

Self-Assembly of the Second Transmembrane Domain of hCtr1 in Micelles and Interaction with Silver Ion

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Supporting Information

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Table S1 NMR restraints used in the structure calculation and statistical data of 20 structures with the lowest target functions for 1 mM TMD2-1 in 120 mM SDS-d₂₅ micelles in the absence and presence of 2 mM AgNO₃ at pH 6, 25°C.

	-Ag	+ Ag
Average target functions (Å ²)	0.11±0.04	0.14±0.03
Number of nonredundant distance restraints	322	239
Intraresidual (i-j =0)	158	119
Sequential (i-j =1)	77	59
Medium (i-j ≤4)	86	60
Long range (i-j >4)	1	1
Average sum of distance restraint violations (Å)	0.9±0.2	1.3±0.2
Average max. distance restraint violation (Å)	0.17±0.05	0.2±0.02
Average sum of torsion angle restraint violations (°)	0.0±0.0	0.0±0.0
Average max. of torsion angle restraint violation (°)	0.0±0.0	0.0±0.0
RMS deviation from the mean structure (Å)		
All residues		
Backbone heavy atoms	1.32±0.37	1.57±0.43
All heavy atoms	2.34±0.51	2.55±0.52
Residues in helix region	4-26	4-26
Backbone heavy atoms	0.90±0.23	0.89±0.29
All heavy atoms	1.80±0.35	1.57±0.34
Ramachandran plot statistics (for each helix span)		
Residues in most favored region (%)	74.3	74.3
Residues in additionally allowed region (%)	23.9	20.2
Residues in generously allowed region (%)	1.7	5.5
Residues in disallowed region (%)	0.0	0.0

Table S2 Proton chemical shifts of 1 mM TMD2-1 in 120 mM SDS-d₂₅ micelles in the absence and presence of 2 mM AgNO₃ at pH 6, 25°C.

Residue	HN		H α		H β		H γ		H δ		H ε	
	-Ag	+Ag	- Ag	+Ag	- Ag	+Ag	- Ag	+Ag	- Ag	+Ag	- Ag	+Ag
K1	8.723	8.724	4.004	4.002	1.98	1.978	1.511	1.506	1.733	1.738	3.031	3.026
H2	8.721	8.724	5.036	5.035	3.32	3.324			7.34	7.337	- ^a	- ^a
L3	8.373	8.372	4.105	4.103	1.81	1.807	1.65	1.641	0.949	0.951		
L4	8.266	8.266	3.966	3.962	1.735	1.734	1.678	1.668	0.937	0.935		
Q5	7.947	7.955	3.863	3.858	2.1	2.103	2.389	2.388			7.037	7.032
T6	8.146	8.137	4.101	4.097	4.391	4.383	1.318	1.313				
V7	8.503	8.499	3.533	3.533	2.258	2.258	0.986	0.988				
L8	8.47	8.476	3.981	3.979	1.866	1.884	1.593	1.566	0.866	0.851		
H9	8.153	8.156	4.586	4.579	3.544	3.54			7.281	7.276	- ^a	- ^a
I10	8.299	8.29	3.499	3.493	2.093	2.094	1.32	1.315	0.854	0.85		
I11	8.3	8.288	3.5	3.495	2.024	2.023	1.248	1.251	0.761	0.757		
Q12	8.362	8.371	3.793	3.774	2.246	2.226	2.481	2.462			6.852	6.797
V13	8.156	8.196	3.594	3.591	2.178	2.15	0.895	0.875				
V14	8.386	8.383	3.604	3.601	2.188	2.176	0.949	0.936				
I15	8.754	8.753	3.783	3.783	2.018	2.016	1.31	1.308	0.774	0.772		
S16	8.366	8.372	4.114	4.098	3.975	3.975						
Y17	8.076	8.133	4.295	4.232	3.12	3.174			7.003	6.922	6.674	6.672
F18	8.508	8.415	4.272	4.247	3.212	3.189			7.148	7.159	- ^a	- ^a
L19	8.758	8.776	3.903	3.94	1.945	2	1.398	1.374	0.87	0.869		
M20	7.827	7.971	4.178	4.175	2.265	2.306	2.646	2.969				
L21	8.071	8.247	4.1	3.957	1.835	1.884	1.675	1.615	0.878	0.858		
I22	8.327	8.244	3.65	3.633	1.905	1.901	1.155	1.18	0.657	0.665		
F23	8.559	8.559	4.335	4.262	3.24	3.213			7.264	7.245	- ^a	- ^a
M24	8.511	8.788	4.198	4.165	2.24	2.341	2.752	2.99				
T25	7.924	7.864	3.985	4	4.19	4.182	1.09	1.097				
Y26	8.263	8.187	4.254	4.229	2.99	2.976			7.047	7.029	6.758	6.751
N27	7.923	7.886	4.466	4.448	2.6	2.546			6.852	6.786		
K28	7.719	7.675	4.255	4.242	1.83	1.834	1.459	1.442	1.671	1.668	2.984	2.985
K29	7.76	7.752	4.148	4.145	1.79	1.776	1.407	1.398	1.623	1.614	2.945	2.944

a: The chemical shifts were not assigned.

