

Visualisation and analysis in Mercury – Intermediate level

CCDC Virtual Workshop Spring 2021 – Session 1

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Learning outcomes for today

- Learn how to use advanced Mercury features to analyse structures
- Familiarise yourself with functionalities from the Calculate menu
 - Enabling you to explore structures in more depth
 - Including contacts, planes and centroids
- Familiarise yourself with functionalities from the Display menu
 - including displaying the symmetry elements and voids within a structure

Inside the Cambridge Structural Database

The CSD is a database of all the published organic and metal-organic experimental crystal structures

Organic
43%

Metal-Organic
57%

At least one transition metal,
lanthanide, actinide or any of Al,
Ga, In, Tl, Ge, Sn, Pb, Sb, Bi, Po

Not Polymeric
89%

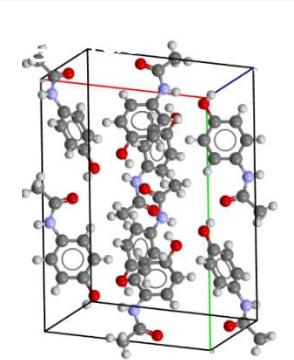
Polymeric: 11%

Single
Component
56%

Multi
Component
44%

Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands

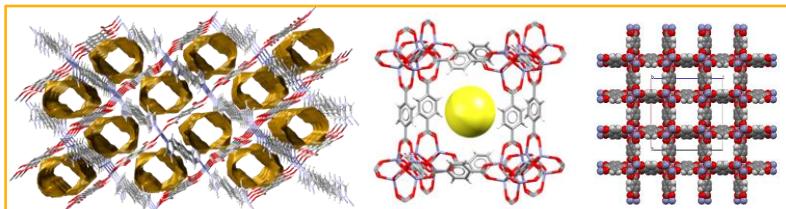


Additional data

- 11,525 polymorph families
- 171,683 melting points
- 909,992 crystal colours
- 778,663 crystal shapes
- 24,916 bioactivity details
- 11,387 natural source data
- > 250,000 oxidation states

Metal-Organic

- Metal Organic Frameworks
- Models for new catalysts
- Porous frameworks for gas storage
- Fundamental chemical bonding

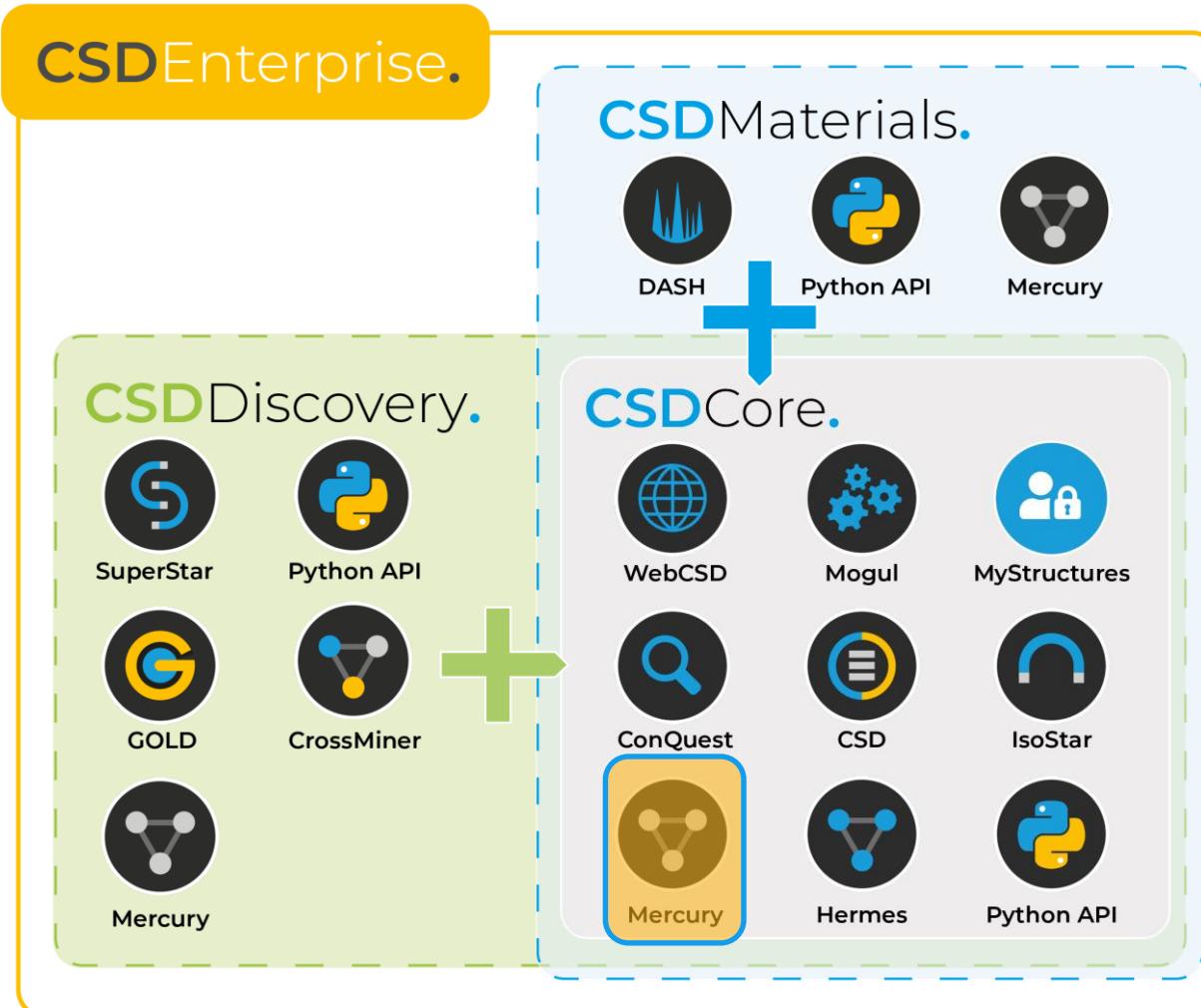


Links and subsets



- DrugBank
- Druglike
- MOFs
- PDB ligands
- PubChem
- ChemSpider
- Pesticide PDB

The CSD Portfolio



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Mercury – Structure visualisation

With Mercury you can:

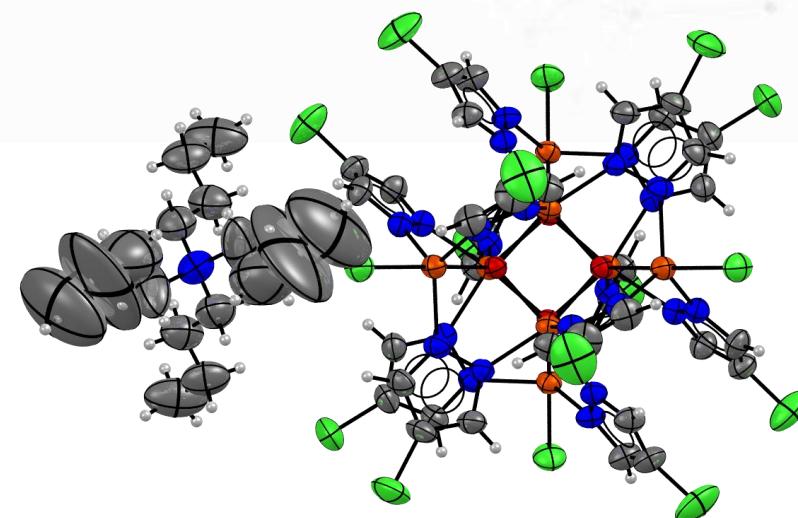
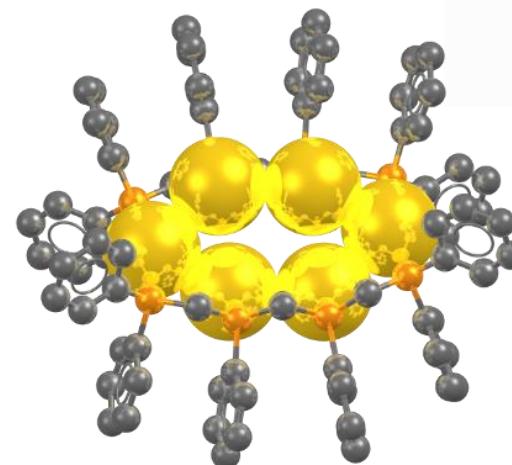
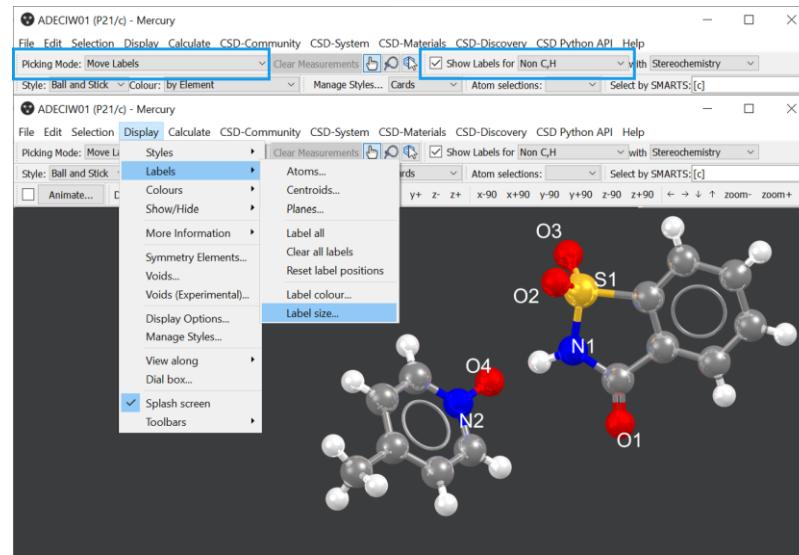
- Explore crystal structures, molecular conformations, crystallographic planes and simulated morphologies
- Generate high quality structural images for effective scientific communication
- Output model files for 3D printing
- Analyse geometries, interactions and the packing inside structures



Structure visualisation – Beginners session

What have we already learnt?

- The basics of the Mercury interface
- Basic options to visualise small molecule crystal structures
- Visualisation of the packing and basic symmetry
- Creation of high resolution publication ready images



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Show One: Mercury Demo

16



AABHTZ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms Clear Measurements Show Labels for All atoms with Atom Label

Style: Ball and Stick Colour: by Element or Suppression Manage Styles... Work Atom selections:

Animate... Default view: b a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+ Select by SMARTS: [c]

Structure Navigator

| Crystal Structures | Spacegroup |
|--------------------|------------|
| AABHTZ | P-1 |
| AACANI10 | P21/c |
| AACANI11 | P21/c |
| AACFAZ | Pbcn |
| AACFAZ10 | Pbcn |
| AACMAL | P21/c |
| AACMHX10 | Pbca |
| AACRHA | Pncm |
| AACRHC | P-1 |
| AACRUB | Cc |
| AACRUB01 | C2/c |
| AADAMC | P21/c |
| AADMKY | P-1 |
| AADMKY10 | P-1 |
| AADRIB | P21 |
| AAGAGG10 | P212121 |
| AAGGAG10 | P21 |

Display Options

Display

Packing
 Asymmetric Unit
 Auto centre

Short Contact < (sum of vdw radii)
 H-Bond Default definition

Options

Show hydrogens
 Show cell axes
 Label atoms

Depth cue
 Z-Clipping
 Stereo

Press the left mouse button and move the mouse to rotate the structure

A reminder: The basics

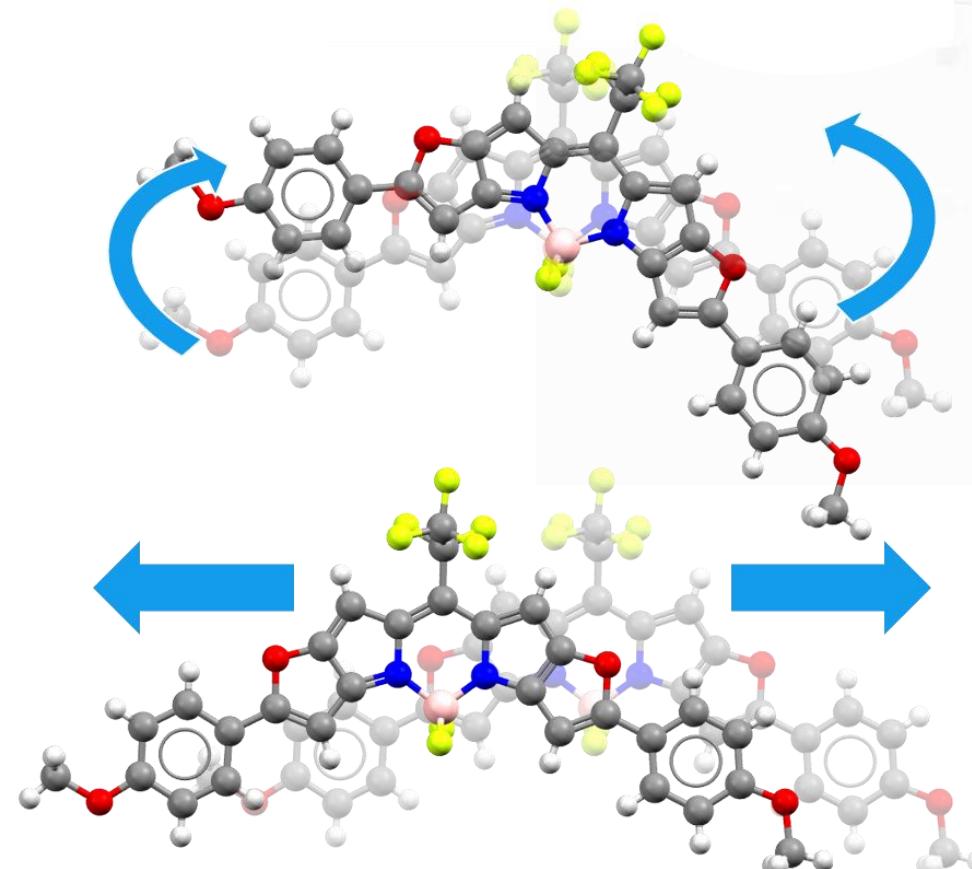
- Left mouse button and move – allows you to rotate structure
- Middle Mouse button and move – allows you to move structure
- Right mouse button and move – allows you to zoom in and out of structure
- **Structure Navigator** – Allows you to view any structure in the CSD



| Structure Navigator | |
|---------------------|------------|
| Type in a refcode | |
| Crystal Structures | Spacegroup |
| AABHTZ | P-1 |
| AACANI10 | P21/c |
| AACANI11 | P21/c |
| AACFAZ | Pbcn |
| AACFAZ10 | Pbcn |
| AACMAL | P21/c |
| AACMHX10 | Pbca |
| AACRHA | Pncm |
| AACRHC | P-1 |
| AACRUB | Cc |
| AACRUB01 | C2/c |
| AADAMC | P21/c |
| AADMKY | P-1 |
| AADMKY10 | P-1 |
| AADRIB | P21 |
| AAGAGG10 | P212121 |
| AAGGAG10 | P21 |

A reminder: The basics

With the keyboard:

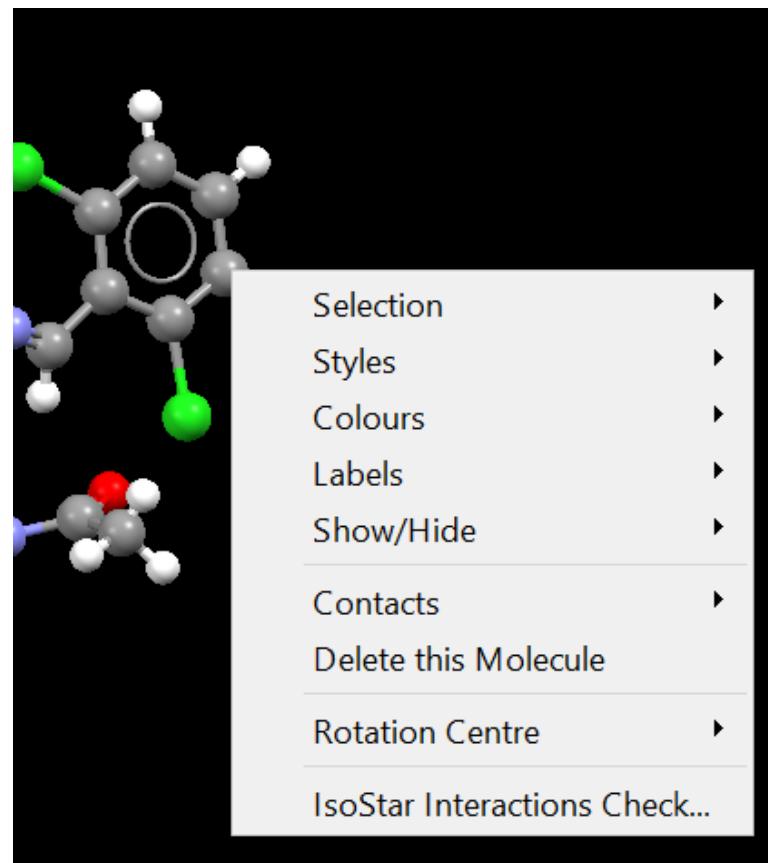


CSD Refcode: GIMXUY

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A reminder: Right mouse click

