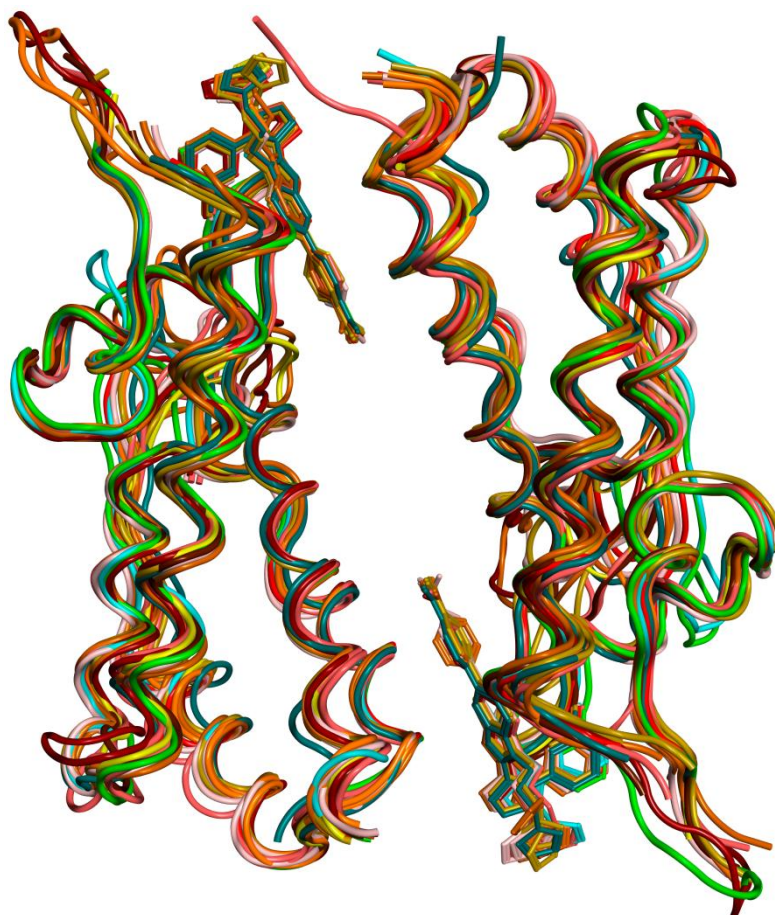


Supplementary Material



Supplementary Figure S1

All-residue C α -based superposition of the 17 CA_{NTD} dimers from the 11 dimer-containing crystal forms described in Table 2 and Figure 3. Backbone traces of the 17 superposed dimers and associated Compound 1 molecules (shown in stick form) are uniformly colored by dimer.

	A1	A2	A3	A4	B1	C1	E1	E2	E3	F1	G1	H1	H2	I1	J1	K1	L1	
A1	0.00	0.81	0.72	0.65	0.73	0.71	0.51	0.40	0.61	0.83	0.95	0.51	0.65	1.20	0.84	0.96	0.86	4.0
A2	0.81	0.00	0.80	0.97	1.06	1.02	0.96	0.83	1.01	0.84	0.88	0.79	0.73	1.22	1.08	1.43	1.05	3.5
A3	0.72	0.80	0.00	0.87	0.94	0.90	0.76	0.74	0.77	0.67	0.99	0.74	0.79	1.26	0.99	1.17	0.96	3.0
A4	0.65	0.97	0.87	0.00	0.94	0.85	0.62	0.68	0.61	0.93	1.10	0.79	0.85	1.30	0.89	0.92	0.94	2.5
B1	0.73	1.06	0.94	0.94	0.00	0.68	0.77	0.70	0.85	1.01	0.95	0.70	0.91	1.20	0.97	1.00	0.83	2.0
C1	0.71	1.02	0.90	0.85	0.68	0.00	0.80	0.68	0.78	0.84	0.94	0.74	0.78	1.00	0.68	1.09	0.43	1.5
E1	0.51	0.96	0.76	0.62	0.77	0.80	0.00	0.41	0.38	0.86	1.11	0.64	0.82	1.35	0.86	0.70	0.93	1.0
E2	0.40	0.83	0.74	0.68	0.70	0.68	0.41	0.00	0.50	0.75	0.93	0.43	0.58	1.14	0.80	0.91	0.78	0.5
E3	0.61	1.01	0.77	0.61	0.85	0.78	0.38	0.50	0.00	0.77	1.10	0.64	0.77	1.21	0.82	0.71	0.83	0.0
F1	0.83	0.84	0.67	0.93	1.01	0.84	0.86	0.75	0.77	0.00	0.94	0.73	0.67	1.03	0.99	1.21	0.78	
G1	0.95	0.88	0.99	1.10	0.95	0.94	1.11	0.93	1.10	0.94	0.00	0.81	0.80	0.94	1.10	1.47	0.91	
H1	0.51	0.79	0.74	0.79	0.70	0.74	0.64	0.43	0.64	0.73	0.81	0.00	0.52	1.04	0.88	1.01	0.79	
H2	0.65	0.73	0.79	0.85	0.91	0.78	0.82	0.58	0.77	0.67	0.80	0.52	0.00	0.88	0.90	1.25	0.77	
I1	1.20	1.22	1.26	1.30	1.20	1.00	1.35	1.14	1.21	1.03	0.94	1.04	0.88	0.00	1.17	1.63	0.84	
J1	0.84	1.08	0.99	0.89	0.97	0.68	0.86	0.80	0.82	0.99	1.10	0.88	0.90	1.17	0.00	1.11	0.79	
K1	0.96	1.43	1.17	0.92	1.00	1.09	0.70	0.91	0.71	1.21	1.47	1.01	1.25	1.63	1.11	0.00	1.16	
L1	0.86	1.05	0.96	0.94	0.83	0.43	0.93	0.78	0.83	0.78	0.91	0.79	0.77	0.84	0.79	1.16	0.00	

RMSD = 0.899 Å

Supplementary Figure S2

Pairwise RMSD values of 17 C α -superposed CA_{NTD} dimers from the 11 dimer-containing crystal forms described in Table 2 and Figure 3. Individual dimers are designated by the crystal form letter of Table 2, followed by the dimer number within that crystal form. RMSD values range from 0.38 Å to 1.63 Å, and average 0.90 Å.