18.728	-14.553	37.382	113	1	7.442	-17.322	39.560
56	1	18.463	-14.947	38.390	114	1	10.298	-16.269	32.232
57	1	18.700	-15.395	36.663	115	1	14.343	-20.942	31.986
58	6	17.669	-13.531	37.004					

Table S9 Cartesian coordinates (Å) of QM-part optimized structure for AR0.6 protein in red state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	18.338	-21.670	38.973	58	1	17.696	-12.650	37.876
2	8	19.488	-21.816	38.568	59	7	16.409	-14.090	37.044
3	7	17.542	-20.656	38.566	60	1	16.168	-14.581	37.921
4	6	16.495	-20.466	37.859	61	1	16.418	-14.818	36.298
5	6	9.435	-17.211	36.497	62	1	15.621	-13.430	36.860
6	6	9.849	-16.016	37.173	63	6	14.416	-15.031	44.830
7	1	9.129	-15.208	37.253	64	1	13.371	-15.356	44.757
8	6	10.413	-18.255	36.343	65	1	15.016	-15.917	45.060
9	1	10.094	-19.153	35.822	66	7	14.858	-14.417	43.591
10	6	11.693	-18.101	36.794	67	1	15.039	-13.412	43.583
11	1	12.424	-18.885	36.640	68	6	14.939	-15.035	42.410
12	6	11.133	-15.871	37.616	69	7	14.686	-16.339	42.303
13	1	11.440	-14.948	38.104	70	1	14.587	-16.943	43.124
14	6	12.108	-16.899	37.442	71	1	14.765	-16.812	41.415
15	6	13.410	-16.662	37.898	72	7	15.238	-14.329	41.322
16	1	13.580	-15.685	38.356	73	1	15.316	-13.325	41.358
17	6	14.554	-17.456	37.921	74	1	15.395	-14.794	40.430
18	8	8.247	-17.342	36.040	75	6	6.951	-18.145	39.095
19	6	15.733	-17.000	38.619	76	1	6.214	-18.724	39.641
20	8	16.035	-15.895	39.124	77	1	7.752	-18.831	38.812
21	7	16.577	-18.087	38.628	78	7	6.332	-17.679	37.832
22	6	15.946	-19.108	37.926	79	1	5.612	-16.945	37.929
23	7	14.758	-18.756	37.492	80	1	7.069	-17.342	37.158
24	6	15.752	-21.522	37.085	81	1	5.915	-18.503	37.351
25	1	14.883	-21.080	36.597	82	6	10.278	-16.465	33.436
26	1	15.378	-22.255	37.809	83	1	10.363	-17.535	33.650
27	6	17.978	-17.923	38.911	84	1	9.344	-16.105	33.871
28	1	18.341	-18.681	39.604	85	6	11.666	-14.462	34.392
29	1	18.080	-16.934	39.371	86	1	11.014	-13.604	34.379
30	6	18.739	-17.981	37.593	87	6	11.449	-15.754	34.006
31	8	18.145	-17.863	36.516	88	7	12.977	-14.391	34.801
32	7	20.059	-18.179	37.647	89	1	13.433	-13.605	35.303
33	1	20.526	-18.260	38.557	90	7	12.641	-16.413	34.196
34	6	20.794	-18.485	36.430	91	1	12.780	-17.426	34.096
35	1	21.842	-18.609	36.719	92	6	13.551	-15.586	34.693
36	6	20.278	-19.794	35.845	93	1	14.567	-15.855	34.969
37	1	20.188	-20.517	36.669	94	6	14.290	-20.037	32.415
38	1	19.272	-19.616	35.453	95	1	13.320	-19.795	31.980
39	8	21.159	-20.230	34.838	96	1	15.072	-19.504	31.867
40	1	20.682	-20.892	34.301	97	6	14.230	-19.522	33.816
41	6	20.718	-17.324	35.423	98	8	13.202	-19.073	34.308
42	8	20.308	-17.472	34.274	99	8	15.365	-19.529	34.506
43	7	21.170	-16.134	35.890	100	1	15.200	-19.131	35.408
44	1	21.522	-16.109	36.849	101	8	16.425	-16.239	35.288
45	6	20.871	-14.871	35.230	102	1	16.857	-16.930	35.828
46	1	19.894	-14.941	34.744	103	1	16.949	-16.268	34.452
47	6	20.863	-13.710	36.249	104	8	8.357	-19.409	34.142
48	1	21.911	-13.412	36.456	105	1	8.205	-18.696	34.786
49	1	20.369	-12.842	35.763	106	1	7.660	-20.067	34.301
50	6	20.203	-13.979	37.609	107	1	17.993	-22.301	39.822
51	1	20.807	-14.714	38.181	108	1	16.342	-22.064	36.334
52	1	20.227	-13.032	38.196	109	1	21.594	-14.643	34.404
53	6	18.765	-14.495	37.552	110	1	14.544	-14.331	45.656
54	1	18.485	-14.846	38.570	111	1	7.339	-17.350	39.728
55	1	18.710	-15.362	36.862	112	1	10.250	-16.266	32.359
56	6	17.742	-13.450	37.140	113	1	14.464	-21.108	32.308
57	1	17.987	-13.014	36.177					