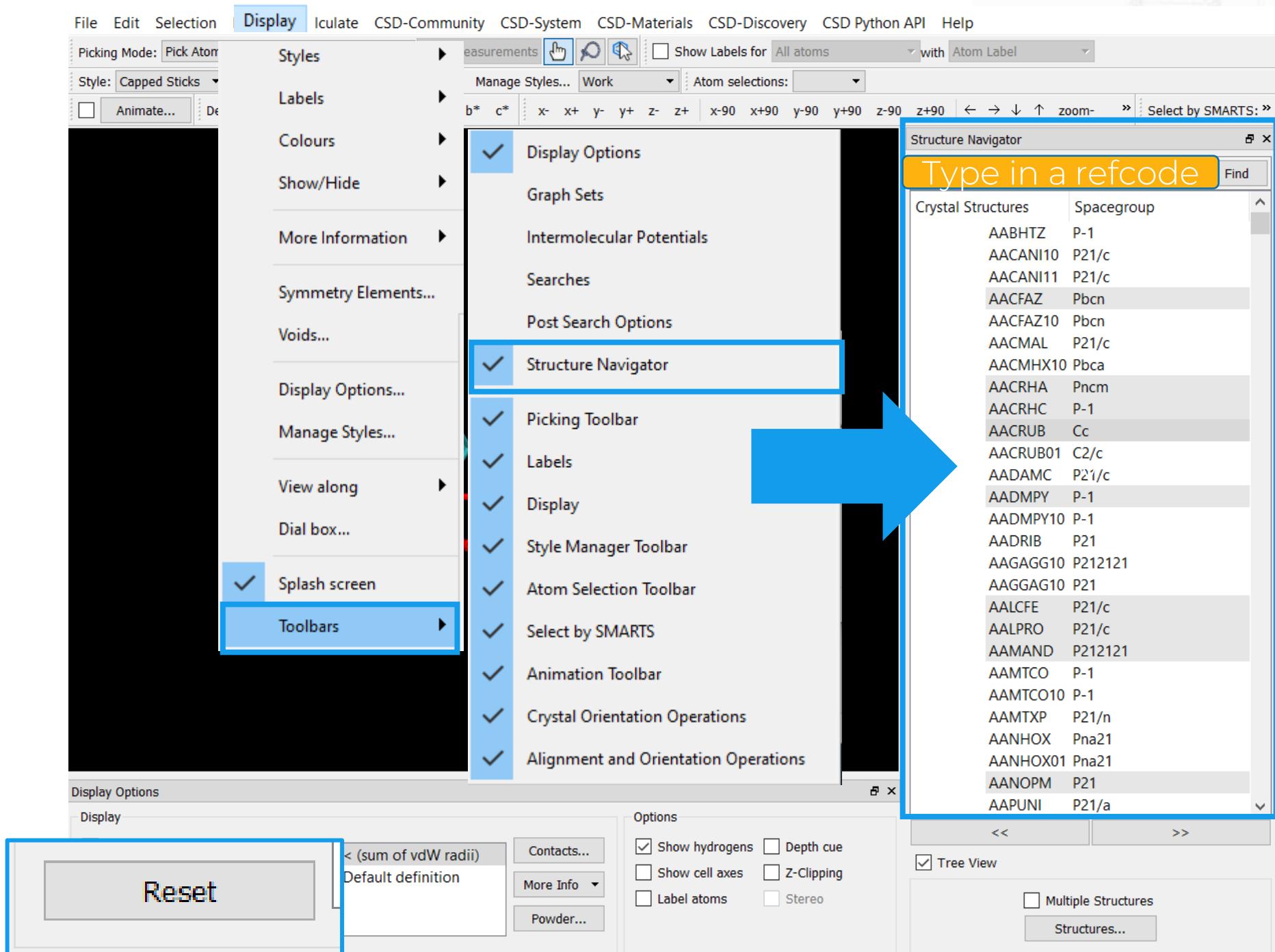
Near a molecule



Away from a molecule



CCDC

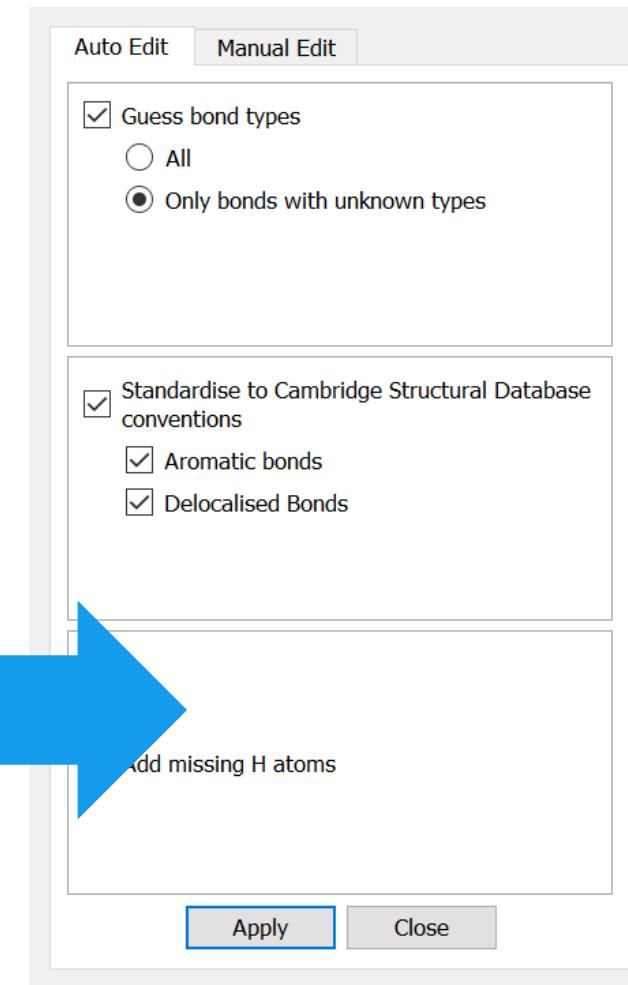
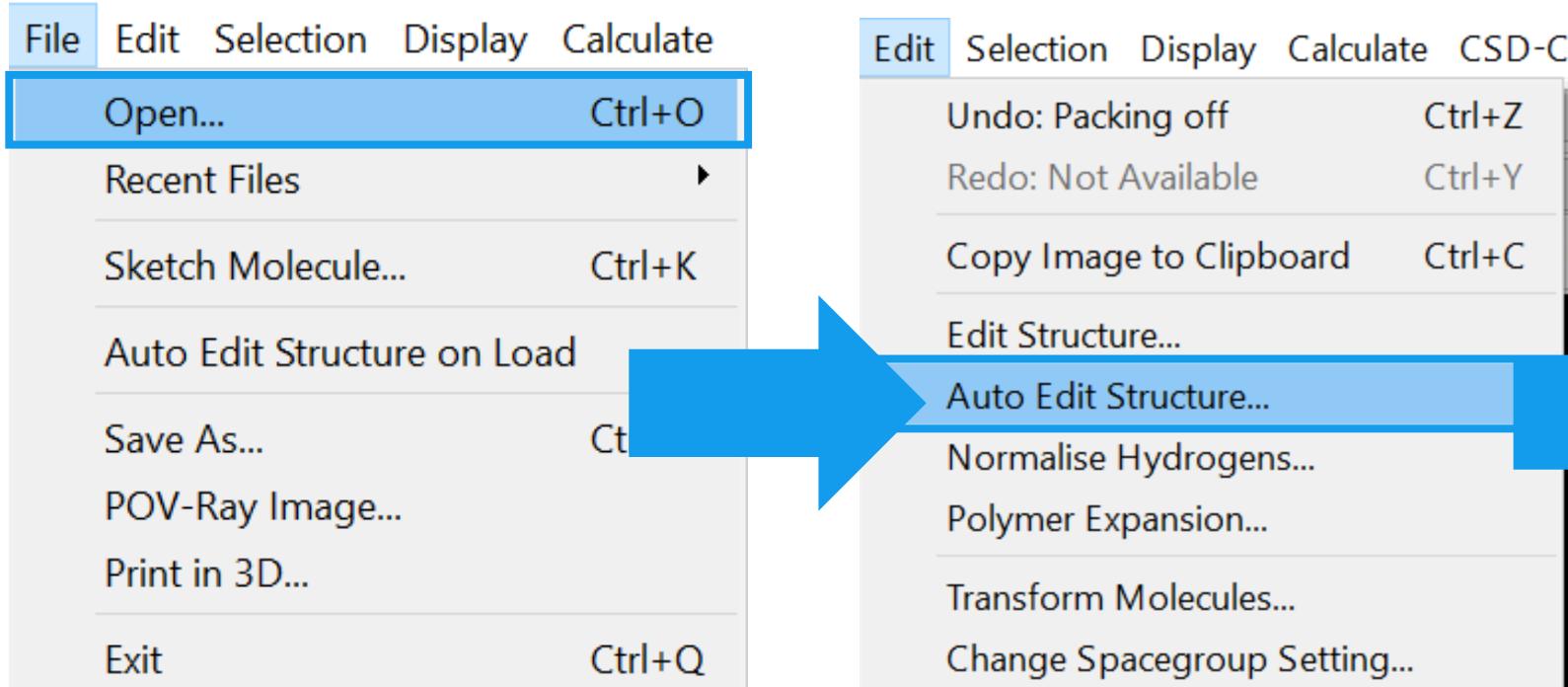


- ## A reminder:
- Recovering Toolbars
 - Resetting view

A reminder: Using your own file

- File > Open – to open one of your own files for example a CIF
- Edit > Auto Edit Structure to assign bond types
- File > Auto Edit Structure on Load to automate

AABHTZ (P-1) - Mercury



Open... Ctrl+O

Recent Files ▶

Sketch Molecule... Ctrl+K

Auto Edit Structure on Load

Save As... Ctrl+S

POV-Ray Image...

Print in 3D...

Exit Ctrl+Q

Mercury Menus

- Mercury for Beginners
- In todays session

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API

Undo: Hide Ctrl+Z

Redo: Enable Contact Definition Ctrl+Y

Copy Image to Clipboard Ctrl+C

▼

Edit Structure...

Auto Edit Structure...

Normalise Hydrogens...

Polymer Expansion...

Transform Molecules...

Change Spacegroup Setting...

Invert Structure

Change Spacegroup to Subgroup...

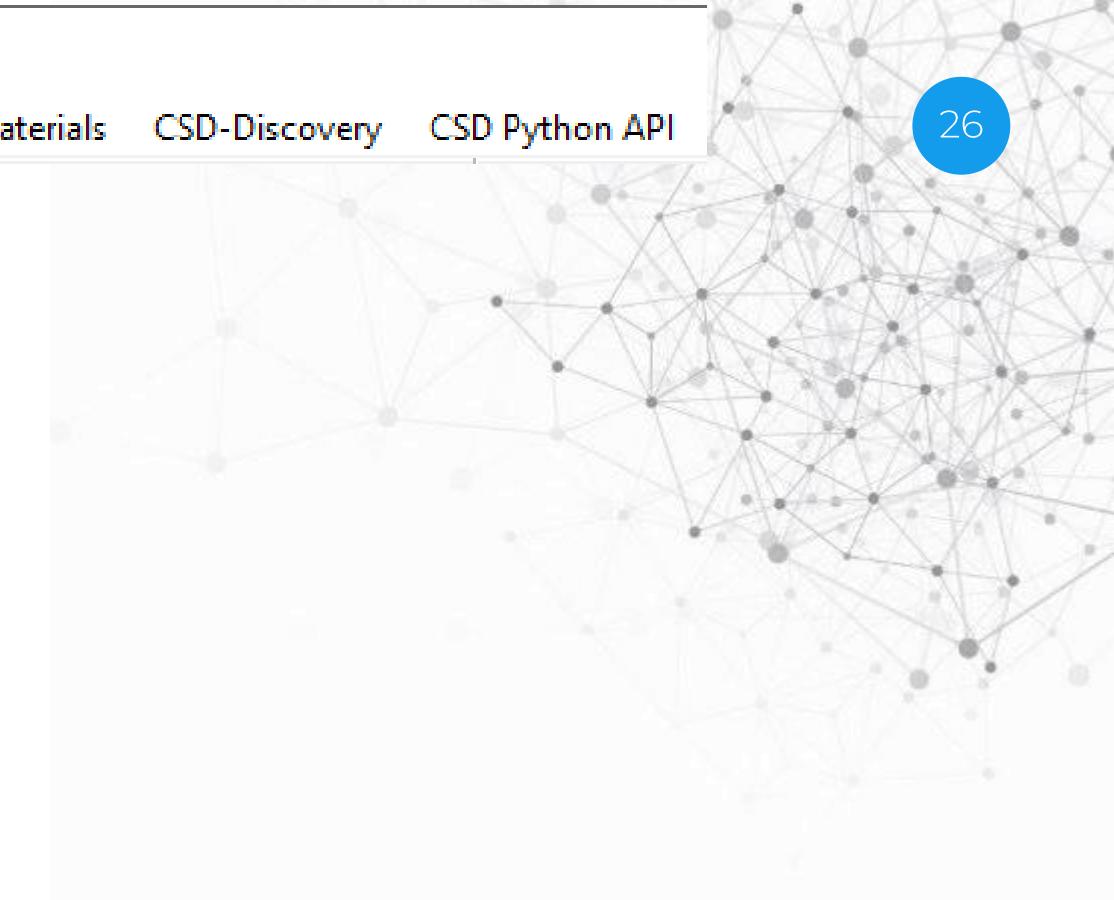


- Undo: Select All Ctrl+A
- Redo: Select Molecules...
- Copy: Select Atoms...
- Select
- Edit Structure
- Auto Edit Deselect All Ctrl+D
- Normal Deselect Molecules...
- Polymers Deselect Atoms...
- Deselect
- Transform
- Change Invert Selection Ctrl+I
- Invert Selection Expand Selection Ctrl+E
- Change Save Current Selection...



- Undo: Hide Styles ▶
- Redo: Enable Conta Labels ▶
- Copy Image to Clip Colours ▶
- Show/Hide ▶
- More Information ▶
- Symmetry Elements...
- Voids...
- Display Options...
- Manage Styles...
- View along ▶
- Dial box...
- Splash screen
- Toolbars ▶

- Undo: Select All St: Centroids...
 - Redo: Select Mc La: Planes...
 - Copy: Select Atc C: Packing/Slicing...
 - Copy: Select Sh: Contacts...
 - ✓ Edit Str M: Molecular Shell...
 - Auto E Deselect / Sy: Graph Sets...
 - Normal Deselect / Vc: Powder Pattern...
 - Polymers Deselect / Di: Structure Overlay...
 - Transfo Deselect / M: Molecule Overlay...
 - Change Invert Sel View along
 - Invert: Expand S Dial box...
 - Change Save Curr Splash screen
- ✓ Toolbars ▾



File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API

- Undo: Select All St: Centroid:  CSD Deposit
- Redo: Select Mc La: Planes...  Access Structures Online
- Copy: Select Atc Cr: Packing/ Open Teaching Database
- Copy: Select Atc Sh: Contacts About Teaching Database
- Edit Str: Deselect / M: Molecule  Launch enCIFer
- Auto E: Deselect / Sy: Graph Se  CellCheckCSD
- Normal: Deselect / Vc: Powder F About CSD-Community
- Polym: Deselect / Di: Structure Overlay...
- Transfo: Deselect / M: Molecule Overlay...
- Change: Invert Sel: View along
- Invert: Expand S: Dial box...
- Change: Save Curr: Splash screen
- Toolbars

File Edit Selection Display Calculate CSD-Community **CSD-Core** CSD-Materials CSD-Discovery CSD Python API

Undo: Select All St: Centroid: CSD Deposit: Launch WebCSD

Redo: Select Mc La: Planes... Access Structure: ConQuest Hit Highlighting...

Copy: Select Atoms Ce: Packing/ Open Teacher: Launch ConQuest

Copy: Select Sh: Contacts About Teacher: Data Analysis Module...

✓ Edit Structure M: Molecule: Launch enCore: Mogul Geometry Check...

Auto E: Deselect / Sy: Graph Set: CellCheckC: Launch Mogul

Normal: Deselect / Vc: Powder F: About CSD-: Mogul Settings...

Polymers: Deselect / Di: Structure Overlay... IsoStar Interaction Check...

Transfcs: Deselect / M: Molecule Overlay... Launch IsoStar

Changes: Invert Selection View along IsoStar Settings...

Invert Selection: Expand Selection Dial box... Select Databases...

Changes: Save Current Splash screen

Toolbars ▾

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API

Undo: Select All St: Centroid: CSD Deposit Laur Search ▶

Redo: Select Mc La: Planes... Access Structure Con Calculations ▶

Copy: Select Atc Cr: Packing/ Open Teach Laur Polymorph Assessment ▶

Copy: Select Sh: Contacts About Teach Data ▶

Edit Structure: M: Molecule Launch enC Mo Full Interaction Maps... ▶

Auto E: Deselect / Sy: Graph Se CellCheckC Laur Hydrate Analyser... ▶

Normal: Deselect / Vc: Powder F About CSD- Mo Solvate Analyser... ▶

Polym: Deselect / Di: Structure Overlay... IsoStr Aromatics Analyser... ▶

Transf: Deselect / M: Molecule Overlay... Laur Conformer Generation... ▶

Change: Invert Selection View along IsoStr Launch DASH

Invert Selection: Expand Selection Dial box... Selection

Change: Save Current Splash screen

Toolbars ▶

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API

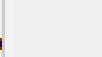
| | | | | | | | |
|----------|----------------|-----|----------------------|------------------|--------|---------------|-----------------------------|
| Undo: | Select All | St: | Centroid: | CSD Deposit | Laur: | Search | Full Interaction Maps... |
| Redo: | Select Mc | La: | Planes... | Access Structure | Con: | Calculate | Conformer Generation... |
| Copy: | Select Atoms | Co: | Packing/ | Open Teacher | Laur: | Polymers | Launch GOLD Docking |
| | Select | Sh: | Shells | About Teacher | Data: | Co-Crys | Launch Protein Interactions |
| ✓ | Edit Structure | M: | Molecules | Launch enC | Mod: | Full Interact | Launch Ligand Overlay |
| Auto E: | Deselect / | Sy: | Graph Set | CellCheckC | Laur: | | |
| Normal: | Deselect / | Vc: | Powder F | About CSD- | Mod: | | Hydrate Analyser... |
| Polym: | Deselect / | Di: | | | IsoSt: | | Solvate Analyser... |
| Transfo: | Deselect | M: | Structure Overlay... | | Laur: | | Aromatics Analyser... |
| Chang: | Invert Sel: | M: | Molecule Overlay... | | IsoSt: | | Conformer Generation... |
| Invert: | Expand Sel: | | View along | | Sele: | | Launch DASH |
| Chang: | Save Curr: | | Dial box... | | | | |



Splash screen



Toolbars

| | | | | | | | | | | |
|----------|------------|-------------------------------------|----------------------|---|------------------|---|---------------|-------------------------|------------------------------|----------|
| File | Edit | Selection | Display | Calculate | CSD-Community | CSD-Core | CSD-Materials | CSD-Discovery | CSD Python API | |
| Undo: | Select All | St: | Centroid: |  | CSD Deposit |  | Laurie | Search | Full Intel | Analysis |
| Redo: | Select Mc | La: | Planes... |  | Access Structure |  | Conform | Calculat | Conform | Reports |
| Copy: | Select Atc | Co: | Packing/ | | Open Teach |  | Laur | Polymor | Launch | Searches |
| | Select | Sh: | Sh: | | About Teach | | Data | | | |
| ✓ | Edit Str | | | M: | Molecular |  | Launch enC | Mo | | |
| Auto E | Deselect / | Sy: | Graph Se |  | CellCheckC |  | Laur | Full Intel | | |
| Normal | Deselect / | Vc: | Powder F | | About CSD- | | Mo | Hydrate Analyser... | | |
| Polym | Deselect / | Di: | | | | | IsoS | Solvate Analyser... | Options... | |
| Transfo | Deselect | M: | Structure Overlay... | | | | Laur | Aromatics Analyser... | CSD Python API Documentation | |
| Chang | Invert Sel | M: | Molecule Overlay... | | | | IsoS | Conformer Generation... | CSD Python API Forum | |
| Invert S | Expand Sel | | View along | | | | Sele | Launch DASH | | |
| Chang | Save Curr | | Dial box... | | | | | | | |
| | | <input checked="" type="checkbox"/> | Splash screen | | | | | | | |
| | | | Toolbars | | | | | | | |

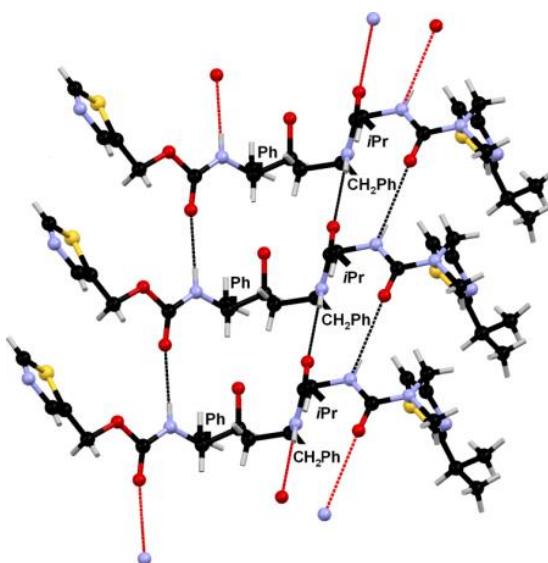
Calculate - Exploring contacts

- Hydrogen bonds and short contacts can help to stabilise a crystal structure
- Different polymorphs with different hydrogen bonding networks often exhibit different properties

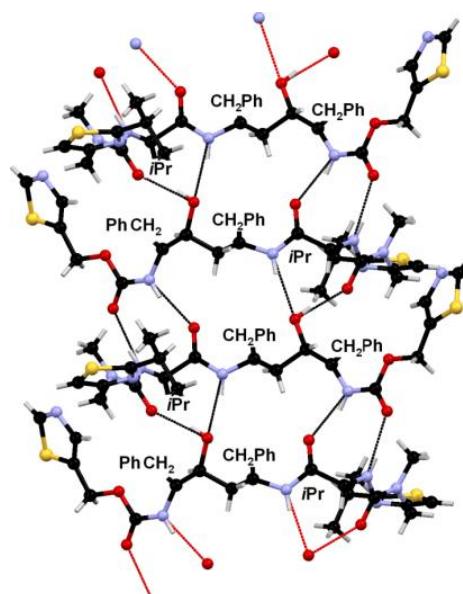


A real-life example...

