BIOLOGICAL
CRYSTALLOGRAPHY

Volume 71 (2015)

Supporting information for article:

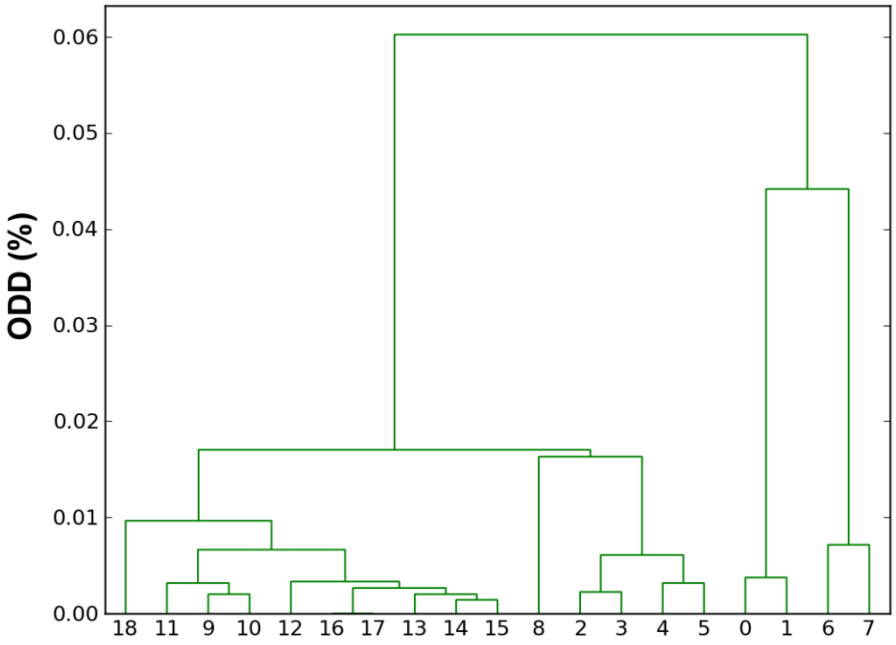
S-SAD phasing of monoclinic histidine kinase from *Brucella abortus* combining data from multiple crystals and orientations: an example of data collection strategy and *a posteriori* analysis of different data combinations

Sebastián Klinke, Nicolas Foos, Jimena J. Rinaldi, Gastón Paris, Fernando A. Goldbaum, Pierre Legrand, Beatriz G. Guimarães and Andrew Thompson

S-SAD phasing of monoclinic histidine kinase from *Brucella abortus* combining data from multiple crystals and orientations: an example of data collection strategy and *a posteriori* analysis of different data combinations.

Sebastián Klinke, Nicolas Foos, Jimena J. Rinaldi, Gastón Paris, Fernando A. Goldbaum, Pierre Legrand, Beatriz G. Guimarães and Andrew Thompson

Supplementary Figures



Supplementary Figure S1. Cluster analysis of the overall diffraction dissimilarity (ODD, %) among data from multi-crystal and multi-orientation data sets. The analysis is based in the procedure described in (Liu *et al.*, 2012). From **0** to **18**, data sets correspond to: **0**, X102a; **1**, X102a-k10; **2**, X104a; **3**, X104a-k10; **4**, X111a; **5**, X111a-inv; **6**, X111b; **7**, X111b-inv; **8**, X111c; **9**, X112a; **10**, X112a-k10; **11**, X112a-kminus10; **12**, X113a; **13**, X113b; **14**, X113b-k10; **15**, X113b-kminus10; **16**, X113a-k10; **17**, X113a-kminus10; **18**, X93a (see the legend of Table 1 and Supplementary Table 1 for a complete description).

Supplementary Tables

Supplementary Table S1. Data collection parameters and statistics from data sets that were not used for the original structure determination of HK and that complement Table 1. In the data set name, positions **a** and **b** refer to translations of the crystal in the X-ray beam, whereas **k** refers to different crystal orientations used (κ offset). Seven additional data sets were collected from four crystals: X93 (single position, single orientation), X102 (single position, 2 orientations), X104 (single position, 2 orientations), and X111 (two positions, single orientation, inverse beam). $\Delta F/\sigma(\Delta F)$ is the average anomalous signal from data truncated to 4.2 Å resolution. The anomalous correlation coefficients are also calculated from data truncated to 4.2 Å.

