Probing the conformation of FhaC with small angle neutron scattering and molecular modeling

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Supplementary file

Content of this file:

Additional supplemental files:

Movie S1. Illustrative movie of the association of 140 detergent molecules to the membrane protein FhaC. FhaC was initially placed in a lipid bilayer, after which selected lipids were replaced by d17-OG detergent molecules. A subsequent molecular dynamics simulation in vacuo, where protein coordinates were removed from the equations of motion, relaxes the detergent into a momentaneous, nonhomogeneous organization around the protein.

Zip S1. Figures accompanying Figure 6. High resolution images that were used to create Figure 6.

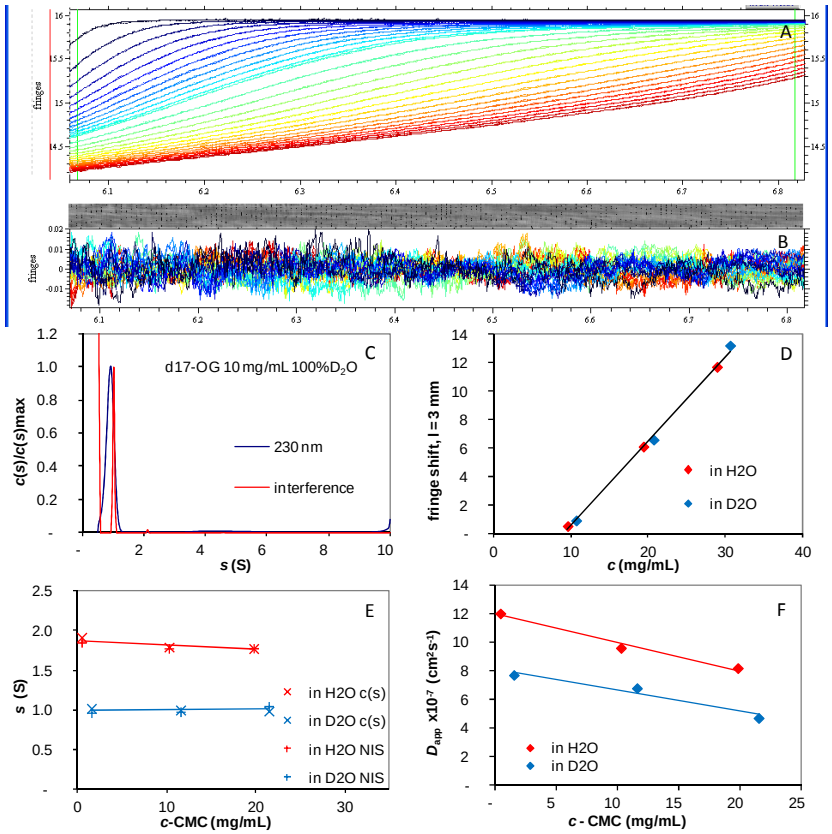

Figure S1. d17-OG characterization by AUC.

Sedimentation velocity was measured during 21 hours at 42000 rpm at 20°C, for samples of d17-OG, at 28.9, 19.4 and 9.6 mg/mL in H_2O and 30.6, 20.7 and 10.7 mg/mL in D_2O, in 3 mm optical path length cells, at 230 nm and using interference optics. The analysis was done with the program SEDFIT v 11.8, in terms of *c*(*s*) analysis and of two non interacting species, *i.e.* monomer and micelle. Panels (A-C) show the *c*(*s*) analysis for d17-OG at 10.7 mg/mL in D_2O. (A): superposition of experimental and fitted sedimentation velocity profiles obtained with interference optics; (B): their differences; (C): superposition of the *c*(*s*) profiles from 230 nm and interference data, showing the micelle at $s \approx 1$ S. In H_2O, $s \approx 1.8$ S. The micelles peak was sometimes splitted. (D): plot of the fringe shift numbers for the micelle as a function of d17-OG concentration. From the mean slope, the refractive index increment $\partial n/\partial c$ and the critical micelle concentration CMC are derived according to e.g. (1). (E): Linear extrapolation of *s* at infinite dilution for d17-OG micelle, leading to *s*°, obtained from interference data analysed in terms of *c*(*s*) and of non-interacting species (NIS). (F): Linear extrapolation of the apparent diffusion coefficients D_{app} at infinite dilution of d17-OG micelle, leading to *D*°, from the non-interacting species analysis of interference data. The diffusion coefficients given by the software are indeed apparent ones, since the boundaries are affected by weak interparticular interactions (2). The obtained numerical values are given in Table SI1.

Table S1. d17-OG characteristics from AUC.

Solvent	$\rho°$	$\eta°$	CMC	+/-	$\partial n/\partial c$	+/-	$s°$	+/-	$D°$	+/-	M_b	+/-	R_H	+/-	M	+/-	N_{agg}	+/-
	g/mL	cp	mM		mL/g		S		x 10^{-7} cm^2 s^{-1}		kDa		nm		kDa			%
H_2O	0.998	1.002	29.5	1.2	0.135	0.005	1.87	0.03	12	1	3.8	0.4	1.8	0	19.8	2.0	64	10
D_2O	1.106	1.250					0.99	0.04	8	1	3.01	0.5	2.1	0	25.6	4.8	83	19

$\rho°$ and $\eta°$ are the solvent density and viscosity. The *cmc* and $\partial n/\partial c$, *s*° and *D*° are derived from Fig. SI1 D-F. The buoyant molar mass, M_b, and hydrodynamic radius, R_H, of the micelle are derived from *s*° and *D*°, according to: $s°/D° = M_b/RT$, and $D° = RT/N_A 6\pi\eta° R_H$, with *R* the gaz constant, *T* the absolute temperature, N_A Avogadro's number. The molar mass *M* and aggregation number, N_{agg}, of the micelles are derived in H_2O from $M_b = M(1-\rho°\bar{v})$, with $\bar{v}$ =0.81 mL/g for d17-OG, calculated assuming the invariance of the molar volumes with deuteration from the value of 0.859 mL/g for n-octyl-glucoside (OG) (3), and the molar mass for d17-OG and OG monomers of 309 and 292.4 g/mole, respectively. In D_2O, we use $M_b = M[(M_D/M) - \rho°\bar{v}]$ (4), with M_D = 313 g/mole the molar mass in D_2O of d17-OG, which has 4 labile Hydrogen atoms. These values are close to that given in litterature for OG: CMC of 18-20 mM, aggregation number of 27-100 or 90, $\partial n/\partial c$ of 0.1159 mL/g (http://www.affymetrix.com and (3)).

