How to analyse molecular geometry with Mogul

CCDC Virtual Workshop Summer 2021 – Session 1

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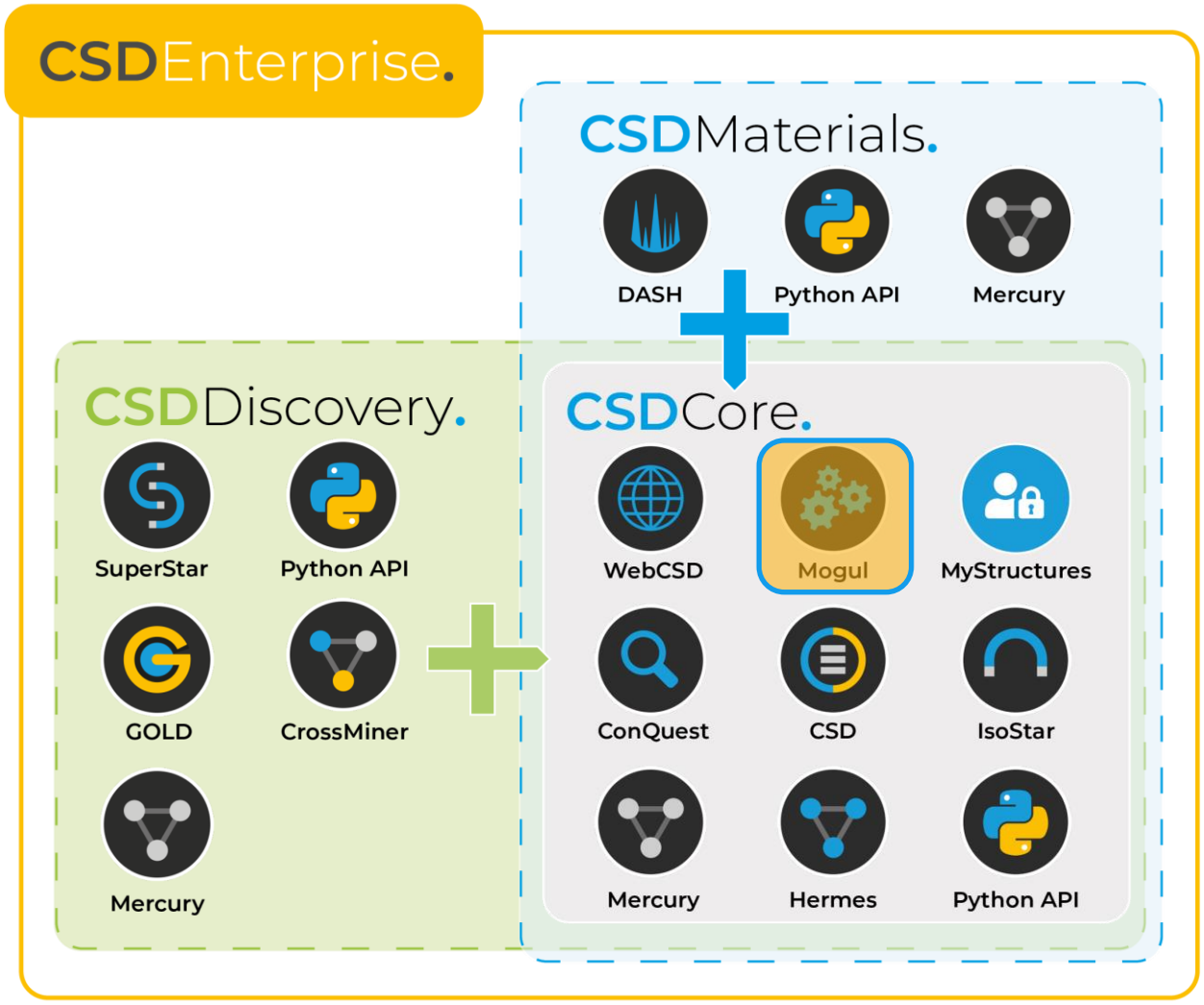
advancing structural science

Learning outcomes for today

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

The CSD software



Professional Services

Research & Knowledge partnerships

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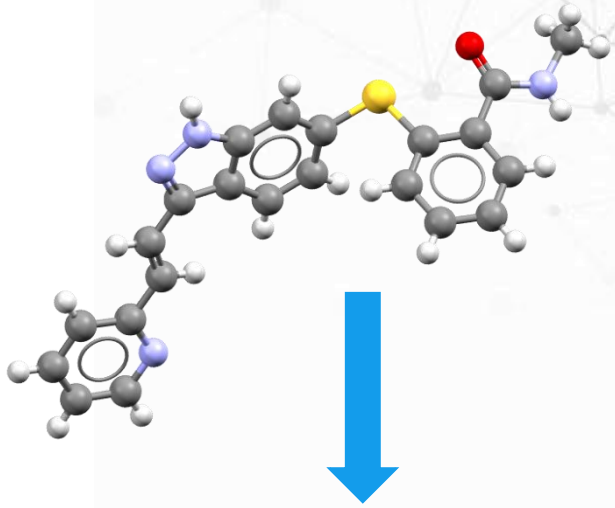
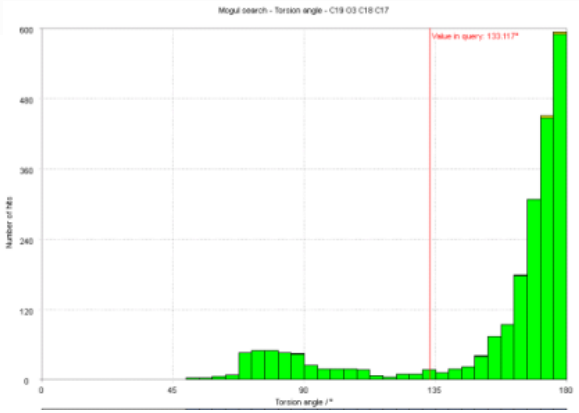
CSD-Core – Conformations

- 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

Bruno *et al., J. Chem. Inf. Comput. Sci.*, 44, 2133-2144, 2004

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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

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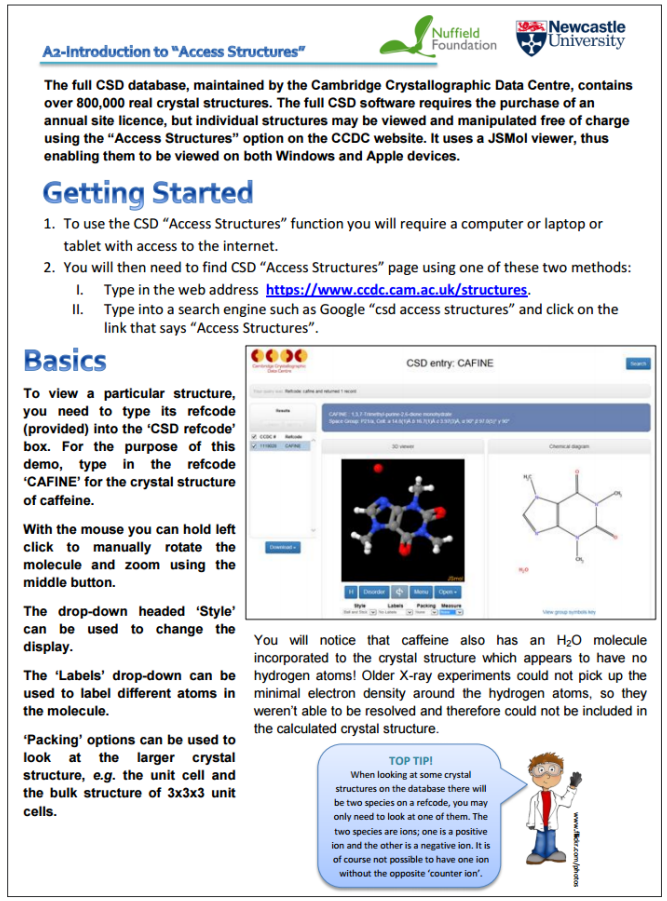
Using Mogul to teach chemistry



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 JSMol viewer, thus enabling them to be viewed on both Windows and Apple devices.

Getting Started

1. To use the CSD "Access Structures" function you will require a computer or laptop or tablet with access to the internet.
2. You will then need to find CSD "Access Structures" page using one of these two methods:
   I. Type in the web address https://www.ccdc.cam.ac.uk/structures.
   II. 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.

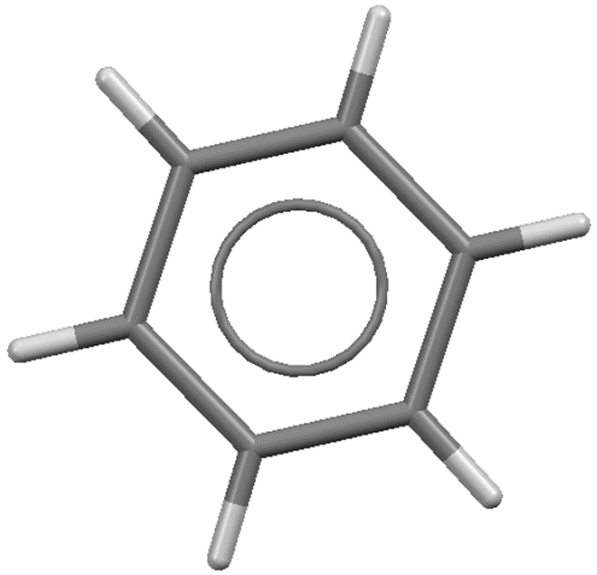
The drop-down headed 'Style' can be used to change the display.

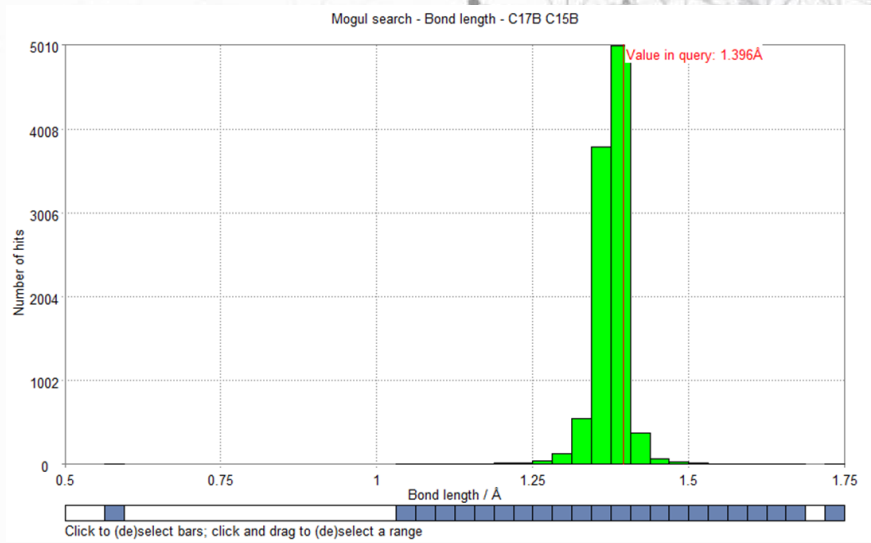
The 'Labels' drop-down can be used to label different atoms in the molecule.

'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.

You will notice that caffeine also has an H_2O molecule incorporated to the crystal structure which appears to have no hydrogen atoms! Older X-ray experiments could not pick up the minimal electron density around the hydrogen atoms, so they weren't able to be resolved and therefore could not be included in the calculated crystal structure.

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

https://www.ccdc.cam.ac.uk/Community/educationalresources/teaching-modules/

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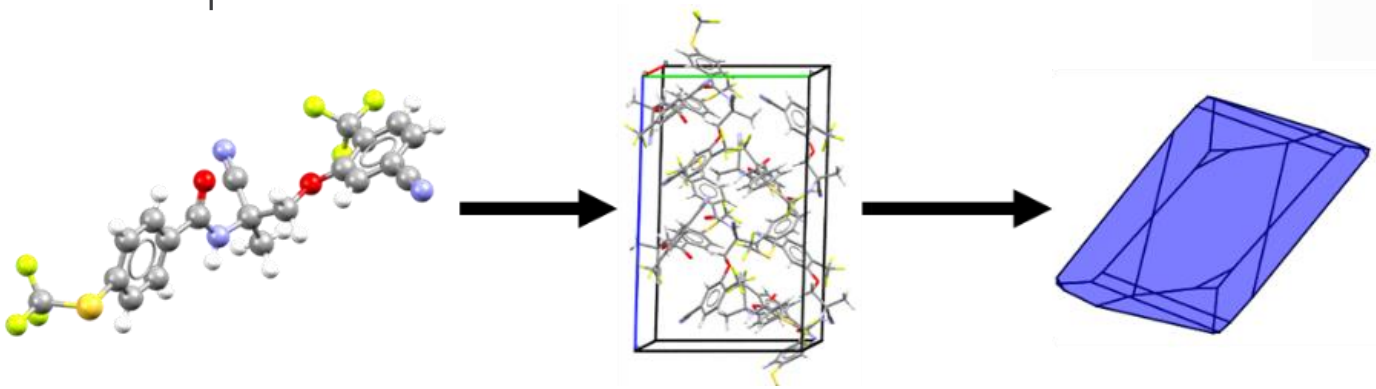
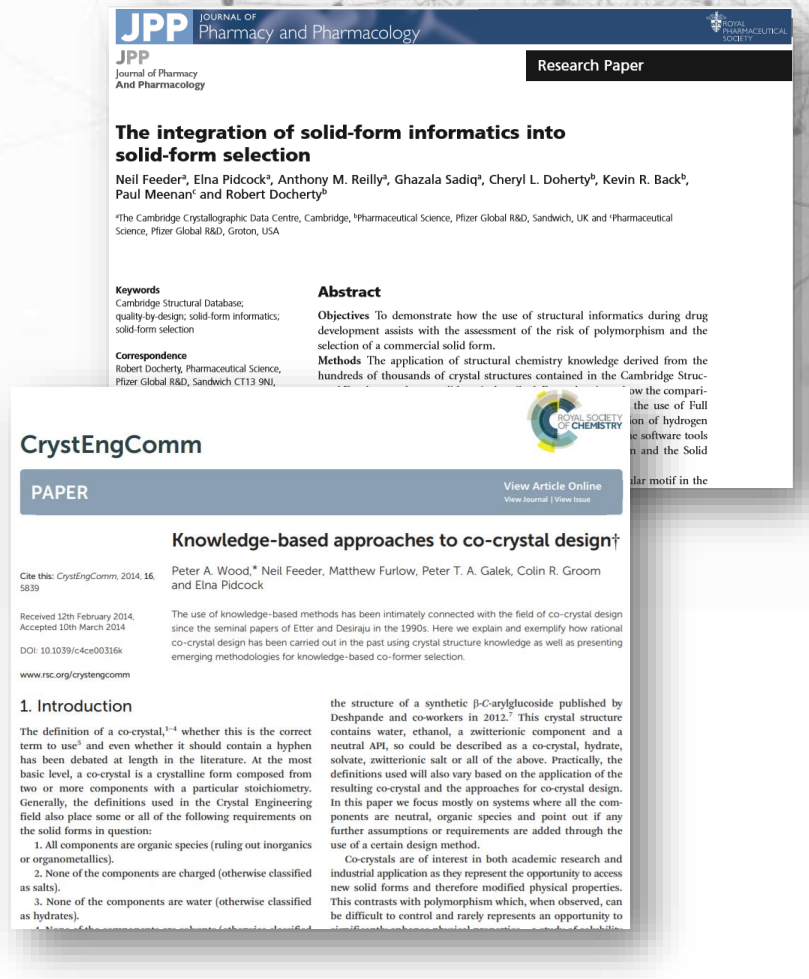
Using Mogul to inform key decisions

