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Supporting information for article:

The non-swapped monomeric structure of the arginine-binding protein from *Thermotoga maritima*

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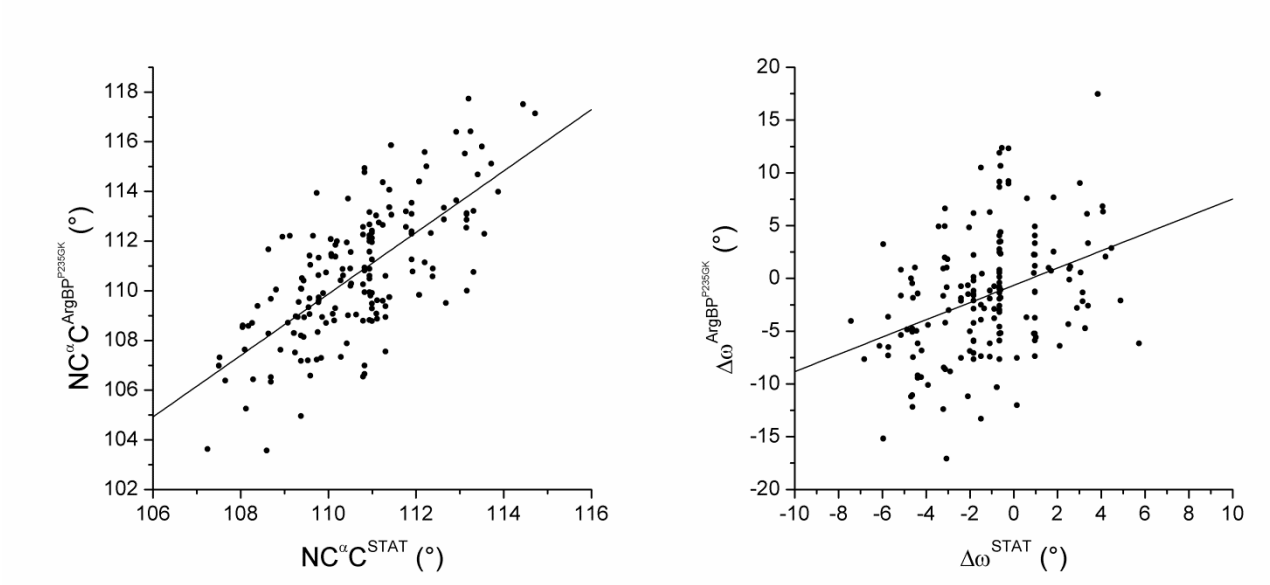

Figure S1 Regression analysis of the variability of geometrical parameters of protein backbone of the ArgBP^{P235GK} crystal structure. In panels A and B is reported the variability of the NC$^{\alpha}$C bond angle and of the deviation from the peptide bond planarity $\Delta\omega=(\omega-180°)\text{mod}360°$ (B), respectively. This analysis has been conducted by plotting the NC$^{\alpha}$C or $\Delta\omega$ values of the ArgBP^{P235GK} structure against the average corresponding values of residues adopting the same (φ, ψ) conformation obtained from databases of well-refined X-ray PDB structures. These protein structures were retrieved from the PDB using the PISCES culling server (http://dunbrack.fccc.edu/PISCES.php) using the following criteria: resolution better than 1.6 Å for bond angles and 1.2 Å for dihedral angles, R-factor ≤ 0.20, and internal sequence identity ≤ 25%. The regression lines are also shown. The correlation coefficient and p-value of the linear fitting are reported in Table S1.

Table S1 Correlation coefficient and p-value of the regression analysis of the variability of some backbone geometrical parameters (bond angles, deviation from peptide bond planarity Δω and carbon carbonyl pyramidalization θ_C) of ArgBP^{P235GK} crystal structure compared to the corresponding parameters derived from datasets of well-refined protein structures (see text and legend of Figure S1 for details).

This analysis clearly indicates that the variability of these parameters agree with that detected in well refined PDB structures.

Geometrical parameter	**Correlation coefficient**	**p-value**
$NC^{\alpha}C$	0.70	$<10^{-10}$
$NC^{\alpha}C^{\beta}$	0.21	$5.6*10^{-3}$
$C^{\beta}C^{\alpha}C$	0.33	$9.0*10^{-6}$
$C^{\alpha}CO$	0.13	$8.8*10^{-2}$
$C^{\alpha}CN_{+1}$	0.40	$8.3*10^{-8}$
OCN_{+1}	0.22	$4.2*10^{-3}$
$C_{-1}NC^{\alpha}$	0.46	$1.5*10^{-10}$
Δω	0.37	$1.0*10^{-6}$
θ_C	0.30	$7.3*10^{-5}$