Volume 79 (2023)

Supporting information for article:

Using graphlet degree vectors to predict atomic displacement parameters in protein structures

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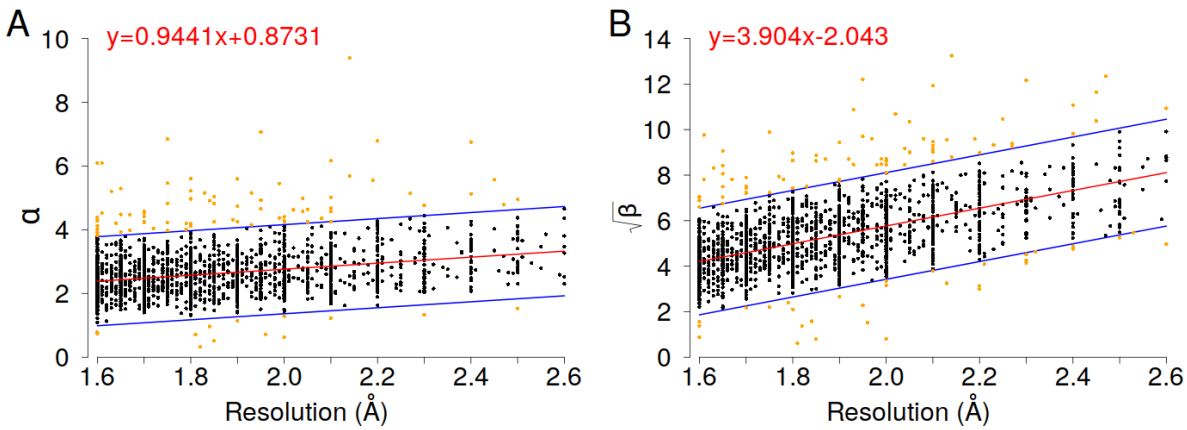


Figure S1 Dependence of the parameters of the SIGD on resolution. The linear fit (red line) of the shape (α) and scale ($\beta^{0.5}$) parameters against resolution is shown. The blue lines correspond to the upper and lower prediction intervals at a confidence level of 95%. The data points falling outside the 95% prediction interval are in orange; they were excluded from the further analysis.

