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**Supporting information for article:**

**Atomic structures of ternary Yb–Cd–Mg icosahedral quasicrystals and a 1/1 approximant**

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## S1. Supporting crystallographic information file

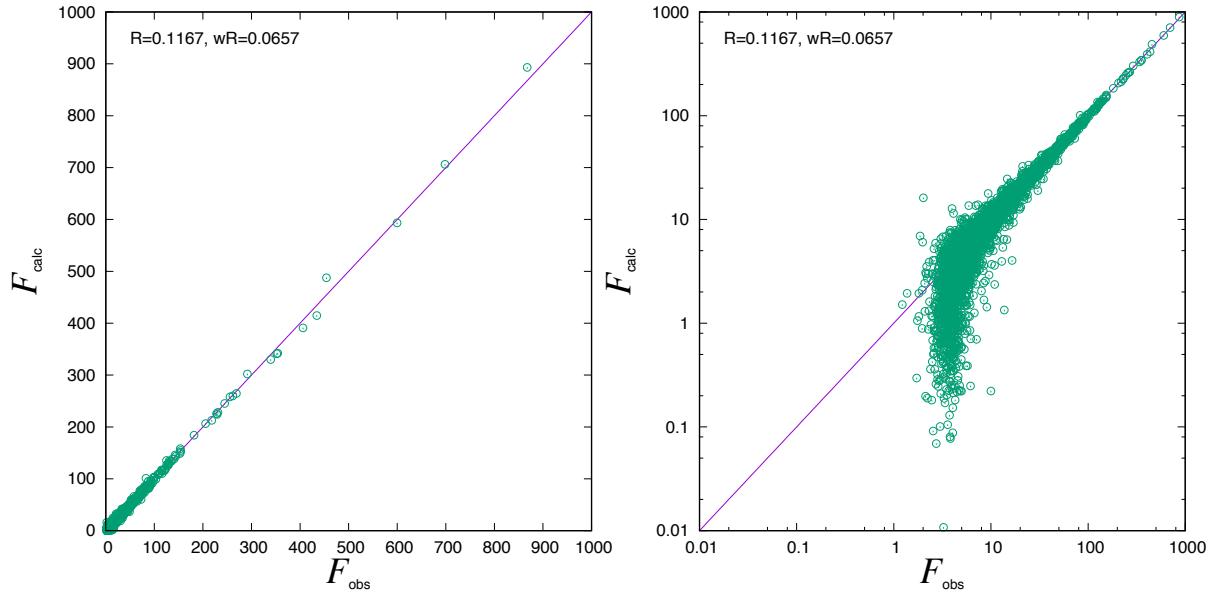
Following five crystallographic information files (CIF) contains atomic coordinates in  $80 \times 80 \times 80$  Å<sup>3</sup> regions for the refined atomic structure for the i-Yb-Cd-Mg quasicrystals.

- **dk5061sup2.cif**: Atomic coordinates for the Yb<sub>15.2</sub>Cd<sub>78.4</sub>Mg<sub>6.4</sub> (sample 2)
- **dk5061sup3.cif**: Atomic coordinates for the Yb<sub>15.5</sub>Cd<sub>68.4</sub>Mg<sub>16.1</sub> (sample 3)
- **dk5061sup4.cif**: Atomic coordinates for the Yb<sub>16.0</sub>Cd<sub>58.7</sub>Mg<sub>25.3</sub> (sample 4)
- **dk5061sup5.cif**: Atomic coordinates for the Yb<sub>15.8</sub>Cd<sub>51.6</sub>Mg<sub>32.5</sub> (sample 5)
- **dk5061sup6.cif**: Atomic coordinates for the Yb<sub>15.1</sub>Cd<sub>38.5</sub>Mg<sub>46.4</sub> (sample 6)

