

# Welcome to CSDU



# Analysing molecular geometries 101 - basics of Mogul



CCDC  
advancing structural science

# Learning outcomes

- How to use the Mogul geometry check from Mercury to assess the geometry of a molecule.
- How to run a geometry check on specific features (for example a torsional angle) of a molecule that you load.
- How to interpret the results obtained.

# The CSD Software

CSDEnterprise.

CSDMaterials.



DASH



Python API



Mercury

CSDDiscovery.



SuperStar



Python API



GOLD



CrossMiner



Mercury

CSDCore.



WebCSd



Mogul



MyStructures



ConQuest



CSD



IsoStar



Mercury



Hermes



Python API



Professional  
Services



Research  
& Knowledge  
partnerships

CSDCommunity.



Mercury



enCIfer



Symmetry



Deposit



CellCheck



Educational



Access

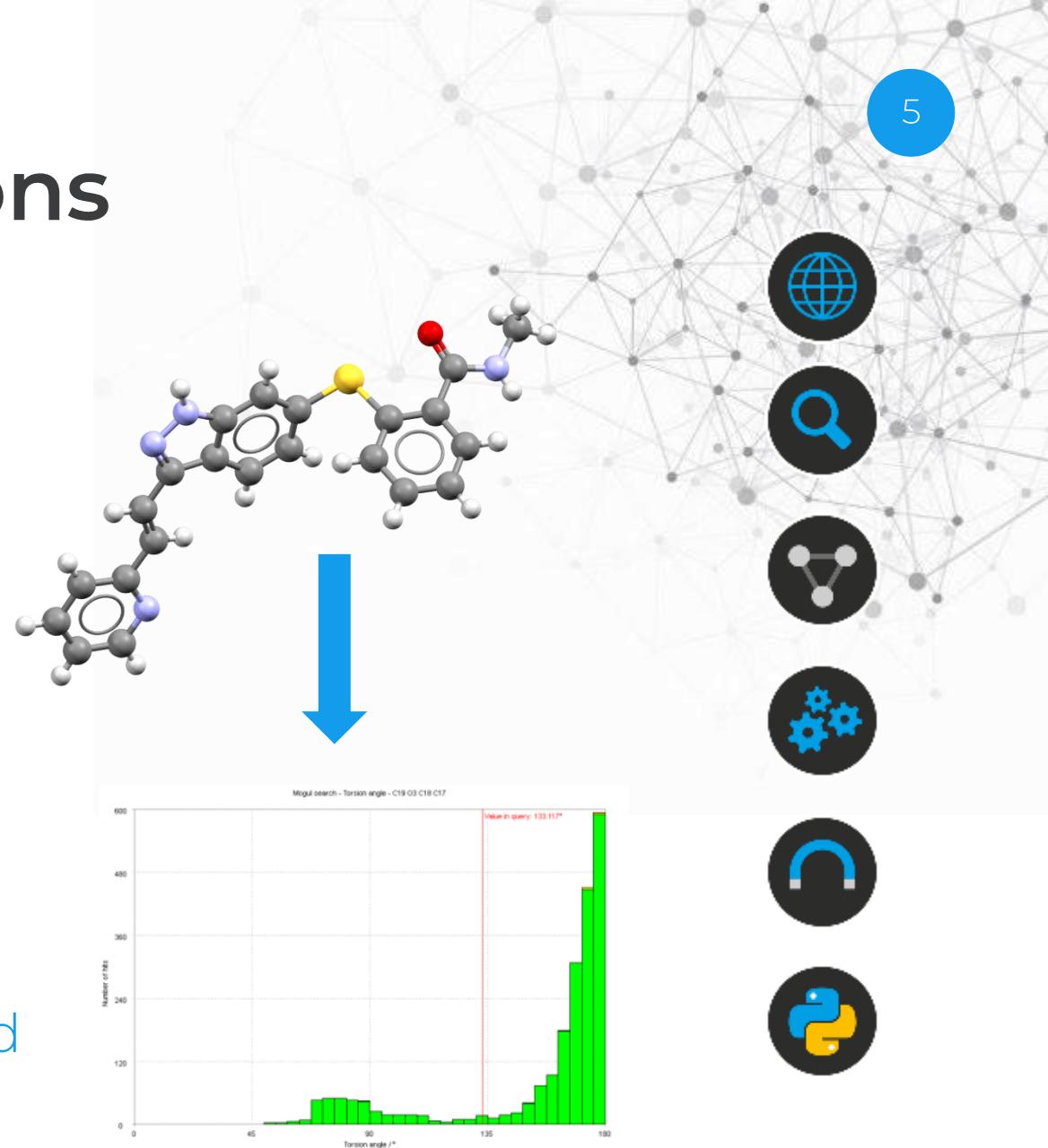


MyStructures

CCDC

# CSD-Core – Conformations

- Mogul provides precise information on preferred molecular geometries
- Validate molecular geometries rapidly using interactive plots & statistics
- Identify any unusual features of a given query structure
- Mine millions of chemically classified bond lengths, angles, torsion angles and ring conformations in the CSD



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# Mogul

- Incorporates **pre-computed libraries** of bond lengths, valence angles, torsion angles and ring conformations **derived entirely from the CSD**
- **Validate complete geometry:** retrieve distributions, and figures of merit for all bonds, angles, torsions and rings in the molecule
- **Fragment Generalisation:** If fragment specified is rare, Mogul will include CSD results from the most similar fragments
- **Hyperlinking to the CSD:** View CSD entries in specific areas of histogram
- **Integration with other software:** Instruction file permits other programs to interact with Mogul

# When could we use Mogul?

- In teaching to help us understand fundamental chemistry
- To help design and assess new materials such as drug molecules
- To validate conformations
  - To analyse calculated conformations
  - To filter out protein-ligand docking solutions with unlikely ligand conformations
- To validate geometries
  - To check molecular dimensions of new crystal structures
- To create restraint data/ligand dictionaries
  - For protein refinement
  - To guide small molecule structure solution from powder diffraction data

# Using Mogul to teach chemistry

[A2-introduction to "Access Structures"](#)

Nuffield Foundation Newcastle University

The full CSD database, maintained by the Cambridge Crystallographic Data Centre, contains over 800,000 real crystal structures. The full CSD software requires the purchase of an annual site licence, but individual structures may be viewed and manipulated free of charge using the "Access Structures" option on the CCDC website. It uses a JSView viewer, thus enabling them to be viewed on both Windows and Apple devices.

## Getting Started

- To use the CSD "Access Structures" function you will require a computer or laptop or tablet with access to the internet.
- You will then need to find CSD "Access Structures" page using one of these two methods:
  - Type in the web address <https://www.ccdc.cam.ac.uk/structures>.
  - Type into a search engine such as Google "csd access structures" and click on the link that says "Access Structures".

## Basics



To view a particular structure, you need to type its refcode (provided) into the 'CSD refcode' box. For the purpose of this demo, type in the refcode 'CAFINE' for the crystal structure of caffeine.

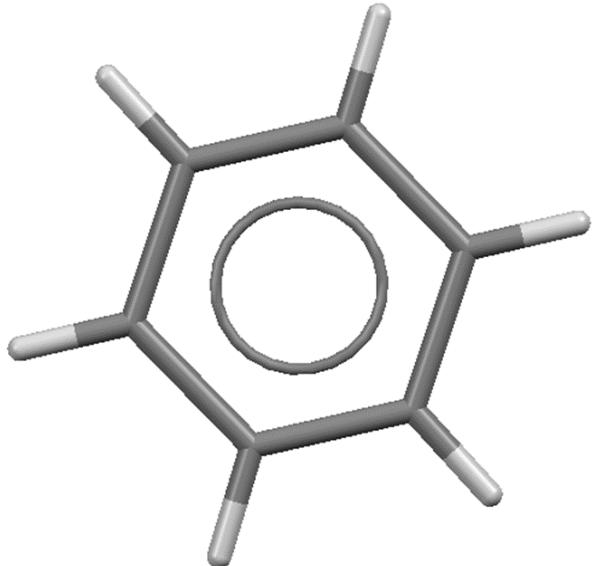
With the mouse you can hold left click to manually rotate the molecule and zoom using the middle button.

The drop-down headed 'Style' can be used to change the display.

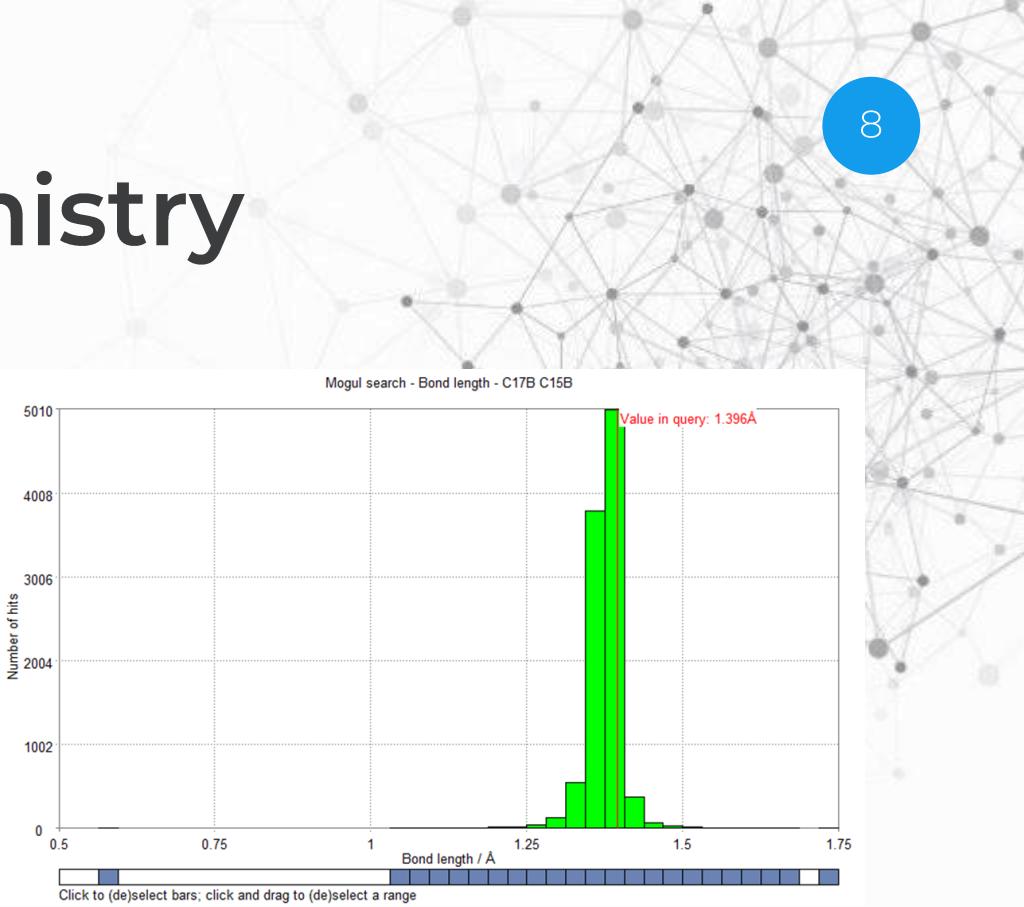
The 'Labels' drop-down can be used to label different atoms in the molecule.

'Packing' options can be used to look at the larger crystal structure, e.g. the unit cell and the bulk structure of 3x3x3 unit cells.

**TOP TIP!**  
When looking at some crystal structures on the database there will be two species on a refcode, you may only need to look at one of them. The two species are ions; one is a positive ion and the other is a negative ion. It is of course not possible to have one ion without the opposite 'counter ion'.