- 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

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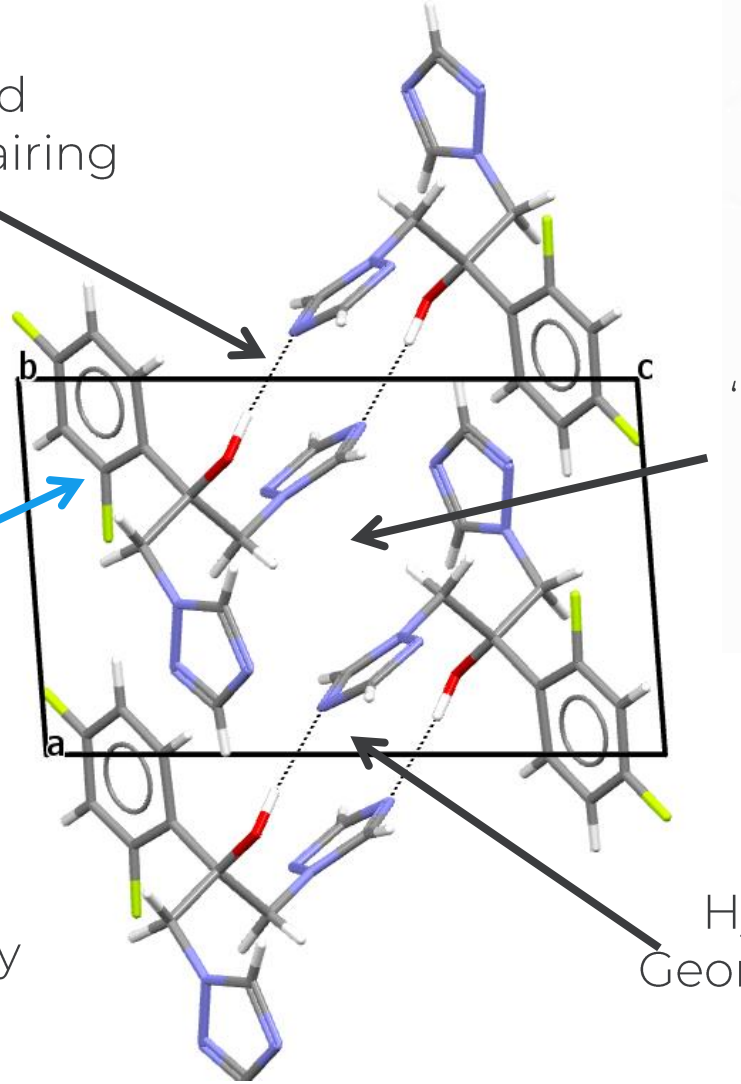
Characteristics that influence stability

Hydrogen Bond
Donor/Acceptor Pairing



'Non-Hydrogen Bond'
Intermolecular
Interactions

Molecular
Conformation

Hydrogen Bond
Geometry, Symmetry
and Motif

We can mine the CSD to identify these intra and intermolecular geometric preferences.

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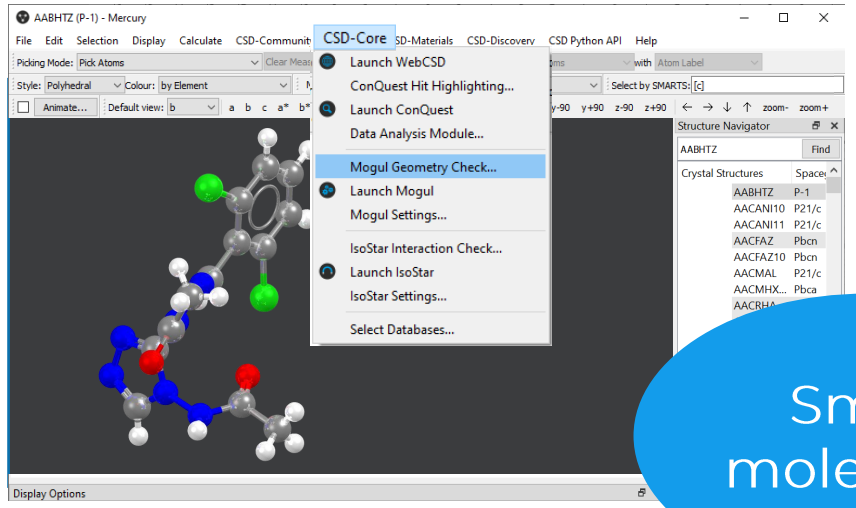
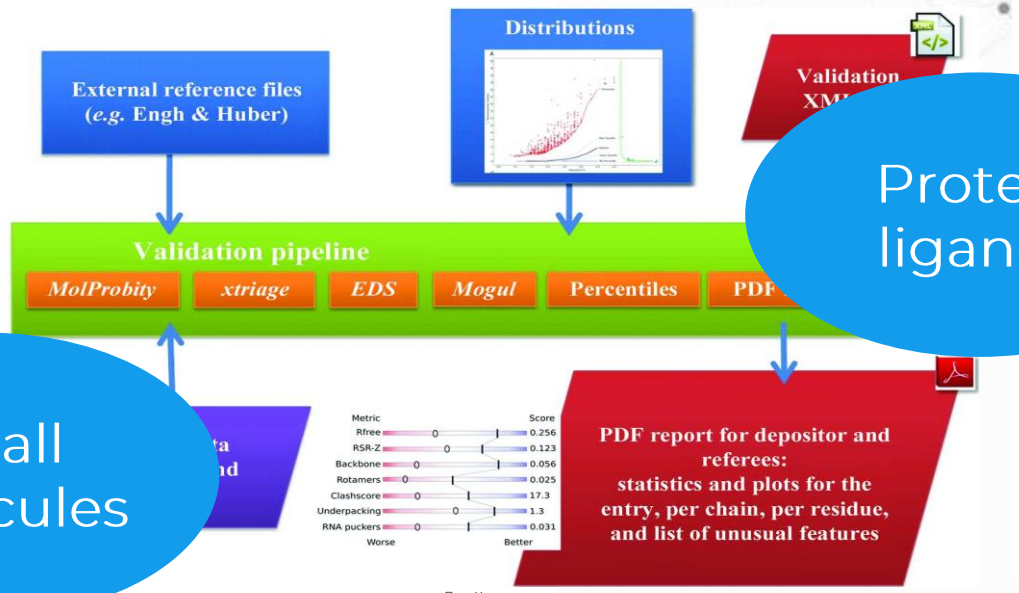
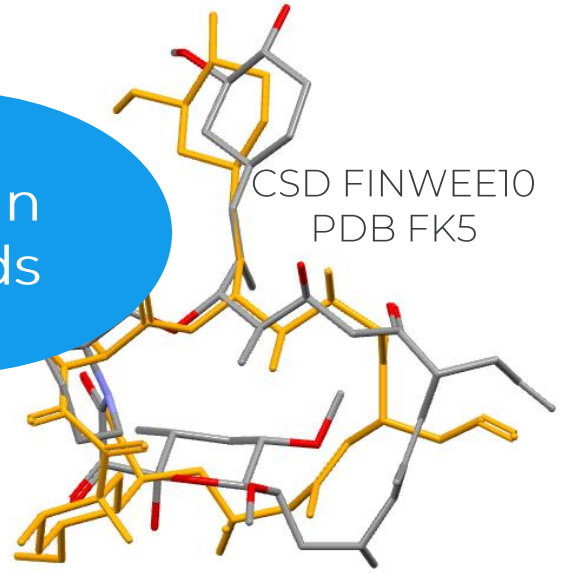
Using Mogul to check new structural data

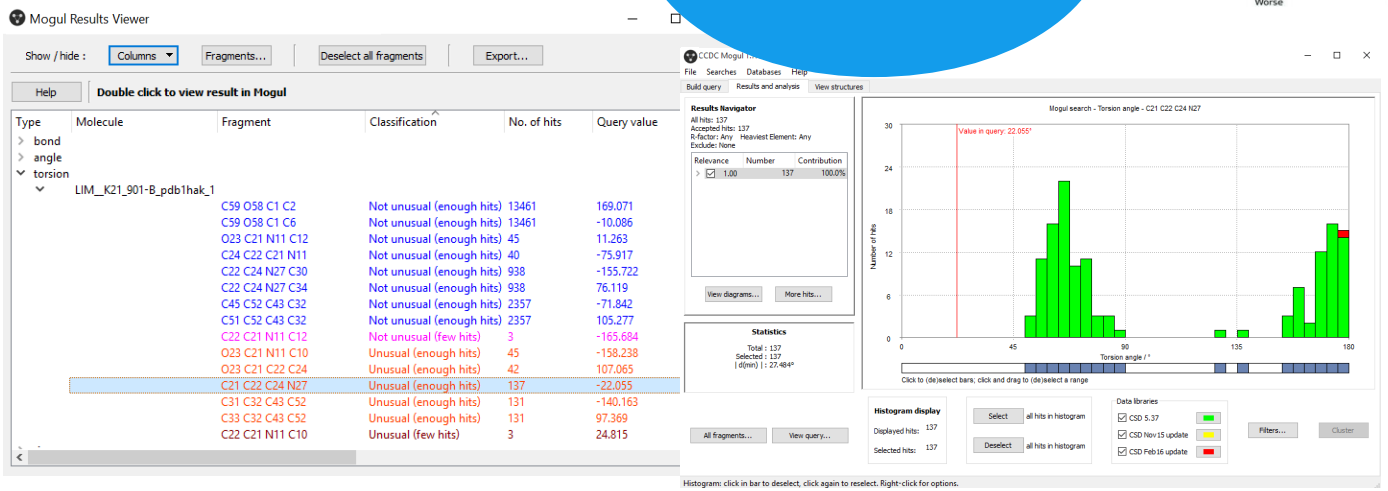


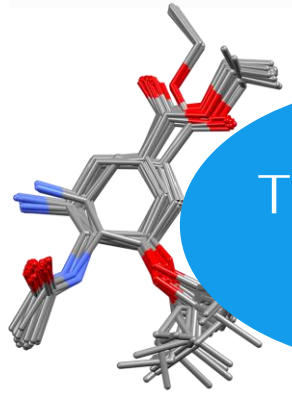


Small molecules

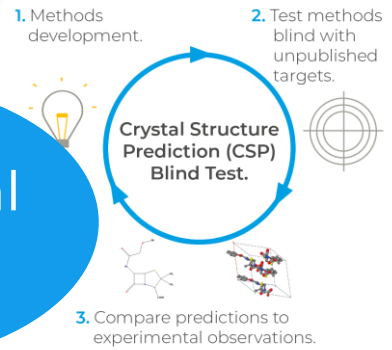
Protein ligands







Theoretical data



I.J.Bruno, G.P.Shields, R.Taylor, *Acta Cryst.* (2011). B67, 333-349 DOI: 10.1107/S0108768111024608

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Chemical coverage - the details....

- 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)

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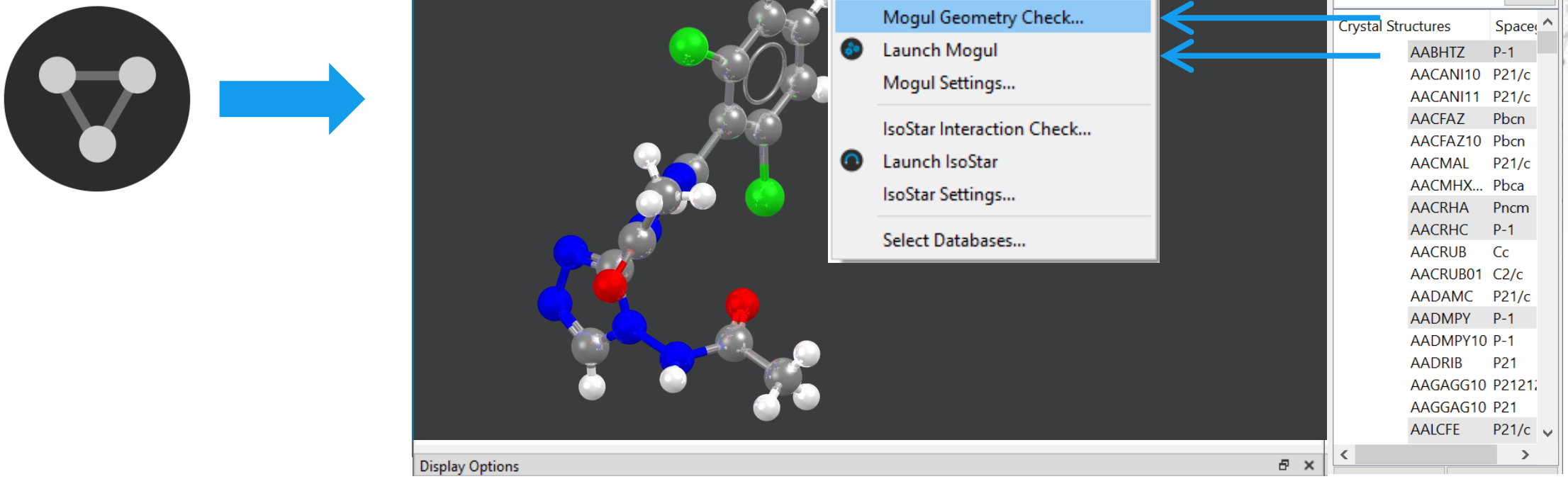
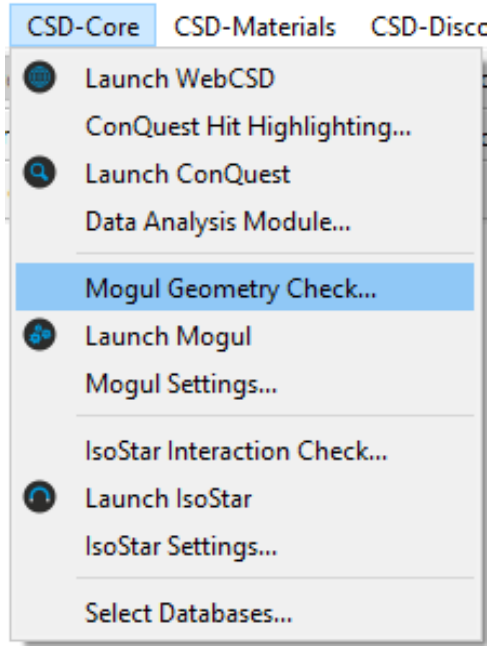
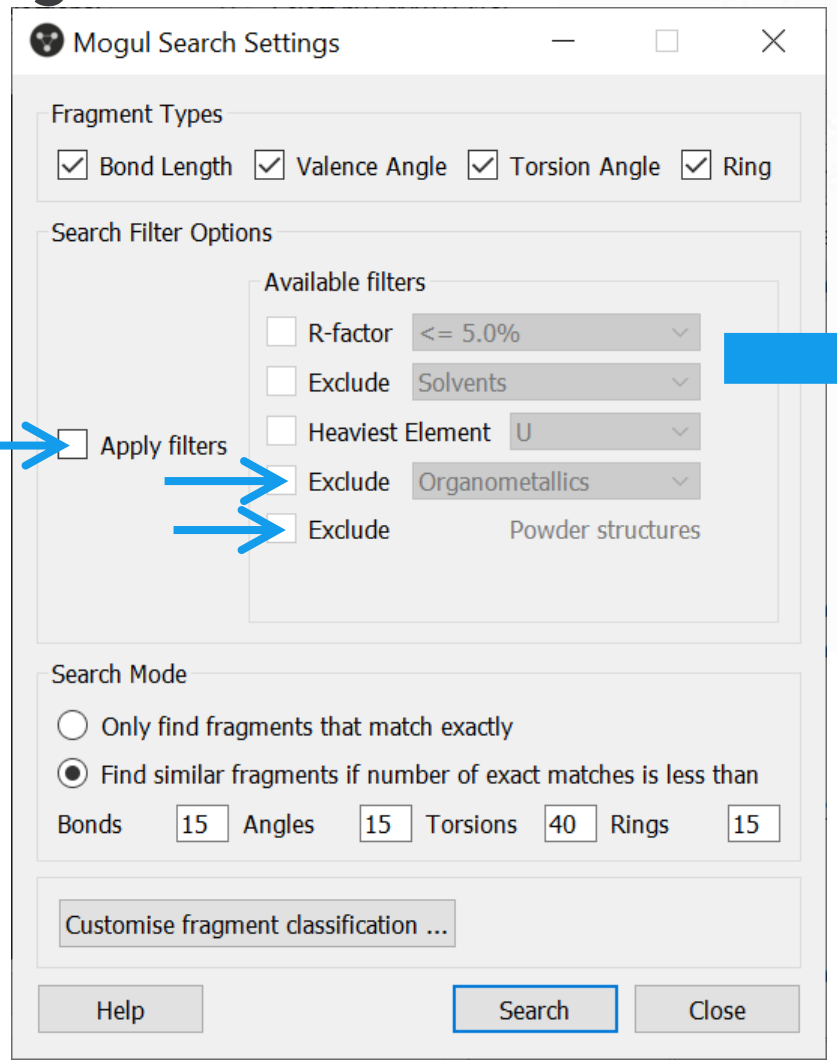
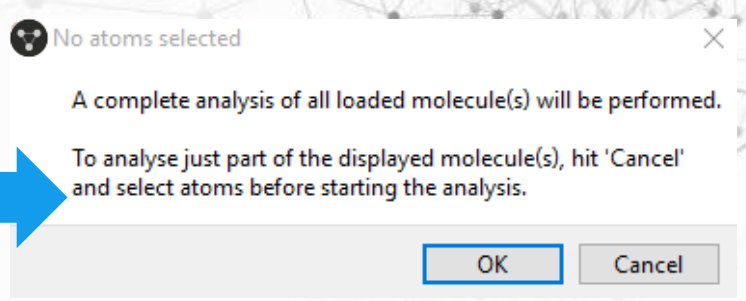
Show One: Mogul – Launch from Mercury