Table S10 Cartesian coordinates (Å) of QM-part optimized structure for AR1.0 protein in green state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	-0.895	9.936	47.011	60	1	0.344	0.684	46.361
2	8	0.039	9.601	46.278	61	7	-1.286	1.568	47.343
3	7	-1.256	9.296	48.135	62	1	-1.669	2.520	47.512
4	1	-2.018	9.685	48.679	63	1	-1.402	0.942	48.166
5	6	-0.451	8.268	48.789	64	1	-1.902	1.166	46.617
6	1	0.437	8.145	48.160	65	6	-8.416	4.430	45.353
7	6	-4.197	3.046	53.745	66	1	-8.993	4.455	46.286
8	6	-4.283	2.142	52.645	67	1	-8.371	5.450	44.961
9	1	-4.675	1.149	52.844	68	7	-7.089	3.889	45.576
10	6	-3.684	4.362	53.487	69	1	-6.910	2.930	45.264
11	1	-3.628	5.044	54.328	70	6	-6.057	4.516	46.134
12	6	-3.251	4.735	52.244	71	7	-6.088	5.824	46.372
13	1	-2.822	5.719	52.071	72	1	-6.815	6.442	46.011
14	6	-3.890	2.533	51.397	73	1	-5.380	6.245	46.974
15	1	-3.956	1.843	50.558	74	7	-4.977	3.801	46.448
16	6	-3.351	3.828	51.155	75	1	-5.091	2.817	46.727
17	6	-2.925	4.103	49.849	76	1	-4.074	4.225	46.633
18	1	-3.176	3.328	49.123	77	6	-7.369	3.611	56.440
19	6	-2.241	5.146	49.263	78	1	-7.091	3.096	57.359
20	8	-4.567	2.695	54.916	79	1	-8.205	4.275	56.639
21	6	-1.980	5.077	47.854	80	7	-6.205	4.403	55.983
22	8	-2.214	4.176	47.009	81	1	-5.451	3.750	55.587
23	7	-1.359	6.264	47.563	82	1	-6.463	5.091	55.246
24	6	-1.188	6.954	48.768	83	1	-5.763	4.947	56.753
25	7	-1.710	6.329	49.779	84	6	-0.943	2.897	54.739
26	6	-0.064	8.726	50.193	85	1	-0.857	3.983	54.640
27	1	0.367	7.887	50.742	86	1	-1.907	2.660	55.198
28	1	-0.971	9.040	50.715	87	6	-1.092	1.014	52.917
29	6	-0.789	6.521	46.277	88	1	-1.468	0.142	53.436
30	1	-1.036	7.522	45.915	89	6	-0.840	2.275	53.387
31	1	-1.216	5.777	45.595	90	7	-0.798	1.034	51.574
32	6	0.719	6.357	46.341	91	1	-0.984	0.312	50.852
33	8	1.275	5.944	47.363	92	7	-0.412	3.007	52.305
34	7	1.417	6.699	45.253	93	1	-0.221	4.031	52.326
35	1	0.940	7.088	44.438	94	6	-0.402	2.253	51.218
36	6	2.857	6.868	45.345	95	1	-0.107	2.605	50.239
37	1	3.243	6.969	44.330	96	6	2.276	6.400	53.552
38	6	3.125	8.143	46.134	97	1	1.870	6.121	54.526
39	1	2.501	8.930	45.688	98	1	3.214	5.867	53.371
40	1	2.772	7.977	47.158	99	6	1.331	5.914	52.499
41	8	4.486	8.484	46.100	100	8	0.205	5.505	52.774
42	1	4.689	8.949	46.930	101	8	1.845	5.892	51.294
43	6	3.504	5.613	45.936	102	1	1.178	5.496	50.663
44	8	4.192	5.645	46.960	103	8	3.619	4.004	49.067
45	7	3.276	4.491	45.220	104	1	3.870	4.639	48.371
46	1	2.785	4.595	44.336	105	1	4.390	3.925	49.649
47	6	3.527	3.153	45.729	106	8	1.021	4.257	49.480
48	1	3.337	3.131	46.806	107	1	0.845	4.838	48.716
49	6	2.657	2.093	45.022	108	1	1.989	4.054	49.380
50	1	3.137	1.804	44.063	109	8	-4.324	1.960	57.548
51	1	2.656	1.183	45.660	110	1	-4.307	2.027	56.582
52	6	1.217	2.475	44.670	111	1	-3.556	1.404	57.763
53	1	1.206	3.334	43.965	112	1	-1.537	10.812	46.778
54	1	0.787	1.609	44.112	113	1	0.654	9.557	50.189
55	6	0.298	2.789	45.852	114	1	4.597	2.850	45.616
56	1	-0.683	3.078	45.412	115	1	-8.918	3.816	44.609
57	1	0.680	3.663	46.415	116	1	-7.661	2.878	55.701
58	6	0.117	1.637	46.836	117	1	-0.150	2.500	55.387
59	1	0.787	1.769	47.686	118	1	2.471	7.471	53.548

