

Appendix

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Appendix Text

The equation for the AICG2+ potential is below.

$$\begin{aligned}
 V_{AICG2+}(R|R_0) = & \sum_i K_{b,i} (b_i - b_{i,0})^2 + V_{loc}^{flp} \\
 & + \sum_{j=i+2} \varepsilon_{loc,ij} \exp\left(-\frac{(r_{ij} - r_{ij0})^2}{2W_{ij}^2}\right) + \sum_{j=i+3} \varepsilon_{loc,ij} \exp\left(-\frac{(\phi_{ij} - \phi_{ij0})^2}{2W_{\phi,ij}^2}\right) \\
 & + \sum_{i < j-3}^{nat\ contact} \varepsilon_{go,ij} \left[5 \left(\frac{r_{ij0}}{r_{ij}}\right)^{12} - 6 \left(\frac{r_{ij0}}{r_{ij}}\right)^{10} \right] + \sum_{i < j-3}^{non-native} \varepsilon_{ev} \left(\frac{d}{r_{ij}}\right)^{12}
 \end{aligned}$$

b_i : bond length between i-th and i+1-th residues.

V_{loc}^{flp} : (Terakawa et al., Biophys J 2011)

r_{ij} : distance between i-th and j-th residues.

ϕ_{ij} : dihedral angle defined as i-th, i+1-th, i+2-th, and i+3-th residues.

$W_{ij}^2, W_{\phi,ij}^2$: widths of the attractive interaction

$K_{b,i}, \varepsilon_{loc,ij}, \varepsilon_{go,ij}$: determined by AMBER force field

ε_{ev}, d : determined from a structural servay.

Each term represents, the elasticity of the virtual bond, the sequence-dependent angle- and dihedral-angle potential, the structure-based local potential between i-th and i+2-th residues, the structure-based local potential for dihedral angles, the Go potential for non-local natively interacting pairs, and the generic repulsion for the rest of the non-local pairs. The vector R represents the $3n_{aa}$ -dimensional Cartesian coordinates of the simulated protein where n_{aa} is the number of the protein amino acids. R_0 is the corresponding coordinates in the reference structure. All variables with the subscript 0 refer to parameters defined by the reference structure (initial structure). The attraction factor mentioned in the main text is “The Go potential for non-local natively interacting pairs” in the AICG2+ equation. The Go potential is already well estimated for the intra-chain interactions, but it needs to be edited for the inter-chain interactions, so we changed these parameters.

The CafeMol manual are written the meaning and the default values of these parameters (<http://www.cafemol.org>).

Appendix Figures

A

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Q22T00_TETTS/1-555      1  ----- MRASSAT----- KSQKDLK TLEEYI HQS KKS NL 29
hsCCDC151/1-595        1  MTS L CRAAS ANAL P QDQAS T S SRVKGR EAS GK P SHLRGKGT AQAWT PGRS KGG S FHR GAGK P S VHS QVA ELHK K I QL 80

Q22T00_TETTS/1-555     30  L E N D R K K I F H K N A E E T K N N M C I E S L K K E N K Q L K T L R D E L I A N K R A S T P G M S K T O G S L V S W S G D I K D E N Y W R K F D E A R H 109
hsCCDC151/1-595     81  L E G D R K A F F E S S W N I K K Q T I S Q L R K E T A L E L K L L D L L K G D E ----- K V V L A V I R E W ----- K W E R P Y L K N E T 146

Q22T00_TETTS/1-555     110  A T ----- K ----- N K K S Q L L Q L O D K L N E V S D A K F G A V E E S P L M R Q I R I L E N R L D K V M I K F N E A G S 164
hsCCDC151/1-595     147  Q A L E H L D H R L R E K V K Q Q N A L R H Q V V L R Q R R L E E L Q L H S L R L L E M - A E A Q N R H E V A K T M N L E N R L E K A Q M K A Q E A E H 225

Q22T00_TETTS/1-555     165  R K K T E E I V K R L K E E R V G Y D N Q L A A I E R S L K G K E H D F E E L L L A H D A T H A K E L A A A L K K Y E H K K A A V R E L K T Y I A E K R 244
hsCCDC151/1-595     226  I T S V L L L K A Y L M D E S L N L E R L D S M E A E V V R T K H E L E A L H V V N Q E A L N A R D I A K N L Q Y L E T L V R E R K K R E R Y I S E C K 305

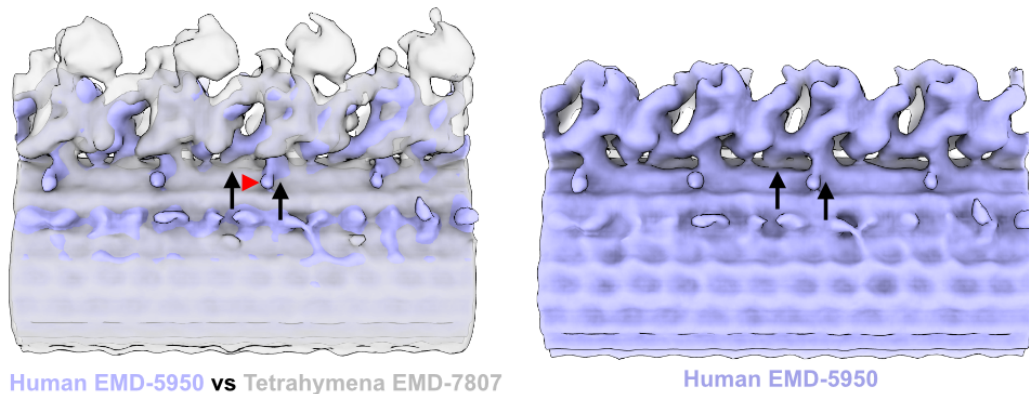
Q22T00_TETTS/1-555     245  K A I E Q R E A V I S R M E K K D K D N D R N L E K S Q A N N L N E L N N Q I E P Q N I - - Q D A T F Q R K L N D Y D E A F R R L Y E A T G V T V N E I 322
hsCCDC151/1-595     306  K R A E K K L E N E R M E R K T H R E ----- H L L Q S D D T I Q D S L H A K E E E L R Q R W S M Y Q M E V I F G R V K D A T G T D E T H S L 374