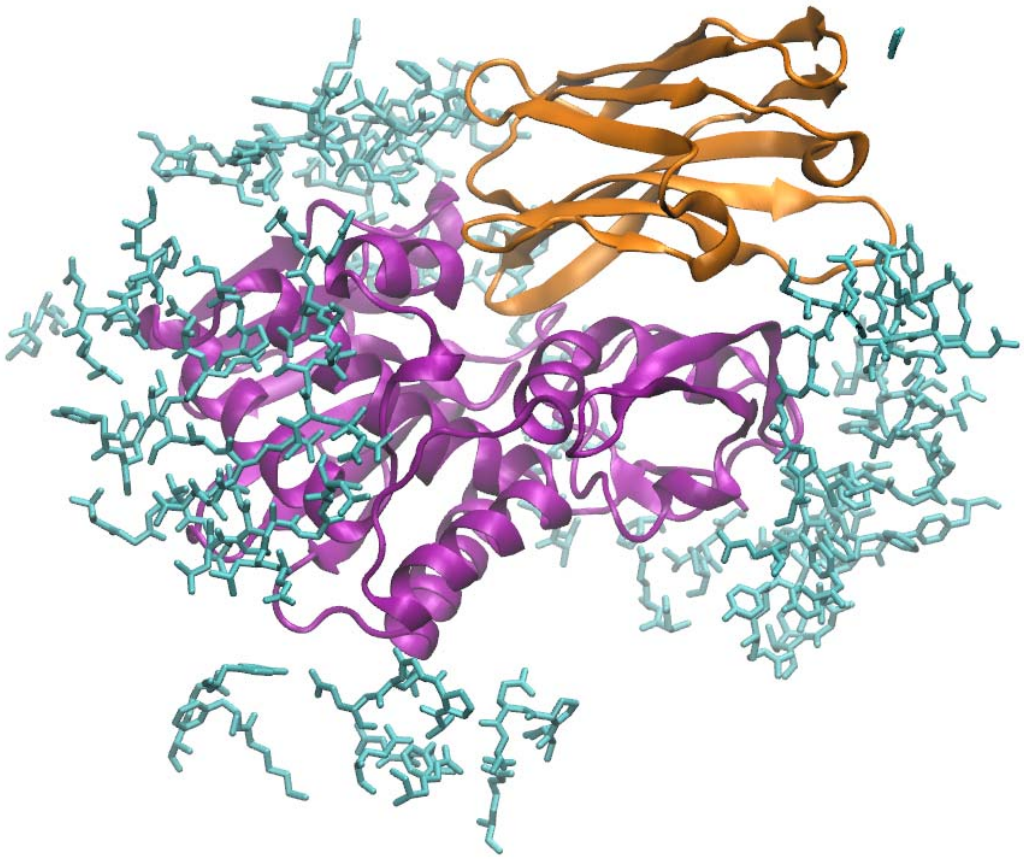
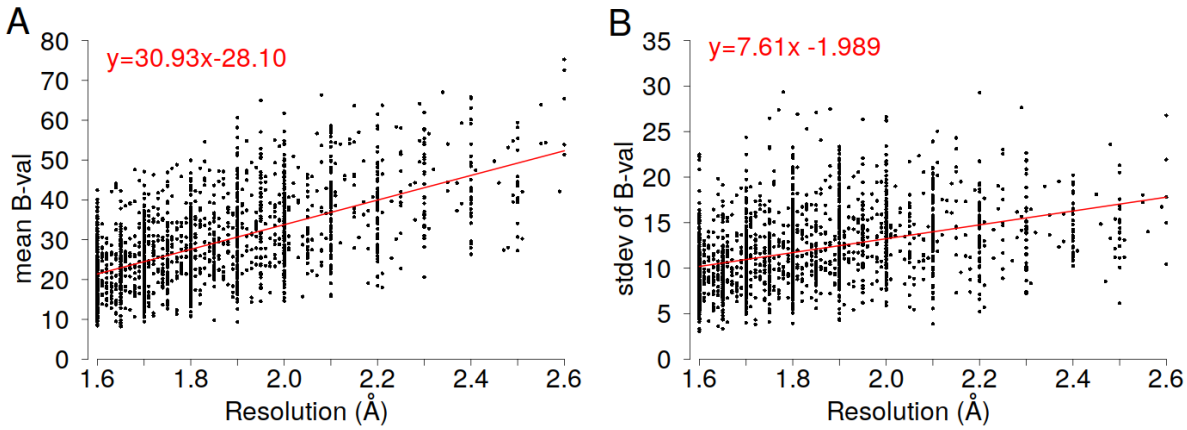


Figure S2 Model with symmetry-related residues. PDB-REDO entry (PDBid: 6obe) is shown as a ribbon, chain A in purple and chain B in orange, while symmetry-related residues are shown as cyan sticks.



Dependence of the mean and standard deviation of the B-value on resolution. The linear regression line of best fit is represented by the red line.

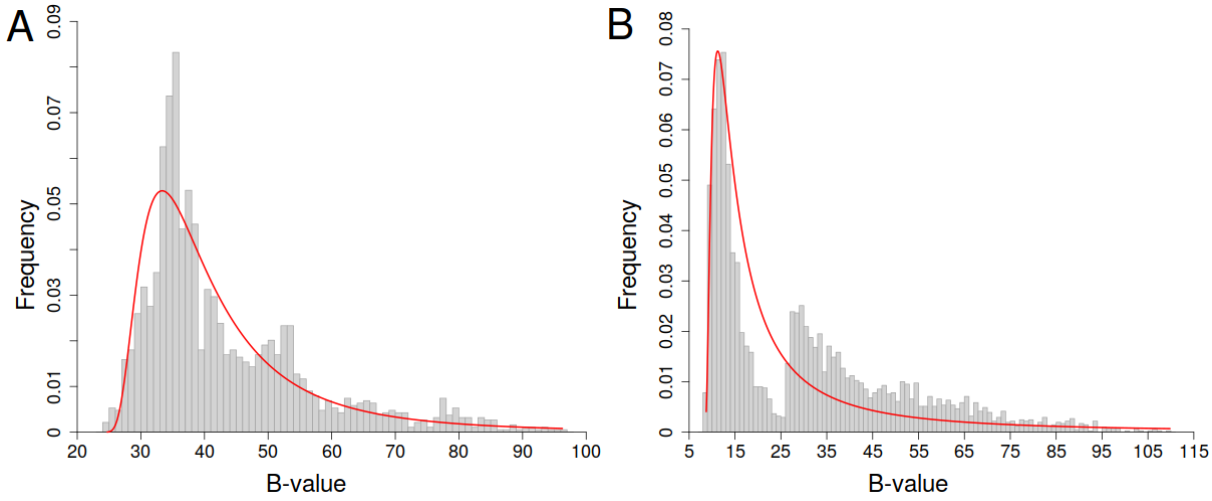


Figure S3 B-value distribution and fitted SIGD (red color) are shown; (A) PDBid: 7upo and (B) PDBid: 4d05.