Table S11 Cartesian coordinates (Å) of QM-part optimized structure for AR1.0 protein in red state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	-0.499	9.967	46.761	59	7	-1.322	1.490	47.282
2	8	0.469	10.130	46.014	60	1	-1.729	2.435	47.447
3	7	-0.728	8.833	47.435	61	1	-1.435	0.862	48.105
4	6	-0.815	8.289	48.586	62	1	-1.926	1.078	46.551
5	6	-4.276	3.129	53.706	63	6	-8.464	4.403	45.250
6	6	-4.348	2.182	52.635	64	1	-9.030	4.428	46.188
7	1	-4.742	1.197	52.864	65	1	-8.425	5.424	44.857
8	6	-3.756	4.439	53.410	66	7	-7.134	3.868	45.462
9	1	-3.712	5.147	54.230	67	1	-6.954	2.909	45.153
10	6	-3.306	4.767	52.164	68	6	-6.116	4.482	46.060
11	1	-2.875	5.744	51.960	69	7	-6.145	5.784	46.323
12	6	-3.939	2.529	51.383	70	1	-6.842	6.422	45.935
13	1	-3.994	1.813	50.565	71	1	-5.463	6.187	46.966
14	6	-3.395	3.819	51.104	72	7	-5.049	3.755	46.389
15	6	-2.969	4.051	49.800	73	1	-5.172	2.772	46.670
16	1	-3.198	3.246	49.100	74	1	-4.143	4.168	46.578
17	6	-2.313	5.099	49.172	75	6	-7.471	3.751	56.420
18	8	-4.656	2.821	54.877	76	1	-7.221	3.280	57.369
19	6	-2.078	4.996	47.759	77	1	-8.320	4.416	56.559
20	8	-2.287	4.050	46.960	78	7	-6.301	4.542	55.971
21	7	-1.532	6.200	47.405	79	1	-5.547	3.900	55.582
22	6	-1.366	6.933	48.586	80	1	-6.551	5.231	55.232
23	7	-1.829	6.303	49.636	81	1	-5.866	5.092	56.742
24	6	-0.472	8.908	49.912	82	6	-0.977	2.942	54.623
25	1	-0.383	8.108	50.647	83	1	-0.845	4.022	54.522
26	1	-1.327	9.533	50.206	84	1	-1.959	2.741	55.059
27	6	-0.917	6.372	46.120	85	6	-1.136	1.052	52.812
28	1	-1.236	7.298	45.640	86	1	-1.533	0.190	53.331
29	1	-1.243	5.517	45.514	87	6	-0.861	2.311	53.277
30	6	0.592	6.330	46.284	88	7	-0.827	1.057	51.473
31	8	1.112	5.934	47.330	89	1	-1.020	0.327	50.759
32	7	1.328	6.716	45.239	90	7	-0.402	3.026	52.197
33	1	0.871	7.086	44.403	91	1	-0.190	4.047	52.216
34	6	2.765	6.870	45.378	92	6	-0.397	2.265	51.115
35	1	3.181	6.991	44.377	93	1	-0.085	2.610	50.140
36	6	3.046	8.116	46.204	94	6	2.156	6.557	53.520
37	1	2.424	8.923	45.799	95	1	1.729	6.271	54.483
38	1	2.703	7.920	47.227	96	1	3.075	5.988	53.351
39	8	4.415	8.430	46.154	97	6	1.227	6.090	52.443
40	1	4.632	8.917	46.968	98	8	0.167	5.525	52.713
41	6	3.392	5.597	45.956	99	8	1.678	6.234	51.222
42	8	4.073	5.612	46.984	100	1	1.030	5.818	50.584
43	7	3.171	4.485	45.222	101	8	3.529	3.994	49.102
44	1	2.677	4.596	44.340	102	1	3.781	4.608	48.388
45	6	3.443	3.144	45.712	103	1	4.306	3.929	49.680
46	1	3.248	3.101	46.787	104	8	0.967	4.414	49.552
47	6	2.601	2.077	44.982	105	1	0.779	4.912	48.733
48	1	3.095	1.806	44.025	106	1	1.931	4.184	49.458
49	1	2.609	1.161	45.610	107	8	-4.476	2.075	57.517
50	6	1.160	2.437	44.619	108	1	-4.442	2.119	56.551
51	1	1.141	3.295	43.913	109	1	-3.755	1.464	57.751
52	1	0.742	1.565	44.061	110	1	-1.298	10.740	46.757
53	6	0.235	2.743	45.797	111	1	0.433	9.530	49.950
54	1	-0.750	3.007	45.353	112	1	4.518	2.858	45.601
55	1	0.599	3.629	46.354	113	1	-8.971	3.783	44.513
56	6	0.081	1.595	46.790	114	1	-7.729	2.984	55.702
57	1	0.739	1.757	47.645	115	1	-0.219	2.518	55.294
58	1	0.345	0.645	46.329	116	1	2.398	7.619	53.536