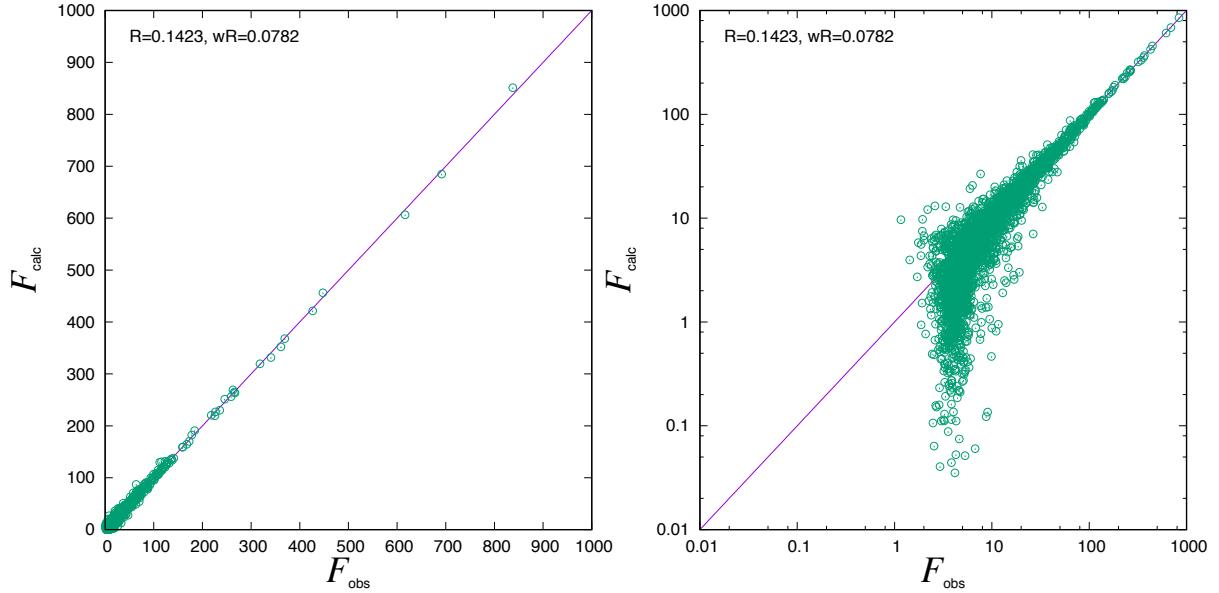
Following five files contains structure factors for i-Yb-Cd-Mg quasicrystals with indices in both six indices by Elser (1985), h<sub>i</sub> (i = 1, ..., 6) and six indices by Cahn *et al.* (1986), n<sub>i</sub> (i = 1, ..., 6), together with cubic indices by Cahn *et al.* (1986), h/h', k/k' l/l'. The parallel and perpendicular components of the Bragg reflections,  $Q_{\text{par}}$  and  $Q_{\text{perp}}$ , are presented in reciprocal lattice units (r.l.u).

- **dk5061sup7.hkl**: structure factors for the Yb<sub>15.2</sub>Cd<sub>78.4</sub>Mg<sub>6.4</sub> (sample 2)
- **dk5061sup8.hkl**: structure factors for the Yb<sub>15.5</sub>Cd<sub>68.4</sub>Mg<sub>16.1</sub> (sample 3)
- **dk5061sup9.hkl**: structure factors for the Yb<sub>16.0</sub>Cd<sub>58.7</sub>Mg<sub>25.3</sub> (sample 4)
- **dk5061sup10.hkl**: structure factors for the Yb<sub>15.8</sub>Cd<sub>51.6</sub>Mg<sub>32.5</sub> (sample 5)
- **dk5061sup11.hkl**: structure factors for the Yb<sub>15.1</sub>Cd<sub>38.5</sub>Mg<sub>46.4</sub> (sample 6)

