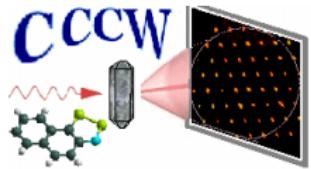


Canadian National Committee
for Crystallography
<http://xtallography.ca/>

OLEX2 – Modeling disorder: Fixed positions

Louise Dawe
Wilfrid Laurier University



Canadian National Committee
for Crystallography
<http://xtallography.ca/>

Data from Charlotte Stern

Check out the OLEX2 youtube channel for an alternate way to tackle this:

<https://www.youtube.com/watch?v=LkIP0s-KEFQ>

Another good resource:

<http://web.mit.edu/pmueller/www/ACA2007/WK01/Disorder.pdf>

Navigate to SplittingCF3 folder.
File → Open “Example5.ins”

Olex2

File Edit View Structure Mode Tools Model Select Help

Open

C:\Users\Lou\Desktop\CCCW17\Olex2 Workshop\Example 0 - Structure Solution\Example0
C:\Users\Lou\Desktop\Maly_June_2017\Maly_June_2017\n16053 Report Stuff\n16053_CIF.cif
C:\Users\Lou\Desktop\Old Data\b16146\June_2017\Crystal_1\b16146_crystal1
C:\Users\Lou\Desktop\Old Data\b16146\June_2017\Crystal_1\b16146_crystal1.p4p
C:\Users\Lou\Desktop\Old Data\b16146\June_2017\Crystal_2\b16146_crystal2
C:\Users\Lou\Desktop\Old Data\b16146\June_2017\Crystal_2\b16146_crystal2.p4p
C:\Users\Lou\Desktop\Old Data\b16146\twin\b16146
C:\Users\Lou\Desktop\Old Data\b16146\twin\b16146.p4p

Save (Ctrl+S)
Save With Sorting
Save model as .. (Ctrl+Shift+S)
Close
Exit

Loading AutoChem_40 (Version Sun May 20 16:49:29 2018) Welcome to Olex2

We are grateful to our users for testing and supporting Olex2
Please find the link to credits in the About box

Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program (2009). J. Appl. Cryst., 42, 339-341.

Loading HARp (Version Sun May 20 16:49:43 2018) OK.

File is closed

>>

1.2 5155

OLEX²

Welcome to Olex2! CHANGELOG Open
Sucrose THPP Co110 ZP2 Water 183 Timmy
Documentation: Online | Static PDF | All Inline Help

Tutorials

Extension Modules

Settings

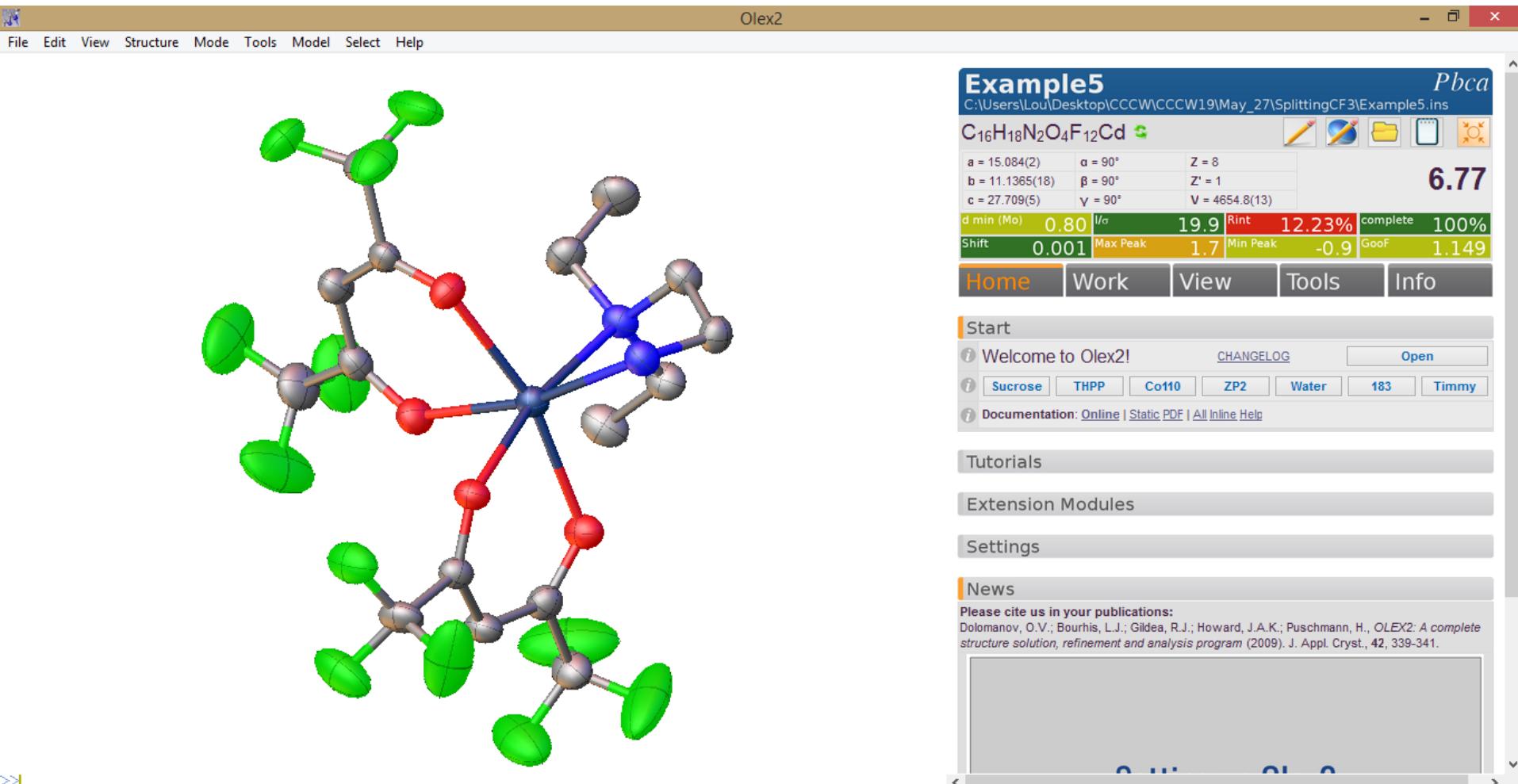
News
Please cite us in your publications:
Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program (2009). J. Appl. Cryst., 42, 339-341.

