

**Structure, Volume 26**

**Supplemental Information**

**Solution Structures of Engineered Vault Particles**

**Ke Ding, Xing Zhang, Jan Mrazek, Valerie A. Kickhoefer, Mason Lai, Hwee L. Ng, Otto O. Yang, Leonard H. Rome, and Z. Hong Zhou**

# **Solution structures of engineered vault particles**

**Ke Ding, Xing Zhang, Jan Mrazek, Valerie A. Kickhoefer, Mason Lai, Hwee L. Ng, Otto**

**O. Yang, Leonard H. Rome, Z. Hong Zhou**

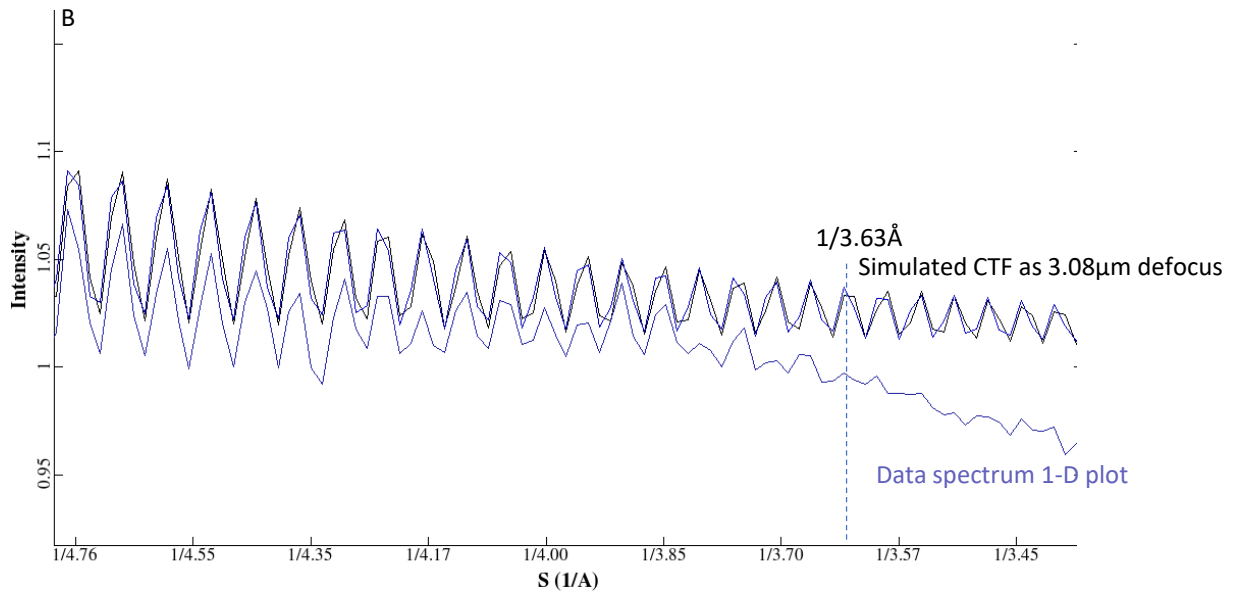
## **Inventory of Supplementary Information**

Two supplementary figures (Figure S1 related to Figure 1, Figure S2 related to star methods)

One supplementary table (Table S1 related to star methods)

One supplementary movie (Movie S1 related to Figure 3, showing MVP conformation changes between the two conformers of vault in solution)