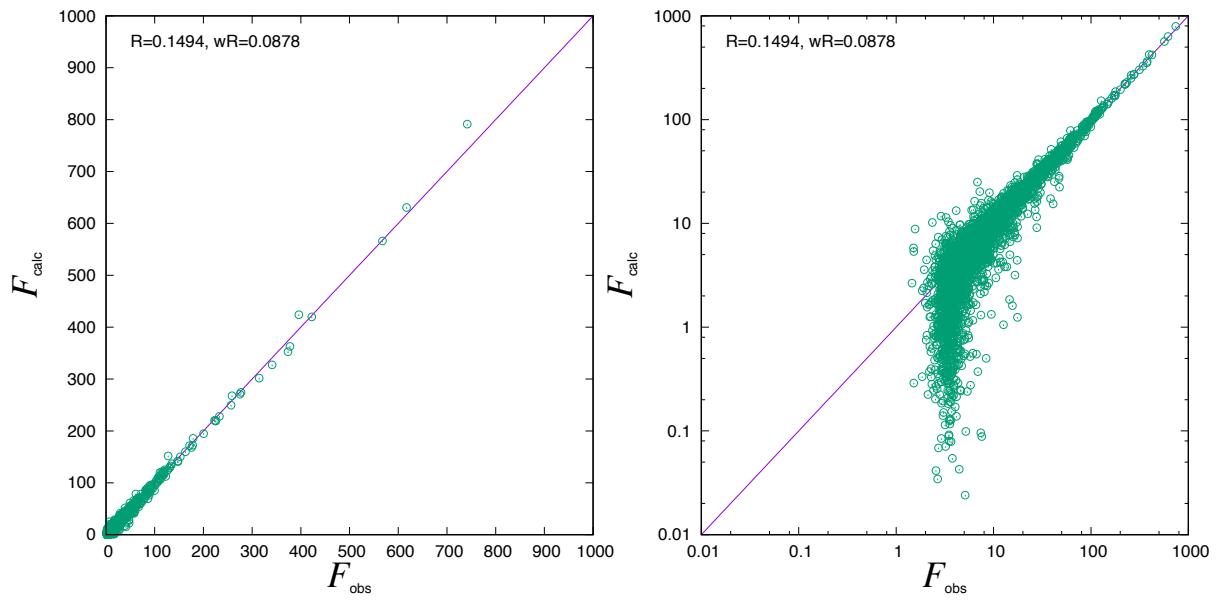
**dk5061sup12.cif** contains crystallographic information for the refined atomic structure for the Yb-Cd-Mg 1/1 approximant (sample 8), and **dk5061sup13.fcf** contains structure factors for the approximant.