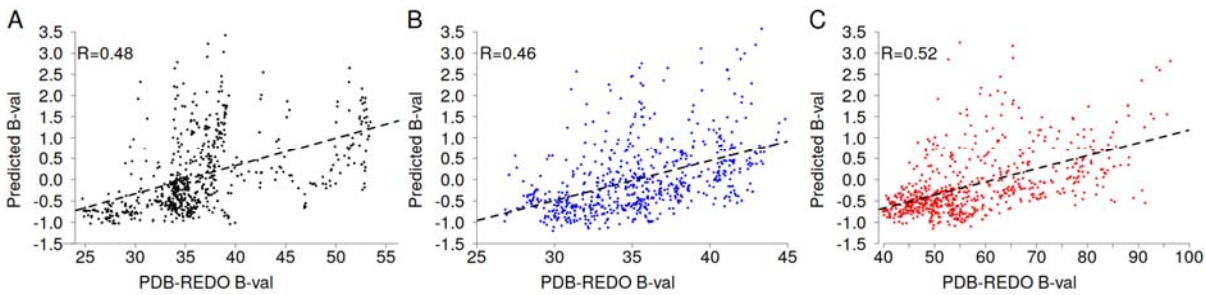


Figure S4 Scatter plot of the predicted versus PDB-REDO B-values of ABC-type heterotrimeric protein (PDBid: 7upo); (A) chain A, (B) chain B and (C) chain C.

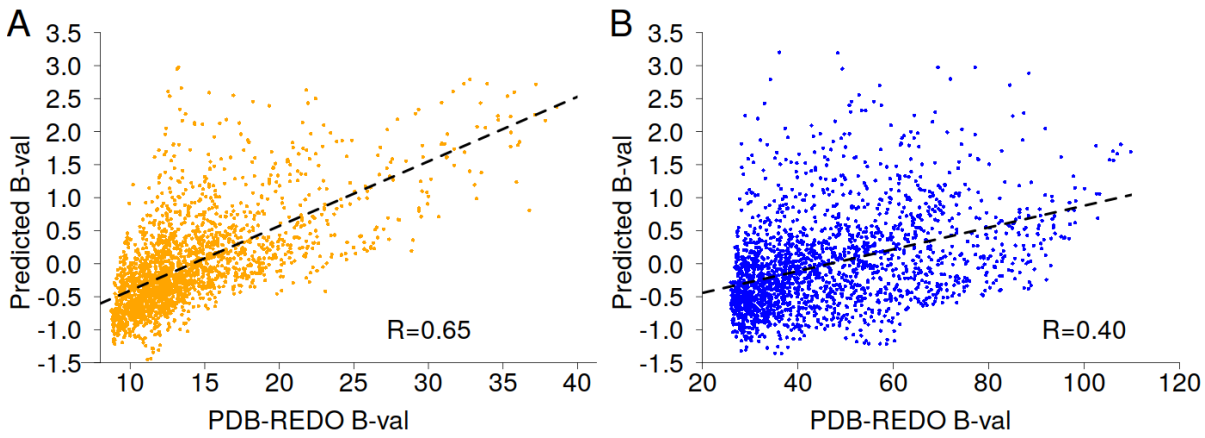


Figure S5 Scatter plot of the predicted versus PDB-REDO B-values of the enzyme-adenylate complex (PDBid: 4d05); (A) chain A and (B) chain B.

Table S1 Pairwise comparison of the heterotrimeric chains: A, B, and C (PDBid: 7upo).

The upper right triangle is the pairwise template modeling score (or TM-score), the bottom left is the pairwise sequence identity (%).

chain	A	B	C
A	/	0.79	0.71
B	30	/	0.64
C	32	18	/