Crystal	X111	X111	X104	X104	X102	X102	X93
Data set name	a	b	a	ak10	a	ak10	a
κ angle (º)	0	0	0	10	0	10	10
Total range (º)	200 + 200	240 + 240	400	400	500	400	400
Unit-cell parameters							
a (Å)	72.3	72.1	72.3	72.3	72.1	72.1	72.1
b (Å)	108.8	108.3	109.2	109.2	108.4	108.4	108.6
c (Å)	73.3	73.1	73.3	73.4	73.1	73.2	73.2
β (º)	103.3	103.1	103.1	103.2	103.5	103.5	103.5
Resolution (Å)	50.0-3.10	50.0-3.00	50.0-3.00	50.0-3.00	50.0-3.05	50.0-3.08	50.0-2.85
(Last shell) (Å)	(3.17-3.10)	(3.07-3.00)	(3.18-3.00)	(3.18-3.00)	(3.23-3.05)	(3.27-3.08)	(3.02-2.85)
Unique reflections	38646 (2659)	42393 (2827)	42150 (6560)	42198 (6578)	40394 (6267)	38656 (5809)	50135 (7999)
Average multiplicity	3.8 (3.5)	4.5 (4.2)	3.9 (3.8)	3.9 (3.8)	4.8 (4.7)	3.8 (3.7)	3.8 (3.7)
Completeness (%)	97.4 (90.6)	97.6 (88.7)	96.5 (93.2)	96.5 (93.4)	98.0 (94.9)	97.2 (90.3)	99.3 (97.9)
R_{meas} (%)	5.1 (77.8)	6.3 (90.9)	5.4 (104.0)	5.3 (103.8)	5.8 (116.4)	5.8 (96.8)	5.6 (81.5)
$CC_{1/2}$ (%)	100.0 (88.5)	99.9 (90.8)	99.9 (85.5)	100.0 (84.4)	99.9 (87.1)	99.9 (88.5)	99.9 (87.7)
$\langle I/\sigma(I)\rangle$	17.4 (1.9)	14.6 (1.7)	18.6 (1.5)	18.7 (1.4)	18.2 (1.4)	16.0 (1.5)	14.1 (1.6)
Anomalous CC (%)	21	27	25	27	41	41	27
$\Delta F/\sigma(\Delta F)$	1.10	1.12	1.11	1.14	1.34	1.32	1.08

Supplementary Table 2. Refinement and validation statistics.

Data set name	NATIVE 1	NATIVE 2
Refinement	*(partial)*	
Resolution range (Å)	33.8-2.70	48.6-2.51
Number of protein atoms	5287	5614
Number of ligand atoms	125	126
Number of water molecules	-	-
R	0.238	0.202
R_{free}	0.267	0.242
Rms deviations from ideal values [a]		
Bond lengths (Å)	0.010	0.010
Bond angles (º)	1.3	1.2
B-factor (average, $Å^2$)	107	74
MolProbity validation [b]		
Clashscore		6.77
Poor rotamers (%)		10.6
Ramachandran plot		
Favoured (%)		95.8
Allowed (%)		4.1
Disallowed (%)		0.1

[a] (Engh & Huber, 1991)
[b] (Chen *et al.*, 2010)

References, supplementary material

Chen, V. B., Arendall, W. B., 3rd, Headd, J. J., Keedy, D. A., Immormino, R. M., Kapral, G. J., Murray, L. W., Richardson, J. S. & Richardson, D. C. (2010). *Acta crystallographica. Section D, Biological crystallography* **66**, 12-21.

Engh, R. A. & Huber, R. (1991). *Acta Crystallogr A* **47**, 392-400.

Liu, Q., Dahmane, T., Zhang, Z., Assur, Z., Brasch, J., Shapiro, L., Mancia, F. & Hendrickson, W. A. (2012). *Science* **336**, 1033-1037.