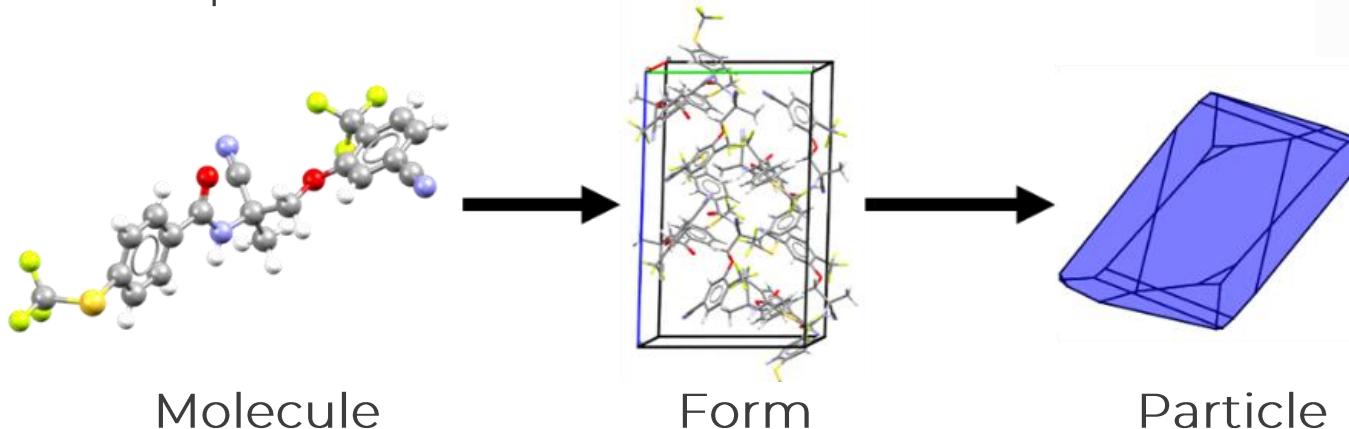


- Distance is about 1.38 Å
- Taken from over 450,000 benzene rings in reported in the CSD



# Using Mogul to inform key decisions

- The term “solid form informatics” was first introduced in mid-2000s
  - Use of structural knowledge to inform key decisions in pharmaceutical development*
- Now a key part of the solid form development workflow at most major pharmaceutical companies



Robert Docherty et al *Journal of Pharmacy and Pharmacology*, (2015) 67, 857. doi:10.1111/jphp.12394.  
 Taylor et al. *J. Chem. Inf. Model.*, (2014) 54 (9), 2500. Wood, P. A. et al. *CrystEngComm* (2013) 15, 65

**JPP** JOURNAL OF  
Pharmacy and Pharmacology

**JPP**  
Journal of Pharmacy  
And Pharmacology

**Research Paper**

**The integration of solid-form informatics into solid-form selection**

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<sup>a</sup>The Cambridge Crystallographic Data Centre, Cambridge, <sup>b</sup>Pharmaceutical Science, Pfizer Global R&D, Sandwich, UK and <sup>c</sup>Pharmaceutical Science, Pfizer Global R&D, Groton, USA

**Keywords**  
Cambridge Structural Database; quality-by-design; solid-form informatics; solid-form selection

**Correspondence**  
Robert Docherty, Pharmaceutical Science, Pfizer Global R&D, Sandwich CT13 9NJ, United Kingdom

**Abstract**  
Objectives To demonstrate how the use of structural informatics during drug development assists with the assessment of the risk of polymorphism and the selection of a commercial solid form.  
Methods The application of structural chemistry knowledge derived from the hundreds of thousands of crystal structures contained in the Cambridge Structural Database to predict polymorphism risk and to support the selection of a commercial solid form. The use of solid-form informatics to predict polymorphism risk and to support the selection of a commercial solid form. The use of solid-form informatics to predict polymorphism risk and to support the selection of a commercial solid form.

**CrystEngComm**

**PAPER**

**Knowledge-based approaches to co-crystal design†**

Cite this: CrystEngComm, 2014, 16, 5839  
Peter A. Wood,\* Neil Feeder, Matthew Furlow, Peter T. A. Galek, Colin R. Groom and Elna Pidcock

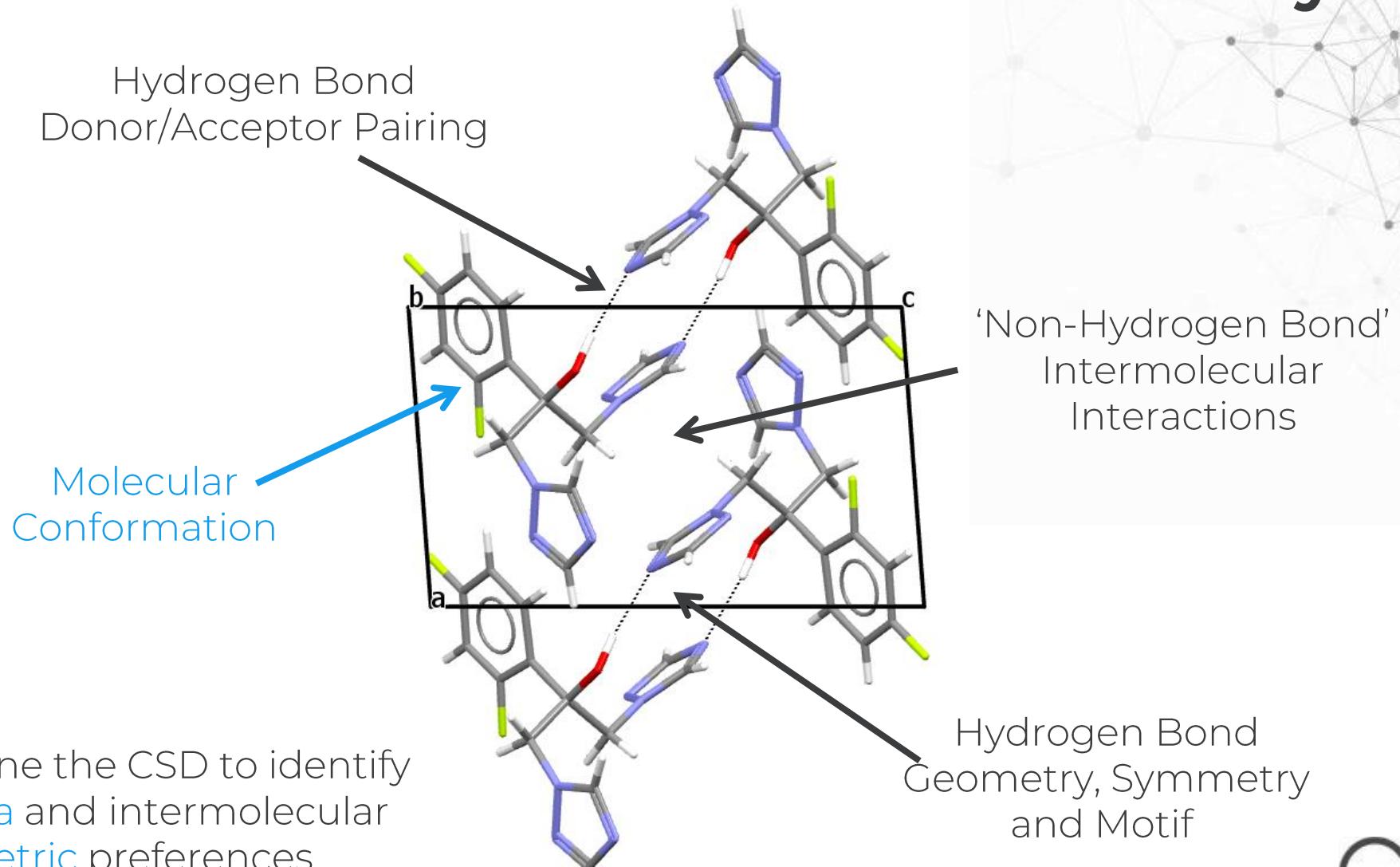
Received 12th February 2014,  
Accepted 10th March 2014  
DOI: 10.1039/c4ce00316k  
[www.rsc.org/crystengcomm](http://www.rsc.org/crystengcomm)

**1. Introduction**  
The definition of a co-crystal,<sup>1,2</sup> whether this is the correct term to use<sup>3</sup> and even whether it should contain a hyphen has been debated at length in the literature. At the most basic level, a co-crystal is a crystalline form composed from two or more components with a particular stoichiometry. Generally, the definitions used in the Crystalline Engineering field also place some or all of the following requirements on the solid forms in question:  
 1. All components are organic species (ruling out inorganics or organometallics).  
 2. None of the components are charged (otherwise classified as salts).  
 3. None of the components are water (otherwise classified as hydrates).

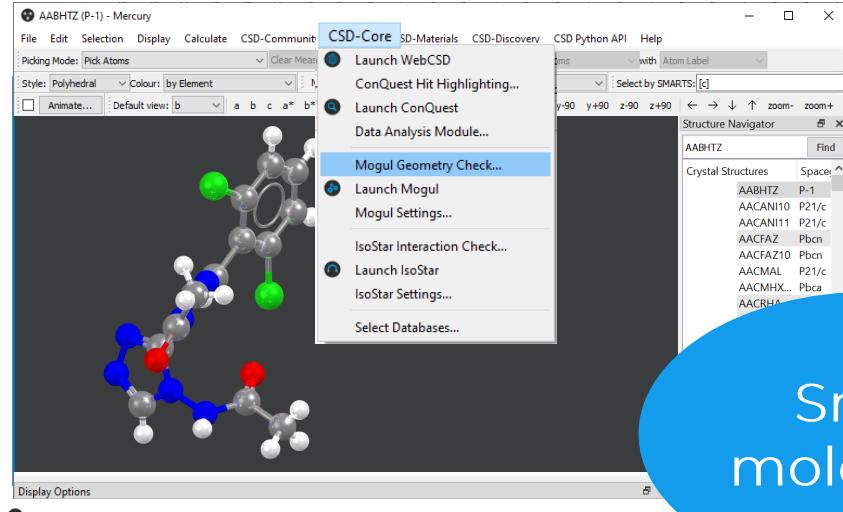
The use of knowledge-based methods has been intimately connected with the field of co-crystal design since the seminal papers of Etter and Desiraju in the 1990s. Here we explain and exemplify how rational co-crystal design has been carried out in the past using crystal structure knowledge as well as presenting emerging methodologies for knowledge-based co-former selection.

