

Acta Crystallographica Section D Biological Crystallography addenda and errata

ISSN 0907-4449

## Novel c-di-GMP recognition modes of the mouse innate immune adaptor protein STING. Corrigendum

Ko-Hsin Chin,<sup>a</sup> Zhi-Le Tu,<sup>b</sup> Yi-Che Su,<sup>b</sup> Yu-Jen Yu,<sup>b</sup> Hui-Chen Chen,<sup>c</sup> Yuan-Chao Lo,<sup>d</sup> Chin-Pan Chen,<sup>d</sup> Glen N. Barber,<sup>e</sup> Mary Lay-Cheng Chuah,<sup>f</sup> Zhao-Xun Liang<sup>f</sup> and Shan-Ho Chou<sup>a,b,c</sup>\*

<sup>a</sup>Agricultural Biotechnology Center, National Chung Hsing University, Taichung 40227, Taiwan, <sup>b</sup>Institute of Biochemistry, National Chung Hsing University, Taichung 40227, Taiwan, <sup>c</sup>Graduate Institute of Basic Medical Science, China Medical University, Taichung 40402, Taiwan, <sup>d</sup>Institute of Biomedical Sciences, Academia Sinica, Taipei 115, Taiwan, <sup>e</sup>Department of Cell Biology, University of Miami School of Medicine, Miami, Florida, USA, and <sup>f</sup>School of Biological Sciences, Nanyang Technological University, Singapore 637551, Singapore

Correspondence e-mail: shchou@nchu.edu.tw

The two structures reported in the article by Chin *et al.* [(2013). *Acta Cryst.* **D69**, 352–366] have been further refined and corrected.

The original structures reported in the article by Chin *et al.* (2013) were incorrectly modeled in the C-terminal region, and contained some notable geometrical deviations. The structures have now been corrected, refined again and validated with *MolProbity* (Chen *et al.*, 2010). The improved structures have been re-deposited in the PDB with the same PDB codes (mSTING-CTD, 4g3l and mSTING-CTD-c-di-GMP complex, 4g4d). A corrected Table 1 is given below. The conclusions of the paper are not changed by these corrections.

## References

Chen, V. B., Arendall, W. B., Headd, J. J., Keedy, D. A., Immormino, R. M., Kapral, G. J., Murray, L. W., Richardson, J. S. & Richardson, D. C. (2010). *Acta Cryst.* D66, 12–21.

Chin, K.-H., Tu, Z.-L., Su, Y.-C., Yu, Y.-J., Chen, H.-C., Lo, Y.-C., Chen, C.-P., Barber, G. N., Chuah, M. L.-C., Liang, Z.-X. & Chou, S.-H. (2013). *Acta Cryst.* D69, 352–366.

 Table 1

 Summary of the crystallographic data for mSTING and the mSTING-c-di-GMP complex.

Values in parentheses are for the outermost shell.

	Native	SeMet-mSTING	mSTING-c-di-GMP
Beamline	BL13C1	BL13B1	SP44XU
Wavelength (Å)	0.97622	0.97898	0.99808
Space group	P3 <sub>1</sub>	P3 <sub>1</sub>	P3 <sub>1</sub>
Unit-cell parameters	a = b = 78.619,	a = b = 78.493,	a = b = 79.058,
$(\mathring{\mathrm{A}},{}^{\circ})$	c = 50.418,	c = 50.409,	c = 49.693,
	$\alpha = \beta = 90$ ,	$\alpha = \beta = 90,$	$\alpha = \beta = 90$ ,
	$\gamma = 120$	$\gamma = 120$	$\gamma = 120$
Resolution range (Å)	30-2.39 (2.48-2.39)	30-2.20 (2.28-2.20)	30-2.36 (2.44-2.36)
Total observations	44542 (4387)	125788 (12546)	41778 (5210)
Unique observations	13794 (1371)	17676 (1767)	14245 (1444)
Multiplicity	3.2 (3.2)	7.1 (7.1)	2.9 (2.9)
Completeness (%)	100 (100)	100 (100)	99.6 (100)
$R_{\text{merge}}$ † (%)	6.1 (59.5)	6.5 (44.7)	3.9 (41.0)
$\langle I/\sigma(I)\rangle$	19.4 (2.3)	23.8 (4.9)	17.4 (2.8)
$R_{\text{free}}$ test-set size (%)	5	5	5
Refinement statistics			
$R_{\text{cryst}} \ddagger / R_{\text{free}} $ (%)	22.5/25.1	19.3/25.1	19.7/26.3
Model content			
Protein residues	370	368	352
c-di-GMP molecules	0	0	1
Mg <sup>2+</sup> ions	2	2	0
Waters	205	158	124
Average B factors ( $\mathring{A}^2$ )			
Backbone atoms	41.8	43.7	41.8
Side-chain atoms	43.6	45.2	44.6
Water O atoms	52.9	51.3	53.1
c-di-GMP molecules			58.9
Ramachandran plot¶, residues in (%)			
Most favourable regions	93.1	97.1	93.3
Additionally allowed regions	0.9	2.9	6.1
Outliers		0	0.6
Rotamer outliers (%)		2.8	0.9
R.m.s.d. from ideal geometry			
Bonds (Å)	0.008	0.0077	0.008
Angles (°)	1.50	1.14	1.20

<sup>†</sup>  $R_{\text{merge}} = \sum_{hkl} \sum_{i} |I_i(hkl) - \langle I(hkl)\rangle|/\sum_{hkl} \sum_{i} I_i(hkl)$ . ‡  $R_{\text{cryst}} = \sum_{hkl} ||F_{\text{obs}}| - |F_{\text{calc}}||/\sum_{hkl} ||F_{\text{obs}}||$ , where  $F_{\text{calc}}$  and  $F_{\text{obs}}$  are the calculated and observed structure-factor amplitudes, respectively. §  $R_{\text{free}}$  is the same as  $R_{\text{cryst}}$  but for 5.0% of the total reflections chosen at random and omitted from refinement. ¶ The percentages of residues located in the most favourable, additionally allowed regions and outliers were calculated using the MolProbity program with the default parameters (Chen et~al., 2010).