

Figure S1. Related to Figure 2. (A) Icosahedron surface (gray surface) fitted to SGIV map (blue surface). The icosahedron is close to the outer shell at the vertices and along the edges of the icosahedron's triangular faces, but appears well under the outer shell in the middle of the triangle (marked with an X). (B) After a spherical factor (0.2) is applied to the icosahedron - the surface is now closer to the outer shell in the middle of the triangle, but has moved too far out along the triangular edges (marked with X). (C) The deformed icosahedron created with iSeg – the edges of each icosahedral triangle is held fixed while the centers are pushed outwards. The deformed icosahedron now more closely matches the outer shell. (D) Plot of cross-correlations at various radii between SGIV map and (1) icosahedral surface (dotted) and (2) deformed icosahedral surface (solid). Cross-correlations using the deformed icosahedral surface are higher at peaks and lower in valleys, matching the layers in the map more accurately.

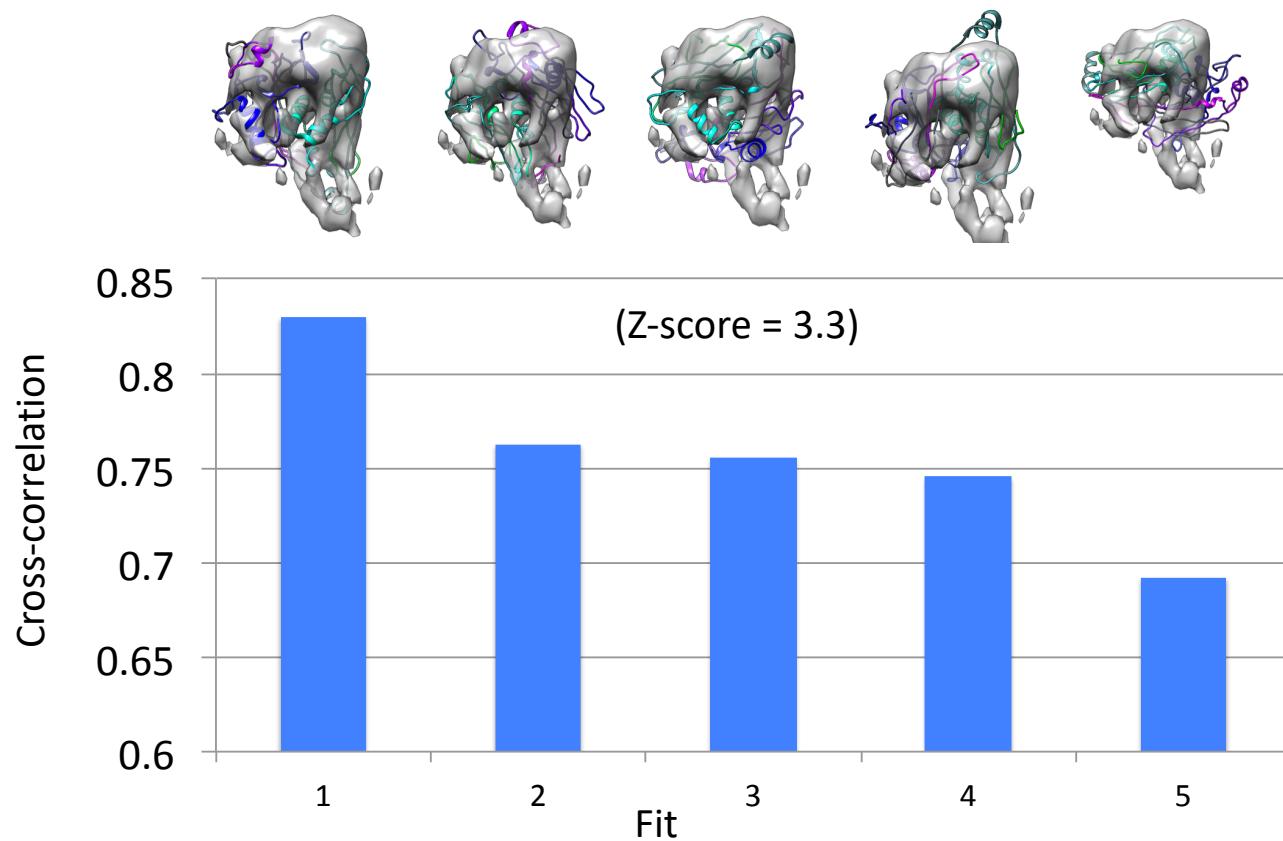


Figure S2. Related to Figure 6A. Rigid fits of Vp54 X-ray model (PDB:1m3y) to the segmented map of a single coat protein from SGIV. For the top fit, 1, the model fits well into the map, with secondary structures including beta sheets and alpha helices matching similar features in the map. Other fits (2-5) have lower cross correlation scores and in these positions, the model does not match the map as well.

