

Re-refinement of 4g4a: room-temperature X-ray diffraction study of cisplatin and its binding to His15 of HEWL after 14 months chemical exposure in the presence of DMSO

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A re-refinement of 4g4a, the room-temperature X-ray diffraction study of cisplatin and its binding to His15 of HEWL after 14 months chemical exposure in the presence of DMSO is published as an addendum to Tanley *et al.* [(2012), *Acta Cryst. F* **68**, 1300–1306]. This example illustrates the benefits of sharing raw diffraction images, as well as structure factors and molecular coordinates, as the diffraction resolution of the study is now much improved at 1.70 Å.

We have re-refined our previously published room temperature crystal structure of cisplatin binding to hen egg lysozyme (PDB entry 4g4a; Tanley *et al.*, 2012) at a resolution of 1.7 Å. This structure was originally refined by us at 2.4 Å resolution and subsequently re-refined by Shabalina *et al.* (2015) to 2.0 Å resolution. Both studies extended the diffraction resolution by reprocessing subsets of the same data set's raw diffraction images [originally held at Utrecht University; Tanley *et al.* (2013) and which are now accessible at the University of Manchester (Tanley & Helliwell, 2015)]. Shabalina *et al.* (2015) (PDB code 4yen) interpreted the platinum coordination spheres as [PtCl₃His15] for the platinum ion (Pt^δ) coordinated

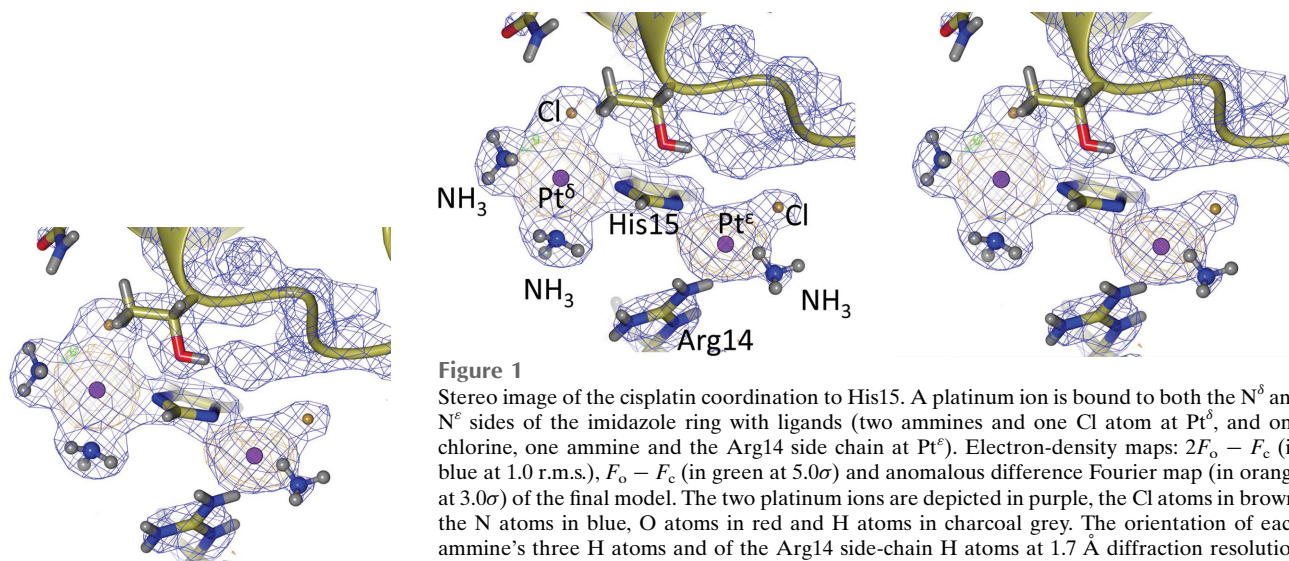


Figure 1

Stereo image of the cisplatin coordination to His15. A platinum ion is bound to both the N^δ and N^ε sides of the imidazole ring with ligands (two ammines and one Cl atom at Pt^δ, and one chlorine, one ammine and the Arg14 side chain at Pt^ε). Electron-density maps: $2F_o - F_c$ (in blue at 1.0 r.m.s.), $F_o - F_c$ (in green at 5.0σ) and anomalous difference Fourier map (in orange at 3.0σ) of the final model. The two platinum ions are depicted in purple, the Cl atoms in brown, the N atoms in blue, O atoms in red and H atoms in charcoal grey. The orientation of each ammine's three H atoms and of the Arg14 side-chain H atoms at 1.7 Å diffraction resolution are obviously approximate (the Arg14 side-chain nitrogen closest to the Pt^ε in particular would present a lone pair of electrons to the metal atom). This figure was prepared using *CCP4mg* (McNicholas *et al.*, 2011).

to N^δ of His15 and [PtCl₂His15Arg14] for the second platinum ion (Pt^ε) bound to His15-N^ε. A re-refinement of 4g4a at the extended resolution of 1.7 Å presented here gives improved clarity, and a small spread of *B* factors, of the Pt ligand assignments which are [PtCINH₃NH₃His15] for Pt^δ, and [PtCINH₃His15Arg14] for Pt^ε; see Fig. 1. Details are provided in the Supporting Information.

The following references are cited in the Supporting Information for this article: Afonine *et al.* (2012); Casini *et al.* (2007); Diederichs & Karplus (2013); Joosten *et al.* (2014); Murshudov *et al.* (1997); Schreurs *et al.* (2010); Tanley, Schreurs, Kroon-Batenburg, Meredith *et al.* (2012); Tanley *et al.* (2015).

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