Can structural knowledge mitigate risk?



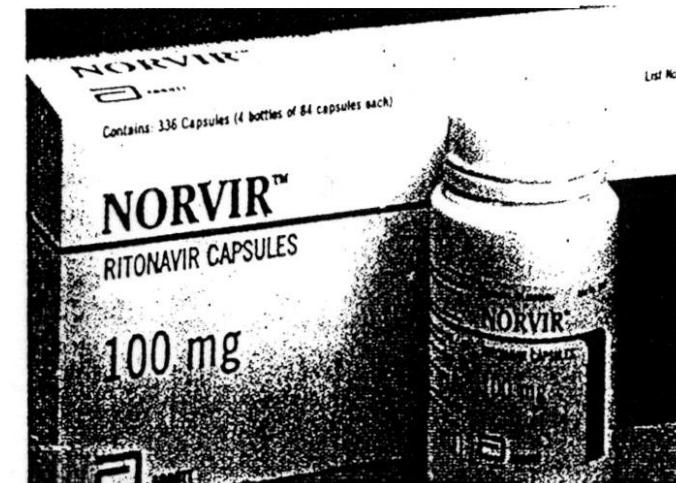
Different interactions



Different solubility
Different stability

Bauer et al. *Pharm. Res.*, (2001) 859, DOI:10.1039/B910882C

Manufacturing problems hit Abbott's HIV drug ritonavir



Capsules of Abbott Laboratories' protease inhibitor Norvir (ritonavir) are likely to become unavailable by the middle of August. The company has a problem with the manufacture of the anti-HIV capsules which it cannot resolve at present.

The problem relates to "undesirable" crystal formation. Abbott says that a series of capsules from a number of marketed batches of capsules were examined and there was no

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HXACAN (Pcab) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Expand Contacts Clear Measurements Show Labels for All atoms with Atom Label

Style: Ball and Stick Colour: by Element Manage Styles... Publication Atom selections:

Animate... Default view: b a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+ Select by SMARTS: >>

Structure Navigator

Hydrogen Bonds are donor-acceptor interactions involving hydrogen atoms.

Learn more in the Glossary on the handout.

Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre
- Short Contact < (sum of vdW radii)
- H-Bond Default definition

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

<< >> Tree View

Multiple Structures Structures...

CDC

Click on a red contact to see the whole molecule

HXACAN (Pcab) - Mercury

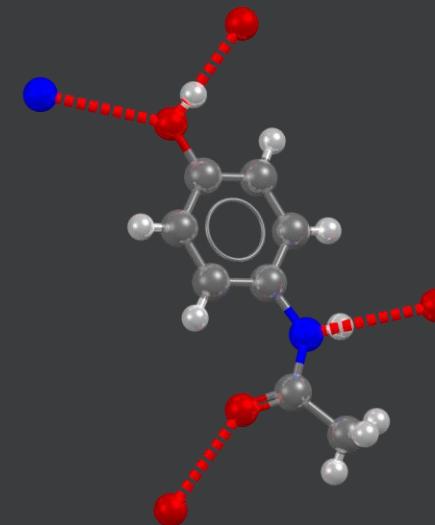
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Expand Contacts Clear Measurements Show Labels for All atoms

Style: Ball and Stick Colour: by Element Manage Styles... Publication Atom selections

Animate... Default view: b a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90

Click on “Default definition” to change the default H-bond definition



Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre

| | |
|--|---------------------------|
| <input type="checkbox"/> Short Contact | < (sum of vdW radii) |
| <input checked="" type="checkbox"/> H-Bond | Default definition |

Options

- Show hydrogens
- Label atoms

Click on a red contact to see the whole molecule

Define H-bonds

Select options and click OK or Apply when done

Require hydrogen atom to be present

D-H...A angle >= 120.0 degrees

Donor atom types:

- all donors
- nitrogen
 - metal bound N
 - imine N
 - aromatic (6-ring) N
 - amide or thioamide N
 - planar N
 - pyramidal N
 - ammonium N (NH₄⁺, RNH)

Acceptor atom types:

- all acceptors
- nitrogen
 - metal bound N
 - terminal N (cyano, etc.)
 - aromatic (6-ring) N
 - other 2-coordinate N
 - 3-coordinate N
 - unclassified N
 - oxygen

WARNING: atom types may not be classified properly for non-Cambridge Structural Database structures

Contact distance range

Actual distance VdW distance

Minimum = sum of vdW radii minus 5.00

Maximum = sum of vdW radii plus 0.00

Intermolecular

Intramolecular: Donor and Acceptor separated by > 3 bonds

OK

HXACAN (Pcab) - Mercury

Picking Mode: Expand Contacts

Style: Ball and Stick **Colour:** by Element

Atom selections:

Select by SMARTS:

Structure Navigator

HXACAN

Crystal Structures

- HXACAN
- HXACAN
- HXACAN
- HXACAN
- HXACAN

Selection

Styles

Colours

Labels

Show/Hide

Contacts

Delete this Molecule

Rotation Centre

IsoStar Interactions Check...

Expand All

Expand Contact

Expand Contacts from this Atom

Expand Contacts from this Molecule

Find Contacts from this Atom

Find Contacts from this Molecule

Delete Hanging Contacts

Delete Contact

Delete Contacts from this Atom

Delete Contacts from this Molecule

Delete this Molecule

Reset Contacts

Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre

Short Contact < (sum of vdW radii)

H-Bond Default definition

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Contacts...

More Info

Powder...

Reset

Click on a red contact to see the whole molecule

Left click on the atoms at the end of the dashed lines (known as hanging contacts) to expand the network

Right click on hanging contacts to see more advanced options including delete hanging contacts

HXACAN (Pcab) - Mercury

File Edit Selection **Display** Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: E S A

Style: Ball and Stick Animate...

Styles ▾

- Wireframe
- Stick
- Ball and stick
- Spacefill
- Ellipsoid
- Polyhedral
- Stick settings...
- Ball and Stick settings...
- Spacefill settings...
- Ellipsoid settings...
- Polyhedral settings...
- Contact settings... **Selected**
- Measurement settings...
- Selected atoms...
- Bonds...
- Contacts...
- Display Bond Types
- Display Aromatic Rings

Options

- Show hydrogens Depth cue
- Show cell axes Z-Clipping
- Label atoms Stereo

Show Labels for All atoms with Atom Label

Contact Display Options

Contact Radius (Angstroms) 0.25

Defaults Close

Structure Navigator

HXACAN

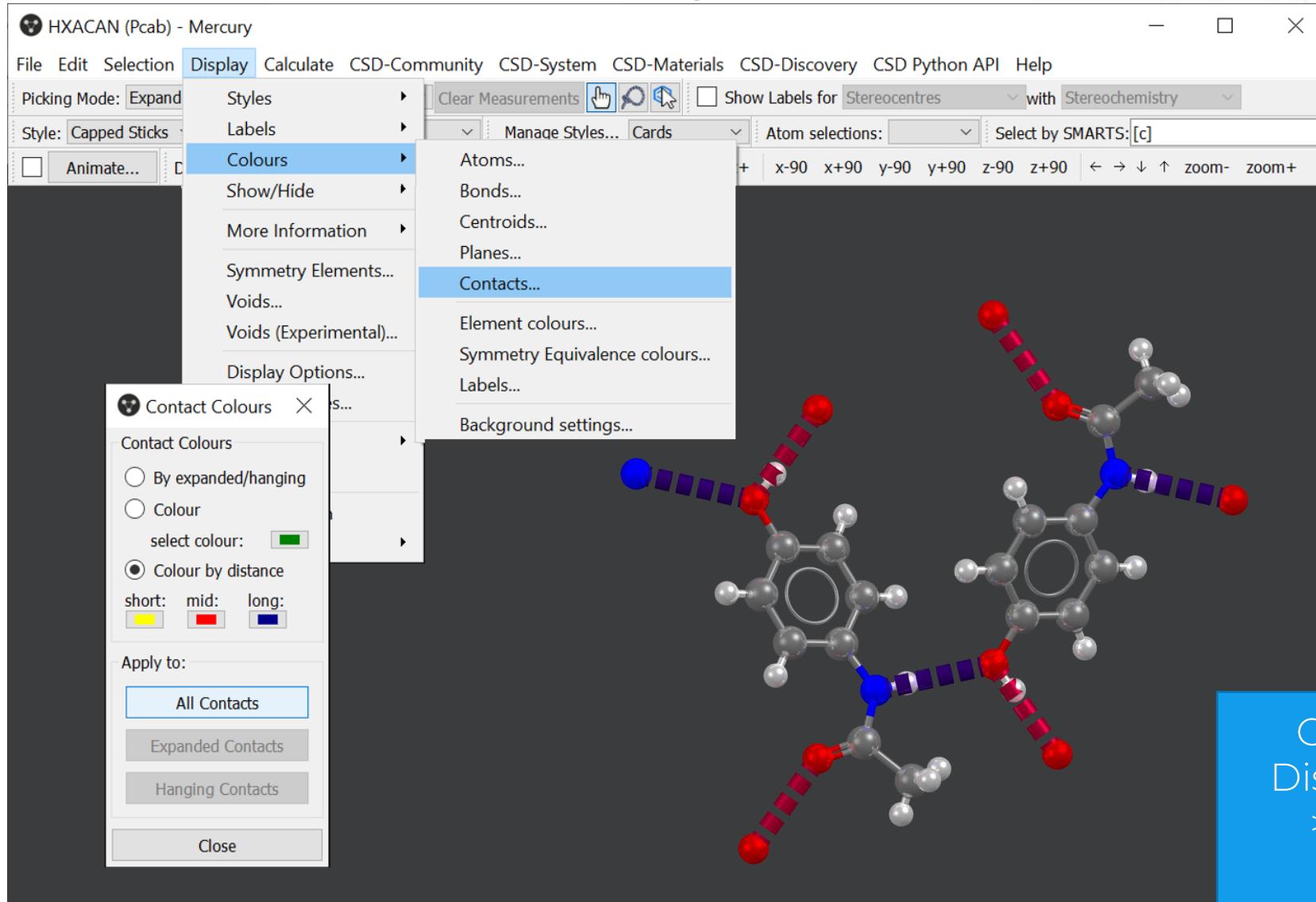
Crystal Structures

- HXACAN
- HXACAN01
- HXACAN02
- HXACAN03
- HXACAN04
- HXACAN05**
- HXACAN06
- HXACAN07
- HXACAN08
- HXACAN09
- HXACAN10
- HXACAN11
- HXACAN12
- HXACAN13
- HXACAN14
- HXACAN15
- HXACAN16
- HXACAN17
- HXACAN18
- HXACAN19
- HXACAN20

Click on a red contact to see the whole molecule

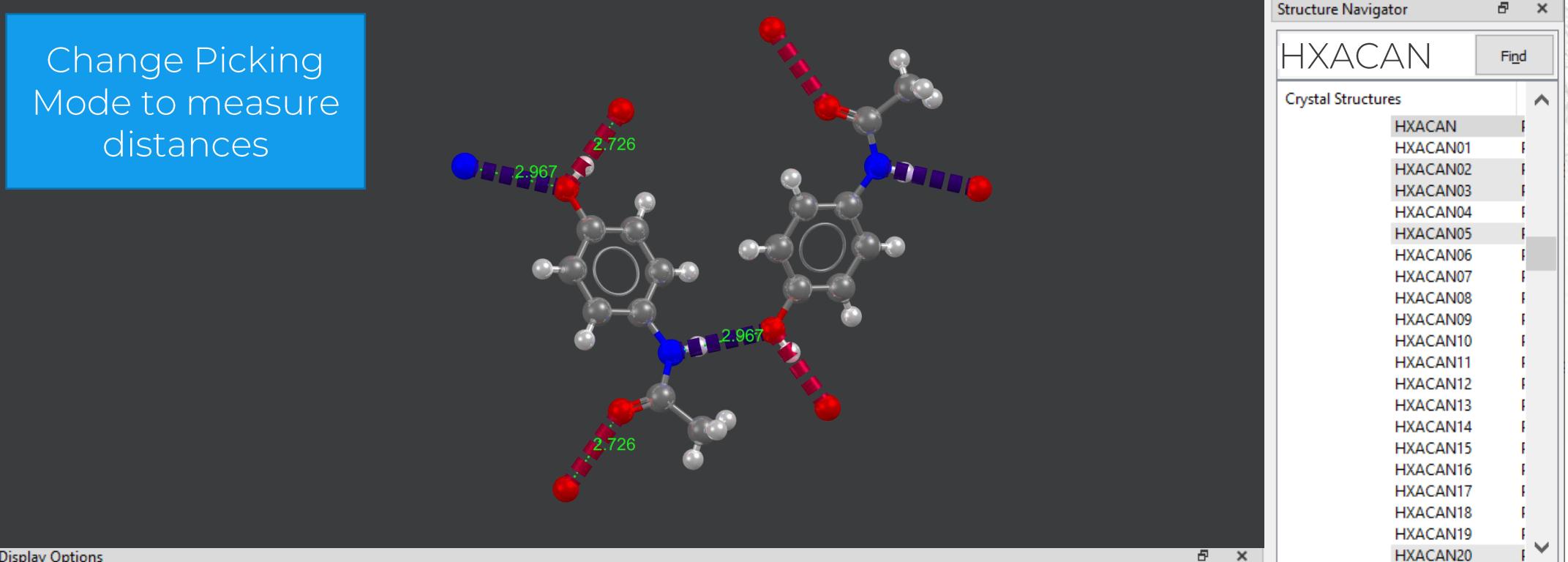
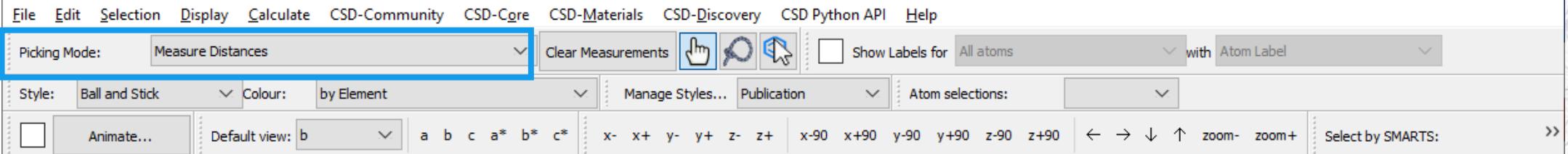
Change bond thickness by
Display>Styles>Contact
settings...

Colour H-bonds by distance



CSD Refcode:
HXACAN

Change bond colours by
Display>Colours>Contacts...
>colour by distance>All
contacts



Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre

Short Contact < (sum of vdW radii)

H-Bond Default definition

Options

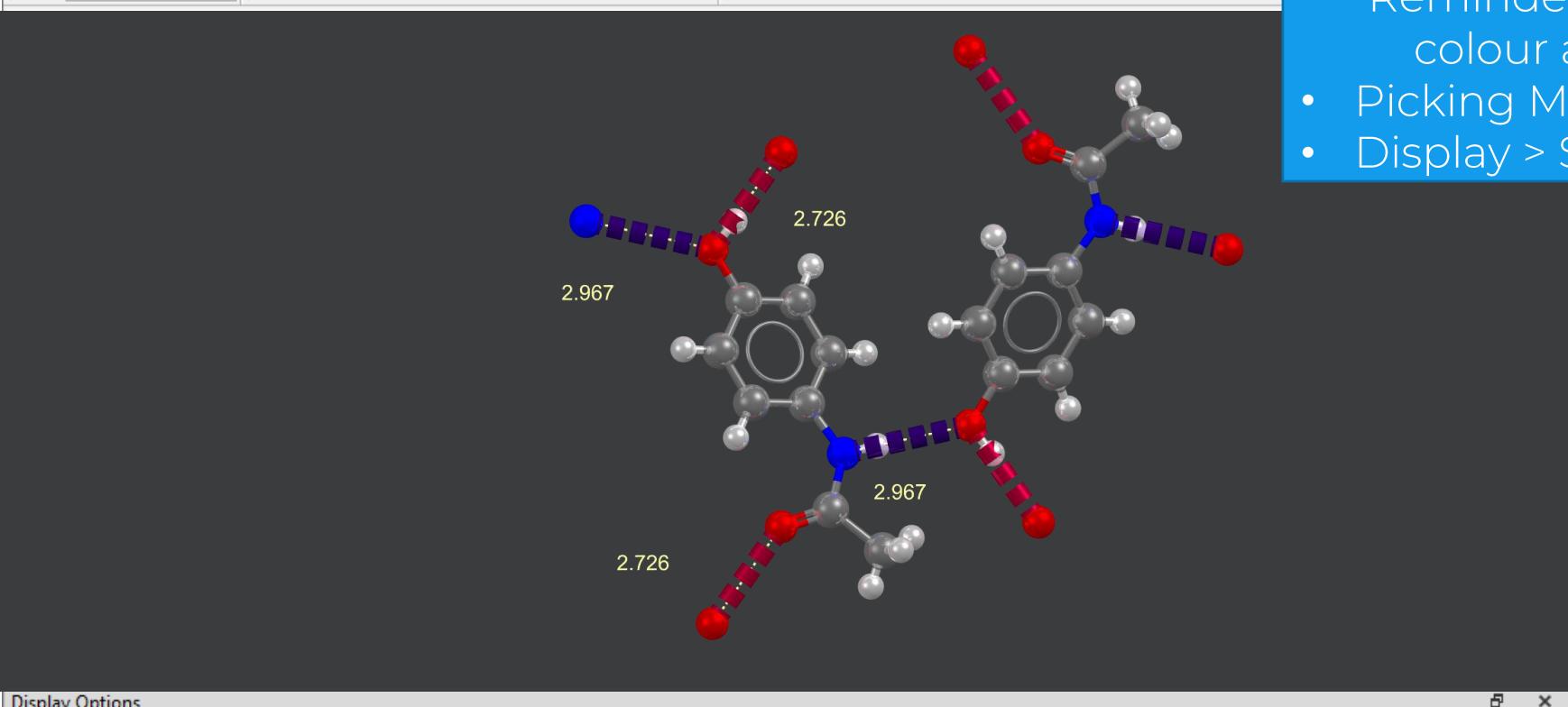
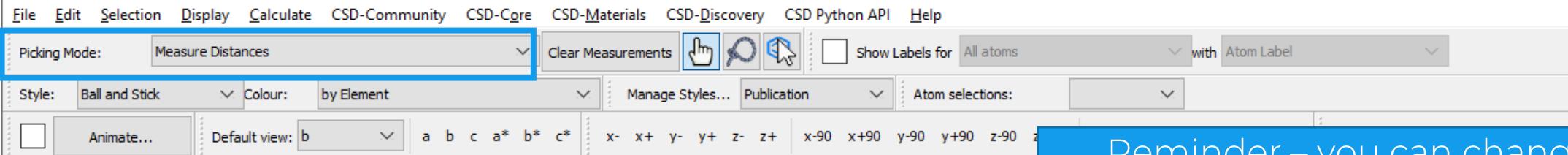
- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Contacts... More Info Powder...