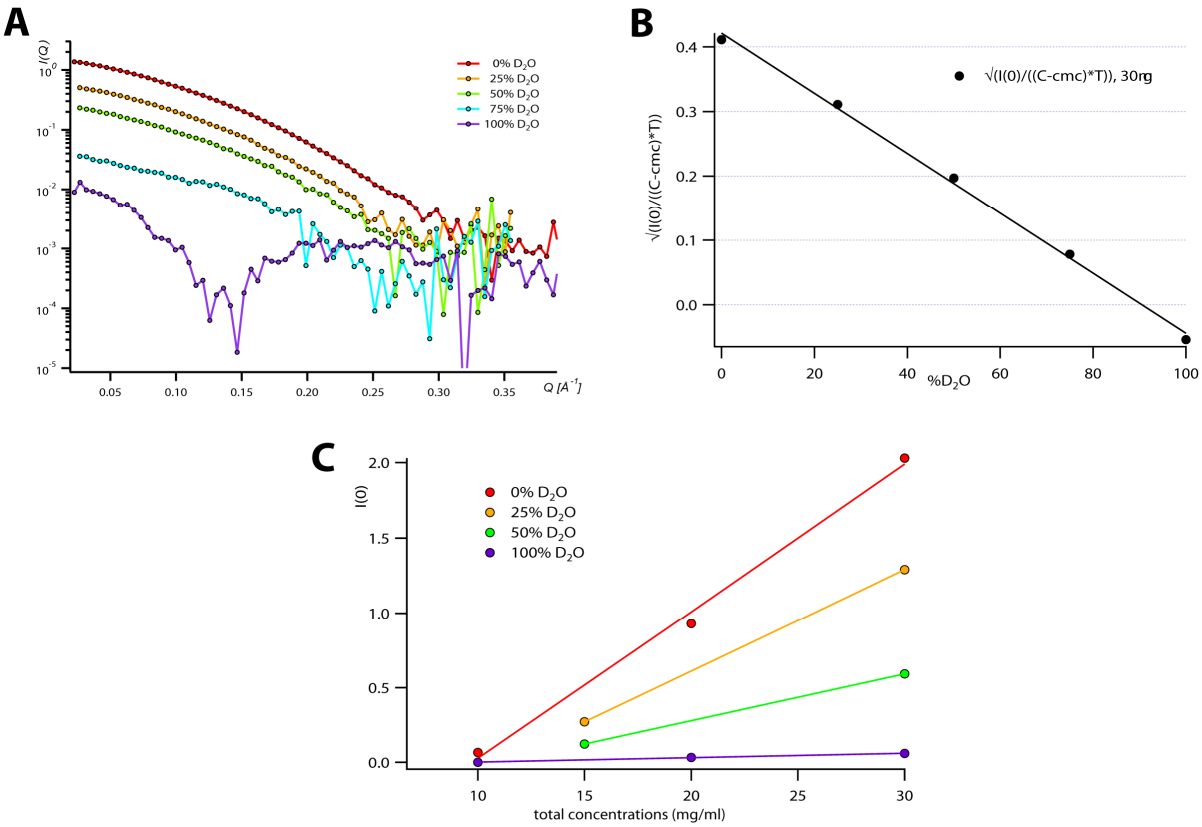

Figure S2. SANS of d17-OG. A) SANS curves at 30 mg/ml as a function of contrast, B) determination of the contrast match point (CMP) from the *I*(0) intensities at 30 mg/ml, C) determination of the critical micelle concentration (CCM) of d17-OG from the *I*(0) intensities as a function of contrast.

Table S2. Complete overview over all WT FhaC detergent models and their respective χ^2 fit values with the program CRYSON.

	WT$_0$		WT$_1$		WT$_2$	
	42% D2O	*90% D2O*	*42% D2O*	*90% D2O*	*42% D2O*	*90% D2O*
120	4,14	1,861	8,343	3,284	3,297	2,166
	6,18	2,11	6,376	1,916	5,414	1,964
	8,12	1,33	4,239	1,844	2,369	2,396
	5,71	2,413	13,72	2,876	6,829	2,159
	9,06	1,787	5,404	1,558	5,287	2,289
	4,53	2,341	3,683	1,962	4,333	2,581
	5,24	1,73	3,202	2,21	5,102	2,257
	6,24	2,249	11,732	2,96	3,838	2,123
	7,48	1,338	4,663	1,974	1,437	2,265
	6,24	1,325	6,169	2,446	4,33	2,08
	7,04	1,354	7,034	1,889	5,353	2,423
	4,91	2,228	5,344	2,071	8,221	2,405
	9,15	2,148	9,803	2,673	8,693	2,061
	8,89	2,069	5,954	2,432	6,047	2,794
	6,54	1,535	5,313	2,794	3,544	2,907
	6,56	1,289	5,276	2,426	2,011	2,009
	2,35	1,561	8,769	2,986	6,979	2,309
	6,55	2,262	4,598	1,988	5,1	2,117
	5,09	2,408	2,921	1,815	5,058	2,673

