Visualizing and assessing hydrogen bonds in crystal structures using Hydrogen Bond Statistics

CCDC Virtual Workshop October 2022

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October 2022

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advancing structural science

Learning outcomes for today

- The basics of hydrogen bond visualization in Mercury:
  - Changing the definition of donors and acceptors
  - How to visualize H-bonds patterns and networks
  - Some tips and tricks for visualising and displaying H-bonds effectively
- How to assess hydrogen bonds using the Hydrogen Bond Statistics tool:
  - Familiarity with the tool and how the statistics are generated
  - When to use the tool and how to interpret the results
  - How to perform in depth analysis of hydrogen bonds in structures and what it can tell us about the system
- What other tools in the CSD Portfolio can complement Hydrogen Bond Statistics

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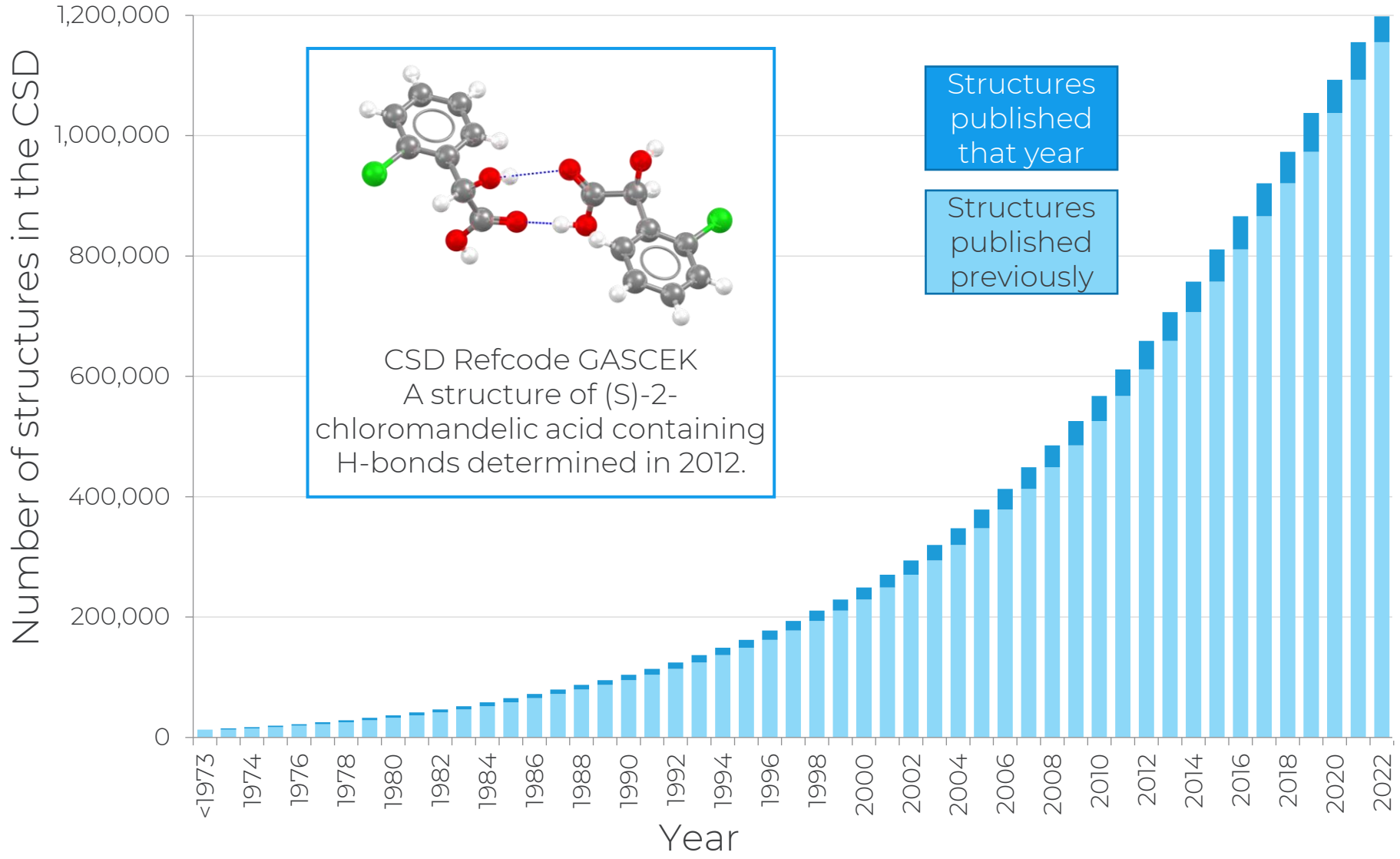
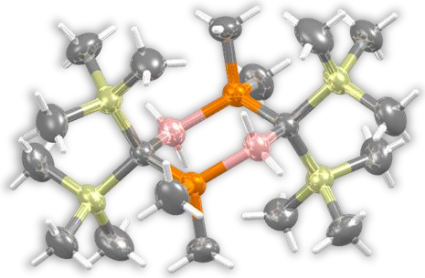
The Cambridge Structural Database



- Every published structure
  - Inc. ASAP & early view
  - CSD Communications
  - Patents
  - University repositories
  - Thesis
- Every entry enriched and annotated by experts
- Discoverability of data and knowledge
- Sustainable for over 57 years
- A trusted CoreTrustSeal repository

Certified as Trustworthy by CoreTrustSeal

CSD Refcodes



CSD Refcode - ELOFUJ

What is ELOFUJ?

- A CSD Refcode
- A database reference code
- Containing 6-8 characters
- Used to identify entries in the CSD

Refcode families

- The same substances are assigned the *same* 6 letter code plus an additional 2 numbers
  - Polymorphs
  - New determinations or re-refinements of the same substance
  - Determinations at different temperatures/pressures
- Stereoisomers or different solvates, co-crystals, etc. are assigned *different* refcode families

Some of our favourite refcodes are: KITTEN, BATMAN, DISNEY, GAUTAM, GLYCIN, What are yours?

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%

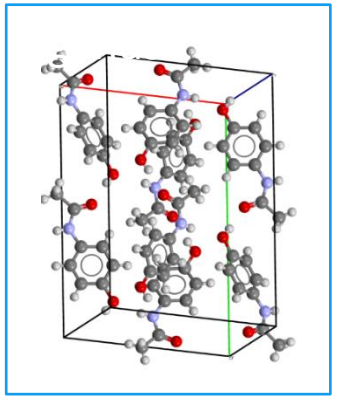
Polymeric: 11%

Single Component
56%

Multi Component
44%

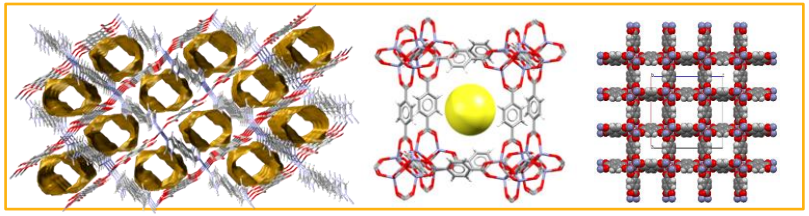
Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



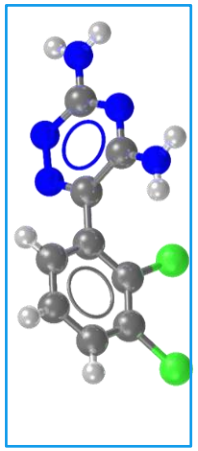
Metal-Organic

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



Additional data

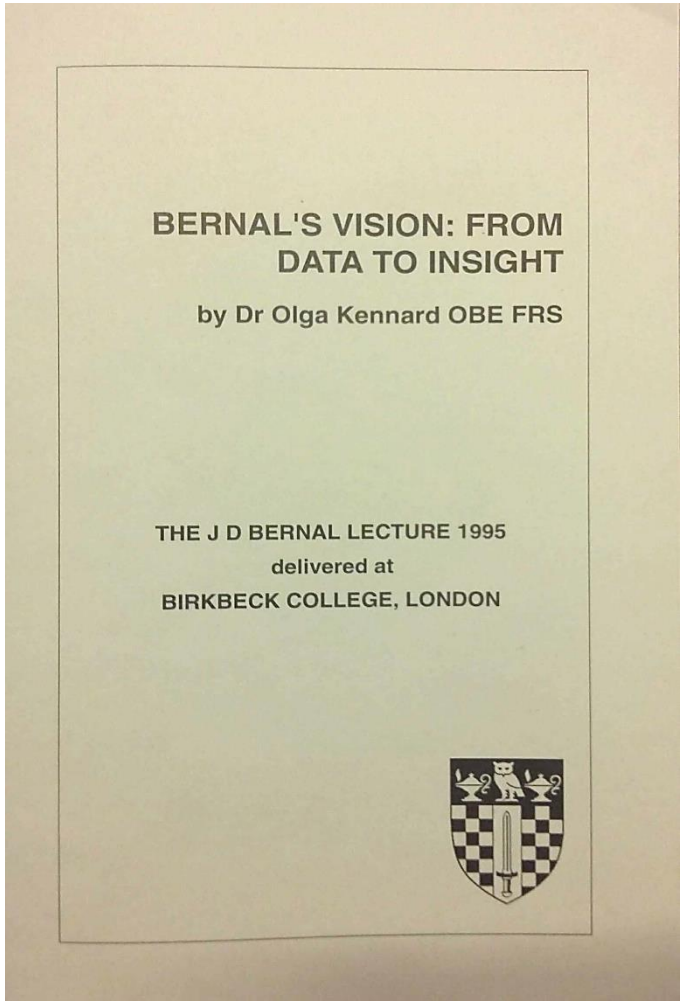
- >12,000 polymorph families
- >175,000 melting points
- >1 million crystal colours
- >900,000 crystal shapes
- > 29,000 bioactivity details
- >12,000 natural source data
- > 250,000 oxidation states



Links and subsets

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

The vision



BERNAL'S VISION: FROM DATA TO INSIGHT

by Dr Olga Kennard OBE FRS

THE J D BERNAL LECTURE 1995
delivered at
BIRKBECK COLLEGE, LONDON

We clearly recognised even in those early days, that data banks have three principal functions. Firstly they must gather together existing knowledge and make it readily available to the scientific community. Secondly they can be used to reduce a large number of observations to a small set of constants and rules, and in this way transform a data base to a knowledge base. Such a knowledge base may obviate the need for further individual experiments in specific areas. Thirdly, they facilitate the comparison and collective analysis of individual results to gain insight into new or as yet unexplained phenomena. These ideas have been at the heart of the work of the Cambridge Crystallographic Data Centre and the driving force for improving methods of data collection, storage and dissemination. Most importantly they influenced development of computer programs and methodologies which are needed for the analysis and transformation of the accumulated information. (5)

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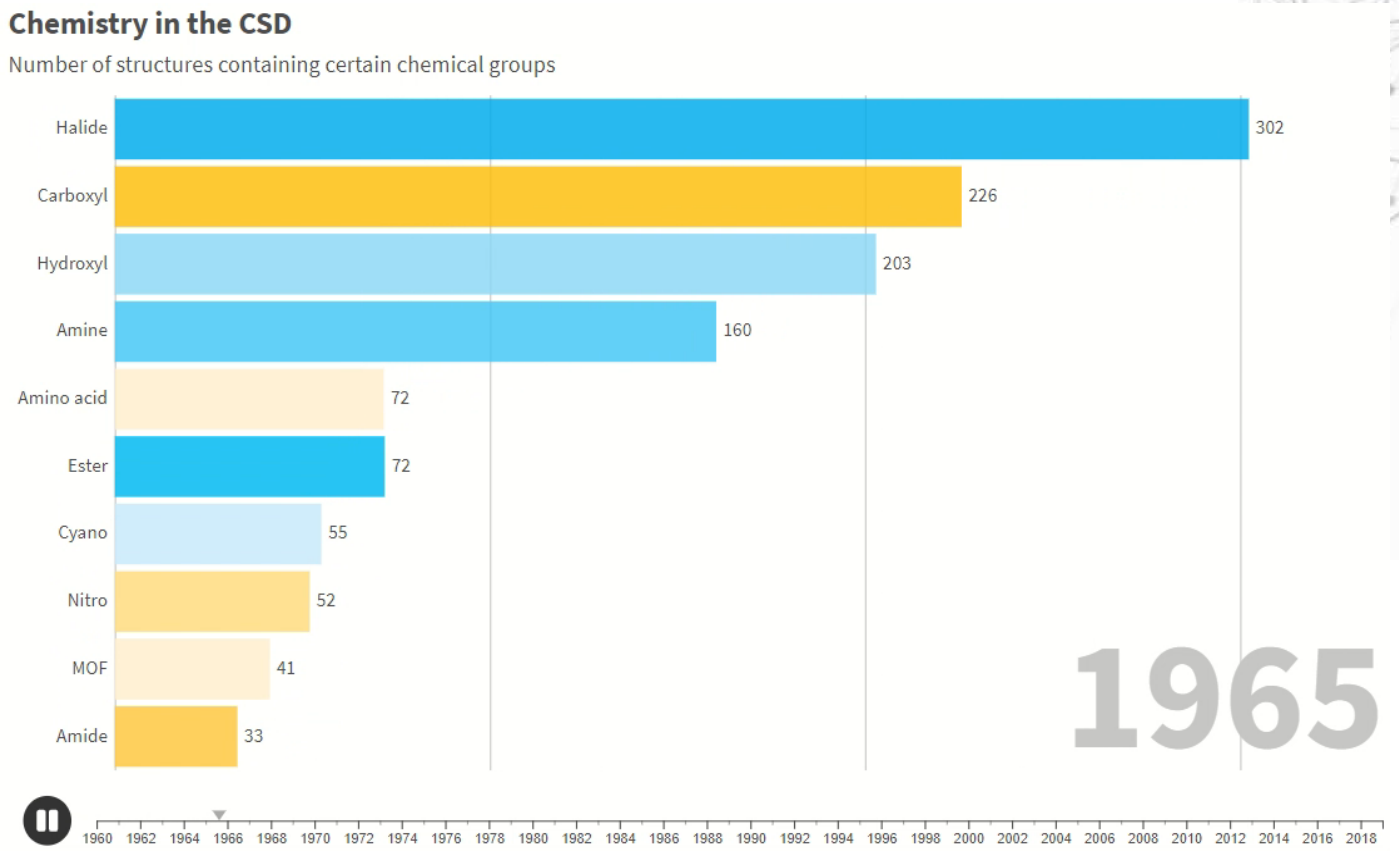
Exploring the CSD

- > 1 million structures
  - > 94M 3D coordinates
- > 28 million bond lengths
  - > 2M unique distributions
- > 40 million valence angles
  - > 3M unique distributions
- > 14 million torsion angles
  - > 800K unique distributions
- > 2 million rings
  - > 400K unique distributions



Images and graphics created using the CSD Python API and Flourish

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Software to gain new insights

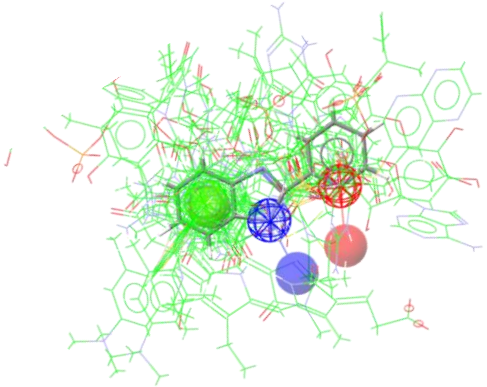
CSDCore.

Search, visualise, analyse and communicate structural data

Insights into molecular and crystal shape and interactions

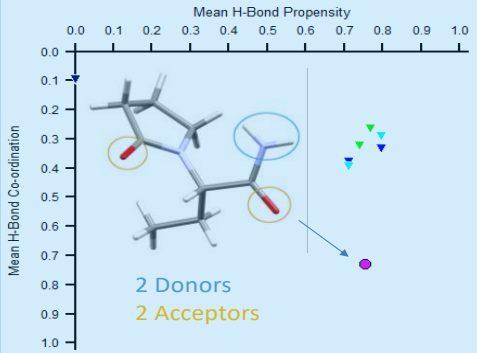
CSDDiscovery.

Design of new molecules



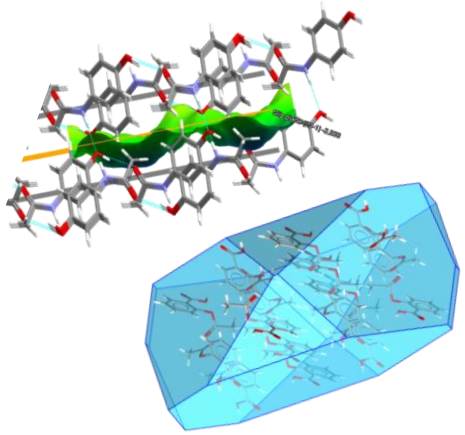
CSDMaterials.

Assessment of solid form stability and properties



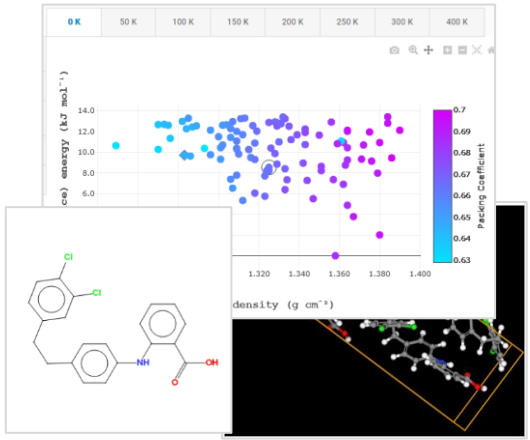
CSDParticle.

