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Supporting information for article:

Daliranite, PbHgAs2S5: determination of the incommensurately modulated structure and revision of the chemical formula

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Supporting information

S1. Supplementary Figures

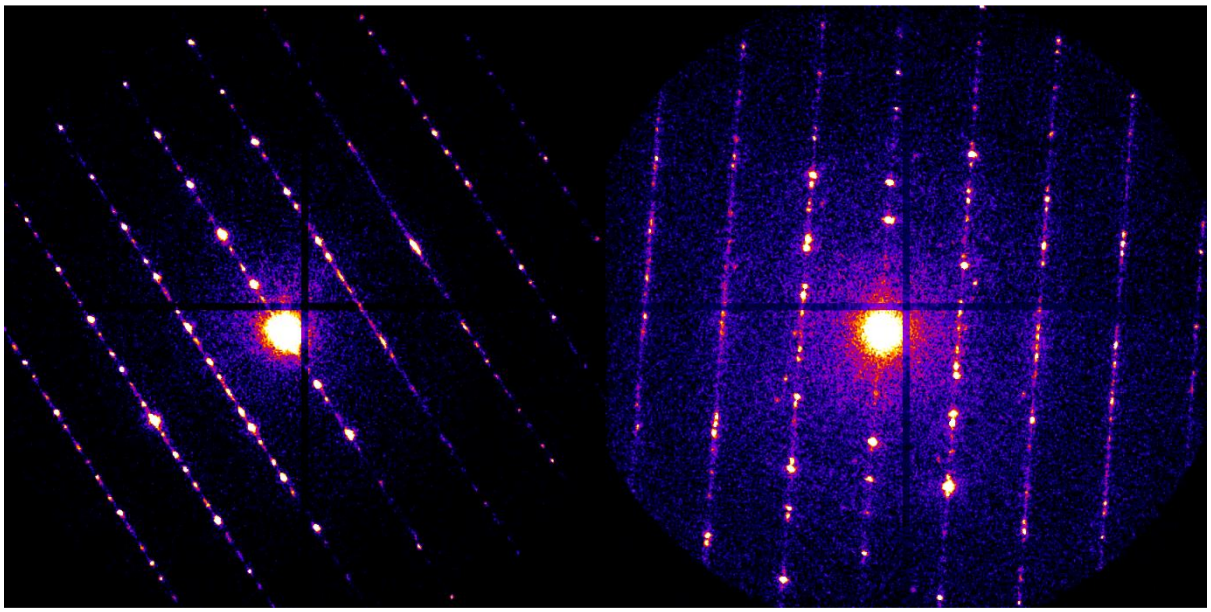

Figure S1 Diffraction patterns collected during two 3D ED data collections on two different crystals of daliranite showing streaking along the modulation direction, due to disorder in the structure.

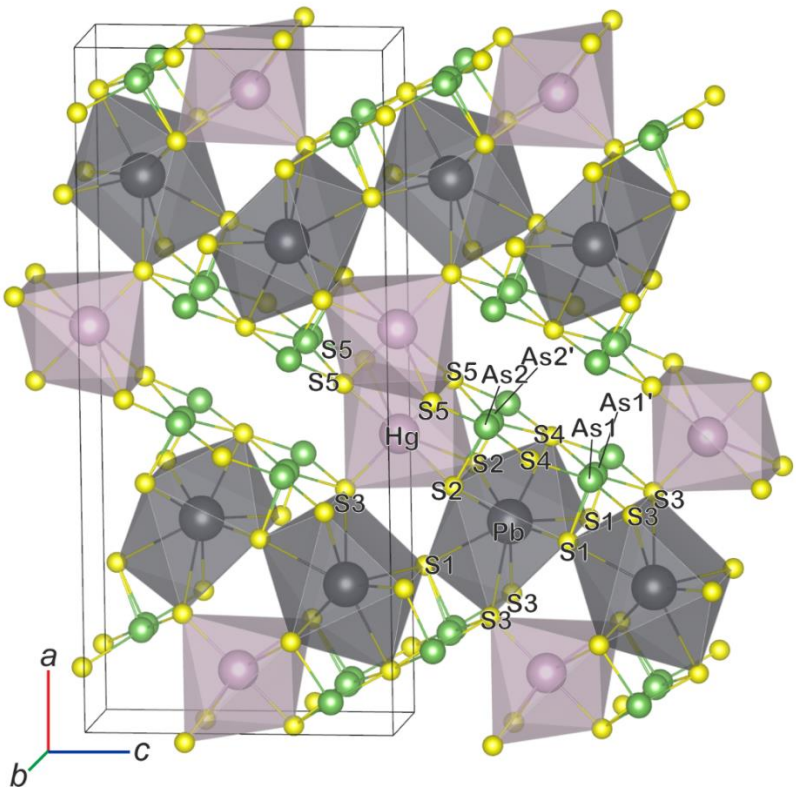

Figure S2 Crystal packing of daliranite with atom labelling scheme.

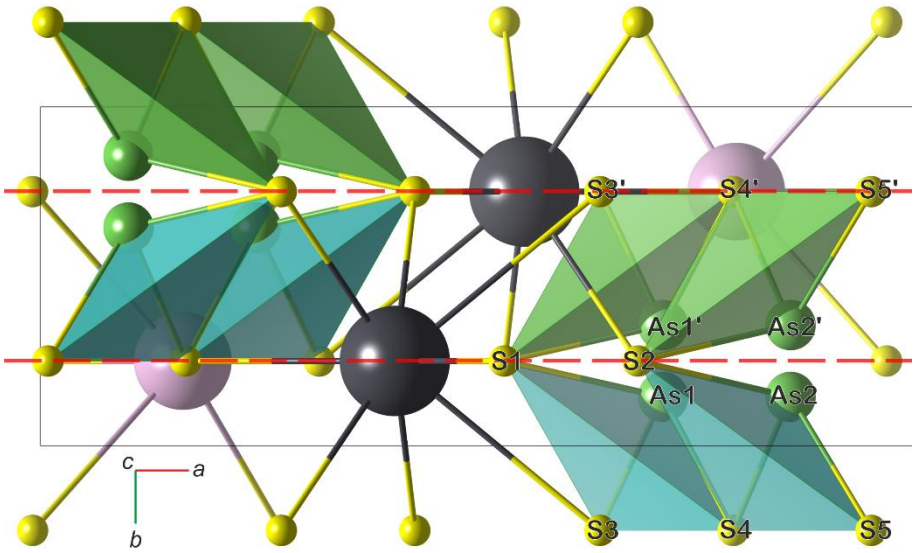

Figure S3 Detail of the disordered model showing each of the As sites split over two equivalent positions above and below the mirror plane (red dashed line). Blue and green polyhedra highlight the alternative coordination geometries resulting from the occupancy of one or the other site. Such symmetry equivalent sites have equal probability but cannot be occupied simultaneously and the occupation periodicity is described by the modulation.