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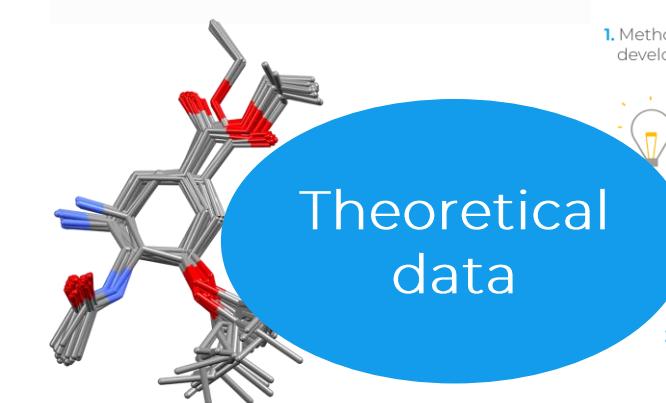
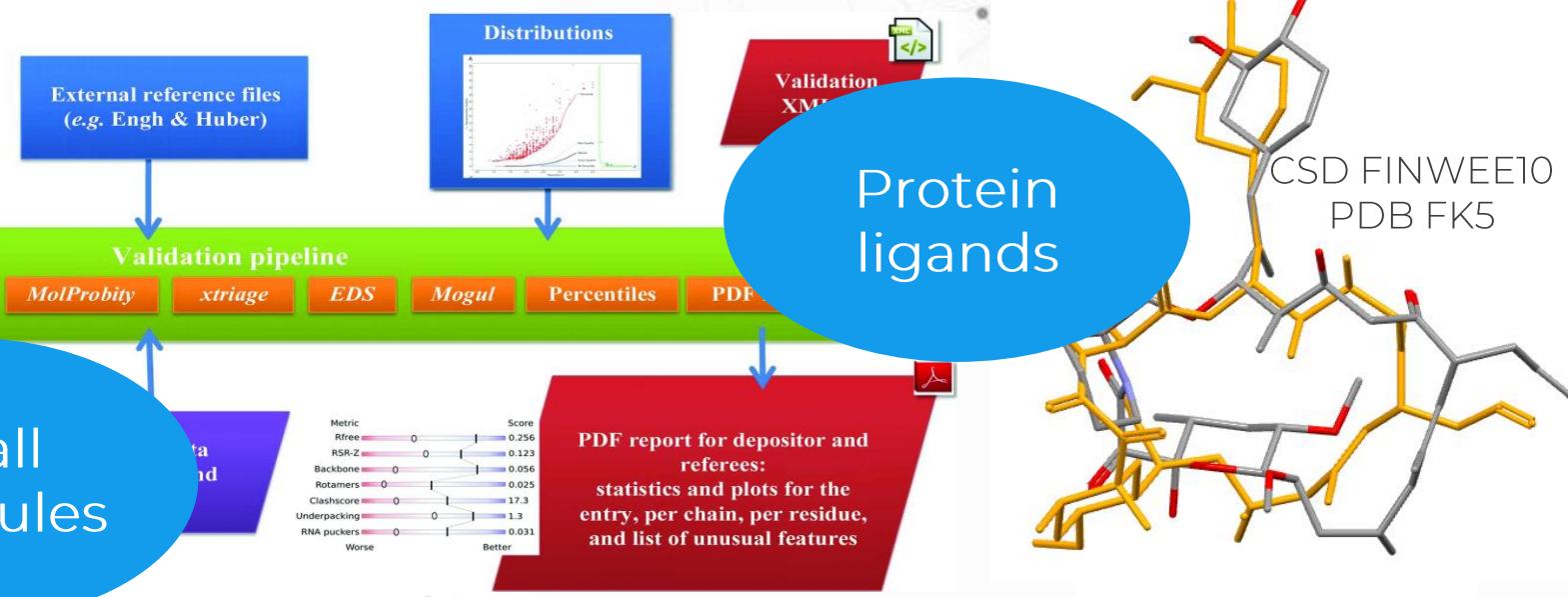
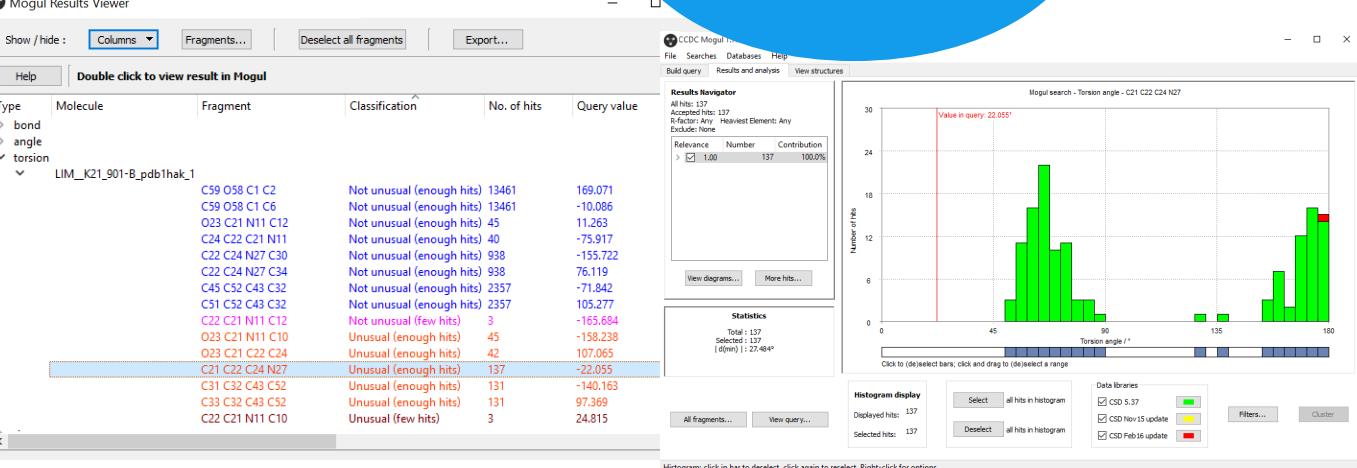
# Characteristics that influence stability



# Using Mogul to check new structural data



Small molecules



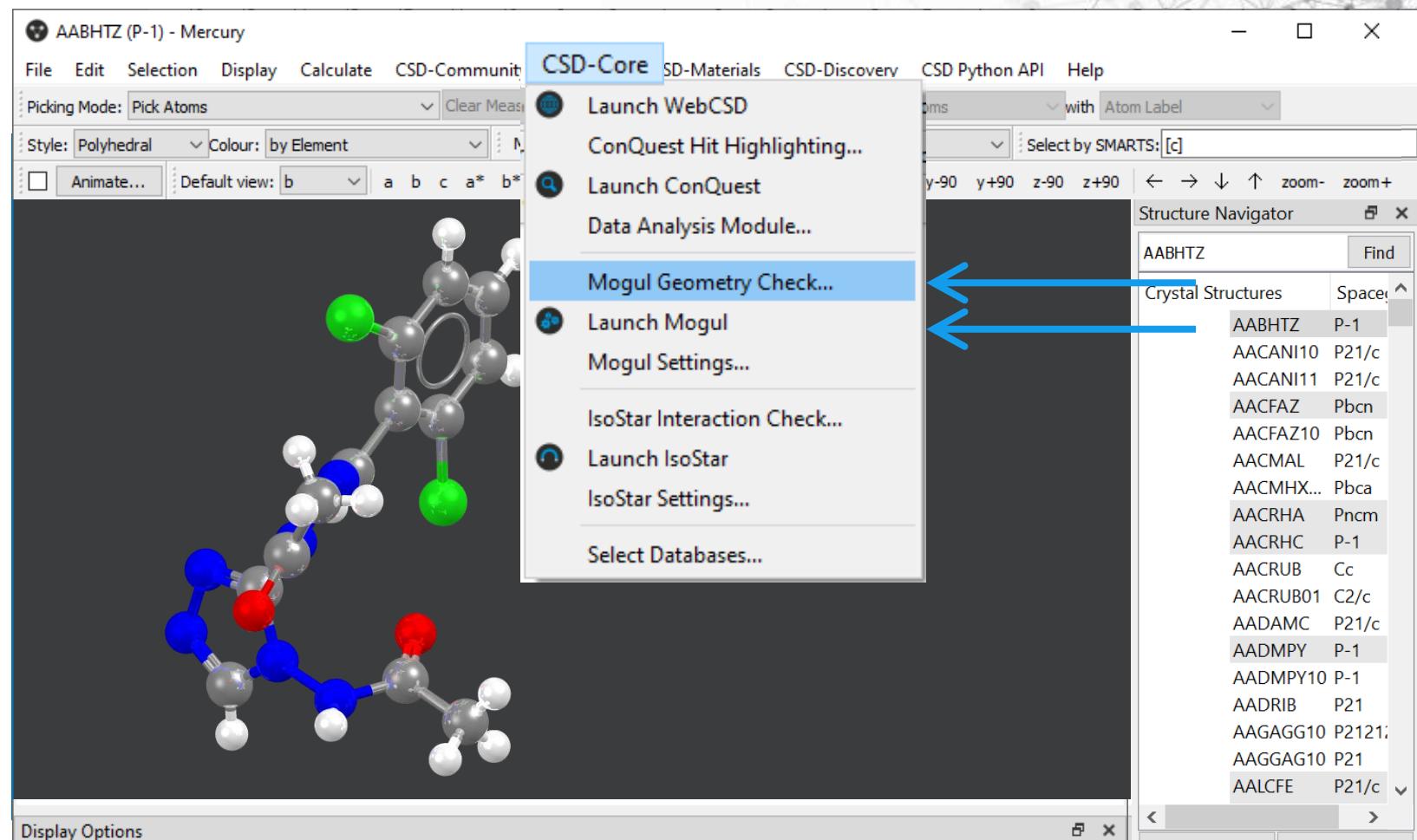
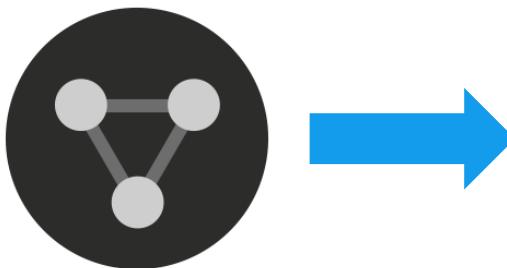
1. Methods development.
  2. Test methods blind with unpublished targets.
  3. Compare predictions to experimental observations.
- Crystal Structure Prediction (CSP) Blind Test.

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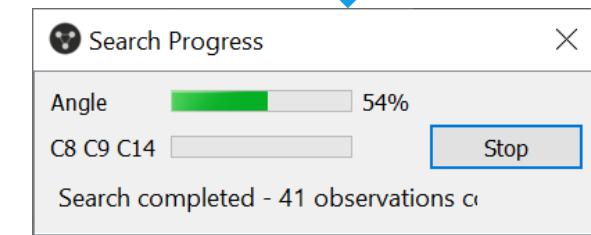
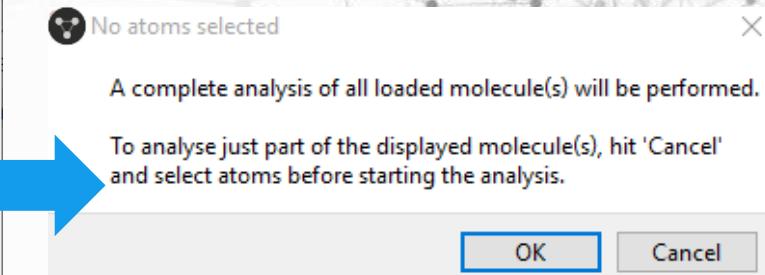
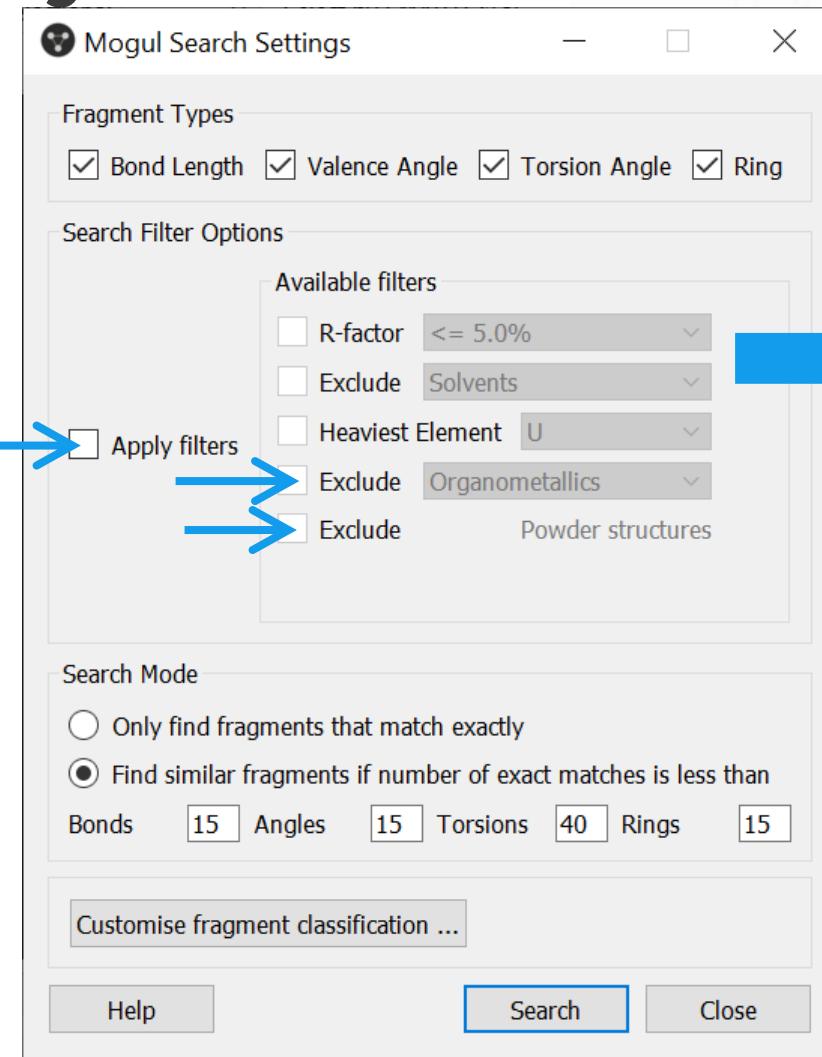
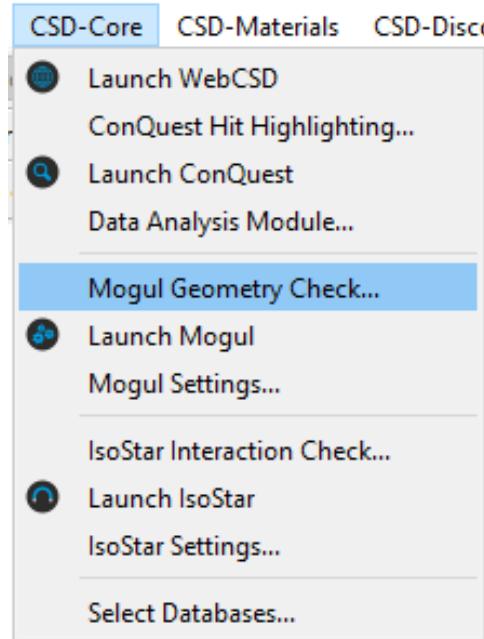
# Chemical coverage - the details....