	4,19	2,002	3,571	2,117	7,911	2,433
	6,21	**1,867**	**6,3057**	**2,31105**	**5,05765**	**2,32055**
125	3,833	1,532	4,623	2,214	5,075	2,197
	4,156	1,578	6,225	2,034	5,356	2,271
	4,814	1,398	4,902	1,812	4,973	2,515
	6,558	2,211	5,646	2,068	3,721	2,335
	4,441	1,789	5,12	2,326	4,769	2,336
	4,002	2,311	8,151	2,616	4,432	2,256
	4,518	1,826	5,063	2,251	5,417	2,71
	4,695	1,694	3,48	2,278	4,62	2,266
	5,651	1,28	7,25	2,409	4,86	2,295
	6,528	1,217	10,134	3,021	6,963	2,316
	6,677	2,245	11,386	3,302	4,638	2,389
	8,831	1,452	8,639	3,396	6,693	2,6
	1,947	1,929	8,716	3,012	3,156	2,429
	7,212	1,545	5,862	2,309	7,623	1,813
	5,679	1,699	4,936	1,925	5,274	1,902
	6,424	1,461	3,771	1,991	6,087	1,7
	5,113	1,77	7,772	3,267	3,066	1,866
	4,555	1,448	9,25	2,761	5,005	2,322
	4,928	2,015	5,305	2,234	5,303	2,825
	4,53	1,543	4,543	2,56	5,719	2,025
	5,25	**1,70**	**6,5387**	**2,4893**	**5,1375**	**2,2684**
130	6,124	1,288	4,468	2,06	4,547	2,085
	1,662	2,09	8,201	2,657	5,616	2,737
	6,374	1,377	3,216	2,404	6,672	2,562
	4,818	2,42	8,2	1,964	6,916	1,907
	7,365	2,038	7,889	3,588	2,728	1,99
	4,876	1,265	6,549	2,643	4,517	1,699
	2,495	2,546	7,099	2,013	6,418	2,307
	7,233	1,309	4,531	1,729	1,953	2,113
	9,079	1,306	6,134	2,727	1,647	2,141
	5,956	1,477	5,246	2,304	5,184	1,878
	3,607	2,452	6,588	2,493	5,534	2,512
	7,257	1,456	8,848	2,587	3,844	2,245
	1,626	2,434	5,32	2,058	6,243	2,428
	4,655	1,696	4,927	2,343	5,916	2,549
	2,873	1,841	2,513	1,643	2,567	2,742
	3,998	1,379	6,359	2,799	3,887	2,13
	6,307	1,584	9,57	1,966	1,974	2,22
	3,371	1,928	8,198	2,767	5,851	2,042
	4,514	1,339	6,136	3,062	5,767	2,501
	6,333	1,723	3,755	2,297	9,559	2,463
	5,02615	**1,7474**	**6,18735**	**2,4052**	**4,867**	**2,26255**
135	4,665	1,298	6,282	2,3	7,225	2,606
	3,316	1,924	3,746	1,262	6,357	2,285
	7,203	1,573	6,673	2,449	5,866	2,461
	2,714	1,552	4,734	1,652	5,919	1,944
	2,555	2,49	4,78	2,527	3,815	2,268
	4,228	1,432	6,352	1,887	6,964	2,389
	3,04	2,115	8,254	2,212	2,172	2,296
	6,888	1,655	4,941	1,453	4,941	2,33
	7,587	1,558	6,393	2,586	4,279	2,635
	6,467	2,035	6,633	2,623	4,693	2,14
	3,542	1,734	4,854	1,836	3,242	1,753
	7,069	1,357	7,208	3,267	5,569	2,646
	3,478	1,965	9,464	2,479	5,435	2,441
	3,534	1,559	5,652	1,801	5,882	2,708
	3,014	2,218	3,861	1,657	7,559	2,521
	8,669	1,854	10,416	2,254	1,759	2,812
	7,107	1,921	5,741	1,927	5,31	1,964
	3,467	1,704	5,296	2,345	3,141	1,963

	3,273	1,89	7,51	2,823	7,689	2,262
	4,542	1,408	3,453	2,467	4,419	2,274
	4,8179	**1,7621**	**6,11215**	**2,19035**	**5,1118**	**2,3349**
140	5,408	1,553	6,48	2,683	3,395	1,825
	2,311	1,883	5,493	1,887	6,908	2,527
	7,352	1,167	7,763	2,659	3,169	1,863
	6,947	1,516	7,172	2,387	3,205	2,351
	2,726	2,763	5,491	2,125	6,5	2,218
	7,2	2,213	6,122	2,435	4,91	2,616
	3,777	2,094	7,339	2,208	3,71	2,008
	4,551	1,818	3,624	1,936	3,659	2,453
	4,157	1,546	7,947	2,047	6,064	2,405
	6,69	1,53	9,528	2,377	5,459	2,469
	6,515	1,466	5,67	2,108	5,45	2,155
	9,957	1,44	4,911	2,533	4,765	2,194
	5,432	2,047	6,521	2,283	3,628	2,121
	2,058	2,022	2,24	1,322	5,253	2,133
	8,015	1,846	7,111	2,719	3,616	2,747
	6,951	1,264	5,497	1,898	1,907	2,176
	5,446	1,928	10,088	2,778	2,792	2,232
	2,648	2,059	9,216	2,808	2,83	2,261
	5,914	1,725	4,876	2,419	4,95	2,319
	9,354	1,617	5,486	3,095	5,56	2,117
	5,67	**1,77485**	**6,42875**	**2,33535**	**4,3865**	**2,2595**
145	5,326	1,616	9,754	3,52	4,262	2,533
	4,471	2,382	3,292	2,067	7,31	2,283
	5,187	1,743	8,456	3,872	4,195	2,085
	5,909	2,251	5,861	2,067	7,602	2,02
	6,214	1,659	4,892	2,31	3,589	2,243
	4,019	1,921	6,981	2,147	5,119	3,18
	2,225	1,79	5,087	1,981	4,713	2,407
	3,733	1,991	6,691	3,102	7,313	2,346
	5,82	1,24	9,69	3,417	2,46	2,012
	5,719	1,726	7,959	2,981	3,252	2,628
	6,739	1,617	6,793	2,432	5,669	2,697
	5,297	1,458	5,613	2,108	4,717	2,724
	6,547	2,043	7,451	2,336	8,197	2,001
	2,512	2,118	1,727	1,281	5,756	2,42
	5,703	1,862	3,086	1,662	2,541	2,32
	5,456	1,717	6,922	3,446	2,979	1,651
	5,132	1,942	9,72	2,965	6,234	2,262
	2,857	2,771	5,343	2,466	3,989	2,424
	7,457	1,888	9,08	3,005	4,108	2,758
	8,037	1,486	5,506	2,713	5,301	2,304
	5,218	**1,86105**	**6,4952**	**2,5939**	**4,9653**	**2,3649**
150	7,92	1,374	4,332	2,642	4,704	2,739
	4,487	2,141	6,897	2,164	7,967	2,777
	7,526	1,367	5,87	2,795	4,772	2,403
	5,707	1,476	10,653	2,557	6,358	2,049
	6,394	1,823	4,964	2,51	4,634	2,434
	5,898	1,899	5,556	2,378	6,555	2,183
	2,006	2,054	4,879	2,325	5,434	3,03
	4,709	1,416	4,987	2,559	5,895	2,516
	5,88	1,722	8,98	2,353	2,707	3,068
	5,365	1,356	6,189	2,215	6,426	2,086
	6,601	1,625	5,57	1,846	6,419	2,836
	9,102	1,774	8,157	2,545	6,996	2,081
	3,901	2,483	6,242	1,823	5,682	2,472
	1,609	2,543	8,513	2,297	5,513	2,587
	5,331	1,233	7,385	2,969	2,549	2,431
	5,689	1,749	8,065	2,007	2,431	2,263
	5,11	1,556	12,873	3,516	2,835	2,326