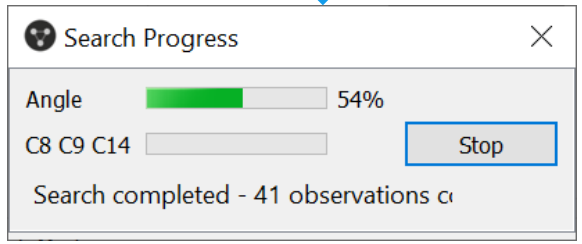


Mogul Geometry Check









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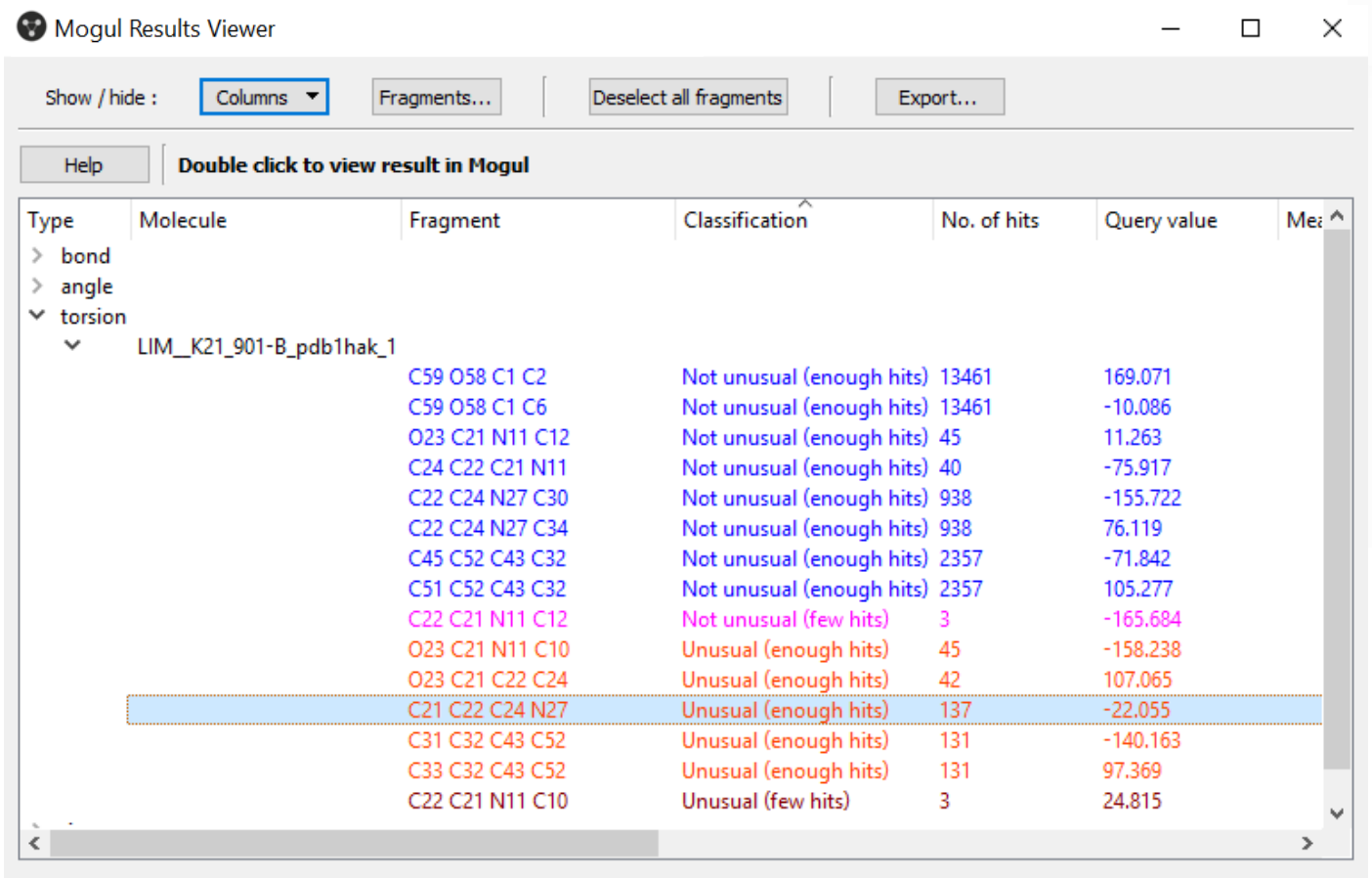
Mogul Geometry Check - Results



Type	Molecule	Fragment	Classification	No. of hits	Query value
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.

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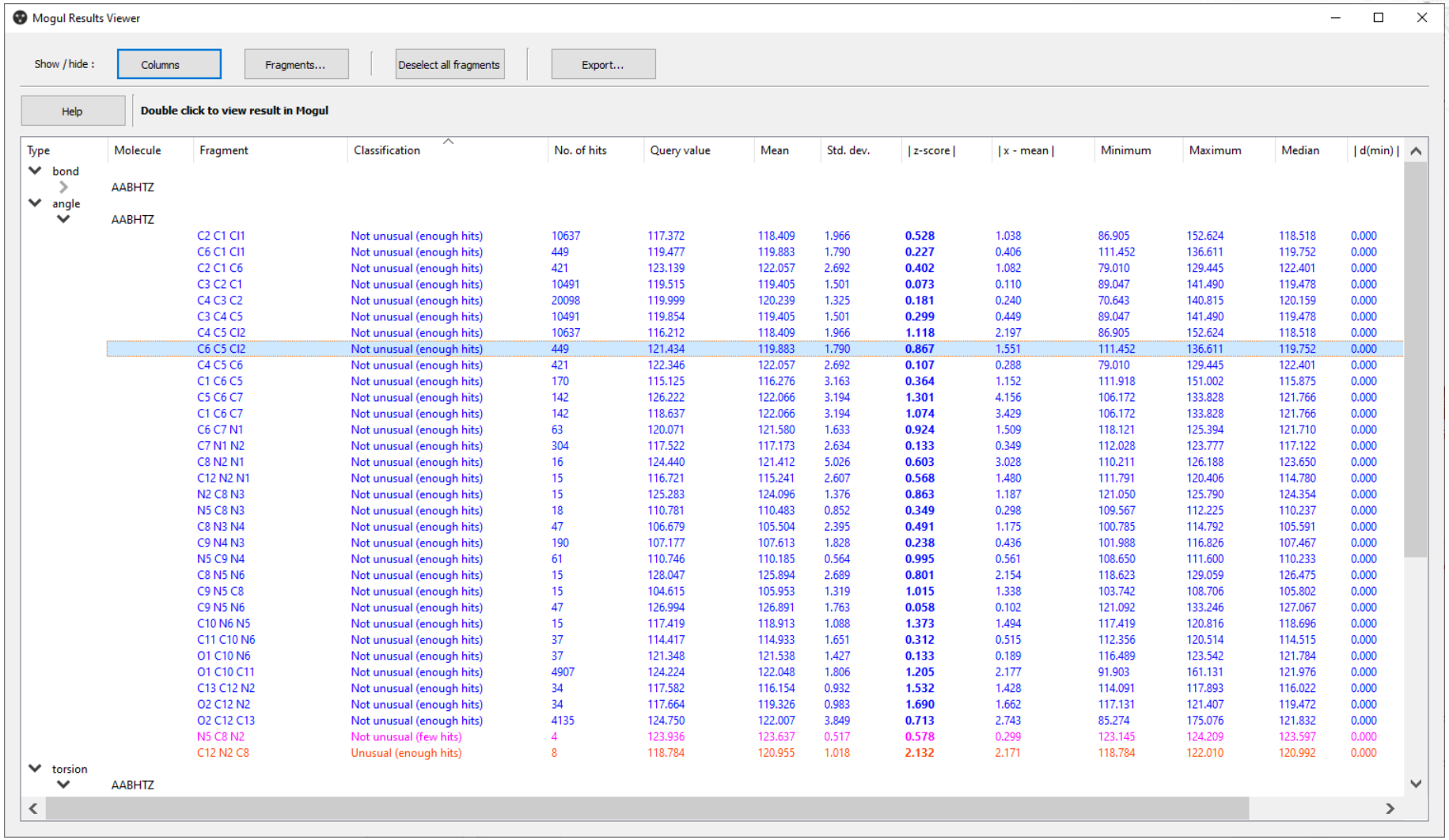
Mogul Geometry Check - Results



Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	| z-score |	| x - mean |	Minimum	Maximum	Median	| d(min) |
bond													
	AABHTZ												
angle													
	AABHTZ												
		C2 C1 Cl1	Not unusual (enough hits)	10637	117.372	118.409	1.966	**0.528**	1.038	86.905	152.624	118.518	0.000
		C6 C1 Cl1	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 Cl2	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 Cl2	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
torsion													
	AABHTZ												

