The Structure of Metal Binding Domain 1 of the Copper Transporter ATP7B Reveals Mechanism of a Singular Wilson Disease Mutation.

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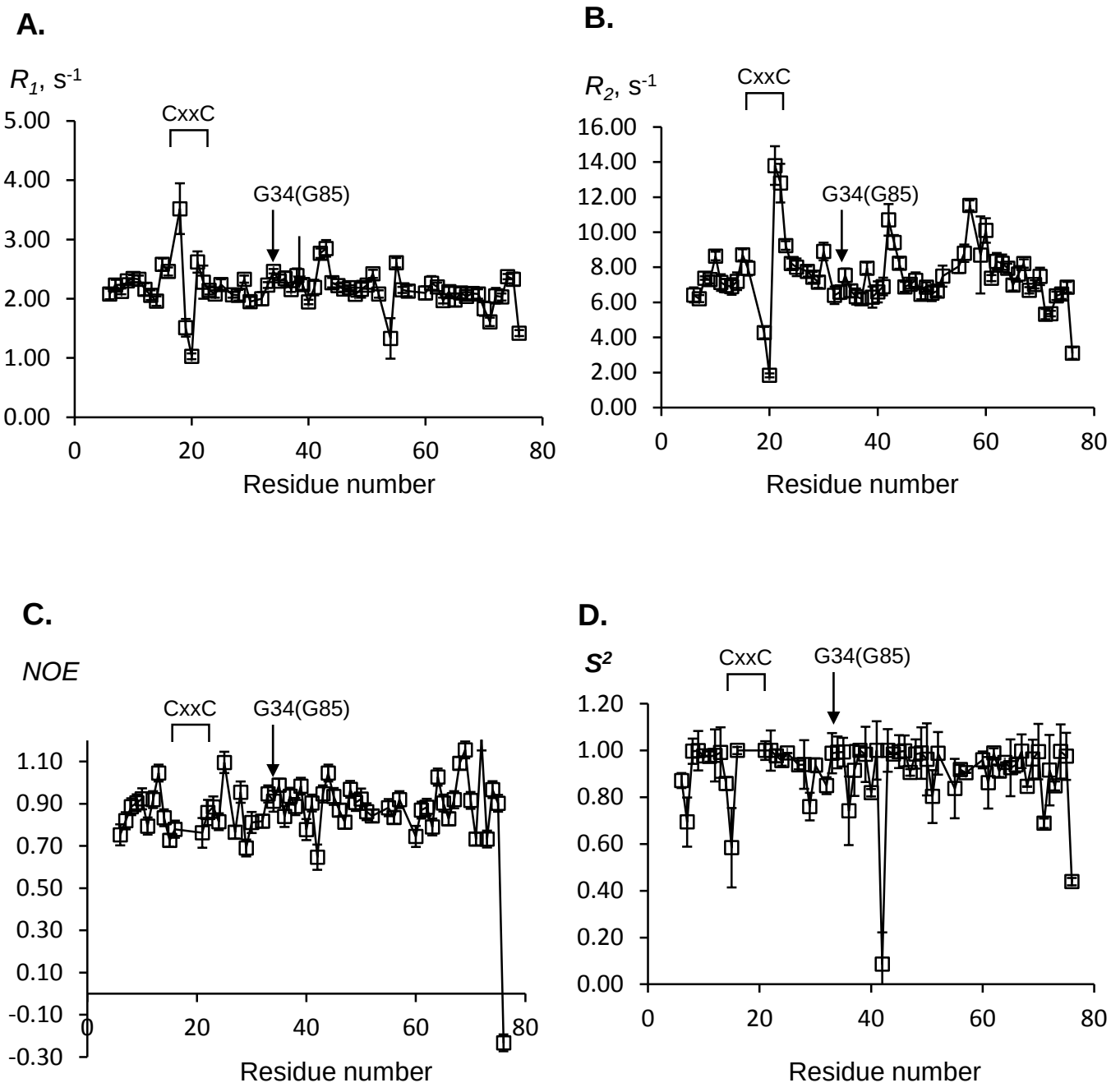
Supplementary information

Table S1: Statistics for structure calculation of MBD1.

Parameter	Value
Total number of NOE distance restraints	628
Intra-residue	305
Sequential (|i – j| = 1)	143
Medium range (|i – j| < 5)	49
Long range (|i – j| > = 5)	91
Hydrogen bond restraints	40
Dihedral angle constraints	119
Phi (ϕ)	54
Psi (ψ)	65
RMSD for bond angles (°)	0.6
RMSD for bond lengths (Å)	0.008
RMSD from experimental restraints	
NOE (Å)	0.016 ± 0.002
Dihedral angles (°)	0.452 ± 0.008
Mean NOE violations larger than 0.25 Å	0
Maximum NOE violation (Å)	0.27
Average RMSD to the mean (Å)	
Backbone	0.59±0.16
All heavy atoms	1.15±0.23
PROCHECK Z-scores (ϕ an ψ/all dihedral angles)	1.14/1.12
MolProbity clash score/Z-score	13.88/-0.86
Ramachandran plot summary from PROCHECK (%)	
Residues in most favorable regions	97.3
Residues in additionally allowed regions	2.7
Residues in disallowed regions	0.0
Ramachandran plot summary from MolProbity (%)	
Residues in most favorable regions	99.4
Residues in additionally allowed regions	0.6
Residues in disallowed regions	0.0
Average number of angle constraint violations per conformer (>5°)	0

Fig. S1



MBD1 dynamics. Relaxation rates R_1 (**A**) and R_2 (**B**), heteronuclear ^{15}N-{^{1}H} NOEs (**C**), and order parameter S^2 (**D**) plotted as functions of residue number. Data points for G34, corresponding to G85 in the full-length ATP7B are marked with an arrow, and data points for the residues in the conserved copper binding motif (C18 to C21 in MBD1, corresponding to C69 to C72 in the full length ATP7B) with a square bracket.