	4,133	2,229	6,408	2,964	5,052	2,429
	5,354	1,613	8,82	1,955	8,36	2,749
	6,612	1,266	4,645	2,226	3,794	2,689
	5,4667	**1,73495**	**6,99925**	**2,4323**	**5,25415**	**2,5074**
155	4,519	1,44	9,026	3,622	4,172	2,475
	2,496	2,151	3,488	1,224	7,394	2,242
	9,034	1,298	7,862	2,489	2,578	3,027
	8,273	1,306	6,783	1,998	10,361	2,752
	3,024	2,875	5,1	1,991	6,289	1,883
	7,775	1,968	7,643	2,565	5,108	2,299
	4,136	1,97	11,458	3,21	5,31	2,977
	5,372	1,488	8,732	2,805	2,711	3,133
	4,699	1,98	5,466	2,87	2,853	2,625
	6,668	1,187	6,213	2,929	4,983	2,441
	5,305	1,531	3,572	2,599	3,763	2,306
	7,414	1,431	3,211	1,659	4,802	2,946
	3,482	2,44	7,069	2,527	6,865	2,158
	2,941	1,639	4,483	1,645	4,746	2,963
	3,984	1,952	5,631	2,008	5,501	2,853
	6,25	1,377	6,678	2,856	3,993	3,023
	4,339	1,623	7,29	2,39	3,102	2,799
	2,938	1,817	6,051	3,673	3,535	2,272
	10,773	1,425	6,06	2,305	6,168	2,212
	12,115	1,3	8,28	3,613	7,68	2,049
	5,77685	**1,7099**	**6,5048**	**2,5489**	**5,0957**	**2,57175**
160	5,159	1,849	3,582	2,393	5,713	2,043
	6,829	2,011	5,15	2,123	3,174	2,854
	5,66	2,088	2,518	2	3,207	2,891
	5,041	1,663	9,276	2,482	4,127	2,233
	3,388	2,459	5,792	2,078	7,276	2,113
	4,19	2,382	7,053	2,412	6,265	3,591
	6,043	1,399	6,18	2,622	5,829	2,62
	4,347	1,39	8,657	2,073	5,639	3,287
	4,291	1,745	10,187	2,838	10,111	2,39
	5,988	1,35	8,239	2,696	4,218	2,43
	4,597	1,909	4,11	1,643	4,55	2,279
	6,85	1,905	3,737	1,371	5,869	2,695
	3,658	2,328	6,737	2,773	2,943	2,346
	5,976	1,719	4,063	1,827	5,277	2,005
	6,57	1,79	5,567	2,793	2,322	2,935
	5,063	2,032	7,998	2,257	4,315	2,569
	6,799	1,55	10,633	2,923	4,174	2,03
	3,395	2,362	4,425	1,854	3,312	2,637
	2,504	2,461	6,226	2,536	6,502	2,241
	6,686	1,454	5,306	1,768	5,454	2,646
	5,1517	**1,8923**	**6,2718**	**2,2731**	**5,01385**	**2,54175**

Table S3. Complete overview over all FhaC-ΔH1 models and their respective χ^2 fit values with the program CRYSON.

	ΔH_{10}		ΔH_{11}		ΔH_{12}	
	42% D2O	***90% D2O***	***42% D2O***	***90% D2O***	***42% D2O***	***90% D2O***
120	2,79	0,971	3,034	0,885	3,097	0,76
	2,82	0,93	2,565	0,829	3,992	0,764
	2,34	0,963	5,658	0,636	3,404	0,677
	3,21	1,146	2,734	0,681	2,762	0,883
	3,70	1,053	2,944	0,743	3,337	0,712
	3,55	0,903	2,758	0,833	2,769	0,765
	4,34	0,917	1,944	0,832	2,607	0,784