- Based on data in the CSD - organic and metal-organic experimental structures
  - Bond Lengths
  - Valence angles
  - Torsion angles
  - Rings
- Large distributions are reduced by random selection
- Bond fragments and rings involving metals are characterised in exactly the same way as organic fragments
- The following are not included:
  - Bonds, angles & torsions involving H atoms
  - Valence angles & torsions involving metals
  - Cyclic torsions of rings less than 8 atoms
  - Rings containing less than 5 atoms (fused and bridged rings are included)

# Show One: Mogul – Launch from Mercury



# Mogul Geometry Check



# Mogul Geometry Check - Results

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
> bond						
> angle						
✓ torsion						
✓ LIM_K21_901-B_pdb1hak_1						
	C59 O58 C1 C2		Not unusual (enough hits)	13461	169.071	
	C59 O58 C1 C6		Not unusual (enough hits)	13461	-10.086	
	O23 C21 N11 C12		Not unusual (enough hits)	45	11.263	
	C24 C22 C21 N11		Not unusual (enough hits)	40	-75.917	
	C22 C24 N27 C30		Not unusual (enough hits)	938	-155.722	
	C22 C24 N27 C34		Not unusual (enough hits)	938	76.119	
	C45 C52 C43 C32		Not unusual (enough hits)	2357	-71.842	
	C51 C52 C43 C32		Not unusual (enough hits)	2357	105.277	
	C22 C21 N11 C12		Not unusual (few hits)	3	-165.684	
	O23 C21 N11 C10		Unusual (enough hits)	45	-158.238	
	O23 C21 C22 C24		Unusual (enough hits)	42	107.065	
	C21 C22 C24 N27		Unusual (enough hits)	137	-22.055	
	C31 C32 C43 C52		Unusual (enough hits)	131	-140.163	
	C33 C32 C43 C52		Unusual (enough hits)	131	97.369	
	C22 C21 N11 C10		Unusual (few hits)	3	24.815	

## Colour code:

- **Blue**: It is **not unusual** value in the CSD and there are **enough data** in the CSD for comparison.
- **Pink**: It is **not unusual** value in the CSD, but there are only **few data** in the CSD for comparison.
- **Orange**: It is an **unusual** value in the CSD and there are **enough data** in the CSD for comparison.
- **Brown**: It is an **unusual** value in the CSD, but there are only **few data** in the CSD for comparison.

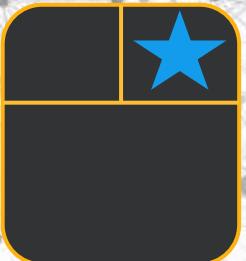
# Mogul Geometry Check - Results

Mogul Results Viewer

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

Help Double click to view result in Mogul

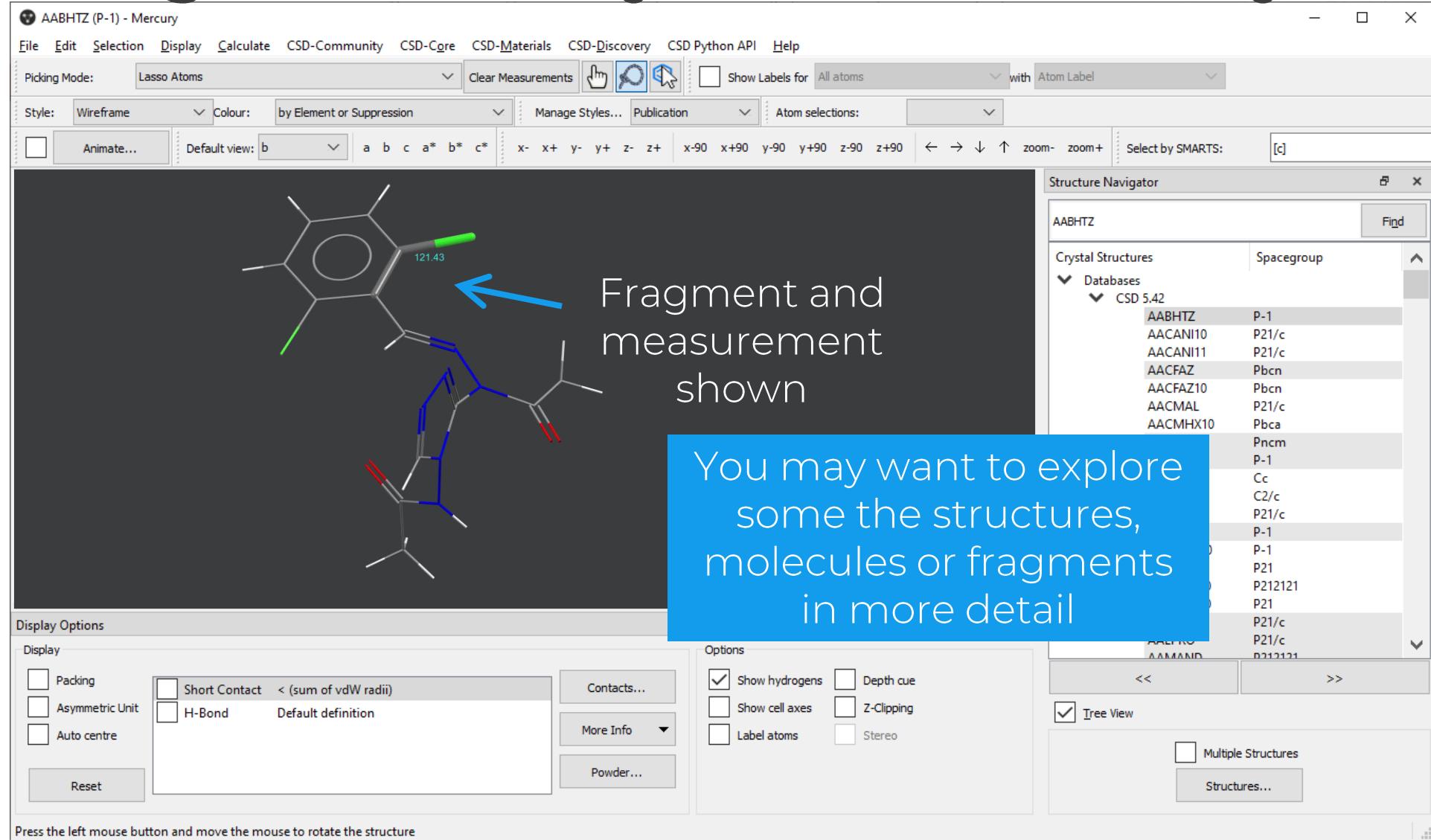
Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median	d(min)
bond	AABHTZ	C2 C1 C11	Not unusual (enough hits)	10637	117.372	118.409	1.966	0.528	1.038	86.905	152.624	118.518	0.000
angle	AABHTZ	C6 C1 C11	Not unusual (enough hits)	449	119.477	119.883	1.790	0.227	0.406	111.452	136.611	119.752	0.000
		C2 C1 C6	Not unusual (enough hits)	421	123.139	122.057	2.692	0.402	1.082	79.010	129.445	122.401	0.000
		C3 C2 C1	Not unusual (enough hits)	10491	119.515	119.405	1.501	0.073	0.110	89.047	141.490	119.478	0.000
		C4 C3 C2	Not unusual (enough hits)	20098	119.999	120.239	1.325	0.181	0.240	70.643	140.815	120.159	0.000
		C3 C4 C5	Not unusual (enough hits)	10491	119.854	119.405	1.501	0.299	0.449	89.047	141.490	119.478	0.000
		C4 C5 C12	Not unusual (enough hits)	10637	116.212	118.409	1.966	1.118	2.197	86.905	152.624	118.518	0.000
		C6 C5 C12	Not unusual (enough hits)	449	121.434	119.883	1.790	0.867	1.551	111.452	136.611	119.752	0.000
		C4 C5 C6	Not unusual (enough hits)	421	122.346	122.057	2.692	0.107	0.288	79.010	129.445	122.401	0.000
		C1 C6 C5	Not unusual (enough hits)	170	115.125	116.276	3.163	0.364	1.152	111.918	151.002	115.875	0.000
		C5 C6 C7	Not unusual (enough hits)	142	126.222	122.066	3.194	1.301	4.156	106.172	133.828	121.766	0.000
		C1 C6 C7	Not unusual (enough hits)	142	118.637	122.066	3.194	1.074	3.429	106.172	133.828	121.766	0.000
		C6 C7 N1	Not unusual (enough hits)	63	120.071	121.580	1.633	0.924	1.509	118.121	125.394	121.710	0.000
		C7 N1 N2	Not unusual (enough hits)	304	117.522	117.173	2.634	0.133	0.349	112.028	123.777	117.122	0.000
		C8 N2 N1	Not unusual (enough hits)	16	124.440	121.412	5.026	0.603	3.028	110.211	126.188	123.650	0.000
		C12 N2 N1	Not unusual (enough hits)	15	116.721	115.241	2.607	0.568	1.480	111.791	120.406	114.780	0.000
		N2 C8 N3	Not unusual (enough hits)	15	125.283	124.096	1.376	0.863	1.187	121.050	125.790	124.354	0.000
		N5 C8 N3	Not unusual (enough hits)	18	110.781	110.483	0.852	0.349	0.298	109.567	112.225	110.237	0.000
		C8 N3 N4	Not unusual (enough hits)	47	106.679	105.504	2.395	0.491	1.175	100.785	114.792	105.591	0.000
		C9 N4 N3	Not unusual (enough hits)	190	107.177	107.613	1.828	0.238	0.436	101.988	116.826	107.467	0.000
		N5 C9 N4	Not unusual (enough hits)	61	110.746	110.185	0.564	0.995	0.561	108.650	111.600	110.233	0.000
		C8 N5 N6	Not unusual (enough hits)	15	128.047	125.894	2.689	0.801	2.154	118.623	129.059	126.475	0.000
		C9 N5 C8	Not unusual (enough hits)	15	104.615	105.953	1.319	1.015	1.338	103.742	108.706	105.802	0.000
		C9 N5 N6	Not unusual (enough hits)	47	126.994	126.891	1.763	0.058	0.102	121.092	133.246	127.067	0.000
		C10 N6 N5	Not unusual (enough hits)	15	117.419	118.913	1.088	1.373	1.494	117.419	120.816	118.696	0.000
		C11 C10 N6	Not unusual (enough hits)	37	114.417	114.933	1.651	0.312	0.515	112.356	120.514	114.515	0.000
		O1 C10 N6	Not unusual (enough hits)	37	121.348	121.538	1.427	0.133	0.189	116.489	123.542	121.784	0.000
		O1 C10 C11	Not unusual (enough hits)	4907	124.224	122.048	1.806	1.205	2.177	91.903	161.131	121.976	0.000
		C13 C12 N2	Not unusual (enough hits)	34	117.582	116.154	0.932	1.532	1.428	114.091	117.893	116.022	0.000
		O2 C12 N2	Not unusual (enough hits)	34	117.664	119.326	0.983	1.690	1.662	117.131	121.407	119.472	0.000
		O2 C12 C13	Not unusual (enough hits)	4135	124.750	122.007	3.849	0.713	2.743	85.274	175.076	121.832	0.000
		N5 C8 N2	Not unusual (few hits)	4	123.936	123.637	0.517	0.578	0.299	123.145	124.209	123.597	0.000
		C12 N2 C8	Unusual (enough hits)	8	118.784	120.955	1.018	2.132	2.171	118.784	122.010	120.992	0.000