Reset

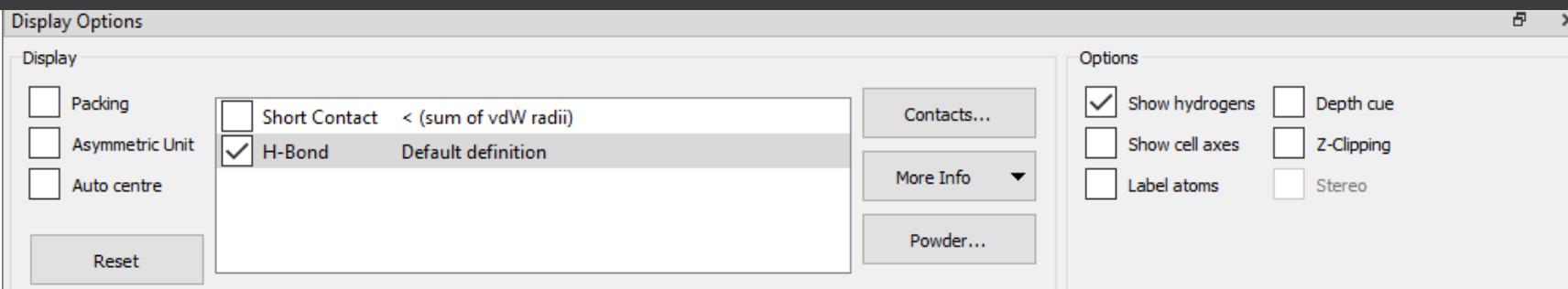
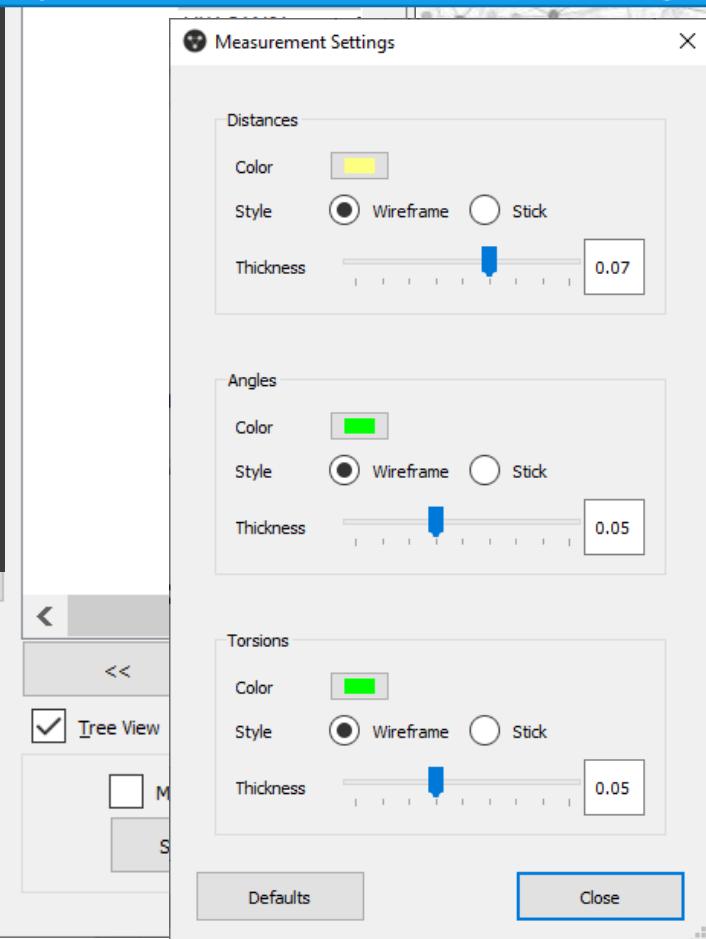
Click on a red contact to see the whole molecule

The 'Display Options' dialog box contains sections for 'Display' and 'Options'. Under 'Display', there are checkboxes for 'Packing', 'Asymmetric Unit', and 'Auto centre'. Under 'Options', there are checkboxes for 'Short Contact' (disabled), 'H-Bond' (selected), 'Show hydrogens' (selected), 'Depth cue', 'Show cell axes', 'Z-Clipping', 'Label atoms', and 'Stereo'. Buttons for 'Contacts...', 'More Info', and 'Powder...' are also present.



Reminder – you can change position, colour and size of distance labels

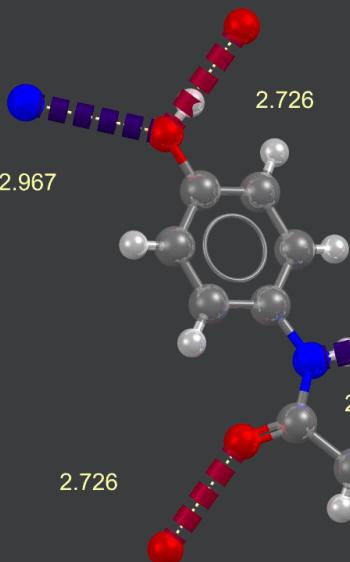
- Picking Mode > Move Labels
- Display > Styles > Measurement settings



Click on a red contact to see the whole molecule

Picking Mode: Measure Distances Clear Measurements Show Labels for All atoms with Atom Label

Style: Ball and Stick Colour: by Element Manage Styles... Publication Atom selections:

 Animate... Default view: b

HXACAN

Current structure: HXACAN

[Customise...](#)[Structure](#)[Diagram](#)[Atoms](#)[Bonds](#)[Contacts](#)[All Angles](#)[All Torsions](#)

Right-click on a contact for options. Click on a column heading to sort rows.

[Save...](#)

| Number | Atom1 | Atom2 | Length | Length-VdW | Symm. op. 1 | Symm. op. 2 | Expanded | Xorth1 | Yorth1 | Zorth1 | Xorth2 | Yorth2 | Zorth2 |
|--------|-------|-------|--------|------------|-------------|----------------|----------|--------|--------|--------|--------|--------|--------|
| 1 | ■ 01 | ■ O2 | 2.726 | -0.314 | x,y,z | x,-1/2+y,1/2-z | No | 3.1047 | 2.2725 | 1.9872 | 4.6854 | 0.0515 | 2.0050 |
| 2 | ■ 01 | ■ N1 | 2.967 | -0.103 | x,y,z | -1/2+x,1/2-y,z | No | 3.1047 | 2.2725 | 1.9872 | 0.2137 | 1.6254 | 2.1528 |

To explore contacts more:

- More Info > Contact List

[Close](#)

Display Options

Display

 Packing Asymmetric Unit Auto centre Short Contact < (sum of vdW radii) H-Bond Default definition[Contact...](#)[More Info](#)[Powder...](#) Show hydrogens Show cell axes Label atoms Depth cue Z-Clipping Stereo

<<

>>

 Tree View Multiple Structures[Structures...](#)

HXACAN (Pcab) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Expand Contacts

Style: Ball and Stick

Animate... Defa

Centroids... Planes... Packing/Slicing... Contacts... Molecular Shell... Graph Sets... Pattern... Overlay... Overlay...

Other ways to expand contacts or change definition

Clear Measurements Show Labels for All atoms

Contacts

Find Contacts Build Network

Contact name Details

Short Contact < (sum of vdW radii)

H-Bond Default definition

Add Edit... Copy Delete

OK Cancel

Build network of contacts

Expand All Expand Picked

Delete Delete Hanging Delete Picked

Undo Clear

Show cell axes

OK Cancel

Define Short Contacts

Select options and click OK or Apply when done

Find contacts shorter than the sum of the vdW radii minus 0.00

Intermolecular

Intramolecular separated by > 3 bonds

Default Cancel Apply OK

Display Options

Display

Packing Short Contact < (sum of vdw radii)

Asymmetric Unit H-Bond Default def

Auto centre

Reset

Click on a red contact to see the whole molecule

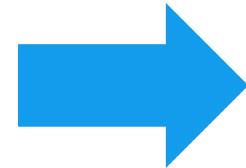
Reminder - left click on hanging contacts will also expand the network

Reminder - right click on hanging contacts will also give you more options

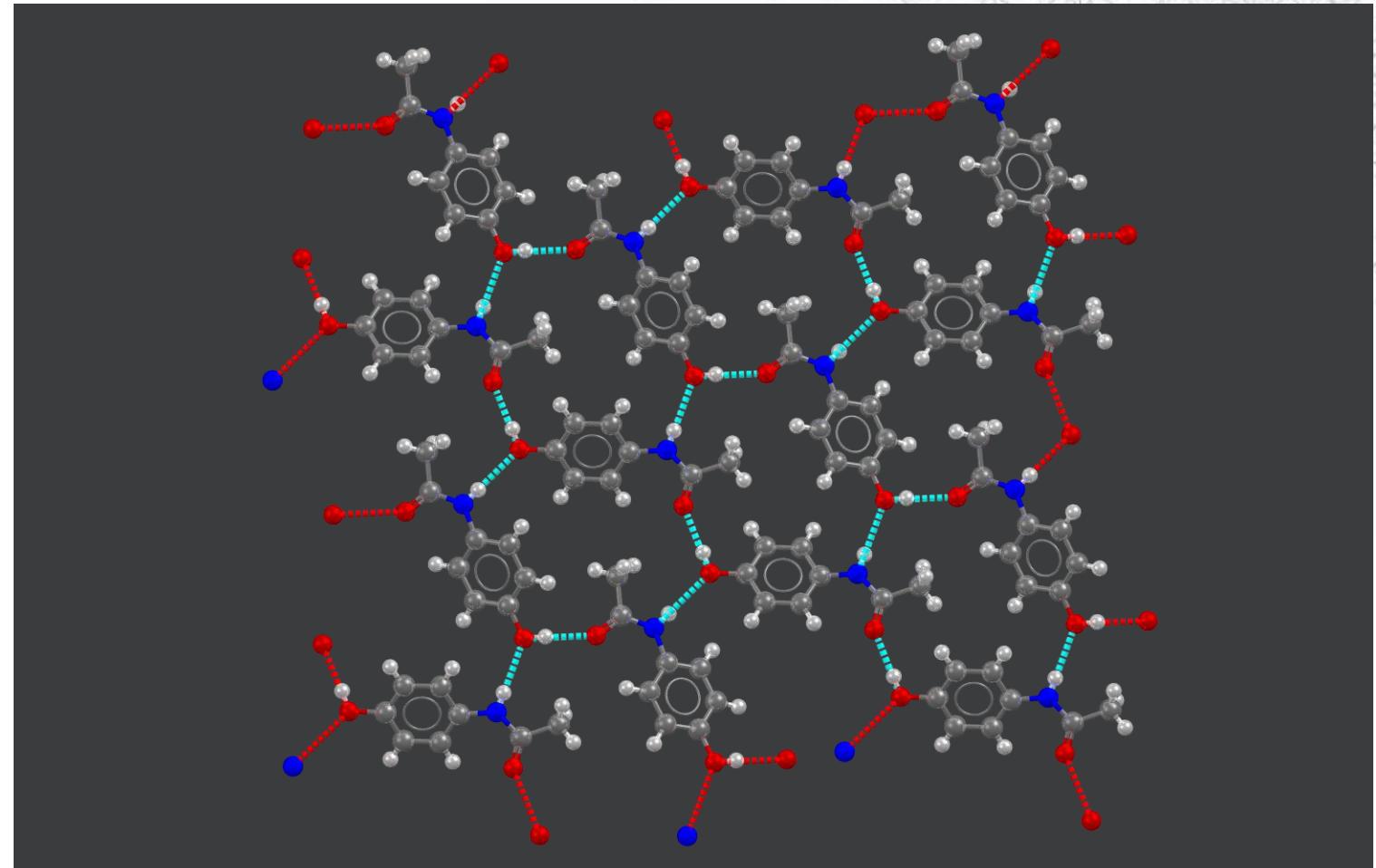
Blue arrows highlight the 'Edit...' button in the 'Contacts' dialog, the 'Edit...' button in the 'Define Short Contacts' dialog, and the 'Edit...' button in the 'Find Contacts' dialog.

Building the H-bond network

You can continue to expand the H-bond network to explore the 1D, 2D or 3D nature of the network



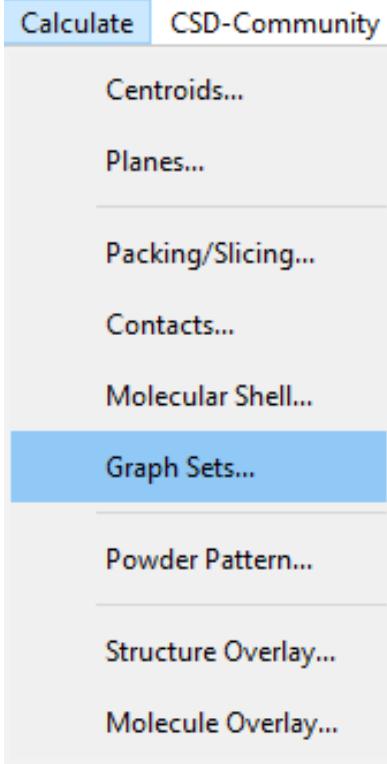
What type of network do you observe for HXACAN?



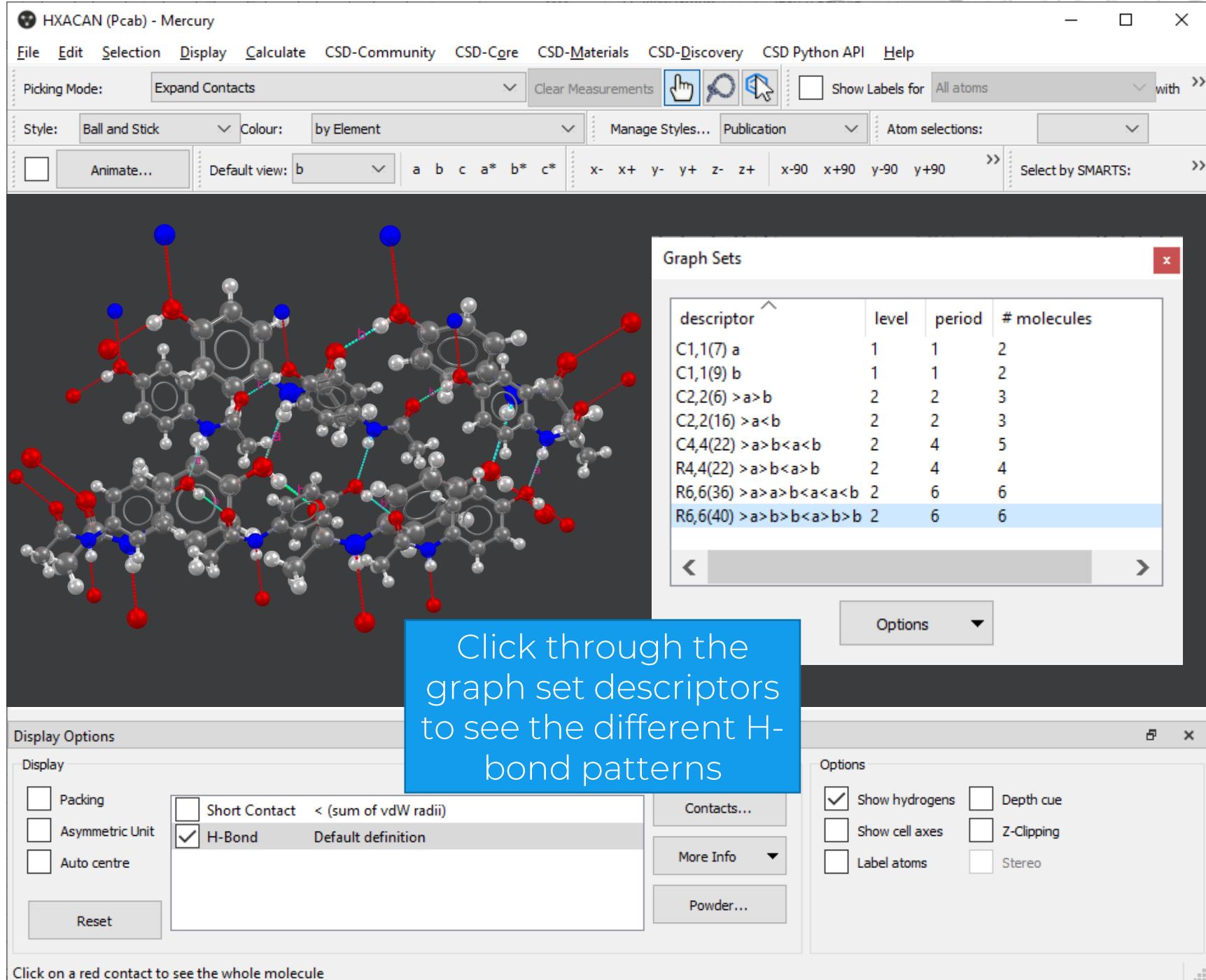
CSD Refcode: HXACAN

CCDC

Graph Sets



Graph Sets describe the H-bonds pattern.
Learn more in the *Glossary* on the handout.



