

UC San Diego

UC San Diego Previously Published Works

Title

Difference distance map data of alternative crystal forms of UlaA

Permalink

<https://escholarship.org/uc/item/8bs3k48f>

Authors

Vastermark, Ake

Driker, Adelle

Weng, Jingwei

et al.

Publication Date

2017-02-01

DOI

10.1016/j.dib.2016.11.087

Peer reviewed



ELSEVIER

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Difference distance map data of alternative crystal forms of UlaA

Ake Vastermark^{a,*}, Adelle Driker^a, Jingwei Weng^b,
Xiaochun Li^c, Jiawei Wang^d, Milton H. Saier Jr.^a^a Department of Molecular Biology, University of California at San Diego, La Jolla, CA 92093-0116, USA^b Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Department of Chemistry and Institute of Biomedical Sciences, Fudan University, Shanghai, People's Republic of China^c Laboratory of Cell Biology, Howard Hughes Medical Institute, The Rockefeller University, New York, New York 10065, USA^d State Key Laboratory of Biomembrane and Membrane Biotechnology, School of Life Sciences, Tsinghua University, Beijing, People's Republic of China

ARTICLE INFO

Article history:

Received 6 October 2016

Received in revised form

18 November 2016

Accepted 23 November 2016

Available online 3 December 2016

ABSTRACT

We introduce the value of information obtained by comparing alternative crystal forms of the same sub-state (of outward open UlaA, our example protein), which is found in the same lattice configuration but different space groups. We compare instability estimates obtained using this new method (alternative crystal forms) with temperature factors. Using a transport assay result, we correlate observations for two homologous secondary structure elements, and show that the alternative states method for obtaining instability estimates provide differentiating information about an important and immobilized mid-TMS region. The data presented in this article are related to the article entitled “The V-motifs facilitate the substrate capturing step of the PTS elevator mechanism” (A. Vastermark, A. Driker, J. Weng, X. Li, J. Wang, M.H. Saier Jr., 2016).

© 2016 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

DOI of original article: <http://dx.doi.org/10.1016/j.jsb.2016.10.002>

Abbreviations: C2A, P2₁A, Space group names; APC, Amino acid-Polyamine organoCation superfamily of secondary carriers; PTS, Bacterial Phospho-Transferase System; NMA, Normal Mode Analysis

* Corresponding author.

E-mail address: msaier@ucsd.edu (A. Vastermark).

<http://dx.doi.org/10.1016/j.dib.2016.11.087>

2352-3409/© 2016 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

Specifications Table

Subject area	Physics
More specific subject area	Biophysics, bioinformatics
Type of data	3 tables, 3 molecular graphics, 1 alignment, 1 graph, 1 schematic figure, 5 distance maps
How data was acquired	Secondary analyses of published data
Data format	Raw (Figs. 2, 4, 9–12, Tables 2–3), Analyzed (Fig 1, 3, 5–8, Table 1)
Experimental factors	Secondary analyses of published data, distance maps
Experimental features	Computational analysis
Data source location	The data are accessible within the article
Data accessibility	The data are accessible within the article

Value of the data

- Alternative crystal forms of outward open UlaA structure is valuable to interpret MD simulation of MalT substrate catching step, constituting 25% of the “elevator mechanism” of the PTS group translocation process.
- The strength of the alt. crystal data might be that it represents two real low energy collective states [1] that the protein prefers, in the crystal hindering environment.

