**Supplemental Material**

**Supplemental Movie S1. The E153/R210 interactions persist during HK97 capsid maturation.** This interpolated atomic model movie shows the changes that occur during HK97 maturation and in particular illustrates that the ionic interactions between E153 and R210 on adjacent subunits in HK97 capsomers persists from prohead to mature head. The movie was derived from 5 crystal structures, using linear interpolation followed by energy minimization between each step [1]. The PDB files used for this movie are listed below. Note that 2FSY & 2FS3 are very similar. For each section the number of atoms in the two models was matched by deleting the parts that are not present in both models to enable successful interpolation. The result is that some sections of the models appear suddenly when the sections that were deleted are restored to a truncated structure for the following step. The movie illustrates expansion from Prohead II all the way to Head II and then reverses and returns to the beginning.

| PDB | description | resolution |
|---|---|---|
| 3E8K | Crystal structure of HK97 Prohead II (has mcp with truncated E-loop) | 3.65 Å |
| 2FSY | Bacteriophage HK97 pepsin-treated EXPANSION INTERMEDIATE IV | 3.80 Å |
| 2FS3 | Bacteriophage HK97 K169Y HEAD I (mutant that can't crosslink) | 4.20 Å |
| 2FT1 | Bacteriophage HK97 “HEAD II” (almost HII - pentons slightly recessed) | 3.90 Å |
| 1OHG | Bacteriophage HK97 mature empty capsid (genuine refined HEAD II) | 3.45 Å |

**Supplemental Movie S2. Movie showing how the E153/R210 interactions may play their important roles during HK97 prohead assembly.** A hypothetical model of the beginnings of HK97 capsid assembly in which a hexon in a symmetric configuration adopts its characteristic asymmetric shape via changes induced by assembly. In this scheme, the shape changes of the subunits of the hexon are partly limited by contacts between residues D231 and K178. The subunits are also constrained by the interactions of the other residues highlighted in the movie, which make ionic interactions that are maintained during assembly. Importantly, the movie shows how the E153 - R210 salt bridge acts as a pivoting point of contact during this process.

The symmetric hexon model was made from 6 copies of the F chain from PDB ID: 3E8K (Prohead II). All PDB chains were modified to have the same length for ease of manipulation and for successful interpolation using the Morph Server [1]

**Supplemental Table 1**. **E-loop-to-adjacent subunit interactions in capsid PDB models and potential analogs of the HK97 E153-R210 ionic interaction**. The PDB files listed were opened in Chimera [2] and the disposition of the E-Loop was evaluated and recorded. In virtually all cases the E-loops overlap the adjacent subunit in each capsomer. Models with sidechains were examined further by visualizing all charged residues in the hexamer of the asymmetric unit and looking for any potential ionic interactions between the E-loop and the adjacent subunit in the model. These interactions were noted in the table, where the residues observed to interact were placed on the same line in different columns. In most cases a penton was built to see if the same potential interactions exist there as well. Figure panels showing two subunits from the model's hexon were prepared and are shown in Figure 9. Side chains involved in the listed potential side chain interactions are shown in space-filling mode in the figure.

| system geometry | PDB ID resolution | notes | E-loop residues | back-bone helix residues | P-domain residue or Extra Notes |
|---|---|---|---|---|---|
| HK97 head, etc. | 1OHG 3.45 Å | E-loop overlaps adjacent P-domain | E153 | R210 | |
| T4 penton protein in crystal | 1YUE 2.9Å | Insertion Domain located in distal E-loop binds to adjacent A- & P-domains | 82-142 | | in 6 subunit per turn $P6_5$ helix |
| T7 prohead T=7 | 3J7V | E-loop overlaps adjacent P-domain (R42 in N-arm closer than R68) | R68 | E128 | in some hexon pairs |
| T7 mature T=7 | 3J7X | E-loop overlaps adjacent P-domain | R68 | E128 | 5-6Å |
| P22 prohead T=7 -mature | 2xyy 3.8Å 2xyz 4.0Å | E-loop overlaps adjacent P-domain in hexon & penton C-alpha | *54, 58, 59*? | *101, 102, 109, 110?* | residues guessed from models without explicit side chains |
| P22 mature T=7 | 5UU5 3.3A | E-loop overlaps adjacent P-domain | E52 E54 E59 E72 | R109 K110 K118 R102 | D83 |

| | | | | | |
|---|---|---|---|---|---|
| Sf6<br>T=7 mature | 5L35<br>2.9Å | E-loop overlaps adjacent P-domain | R60<br>K71 | E123 | <br>E92 |
| epsilon15<br>T=7 mature | 3J40<br>4.5Å | E-loop overlaps adjacent P-domain and beyond. (positions not consistant in model) | E62? | K124? | 3.3-9 Å in model |
| BPP-1<br>T=7 mature | 3J4U<br>3.7Å | E-loop overlaps adjacent P-domain | R58<br>R67 | E114 | <br>E91 |
| ATCCclear<br>T=7 mature | 3JB5<br>3.7Å | E-loop overlaps adjacent P-domain | K65 | | E285 |
| ϕ29<br>T=3 mature | 1YXN<br>7.9Å | E-loop reaches to adjacent P-domain in model, but the density for the E-loop is weak. C-alpha only | | | |
| P-SSP7<br>T=7 mature | 2XD8<br>4.6Å | E-loop overlaps adjacent P-domain C-alpha only | | | |
| SPP1<br>T=7 mature | 4AN5<br>8.8Å | E-loops truncated in model just before overlapping adacent backbone helix, C-alpha only | | | |
| Pyrococcus encapsulin<br>T=3 | 2E0Z<br>3.6Å | E-loop overlaps adjacent P-domain, consistant | D153<br>R156 | | K171<br>D322 |
| Myxococcus encapsulin<br>T=3 | 4PT2<br>4.6Å | E-loop overlaps adjacent P-domain, [contacts adjacent and distal capsomers] | E71 or E69 | | K90 |
| Thermotoga encapsulin<br>T=1 | 3DKT<br>3.1Å | E-loop contacts adjacent P-domain and overlaps neighboring capsomer | E-loop has no charged residues | | |

[1] Krebs WG, Gerstein M. The morph server: a standardized system for analyzing and visualizing macromolecular motions in a database framework. Nucleic acids research. 2000;28:1665-75.
[2] Pettersen EF, Goddard TD, Huang CC, Couch GS, Greenblatt DM, Meng EC, et al. UCSF Chimera--a visualization system for exploratory research and analysis. J Comput Chem. 2004;25:1605-12.