Finding short contacts

The screenshot shows the Mercury software interface. The top menu bar includes File, Edit, Selection, Display, Calculate, CSD-Community, CSD-Core, CSD-Materials, CSD-Discovery, CSD Python API, and Help. The Picking Mode dropdown is set to "Expand Contacts". The Style dropdown is set to "Ball and Stick". The Colour dropdown is set to "by Element". The main window displays a molecular structure with red dashed lines representing short contacts.

Short contacts
are contacts
shorter than the
sum of van der
Waals (vdW)
radii

Learn more in the
Glossary on the
handout.

The screenshot shows the "Display Options" dialog in the Mercury software. Under the "Display" section, the "Short Contact" checkbox is checked and highlighted with a blue border. Other options like "Packing", "Asymmetric Unit", and "Auto centre" are unchecked. A large blue arrow points from this dialog to the "Define Short Contacts" dialog.

Colour contacts by colour
Display > Colours >
Contacts...

Define short contacts by
Calculate > Contacts >
Edit...

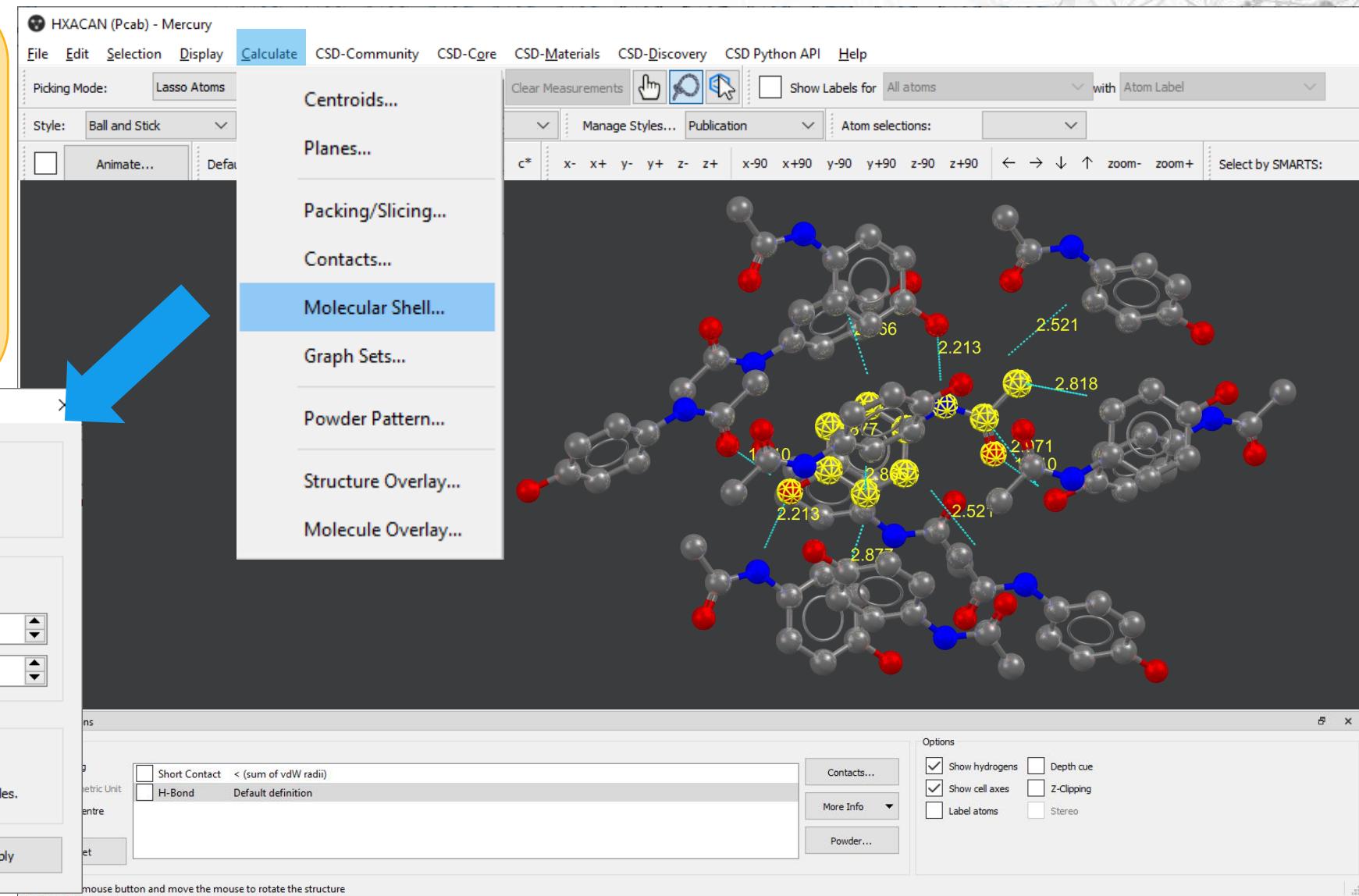
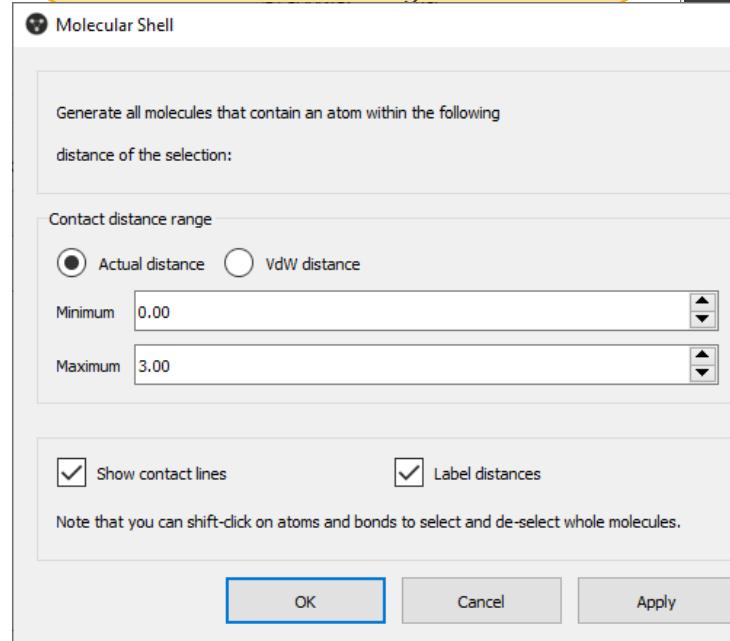
The screenshot shows two dialog boxes. The first is "Contact Colours" which allows coloring contacts by expanded/hanging, colour, or distance. The second is "Define Short Contacts" which allows defining contacts shorter than the sum of vdW radii, selecting intermolecular or intramolecular contacts, and specifying the number of bonds between atoms.

Exploring Molecular Shells

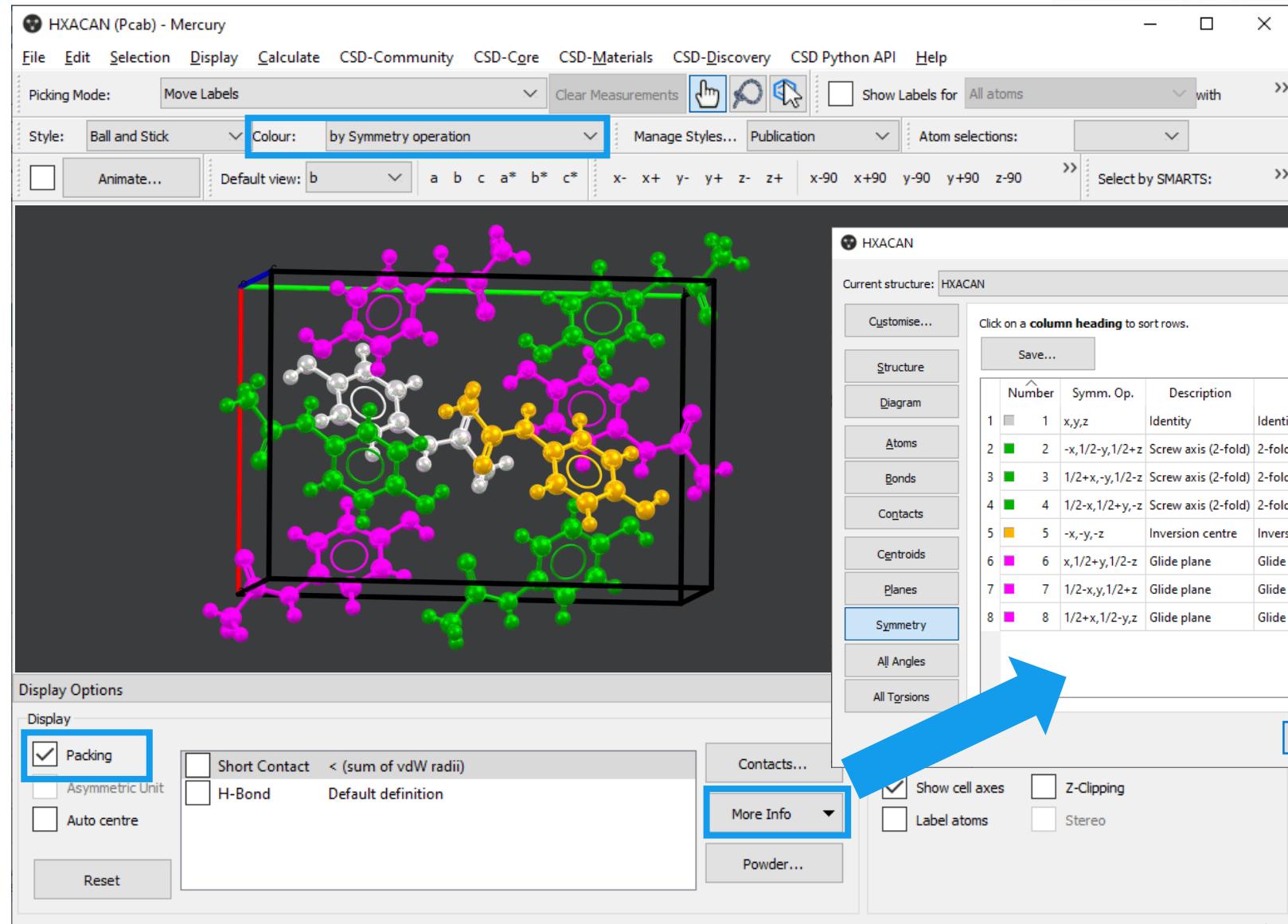
Molecular shells

contain atoms within a set distance from a selection (in some fields: “coordination sphere”).

Learn more in the *Glossary*.



Exploring symmetry



CSD Refcode:
HXACAN

CCDC

To show or remove symmetry elements

Symmetry Elements

Show Symmetry Elements

Show Inversions

Show Colour Size 0.25

Show Axes

Show proper rotation axes

Show screw axes

Show rotoinversion axes

2-fold Colour 3-fold Colour
4-fold Colour 6-fold Colour

Show Glide & Mirror Planes

Show mirrors Colour 0.68

Show glides Colour 0.17

Shadows

Defaults OK Reset

Display

Picking Mode:

Style: Ball and Stick

Styles Labels Colours Show/Hide More Information Symmetry Elements... Voids... Display Options... Manage Styles... View along Dial box... Splash screen Toolbars

Clear Measurements Atom selections:

Operation: Atom selections:

a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90

Select by SMARTS:

Chemical structure visualization showing molecules in a unit cell with symmetry elements highlighted.

Options

Show hydrogens Depth cue
Show cell axes Z-Clipping
Label atoms Stereo

HXACAN (Pcab) - Mercury

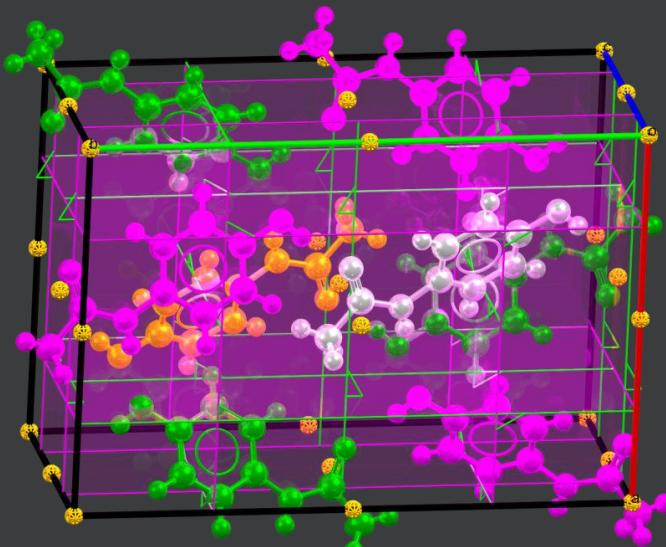
[File](#) [Edit](#) [Selection](#) [Display](#) [Calculate](#) [CSD-Community](#) [CSD-Core](#) [CSD-Materials](#) [CSD-Discovery](#) [CSD Python API](#) [Help](#)Picking Mode: [Move Labels](#) Clear Measurements Show Labels for All atoms with Atom LabelStyle: [Ball and Stick](#) Colour: by Symmetry operation Manage Styles... Publication Atom selections: Animate...

Default view: b a b c a* b* c*

x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90

< > ↓ ↑ zoom- zoom+

Select by SMARTS: [c]



Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre

| | |
|---|-------------|
| <input type="checkbox"/> Short Contact < (sum of vdW radii) | Contacts... |
| <input type="checkbox"/> H-Bond Default definition | More Info ▾ |
| | Powder... |

[Reset](#)

Press the left mouse button and move the mouse to rotate the structure

Why not explore what
H-bond networks and
symmetry the other
paracetamol
structures have

Structure Navigator

HXACAN

Find

Crystal Structures

Spacegroup

| Crystal Structure | Spacegroup |
|-------------------|------------|
| HXACAN | Pcab |
| HXACAN01 | P21/a |
| HXACAN02 | P21/c |
| HXACAN03 | P21/n |
| HXACAN04 | P21/n |
| HXACAN05 | P21/a |
| HXACAN06 | P21/a |
| HXACAN07 | P21/n |
| HXACAN08 | Pbca |
| HXACAN09 | P21/n |
| HXACAN10 | P21/n |
| HXACAN11 | P21/n |
| HXACAN12 | P21/n |
| HXACAN13 | P21/a |
| HXACAN14 | P21/a |
| HXACAN15 | P21/a |
| HXACAN16 | P21/a |
| HXACAN17 | P21/a |
| HXACAN18 | P21/a |