Anticipate particle properties and behaviour



CSDTheory.

Insights from predicted structure landscapes



Medicinal & Computational Chemists ♦ Crystallographers & Structural Biologists ♦ Solid Form & Crystallisation Scientists

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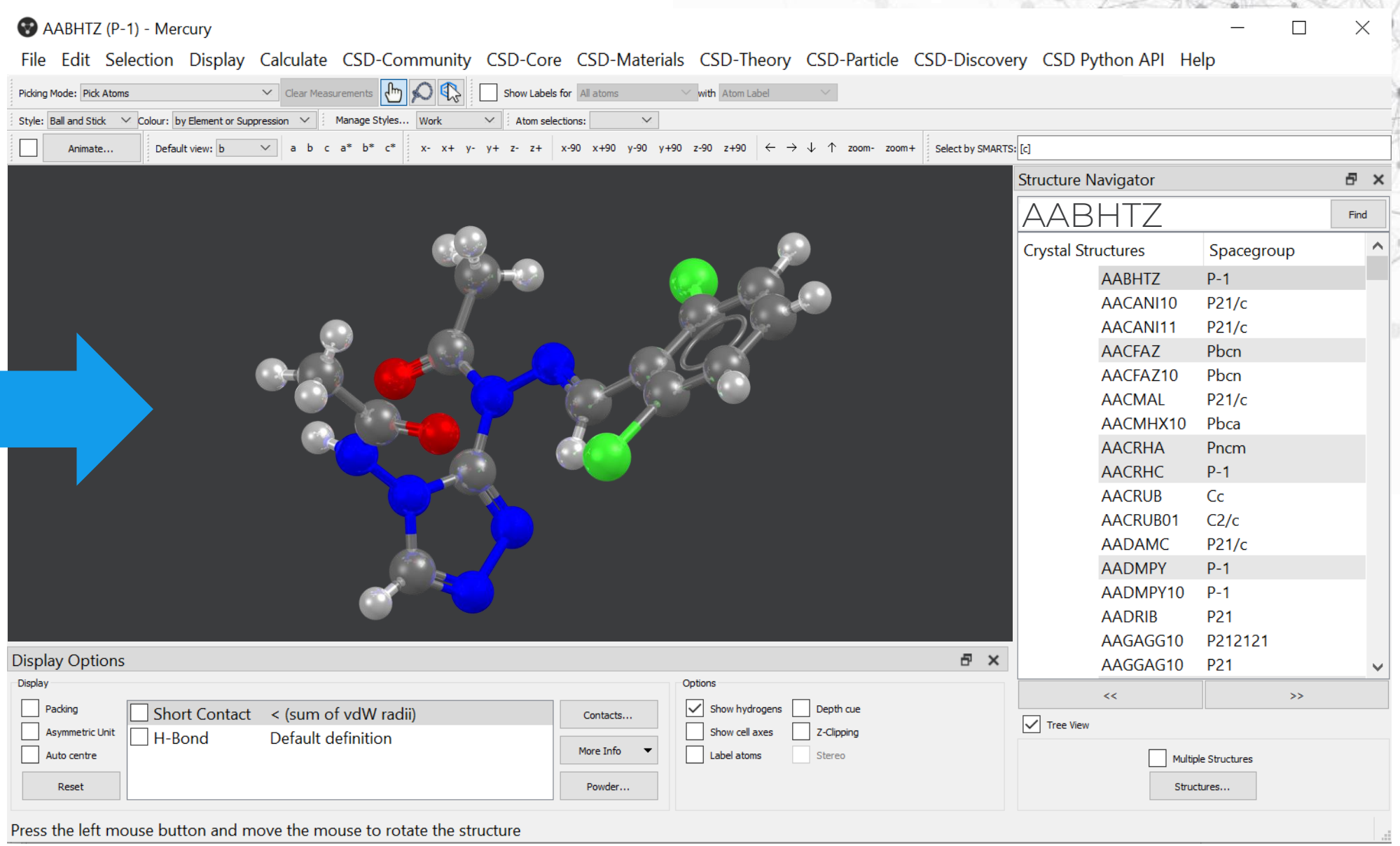
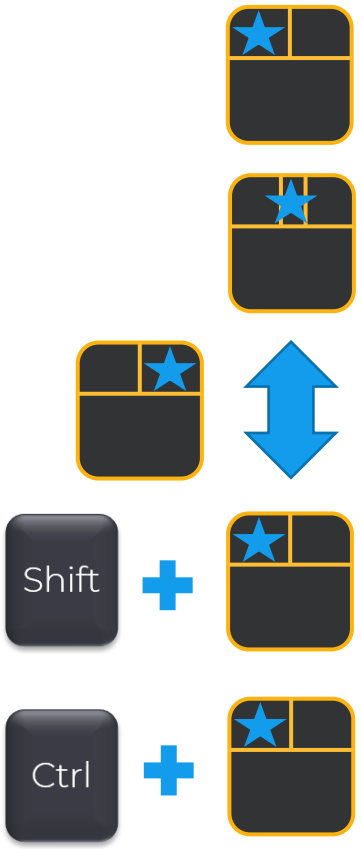
Exploring hydrogen bonds through Mercury

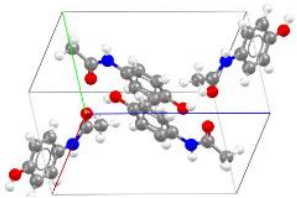


Reminder: Basic navigation in Mercury



- Left mouse button and move – rotate molecules
- Middle Mouse wheel – move molecules up and down
- Right mouse button and move up and down – zoom in and out of molecules
- Shift + Left mouse button and move - rotate in the plane molecules
- Ctrl + Left mouse button and move - translate molecules

Visualisation 101 - Visualising structural chemistry data with Mercury



Begin module

Learn more in this CSDU on-demand course

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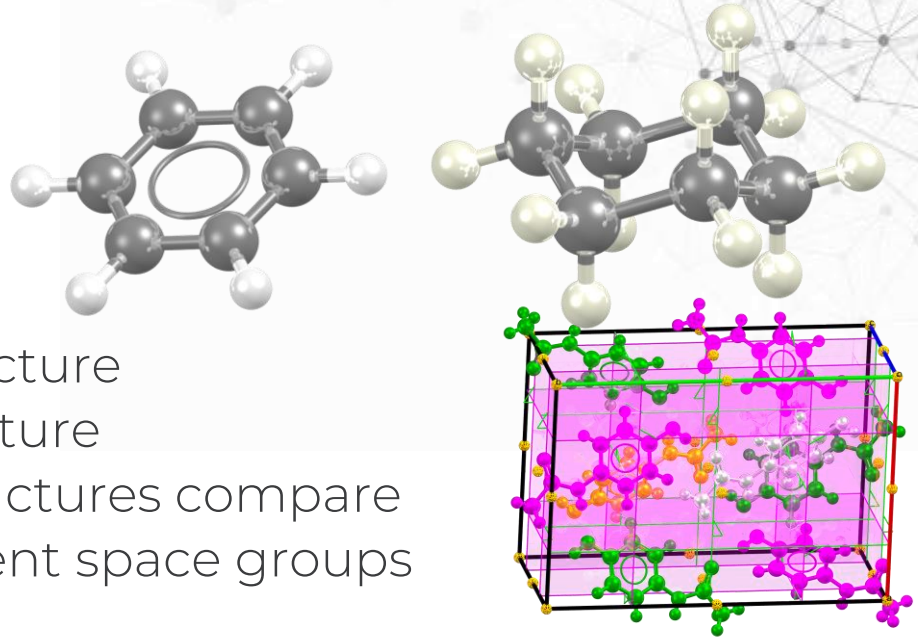
From visualisation to deeper understanding

By exploring 3D structures, we can gain a deeper understanding of:

- Chemistry:
  - The geometry of molecules
  - The geometry around metals
- Solid forms:
  - How molecules pack together
  - What voids and channels exist within a structure
  - What interactions help to stabilise the structure
  - How solid forms including polymorphic structures compare
  - The symmetry within a structure and different space groups
- Data validation:
  - Validate a structural model compared to 1.1 million structures in the CSD



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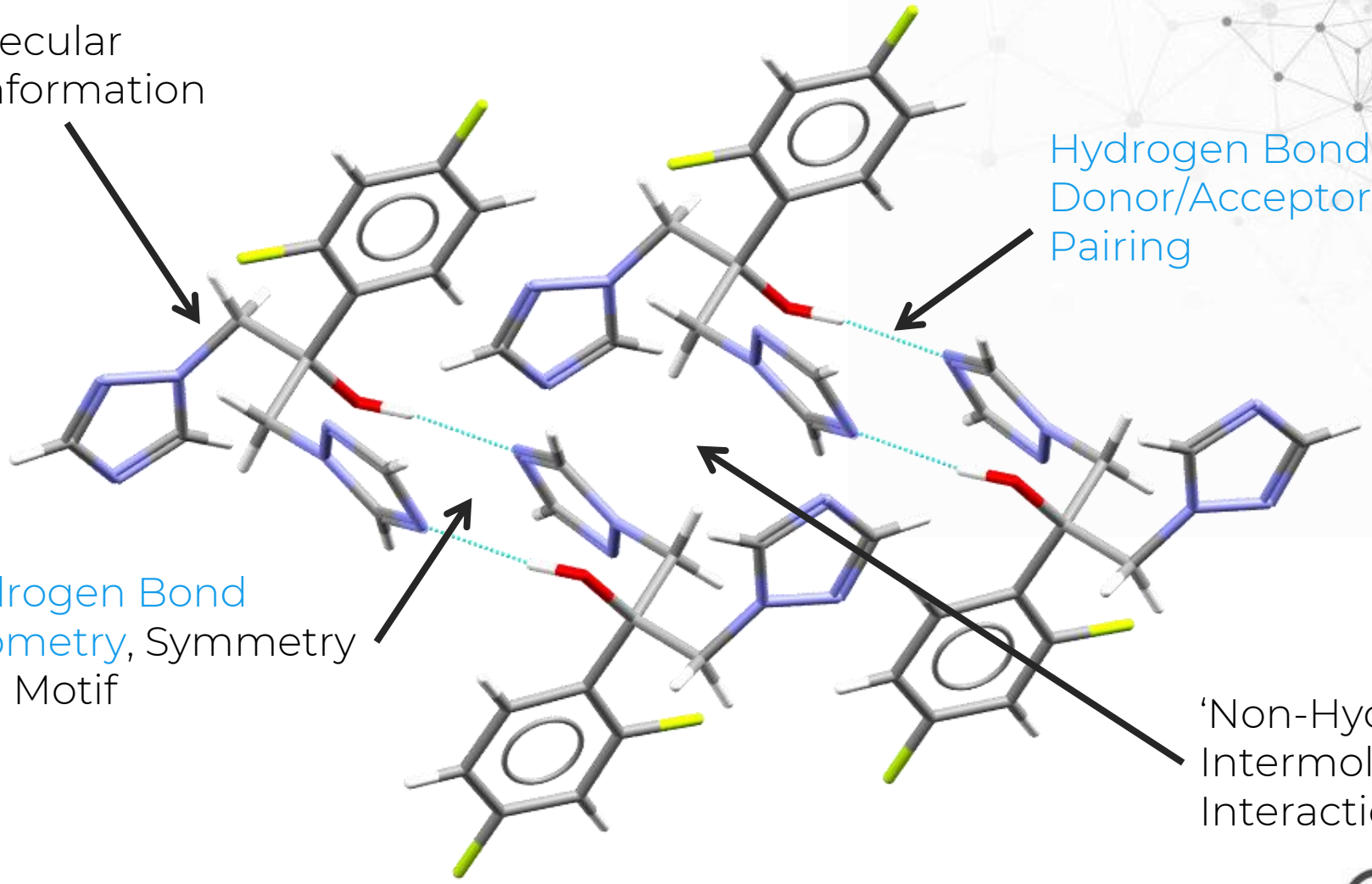
Characteristics that influence stability



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Hydrogen bonds

- Common in organic crystal structures and known for around a century.
  - What defines a hydrogen bond?
  - Where is the dividing line between hydrogen bond and van der Waals contact?

- How can the CSD be used?
  - Theoretical calculations tend to correlate very well with experimental database statistics and this is true in particular for interactions.
  - Exploring hydrogen bond energies – hydrogen bond energies are more sensitive to *angle than distance*.
  - To help us understand how changes in hydrogen bond networks impact the properties of a crystal.
  - If analysing a structure for hydrogen bonds using Mercury we can endeavour to "*look for them and to look at them*".

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What are they and why are they important?

- Primarily an electrostatic force interaction
  - Between an electronegative donor attached to a H-atom and an electronegative acceptor with a lone pair of electrons.
- Somewhat stronger than a van der Waals interaction, and weaker than fully covalent or ionic bonds.
- Found in many substances including water, DNA, proteins and wool.
- Key to the design of drugs:
  - Lipinski's rule of five – states that orally active drugs in general have no more than one violation of a number of criteria including:
    - No more 5 hydrogen bond donors
    - No more than 10 hydrogen bond acceptors

Definition of the hydrogen bond (IUPAC Recommendations 2011), *Pure Appl. Chem.*, 83, 8, 1637–1641, 2011

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What do we mean by a hydrogen bond?

- A hydrogen bond is described as *D*-*H*···*A*, where:
  - *D* = donor, *H* = hydrogen and *A* = acceptor.
- Our default definition of a hydrogen bond:
  - *D* must be a nitrogen, oxygen or sulphur covalently bound to ≥ one hydrogen.
    - Note: H-bonds will still be found even if the 3D coords for the *H* were not determined.
  - A must be a nitrogen, oxygen, sulphur or halogen with at least one lone pair.
    - e.g. pyramidal trigonal nitrogen is regarded as an acceptor but planar trigonal nitrogen is not.
  - *D*···*A* distance must be less than the sum of van der Waals Radii of the *D* and *A* atoms
  - The contact may be intermolecular, or intramolecular involving donor and acceptor atoms separated by at least 3 covalent bonds within the molecule.

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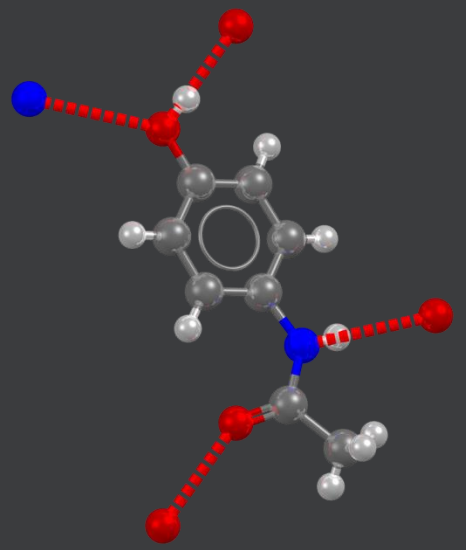
Visualising hydrogen bonds



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

Tick ‘Require hydrogen atom to be present’

HXACAN (Pcab) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle 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

HXACAN

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+ R

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

Default | Cancel | Apply | OK

Display Options

Display

Packing | Asymmetric Unit | Auto centre | Reset

Short Contact < (sum of vdW radii)

H-Bond Default definition

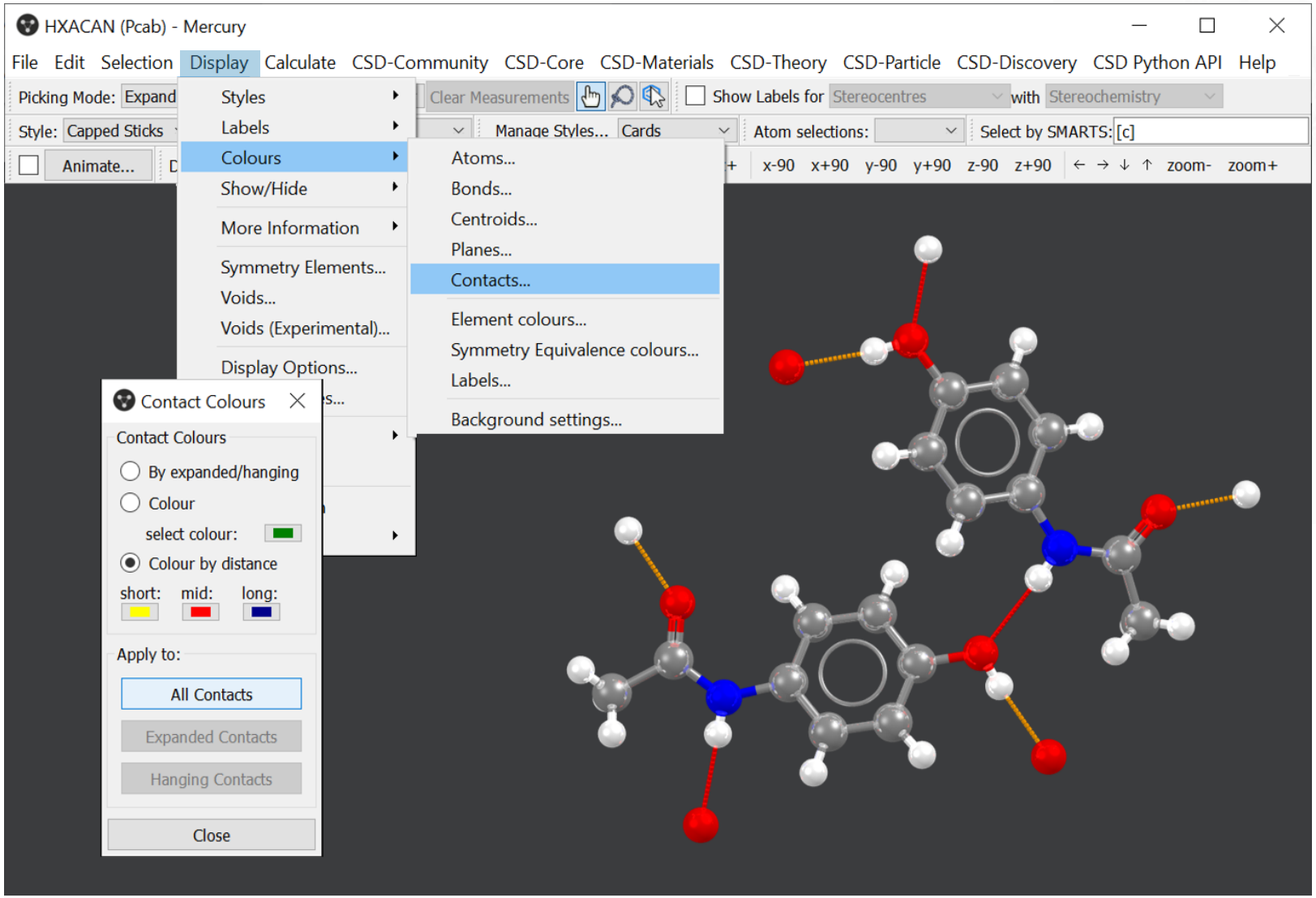
Contacts... | More Info | Powder...