	2,45	0,887	4,028	0,559	3,833	0,598
	3,91	1,058	3,701	0,59	2,425	0,98
	4,43	0,791	3,919	0,798	2,067	0,865
	2,84	1,008	2,424	0,802	4,602	0,795
	3,23	0,719	2,025	0,831	3,745	0,72
	1,96	0,823	2,039	0,82	2,892	0,818
	5,64	0,59	5,563	0,574	4,39	0,861
	3,53	1,053	4,64	0,979	3,429	0,893
	3,43	0,793	2,71	0,832	3,033	0,916
	2,30	0,984	2,814	0,67	3,906	0,912
	3,08	0,799	3,7	0,788	2,867	0,853
	5,23	0,816	2,561	0,94	2,897	0,778
	4,67	0,62	1,421	0,756	2,329	0,921
	3,47205	**0,8912**	**3,1591**	**0,7689**	**3,21915**	**0,81275**
125	3,554	0,971	1,962	0,913	3,795	0,701
	3,815	1,059	3,688	0,614	2,728	0,798
	4,481	0,873	4,584	0,527	3,161	0,876
	3,925	0,99	3,168	0,528	3,72	0,867
	3,704	0,818	3,529	0,755	1,771	0,773
	5,063	0,914	1,451	0,96	4,579	0,844
	2,92	1,024	3,303	0,835	5,646	0,781
	2,405	0,936	1,304	0,596	2,179	0,683
	3,039	0,862	2,443	0,719	4,208	1,026
	4,155	0,668	3,445	0,657	4,249	0,741
	3,373	1,182	1,935	1,194	3,306	0,838
	5,268	0,966	3,572	0,705	3,734	0,663
	4,609	0,732	4,512	0,583	2,89	0,865
	5,685	0,831	4,656	0,56	1,572	0,895
	3,189	0,911	3,114	0,861	3,604	0,679
	4,897	0,994	2,061	0,859	4,286	0,676
	4,45	0,734	2,352	0,722	1,923	1,114
	3,917	0,862	4,515	0,665	3,885	0,93
	3,831	1,143	3,272	0,679	3,825	0,766
	4,298	0,98	2,923	0,9	3,077	0,953
	4,0289	**0,9225**	**3,08945**	**0,7416**	**3,4069**	**0,82345**
130	3,405	1,059	3,331	0,679	3,304	0,802
	3,637	0,714	3,586	0,692	3,4	0,795
	3,366	1,114	3,191	0,599	2,816	1,043
	3,937	1,007	1,608	1,105	4,354	0,642
	4,15	0,907	3,146	0,781	3,973	0,831
	3,595	1,238	1,775	1,195	3,005	0,869
	4,406	0,971	1,647	1,083	3,482	0,955
	2,512	0,825	2,426	0,747	3,581	0,596
	4,551	0,831	3,413	0,651	3,573	0,972
	4,146	0,826	4,221	0,668	3,691	0,837
	3,541	0,828	2,145	1,029	3,36	0,783
	4,274	0,764	4,087	0,691	3,481	0,774
	3,592	0,809	3,183	0,918	3,374	0,845
	4,859	0,796	3,992	0,698	2,055	0,826
	5,803	0,849	3,191	0,801	2,098	1,093
	3,119	1,057	1,353	0,688	4,322	0,683
	4,752	0,681	2,95	0,885	2,522	0,766
	4,561	0,773	4,679	0,589	3,249	0,983
	2,484	1,158	5,477	0,67	3,273	0,803

	5,504	0,872	1,593	0,715	2,071	0,922
	4,0097	**0,90395**	**3,0497**	**0,7942**	**3,2492**	**0,841**
135	3,629	0,821	2,885	0,818	3,434	0,931
	3,023	1,068	3,571	0,55	3,894	0,685
	4,225	0,854	1,84	0,886	2,921	0,759
	2,704	1,074	1,808	0,891	3,622	0,875
	4,1	1,1	4,636	0,811	2,65	0,709
	3,946	1,017	2,401	0,949	2,821	0,678
	3,194	1,016	1,662	1,18	3,475	0,746
	3,886	1,044	3,439	0,668	3,393	0,67
	3,819	1,006	3,536	0,643	3,469	0,771
	2,692	1,171	1,543	0,787	2,397	0,801
	3,261	1,063	1,98	1,013	3,936	0,702
	3,142	0,999	3,733	0,68	3,149	0,671
	3,347	1,113	2,44	0,945	3,379	0,855
	5,543	0,694	3,287	0,829	4,671	0,717
	3,971	0,722	1,901	1,05	3,444	0,811
	4,501	0,648	2,983	0,86	3,94	0,699
	3,519	0,926	3,955	0,564	3,89	0,683
	4,247	1,11	2,833	0,622	4,177	0,983
	3,024	1,139	3,865	0,669	2,587	0,978
	4,921	0,99	1,445	1,208	3,069	0,9
	3,7347	**0,97875**	**2,78715**	**0,83115**	**3,4159**	**0,7812**
140	3,909	1,232	2,09	1,054	2,166	0,873
	3,599	0,917	2,42	1,026	2,704	0,816
	3,036	1,097	1,979	1,091	3,949	0,789
	3,664	1,157	1,507	1,02	3,872	0,772
	3,411	1,094	3,119	0,649	2,788	0,709
	2,896	1,03	3,495	0,934	2,792	0,786
	3,508	1,025	2,055	1,204	3,876	1,017
	2,7	1,107	2,464	1,009	2,245	0,807
	2,593	1,229	2,792	0,797	3,64	0,858
	1,828	1,098	3,965	0,816	1,944	0,854
	3,651	1,244	3,354	1,264	3,962	0,768
	4,26	0,918	1,393	0,947	3,203	0,959
	3,6	1,227	3,33	0,873	2,903	1,178
	4,071	0,904	2,711	0,946	2,863	0,684
	3,728	0,806	1,813	1,245	3,7	0,807
	4,082	0,744	2,494	0,766	2,279	0,744
	2,379	0,978	2,642	0,992	2,327	0,852
	4,758	0,912	1,83	0,883	2,403	0,946
	3,712	1,053	2,975	0,993	3,384	0,938
	2,252	1,253	0,788	0,98	1,557	0,886
	3,38185	**1,05125**	**2,4608**	**0,97445**	**2,92785**	**0,85215**
145	2,412	1,207	1,385	0,893	3,851	0,824
	3,667	0,95	2,498	0,791	3,111	0,753
	2,939	1,225	3,494	0,76	3,367	0,969
	4,413	1,147	2,776	0,829	2,8	0,894
	2,058	1,179	3,887	0,697	1,925	0,804
	3,207	1,194	1,875	1,038	2,817	0,664
	1,589	1,262	2,43	1,018	3,998	0,655
	4,114	0,998	2,411	0,744	3,197	0,713
	2,391	0,972	2,157	1,074	2,547	0,982
	4,586	0,796	3,629	0,952	2,875	0,87