Single click on a row to view result in Mercury

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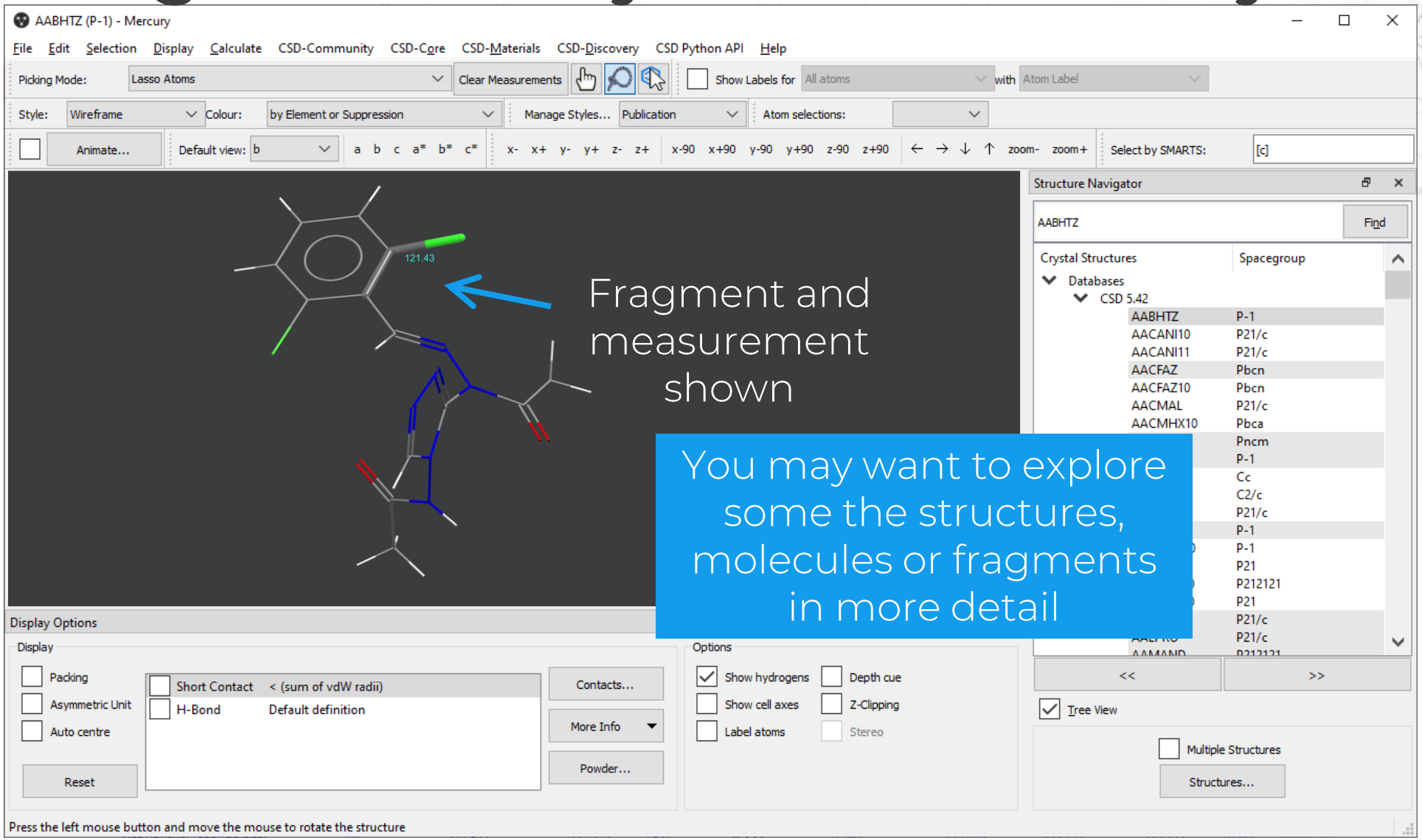
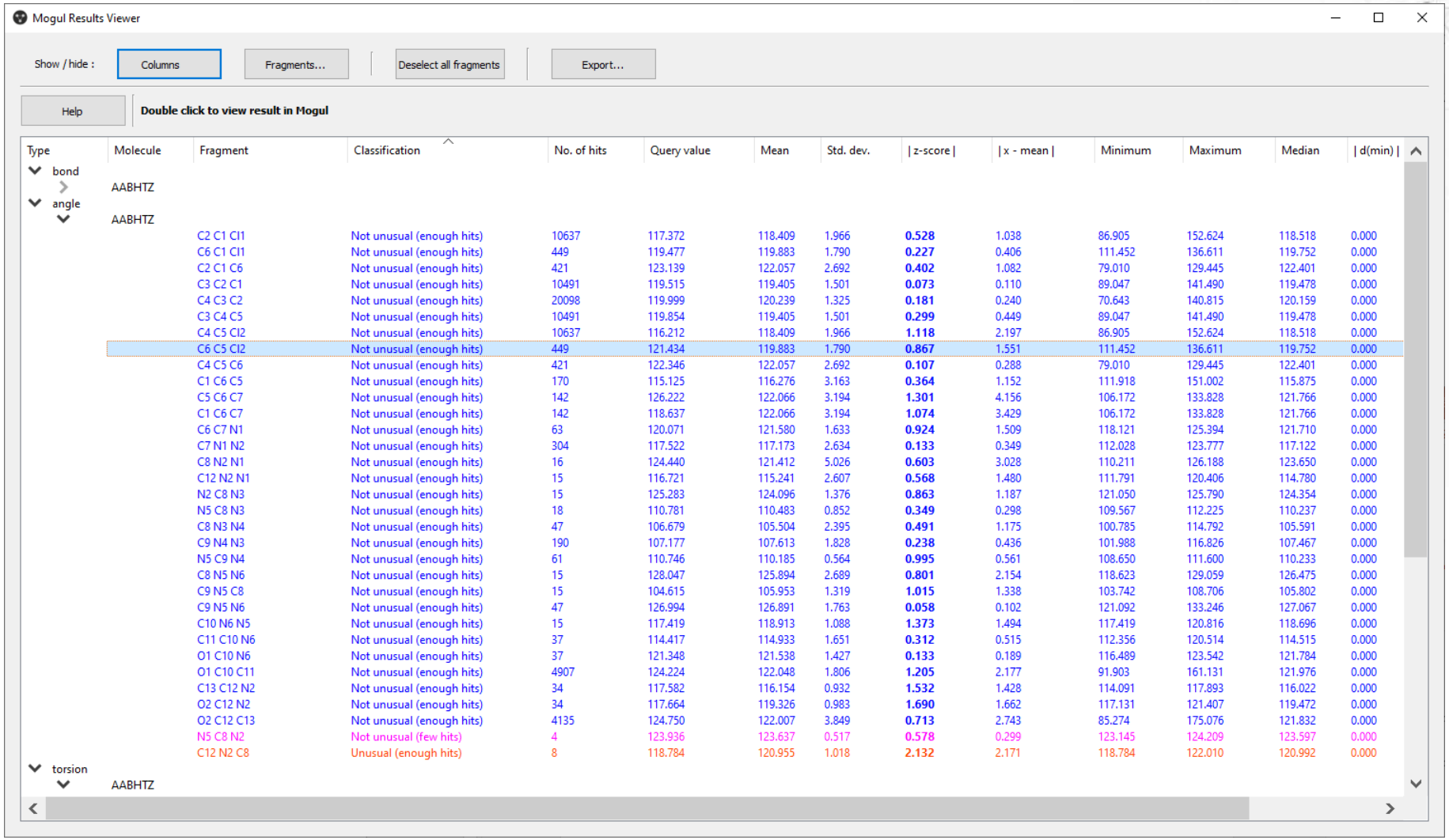
Mogul Geometry Check – Mercury view



Mogul Geometry Check - Results



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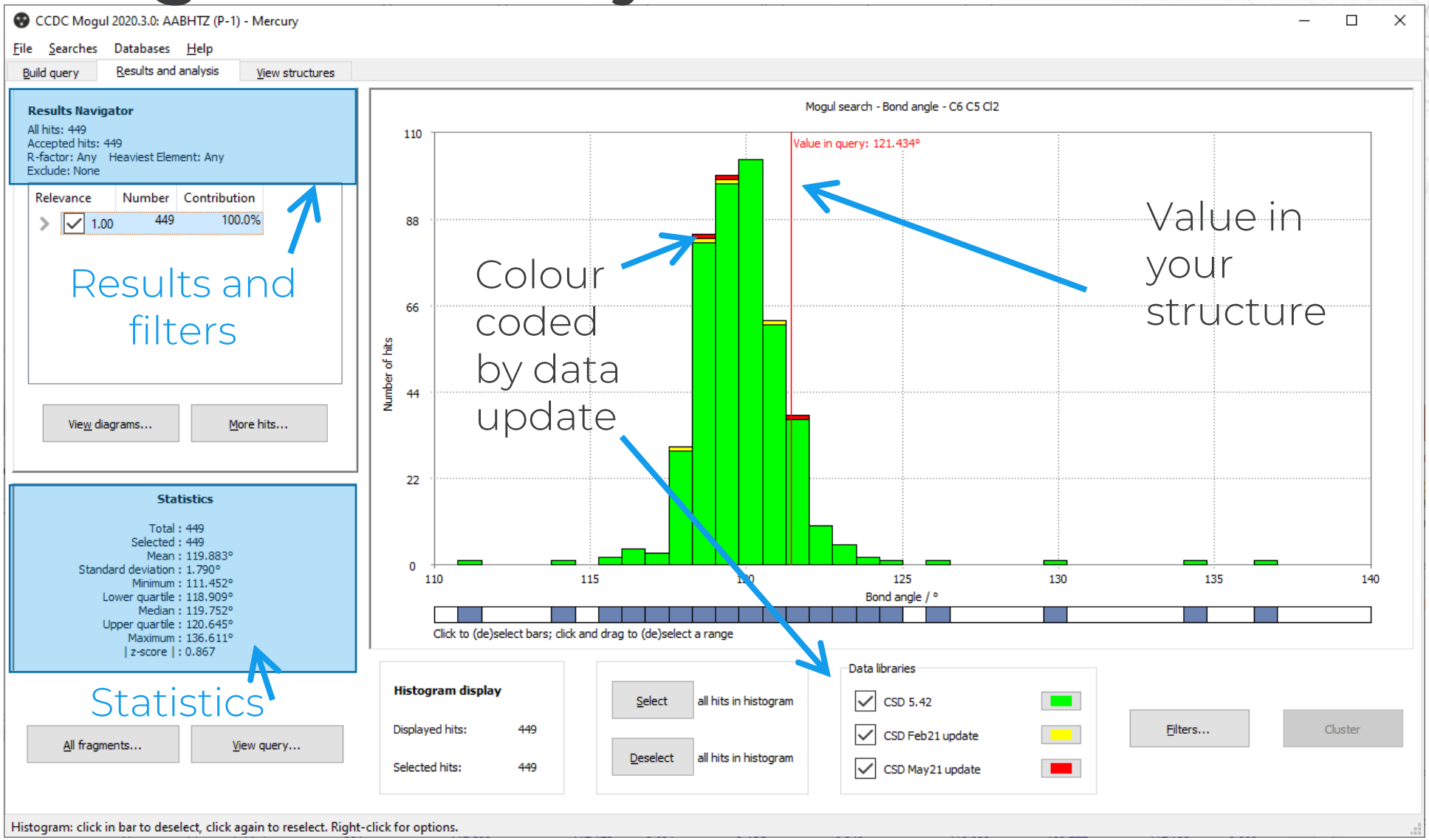
		C5 C6 C7	Not unusual (enough hits)	142	126.222	122.066	3.194	**1.301**	4.156	106.172	133.828	121.766	0.000
		C1 C6 C7	Not unusual (enough hits)	142	118.637	122.066	3.194	**1.074**	3.429	106.172	133.828	121.766	0.000
		C6 C7 N1	Not unusual (enough hits)	63	120.071	121.580	1.633	**0.924**	1.509	118.121	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
torsion													
	AABHTZ												

Double click on a row to view result in Mogul

CCDC

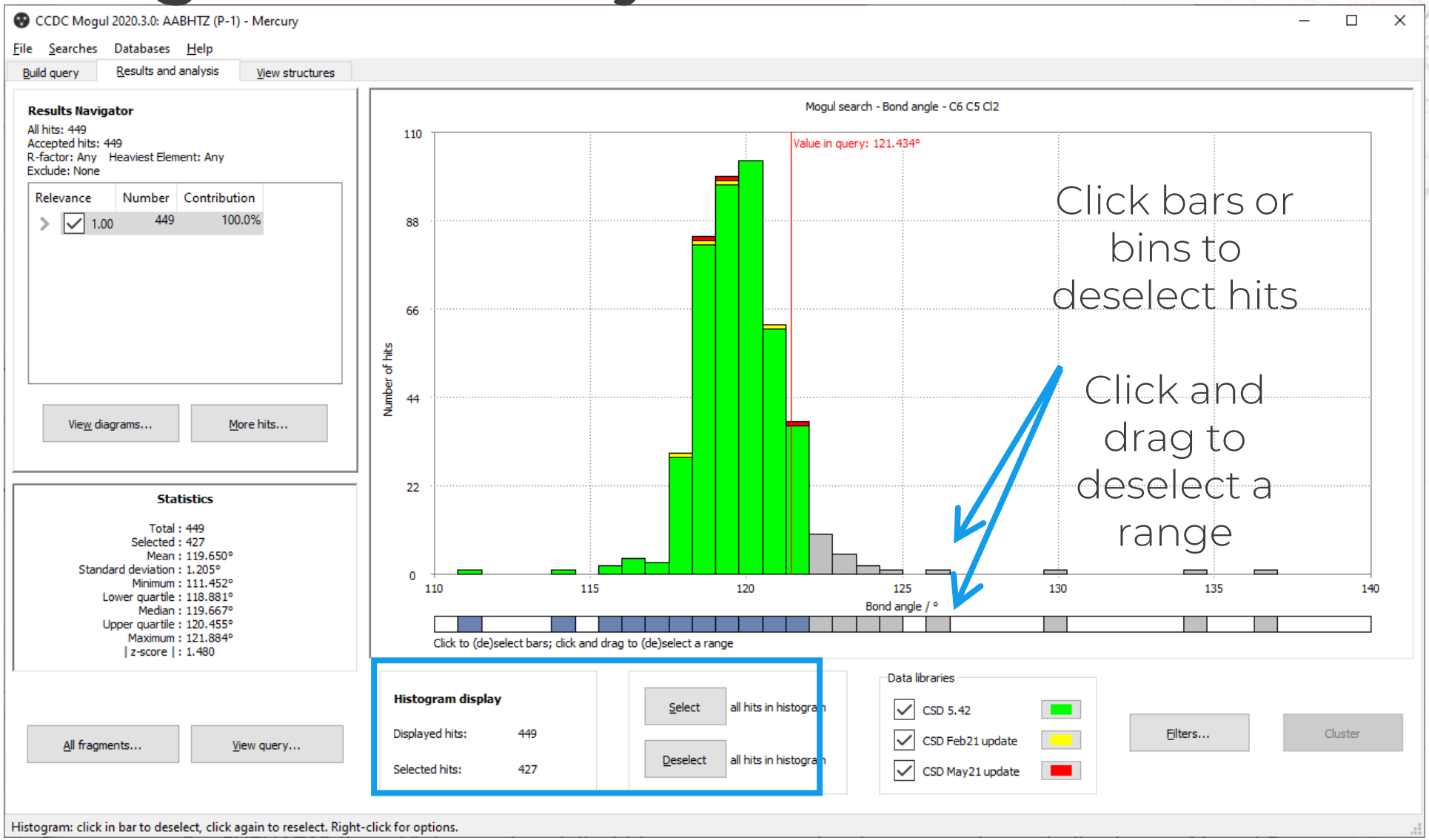
Mogul Geometry Check – Results



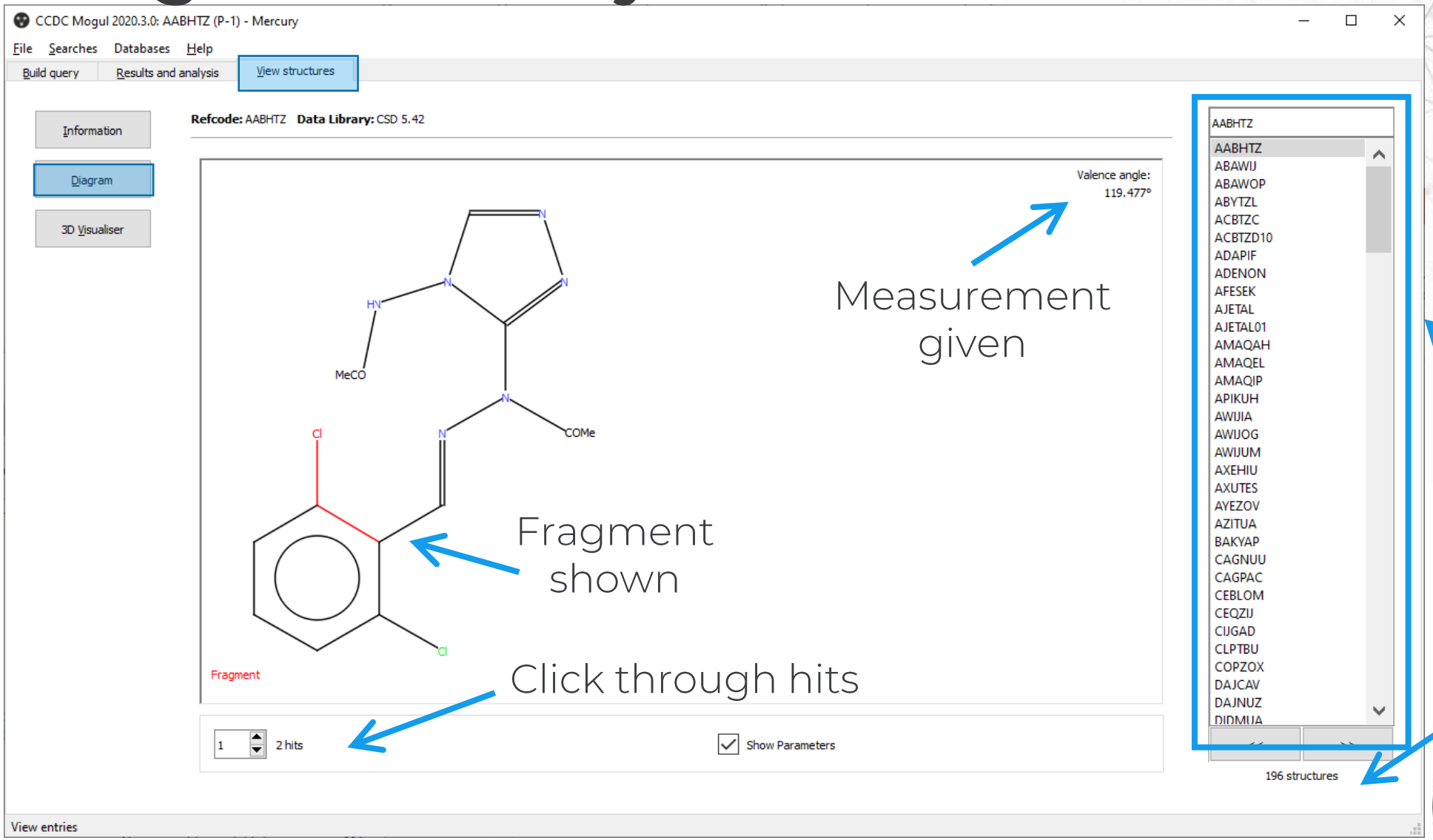
Histogram built with data from structures in the CSD