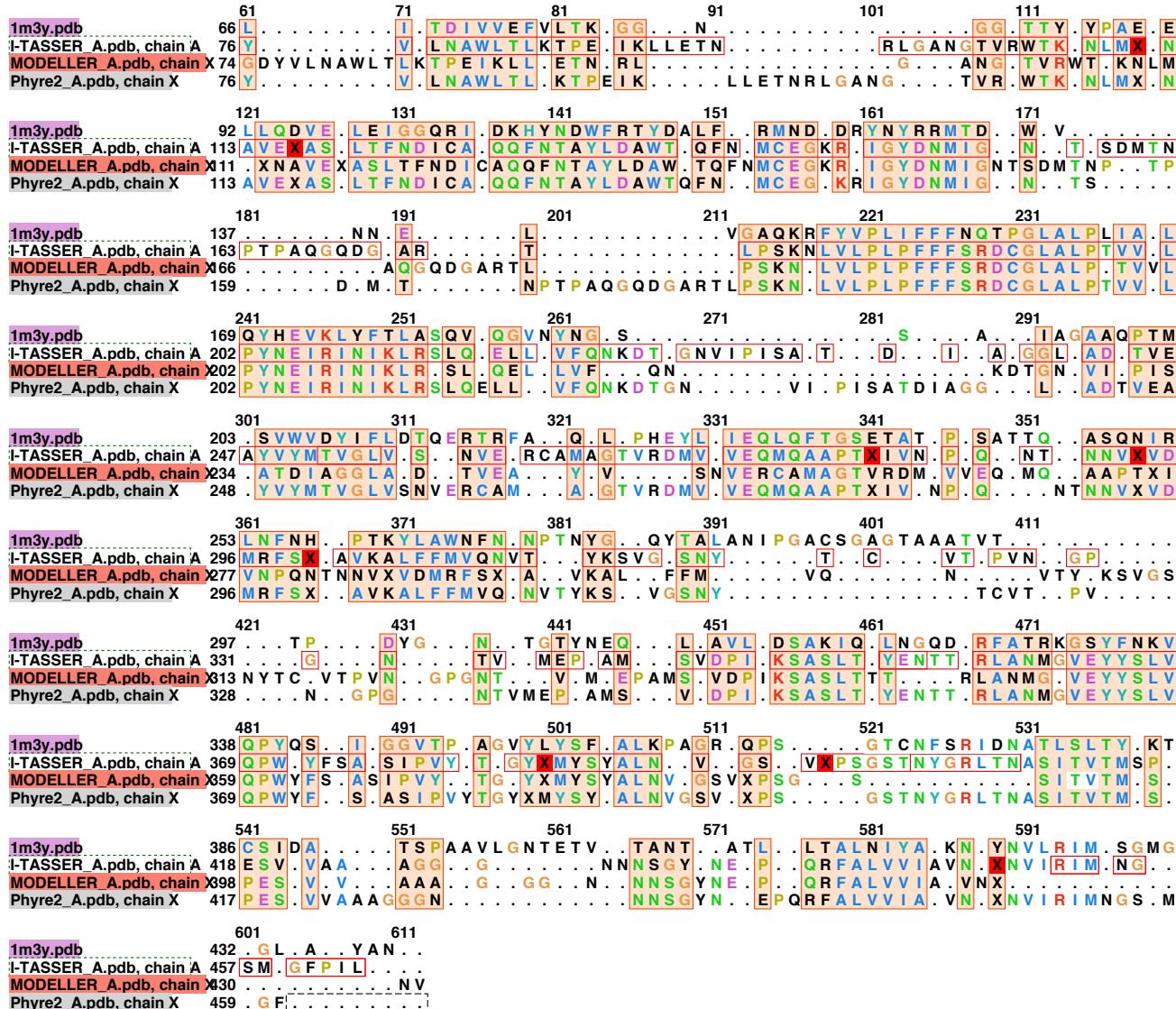


Figure S3. Related to Figure 7B. Multiple sequence alignment of Vp54 crystal model (PDB:1m3y) and comparative models generated by I-TASSER, MODELLER, and Phyre2. The alignment was performed using MatchMaker tool in UCSF Chimera.

All-Atom Contacts	Clashscore, all atoms:	5.41	93 rd percentile* (N=1784, all resolutions)	
Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.				
Protein Geometry	Poor rotamers	20	1.98%	Goal: <0.3%
	Favored rotamers	848	83.88%	Goal: >98%
	Ramachandran outliers	17	1.36%	Goal: <0.05%
	Ramachandran favored	1023	81.77%	Goal: >98%
	MolProbity score^	2.23		63 rd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 9876	0.00%	Goal: 0%
	Bad angles:	0 / 13485	0.00%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 72	0.00%	Expected: ≤1 per chain, or ≤5%

All-Atom Contacts	Clashscore, all atoms:	26.68	14 th percentile* (N=715, 2.00Å ± 0.25Å)	
Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.				
Protein Geometry	Poor rotamers	28	8.59%	Goal: <0.3%
	Favored rotamers	274	84.05%	Goal: >98%
	Ramachandran outliers	4	1.01%	Goal: <0.05%
	Ramachandran favored	364	92.15%	Goal: >98%
	MolProbity score^	3.10		7 th percentile* (N=12522, 2.00Å ± 0.25Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 3155	0.00%	Goal: 0%
	Bad angles:	1 / 4302	0.02%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 16	0.00%	Expected: ≤1 per chain, or ≤5%

Figure S4. Related to Figure 7. Top: Molprobity statistics for the comparative model from Phyre2, after flexible fitting and phenix.geometry_minimization. Bottom: Molprobity statistics for X-ray model (PDB:1m3y) on which the comparative model is based.