<<

>>

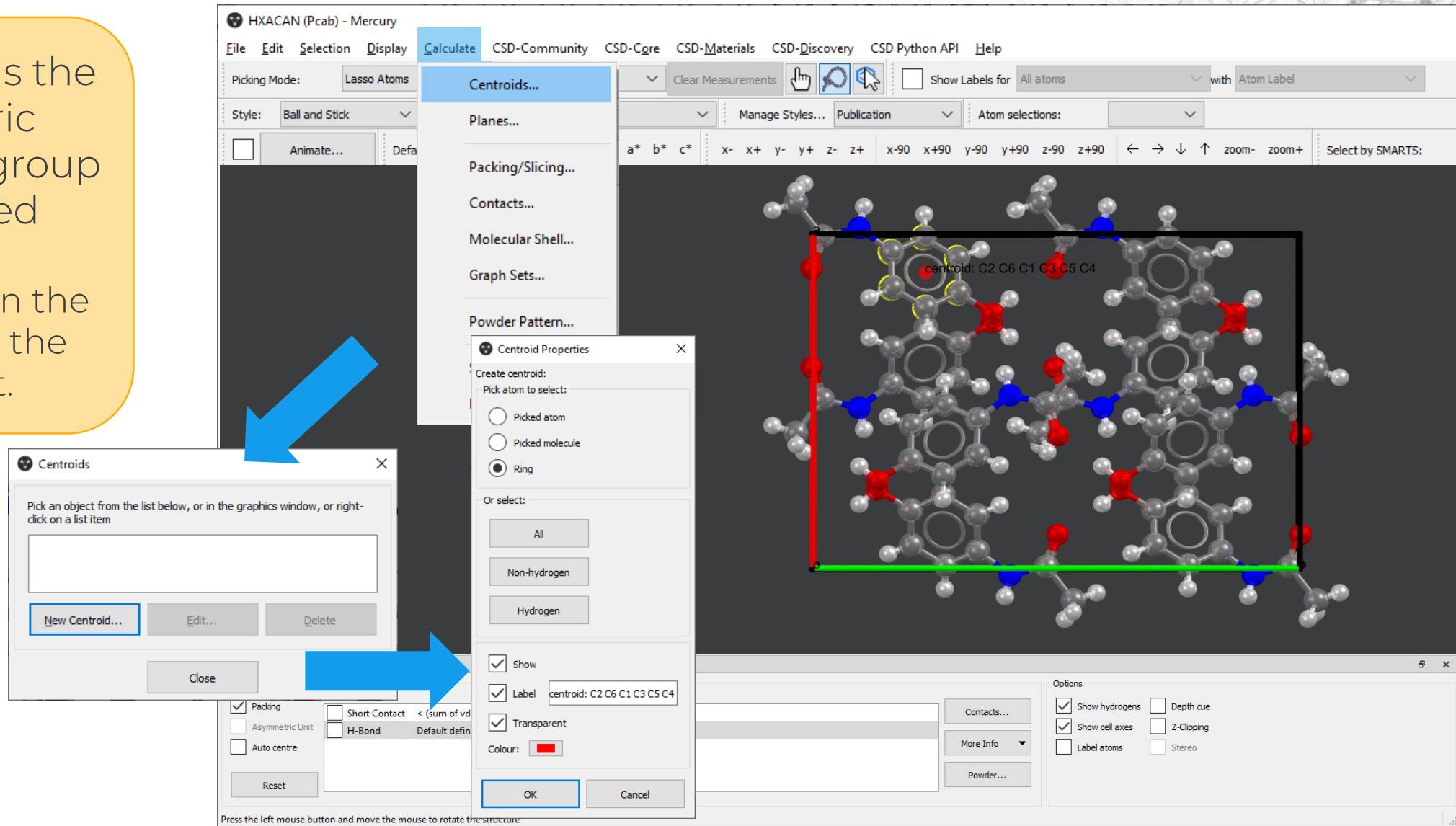
See View

| |
|--|
| <input type="checkbox"/> Multiple Structures |
| Structures... |

CCDC

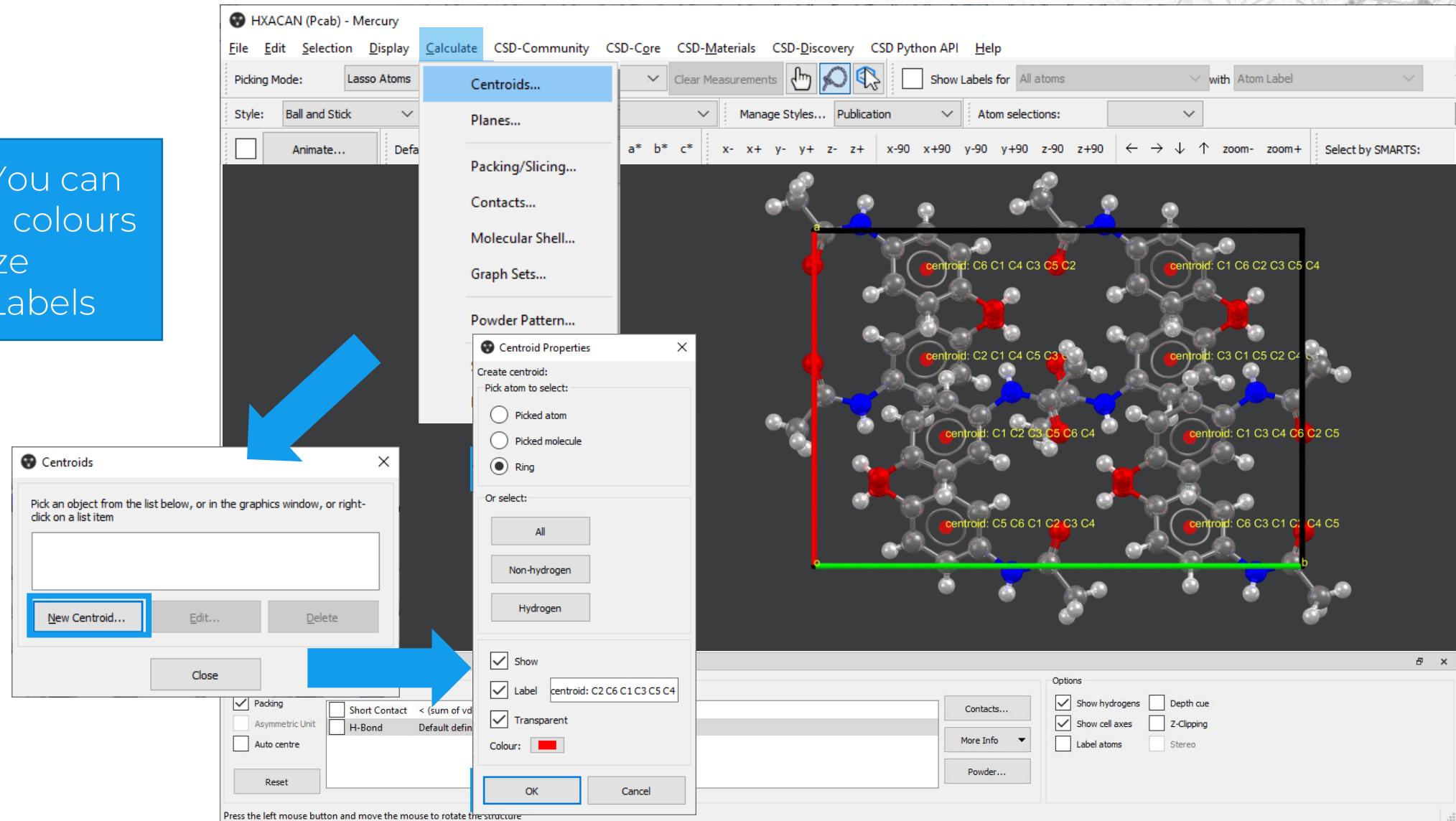
Calculating centroids

A **centroid** is the geometric centre of a group of selected atoms
Learn more in the *Glossary* on the handout.



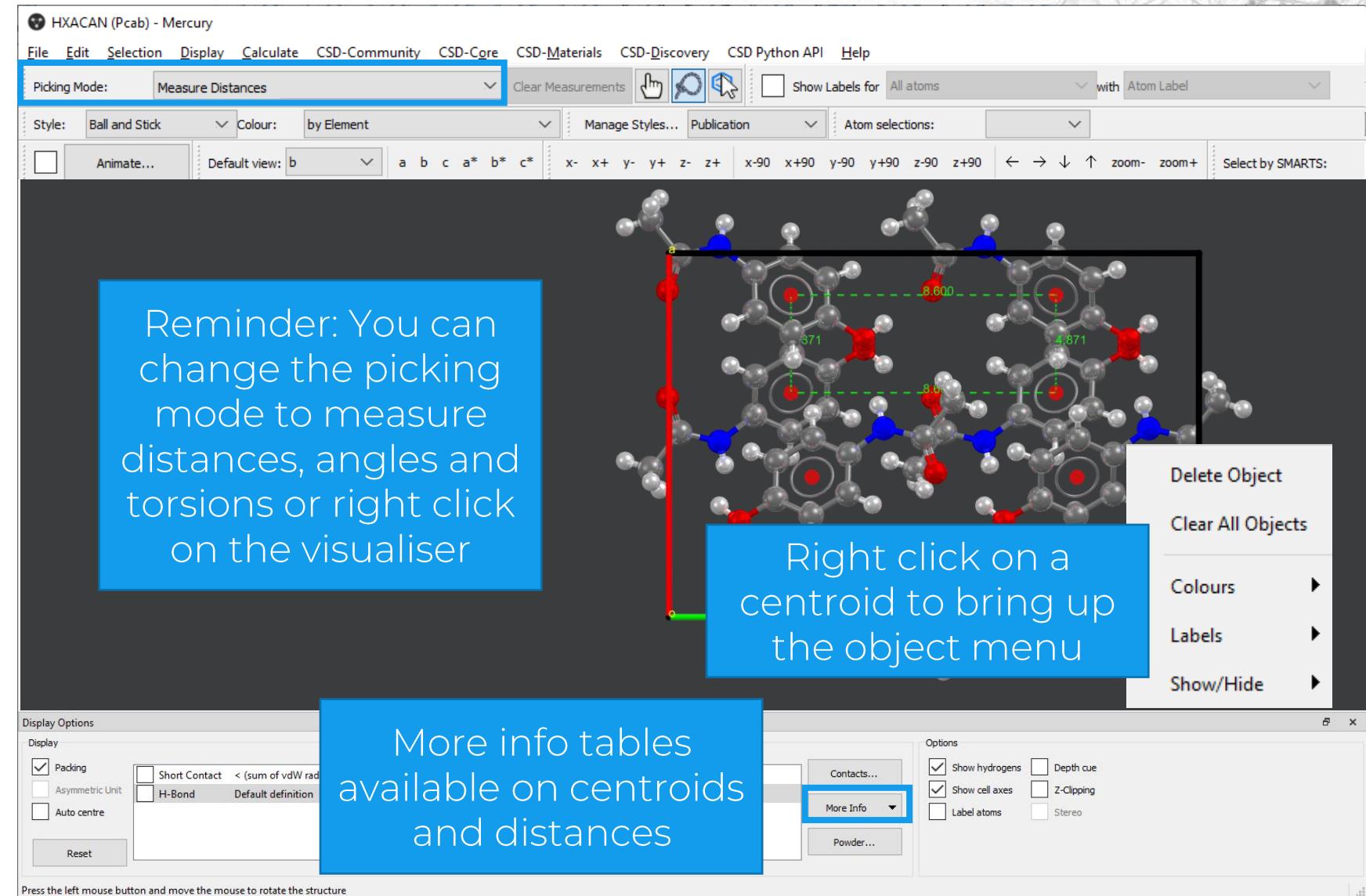
Calculating centroids

Reminder: You can change label colours and size
Display > Labels

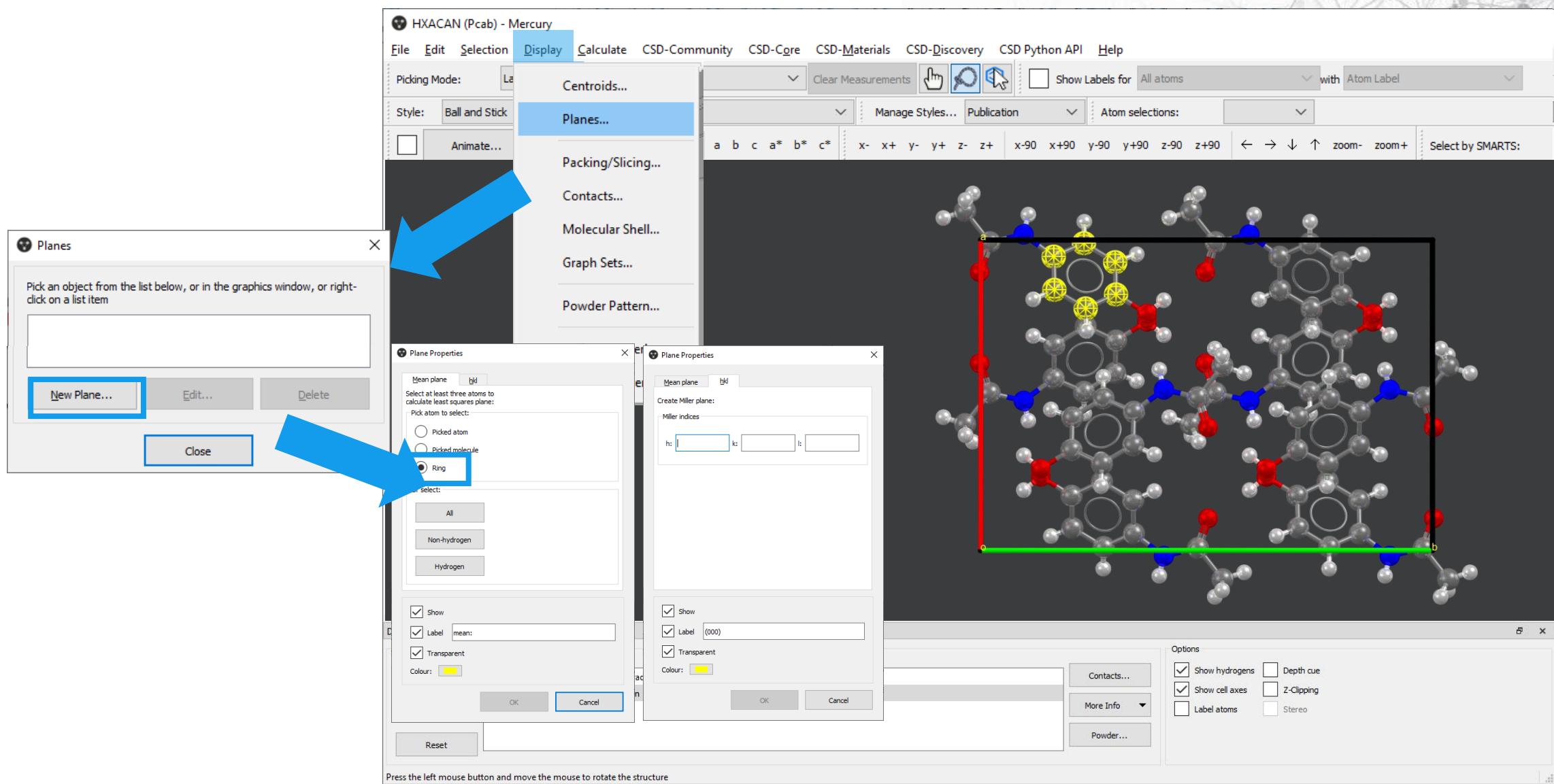


Measuring distances between centroids

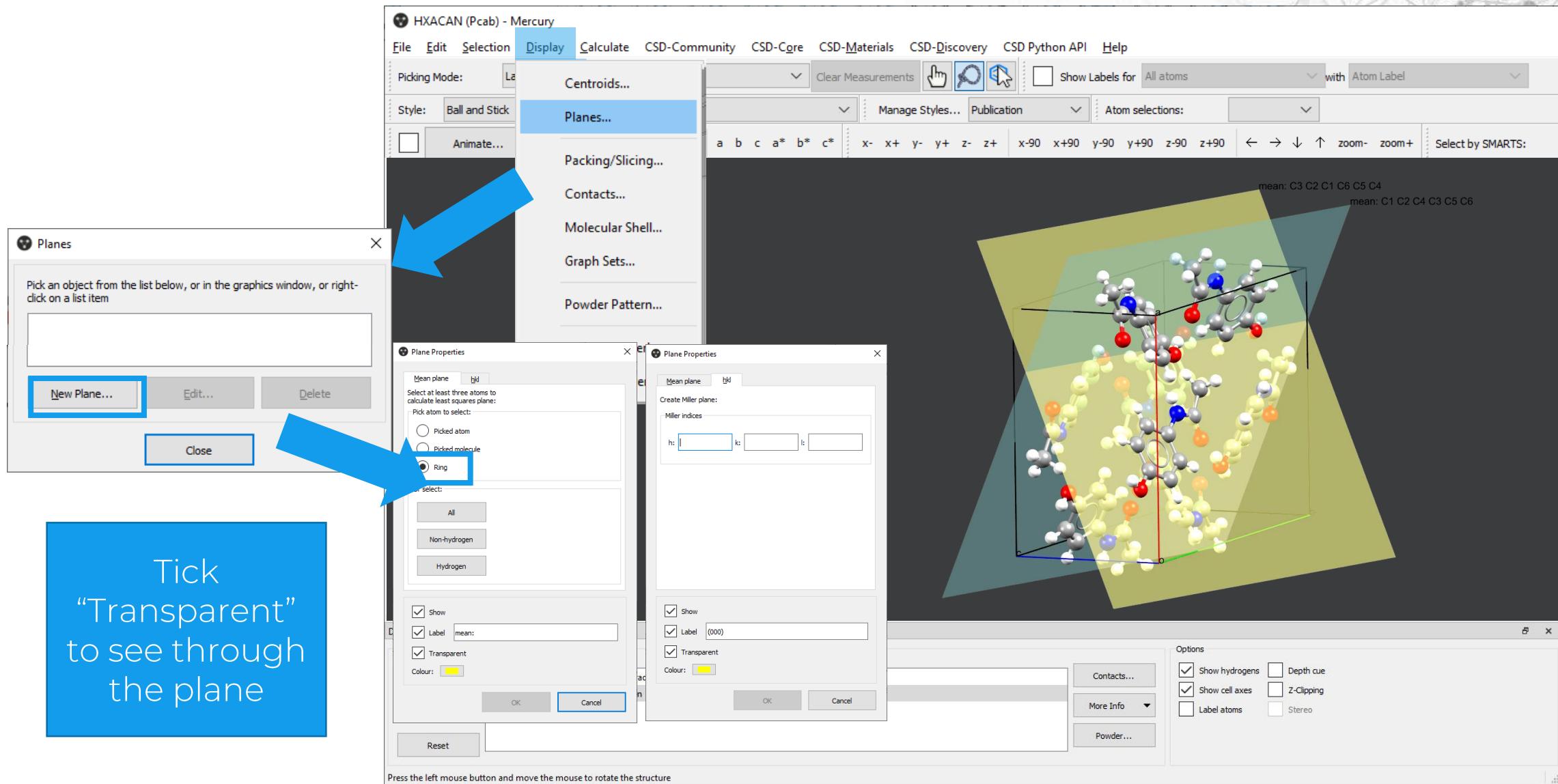
Why not explore how the distance and angles between the ring centroids differ in the other paracetamol structures



Calculating planes



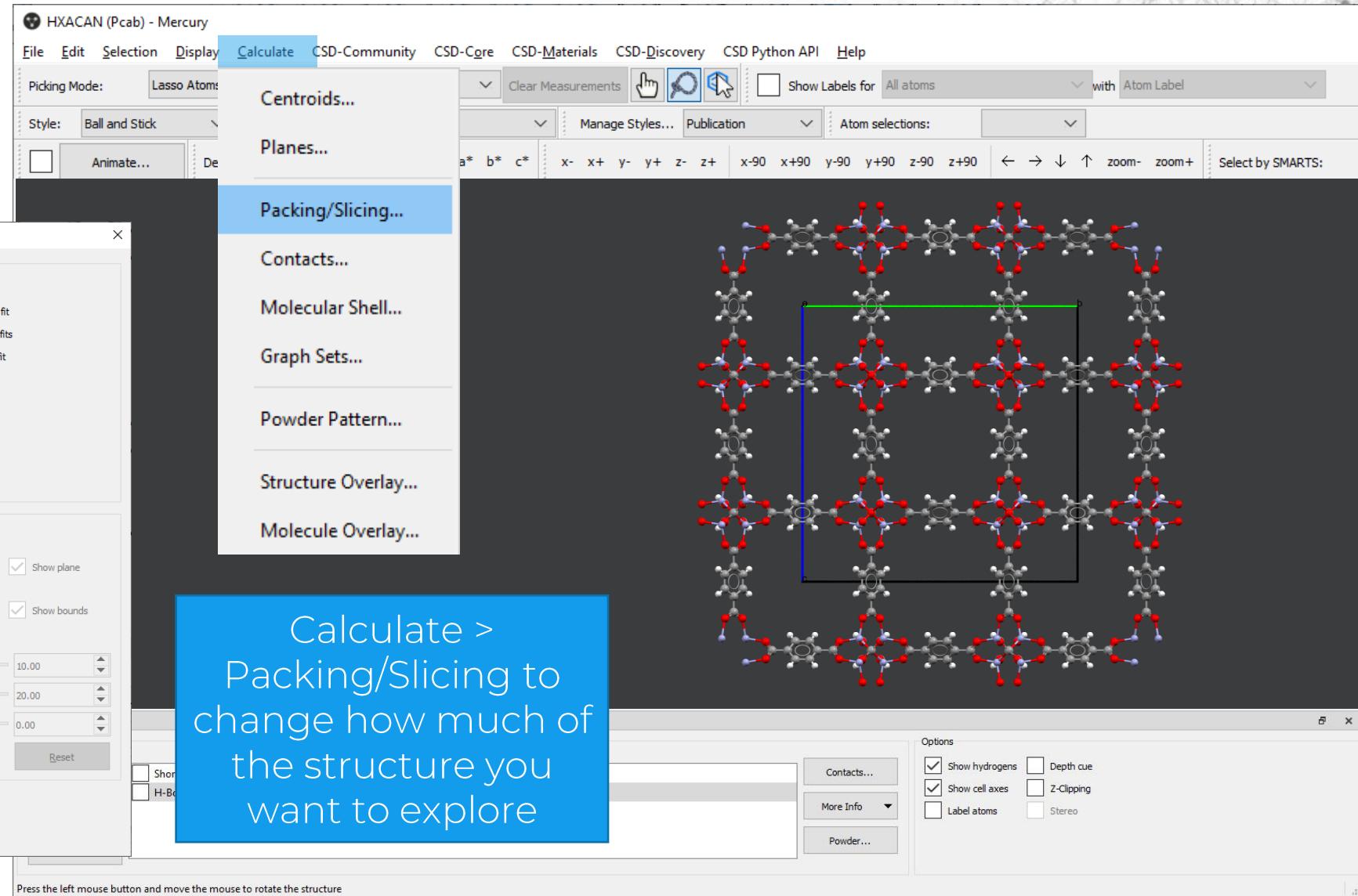
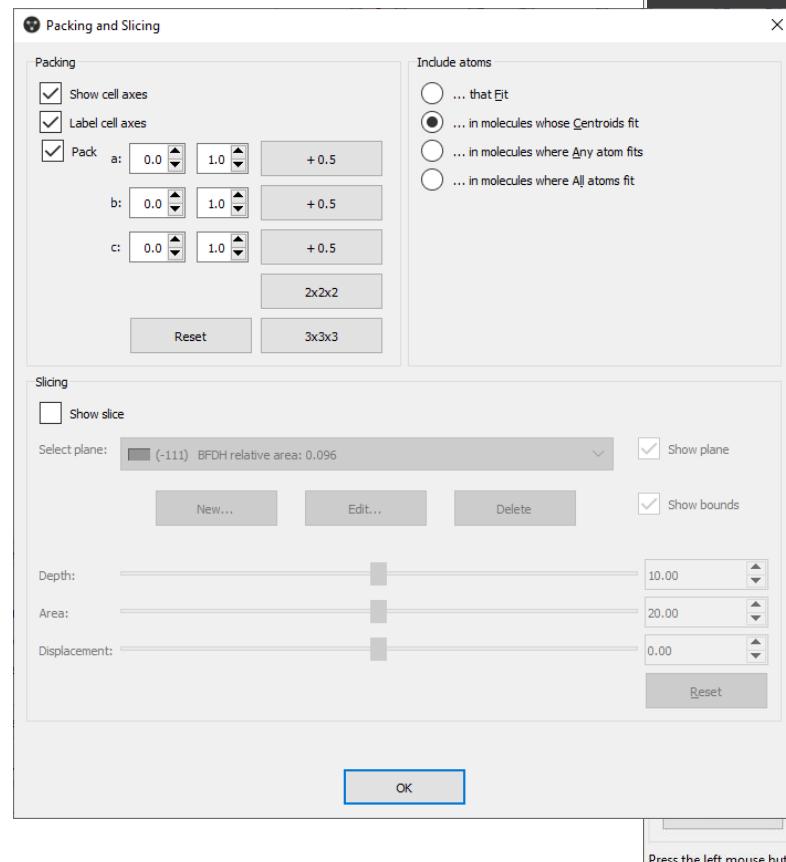
Calculating planes