Options

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

Click on a red contact to see the whole molecule

Colouring hydrogen bonds by distance



Display
> Colours > Contacts
> Colour by distance

CSD Refcode:
HXACAN

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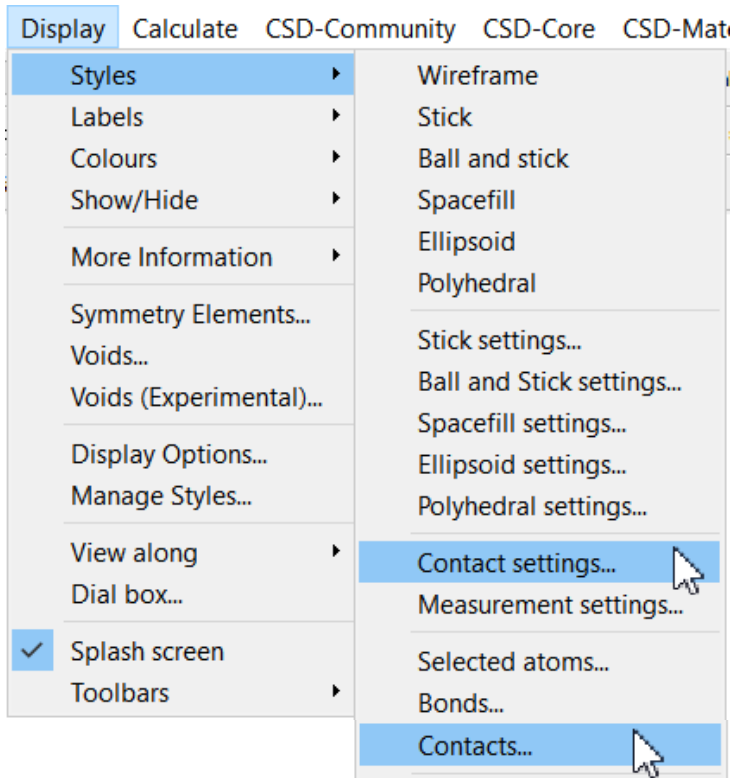
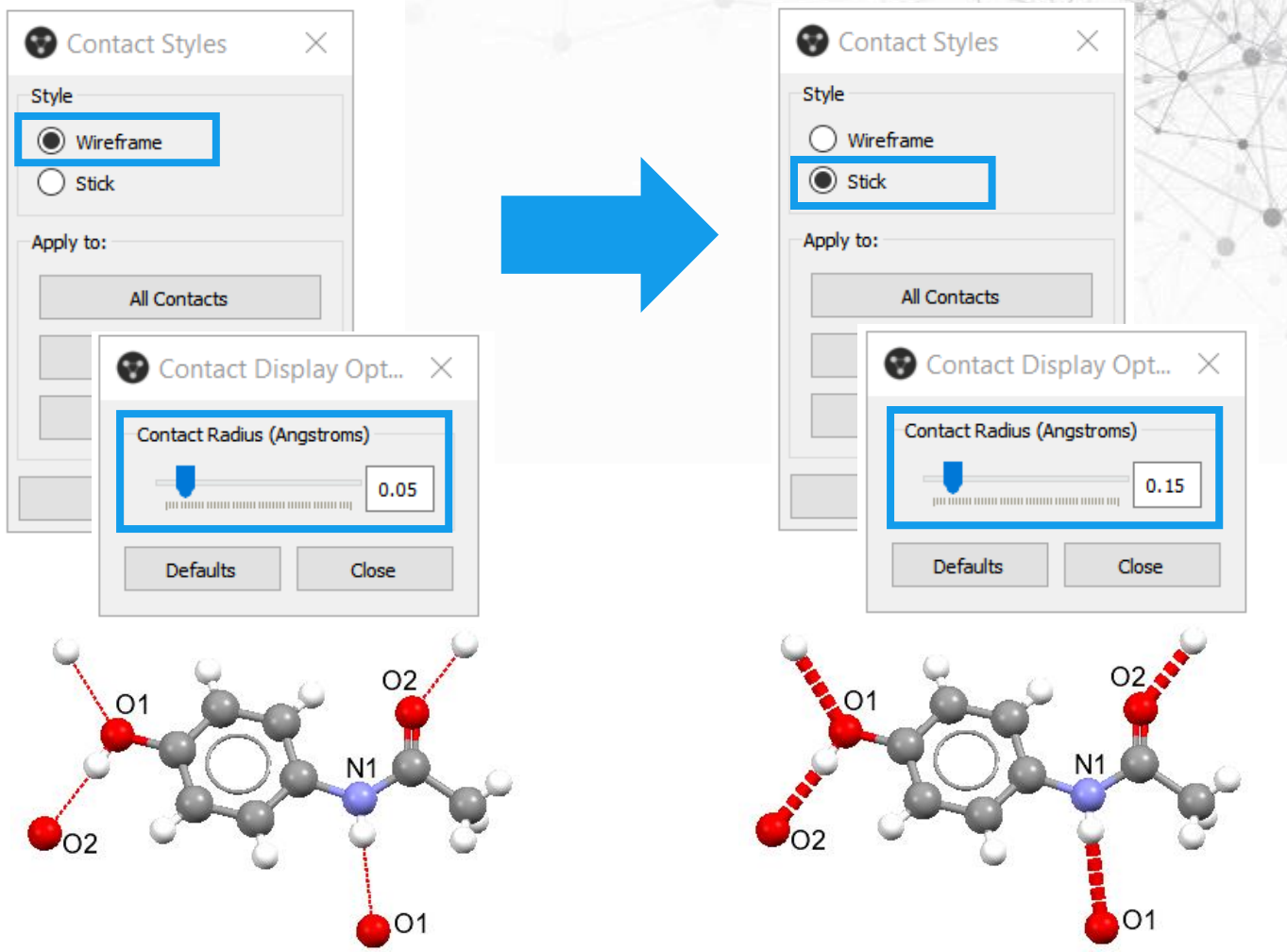
Hydrogen bond style

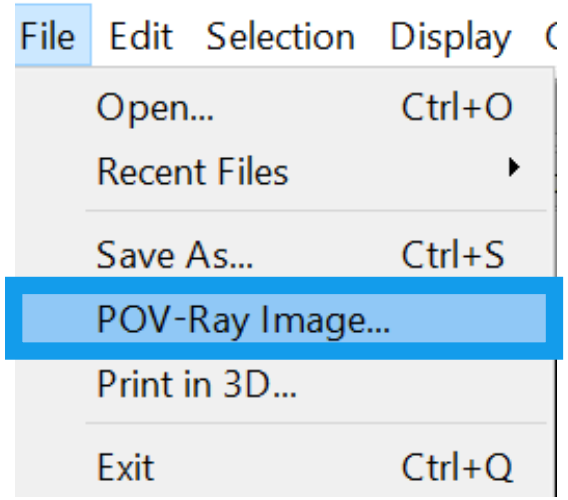
Display > Styles > Contacts
Display > Styles > Contact settings

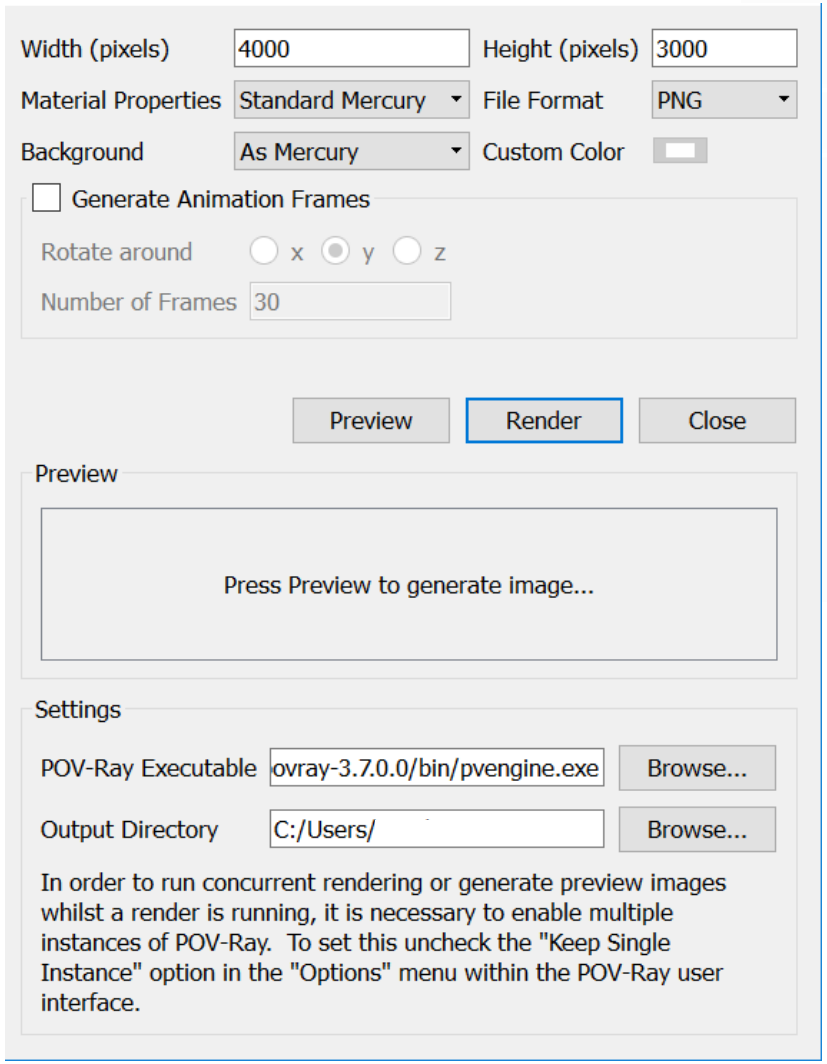
- Change contact style to stick (from default wireframe)
- Change radius of stick to vary thickness / number of segments





More style options via POV-Ray….





File > POV-Ray Image

- Resolution (W x H)
- Material Properties
- Background
- Output directory

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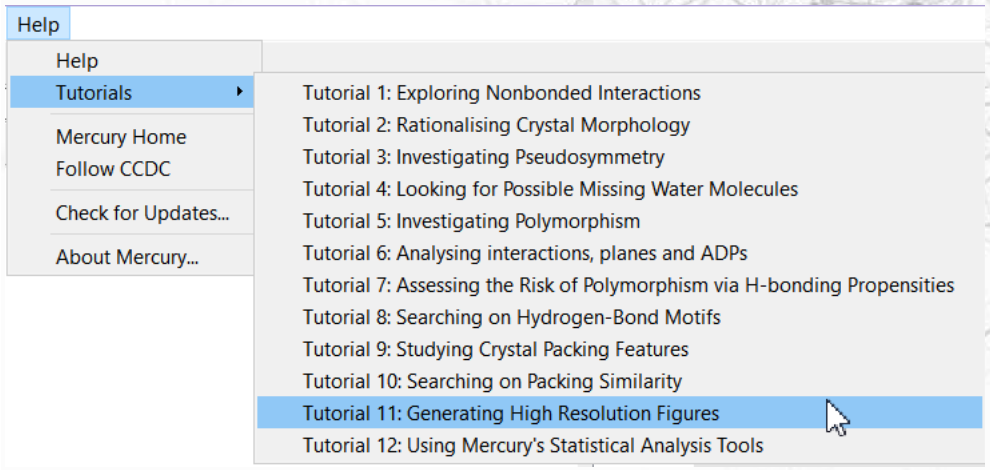
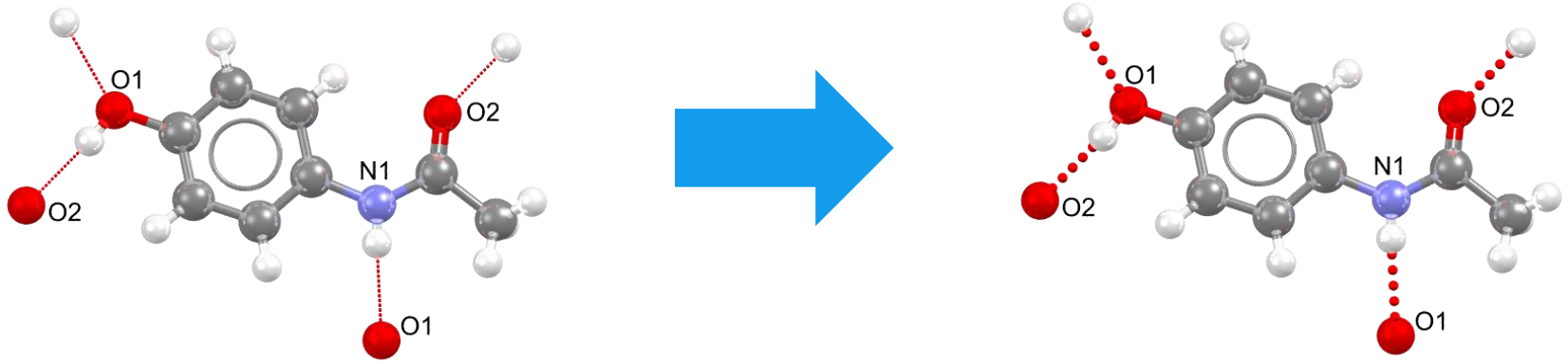
Changing hydrogen bond style in POV-Ray

- Tutorial 11 in Mercury
- ccdc_macro_overrides.inc file
  - Created when a POV-Ray image is saved
  - Controls style for images
- Open and edit in a text editor
- Save POV-Ray image from Mercury into directory containing your ccdc_macro_overrides.inc file





Example in turorial11.inc file to change H-bond display type

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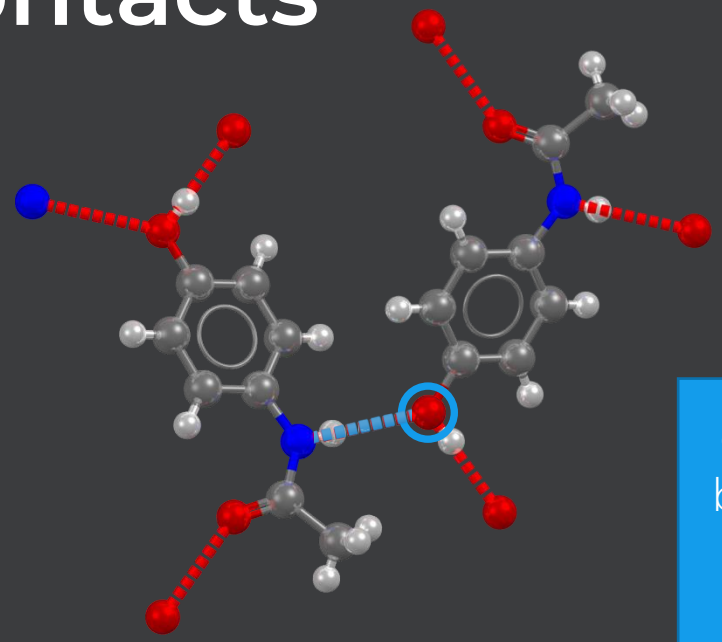
Expand contacts



Select ‘Expand Contacts’ picking mode then left click on atoms at end of dashed lines (hanging contacts) to expand network

Colour changes to blue for connected (non-hanging) hydrogen bonds

Right click on a molecule or hanging contact to see more advanced options including delete hanging contacts or expand contacts

HXACAN (Pcab) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle 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