CCDC

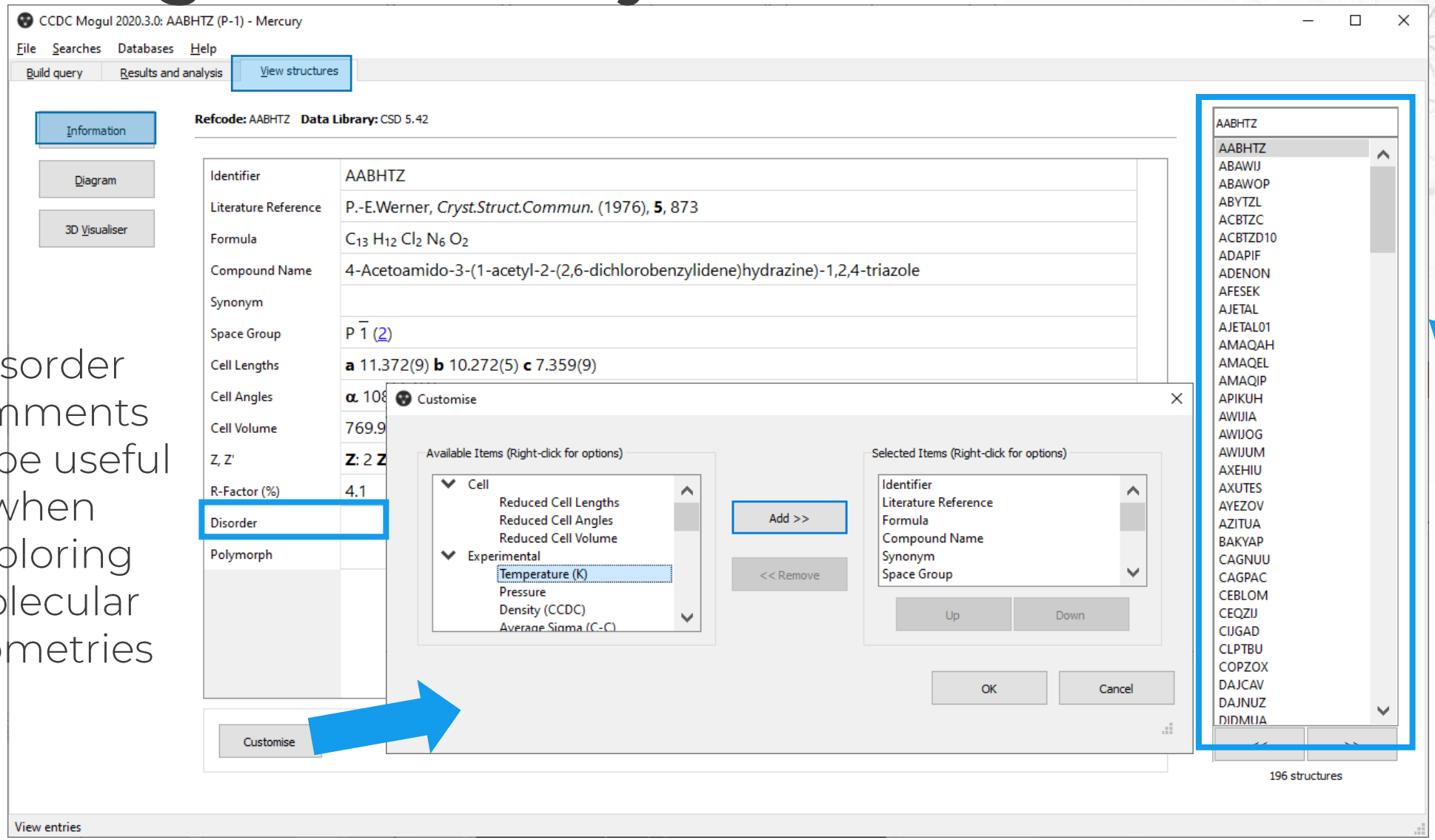
Mogul Geometry Check – Results



Mogul Geometry Check – View structures



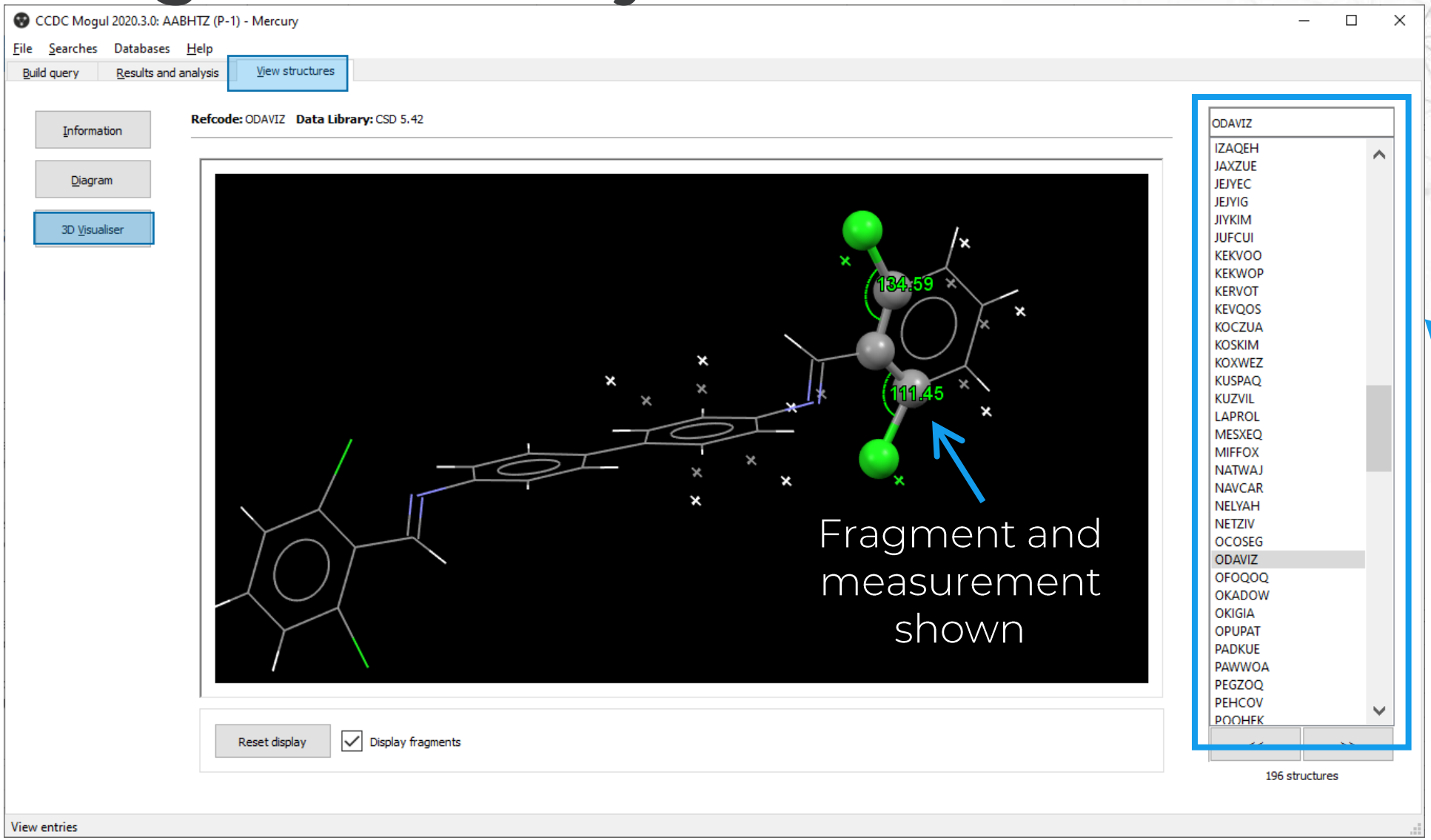
Mogul Geometry Check – View structures



Disorder comments can be useful when exploring molecular geometries

Click through the refcode list

Mogul Geometry Check – View structures



Click through the refcode list

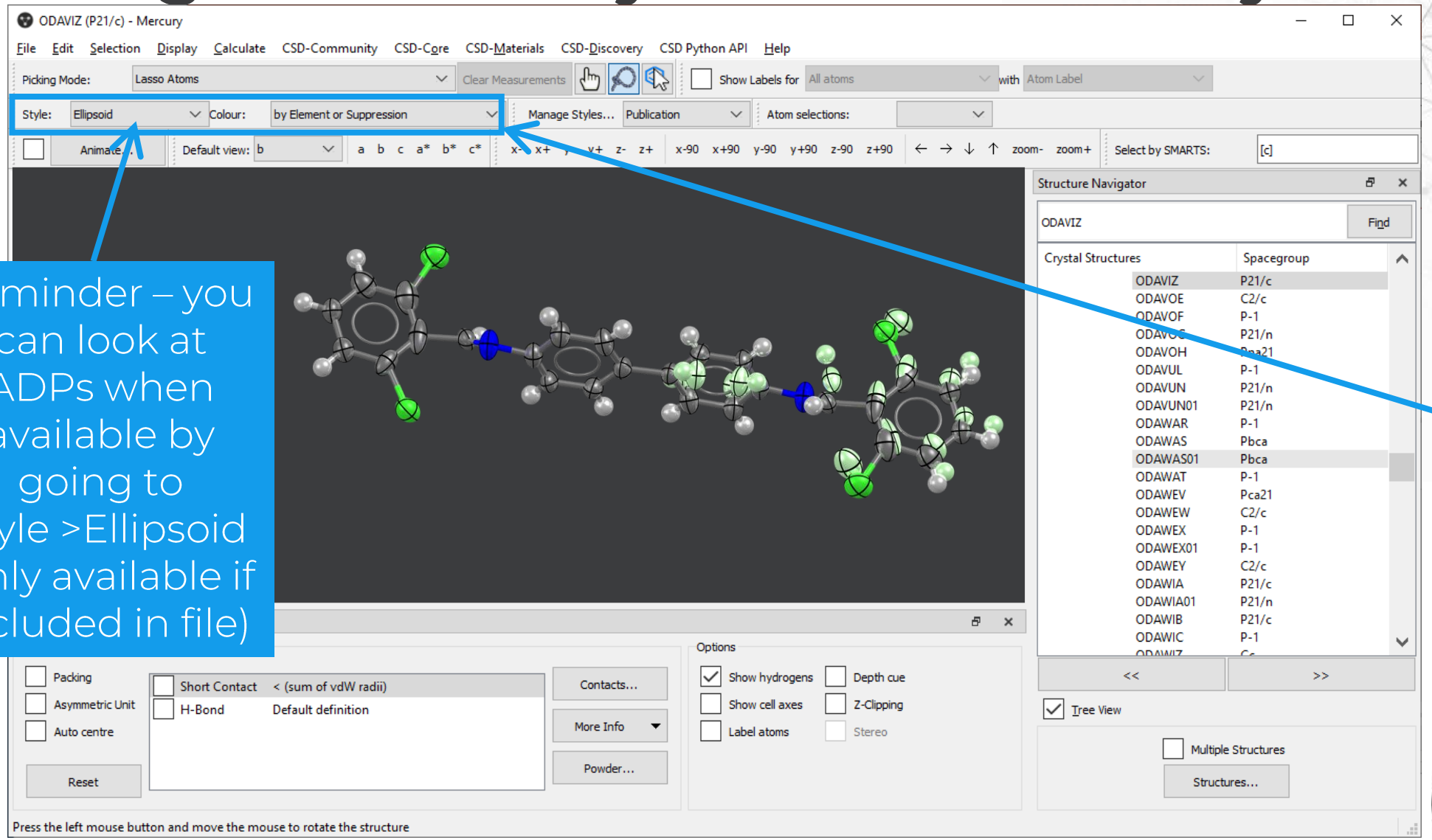
CCDC

Mogul Geometry Check – Mercury view

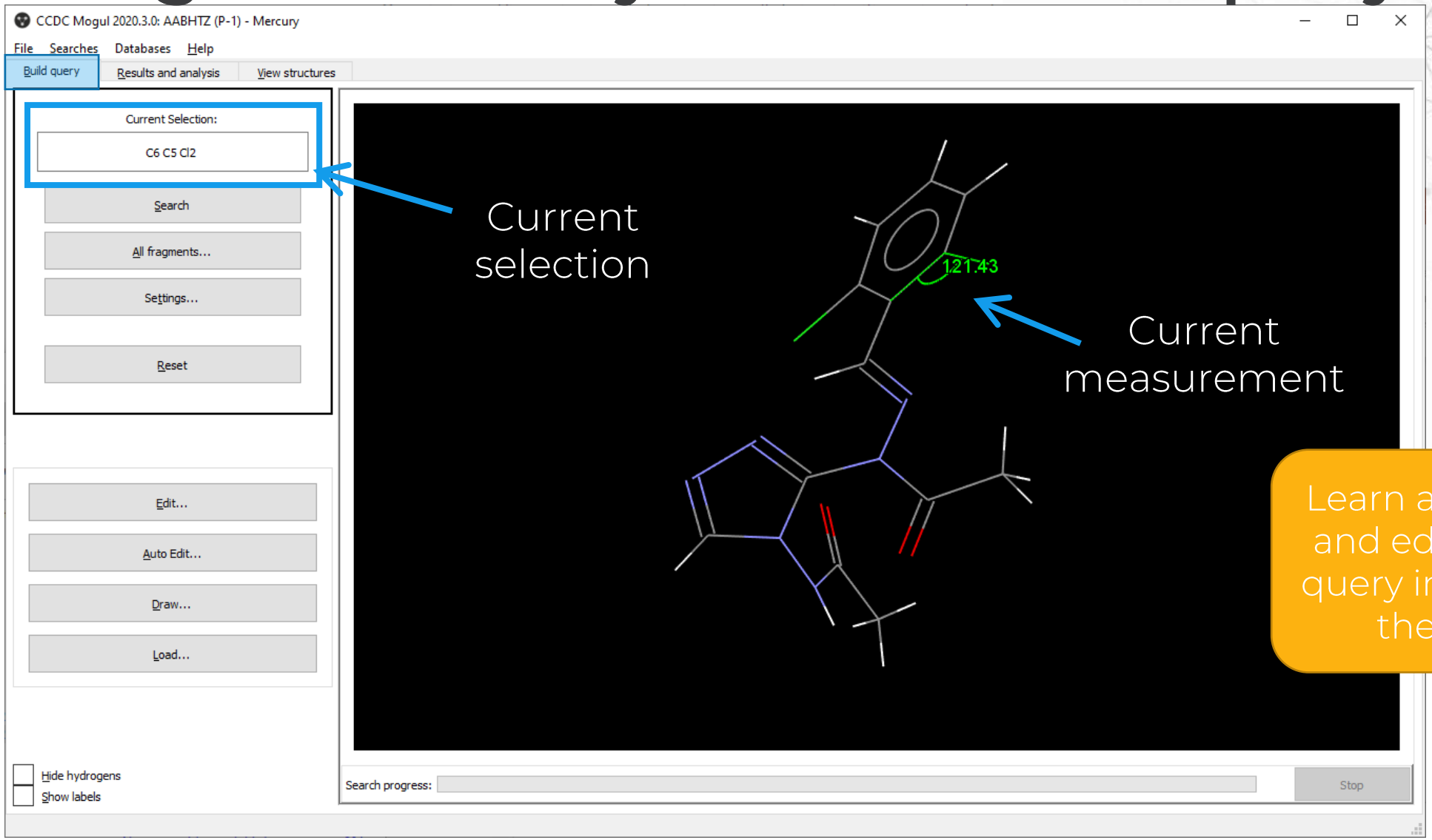
CSD Refcode
ODAVIZ