Table S12 Cartesian coordinates (Å) of QM-part optimized structure for AR1.6 protein in green state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	19.153	22.269	27.398	59	1	26.354	27.528	29.003
2	8	19.316	23.253	26.667	60	1	27.293	26.279	28.187
3	7	19.639	22.143	28.639	61	7	26.069	25.594	29.765
4	1	19.408	21.292	29.143	62	1	25.210	25.920	30.243
5	6	20.145	23.240	29.469	63	1	26.831	25.532	30.468
6	1	20.043	24.151	28.873	64	1	25.887	24.635	29.425
7	6	24.814	20.958	35.533	65	6	27.435	17.970	27.213
8	6	25.973	21.357	34.789	66	1	27.483	17.377	28.130
9	1	26.930	21.268	35.294	67	1	26.477	17.765	26.738
10	6	23.541	21.103	34.871	68	7	27.598	19.384	27.489
11	1	22.653	20.806	35.424	69	1	28.545	19.768	27.413
12	6	23.451	21.607	33.600	70	6	26.655	20.174	28.007
13	1	22.493	21.710	33.100	71	7	25.385	19.764	28.050
14	6	25.872	21.808	33.500	72	1	25.036	19.037	27.424
15	1	26.763	22.070	32.932	73	1	24.670	20.307	28.517
16	6	24.611	21.968	32.863	74	7	26.978	21.354	28.527
17	6	24.585	22.442	31.536	75	1	27.952	21.638	28.634
18	1	25.566	22.590	31.079	76	1	26.262	22.075	28.627
19	6	23.542	22.741	30.684	77	6	24.055	17.441	35.443
20	8	24.916	20.485	36.711	78	1	23.732	16.403	35.507
21	6	23.811	23.092	29.311	79	1	23.342	17.975	34.812
22	8	24.879	23.270	28.680	80	7	23.985	18.047	36.791
23	7	22.561	23.235	28.752	81	1	24.401	19.039	36.805
24	6	21.617	23.054	29.760	82	1	22.984	18.181	37.044
25	7	22.159	22.744	30.900	83	1	24.448	17.457	37.504
26	6	19.309	23.335	30.735	84	6	23.774	23.892	36.607
27	1	19.801	24.013	31.427	85	1	22.824	23.479	36.255
28	1	19.285	22.351	31.215	86	1	24.380	23.061	36.975
29	6	22.366	23.806	27.456	87	6	25.728	24.643	35.031
30	1	21.672	23.212	26.856	88	1	26.642	24.314	35.498
31	1	23.348	23.816	26.969	89	6	24.435	24.566	35.458
32	6	21.836	25.223	27.604	90	7	25.709	25.277	33.811
33	8	21.893	25.814	28.685	91	1	26.518	25.396	33.161
34	7	21.264	25.772	26.530	92	7	23.680	25.186	34.484
35	1	21.260	25.276	25.641	93	1	22.676	25.387	34.603
36	6	20.524	27.021	26.635	94	6	24.460	25.596	33.488
37	1	20.375	27.366	25.614	95	1	24.123	26.030	32.551
38	6	19.154	26.768	27.256	96	6	19.143	26.413	33.694
39	1	19.273	26.406	28.283	97	1	19.296	27.399	34.131
40	1	18.604	27.710	27.304	98	1	19.309	26.512	32.613
41	8	18.416	25.868	26.462	99	6	20.246	25.514	34.157
42	1	18.778	24.974	26.587	100	8	21.022	25.740	35.073
43	6	21.335	28.080	27.385	101	8	20.385	24.439	33.380
44	8	20.944	28.602	28.428	102	1	21.182	23.918	33.685
45	7	22.504	28.419	26.788	103	8	19.910	26.957	30.522
46	1	22.694	27.990	25.875	104	1	19.010	27.291	30.336
47	6	23.601	29.042	27.515	105	1	20.420	27.305	29.771
48	1	23.623	28.656	28.538	106	8	23.594	26.504	30.696
49	6	24.951	28.763	26.817	107	1	23.093	27.265	31.070
50	1	25.008	29.369	25.891	108	1	22.940	26.053	30.132
51	1	25.754	29.123	27.494	109	1	18.576	21.382	27.046
52	6	25.258	27.311	26.429	110	1	18.283	23.699	30.586
53	1	24.547	26.965	25.648	111	1	23.473	30.148	27.616
54	1	26.273	27.287	25.968	112	1	28.175	17.627	26.501
55	6	25.216	26.325	27.595	113	1	25.045	17.492	34.998
56	1	25.304	25.294	27.186	114	1	23.623	24.580	37.440
57	1	24.231	26.415	28.095	115	1	18.110	26.053	33.819
58	6	26.325	26.511	28.623					