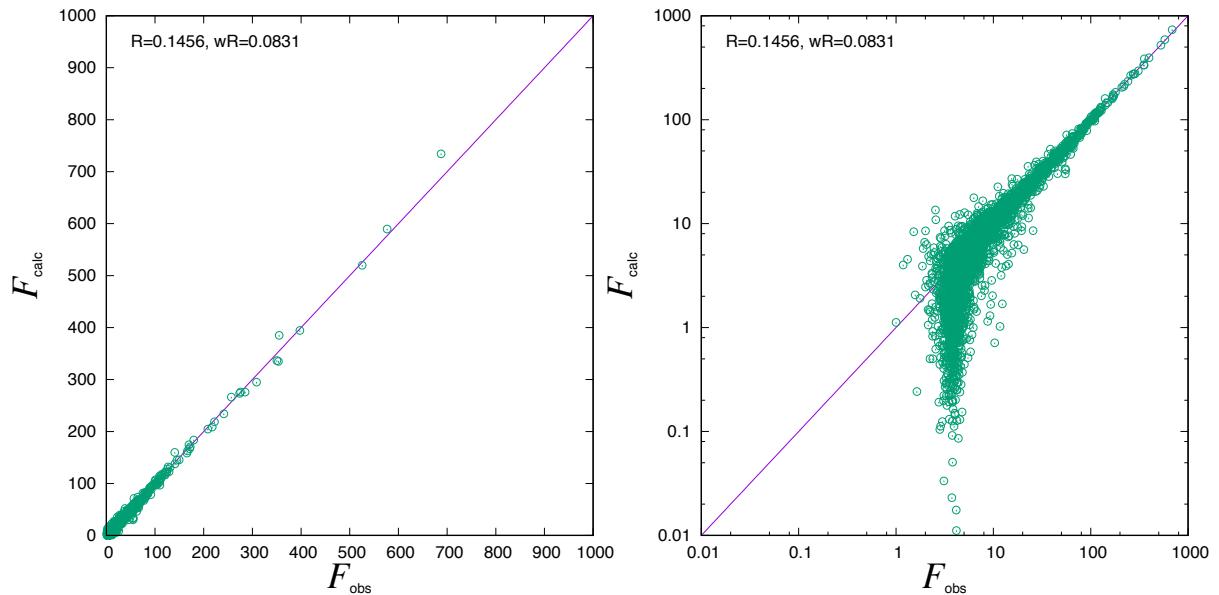
**Figure S1** Normal (left) and logarithmic (right)  $F_{\text{calc}}$  versus  $F_{\text{obs}}$  plots of the structure refinement for the  $\text{Yb}_{15.2}\text{Cd}_{78.4}\text{Mg}_{6.4}$  (sample 2).



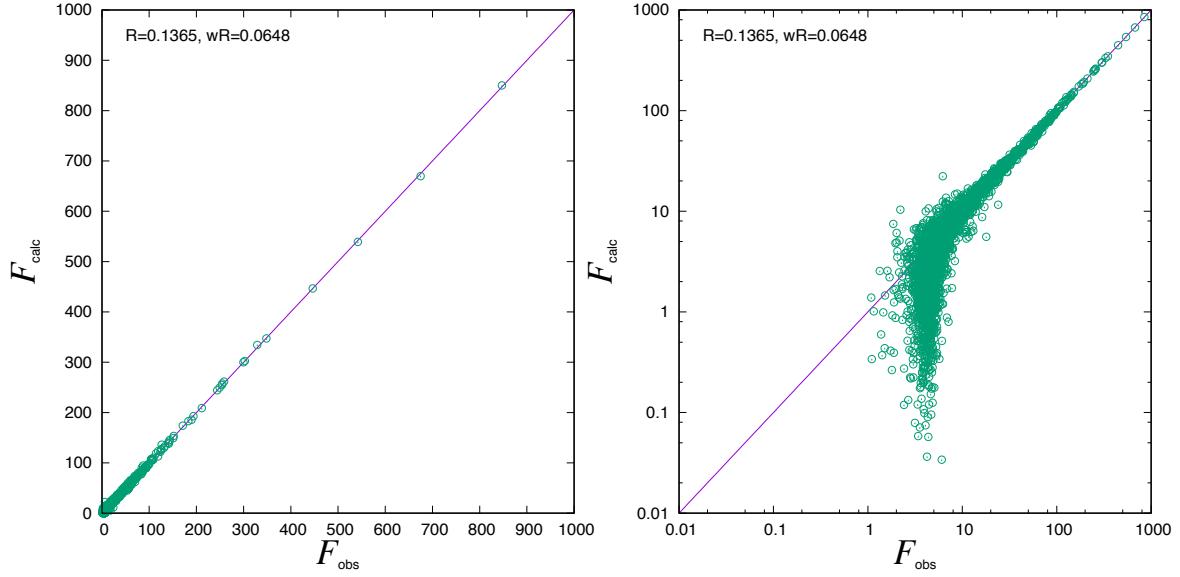
**Figure S2** Normal (left) and logarithmic (right)  $F_{\text{calc}}$  versus  $F_{\text{obs}}$  plots of the structure refinement for the  $\text{Yb}_{15.5}\text{Cd}_{68.4}\text{Mg}_{16.1}$  (sample 3).