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

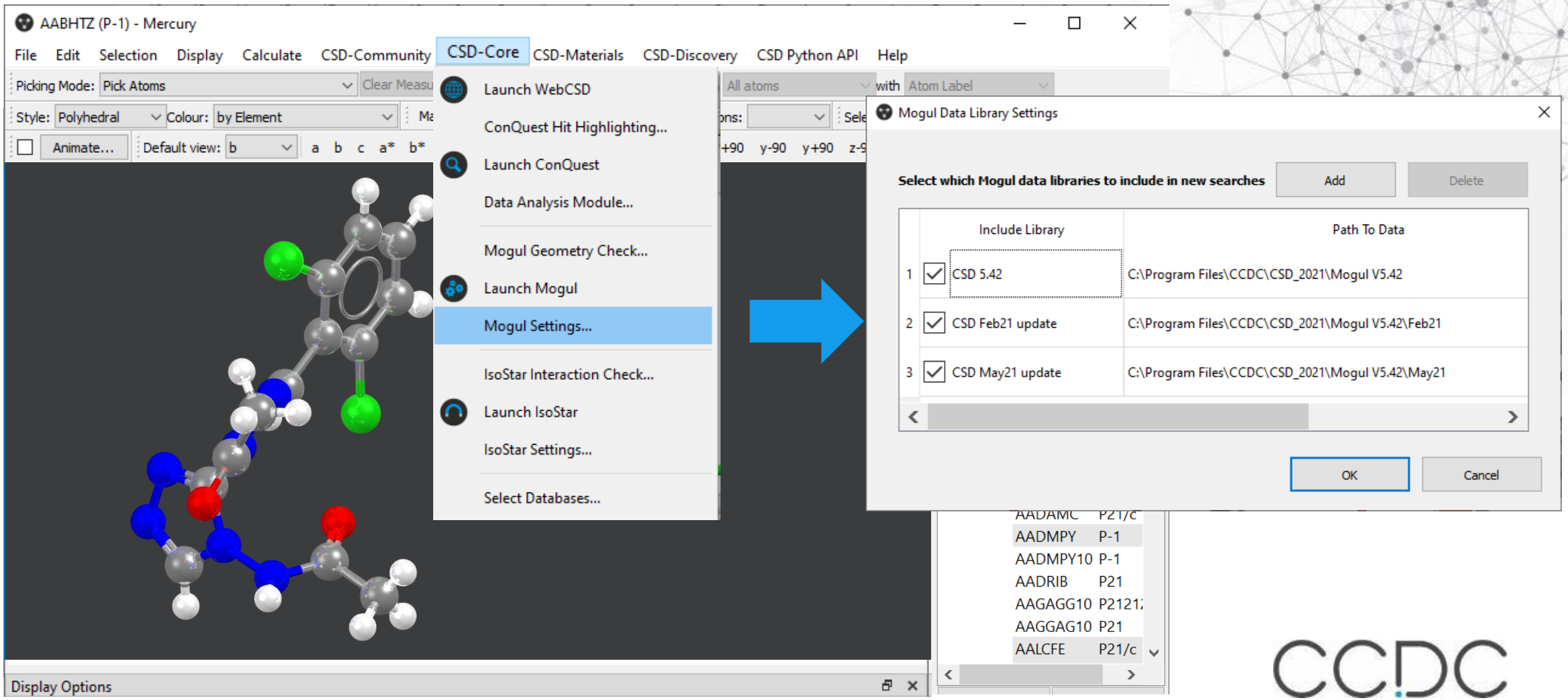


Mogul Geometry Check – Build query

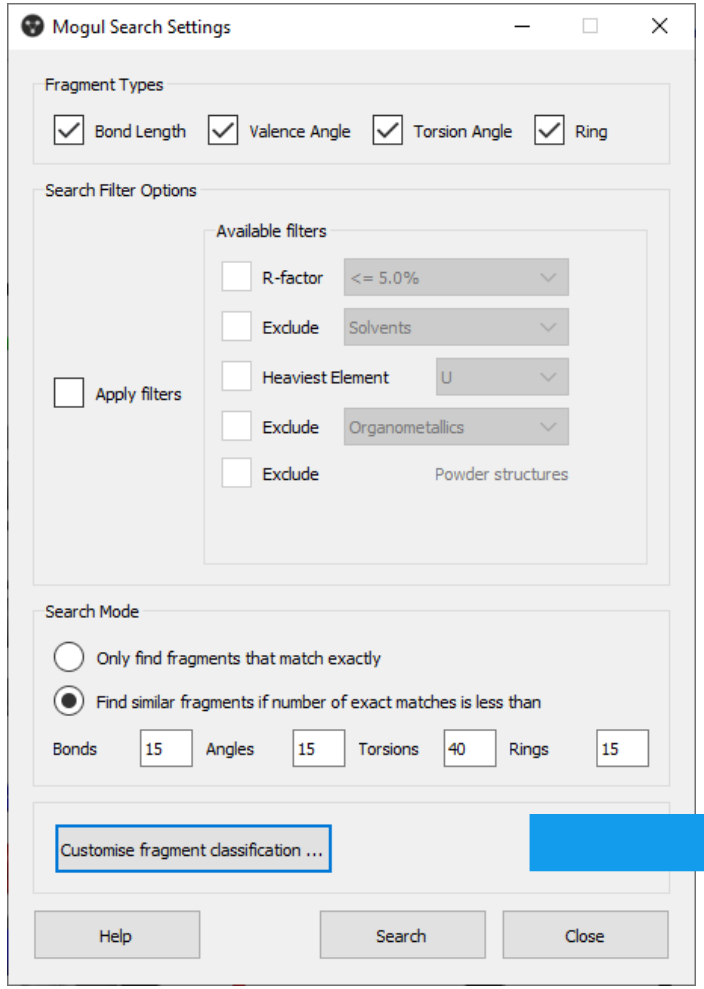


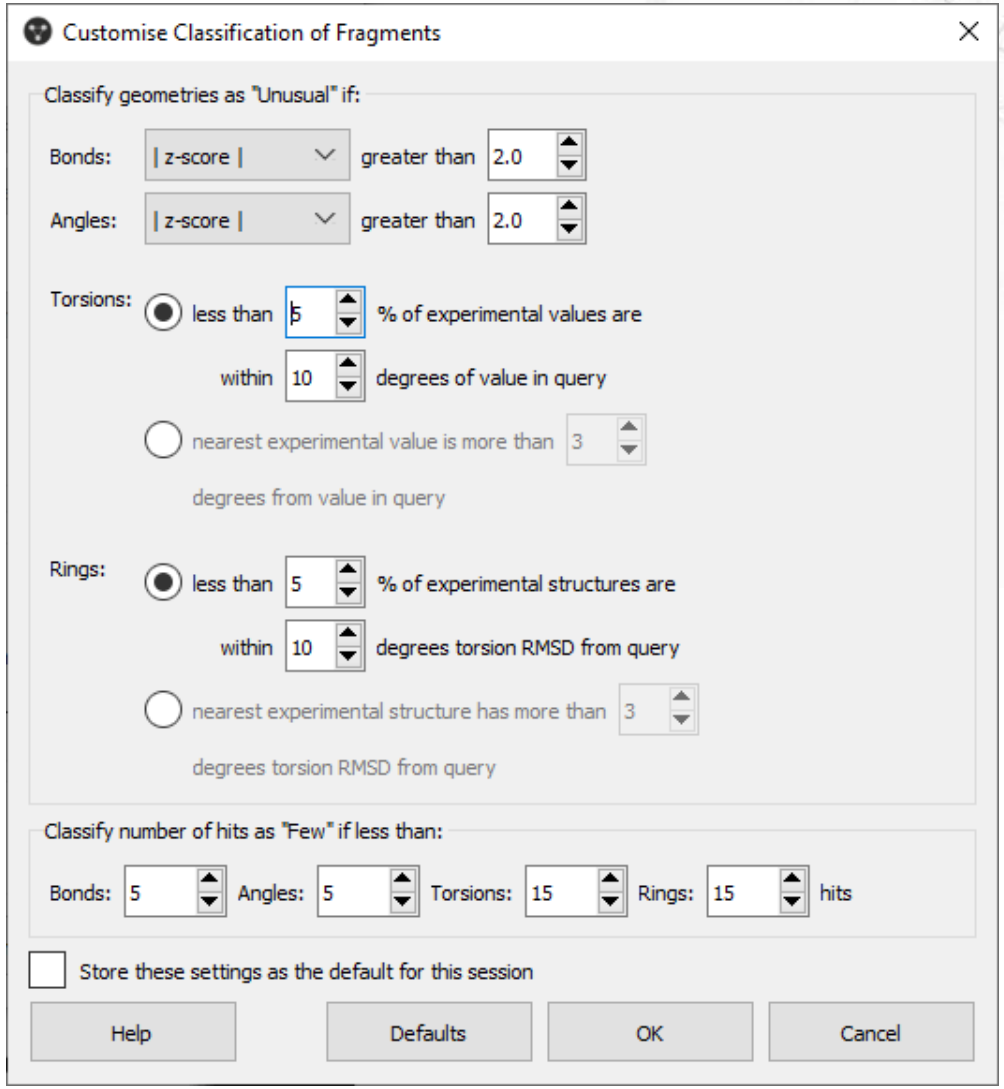
Learn about building and editing a Mogul query in Exercise 2 of the handout.

Mogul Settings



Customise fragment classification

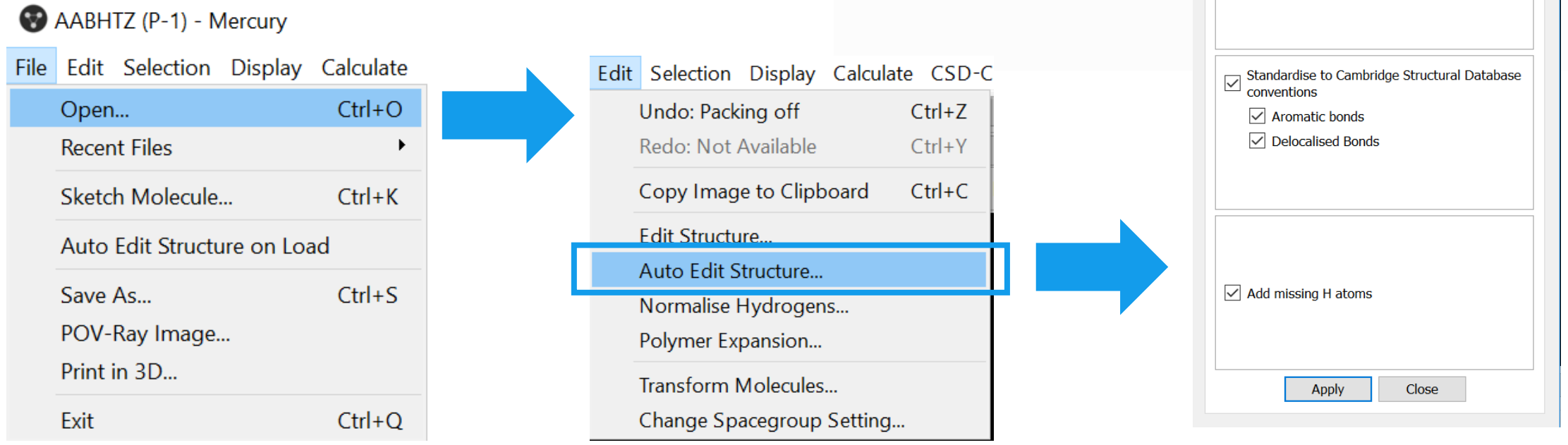




Using Mogul to check a new structure

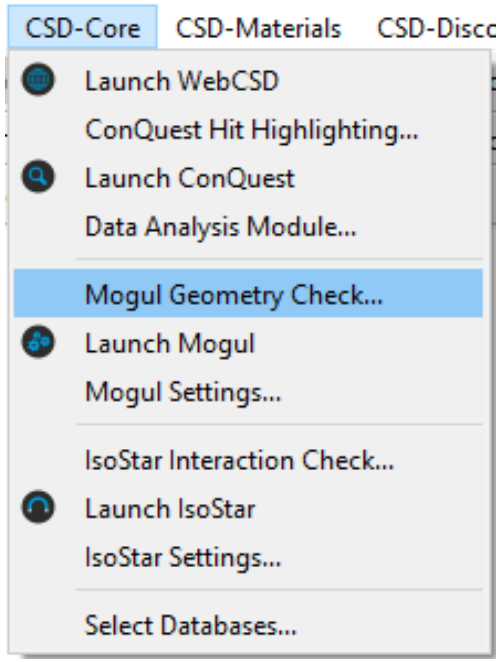
1. Load your structure in Mercury
   - Do you remember how to do it from the Visualisation session?