	1,733	1,288	3,388	1,167	3,794	0,751
	4,366	1,064	2,909	0,916	4,698	0,711
	2,341	0,971	1,596	0,792	4,247	0,776
	5,659	0,736	5,673	0,634	3,307	0,672
	2,31	1,376	1,372	0,968	4,122	0,636
	4,767	1,068	2,309	0,712	5,156	0,654
	2,713	0,804	2,573	0,871	3,476	0,763
	5,177	0,824	4,915	0,682	2,794	0,88
	4,245	0,956	3,609	1,047	4,092	0,879
	4,735	0,788	1,91	1,32	1,938	0,708
	3,4711	**1,04025**	**2,8398**	**0,89525**	**3,4056**	**0,7779**
150	3,337	1,045	2,705	0,831	3,079	0,702
	3,232	1,113	4,184	0,759	2,801	0,739
	4,139	1,224	1,463	1,128	3,992	0,825
	5,561	1,321	2,716	0,845	3,43	0,708
	3,573	1,035	2,08	0,932	2,103	1,024
	4,398	1,358	2,825	0,923	2,562	0,799
	4,725	0,817	1,69	1,001	2,208	0,942
	3,074	1,223	2,524	1,101	2,821	0,752
	5,888	0,77	2,287	0,928	2,358	0,938
	3,882	1,118	2,002	1,3	1,912	0,777
	3,426	1,199	2,151	1,329	4,048	0,846
	2,652	1,041	3,445	0,801	3,57	0,785
	3,019	1,256	2,36	1,152	2,066	1,019
	3,787	0,923	1,279	1,272	3,503	0,729
	3,242	1,143	2,591	1,154	2,731	0,77
	3,109	1,164	2,084	0,926	4,527	0,769
	2,316	1,061	1,093	1,285	3,228	0,743
	4,197	1,126	4,024	0,871	3,226	0,792
	3,776	1,008	3,527	0,917	1,188	1,172
	3,999	0,96	2,397	0,998	2,337	1,058
	3,7666	**1,09525**	**2,47135**	**1,02265**	**2,8845**	**0,84445**
155	4,813	0,725	3,388	1,08	2,997	1,007
	3,047	0,954	3,338	0,816	2,418	0,973
	2,656	0,896	1,455	0,985	2,882	1,027
	2,502	1,159	1,052	1,038	3,19	0,961
	2,264	1,587	1,933	1,111	1,193	1,018
	2,76	1,044	3,04	1,029	2,592	0,639
	3,25	1,281	1,728	1,012	3,347	1,034
	4,307	0,877	2,52	0,98	3,025	0,767
	3,69	0,813	2,612	0,896	1,427	1,01
	4,564	0,775	3,47	1,053	2,746	0,912
	3,288	1,211	2,707	1,146	3,181	0,804
	3,173	1,549	2,256	0,89	3,65	0,636
	2,085	1,139	2,686	1,17	3,199	0,959
	4,274	1,094	3,518	0,836	2,739	0,694
	3,887	0,994	2,967	1,06	2,986	0,782
	2,557	1,08	2,837	0,952	3,039	0,754
	2,687	1,317	1,482	1,241	3,454	0,725
	3	1,25	2,19	0,789	2,592	0,903
	3,469	1,209	3,415	0,973	4,336	1,089
	5,188	0,812	1,809	1,043	3,095	1,041
	3,37305	**1,0883**	**2,52015**	**1,005**	**2,9044**	**0,88675**
160	2,973	1,007	3,519	1,296	1,734	1,095

4,546	0,683	4,705	0,908	3,416	0,931
3,783	1,18	4,175	0,904	2,953	1,303
3,083	1,245	1,996	1,018	2,863	0,832
2,141	1,444	1,441	1,121	2,849	0,892
2,355	1,035	2,66	0,937	1,68	0,773
4,323	1,121	1,981	1,333	2,979	1,042
2,859	0,962	2,988	1,083	2,656	0,72
3,327	1,076	1,991	1,081	1,986	1,005
3,692	0,812	2,124	1,407	2,988	0,913
1,964	1,316	4,015	0,965	4,048	0,808
3,073	1,453	2,347	1,272	3,529	0,741
2,12	1,4	2,253	1,119	4,679	0,943
3,818	1,207	2,719	0,979	2,124	0,961
2,551	1,566	1,516	1,324	2,89	0,781
4,13	0,92	2,118	1,194	2,894	0,699
2,827	1,136	1,23	1,198	2,657	1,013
3,806	1,036	2,942	0,786	3,226	0,702
3,784	1,301	3,052	1,115	3,201	0,881
3,162	1,144	1,31	1,018	2,881	0,914
3,21585	**1,1522**	**2,5541**	**1,1029**	**2,91165**	**0,89745**