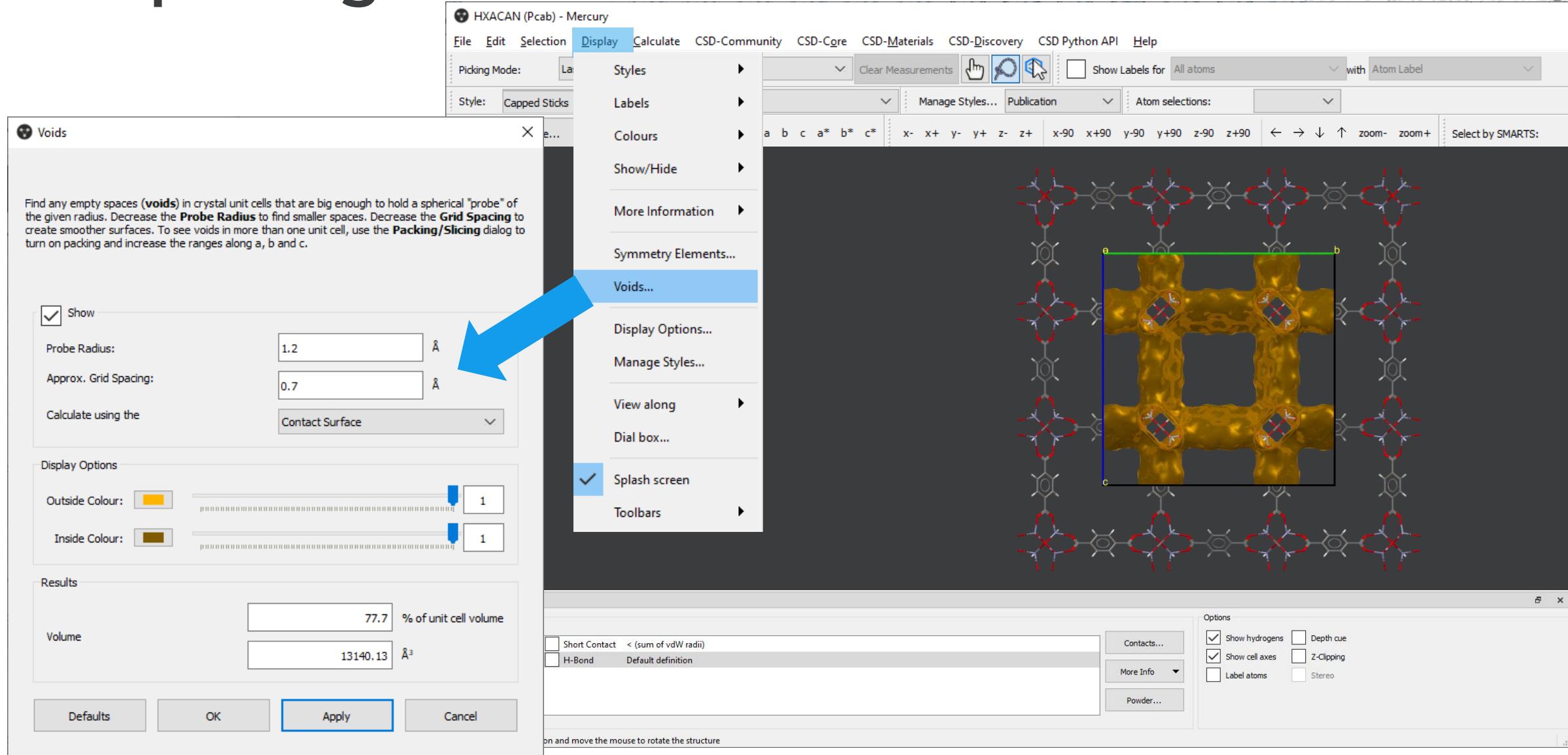
Tick
“Transparent”
to see through
the plane

Exploring voids

CSD Refcode: SAHYIK



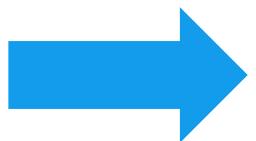
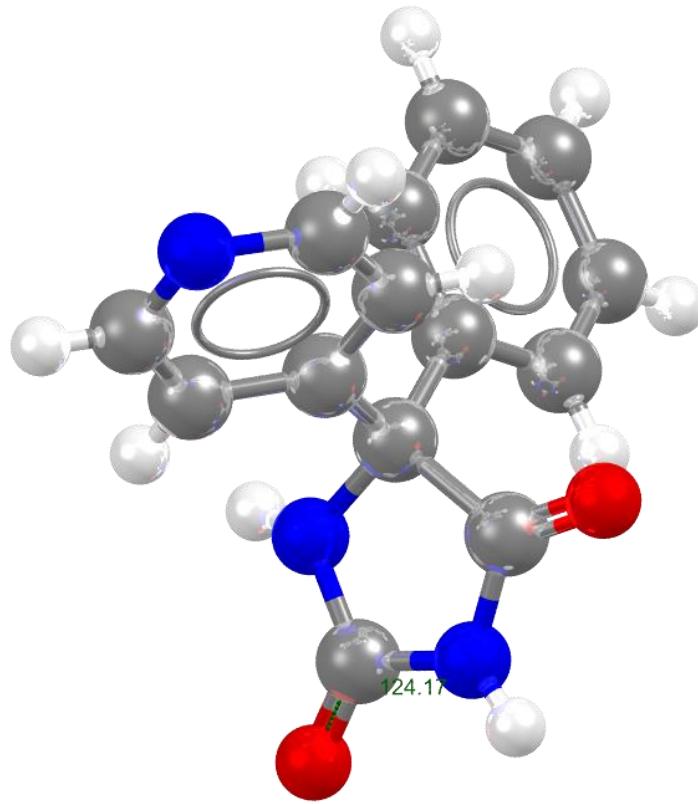
Exploring voids



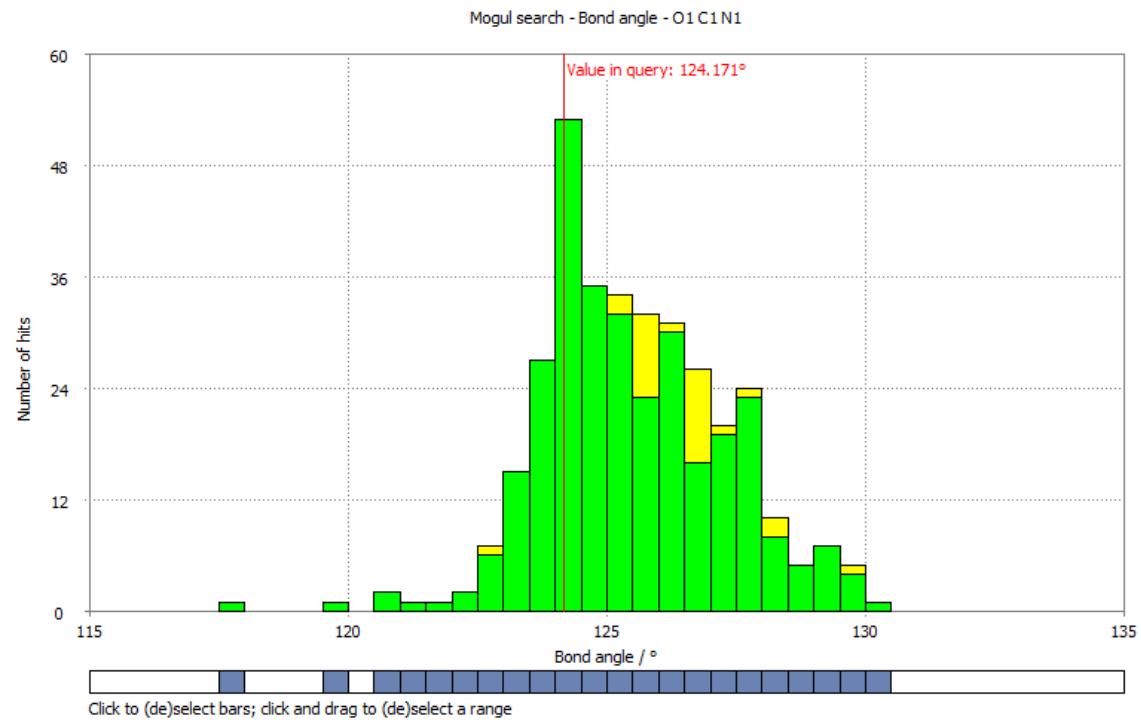
Explore More!

- So far we have explored the backbone of the Mercury analysis tools.
- You can also find a range of more advanced tools you can use to gain more insights into your structures.
- Lets explore a selection of these that either complement or are built on the ones discussed in this session.

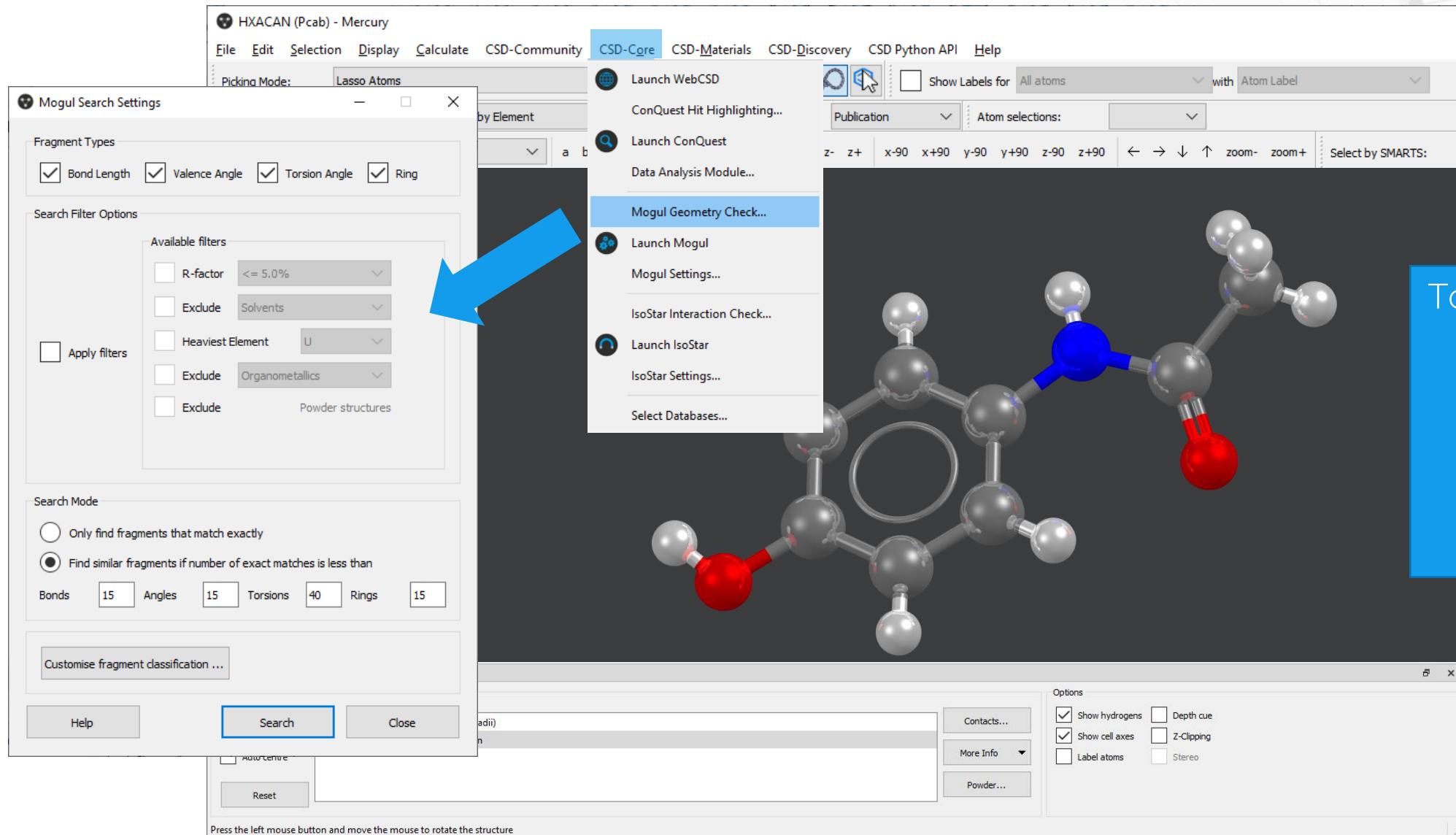
Measurements of bonds, angles, and torsions



Mogul



Measurements of bonds, angles, and torsions



CCDC

Measurements of bonds, angles, and torsions

Mogul Results Viewer

Show / hide : Columns Fragments... Deselect all fragments Export...

Help Double click to view result in Mogul

| Type | Molecule | Fragment | Classification | No. of hits | Query value | Mean | Std. dev. | z-score | x - mean | Minimum | Maximum | Median | d(min) | Loc |
|---------|----------|-------------------|---------------------------|-------------|-------------|---------|-----------|---------|----------|---------|---------|--------|--------|-----|
| bond | HXACAN | C2 C1 | Not unusual (enough hits) | 11501 | 1.392 | 1.388 | 0.017 | 0.267 | 0.004 | 1.129 | 1.577 | 1.389 | 0.000 | |
| | | C3 C2 | Not unusual (enough hits) | 20000 | 1.385 | 1.383 | 0.017 | 0.089 | 0.002 | 0.882 | 1.646 | 1.384 | 0.000 | |
| | | C3 C4 | Not unusual (enough hits) | 10415 | 1.381 | 1.385 | 0.019 | 0.211 | | | | | | |
| | | C5 C4 | Not unusual (enough hits) | 10415 | 1.379 | 1.385 | 0.019 | 0.323 | | | | | | |
| | | C6 C5 | Not unusual (enough hits) | 20000 | 1.391 | 1.383 | 0.017 | 0.455 | | | | | | |
| | | C6 C1 | Not unusual (enough hits) | 11501 | 1.386 | 1.388 | 0.017 | 0.140 | | | | | | |
| | | C8 C7 | Not unusual (enough hits) | 4811 | 1.510 | 1.501 | 0.021 | 0.452 | | | | | | |
| | | C1 N1 | Not unusual (enough hits) | 10620 | 1.424 | 1.412 | 0.020 | 0.583 | | | | | | |
| | | O1 C4 | Not unusual (enough hits) | 10295 | 1.381 | 1.365 | 0.023 | 0.663 | | | | | | |
| | | O2 C7 | Not unusual (enough hits) | 4811 | 1.223 | 1.228 | 0.022 | 0.238 | | | | | | |
| | | C7 N1 | Not unusual (enough hits) | 1693 | 1.342 | 1.355 | 0.018 | 0.705 | | | | | | |
| angle | HXACAN | C6 C1 C2 | Not unusual (enough hits) | 10675 | 119.757 | 119.032 | 1.344 | 0.539 | | | | | | |
| | | C2 C1 N1 | Not unusual (enough hits) | 11020 | 123.755 | 120.413 | 3.361 | 0.994 | | | | | | |
| | | C6 C1 N1 | Not unusual (enough hits) | 11020 | 116.457 | 120.413 | 3.361 | 1.177 | | | | | | |
| | | C3 C2 C1 | Not unusual (enough hits) | 10777 | 119.355 | 120.297 | 1.136 | 0.829 | | | | | | |
| | | C2 C3 C4 | Not unusual (enough hits) | 10375 | 120.688 | 119.875 | 1.078 | 0.754 | | | | | | |
| | | C5 C4 C3 | Not unusual (enough hits) | 8456 | 120.163 | 119.769 | 1.635 | 0.241 | | | | | | |
| | | O1 C4 C3 | Not unusual (enough hits) | 10415 | 118.961 | 120.007 | 2.809 | 0.373 | | | | | | |
| | | O1 C4 C5 | Not unusual (enough hits) | 10415 | 120.875 | 120.007 | 2.809 | 0.309 | | | | | | |
| | | C6 C5 C4 | Not unusual (enough hits) | 10375 | 119.547 | 119.875 | 1.078 | 0.305 | | | | | | |
| | | C5 C6 C1 | Not unusual (enough hits) | 10777 | 120.398 | 120.297 | 1.136 | 0.089 | | | | | | |
| | | O2 C7 C8 | Not unusual (enough hits) | 4811 | 122.654 | 122.058 | 1.810 | 0.329 | | | | | | |
| | | C8 C7 N1 | Not unusual (enough hits) | 1693 | 114.596 | 114.988 | 1.445 | 0.271 | | | | | | |
| | | O2 C7 N1 | Not unusual (enough hits) | 1693 | 122.746 | 123.042 | 1.307 | 0.227 | | | | | | |
| | | C1 N1 C7 | Not unusual (enough hits) | 771 | 129.809 | 127.998 | 1.790 | 1.012 | | | | | | |
| torsion | HXACAN | C2 C1 N1 C7 | Not unusual (enough hits) | 10557 | 17.826 | | | | | | | | | |
| | | C6 C1 N1 C7 | Not unusual (enough hits) | 10557 | -164.222 | | | | | | | | | |
| | | C8 C7 N1 C1 | Not unusual (enough hits) | 1493 | -178.813 | | | | | | | | | |
| | | O2 C7 N1 C1 | Not unusual (enough hits) | 1493 | 0.455 | | | | | | | | | |
| ring | HXACAN | C1 C2 C3 C4 C5 C6 | Not unusual (enough hits) | 1000 | | | | | | | | | | |

< All fragments... View query...

