

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

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

^aAgricultural Biotechnology Center, National Chung Hsing University, Taichung 40227, Taiwan, ^bInstitute of Biochemistry, National Chung Hsing University, Taichung 40227, Taiwan, ^cGraduate Institute of Basic Medical Science, China Medical University, Taichung 40402, Taiwan, ^dInstitute of Biomedical Sciences, Academia Sinica, Taipei 115, Taiwan, ^eDepartment of Cell Biology, University of Miami School of Medicine, Miami, Florida, USA, and ^fSchool of Biological Sciences, Nanyang Technological University, Singapore 637551, Singapore

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

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	<i>P</i> 3 ₁	<i>P</i> 3 ₁	<i>P</i> 3 ₁
Unit-cell parameters (Å, °)	<i>a</i> = <i>b</i> = 78.619, <i>c</i> = 50.418, $\alpha = \beta = 90$, $\gamma = 120$	<i>a</i> = <i>b</i> = 78.493, <i>c</i> = 50.409, $\alpha = \beta = 90$, $\gamma = 120$	<i>a</i> = <i>b</i> = 79.058, <i>c</i> = 49.693, $\alpha = \beta = 90$, $\gamma = 120$
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)
<i>R</i> _{merge} [†] (%)	6.1 (59.5)	6.5 (44.7)	3.9 (41.0)
<i>I</i> / σ (<i>I</i>)	19.4 (2.3)	23.8 (4.9)	17.4 (2.8)
<i>R</i> _{free} test-set size (%)	5	5	5
Refinement statistics			
<i>R</i> _{cryst} / <i>R</i> _{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 ²⁺ ions	2	2	0
Waters	205	158	124
Average <i>B</i> factors (Å 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	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

[†] $R_{\text{merge}} = \sum_{hkl} \sum_i |I_i(hkl) - \langle I(hkl) \rangle| / \sum_{hkl} \sum_i I_i(hkl)$. [‡] $R_{\text{cryst}} = \sum_{hkl} (|F_{\text{obs}}| - |F_{\text{calc}}|) / \sum_{hkl} |F_{\text{obs}}|$, where F_{calc} and F_{obs} are the calculated and observed structure-factor amplitudes, respectively. [§] R_{free} is the same as R_{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).

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.