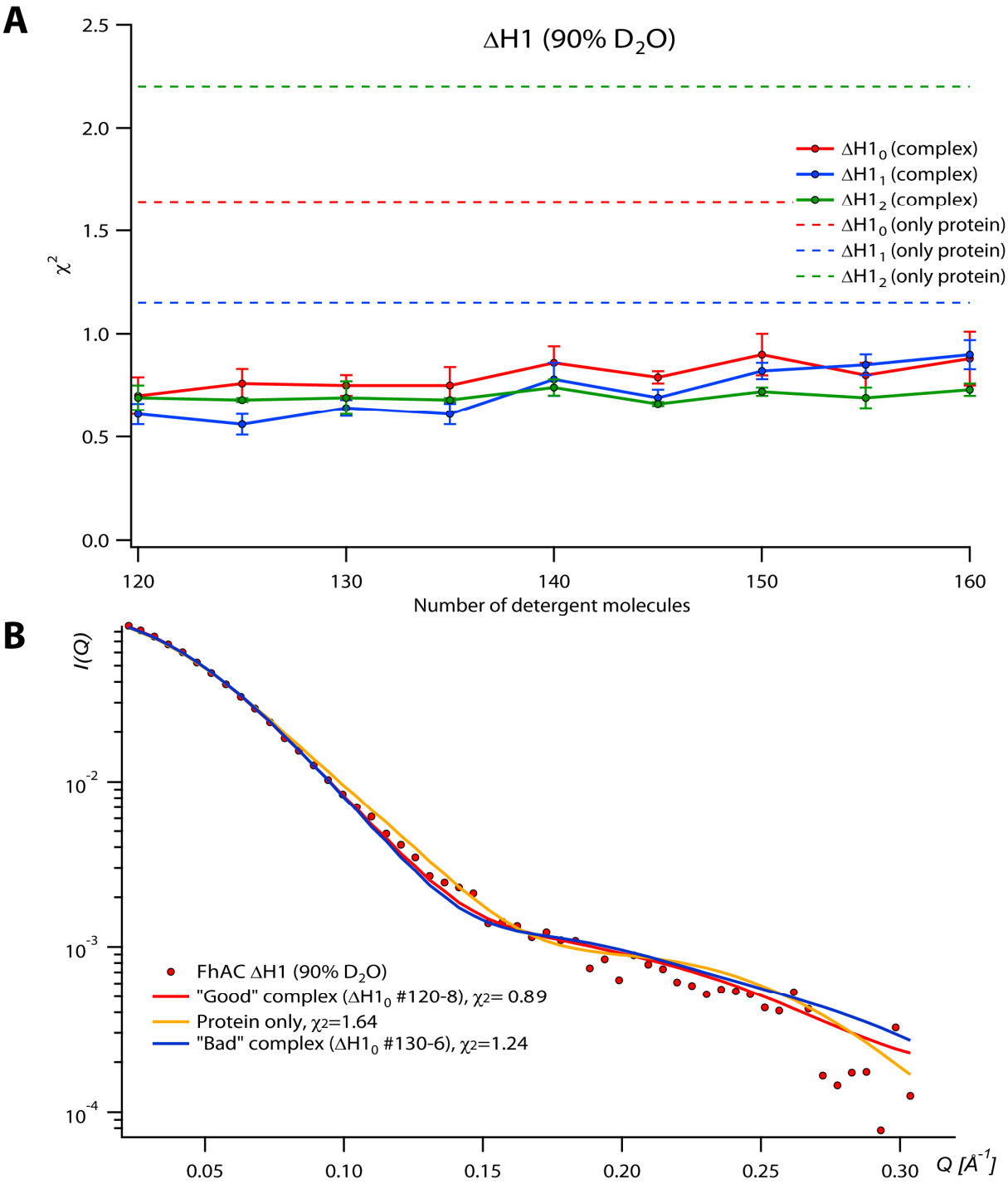

Figure S3. Modeling detergent- FhaC-ΔH1 complexes at 90% D_2O.
A: χ^2 versus detergent number. B: superposition of experiment and modeled $I(0)$.

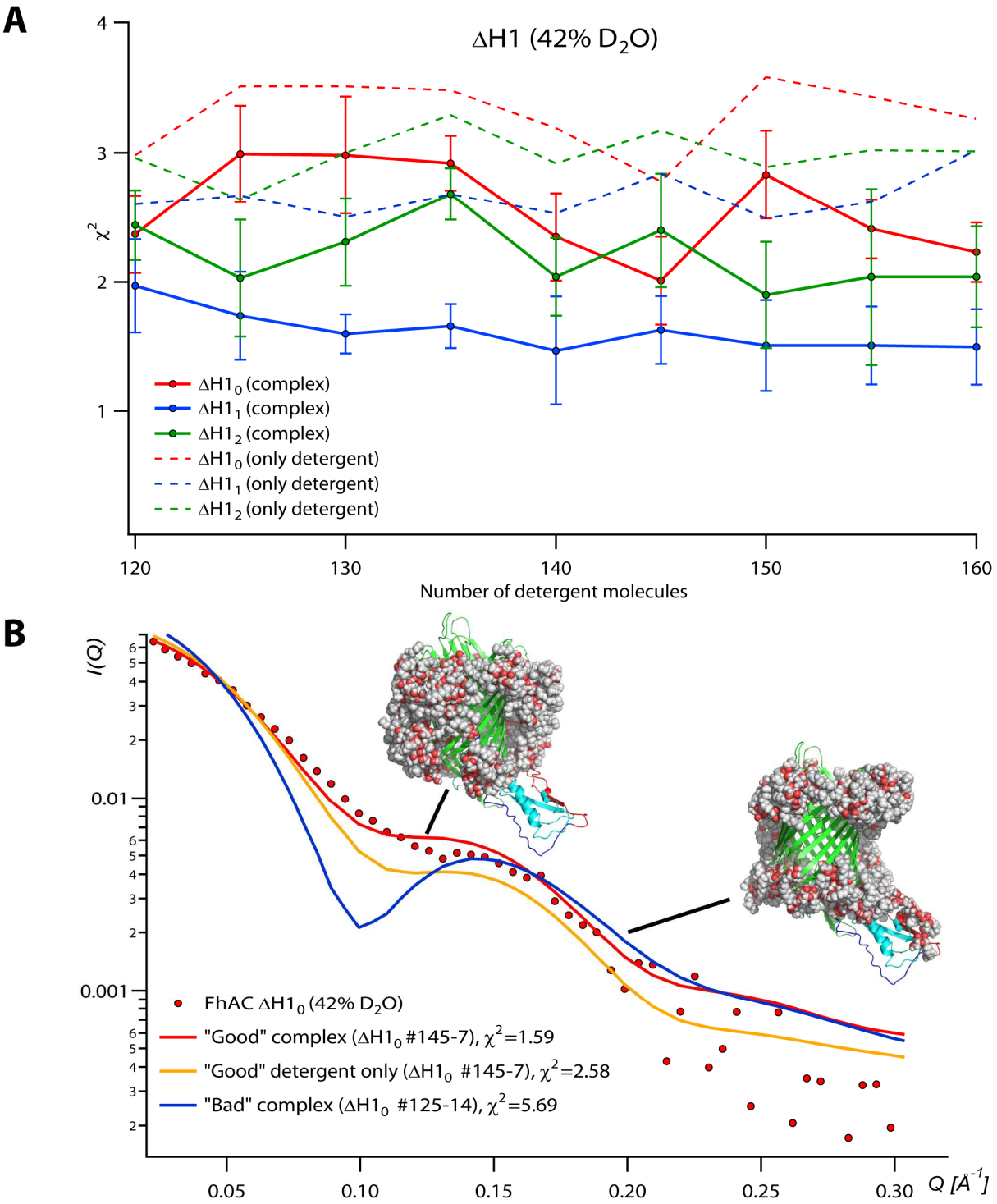

Figure S4. Modeling detergent- FhaC-ΔH1 complexes at 42% D_2O.
A: χ^2 versus detergent number. B: superposition of experimental and modeled $I(0)$ from $\Delta H1_0$.

Table S4. Overview over the 100 WT FhaC models with a reduced detergent belt (140 detergent molecules out of an initial 200) and their respective χ^2 fit values with the program CRYSON.