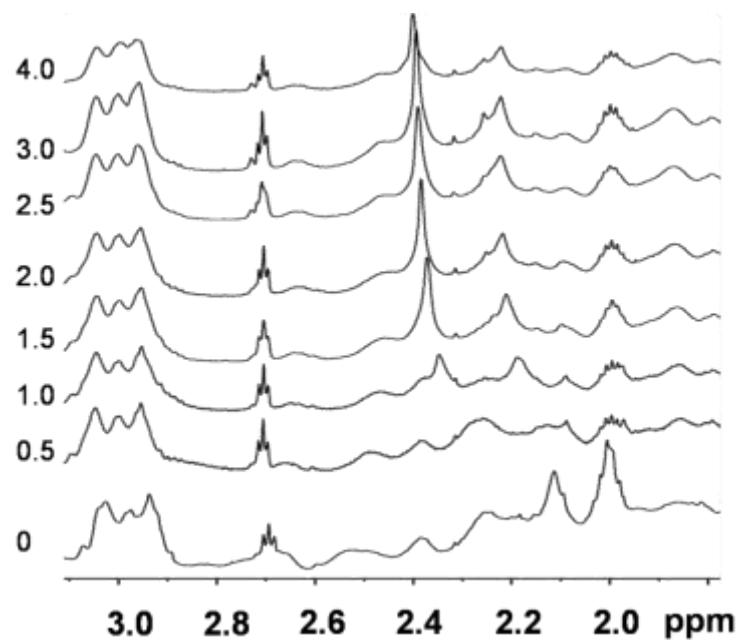


Figure S1 ¹H-NMR spectra of 1 mM TMD2-1 in 120 mM SDS-d₂₅ micelles at pH 6 titrated by AgNO_3 (0 – 4.0 eq.) at 25°C.

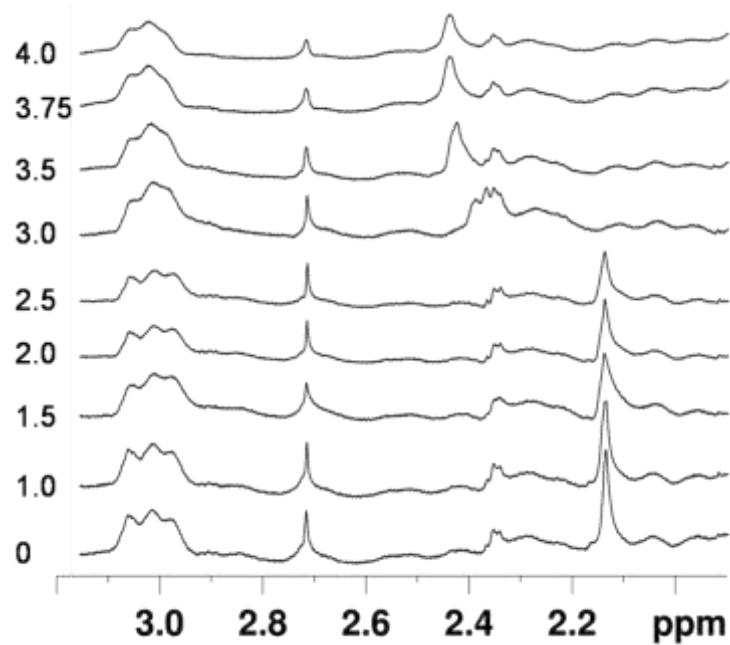


Figure S2 ^1H -NMR spectra of 1 mM M20L-1 in 120 mM SDS- d_{25} micelles at pH 6 titrated by AgNO_3 (0 – 4.0 eq.) at 25 °C.

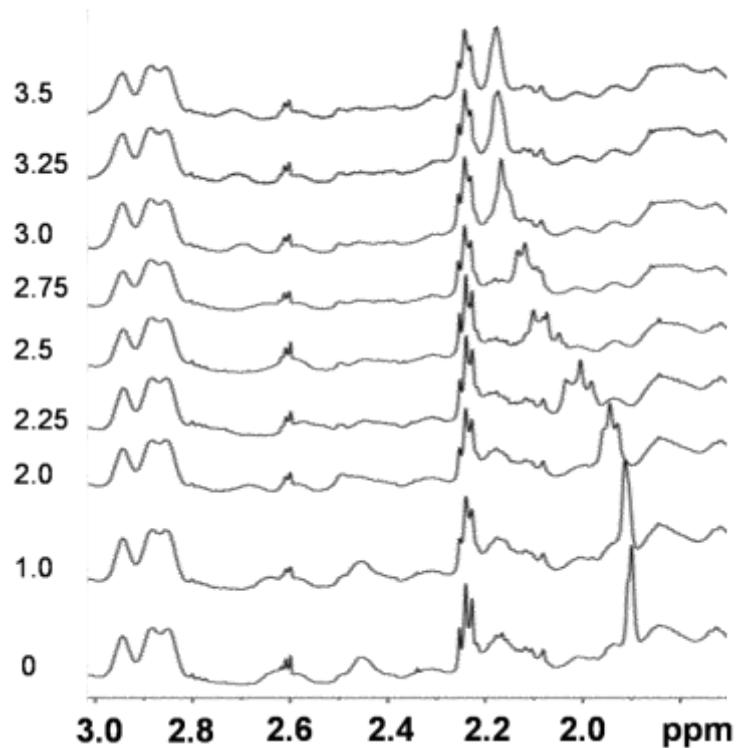


Figure S3 ¹H-NMR spectra of 1 mM M24L-1 in 120 mM SDS-d₂₅ micelles at pH 6 titrated by AgNO_3 (0 – 3.5 eq.) at 25°C.