CCDC Mogul 2020.3: HXACAN (Pcab) - Mercury

File Searches Databases Help

Build query Results and analysis View structures

Results Navigator

All hits: 8456 Accepted hits: 8456 R-factor: Any Heaviest Element: Any Exclude: None

| Relevance | Number | Contribution |
|---------------------------------------|--------|--------------|
| > <input checked="" type="checkbox"/> | 1.00 | 8456 100.0% |

View diagrams... More hits...

Statistics

Total : 8456 Selected : 8456 Mean : 119.759° Standard deviation : 1.635° Minimum : 64.314° Lower quartile : 119.268° Median : 119.719° Upper quartile : 120.154° Maximum : 139.970° |z-score| : 0.241

Number of hits

Mogul search - Bond angle - C5 C4 C3

Bond angle / °

Value in query: 120.163°

120.16

Click to (de)select bars; click and drag to (de)select a range

Histogram display

Displayed hits: 8456 Selected hits: 8456

Select all hits in histogram Deselect all hits in histogram

Data libraries

CSD 5.4.2 CSD Feb21 update

Filters... Cluster

Histogram: click in bar to deselect, click again to reselect. Right-click for options.

Creating reports

Molecular Geometry Report for HXACAN

Crystal Structure Report for HXACAN

Volume and Packing Analysis

Fractional Atom Coordinates

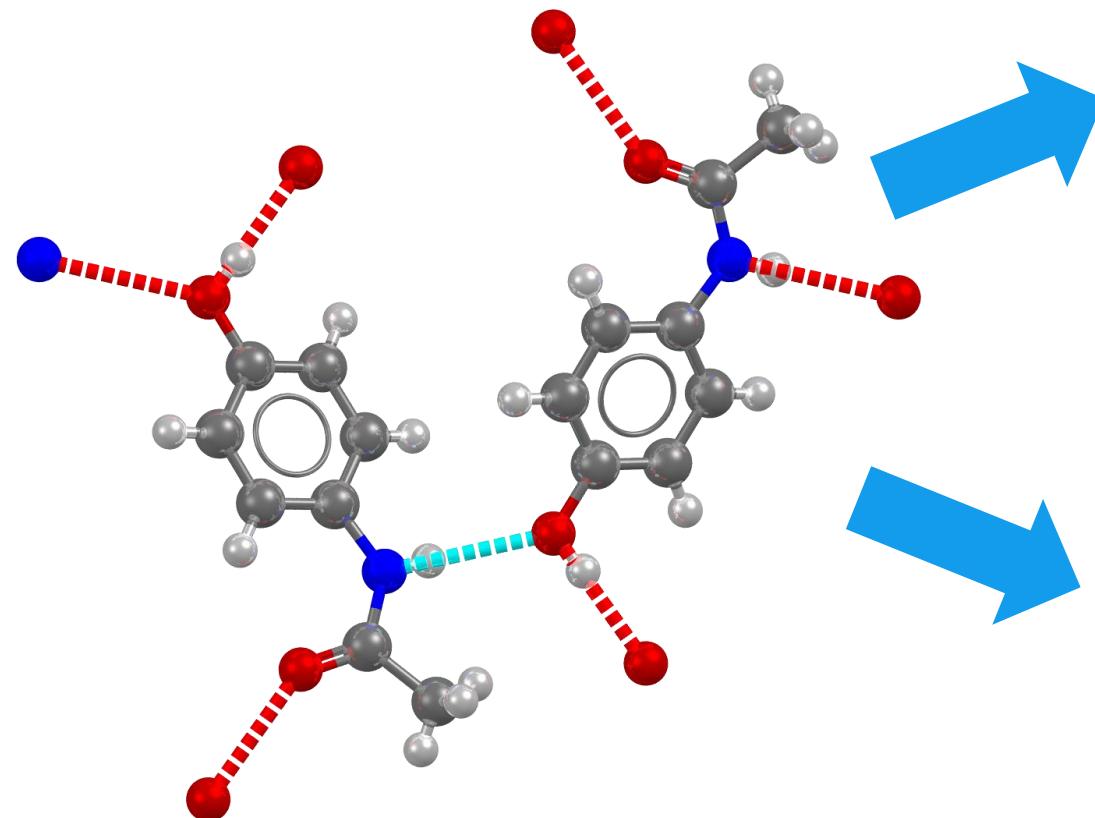
CCDC advancing structural science

CSD Python API

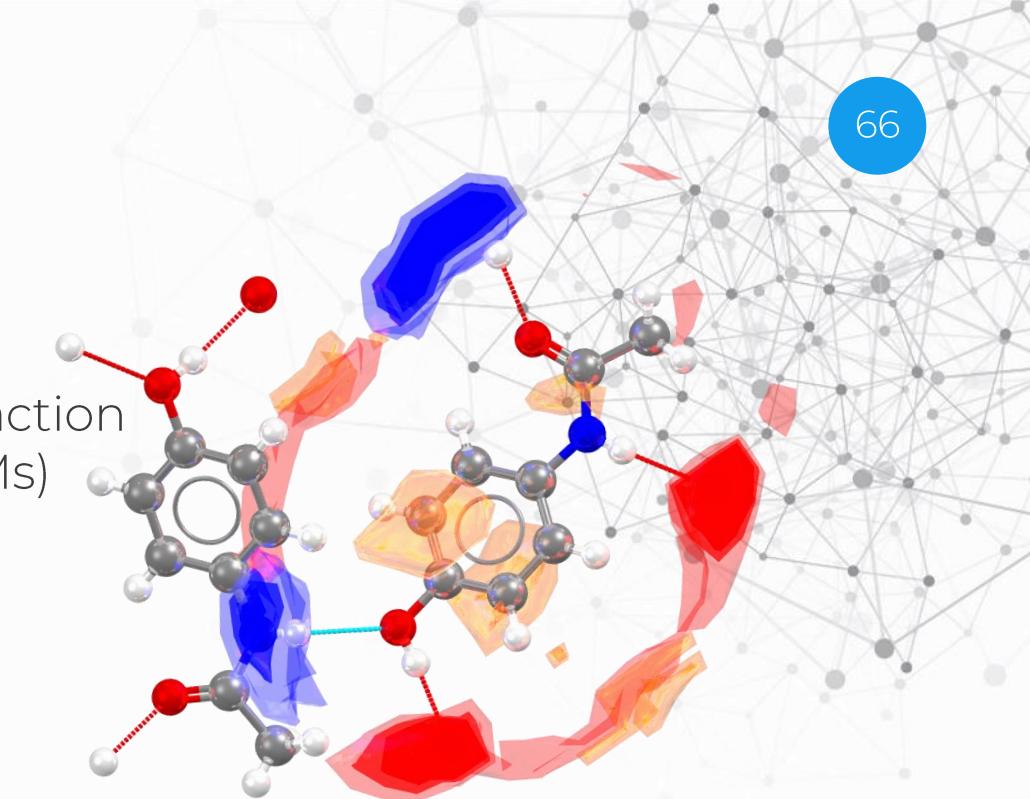
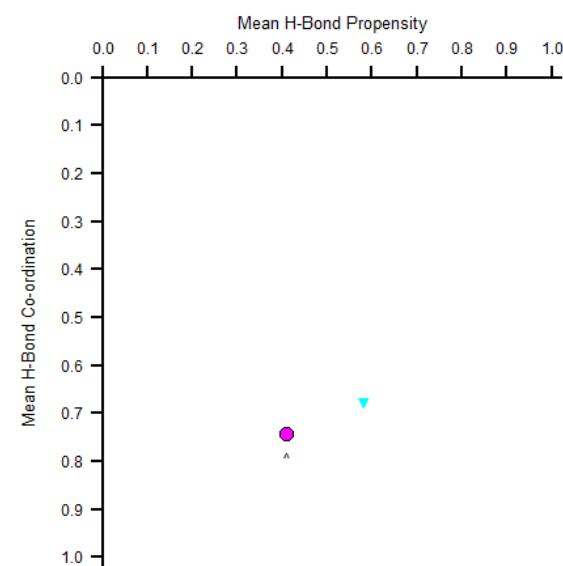
- Analysis
- Reports
- Searches
- user_support.py
- welcome.py
- calculate_CSD_diversity_score.py
- Options...
- CSD Python API Documentation
- CSD Python API Forum

Learn more in our CSD Python API CCDC workshop!

Hydrogen Bonds



Full Interaction
Maps (FIMs)



Hydrogen Bond
Propensity (HBPs)

Creating a FIMs and HBPs

HXACAN (Pcab) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Lasso Atoms

Style: Ball and Stick Colour: by Element

Atom selections: y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+ Select by SMARTS:

Labels for All atoms with Atom Label

Search Calculations Polymorph Assessment Co-Crystal Design Full Interaction Maps... Hydrate Analyser... Solvate Analyser... Aromatics Analyser... Conformer Generation... Launch DASH

Hydrogen Bond Propensities... H-bond Coordination Quick-view...

Full Interaction Maps

Options Maps Hotspots Log Files

Map Contour Levels

- Display first contour with initial level of 2.0
- Display second contour with initial level of 4.0
- Display third contour with initial level of 6.0

Hotspots

Generate hotspots in the map

Probe

- Uncharged NH Nitrogen
- Charged NH Nitrogen
- RNH₃ Nitrogen
- Alcohol Oxygen
- Carbonyl Oxygen
- Water Oxygen
- Oxygen Atom
- Methyl Carbon
- Aromatic CH Carbon
- C-F Fluorine

Col

Defaults

Calculate Maps Clear Maps & Hotspots Load Maps... Save Maps... Contacts... More Info Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Reset

Press the left mouse button and move the mouse to rotate the structure

<https://www.ccdc.cam.ac.uk/Community/blog/getting-started-with-FIMs/>

FIMs enable you to generate a 3D interaction map around a molecule representing regions of higher probability to find interactions with certain functional groups

Getting started with Full Interaction Maps

Ilaria Gimondi – February 15, 2021

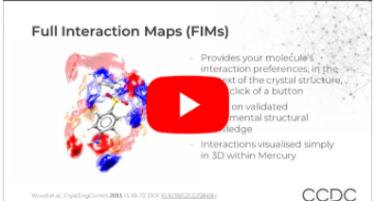
Our collection of educational resources has been growing throughout 2020, welcoming new How to videos (on our YouTube and LinkedIn channels), new self-guided workshops and updates to our existing material. We also added a feedback survey for you to fill in at the end of each workshop to let us know how we are doing and how we can improve.

This month we include in our collections 2 new resources, both about Full Interaction Maps (FIMs, for short): an educational video to write a blog about FIMs, and the first steps to

How do FIMs work?

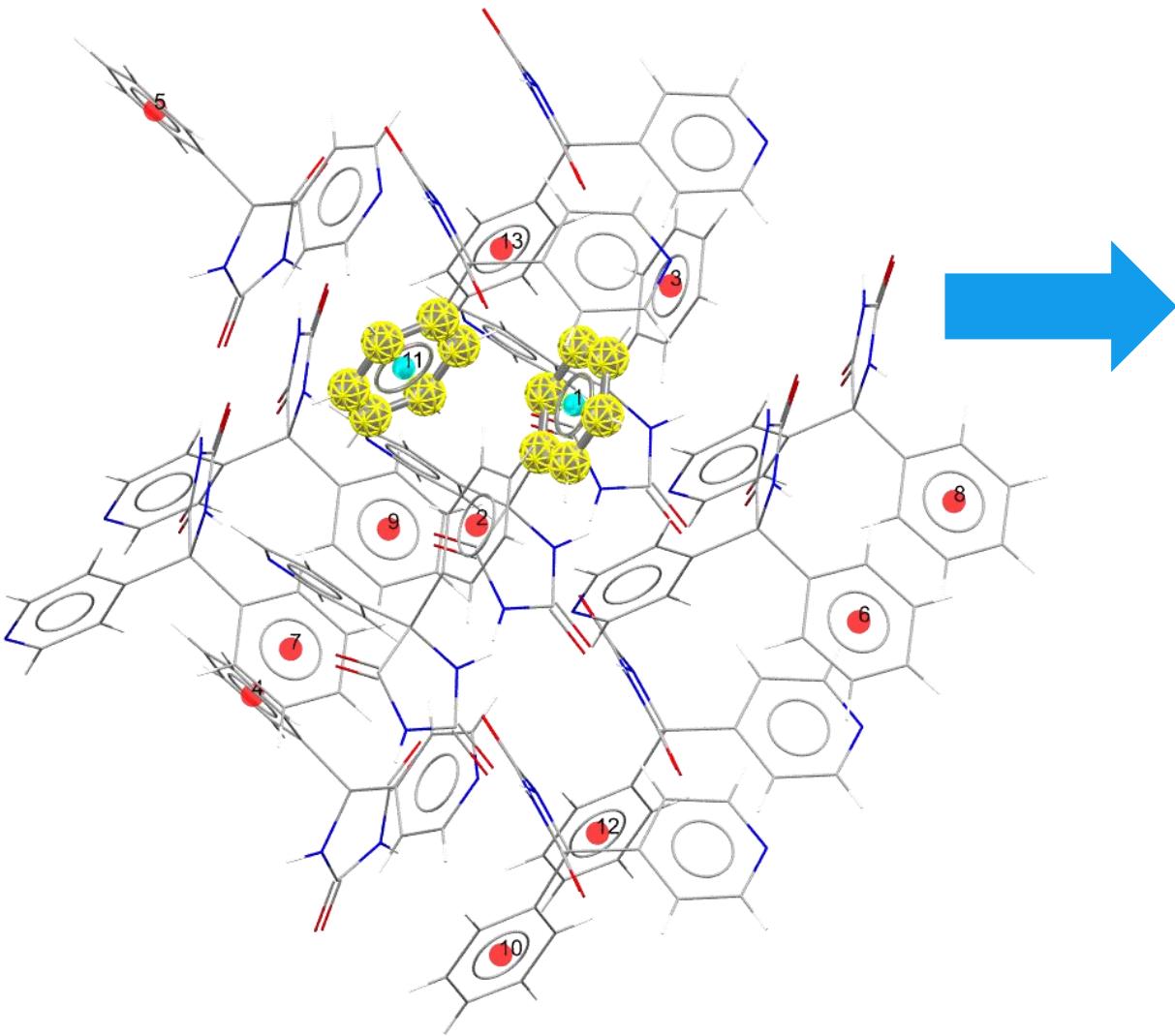
Full Interaction Maps represent regions of higher probability to find interactions with certain functional groups we made it available.

A great way to get started with FIMs is to show you how FIMs work, together with few examples that will give you an idea about insightful information that FIMs can provide on your molecules, crystal structures, and ligand interactions. Our new educational video on FIMs aims exactly at this.



Click on the image to watch the video on YouTube.

Centroids, orientations and interactions



Aromatics Analyser

Aromatics Analyser... GODRAS

Select atoms in just **one** molecule

| | Centroid1 | Centroid2 | Distance | Relative Orientation | Inter-molecular | Score | Assessment |
|---|-----------|-----------|----------|----------------------|-----------------|-------|------------|
| 1 | 1 | 11 | 4.91 | 67.32 | Yes | 8.9 | Strong |
| 2 | 1 | 13 | 4.91 | 67.32 | Yes | 8.9 | Strong |
| 3 | 1 | 2 | 7.27 | 0 | Yes | 1.5 | Weak |
| 4 | 1 | 3 | 7.27 | 0 | Yes | 1.5 | Weak |
| 5 | 1 | 6 | 8.07 | 77.39 | Yes | 0.8 | Weak |
| 6 | 1 | 7 | 8.07 | 77.39 | Yes | 0.8 | Weak |
| 7 | 1 | 8 | 9.16 | 77.39 | Yes | 0.4 | Weak |

Include Intramolecular pairs Exclude symmetry equivalent interactions

Calculate Export Atom info Close

Using the Aromatics Analyser

A previous CCDC virtual workshop covered our Aromatic Analyser in full

The image shows the Mercury software interface. On the left, a dialog box titled "Aromatics Analyser... HXACAN" displays a table of interactions between atoms in a molecule. The columns include Centroid1, Centroid2, Distance, Relative Orientation, Inter-molecular, Score, and Assessment. The Assessment column uses color coding: green for Strong, light green for Moderate, and light blue for Weak. A large blue arrow points from this dialog to the "Aromatics Analyser..." option in the "CSD-Materials" dropdown menu on the right. The main window on the right shows a ball-and-stick model of a molecule with aromatic rings highlighted in red and numbered 1 through 13. The "Aromatics Analyser" menu also includes options for Conformer Generation and Launch DASH.

| | Centroid1 | Centroid2 | Distance | Relative Orientation | Inter-molecular | Score | Assessment |
|---|-----------|-----------|----------|----------------------|-----------------|-------|------------|
| 1 | 1 | 2 | 4.65 | 58.43 | Yes | 8.9 | Strong |
| 2 | 1 | 10 | 4.87 | 50.79 | Yes | 8 | Strong |
| 3 | 1 | 12 | 5.94 | 26.95 | Yes | 5.9 | Moderate |
| 4 | 1 | 7 | 8.93 | 0 | Yes | 0.6 | Weak |
| 5 | 1 | 8 | 8.6 | 58.43 | Yes | 0.6 | Weak |
| 6 | 1 | 6 | 9.38 | 0 | Yes | 0.4 | Weak |
| 7 | 1 | 4 | 9.88 | 50.79 | Yes | 0.2 | Weak |

Include Intramolecular pairs Exclude symmetry equivalent interactions

Buttons: Calculate, Export (highlighted), Atom info, Reset, Close

Text at bottom: Press the left mouse button and move the mouse to rotate the structure

Right side controls:

- Show hydrogens, Show cell axes, Label atoms
- Depth cue, Z-Clipping, Stereo
- Contacts..., More Info, Powder...