	WT_0 reduced belt	
	42% D_2O	*90% D_2O*
140	1.153	1.896
	5.292	1.611
	5.785	1.228
	4.551	1.434
	3.746	2.14
	2.562	1.464
	2.157	2.165
	4.062	2.214
	3.878	1.77
	2.546	1.639
	2.242	1.593
	4.05	1.655
	4.242	1.792
	5.062	1.693
	5.407	1.194
	4.009	1.63
	6.263	1.308
	3.269	1.745
	1.887	2.654
	7.58	1.604
	3.723	1.573
	4.969	1.357
	4.824	1.389
	4.957	1.526
	5.9	1.189
	6.227	1.772
	3.259	1.461
	4.58	1.24
	4.432	1.743
	4.231	1.728
	4.947	1.607
	2.88	1.888
	2.981	1.683
	5.474	1.735
	2.85	1.344
	6.094	1.876
	2.442	1.595
	3.968	1.567
	6.485	1.473
	3.243	1.727
	1.153	1.896
	5.292	1.611
	3.442	2.782
	3.187	1.453
	3.746	2.14
	2.562	1.464
	2.336	1.522
	3.366	1.902
	3.955	1.696
	4.319	1.376
	4.472	2.012
	5.666	1.642
	3.387	1.906
	5.558	1.647
	5.407	1.194
	3.264	1.643
	2.944	1.429
	3.408	1.399
	4.33	1.537

	5.108	1.645
	6.945	1.26
	2.421	1.43
	4.824	1.389
	4.895	1.741
	3.218	1.836
	3.765	1.633
	6.514	2.12
	4.58	1.24
	6.833	1.282
	2.255	1.602
	2.077	2.423
	2.88	1.888
	6.79	1.262
	7.952	1.403
	3.636	2.064
	6.094	1.876
	2.67	2.562
	2.368	1.834
	5.58	1.653
	2.931	2.167
	2.245	1.871
	5.415	1.493
	4.306	1.843
	3.569	1.612
	5.191	1.078
	2.562	1.464
	4.688	1.89
	4.493	1.468
	2.875	2.178
	2.876	1.481
	4.746	1.274
	4.258	1.839
	4.403	1.597
	2.355	1.701
	6.368	2.116
	4.009	1.63
	2.944	1.429
	4.621	1.834
	4.255	1.257
	4.327	1.357
	4.15	**1.67**

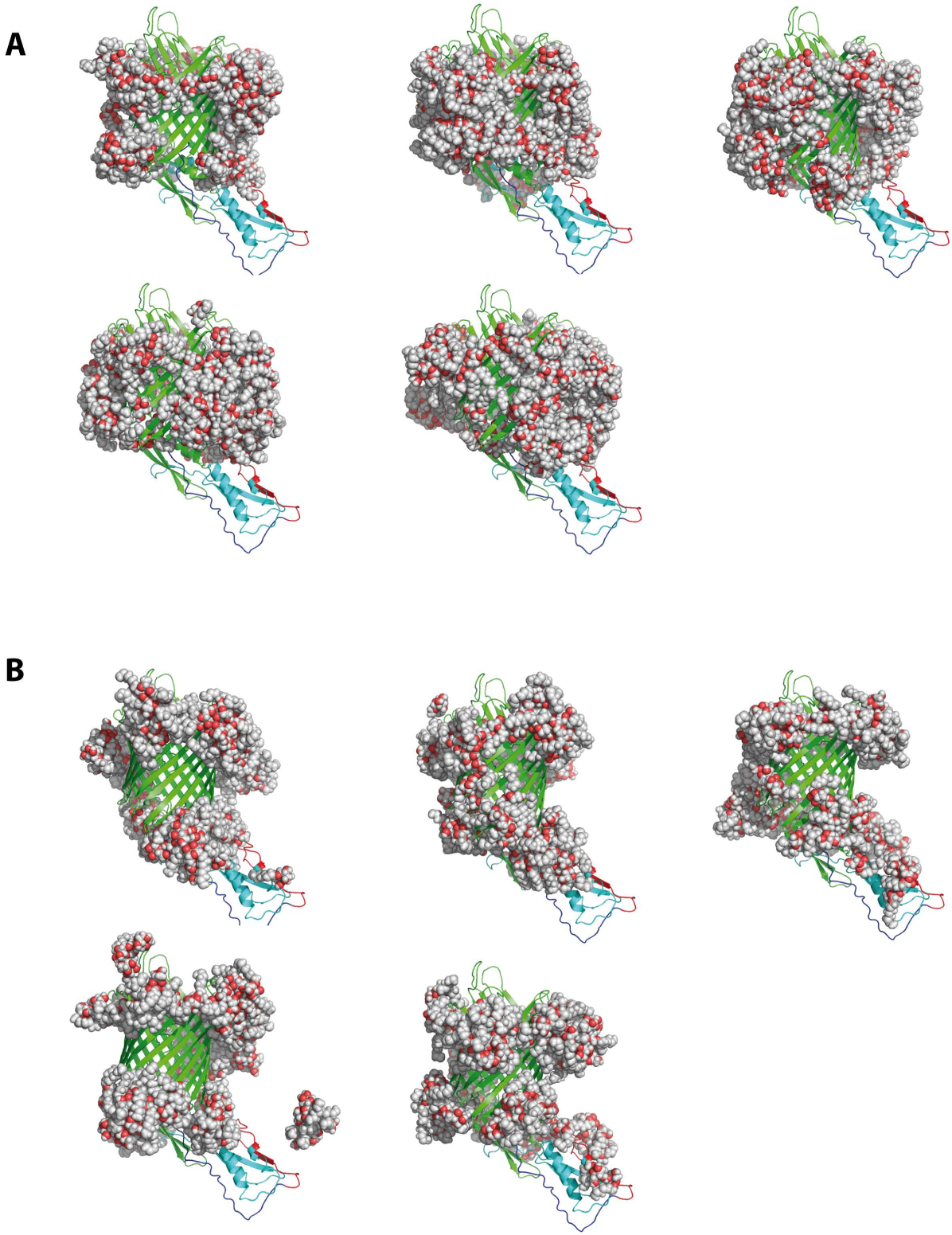

Figure S5. FhaC-ΔH1 -detergent models corresponding to good (A) and bad (B) fits.

Supporting references.

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