

CSD-Community

CSD-Enterprise

Data

CSD deposited and curated data	✓	✓
CSD teaching resources	✓	✓
Proprietary CSD extension		✓

Deposit

Guided data deposition	✓	✓
CIF syntax check	✓	✓
Reduced cell check	✓	✓
Data validation	✓	✓
CSD DOI and curated CSD entry on publication	✓	✓
Direct publication through <i>CSD Communications</i>	✓	✓
Enhanced data discoverability	✓	✓
Persistent, free storage of your data	✓	✓
Deposition portal allowing you to access, edit and share your deposits	✓	✓

Access

Retrieve via bibliographic info, DOI, CSD identifiers or compound name	✓	✓
Link from published articles and repositories	✓	✓
Publisher referee services	✓	✓

Search

Search by chemical formula, cell parameters, 2D/3D substructure, similarity, and more...		✓
Protein-ligand binding sites		✓

Visualise

3D display and manipulation	✓	✓
High resolution graphics and movie generation	✓	✓
3D printing file output	✓	✓
PXRD pattern simulation	✓	✓
PXRD pattern comparison		✓
Molecule and structure editing	✓	✓
2D diagram generation		✓

Analyse

Plotting and charting		✓
Descriptive statistics		✓
Interactive visualisation		✓
Filtering and categorisation		✓
Reporting		✓

Integrations

CSD Pipeline Pilot Component Collection		✓
CSD KNIME Component Collection		✓

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Conformations

Bond length assessment	✓
Valence angle assessment	✓
Torsion angle assessment	✓
Ring geometry assessment	✓
Conformer generation	✓

Interactions

Fragment interaction maps (IsoStar)	✓
Protein interaction maps (SuperStar)	✓
Full interaction maps	✓

Ligand-based drug discovery

Ligand overlay	✓
Field-based ligand screener	✓
Scaffold hopping	✓

Structure-based drug discovery

Protein-ligand docking	✓
Ensemble docking	✓
Pose analysis	✓
Proprietary structures	✓
Cavity similarity searching	✓

Solid form analysis

Motif searching	✓
Packing feature searching	✓
Crystal packing similarity	✓
Calculations	✓
Hydrogen bond propensity and coordination assessment	✓
Hydrate analysis	✓
Solvate analysis	✓
Aromatic analysis	✓
Co-crystal design	✓
Hydrogen bond statistics assessment	✓

¹Essential curated information for each entry is freely available through Access Structures on the CCDC website. More enhanced curated information is available through CSD-Core, CSD-Discovery, CSD-Materials and CSD-Enterprise

+ Services are available – contact the CCDC for more information