HXACAN

Selection
Styles
Colours
Labels
Show/Hide
Contacts
Delete this Molecule

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
Reset

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

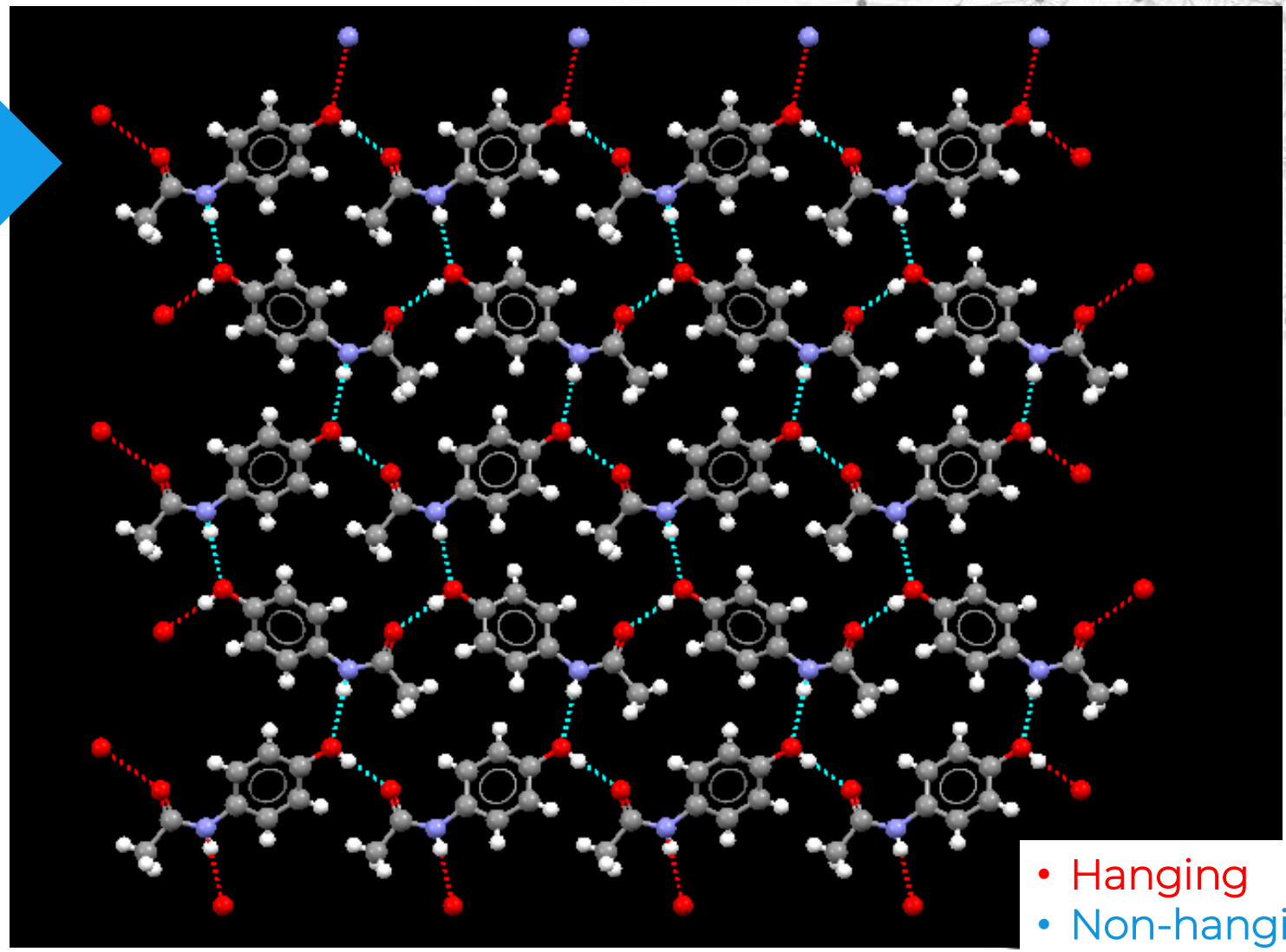
Contacts...
More Info
Powder...

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

Click on a red contact to see the whole molecule

Building a hydrogen bonded network

By clicking on atoms at the end of dashed lines



To expand all hanging contacts:

- Right click on a hanging contact > Expand All

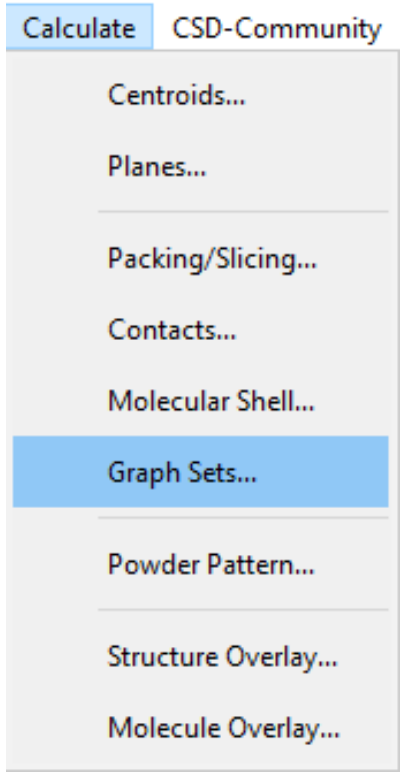
To expand hanging contacts for a specific molecule:

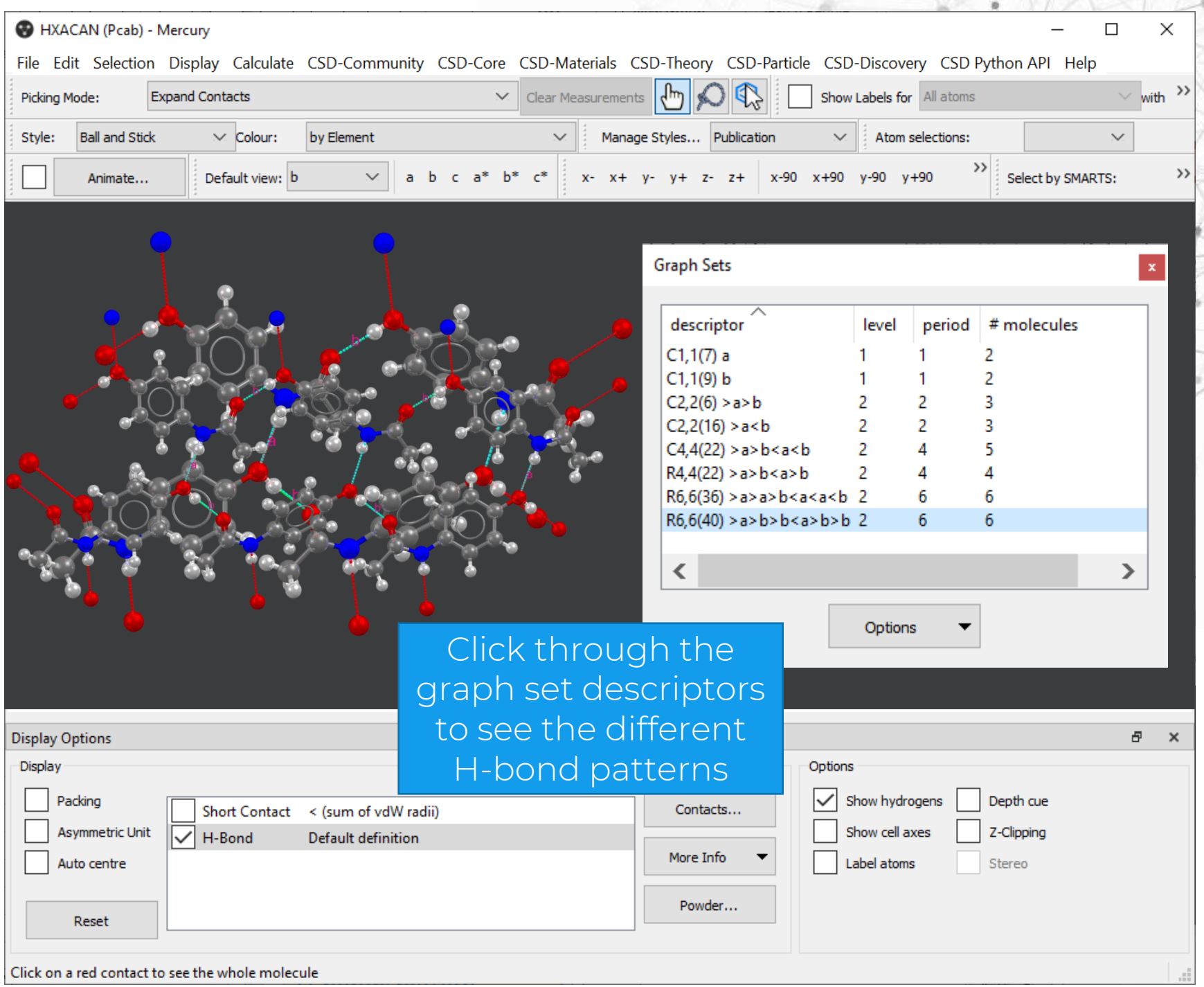
- Right click on a molecule > Contacts > Expand Contacts from this Molecule

- Hanging
- Non-hanging

CSD Refcode: HXACAN

Graph Sets





Click through the graph set descriptors to see the different H-bond patterns

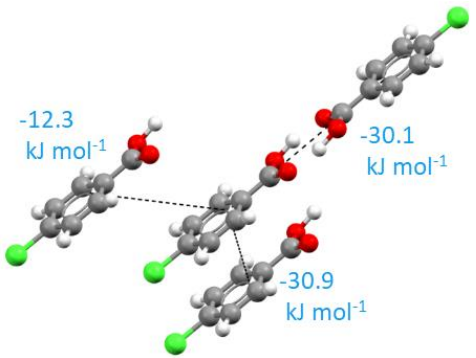
Graph Sets describe the H-bond pattern

Learn more in the *Glossary* on the handout

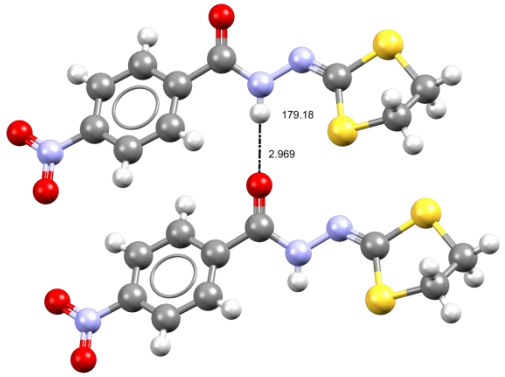
Hydrogen Bond Statistics

- Automatic statistical assessment of geometry of hydrogen bonding intermolecular interactions in context of > 1.1 million structures in CSD
- Determine whether any given hydrogen bond interaction is unusual or not unusual – hydrogen bond geometry can influence stability
- Provides a check when analysing newly solved crystal structures

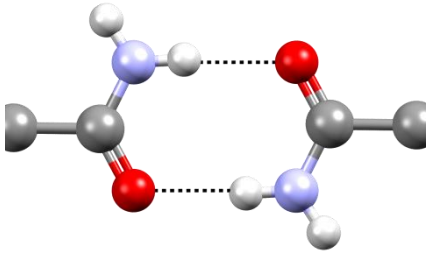
Energy



Geometry



Frequency of occurrence

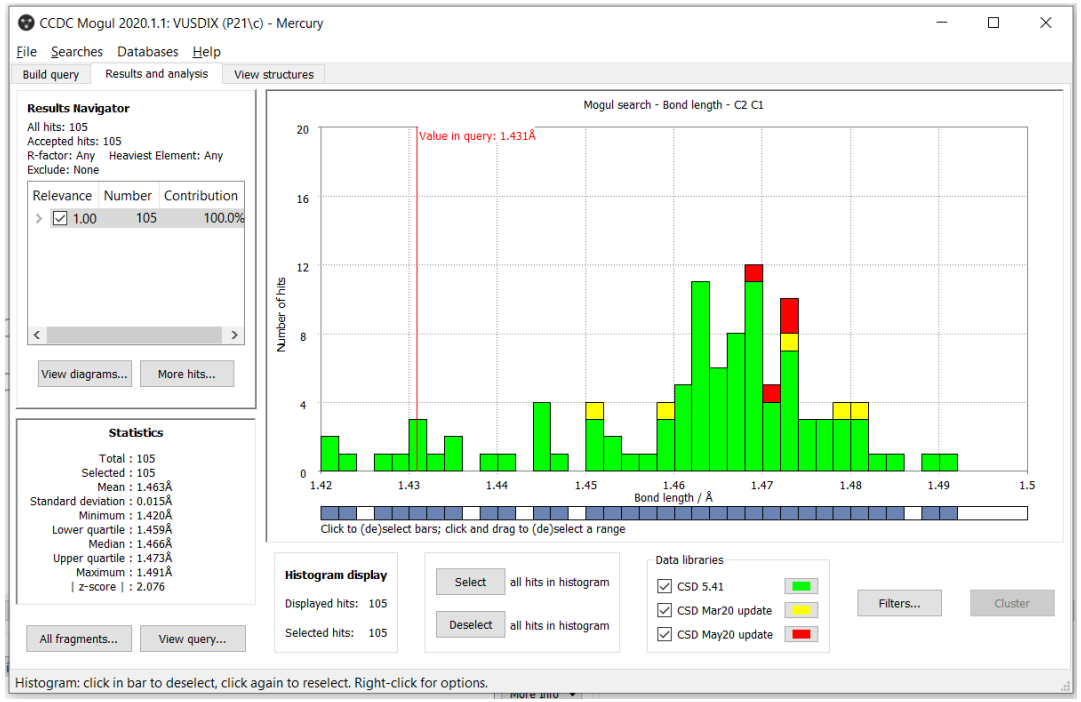


40.2%

Similar to Mogul geometry analysis

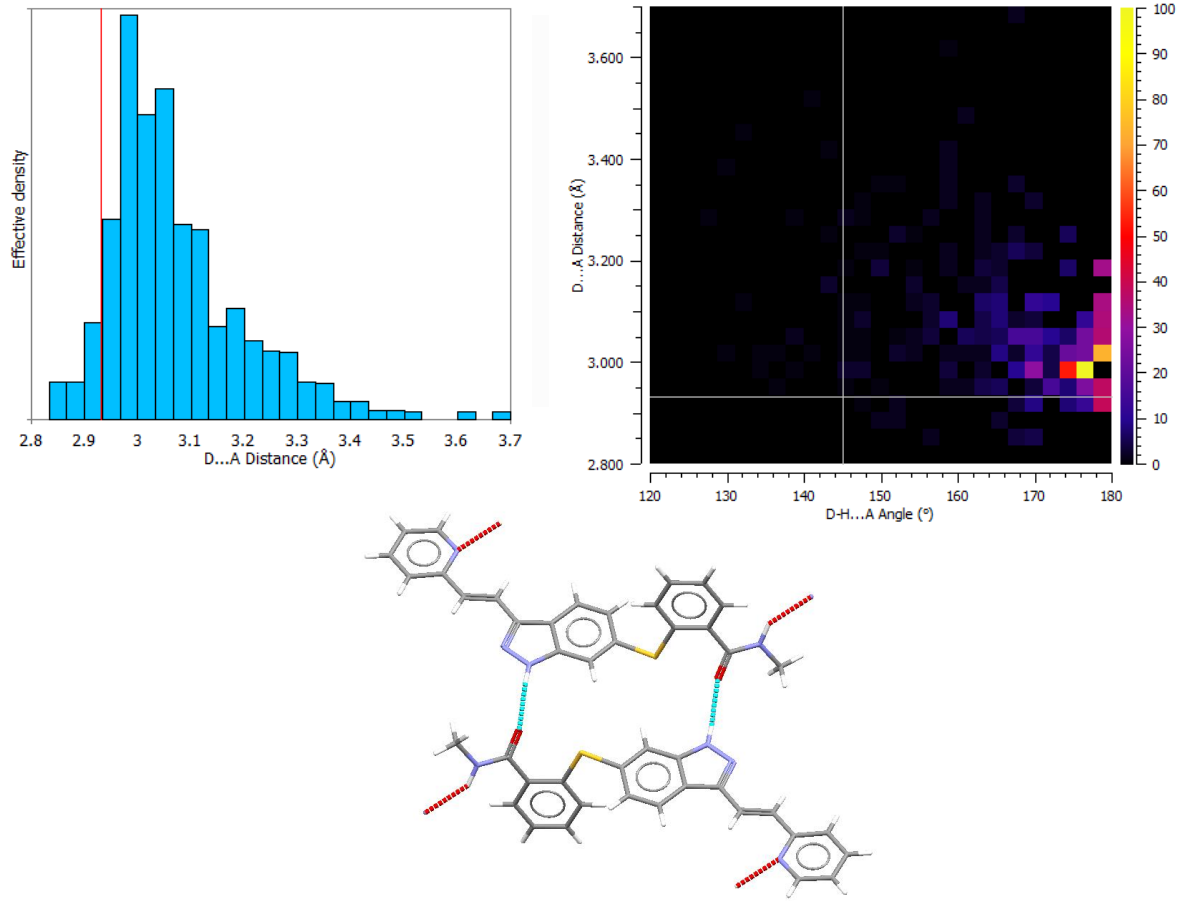
Intramolecular geometry (Mogul):

