

Description of Additional Supplementary Files:

Supplementary Data 1: Custom OEC/OEI restraints file (HR restraints)

Supplementary Data 2: Edits file for ligand environment and Mn-Mn distances for the 2F dataset

Supplementary Data 3: phenix.refine settings file for the 2F dataset

Supplementary Data 4: FBHR file for the 2F dataset