Single click  
on a row to  
view result in  
Mercury

CCDC

# Mogul Geometry Check – Mercury view



# Mogul Geometry Check - Results

Mogul Results Viewer

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

Help Double click to view result in Mogul

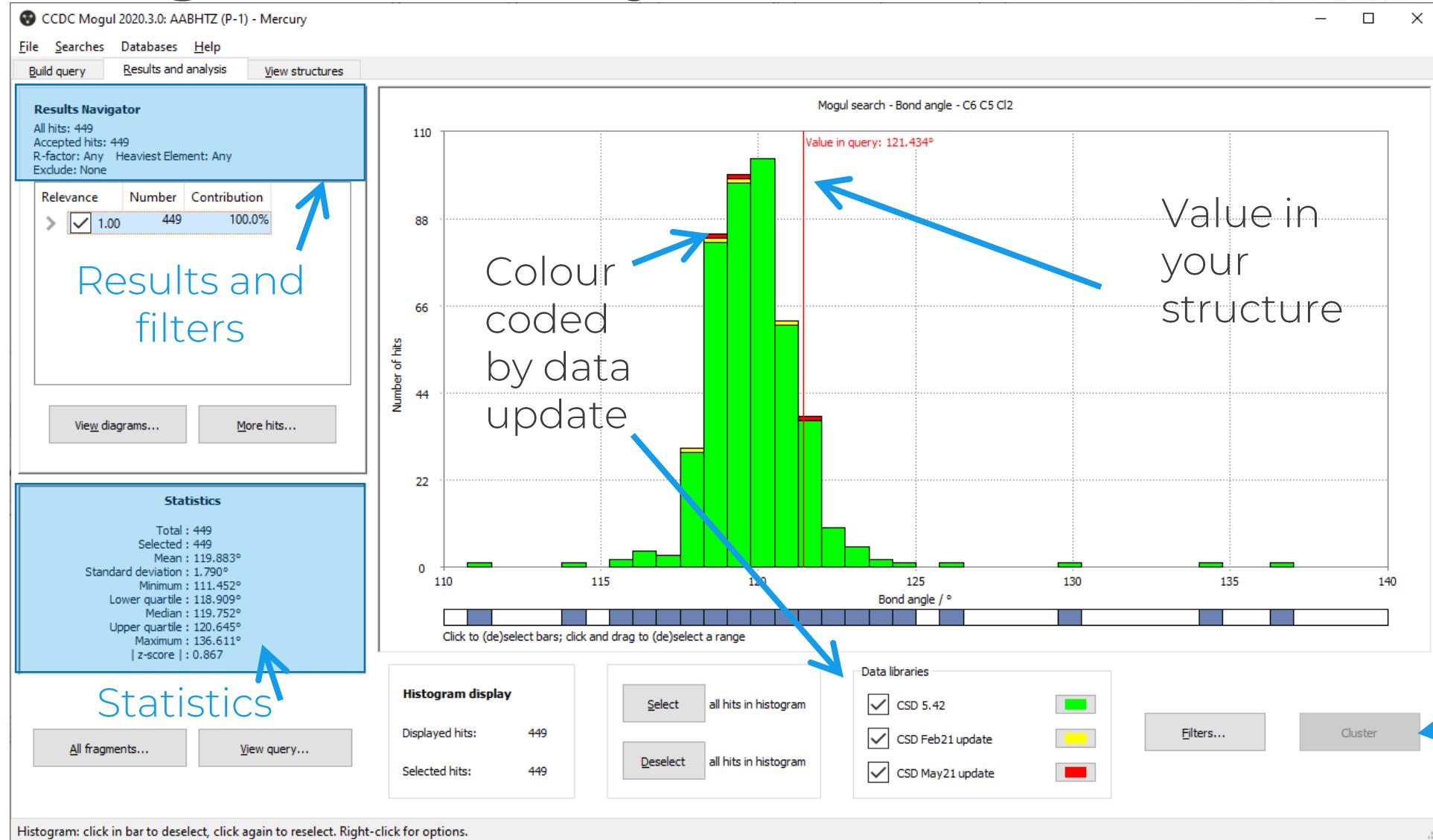
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		C9 N5 C8	Not unusual (enough hits)	15	104.615	105.953	1.319	1.015	1.338	103.742	108.706	105.802	0.000
		C9 N5 N6	Not unusual (enough hits)	47	126.994	126.891	1.763	0.058	0.102	121.092	133.246	127.067	0.000
		C10 N6 N5	Not unusual (enough hits)	15	117.419	118.913	1.088	1.373	1.494	117.419	120.816	118.696	0.000
		C11 C10 N6	Not unusual (enough hits)	37	114.417	114.933	1.651	0.312	0.515	112.356	120.514	114.515	0.000
		O1 C10 N6	Not unusual (enough hits)	37	121.348	121.538	1.427	0.133	0.189	116.489	123.542	121.784	0.000
		O1 C10 C11	Not unusual (enough hits)	4907	124.224	122.048	1.806	1.205	2.177	91.903	161.131	121.976	0.000
		C13 C12 N2	Not unusual (enough hits)	34	117.582	116.154	0.932	1.532	1.428	114.091	117.893	116.022	0.000
		O2 C12 N2	Not unusual (enough hits)	34	117.664	119.326	0.983	1.690	1.662	117.131	121.407	119.472	0.000
		O2 C12 C13	Not unusual (enough hits)	4135	124.750	122.007	3.849	0.713	2.743	85.274	175.076	121.832	0.000
		N5 C8 N2	Not unusual (few hits)	4	123.936	123.637	0.517	0.578	0.299	123.145	124.209	123.597	0.000
		C12 N2 C8	Unusual (enough hits)	8	118.784	120.955	1.018	2.132	2.171	118.784	122.010	120.992	0.000



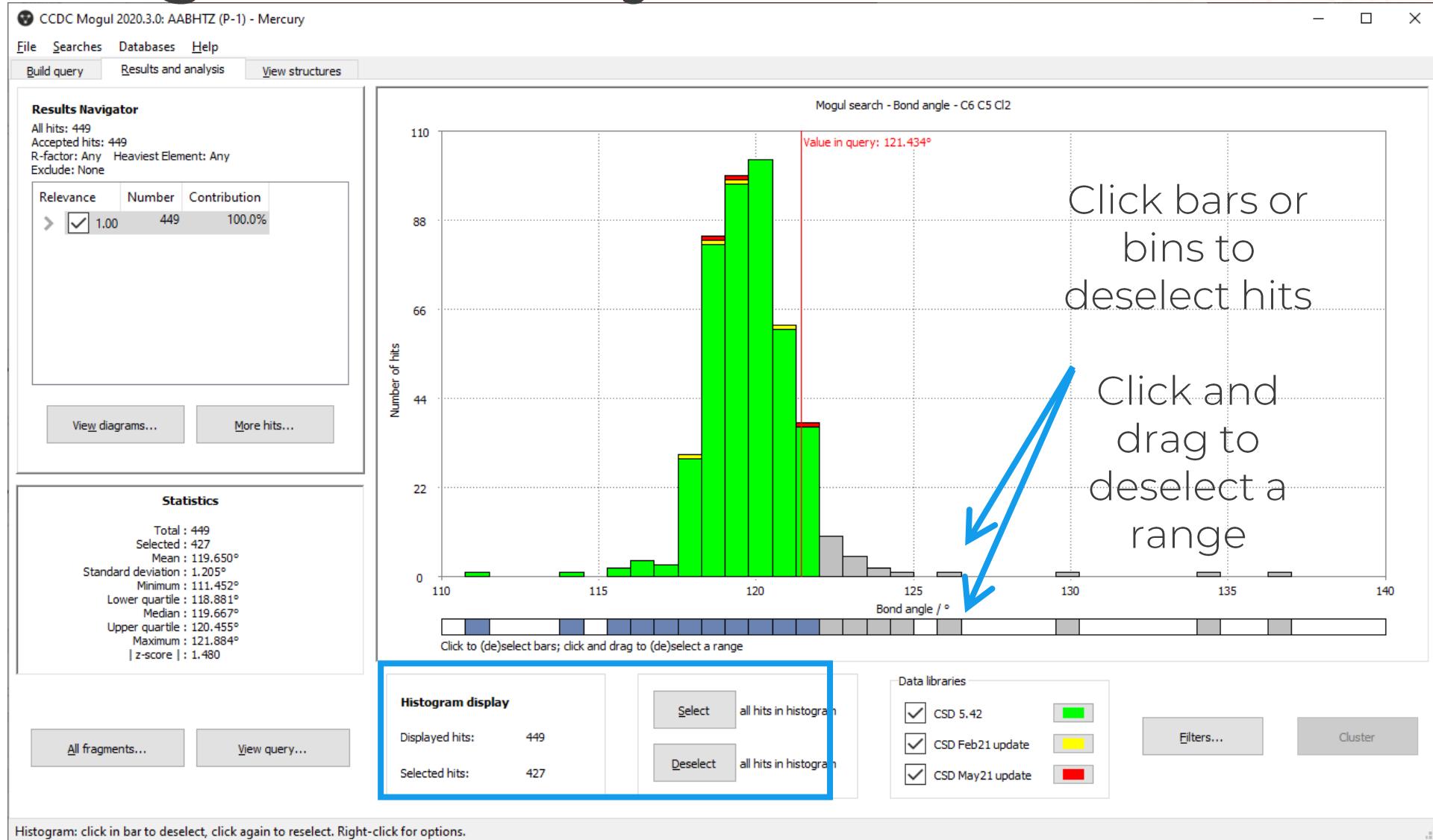
Double click  
on a row to  
view result in  
Mogul

CCDC

# Mogul Geometry Check – Results



# Mogul Geometry Check – Results



CCDC

# Mogul Geometry Check – View structures

CCDC Mogul 2020.3.0: AABHTZ (P-1) - Mercury

File Searches Databases Help

Build query Results and analysis View structures

Refcode: AABHTZ Data Library: CSD 5.42

Information Diagram 3D Visualiser

**Fragment shown**

**Measurement given**

Valence angle: 119.477°

**Click through hits**

1 2 hits

Show Parameters

**Number of structures**

AABHTZ

- AABHTZ
- ABAWIJ
- ABAWOP
- ABYTZL
- ACBTZC
- ACBTZD10
- ADAPIF
- ADENON
- AFESEK
- AJETAL
- AJETAL01
- AMAQAH
- AMAQUEL
- AMAQIP
- APIKUH
- AWIJIA
- AWIJOG
- AWIJUM
- AXEHIU
- AXUTES
- AYEZOV
- AZITUA
- BAKYAP
- CAGNUU
- CAGPAC
- CEBLOM
- CEQZJU
- CIUGAD
- CLPTBU
- COPZOX
- DAJCAV
- DAJNUZ
- DIDMUA

