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RESEARCH ARTICLE

Structures of the CXCR4 Chemokine GPCR with Small-Molecule and Cyclic Peptide Antagonists

Beili Wu¹, Ellen Y. T. Chien¹, Clifford D. Mol¹, Gustavo Fenalti¹, Wei Liu¹, Vsevolod Katritch², ...

[+ See all authors and affiliations](#)

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Abstract

Chemokine receptors are critical regulators of cell migration in the context of immune surveillance, inflammation, and development. The G protein-coupled chemokine receptor CXCR4 is specifically implicated in cancer metastasis and HIV-1 infection. Here we report five independent crystal structures of CXCR4 bound to an antagonist small molecule IT1t and a cyclic peptide CVX15 at 2.5 to 3.2 angstrom resolution. All structures reveal a consistent homodimer with

an interface including helices V and VI that may be involved in regulating signaling. The location and shape of the ligand-binding sites differ from other G protein-coupled receptors and are closer to the extracellular surface. These structures provide new clues about the interactions between CXCR4 and its natural ligand CXCL12, and with the HIV-1 glycoprotein gp120.

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