

## Validation response form

# start Validation Reply Form

\_vrf\_PLAT212\_FCHMAG\_1\_0m

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PROBLEM: ADP of Atom CIW2 is N.P.D. or (nearly) 2D . Please Check

RESPONSE: The occupancy is 0.070(15) and the atom is probably somewhat positionally disordered, NPD is hardly surprising.

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\_vrf\_PLAT220\_FCHMAG\_1\_0m

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PROBLEM: NonSolvent Resd 1 Mn Ueq(max)/Ueq(min) Range 6.3 Ratio

RESPONSE: The coordination of Mn is very unusual here with very long and very short distsnces and it is almost certainly positionally disordered (statically or dynamically), giving rise to large difference between Ueq(max) and Ueq(min).

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\_vrf\_PLAT911\_FCHMAG\_1\_0m

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PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 19 Report

RESPONSE: Checked

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\_vrf\_PLAT976\_FCHMAG\_1\_0m

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PROBLEM: Check Calcd Resid. Dens. 0.70Ang From O1 . -0.41 eA-3

RESPONSE: O1 is bonded to Mn1, and both O1 and Mn1 are significantly (statically or dynamically) positionally disordered. The residual density arises because of the difficulty in modelling such coupled disorder.

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# end Validation Reply Form