- Bond lengths, Valence angles, Torsion angles



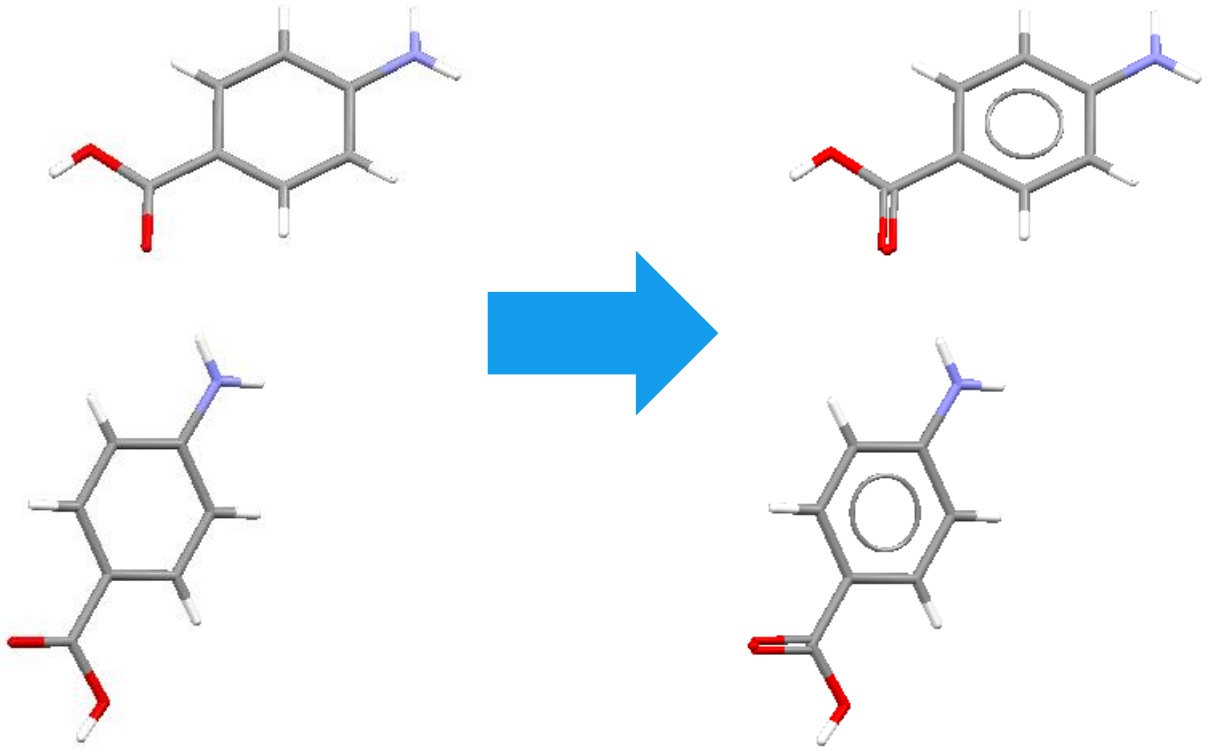
Intermolecular geometry (HBondStats):

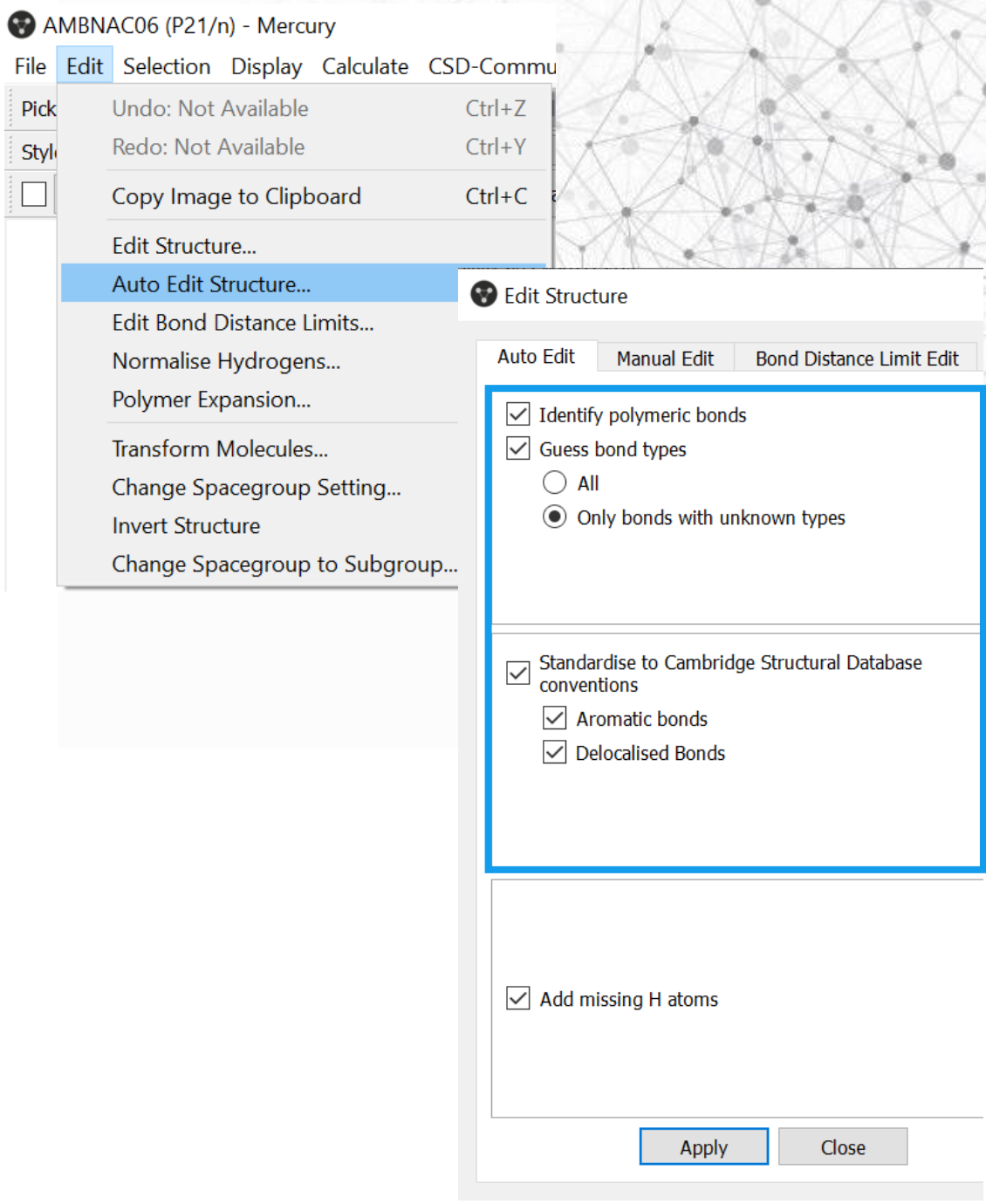
- Hydrogen bond D···A distance, DHA angle



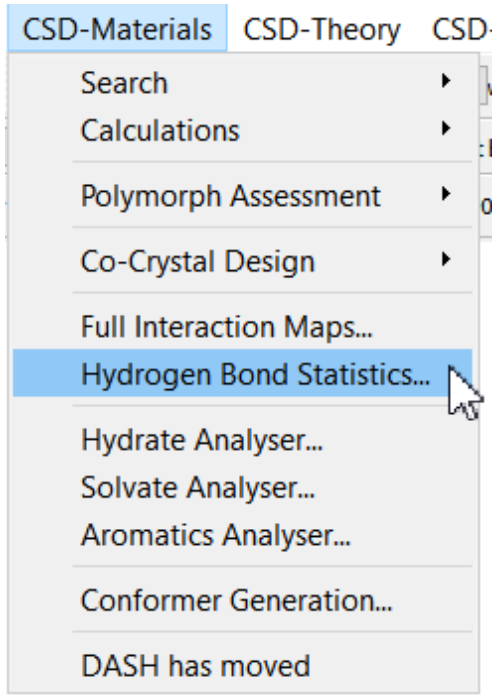
Input

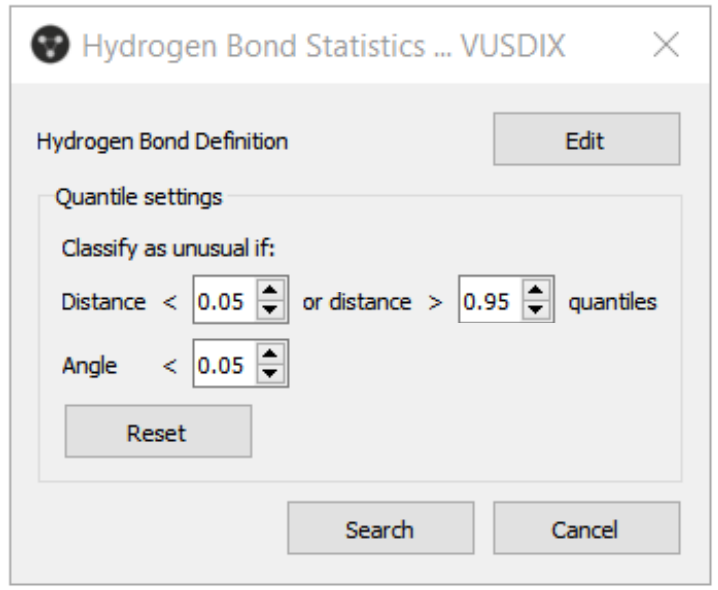
- Uses a crystal structure loaded into Mercury visualizer (e.g. Refcode, cif, mol2)
- For a cif, ensure bond tying is applied





Unusual vs. Not unusual



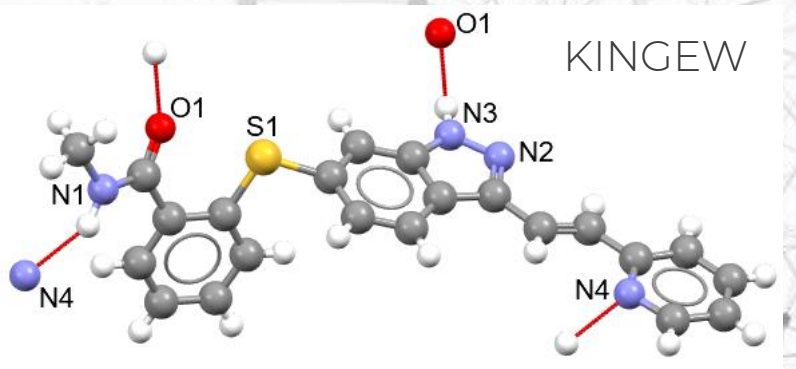


Classification of whether specific hydrogen bond distance or angle is unusual based on quantiles

Unusual if below 5 % of distribution and / or above 95 % (i.e. 5th and 95th percentiles)

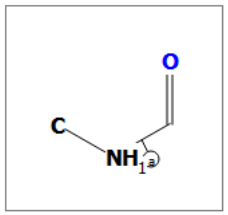
Upper angle quantile removed in next CSD release (end 2022) – so no H-bond angle classed as unusual due to an upper bound

Interactions and statistics



Hydrogen Bond Statistics ... KINGEW

	Donor	Acceptor	Distance D-A	Distance classification	Distance threshold	Distance hits	Distance mean	Distance std. dev.	Distance min.	Distance max.	Angle D-H...A	Angle classification	Angle threshold	Angle hits	Angle mean	Angle std. dev.	Angle min.	Angle max.
1	N1 (amide_carbonyl)	N4 (ar_N_2)	2.93	Not Unusual	(2.93, 3.33)	218	3.08	0.13	2.86	3.67	**145.18**	Unusual	(146.51, 179.23)	218	170.81	10.70	127.88	179.49
2	N3 (pyrazoline_1)	O1 (amide_carbonyl)	2.83	Not Unusual	(2.73, 2.93)	45	2.83	0.14	2.71	3.54	162.92	Not Unusual	(147.16, 179.32)	45	169.10	11.24	132.25	179.32



Export...

Table can be exported as CSV file using **Export** button

Hover to view donor and acceptor functional groups

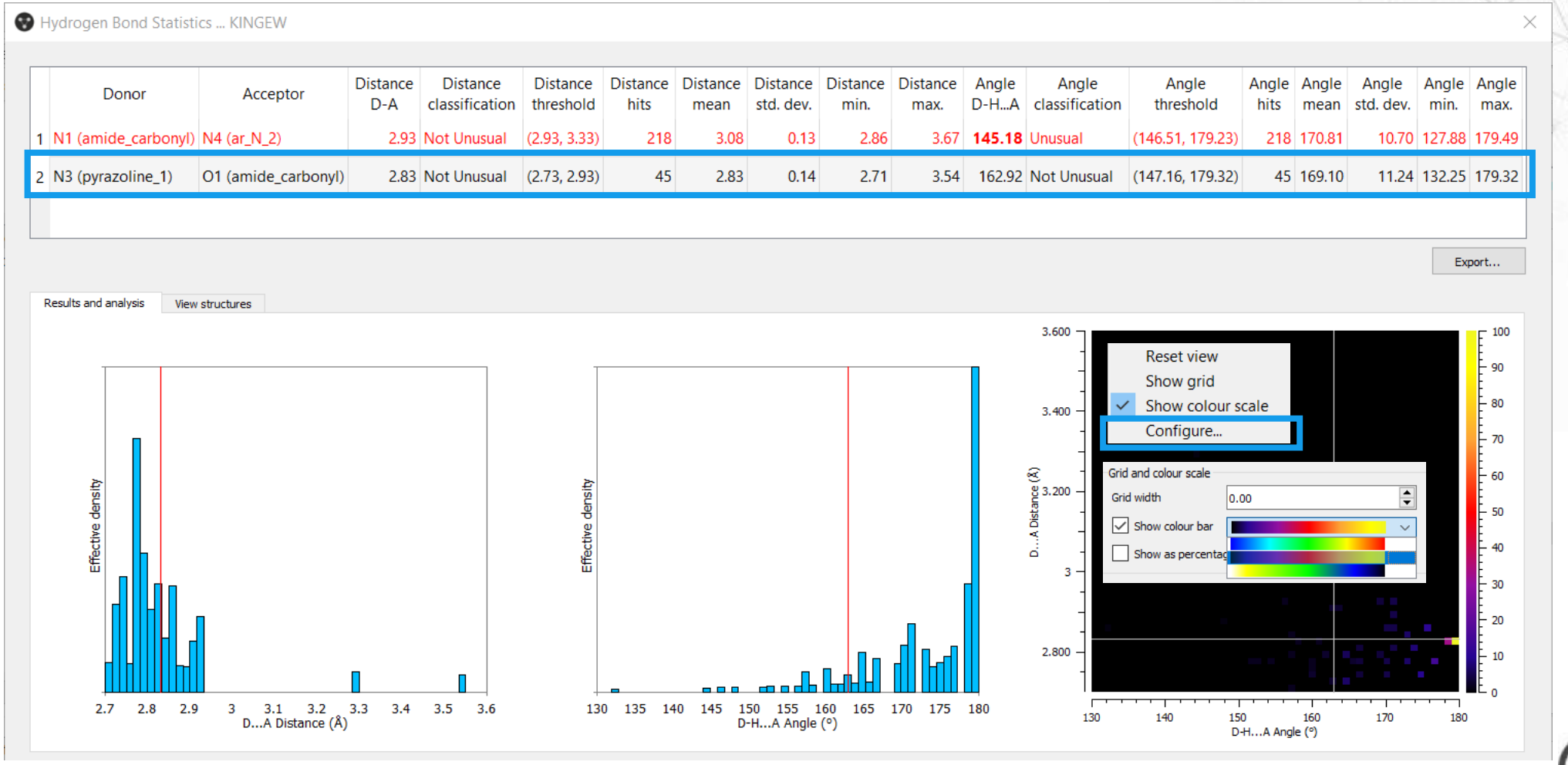
Classification as Not Unusual / Unusual (value outside quantile threshold)

Check enough # hits for confidence in classification

- Row highlighted in red if Distance and / or Angle classed as *Unusual*
- Row in black if both Distance and Angle are *Not Unusual*

Uses Hydrogen Bond Propensity functional group definitions to automatically identify donor/acceptor fragments

Histograms and heat map



Click on row to view histograms, heat map and highlight interaction in 3D viewer of Mercury