Table S13 Cartesian coordinates (Å) of QM-part optimized structure for AR1.6 protein in red state

Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	6	18.853	22.633	27.162	58	1	27.323	26.275	28.200
2	8	18.477	23.473	26.339	59	7	26.069	25.648	29.779
3	7	19.887	22.861	27.995	60	1	25.183	25.967	30.216
4	6	20.145	22.866	29.254	61	1	26.813	25.619	30.504
5	6	24.766	20.851	35.463	62	1	25.908	24.677	29.468
6	6	25.906	21.366	34.752	63	6	27.290	18.010	27.199
7	1	26.858	21.333	35.273	64	1	27.303	17.404	28.109
8	6	23.487	20.921	34.787	65	1	26.339	17.840	26.698
9	1	22.616	20.544	35.317	66	7	27.484	19.416	27.503
10	6	23.376	21.456	33.536	67	1	28.432	19.791	27.403
11	1	22.420	21.501	33.029	68	6	26.575	20.205	28.078
12	6	25.788	21.848	33.483	69	7	25.301	19.816	28.169
13	1	26.660	22.199	32.936	70	1	24.906	19.111	27.543
14	6	24.518	21.937	32.831	71	1	24.630	20.357	28.695
15	6	24.480	22.474	31.544	72	7	26.937	21.370	28.612
16	1	25.459	22.697	31.112	73	1	27.917	21.639	28.686
17	6	23.441	22.761	30.659	74	1	26.240	22.107	28.720
18	8	24.894	20.346	36.617	75	6	24.014	17.293	35.404
19	6	23.766	23.112	29.296	76	1	23.713	16.249	35.472
20	8	24.863	23.325	28.735	77	1	23.304	17.801	34.751
21	7	22.549	23.182	28.660	78	7	23.896	17.914	36.743
22	6	21.561	22.959	29.613	79	1	24.311	18.897	36.753
23	7	22.068	22.709	30.804	80	1	22.888	18.051	36.961
24	6	19.130	22.666	30.332	81	1	24.343	17.341	37.479
25	1	19.609	22.670	31.306	82	6	23.746	23.788	36.550
26	1	18.723	21.664	30.180	83	1	22.786	23.381	36.218
27	6	22.424	23.814	27.374	84	1	24.352	22.957	36.920
28	1	21.823	23.211	26.697	85	6	25.693	24.703	35.045
29	1	23.443	23.910	26.982	86	1	26.608	24.555	35.597
30	6	21.804	25.191	27.565	87	6	24.394	24.447	35.384
31	8	21.835	25.752	28.661	88	7	25.674	25.242	33.781
32	7	21.228	25.758	26.502	89	1	26.499	25.426	33.170
33	1	21.251	25.296	25.594	90	7	23.637	24.858	34.312
34	6	20.535	27.034	26.625	91	1	22.601	24.818	34.287
35	1	20.389	27.393	25.607	92	6	24.419	25.323	33.346
36	6	19.155	26.849	27.244	93	1	24.084	25.667	32.370
37	1	19.254	26.364	28.223	94	6	19.178	26.304	33.518
38	1	18.712	27.834	27.406	95	1	19.469	27.020	34.284
39	8	18.323	26.134	26.370	96	1	19.249	26.808	32.547
40	1	18.554	25.187	26.408	97	6	20.243	25.248	33.497
41	6	21.387	28.069	27.361	98	8	20.947	24.959	34.457
42	8	21.019	28.627	28.396	99	8	20.405	24.699	32.301
43	7	22.560	28.379	26.758	100	1	21.164	24.049	32.341
44	1	22.740	27.945	25.846	101	8	19.821	27.145	30.423
45	6	23.658	29.017	27.469	102	1	18.887	27.356	30.233
46	1	23.690	28.643	28.496	103	1	20.292	27.568	29.683