Q22T00_TETTS/1-555     323  I Q K F T T D E D E S K S L K D L Q R E Y D T I D D K K K Q R D D L K A G L N A L K Y E G N E N N R R K L D E I E - - K N V N A V N K C D K A K L K Y E R 400
hsCCDC151/1-595     375  V R R F L A Q G D I F A Q L E T L K S E N E Q L L V R L K Q E K Q L Q R E L E D L K S G E A T L V S Q Q K L Q A E A Q E R L K K E E R H A E A R D Q L E R 454

Q22T00_TETTS/1-555     401  V S K I L V D V K A G I E H L Y E K L E F Y K L E - - - - G K N I V I T D E T L V E G L S Q I V E K M K I I F Q P V K N D S Y N E D F K T A K G V S 475
hsCCDC151/1-595     455  A L R A M Q V A D S L E H L A S K L I H I T V E D R F A G K E L D - P Q A D N V V N L L G L V E K L L K L Q A Q L - - - - Q G H D V Q M L M C H I A 528

Q22T00_TETTS/1-555     476  Y I N L N L R D K S G R I E S I S K N I R V K L P E K D E E E V S N D E I E D D I D I E T T K L R Q K Y A Q A K Q E A A A N K O K Q L G S T Q Q G R K V 555
hsCCDC151/1-595     529  R - - E F L A S L E G R L P E N T R I A L P L A T S K D K F D E S E E D N E V V I R A S L K I S Q K L I E S H K H R S R S ----- 595
  
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B



Appendix Figure S1. Data related to Docking complex

(A) Sequence alignment of Tetrahymena DC1 (Q22T00_TETTS) and human CCDC151. Blue arrowhead indicates the residues at which early terminations are found in patients with ciliopathy (Hjeij, R. et al., 2014). (B) Overlapping of the tomographic structure of the axonemes from Tetrahymena (EMD-7807, Stoddard, D. et al., 2018) and human (EMD-5950, Lin, J. et al., 2014) (left panel) and the human axoneme alone (right). The two maps are aligned based on the radial spokes on the opposite sides. It is clear that the docking point of the human ODA (black arrows) are different from Tetrahymena ODA. In addition, there is an extra density protruding from the docking complex of humans (red arrowhead).

Appendix Tables

Appendix Table S1: Mass spectrometry of ODA complex components.

MS total spectrum count of ODA components from *Tetrahymena* WT, K40R doublet using native purification and NaCl treatment. In the NaCl treated doublet, most of the DC components were washed out.

Name	Name	UniprotID	K40R	WT	WT (NaCl)
Heavy chain	Dyh3	Q22A67	239,232,229	263,250,245	1,0,0
	Dyh4	I7M9J2	259,241,247	264,255,240	0,0,0
	Dyh5	I7M6H4	223,215,199	239,241,218	2,2,0
Intermediate chain	Dic2	I7M008	36,32,31	38,37,32	6,10,9
	Dic3	Q23FU1	40,38,37	38,39,35	15,11,12
Light chain	Lc3	A4VD75	9,9,7	7,7,6	0,0,0
	Lc4a	Q22C78	5,5,3	3,3,2	0,0,0
	Lc1	I7M1N7	22,22,20	19,17,18	0,0,0
	Lc2a	Q1HGH8	4,4,4	5,5,5	1,3,0
	Lc9	A4VEB3	4,3,3	5,5,3	0,0,0
	Lc8	W7XJB1	5,4,4	3,4,3	0,0,0
	Lc8d	Q24CE5	7,6,5	7,7,5	0,0,0
	Lc8e	Q24DI9	3,2,3	1,3,2	0,0,0
	Lc8f	Q22R86	4,4,5	3,4,5	0,0,0
	Lc10	I7MCM8	2,0,2	0,2,0	0,0,0
	Lc8b	A4VE64	6,6,6	2,2,0	0,0,0

	Lc7	I7MHB1	8,8,8	6,7,7	0,3,3
	Lc7b	Q1HFX1	6,4,5	5,5,4	0,0,0
	Lc7a*	Q1HFX2	4,4,4	3,3,3	0,0,0
	Lc2b*	I7M0N9	4,6,6	4,4,4	0,0,0
	Tct1a*	I7MGG2	0,0,0	0,0,0	0,0,0
	Tct1b*	Q231T5	2,2,2	0,0,0	0,0,0
Docking Complex	DC1	Q22T00	29,26,28	27,26,22	0,0,2
	DC2	Q233H6	20,19,17	24,25,24	0,3,2
	DC3	I7M2C6	15,13,11	17,16,17	4,3,4

* Components do not present in ODA according to Mali et al, (2021).