Right click in heat plot for extra display options/colours

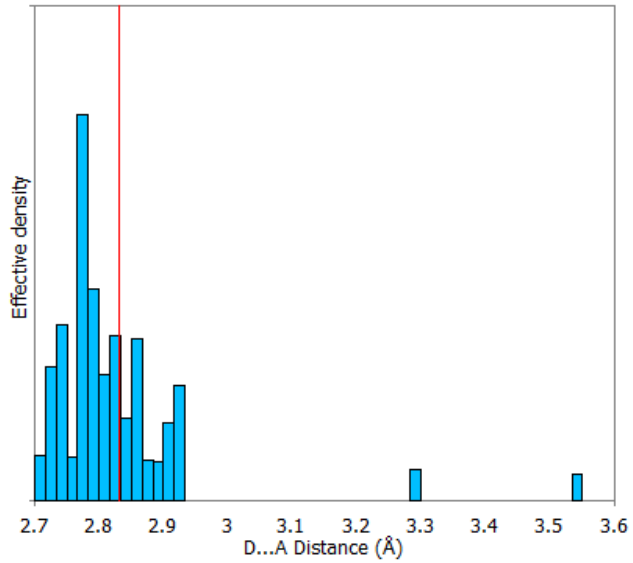
CCDC

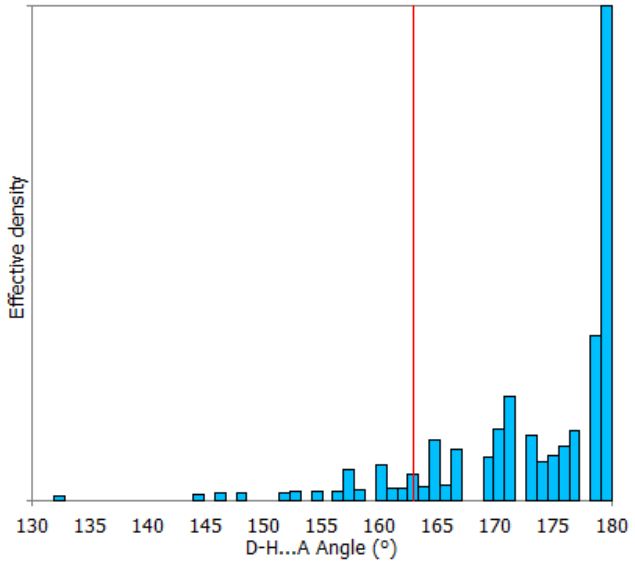
Cone and radial correction

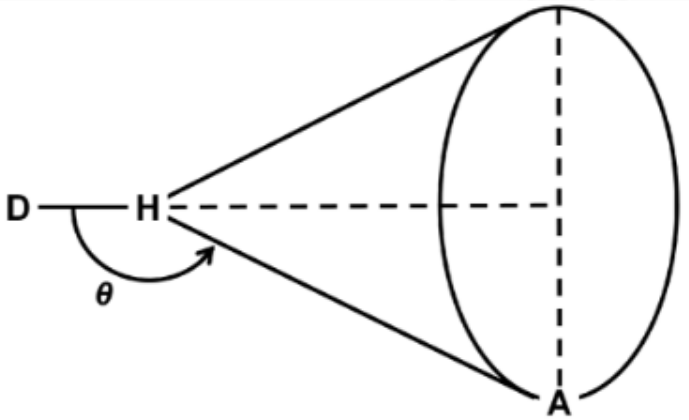
Distribution inherently biased away from 180°

- More linear contacts statistically less likely than bent ones – as θ deviates from linearity, acceptor group sweeps out possible cone of approach that gets progressively larger as angle decreases
- Data corrected (normalised) for this → effective density on *y* axis rather than frequency

Leads to 'Effective Density' on *y* axis for Distance & Angle plots



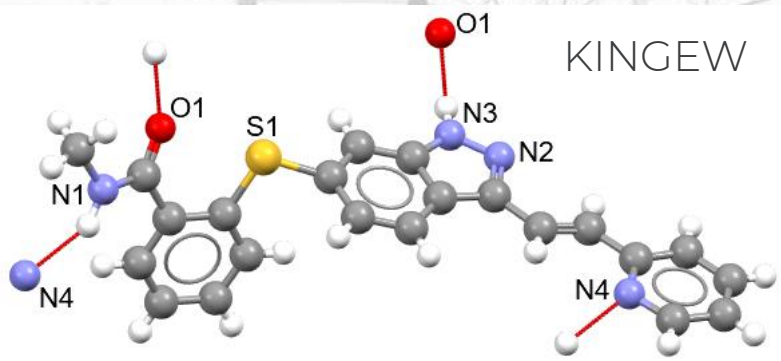




For more information, see: P. A. Wood, F. H. Allen and E. Pidcock, *CrystEngComm*, 2009, **11** 1563-1571

CCDC

Highlighting unusual



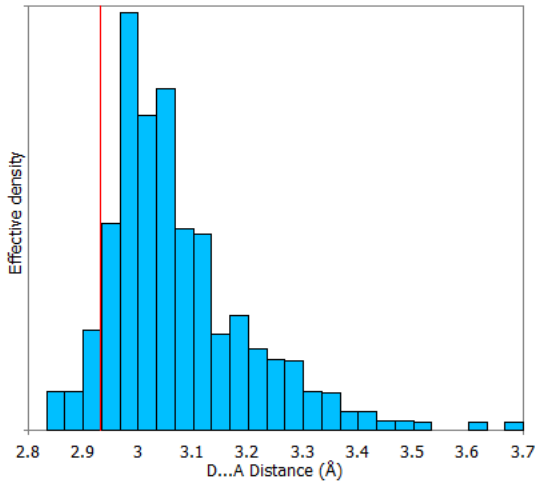
Unusual angle

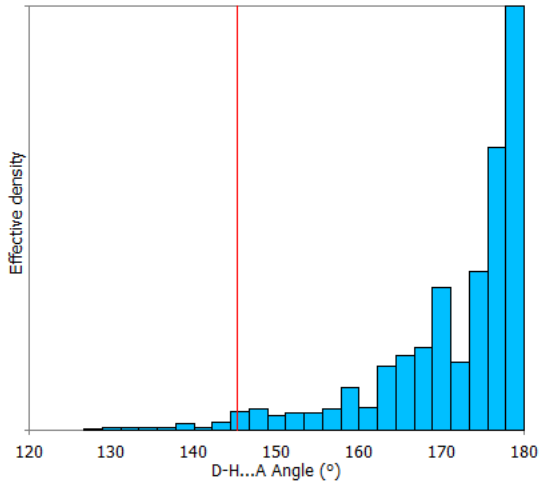
Hydrogen Bond Statistics ... KINGEW

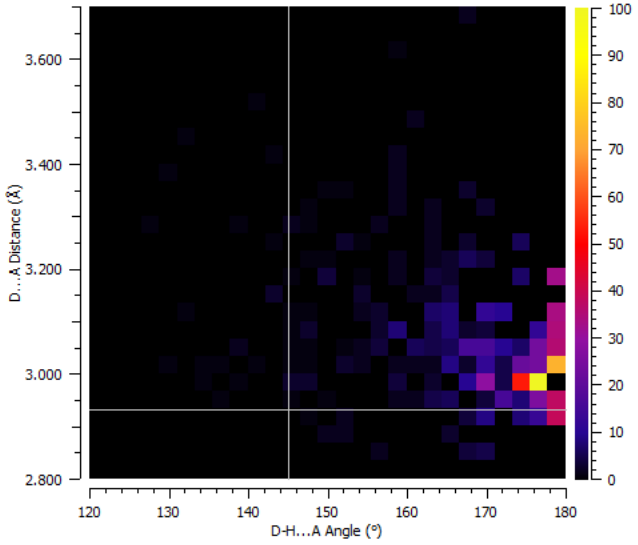
	Donor	Acceptor	Distance D-A	Distance classification	Distance threshold	Distance hits	Distance mean	Distance std. dev.	Distance min.	Distance max.	Angle D-H...A	Angle classification	Angle threshold	Angle hits	Angle mean	Angle std. dev.	Angle min.	Angle max.
1	N1 (amide_carbonyl)	N4 (ar_N_2)	2.93	Not Unusual	(2.93, 3.33)	218	3.08	0.13	2.86	3.67	**145.18**	Unusual	(146.51, 179.23)	218	170.81	10.70	127.88	179.49
2	N3 (pyrazoline_1)	O1 (amide_carbonyl)	2.83	Not Unusual	(2.73, 2.93)	45	2.83	0.14	2.71	3.54	162.92	Not Unusual	(147.16, 179.32)	45	169.10	11.24	132.25	179.32

Export...

Results and analysis | View structures



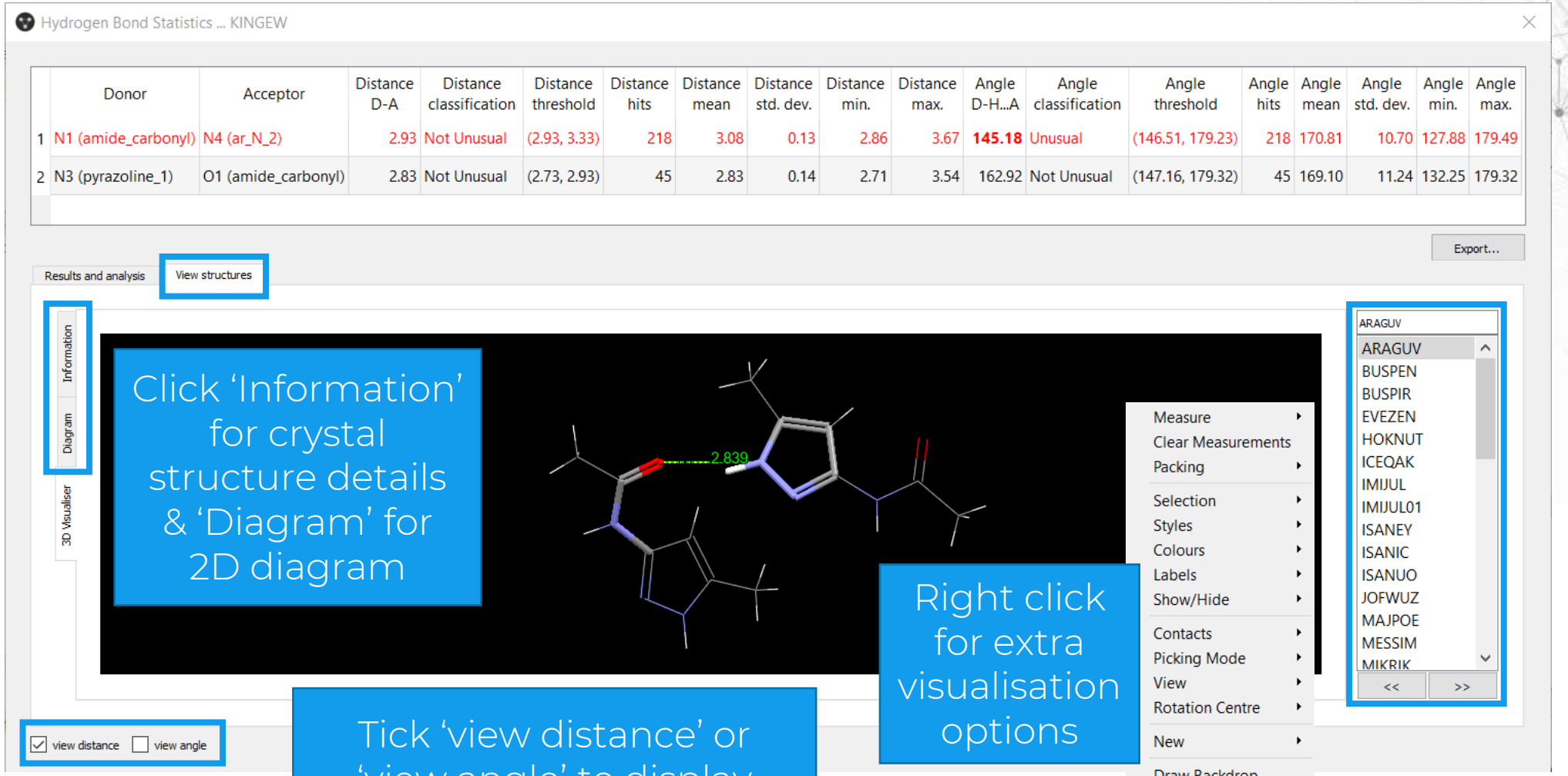




Click View Structures to see the hits

CCDC

Viewing hits



Click 'Information' for crystal structure details & 'Diagram' for 2D diagram

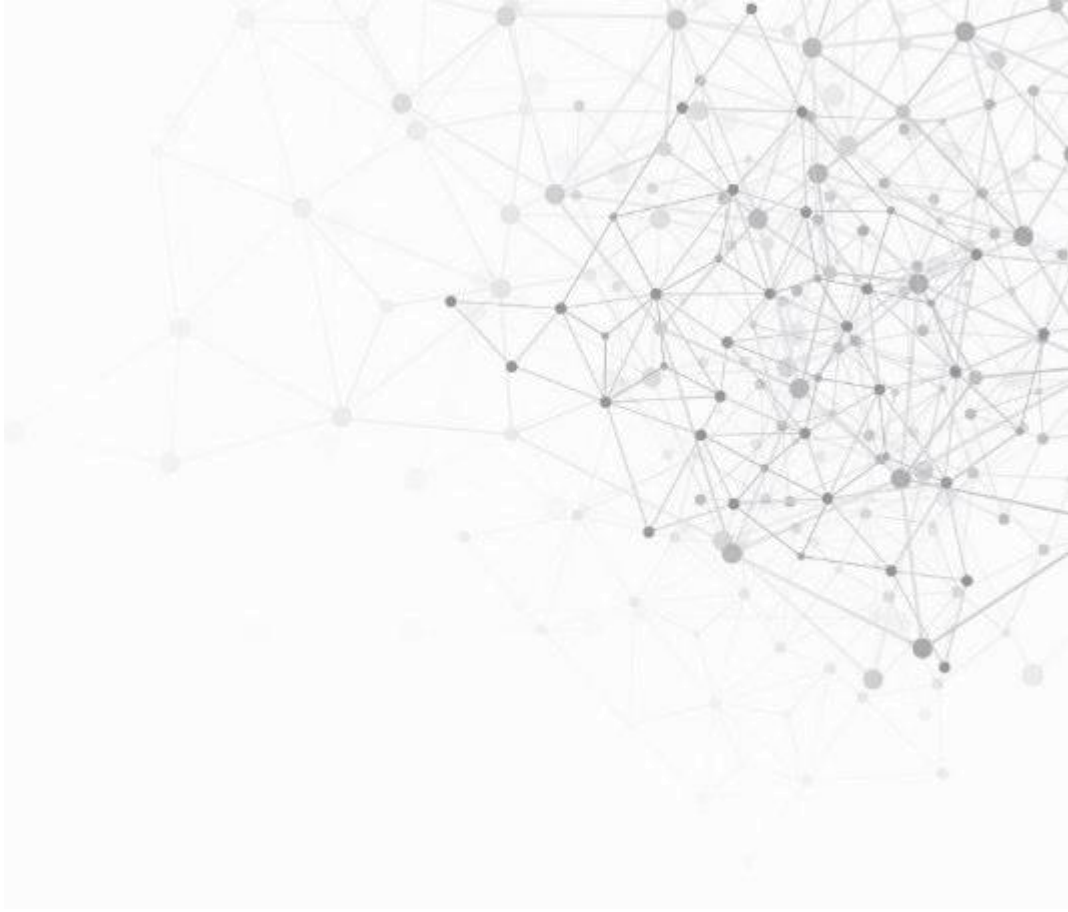
Right click for extra visualisation options

Click through the hits to visualise the structures

Tick 'view distance' or 'view angle' to display relevant values for the hits

CCDC

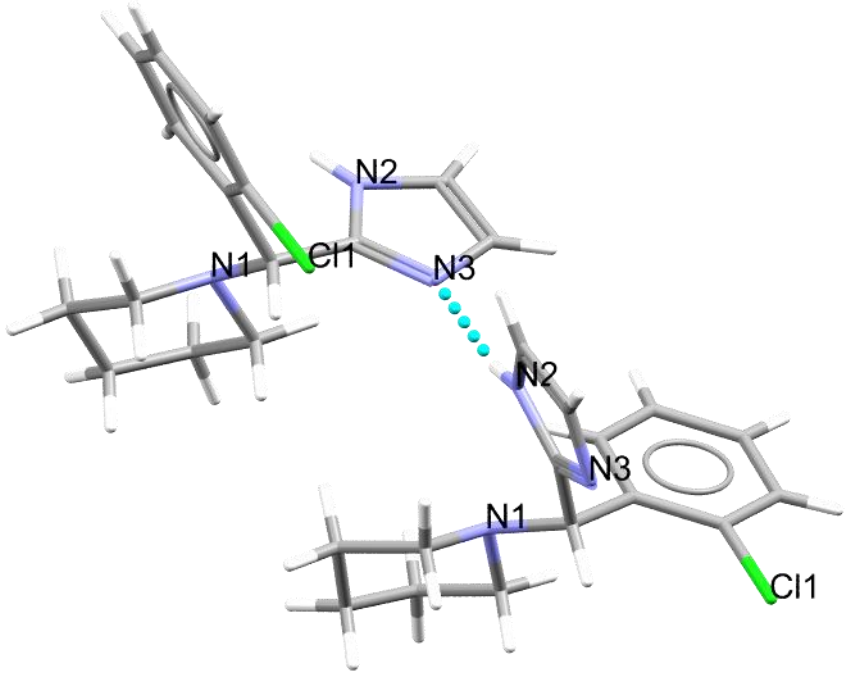
Examples

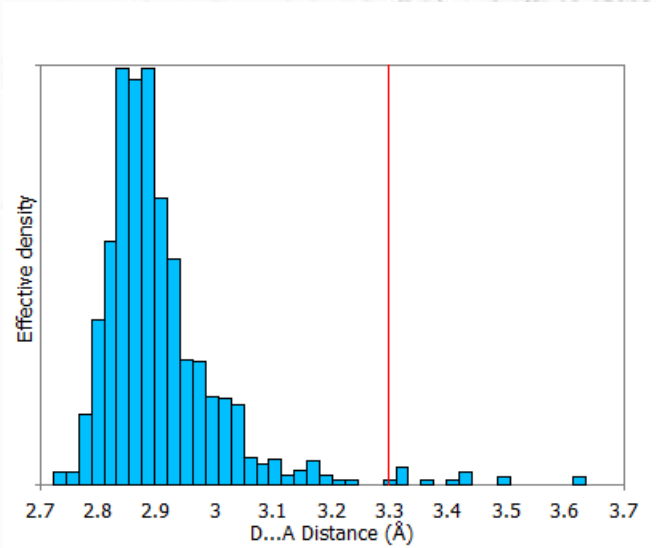


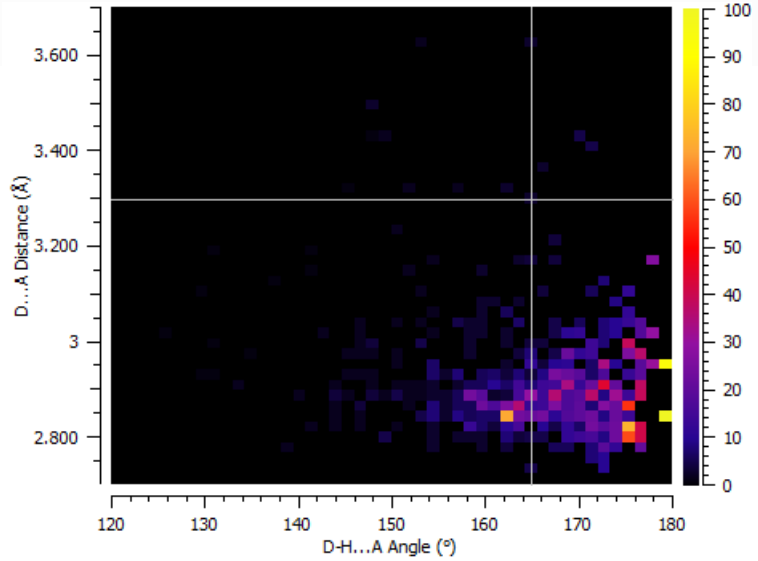
A long hydrogen bond

Donor	Acceptor	Distance D-A	Distance classification	Distance threshold	Angle D-H...A	Angle classification
N2 (imidazole_1)	N3 (imidazole_1)	**3.30**	Unusual	(2.82, 3.11)	165.07	Not Unusual