47	6	25.000	28.736	26.761	104	8	23.531	26.361	30.656
48	1	25.046	29.330	25.827	105	1	23.045	27.116	31.063
49	1	25.808	29.107	27.425	106	1	22.879	25.974	30.038
50	6	25.305	27.279	26.393	107	1	18.390	21.624	27.054
51	1	24.596	26.924	25.613	108	1	18.284	23.361	30.369
52	1	26.322	27.250	25.935	109	1	23.529	30.125	27.564
53	6	25.256	26.311	27.572	110	1	28.044	17.661	26.504
54	1	25.366	25.275	27.179	111	1	25.012	17.364	34.984
55	1	24.260	26.391	28.055	112	1	23.616	24.486	37.382
56	6	26.348	26.525	28.613	113	1	18.137	25.957	33.633
57	1	26.379	27.554	28.957					

Table S14 Cartesian coordinates (Å) of chromophore optimized structure in green and red states

Green state					Red state				
Entry	atom number	x	y	z	Entry	atom number	x	y	z
1	7	-2.343	0.640	1.332	1	7	-3.236	-0.045	-0.186
2	6	-1.937	0.371	-0.053	2	6	-1.991	0.324	0.054
3	6	5.811	1.148	0.307	3	6	5.647	1.263	0.233
4	6	5.977	-0.294	0.421	4	6	5.864	-0.182	0.229
5	1	6.995	-0.660	0.537	5	1	6.897	-0.519	0.257
6	6	4.429	1.586	0.150	6	6	4.246	1.682	0.193
7	1	4.274	2.659	0.057	7	1	4.066	2.753	0.192
8	6	3.378	0.720	0.117	8	6	3.221	0.794	0.157
9	1	2.360	1.079	-0.002	9	1	2.188	1.127	0.126
10	6	4.916	-1.149	0.386	10	6	4.830	-1.059	0.192
11	1	5.080	-2.223	0.475	11	1	5.018	-2.131	0.191
12	6	3.568	-0.695	0.236	12	6	3.458	-0.626	0.157
13	6	2.529	-1.633	0.223	13	6	2.453	-1.578	0.125
14	1	2.824	-2.679	0.321	14	1	2.762	-2.623	0.124
15	6	1.153	-1.483	0.118	15	6	1.053	-1.438	0.097
16	8	6.769	1.943	0.342	16	8	6.581	2.075	0.267
17	6	0.238	-2.612	0.155	17	6	0.167	-2.610	0.067
18	8	0.390	-3.826	0.279	18	8	0.413	-3.809	0.108
19	7	-1.024	-1.988	0.035	19	7	-1.109	-2.041	0.021
20	6	-0.820	-0.627	-0.051	20	6	-0.962	-0.655	0.066
21	7	0.436	-0.295	-0.003	21	7	0.328	-0.305	0.106
22	6	-1.526	1.665	-0.739	22	6	-1.563	1.750	0.282
23	1	-1.311	1.472	-1.792	23	1	-0.476	1.810	0.292
24	1	-0.612	2.057	-0.287	24	1	-1.941	2.116	1.244
25	6	-2.252	-2.725	0.081	25	6	-2.275	-2.887	0.147
26	1	-2.857	-2.438	0.949	26	1	-3.021	-2.383	0.767
27	1	-1.942	-3.771	0.196	27	1	-1.937	-3.809	0.624
28	6	-3.071	-2.616	-1.207	28	6	-2.935	-3.315	-1.171
29	8	-2.656	-3.000	-2.286	29	8	-3.098	-4.495	-1.441
30	7	-4.314	-2.087	-1.024	30	7	-3.325	-2.288	-1.959
31	1	-4.515	-1.525	-0.201	31	1	-3.437	-1.373	-1.515
32	1	-4.848	-1.919	-1.862	32	1	-3.892	-2.534	-2.755
33	6	-3.501	0.252	1.886	33	6	-4.264	0.851	-0.069
34	8	-4.432	-0.312	1.319	34	8	-5.367	0.679	-0.560
35	1	-3.557	0.508	2.961	35	1	-4.066	1.755	0.548
36	1	-2.326	2.407	-0.663	36	1	-1.966	2.403	-0.497
37	1	-1.619	0.991	1.942					
38	1	-2.822	-0.045	-0.540					