196 structures

View entries

CCDC

# Mogul Geometry Check – View structures

CCDC Mogul 2020.3.0: AABHTZ (P-1) - Mercury

File Searches Databases Help

Build query Results and analysis View structures

Refcode: AABHTZ Data Library: CSD 5.42

Information Diagram 3D Visualiser

Identifier	AABHTZ
Literature Reference	P.-E.Werner, <i>Cryst.Struct.Commun.</i> (1976), <b>5</b> , 873
Formula	C <sub>13</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>6</sub> O <sub>2</sub>
Compound Name	4-Acetoamido-3-(1-acetyl-2-(2,6-dichlorobenzylidene)hydrazine)-1,2,4-triazole
Synonym	
Space Group	P 1 (2)
Cell Lengths	a 11.372(9) b 10.272(5) c 7.359(9)
Cell Angles	α 108 °
Cell Volume	769.9
Z, Z'	Z: 2 Z'
R-Factor (%)	4.1
Disorder	
Polymorph	

**Customise**

Available Items (Right-click for options)

- Cell
  - Reduced Cell Lengths
  - Reduced Cell Angles
  - Reduced Cell Volume
- Experimental
  - Temperature (K)
  - Pressure
  - Density (CCDC)
  - Average Sigma (C-C)

Add >> << Remove

Selected Items (Right-click for options)

- Identifier
- Literature Reference
- Formula
- Compound Name
- Synonym
- Space Group

Up Down OK Cancel

Customise

View entries

Disorder  
comments  
can be useful  
when  
exploring  
molecular  
geometries

Click through  
the refcode list

CCDC

# Mogul Geometry Check – View structures

CCDC Mogul 2020.3.0: AABHTZ (P-1) - Mercury

File Searches Databases Help

Build query Results and analysis View structures

Refcode: ODAVIZ Data Library: CSD 5.42

Information Diagram 3D Visualiser

Reset display  Display fragments

View entries

Fragment and measurement shown

ODAVIZ

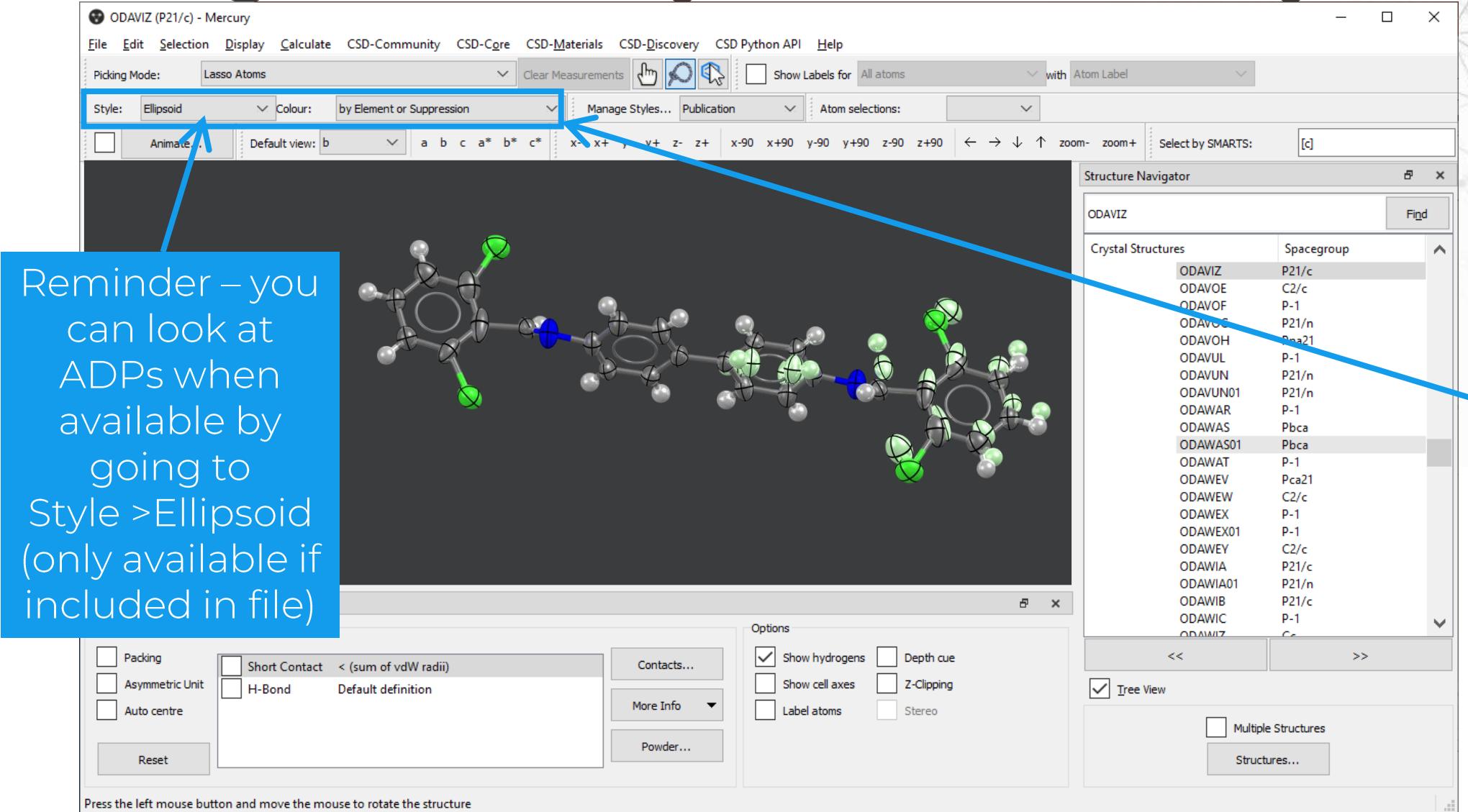
- IZAQEH
- JAXZUE
- JEYVEC
- JEYJIG
- JIYKIM
- JUFCUI
- KEKVOO
- KEKWOP
- KERVOT
- KEVQOS
- KOCZUA
- KOSKIM
- KOXWEZ
- KUSPAQ
- KUZVIL
- LAPROL
- MESSEQ
- MIFFOX
- NATWAJ
- NAVCAR
- NELYAH
- NETZIV
- OCOSEG
- ODAVIZ**
- OFOQOQ
- OKADOW
- OKIGIA
- OPUPAT
- PADKUE
- PAWWOA
- PEGZOQ
- PEHCOV
- POOHFK

196 structures

Click through the refcode list

CCDC

# Mogul Geometry Check – Mercury view



CSD Refcode  
ODAVIZ

Reminder – you can look at ADPs when available by going to Style >Ellipsoid (only available if included in file)

Reminder – disordered atoms in the CSD are often suppressed and can be coloured differently using Colour > by Element or Suppression

CCDC

# Mogul Geometry Check – Build query

CCDC Mogul 2020.3.0: AABHTZ (P-1) - Mercury

File Searches Databases Help

Build query Results and analysis View structures

Current Selection:  
C6 C5 Cl2

Search All fragments... Settings... Reset

Edit... Auto Edit... Draw... Load...

Hide hydrogens Show labels

Search progress: Stop

Current selection

Current measurement

Learn about building and editing a Mogul query in Exercise 2 of the handout.

The screenshot shows the CCDC Mogul software interface. In the top-left corner, the title bar reads "CCDC Mogul 2020.3.0: AABHTZ (P-1) - Mercury". Below the title bar is a menu bar with "File", "Searches", "Databases", and "Help". The "Build query" tab is selected, indicated by a blue border. To its right are "Results and analysis" and "View structures". On the left, there's a sidebar with "Current Selection" set to "C6 C5 Cl2", followed by "Search", "All fragments...", "Settings...", and "Reset" buttons. Below this are "Edit...", "Auto Edit...", "Draw...", and "Load..." buttons. At the bottom left are checkboxes for "Hide hydrogens" and "Show labels". The main workspace is a black area containing a chemical structure. A green line highlights a bond length, which is labeled "121.43". A blue arrow points from the text "Current selection" to the "C6 C5 Cl2" entry in the sidebar. Another blue arrow points from the text "Current measurement" to the highlighted bond length. A yellow callout box in the bottom-right corner contains the text: "Learn about building and editing a Mogul query in Exercise 2 of the handout." At the very bottom of the interface, there's a "Search progress:" bar with a "Stop" button.

# Mogul Settings

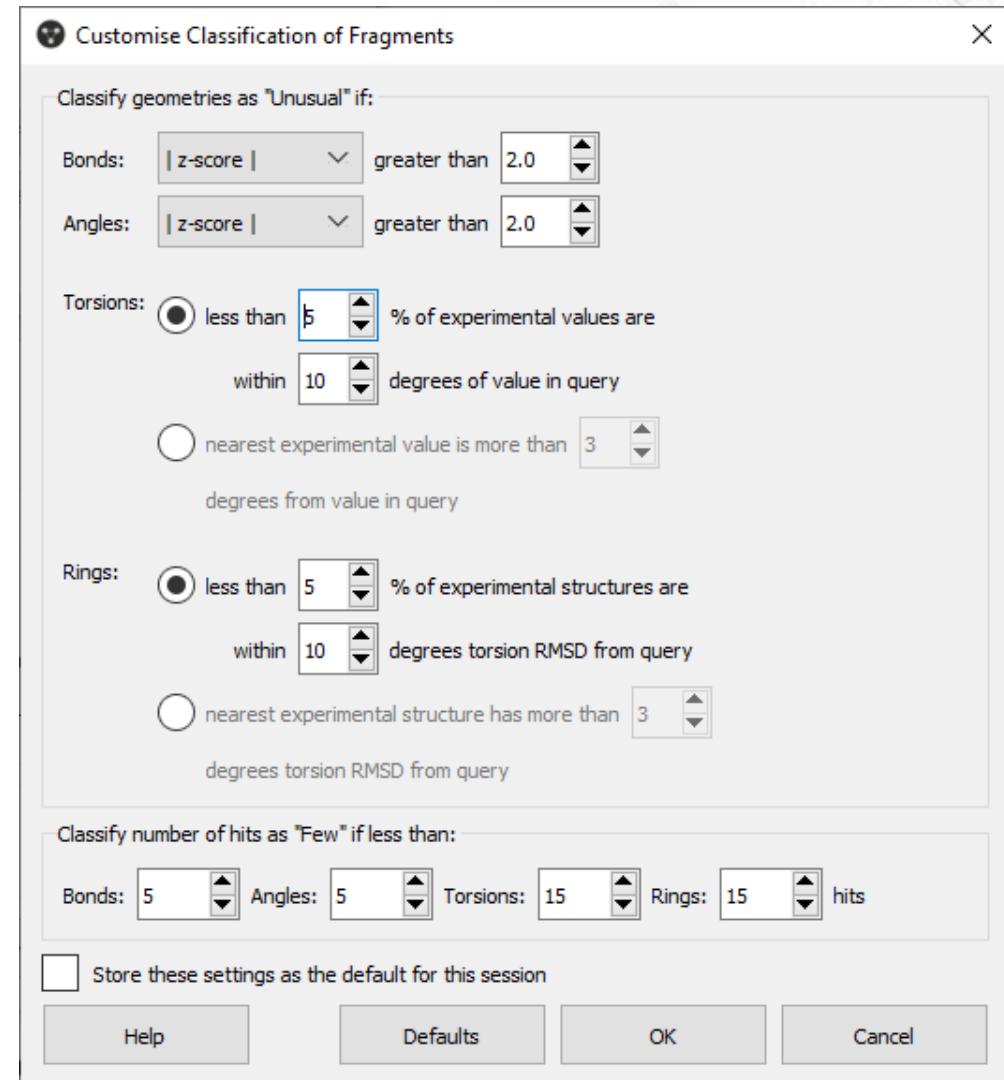
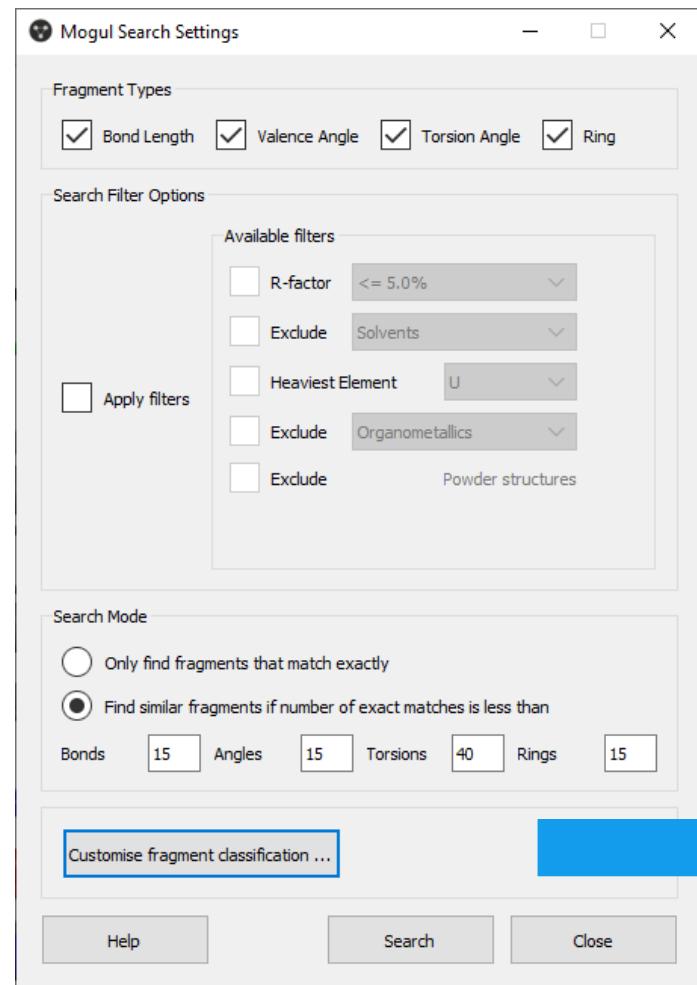
The screenshot shows the CSD Core interface with the following details:

