## **Supplementary Material**

## Solution NMR characterization of WT CXCL8 monomer and dimer binding to CXCR1 N-terminal domain

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**Figure S1.** <sup>1</sup>H-<sup>15</sup>N spectra of CXCL8 monomer variants. Overlay of the 1-66 (black), V27P/E29P (red), and L25Y/V27R (green) monomers at pH 7 in 50 mM sodium phosphate buffer. Characteristic upfield and downfield shifted peaks corresponding to CXCL8 structural fold, and some well dispersed peaks are labelled for comparison. The Q8 peak which is weak in the V27P/E29P spectrum is shown as a red circle at its corresponding position.



**Figure S2.** <sup>1</sup>H-<sup>15</sup>N spectra of CXCL8 monomer variants bound to h21mer. Overlay of the V27P/E29P (black) and L25Y/V27R (red) monomers bound to h21mer at pH 7 in 50 mM sodium phosphate buffer. The signature upfield and downfield shifted peaks corresponding to CXCL8 structural fold, and some representative residues showing binding-induced perturbation are labelled for comparison.