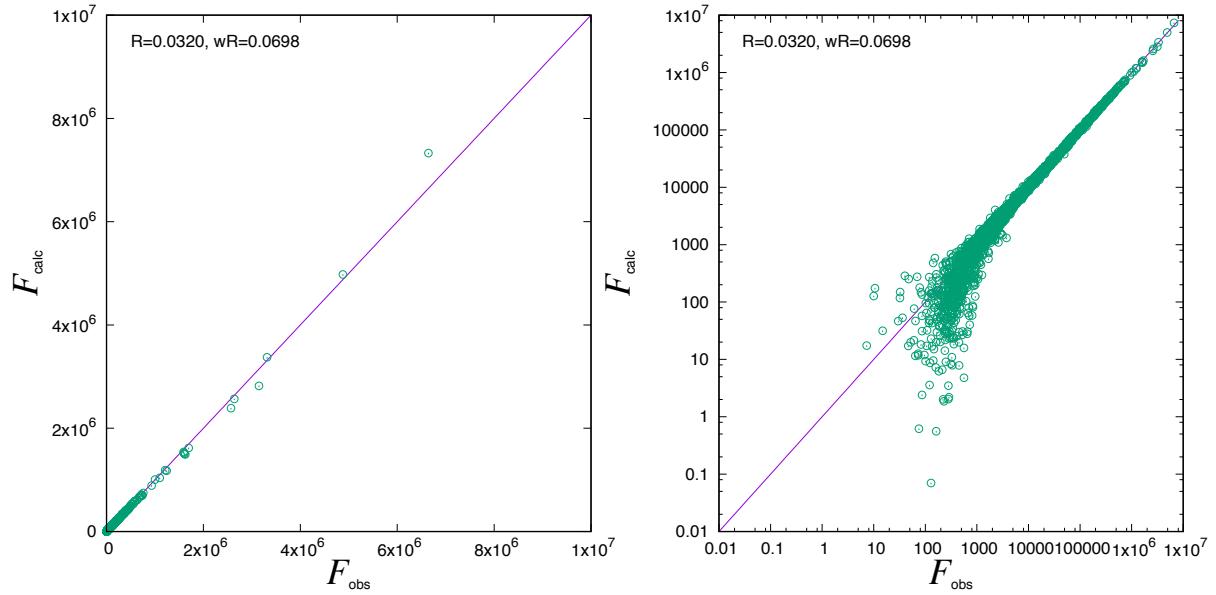
**Figure S3** Normal (left) and logarithmic (right)  $F_{\text{calc}}$  versus  $F_{\text{obs}}$  plots of the structure refinement for the  $\text{Yb}_{16.0}\text{Cd}_{58.7}\text{Mg}_{25.3}$  (sample 4).



**Figure S4** Normal (left) and logarithmic (right)  $F_{\text{calc}}$  versus  $F_{\text{obs}}$  plots of the structure refinement for the  $\text{Yb}_{15.8}\text{Cd}_{51.6}\text{Mg}_{32.5}$  (sample 5).



**Figure S5** Normal (left) and logarithmic (right)  $F_{\text{calc}}$  versus  $F_{\text{obs}}$  plots of the structure refinement for the  $\text{Yb}_{15.1}\text{Cd}_{38.5}\text{Mg}_{46.4}$  (sample 6).



**Figure S6** Normal (left) and logarithmic (right)  $F_{\text{calc}}$  versus  $F_{\text{obs}}$  plots of the structure refinement for the  $\text{Yb}_{13.3}\text{Cd}_{70.3}\text{Mg}_{16.5}$  (sample 8).

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## References

- Cahn, J. W., Shechtman, D., & Gratias, D. (1986). *J. Mater. Res.* **1**, 13-26.  
Elser, V. (1985). *Physical Review B*, **32**(8), 4892–4898.