- Top Bar:** File, Edit, Selection, Display, Calculate, CSD-Community, CSD-Core (highlighted), CSD-Materials, CSD-Discovery, CSD Python API, Help.
- Picking Mode:** Pick Atoms, Clear Measure.
- Style:** Polyhedral, Colour: by Element.
- View Options:** Animate..., Default view: b, a, b, c, a\*, b\*.
- Chemical View:** A 3D molecular model of a complex organic molecule.
- Menu:** CSD-Core dropdown menu with the following items:
  - Launch WebCSD
  - ConQuest Hit Highlighting...
  - Launch ConQuest
  - Data Analysis Module...
  - Mogul Geometry Check...
  - Mogul Settings...** (highlighted)
  - IsoStar Interaction Check...
  - Launch IsoStar
  - IsoStar Settings...
  - Select Databases...
- Central Panel:** A search interface with fields: All atoms, with Atom Label, Options: +90 y-90 y+90 z-90, and a large blue arrow pointing right.
- Right Panel:** Mogul Data Library Settings dialog box.
  - Title:** Mogul Data Library Settings
  - Text:** Select which Mogul data libraries to include in new searches
  - Buttons:** Add, Delete
  - Table:** Includes three entries:

Include Library	Path To Data
1 <input checked="" type="checkbox"/> CSD 5.42	C:\Program Files\CCDC\CSD_2021\Mogul V5.42
2 <input checked="" type="checkbox"/> CSD Feb21 update	C:\Program Files\CCDC\CSD_2021\Mogul V5.42\Feb21
3 <input checked="" type="checkbox"/> CSD May21 update	C:\Program Files\CCDC\CSD_2021\Mogul V5.42\May21
  - Buttons:** OK, Cancel
- Bottom Panel:** A list of database entries:

AADAMLC	P21/C
AADMPLY	P-1
AADMPLY10	P-1
AADRIB	P21
AAGAGG10	P2121
AAGGAG10	P21
AALCFE	P21/c
- Bottom Right:** CCDC logo.

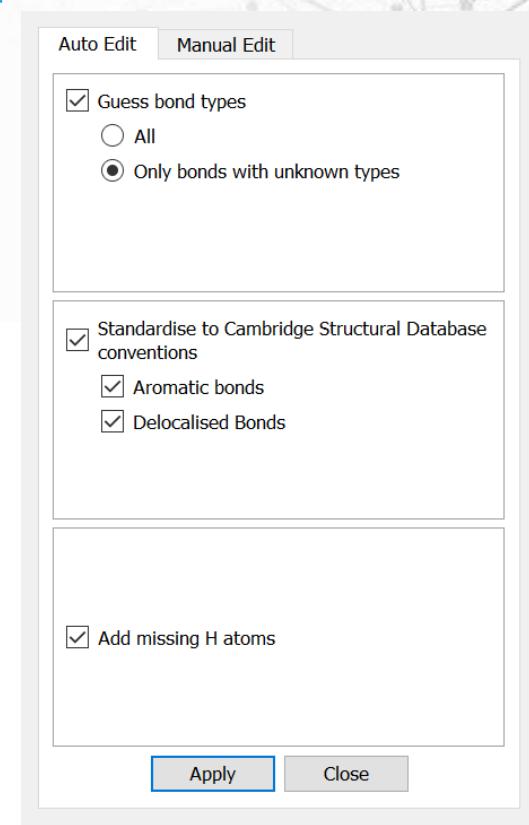
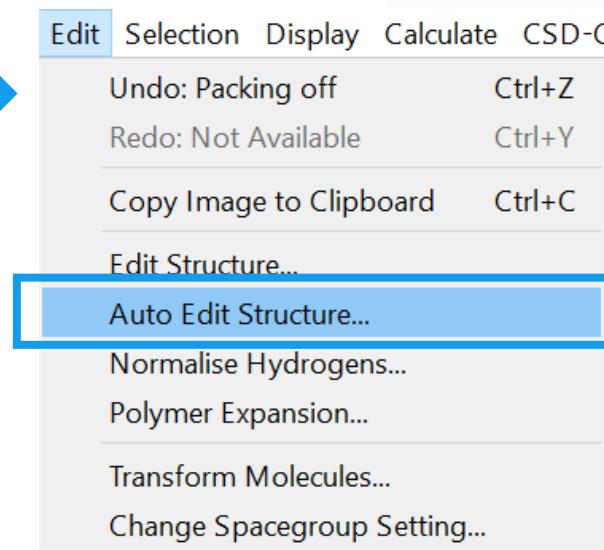
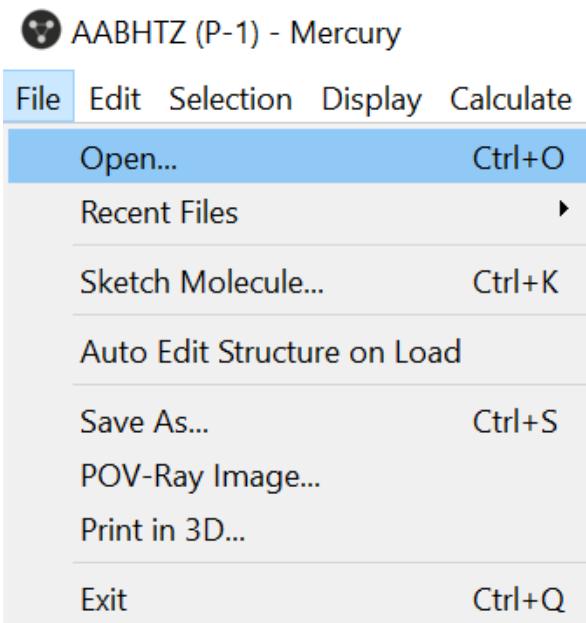
# Customise fragment classification



# Using Mogul to check a new structure

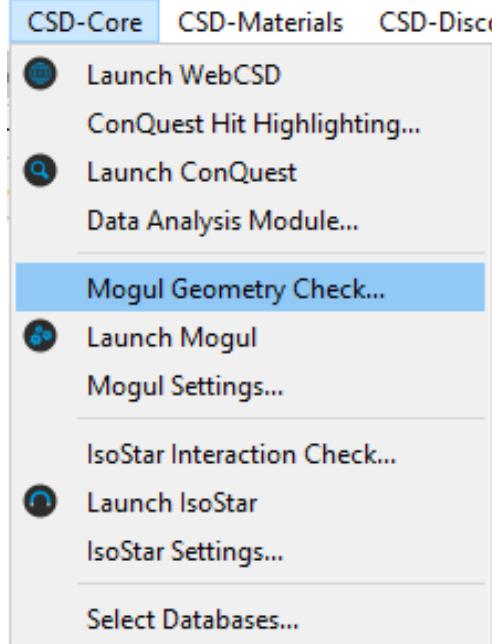
## 1. Load your structure in Mercury

- Do you remember how to do it from the Visualisation session?
- 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



# Using Mogul to check a new structure

2. Repeat the procedure you did before



The screenshot shows the CSD interface with the 'CSD-Core' tab selected. In the main menu, the 'Mogul Geometry Check...' option is highlighted.

**Mogul Results Viewer**

Double click to view result in Mogul

Type	Molecule	Fragment	Classification	No. of hits	Query value	Me:
> bond	C59 O58 C1 C2		Not unusual (enough hits)	13461		
> angle	C59 O58 C1 C6		Not unusual (enough hits)	13461		
▼ torsion	O23 C21 N11 C12		Not unusual (enough hits)	45		
	C24 C22 C21 N11		Not unusual (enough hits)	40		
	C22 C24 N27 C30		Not unusual (enough hits)	938		
	C22 C24 N27 C34		Not unusual (enough hits)	938		
	C45 C52 C43 C32		Not unusual (enough hits)	2357		
	C51 C52 C43 C32		Not unusual (enough hits)	2357		
	C22 C21 N11 C12		Not unusual (few hits)	3		
	O23 C21 N11 C10		Unusual (enough hits)	45		
	O23 C21 C22 C24		Unusual (enough hits)	42		
	C21 C22 C24 N27		Unusual (enough hits)	137		
	C31 C32 C43 C52		Unusual (enough hits)	131		
	C33 C32 C43 C52		Unusual (enough hits)	131		
	C22 C21 N11 C10		Unusual (few hits)	3		

**Results Navigator**

- All Hits: 137
- Accepted hits: 137
- R-factor: Any
- Heaviest Element: Any
- Exclude: None

Relevance	Number	Contribution
<input checked="" type="checkbox"/>	1.00	137 100.0%