**Figure S1** Data quality validation. Related to Figure 1C

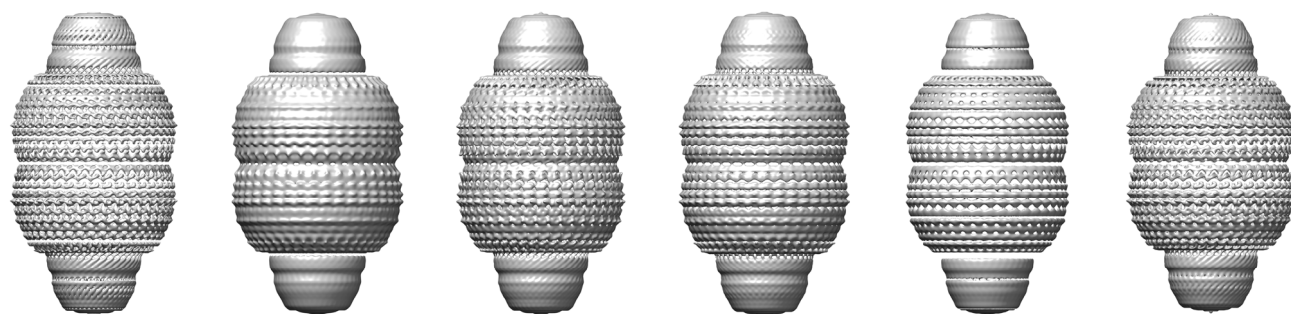


**Figure S1** 1-D plot of a raw micrograph shows that signal is transferred to atomic resolution.

# Figure S2 Classification and refinement process. Related to star methods

32702 particles after 2D classification

3D classification without mask, ask for 6 class



**Class1: 17%**  
9.61Å

Class2: 16%  
11.51Å  
non-chiral

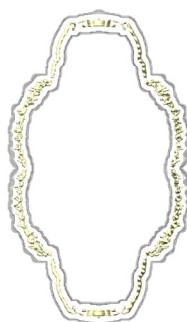
Class3: 19%  
9.91Å

Class4: 19%  
9.91Å  
non-chiral

Class5: 13%  
11.8Å  
non-chiral

**Class6: 16%**  
9.71Å

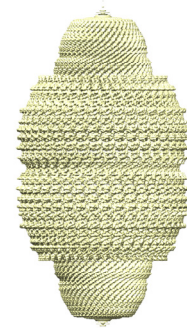
32702 particles after 2D classification  
Direct refinement  
Use **Class1** as initial model



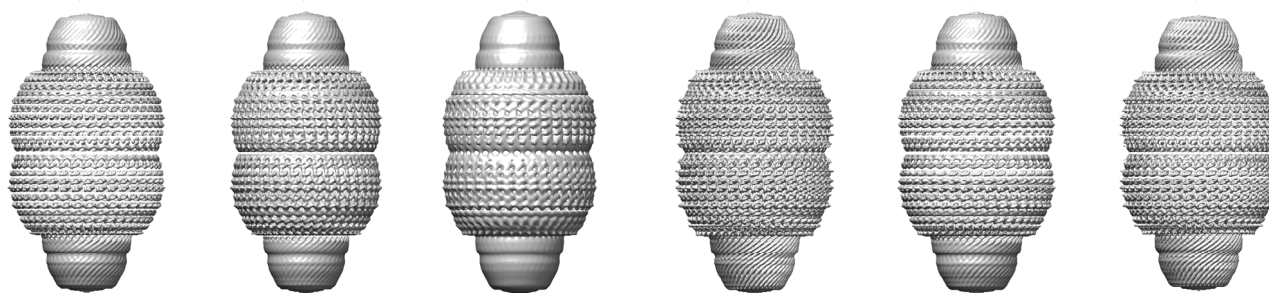
**Structure like conformation 2**  
32702 particles  
Generate a soft mask based on data to keep feature for most conformations

Class3D with mask on 32702 particles

Refinement and local classification after refinement, further remove bad particles



**Conformation 2**  
4.7Å  
2691 particles



Class1: 22%  
9.14Å

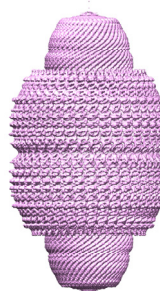
Class2: 9%  
10.13Å

Class3: 6%  
13.91Å

**Class4: 24%**  
7.96Å  
Identical to conformation 2

Class5: 9%  
9.71Å

**Class6: 29%**  
8.1Å



**conformation 1**  
4.9Å  
9669 particles

**Figure S2** Multiple conformations was found in initial classification. Further classification with soft mask was later conducted to increase classification accuracy. Structure chirality and cap-helix quality are major features to distinguish a good 3D class.

**Table S1** Structural statistics of the two conformers.  
Related to star methods.

Conformation ID		# 1	# 2
B-factor for map ( $\text{\AA}^2$ )		-160	-225.5
MapCC (around atoms)		0.763	0.748
Phenix RMSD	Bond ( $\text{\AA}$ )	0.0026	0.0032
	Angles	0.66	0.77
Ramachandran plot (from Phenix)	Outliers	0.77%	0.78%
	Allowed	4.12%	4.18%
	Favored	95.10%	95.04%
All atom clash score		10.94	12.90
$C\alpha$ RMSD Value to PDB 4HL8		1.3 $\text{\AA}$	5.95 $\text{\AA}$
Rotamer outliers		0.00%	0.00%
C-beta deviation		0	0