CCDC
advancing structural science

Engineer New Materials

CSD-Materials

For All Users of CSD-Materials or CSD-Enterprise

For solid-state scientists, the components in CSD-Materials provide solid form informatics capabilities, allowing you to understand and design solid materials such as pharmaceuticals or fine chemicals. The functionality includes sophisticated analysis & prediction of molecular geometry, intermolecular interactions and crystal packing.

There are approximately 150 000 structures in the hydrate subset of the CSD.

Explore with Mercury

- Discover preferred intermolecular interactions and engineer changes to satisfy these requirements using Full Interaction Maps
- Interpret crystal packing and compare with CSD data using powerful Packing Feature, Similarity and Motif searches, Hydrogen Bond Propensity analysis and H-bond Coordination Quick-View
- Understand the effects of hydration on solid forms with Hydrate Analyser
- Explore and analyse complex solvates with the Solvate Analyser
- Explore the structures of potential co-crystals using the Molecular Complementarity tool
- Explore solid-state molecular geometry using the CSD-driven Conformer Generator – unique because the results are derived from all the latest experimental data from the CSD
- Communicate your results with high impact graphics and 3D printing

Connect with the CSD Python API

- Repeatable, precise, programmatic results.
- Create, or download from our portal, CSD-driven analyses and workflows.

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CSD-Materials: From Data to Insights

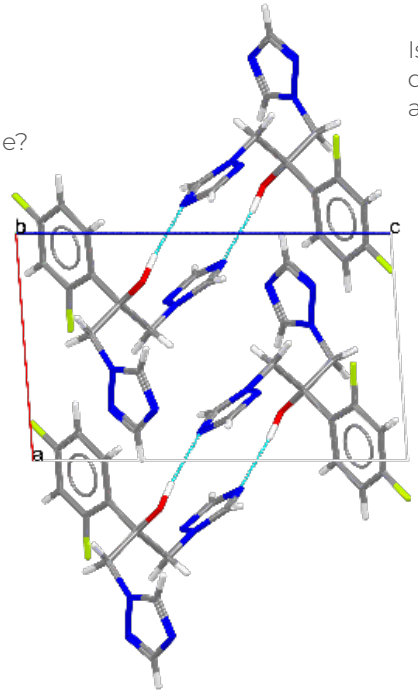
The CSD-Materials software suite includes a range of tools allowing you to derive actionable big-data insights about your solid form.

By drawing on the over 1.1 million published crystal structures in the Cambridge Structural Database (CSD), CSD-Materials allows you to understand the interactions that define your material's behaviour and properties.

Are the H-bond donor/acceptor pairings favourable?

Is my structure correct?

Is the crystal packing efficient? Are there solvent-accessible void spaces?



Is the H-bond geometry distorted? Are the H-bond donors and acceptors accessible?

Is the H-bond coordination of donors/acceptors optimal?

Is the crystal conformation unusual or strained?

CSD-Materials Capabilities:

- Bond length assessment
- Valence angle assessment
- Torsion angle assessment
- Ring geometry assessment
- Conformer generation
- Full interaction maps
- Motif searching
- Packing feature searching
- Crystal packing similarity
- BFDH morphology calculation
- Hydrogen bond propensity and coordination assessment
- Hydrate analysis
- Solvate analysis
- Aromatic analysis
- Co-crystal design
- Hydrogen bond statistics assessment
- Access CSD deposited and curated data
- Search by chemical formula, cell parameters, 2D/3D substructure, similarity, and more
- 3D display and manipulation
- High resolution graphics and frames
- PXRD pattern simulation and comparison
- Plotting and charting
- Descriptive statistics
- Interactive visualization