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**Supporting information for article:**

# Manipulation of an existing crystal form unexpectedly results in interwoven packing networks with pseudo-translational symmetry

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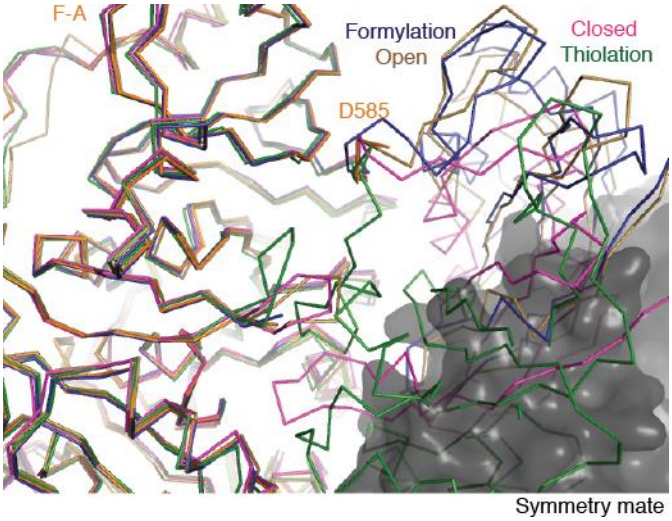


**Figure S1** $A_{sub}$ subdomain disorder in the published crystal structure of the LgrA F-A construct. Only the $A_{core}$ subdomain is well-ordered in the published structure of the full FA construct ((Reimer *et al.*, 2016); PDB ID 5ES6) (shown in orange), allowing modelling up to residue D585 of the hinge region. A symmetry mate (shown as a grey semi-transparent surface) prevents the $A_{sub}$ subdomain from adopting any of its known functional positions. (Formylation: PDB ID 5ES9 chain A – shown in blue; Open and closed: PDB ID 5ES5 chain A and B – shown in magenta, respectively; Thiolation: PDB ID 5ES8 – shown in green).

**Table S1** Surface area buried by each crystal contact.

| **Contact partners** | **Buried surface area per molecule** | **Inter or intra packing network** |
|---|---|---|
| molecule A - molecule C | 1628 Å$^2$ | intra A - C network contact |
| molecule A - molecule C symmetry mate 1 | 598 Å$^2$ | intra A - C network contact |
| molecule A - molecule C symmetry mate 2 | 562 Å$^2$ | intra A - C network contact |
| molecule A - molecule C symmetry mate 3 | 240 Å$^2$ | intra A - C network contact |
| molecule C - molecule B | 206 Å$^2$ | inter AC - BD network contact |
| molecule A - molecule B symmetry mate | 83 Å$^2$ | inter AC - BD network contact |
| | | |
| sum; intra-packing network contacts | 3028 Å$^2$ | intra A - C network contact |
| sum; inter-packing network contacts | 289 Å$^2$ | inter AC - BD network contact |