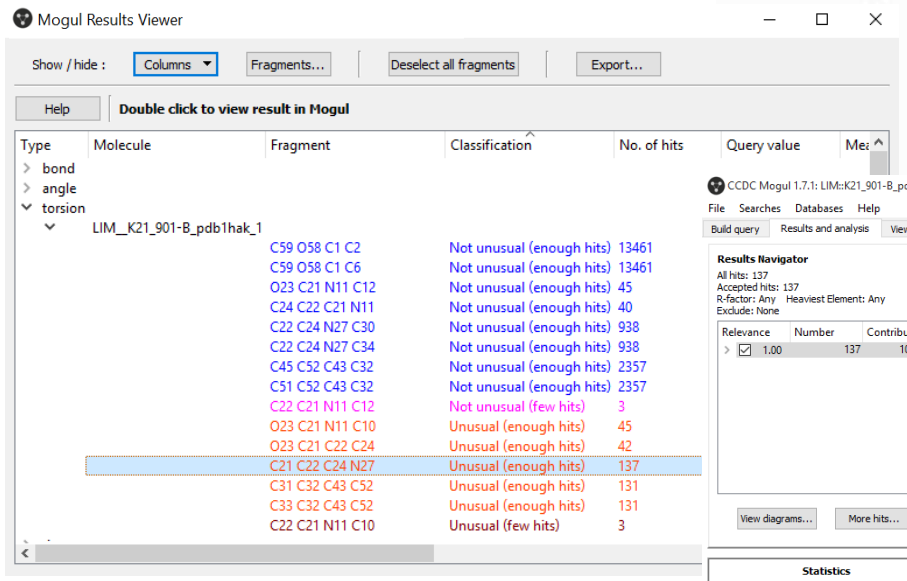
- File > Open – to open one of your own files for example a CIF
- Edit > Auto Edit Structure to assign bond types
- File > Auto Edit Structure on Load to automate

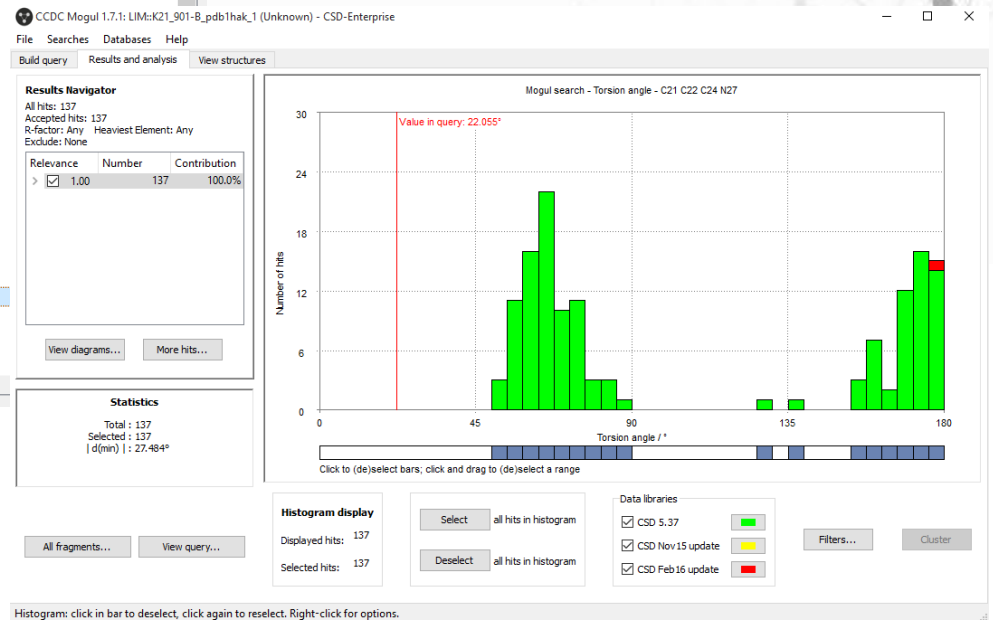


Using Mogul to check a new structure

2. Repeat the procedure you did before







Why use Mogul?

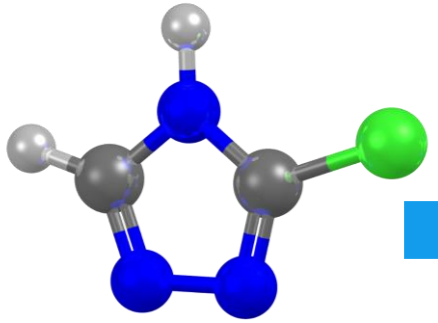
- To enable you to validate the complete geometry of a given query structure and identify any unusual features
  - Could be useful when looking at your own structure or a CSD structure or in fact ligands in the pdb
- To rapidly retrieve geometric data and gain new insights from structures in the CSD

Explore More: More advanced uses

- Not enough time to explore all the insights that you can get from Mogul.
- But here are a selection of:
  - Case studies - Examples from published scientific articles that used Mogul in their work.
  - Other ways you can access Mogul data

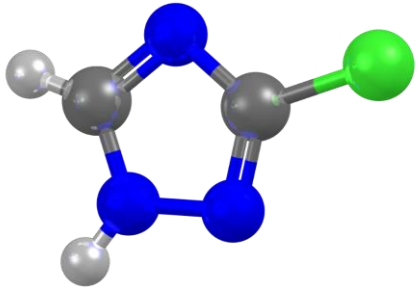
Using Mogul to assign tautomeric forms

CSD CLTRZL

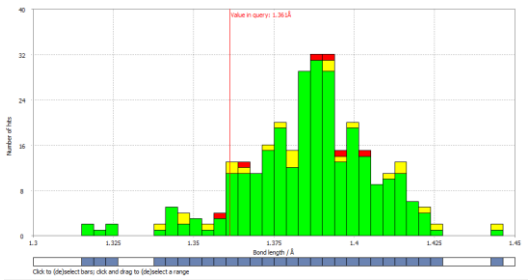


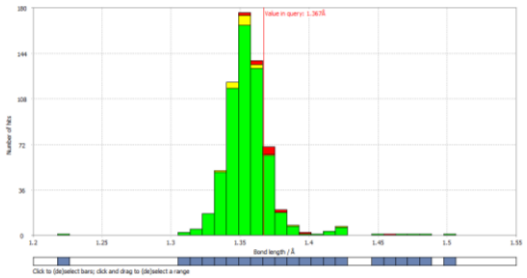
1.361 Å

CSD CLTRZL01



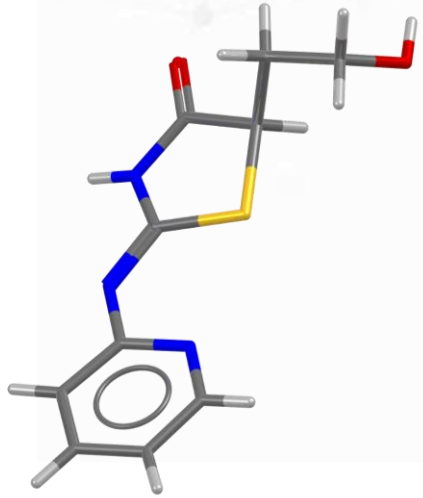
1.367 Å



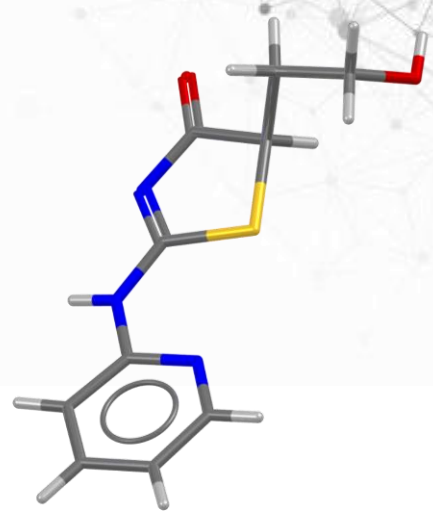


Following Mogul analysis structure re-determined in a different tautomeric form

CSD GACXOZ



CSD LOQBIE

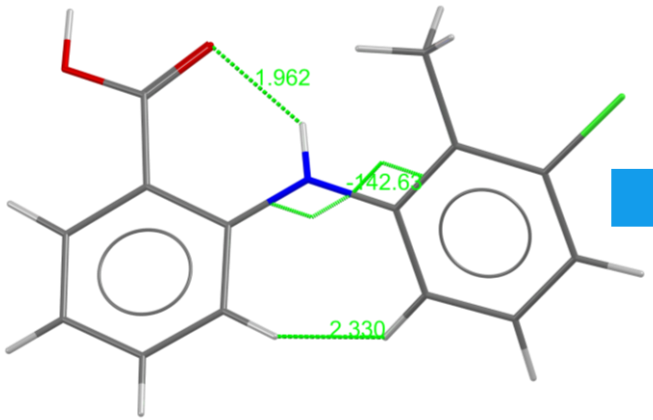


A comparison of the 1,3-thiazol-4-one structures in which *Mogul* queries the C—N bond length of the imine of GACXOZ, but finds all geometrical parameters of the amine version to be within expected limits

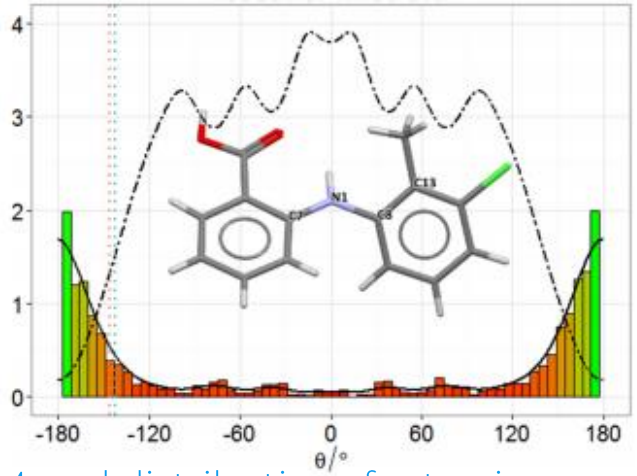
B.Bax, C.Chung, C.Edge, *Acta Cryst. D,* 2017, 73, 131-140, DOI: 10.1107/S2059798316020283
R.Taylor and P.A.Wood, *Chem. Rev.,* 2019, 119, 16, 9427–9477, DOI: 10.1021/acs.chemrev.9b00155

CCDC

Using Mogul to optimise molecular geometries



CSD KAXXAI



Mogul distributions for torsion angle
Solid line = fitted probability density function
Dashed line = derived objective function for use in geometry optimization
Image from DOI: 10.1021/acs.jcim.5b00712

This approach provides average geometric preferences of a molecule according to data in the CSD. It is then possible to exploit this information into an object function to optimise a molecular geometry

Mogul distributions can be converted into smooth, differentiable probability density functions using kernel density estimation. This publication by McCabe *et al.* shows how this approach could be used to drive geometry optimisation of organic molecules

R.Taylor and P.A.Wood, *Chem. Rev.* 2019, 119, 16, 9427–9477, DOI: 10.1021/acs.chemrev.9b00155
J.C.Cole, C.R.Groom, O.Korb, P.McCabe, and G.P.Shields, *J. Chem. Inf. Model.* 2016, 56, 4, 652–661, DOI: 10.1021/acs.jcim.5b00712

CCDC

Using Mogul in powder diffraction

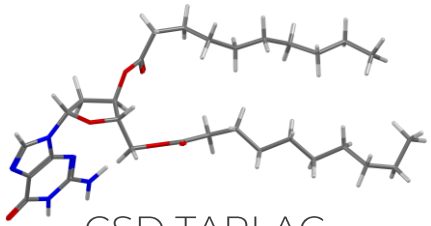
- Powder diffraction patterns have relatively low content information
  - Overlap of reflections
  - Rapid decline in scattering with increasing diffraction angle
- How can the CSD and Mogul help?

By providing sensible geometries for a starting model

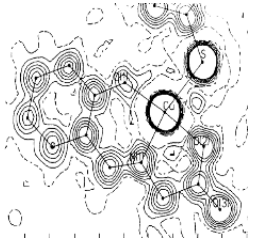
To determine refinement constraints

To help validate the final solution

By using conformational info to reduce the search space



CSD TARLAC

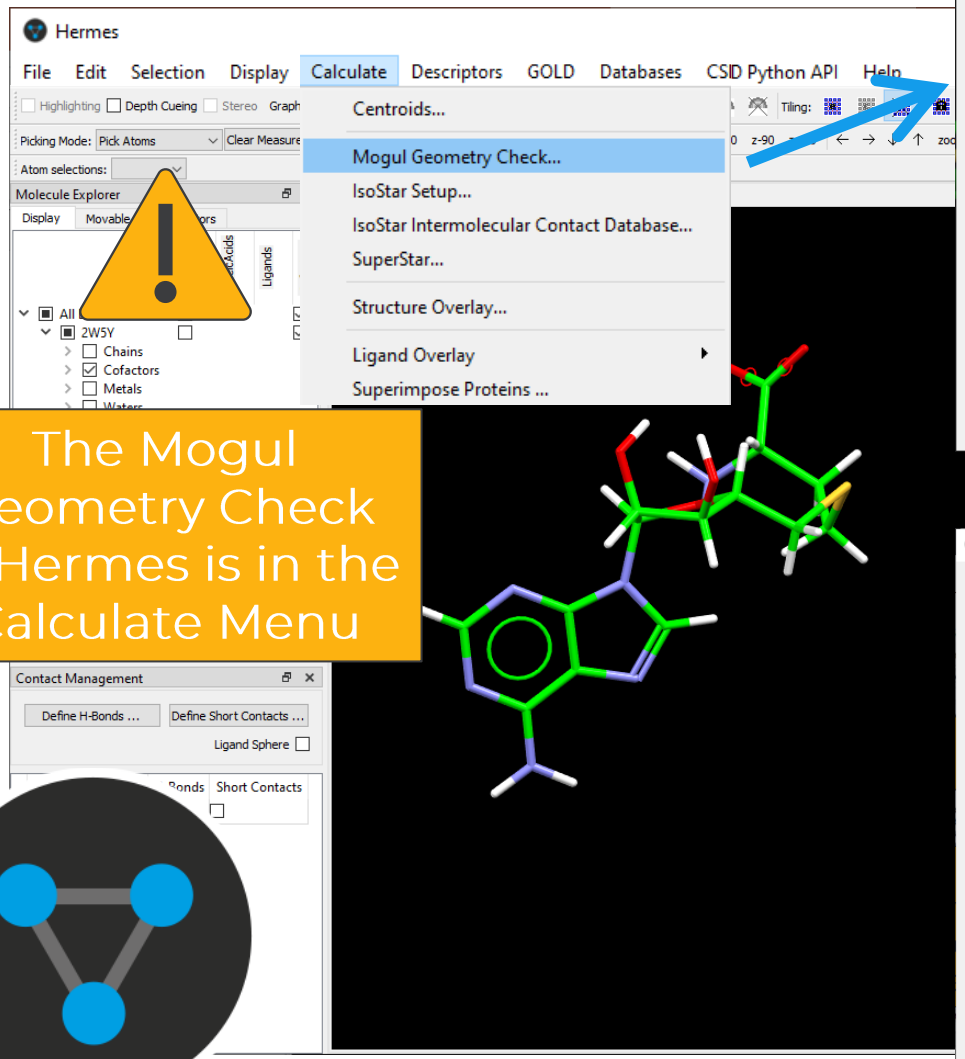


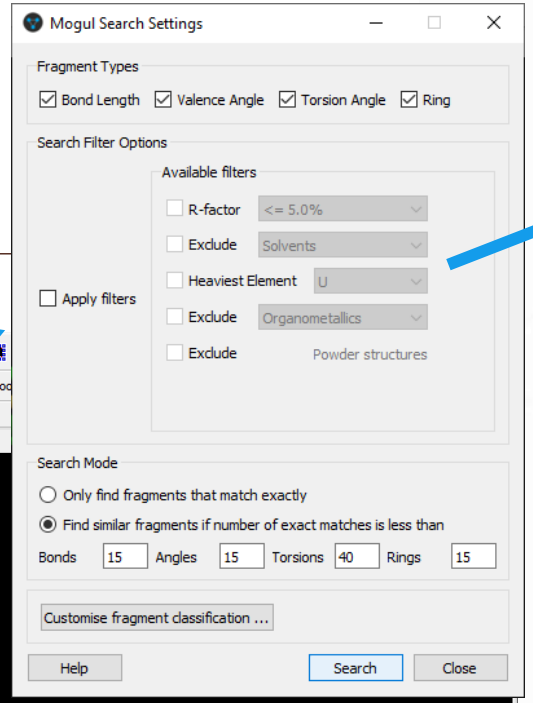
R.Taylor and P.A.Wood, *Chem. Rev.* 2019, 119, 16, 9427–9477, DOI: 10.1021/acs.chemrev.9b00155