References

S1 J. C. Phillips, D. J. Hardy, J. D. C. Maia, J. E. Stone, J. V. Ribeiro, R. C. Bernardi, R. Buch, G. Fiorin, J. Hénin, W. Jiang, R. McGreevy, M. C. R. Melo, B. K. Radak, R. D. Skeel, A. Singharoy, Y. Wang, B. Roux, A. Aksimentiev, Z. Luthey-Schulten, L. V. Kalé, K. Schulten, C. Chipot and E. Tajkhorshid, *J. Chem. Phys.*, 2020, **153**, 044130; https://doi.org/10.1063/5.0014475.

S2 T. Tubiana, J.-C. Carvaillo, Y. Boulard and S. Bressanelli, *J. Chem. Inf. Model.*, 2018, **58**, 2178; https://doi.org/10.1021/acs.jcim.8b00512.

S3 J. H. Ward, Jr., *J. Am. Stat. Assoc.*, 1963, **58**, 236; https://doi.org/10.1080/01621459.1963.10500845.

S4 Y. Lu, M. R. Farrow, P. Fayon, A. J. Logsdail, A. A. Sokol, C. R. A. Catlow, P. Sherwood and T. W. Keal, *J. Chem. Theory Comput.*, 2019, **15**, 1317; https://doi.org/10.1021/acs.jctc.8b01036.

S5 R. B. Best, X. Zhu, J. Shim, P. E. M. Lopes, J. Mittal, M. Feig and A. D. MacKerell, Jr., *J. Chem. Theory Comput.*, 2012, **8**, 3257; https://doi.org/10.1021/ct300400x.

S6 K. Vanommeslaeghe, E. Hatcher, C. Acharya, S. Kundu, S. Zhong, J. Shim, E. Darian, O. Guvench, P. Lopes, I. Vorobyov and A. D. Mackerell, Jr., *J. Comput. Chem.*, 2010, **31**, 671; https://doi.org/10.1002/jcc.21367.

S7 W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey and M. L. Klein, *J. Chem. Phys.*, 1983, **79**, 926; https://doi.org/10.1063/1.445869.

S8 C. Adamo and V. Barone, *Chem. Phys. Lett.*, 1997, **274**, 242; https://doi.org/10.1016/S0009-2614(97)00651-9.

S9 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104; https://doi.org/10.1063/1.3382344.

S10 F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 73; https://doi.org/10.1002/wcms.81.

S11 T. Lu, *J. Chem. Phys.*, 2024, **161**, 082503; https://doi.org/10.1063/5.0216272.

S12 E. D. Glendening, C. R. Landis and F. Weinhold, *J. Comput. Chem.*, 2013, **34**, 1429; https://doi.org/10.1002/jcc.23266.