AQINAQ

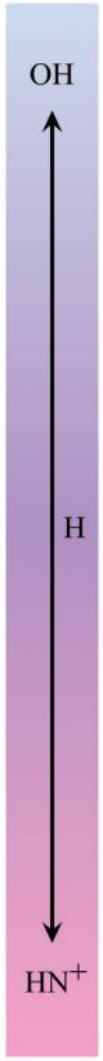




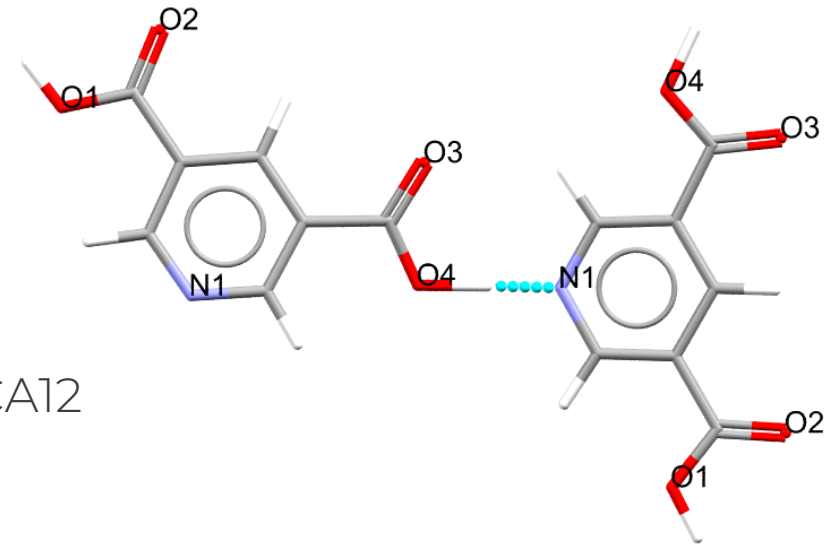


- Angle within usual range, long DA distance for type of interaction

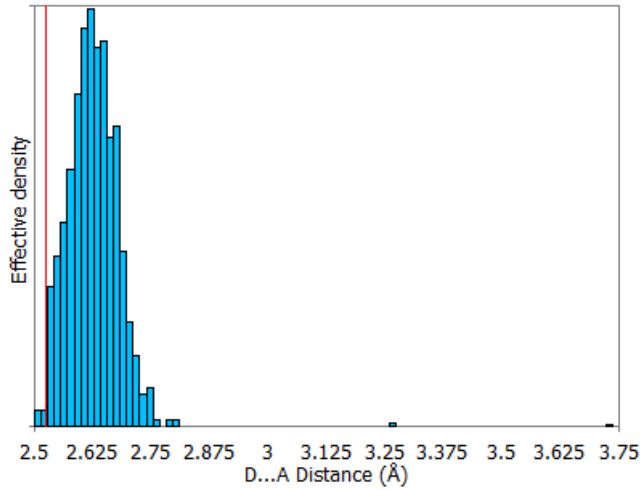
Salt-cocrystal continuum (SSHBs)

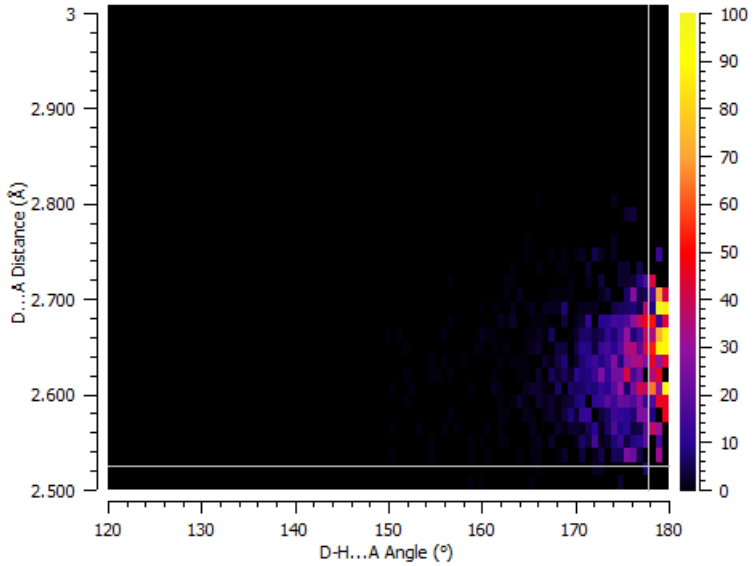


Donor	Acceptor	Distance D-A	Distance classification	Distance threshold	Angle D-H...A	Angle classification
O4 (ar_cooh_1)	N1 (aromatic_nitrogen)	**2.53**	Unusual	(2.54, 2.72)	177.82	Not Unusual



DINICA12





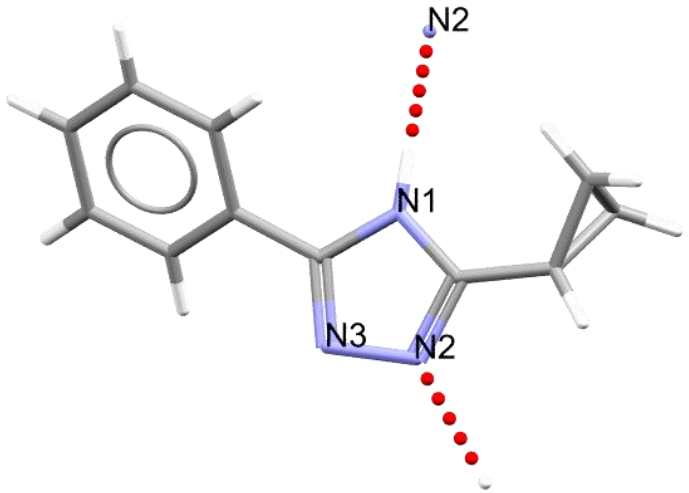
Distance flagged as unusual

- Very short strong H-bond O4···N1, rare case with H located close to middle of donor and acceptor (e.g. centre of salt-cocrystal continuum)

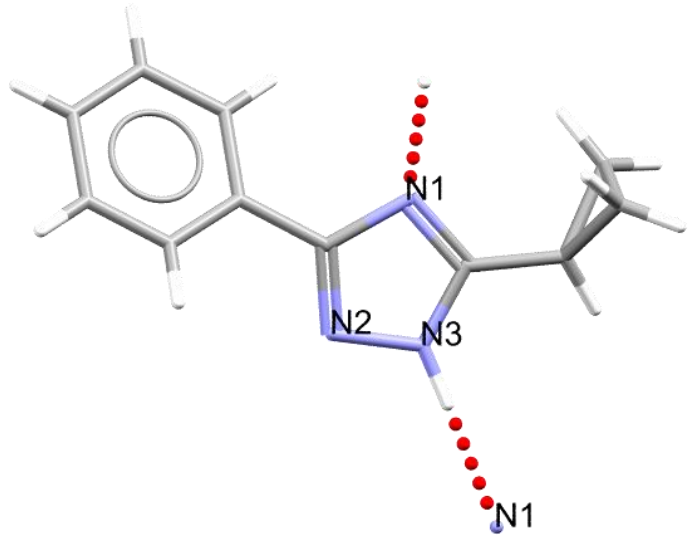
Tautomers

- Automatic recognition of specific functional groups allows easy comparison of statistics for different tautomeric forms
- No need to sketch in ConQuest & set up distance/angle query

JUGYOB



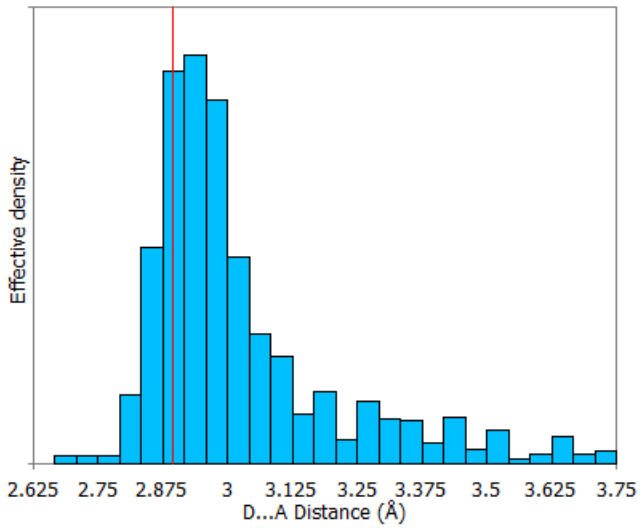
JUGYOB01

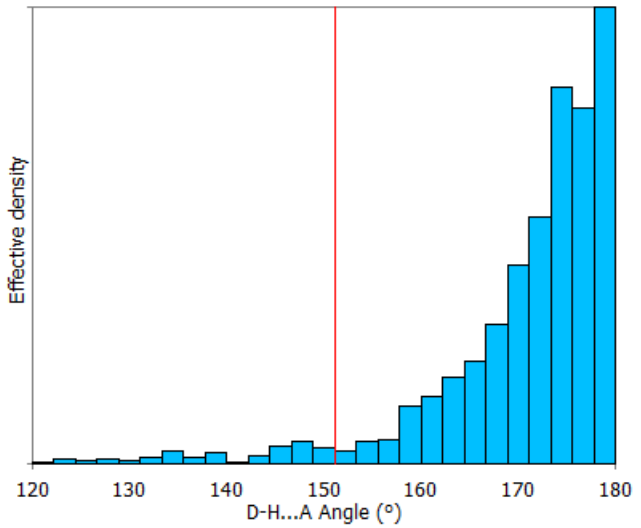


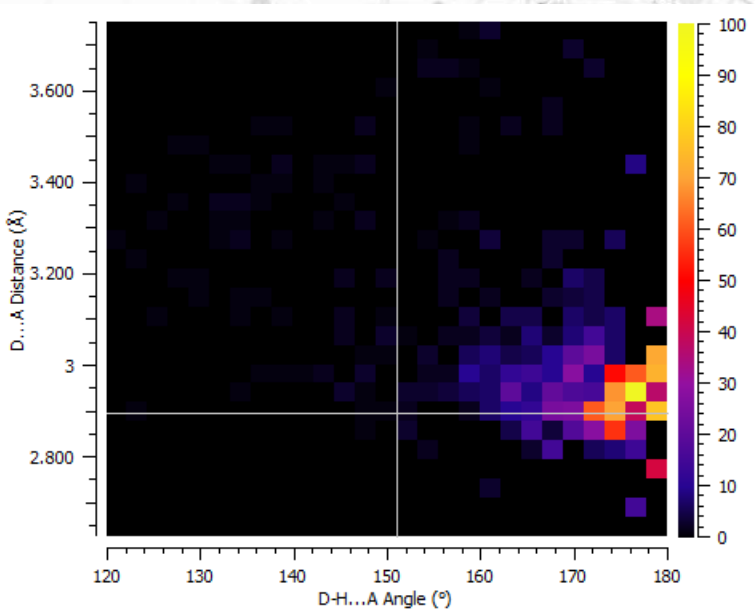
Donor	Acceptor	Distance D-A	Distance classification	Distance threshold	Distance hits	Distance mean	Distance std. dev.	Distance min.	Distance max.	Angle D-H...A	Angle classification	Angle threshold	Angle hits	Angle mean	Angle std. dev.	Angle min.	Angle max.
N1 (sec_amine_pl)	N2 (cyclic_NsingleN)	2.89	Not Unusual	(2.83, 3.43)	362	3.03	0.19	2.70	3.74	151.17	Not Unusual	(143.14, 179.24)	362	169.85	11.55	121.44	179.60
N3 (cyclic_nhn)	N1 (cyclic_n)	2.89	Not Unusual	(2.72, 3.08)	180	2.88	0.11	2.60	3.48	178.65	Not Unusual	(137.96, 179.55)	180	167.73	12.89	120.20	179.55