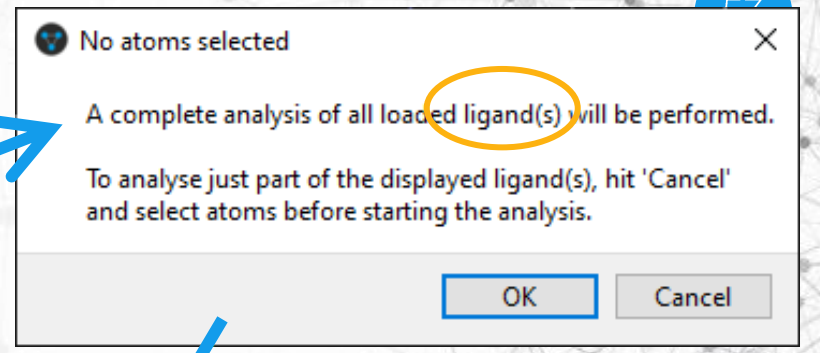
CCDC

In Hermes

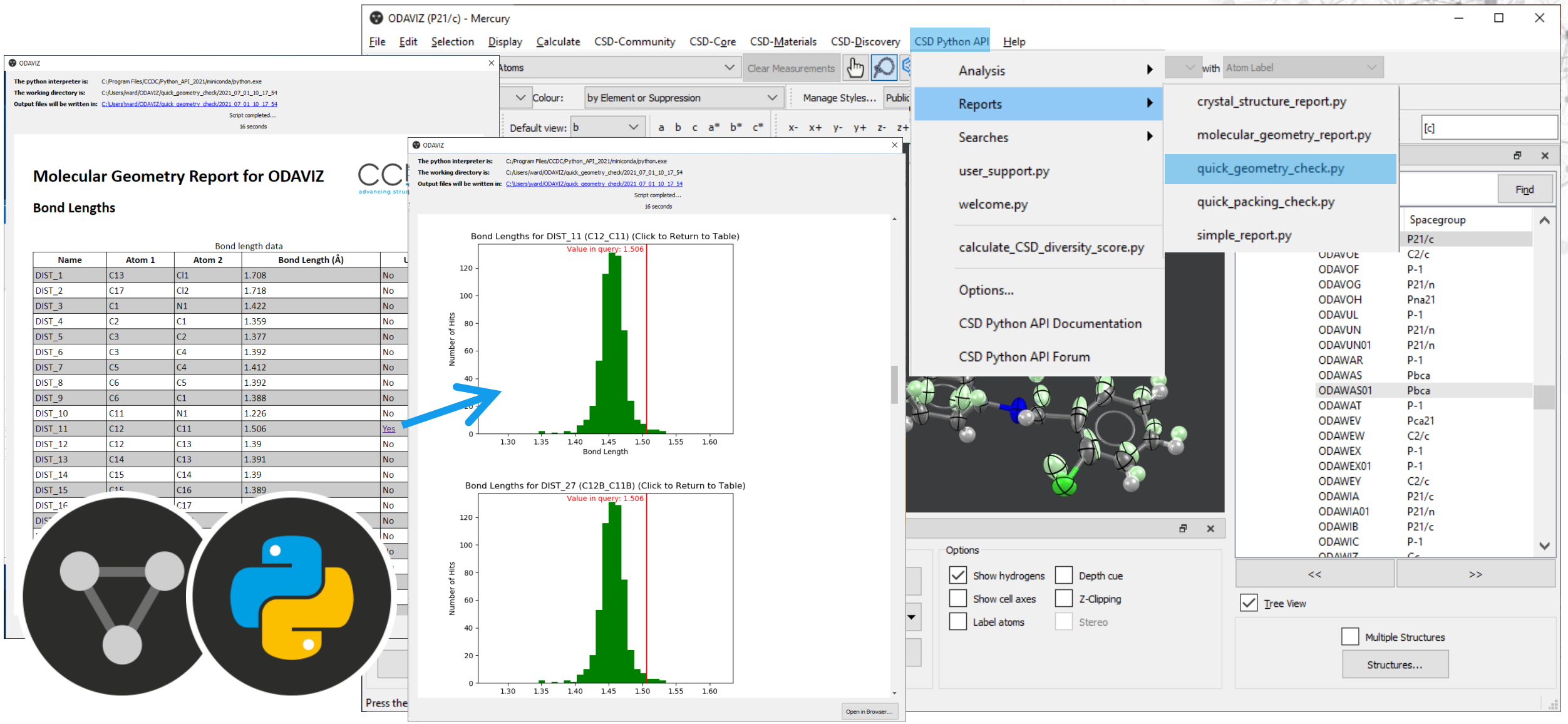
The Mogul Geometry Check in Hermes is in the Calculate Menu







Creating Mogul reports in Mercury



In the CSD Python API

ccdc.conformer.GeometryAnalyser()

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advancing structural science

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Quick search

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Conformer API

Introduction

The `ccdc.conformer` module contains classes concerned with molecular conformations.

The three main classes of the `ccdc.conformer` module are:

- `ccdc.conformer.MoleculeMinimiser`
- `ccdc.conformer.ConformerGenerator`
- `ccdc.conformer.GeometryAnalyser`

A `ccdc.conformer.MoleculeMinimiser` instance can be used to optimise the bond distances and valence angle
3D input molecule using the `ccdc.conformer.MoleculeMinimiser.minimise()` function:

```
from ccdc.conformer import MoleculeMinimiser
molecule_minimiser = MoleculeMinimiser()
minimised_mol = molecule_minimiser.minimise(mol)
```

A `ccdc.conformer.ConformerGenerator` instance can be used to generate a set of conformers for an input mo
using the `ccdc.conformer.ConformerGenerator.generate()` function:

```
from ccdc.conformer import ConformerGenerator
from ccdc.io import MoleculeWriter
conformer_generator = ConformerGenerator()
conformers = conformer_generator.generate(mol)
with MoleculeWriter('conformers.mol2') as mol_writer:
    for c in conformers:
        mol_writer.write(c.molecule)
```

A `ccdc.conformer.GeometryAnalyser` instance can be used to analyse the geometry of an input molecule u
knowledge-based library of intramolecular geometries based on the CSD.

The `ccdc.conformer.GeometryAnalyser` class contains nested classes:

- `ccdc.conformer.GeometryAnalyser.Settings`
- `ccdc.conformer.GeometryAnalyser.Analysis`
- `ccdc.conformer.GeometryAnalyser.AnalysisHit`

The `ccdc.conformer.GeometryAnalyser.analyse_molecule()` function can be used to validate the complete geo
of a given query structure.

```
>>> from ccdc.io import EntryReader
>>> csd_reader = EntryReader('CSD')
>>> yigpio01 = csd_reader.molecule('YIGPIO01')
```

```
>>> from ccdc.conformer import GeometryAnalyser
```


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Quick search

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Molecular geometry analysis

Introduction

The CSD Portfolio contains a knowledge-base of intramolecular geometries. This knowledge-base provides easy and rapid access to millions of chemically classified bond lengths, valence angles, acyclic torsion angles, and ring conformations derived from the CSD.

This enables you to rapidly validate the complete geometry of a given query structure and identify any unusual features without the need to construct complex search queries, or carry out detailed data analyses.

Let us import in the `ccdc.conformer` module.

```
>>> from ccdc import conformer
```

Let us also import the `ccdc.io` module so that we can read in molecules of interest.

```
>>> from ccdc import io
```

Note: For more information on these knowledge-based geometry libraries please see: "Retrieval of Crystallographically-Derived Molecular Geometry Information", I. J. Bruno, J. C. Cole, M. Kessler, Jie Luo, W. D. S. Motherwell, L. H. Purkis, B. R. Smith, R. Taylor, R. I. Cooper, S. E. Harris and A. G. Orpen, J. Chem. Inf. Comput. Sci., 44, 2133-2144, 2004 DOI: 10.1021/ci049780b.

See also: API documentation of the geometry analyser module

The molecular geometry analy

In order to be able to carry out a mol… `ccdc.conformer.GeometryAnalyser` class. Let us cr…

```
>>> engine = conformer.GeometryAnalyser()
```

Note: The most important function of an insta… `ccdc.conformer.GeometryAnalyser.analyse_molecu…` geometry analysed molecule.

Geometry analysis settings

The settings used in a geometry analysis a… `ccdc.conformer.GeometryAnalyser.Settings` class.

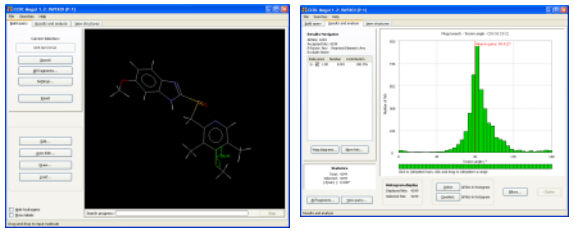
To find out what the current settings are one can make use of the `ccdc.conformer.GeometryAnalyser.Settings.summary()` function.

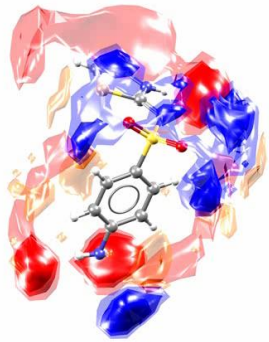
```
>>> print(engine.settings.summary())
Generalisation: True
Impose upper limits: False
Filter rfactor: any
```

Find out more:
The basics of our CSD Python API were covered in our last series of CCDC Virtual workshops!

More tools to assess your structure in CSD-Materials in Mercury

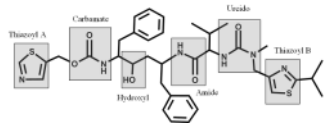
Mogul geometry library



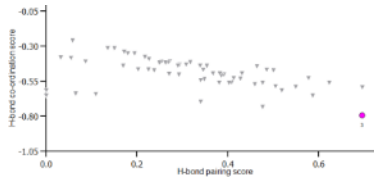


Full Interaction Maps:
3D representation of a map of donor and acceptor atom avai to create an intera network.

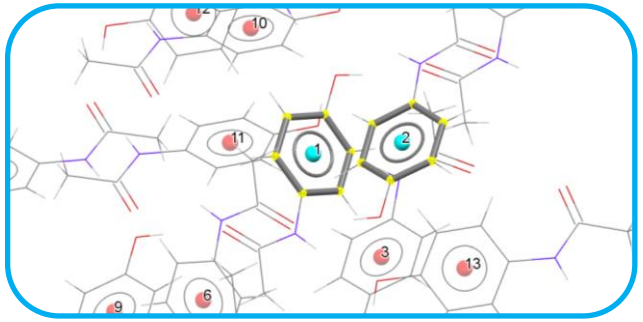
Next week's virtual workshop!



Donor group	Acceptor Group	π	+/− [σ]	Form I	Form II
amide	carbamate	0.618	0.094	×	×
amide	hydroxyl	0.551	0.052	×	✓
carbamate	carbamate	0.538	0.090	✓	×
amide	amide	0.501	0.055	✓	×
carbamate	amide	0.420	0.083	×	✓
hydroxyl	ureido	0.417	0.058	×	✓
ureido	carbamate	0.319	0.086	×	✓
ureido	ureido	0.224	0.044	✓	×
hydroxyl	thiazoyl a	0.114	0.039	✓	×



Hydrogen Bond Propensity:
Evaluation of the relative likelihoods of possible H-bonding networks in any observed polymorphs of a target system.

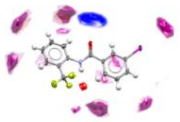


Aromatics Analyser:
Visualisation and identification of aromatic interactions within a crystal structure, and assessing their strength based on their distance and relative orientation.

CCDC

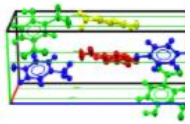
Want to explore more?

Training and Educational Resources



CSD-Materials

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



CSD-Core

Essential crystallographic and structural chemistry capabilities.

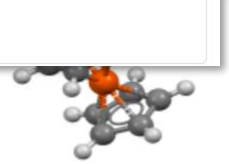
hin the Cambridge Structural Database (CSD) extends far beyond a collection of crystal structures. Knowledge derived from these materials
y, and biology. Chemical and structural concepts are often difficult to grasp without real world, interactive examples for students to explore.

ally produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials
eely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of
n entries are available for free through our Access Structures portal.

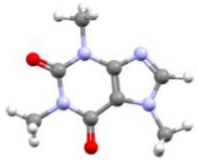
ementary teaching materials, find out more about the Teaching Database **here**. If you have developed your own modules using the CSD and
er community, please contact us at education@ccdc.cam.ac.uk.

from education and outreach at the CCDC, sign up for the Education and Outreach Newsletter **here**.

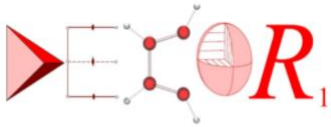
Register for E&O newsletter



Information on the Teaching Subset



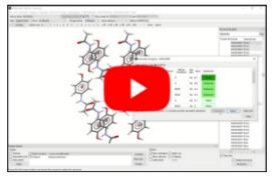
Access a series of teaching modules for use in the classroom



DECOR: Educational Resources for Teaching Crystallography

Self-guided workshops

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

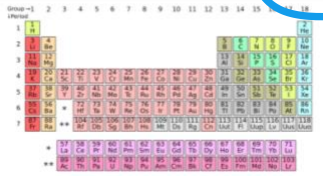


Watch software training and support videos

CSD University modules

On-demand modules with completion certificate

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



Explore the Periodic Table through Crystal Structures

YouTube and LabTube channels

CCDC