1. Data

- **Fig. 1.** Mapping between secondary structural elements.
- **Fig. 2.** Delta distance map, showing 4RP8.C–4RP9 (outward occluded (P2₁B)–outward open (C2A)).
- **Fig. 3, A–B.** Superimposed side view of half space filling Michael Sanner’s molecular surface of the substrate binding space in the C2A (blue) and P2₁A (yellow) states (panel A). Hydrogen bonds coordinate vitamin C in the two conformations (panel B).
- **Fig. 4, A–B.** Variable appearance of Log₁₀-transformed B (temperature) factor of C2A (red and yellow lines) and P2₁A (blue line) crystal forms in the vicinity of pivot residues Gly58 (panel A) and Gly286 (panel B).
- **Fig. 5, A–B.** The side chains coordinating vitamin C are primarily attached to secondary structural elements of the immobile core domains (panel A). They display limited macro-movement during the C2A → P2₁A comparison (panel B).
- **Fig. 6, A–B.** Salt bridges in the C2A and P2₁A crystal forms (A and B) of UlaA.
- **Fig. 7, A–B.** Binary alignment of UlaA and MalT (panel A), and binary alignment of TMS7 region (panel B) of UlaA (sequence A) and MalT (sequence B).
- **Fig. 8.** Nearby (5 Å) atoms of CA of G286 of UlaA (4RP9).
- **Fig. 9, A–D (cartoonwise).** Triplicate 1 (“Rep 1”) of MD simulation of MalT substrate release by TMS7 mechanism (outward open, substrate present).
- **Fig. 10 A–D.** Triplicate 2 (“Rep 2”) of MD simulation of MalT substrate release by TMS7 mechanism (outward open, substrate present).
- **Fig. 11 A–D.** Triplicate 3 (“Rep 3”) of MD simulation of MalT substrate release (by TMS7 mechanism (outward open, substrate present).
- **Fig. 12 A–C.** Δ-distance maps representing the difference between the outward open C2A and P2₁A crystal forms of UlaA, using conditional formatting (panel A), ESCET (panel B), or RR distance maps (panel C).

- **Table 1.** Tabular form of a proposed alignment of secondary structural elements of UlaA and ChbC. This alignment is not “linear” since we cannot rearrange sequential elements.
- **Table 2.** Hydrogen bond distances in the C2A state of the Vitamin C binding site.
- **Table 3.** Hydrogen bond distances in the P2₁A state of the Vitamin C binding site.

2. Experimental design, materials and methods

2.1. Δ -distance maps

Δ -distance maps were calculated as follows. The largest common set of C _{α} atoms was identified from the PDB files of the two conformational states of UlaA. Each state was represented as a matrix of all pairwise distance measurements. Bypassing previous convention (the “inward–outward” convention), the matrix of the state (C2A) was subtracted from the matrix of the (P2₁A) state.

The following parameters were used for ESCET normalization [2]. For 4RP8.A, D_{\min} = 2.36 (resolution), N_{par} = 26604 (number of parameters used in refinement, estimated), N_{obs} = 49177 (number of reflections), Cpl = 96.1 (completeness), R_{free} = 0.239 (free R value; fit to data used in refinement), and R_{all} = 0.199 (R value, working and test set). For 4RP9, D_{\min} = 1.65, N_{par} = 26604, N_{obs} = 71471, Cpl = 94.6, R_{free} = 0.174, and R_{all} = 0.136.

2.2. MD simulations of MalT

A triplicated protein–membrane system was generated with CHARMM membrane builder using 50,000 water molecules, 200–250 ns production runs in the NAMD 2.9 package. Simulations are taken from McCoy et al. MalT structure paper, see original paper for details [3].

Acknowledgments

The work was supported by NIH grants GM077402 and GM094610 (to M.S.) and by funds from Ministry of Science and Technology of China (grant nos. 2011CB911102 and 2015CB910104) and National Natural Science Foundation of China (31321062) to J.W. We are grateful for valuable advice and intellectual contributions (lattice analysis) by Dr Spencer Bliven, Bioinformatics and Systems Biology, University of California at San Diego, La Jolla, CA 92093-0116, USA & National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, MD 20894, USA. We thank Dr. Wonpil Im, Kansas University, for providing the original MalT simulation data.

Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at <http://dx.doi.org/10.1016/j.dib.2016.11.087>.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at <http://dx.doi.org/10.1016/j.dib.2016.11.087>.

References

- [1] A. Vastermark, A. Driker, J. Weng, X. Li, J. Wang, M.H. Saier Jr., The V-motifs facilitate the substrate capturing step of the PTS elevator mechanism, *J. Struct. Biol.* 196 (3) (2016) 496–502.
- [2] T.R. Schneider, Domain identification by iterative analysis of error-scaled difference distance matrices, *Acta Crystallogr. D Biol. Crystallogr.* 60 (2004) 2269–2275.
- [3] J.G. McCoy, Z. Ren, V. Stanevich, J. Lee, S. Mitra, E.J. Levin, S. Poget, M. Quick, W. Im, M. Zhou, The structure of a sugar transporter of the glucose EII^C superfamily provides insight into the elevator mechanism of membrane transport, *Structure* 24 (6) (2016) 956–964.