CCDC

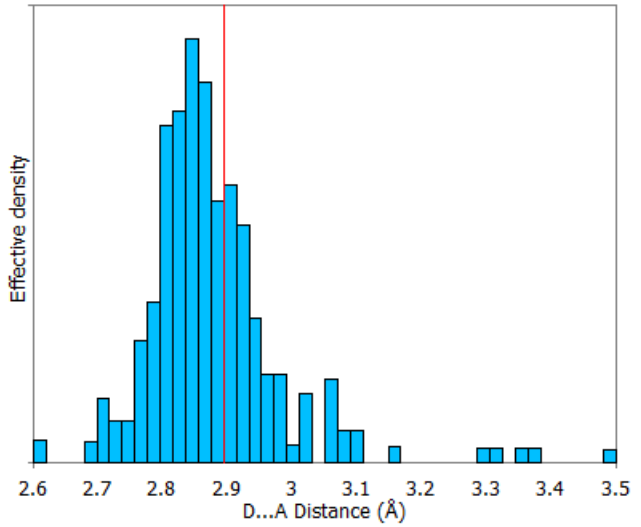
JUGYOB – tautomer #1

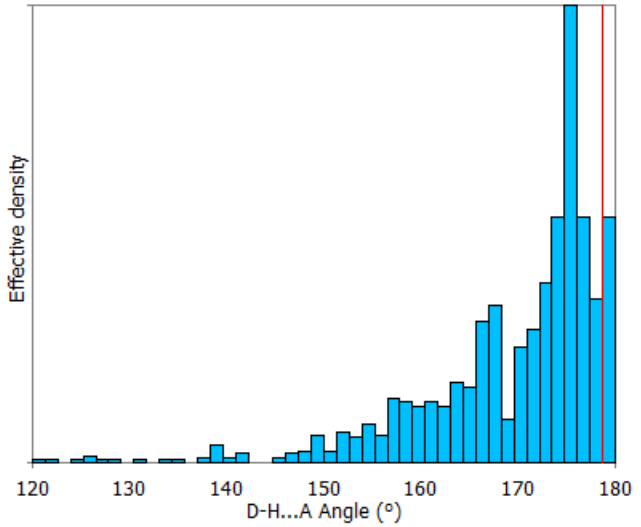


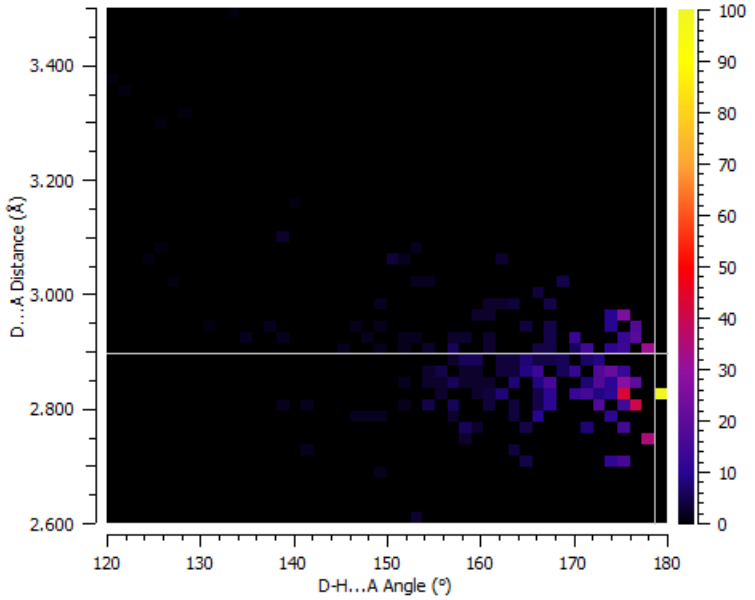




JUGYOB01 – tautomer #2

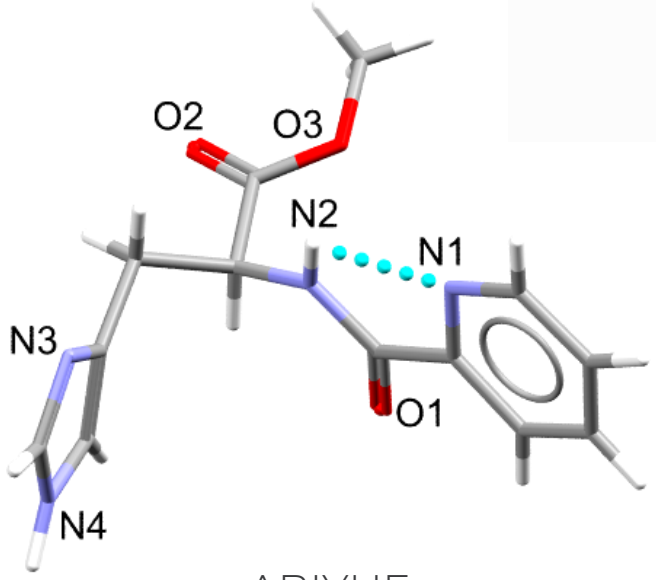




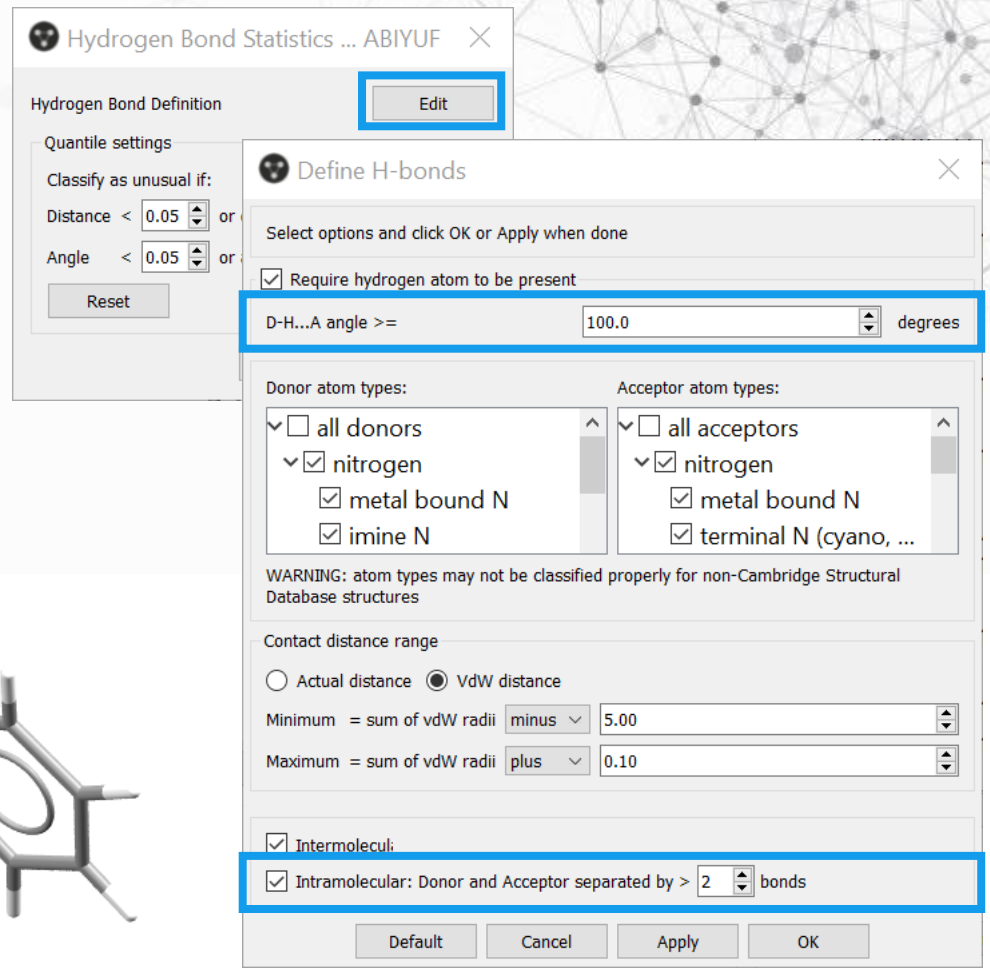


Investigation of acute interaction

- Visual inspection of ABIYUF suggests acute intramolecular interaction N2-N1 (DHA 106.29°, separated by >3 bonds)
- Change H-bond definition to allow this:
  - DHA angle > 100°
  - Intramolecular donor and acceptor separated by > 2 bonds



ABIYUF



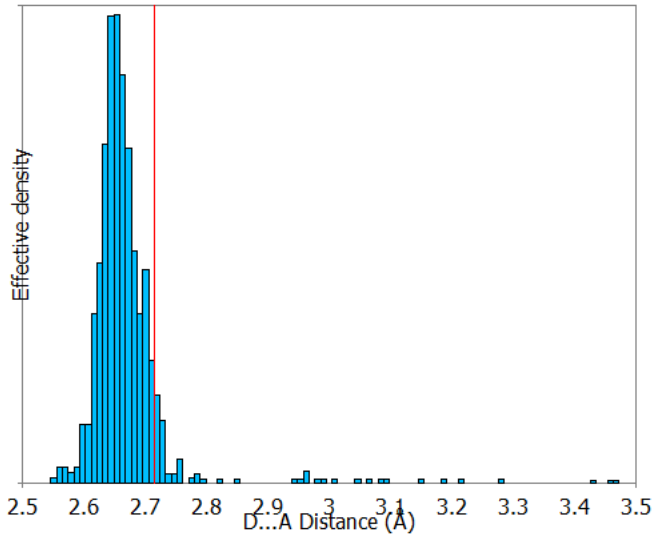
Distance & Angle not unusual for this type of interaction

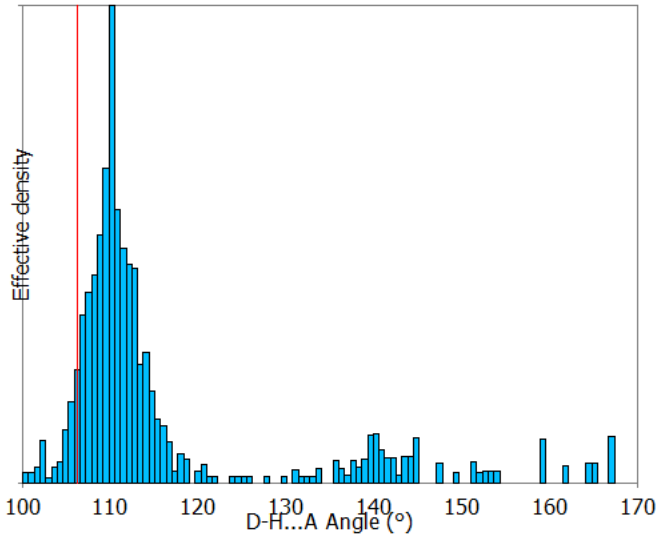
Hydrogen Bond Statistics ... ABIYUF

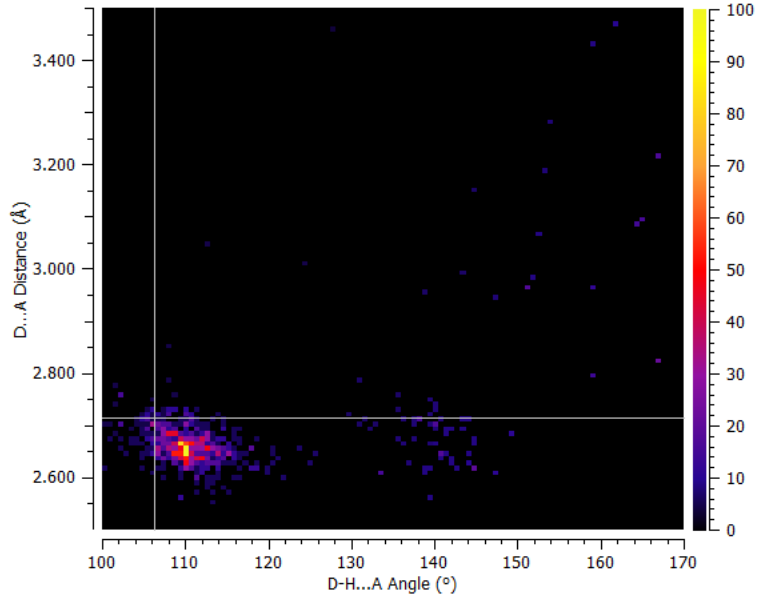
	Donor	Acceptor	Distance D-A	Distance classification	Distance threshold	Distance hits	Distance mean	Distance std. dev.	Distance min.	Distance max.	Angle D-H...A	Angle classification	Angle threshold	Angle hits	Angle mean	Angle std. dev.	Angle min.	Angle max.
1	N2 (amide_carbonyl)	N1 (ar_N_2)	2.71	Not Unusual	(2.64, 2.72)	713	2.67	0.08	2.55	3.47	106.29	Not Unusual	(105.47, 148.29)	713	116.20	14.12	100.38	166.97
2	N2 (amide_carbonyl)	O1 (amide_carbonyl)	3.06	Not Unusual	(2.80, 3.19)	10088	2.94	0.13	2.46	3.79	**132.52**	Unusual	(147.53, 179.38)	10088	167.37	10.55	100.74	179.98
3	N4 (imidazole_2)	N3 (imidazole_2)	2.80	Not Unusual	(2.80, 2.98)	206	2.86	0.07	2.72	3.19	172.57	Not Unusual	(156.25, 179.51)	206	172.73	10.11	105.06	179.75

Export...

Results and analysis | View structures







☑ view distance ☐ view angle

https://www.ccdc.cam.ac.uk/Community/educationalresources/

Want to explore more?

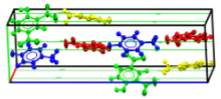
Training and Educational Resources

The wealth of information contained within the Cambridge Structural Database (CSD) extends far beyond a collection of crystal structures. Knowledge derived from these materials informs much of chemistry, biochemistry, and biology. Chemical and structural concepts are often difficult to grasp without real world, interactive examples for students to explore.

The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of course, our database of over one million entries are available for free through our Access Structures portal.

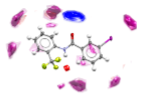
If you are an educator looking for supplementary teaching materials, find out more about the Teaching Database **here**. If you have developed your own modules using the CSD and would like to share them with the broader community, please contact us at education@ccdc.cam.ac.uk.

To keep up to date with the latest news from education and outreach at the CCDC, sign up for the Education and Outreach Newsletter **here**.



CSD-Core

Essential crystallographic and structural chemistry capabilities.

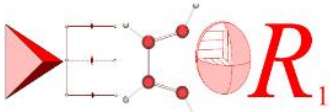


CSD-Materials

Tools to help you to understand your material's behaviours and refine its properties.

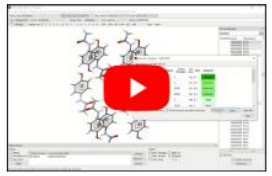
Information on the Teaching Subset

Access a series of teaching modules for use in the classroom



DECOR: Educational Resources for Teaching Crystallography

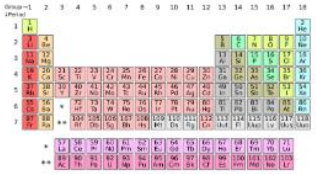
Download a series of self-guided workshop materials for CCDC tools and features



Watch software training and support videos

CSDU modules - Explore our on-demand training courses

Access fun science activities for kids through the CCDC Home learning page



Explore the Periodic Table through Crystal Structures

Bound! a Protein-Drug matching card game

Register for E&O newsletter

On-demand modules with completion certificate

Self-guided workshops

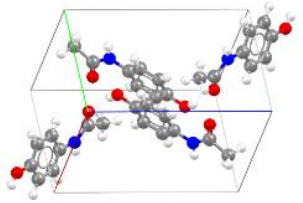
YouTube and LabTube channels

A new docking card game

CSDU

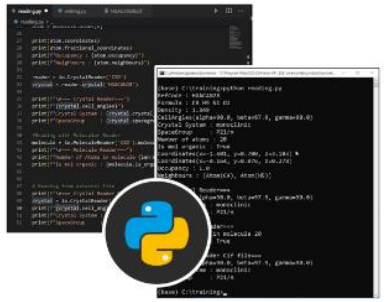
- On-demand modules to learn how to use the CSD Software at your own pace.
- Completion certificate after a final quiz!

Visualisation 101 - Visualising structural chemistry data with Mercury



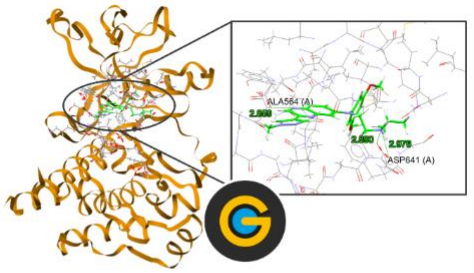
Begin module

Programmatic access to the CSD 101 – CSD Python API



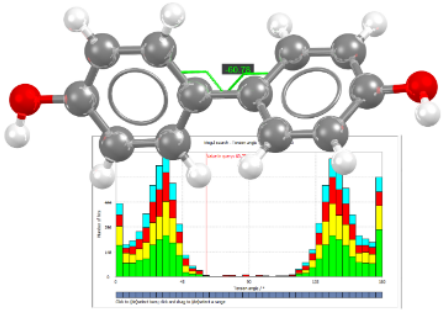
Begin module

Protein-ligand docking 101 - Running a simulation in GOLD



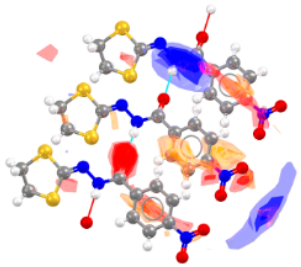
Begin module

Analysing molecular geometries 101 - basics of Mogul



Begin module

Analysing intermolecular interactions 101 - Full Interaction Maps



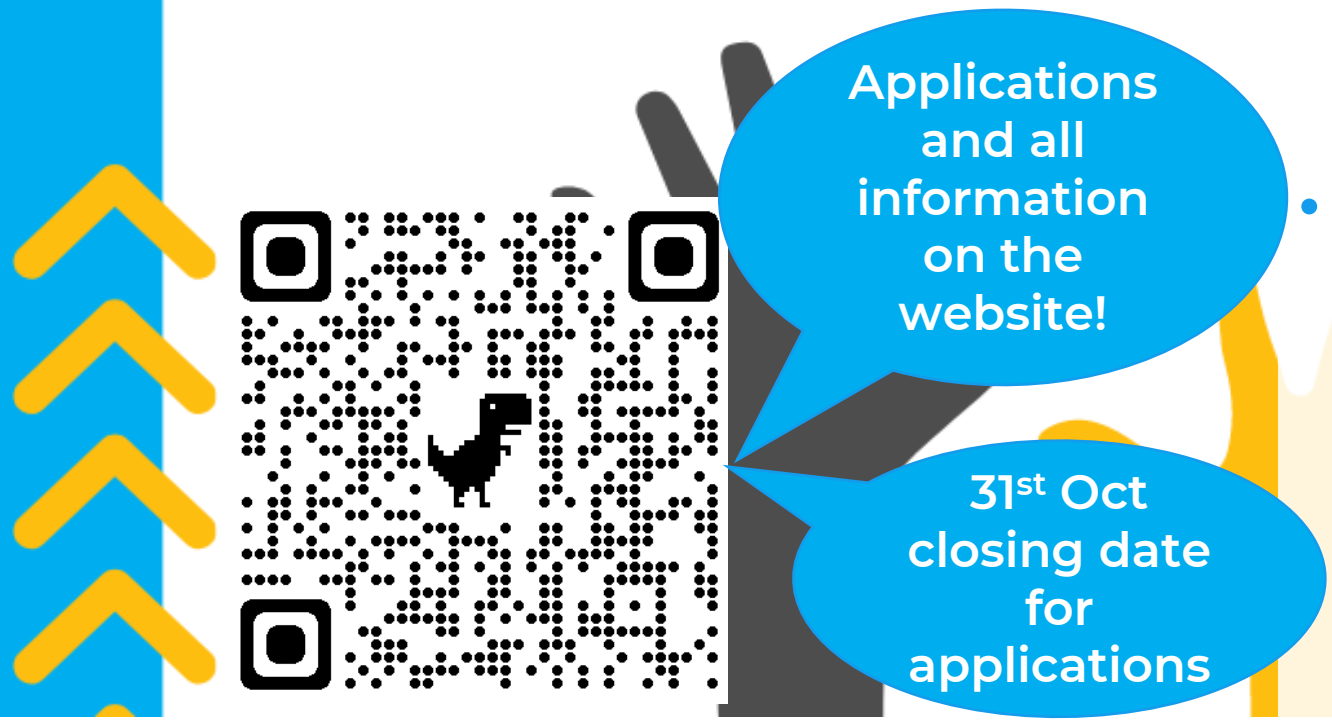
Begin module

https://www.ccdc.cam.ac.uk/Community/educationalresources/CSDU/

CCDC

CCDC Engagement Grants

Engage, inspire, share!



- Do you wish to inspire others with your love of crystallography or structural science?
- CCDC Engagement Grants cover costs for you to produce resources or activities to increase schools and public engagement in crystallography and structural science.

https://www.ccdc.cam.ac.uk/Community/awardsandsponsorship/ccdc-engagement-grants/

CCDC