**Statistics**

- Total : 137
- Selected : 137
- |d(min)| : 27.484°

**Histogram display**

Value in query: 22.055°

Number of hits

Torsion angle /°

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

**Data libraries**

- CSD 5.37
- CSD Nov15 update
- CSD Feb16 update

**Filters...**

**Cluster**

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

# Why use Mogul?

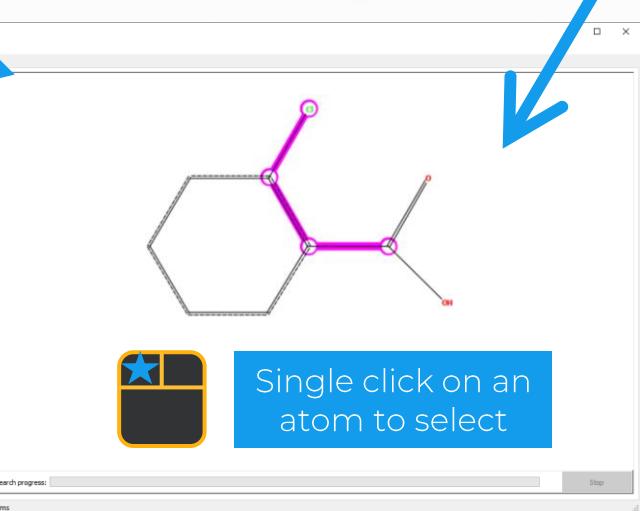
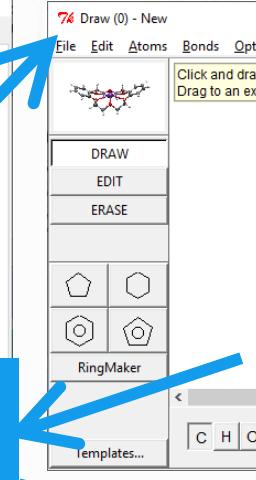
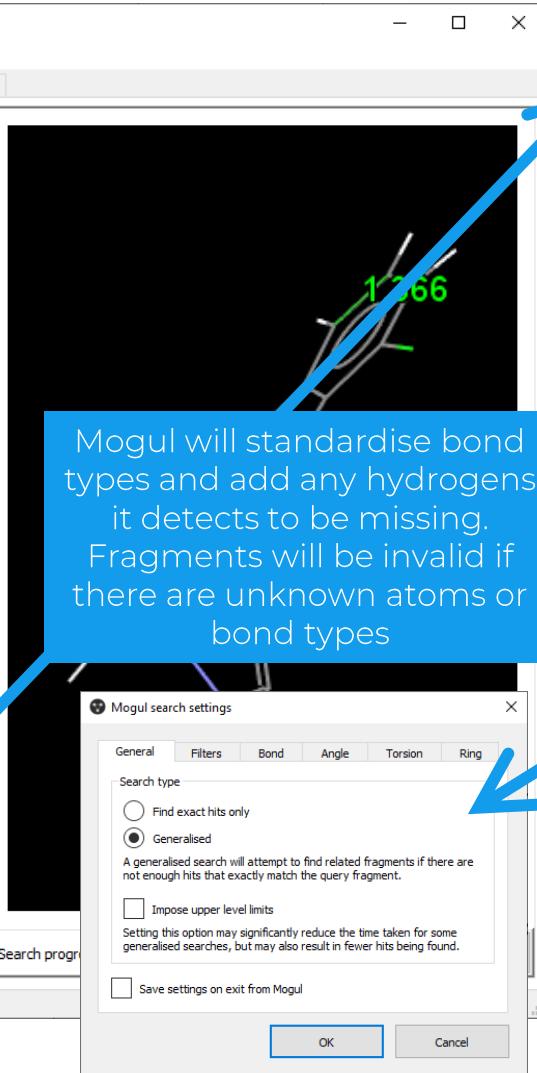
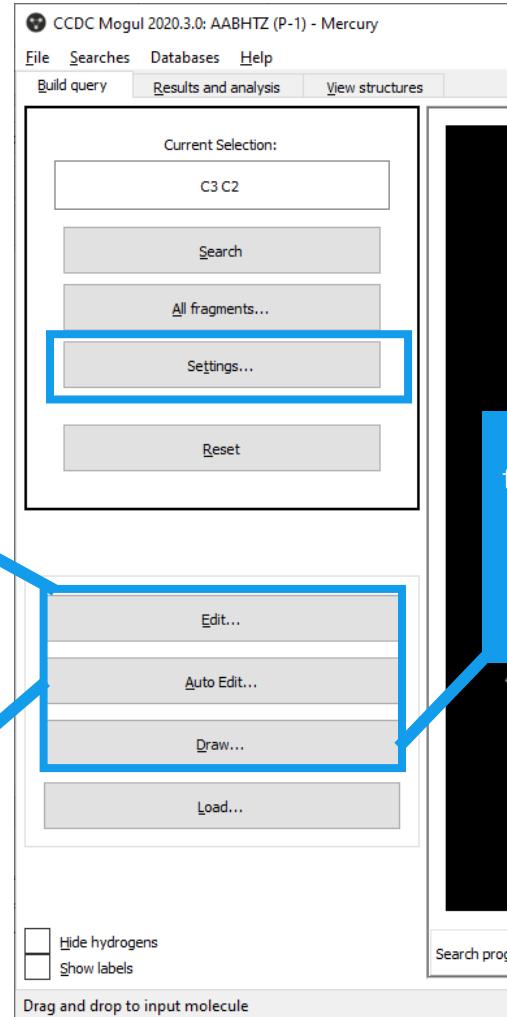
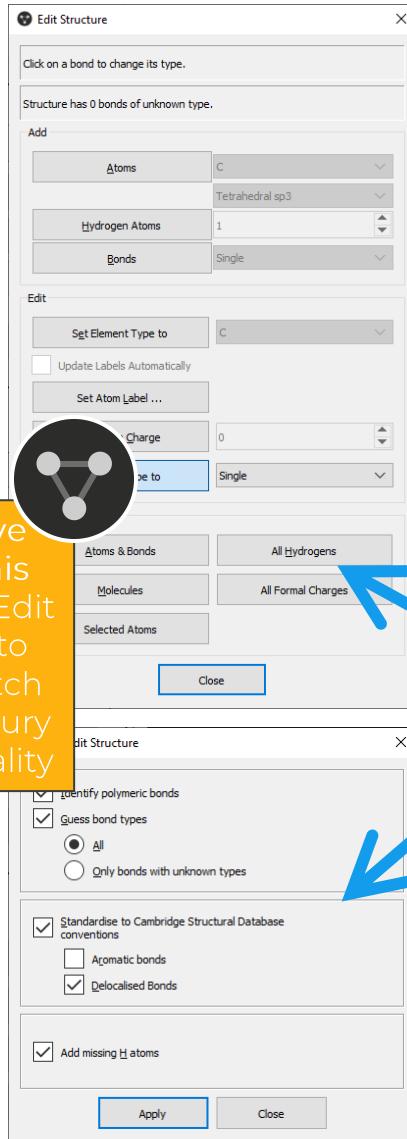
- To enable you to validate the complete geometry of a given query structure and identify any unusual features
  - Could be useful when looking at your own structure or a CSD structure or in fact ligands in the PDB
- To rapidly retrieve geometric data and gain new insights from structures in the CSD

# A few more tips & tricks



# Using the Draw feature in a Mogul Query

We have seen this before - Edit and Auto Edit match the Mercury functionality



We have seen the Draw window before in our ConQuest workshop



# Exporting data from Mogul

The screenshot shows the Mogul Results Viewer interface. At the top, there are buttons for 'Show / hide : Columns', 'Fragments...', 'Deselect all fragments', and 'Export...'. A blue arrow points from the 'Export...' button to a 'Save spreadsheet' dialog box. The dialog shows a file path of 'This PC > Downloads' and a dropdown menu for 'Save as type' with 'Comma-separated (\*.csv)' selected. Another blue arrow points from the 'Save as type' dropdown to a histogram below. The histogram displays the 'Number of hits' on the y-axis (0 to 66) against the 'Bond angle / °' on the x-axis (110 to 140). A red vertical line marks a value of 121.434°. A blue callout box with a star icon indicates that a right-click on the histogram brings up an additional menu. The menu items shown are 'Font...', 'Selection Bar Colour...', 'Deselected Colour...', 'Background Colour...', 'Select All Bars', 'Deselect All Bars', 'Print...', 'Export selected data', and 'Refcode and value only...'. The 'Export selected data' item is highlighted with a blue background.

Mogul Results Viewer

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

Help Double click to view result in Molecule Fragment

Type Molecule Fragment

AABHTZ

C2 C1 C11  
C6 C1 C11  
C2 C1 C6  
C3 C2 C1  
C4 C3 C2  
C3 C4 C5  
C4 C5 C12  
C6 C5 C12  
C4 C5 C6  
C1 C6 C5  
C5 C6 C7  
C1 C6 C7  
C6 C7 N1  
C7 N1 N2  
C8 N2 N1  
C12 N2 N1  
N2 C8 N3  
N5 C8 N3  
C8 N3 N4  
C9 N4 N3  
N5 C9 N4  
C8 N5 N6  
C9 N5 C8

Not unusual (enough hits) 449  
Not unusual (enough hits) 421  
Not unusual (enough hits) 13  
Not unusual (enough hits) 142  
Not unusual (enough hits) 142  
Not unusual (enough hits) 63  
Not unusual (enough hits) 304  
Not unusual (enough hits) 16  
Not unusual (enough hits) 15  
Not unusual (enough hits) 15  
Not unusual (enough hits) 18  
Not unusual (enough hits) 47  
Not unusual (enough hits) 190  
Not unusual (enough hits) 61  
Not unusual (enough hits) 15  
Not unusual (enough hits) 15

Save spreadsheet

This PC > Downloads

File name: Save as type: Comma-separated (\*.csv) Comma-separated (\*.csv) HTML (\*.html) XML (\*.xml)

Save Cancel

Mogul search - Bond angle - C6 C5 Cl2

Value in query: 121.434°

Number of hits

Bond angle / °

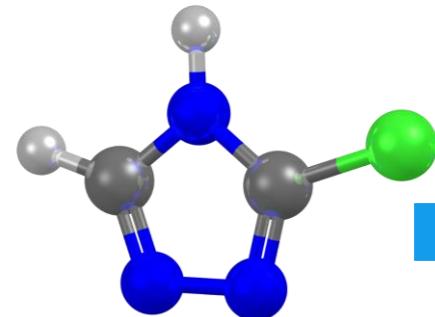
Right click on the histogram to bring up an additional menu

Font...  
Selection Bar Colour...  
Deselected Colour...  
Background Colour...  
Select All Bars  
Deselect All Bars  
Print...  
Export selected data Refcode and value only...

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

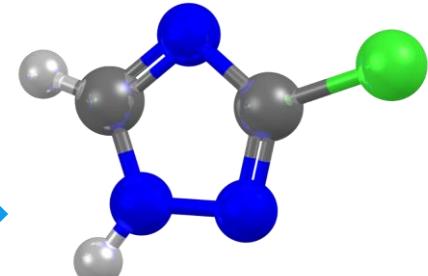
# Using Mogul to assign tautomeric forms

CSD CLTRZL

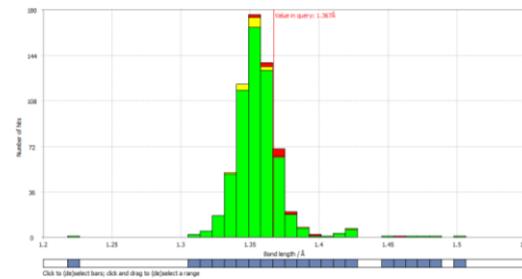
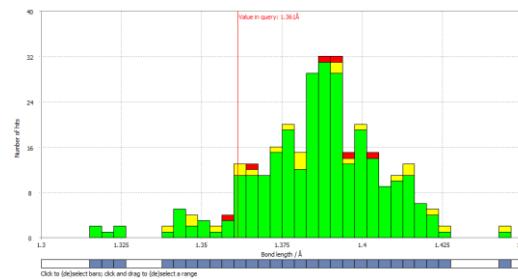


1.361 Å

CSD CLTRZL01

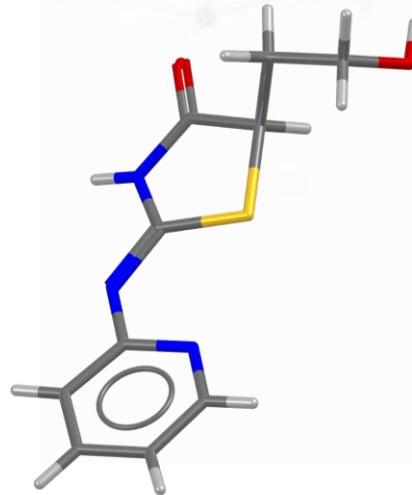


1.367 Å

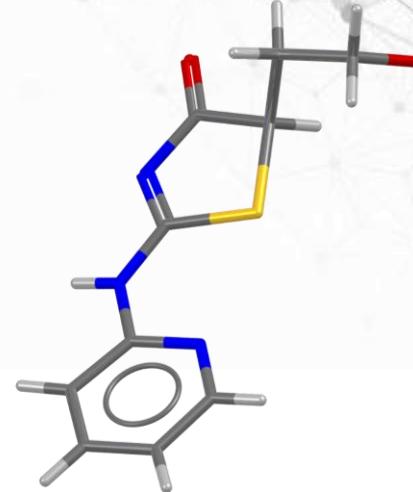


Following Mogul analysis structure re-determined in a different tautomeric form

CSD GACXOZ



CSD LOQBIE



A comparison of the 1,3-thiazol-4-one structures in which Mogul queries the C—N bond length of the imine of GACXOZ, but finds all geometrical parameters of the amine version to be within expected limits