Setting up Olex2
... and everything else you need to get going

OlexSys

Looks like all of our work is done! Coffee?

No hydrogens = No coffee

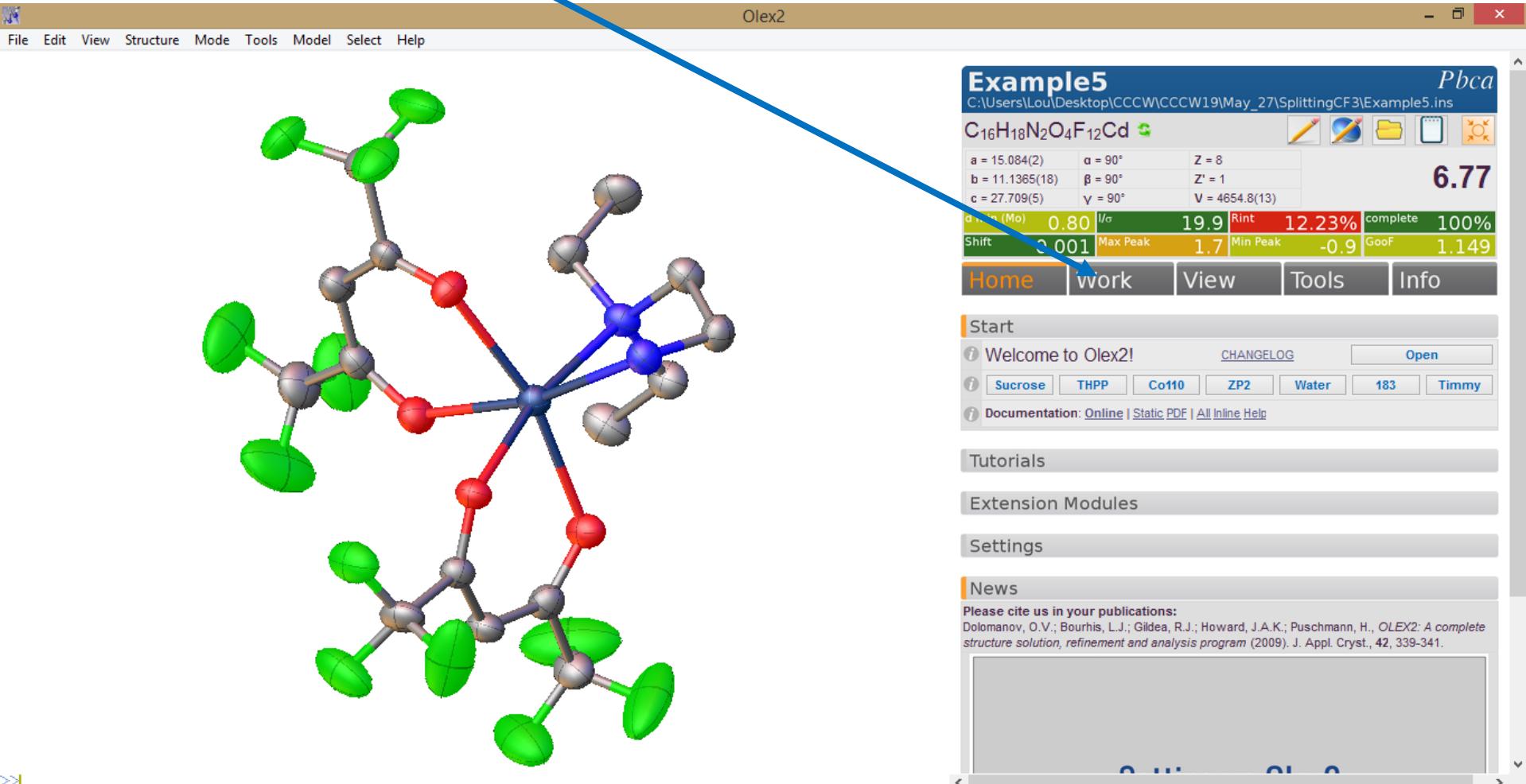


Go to:

Work

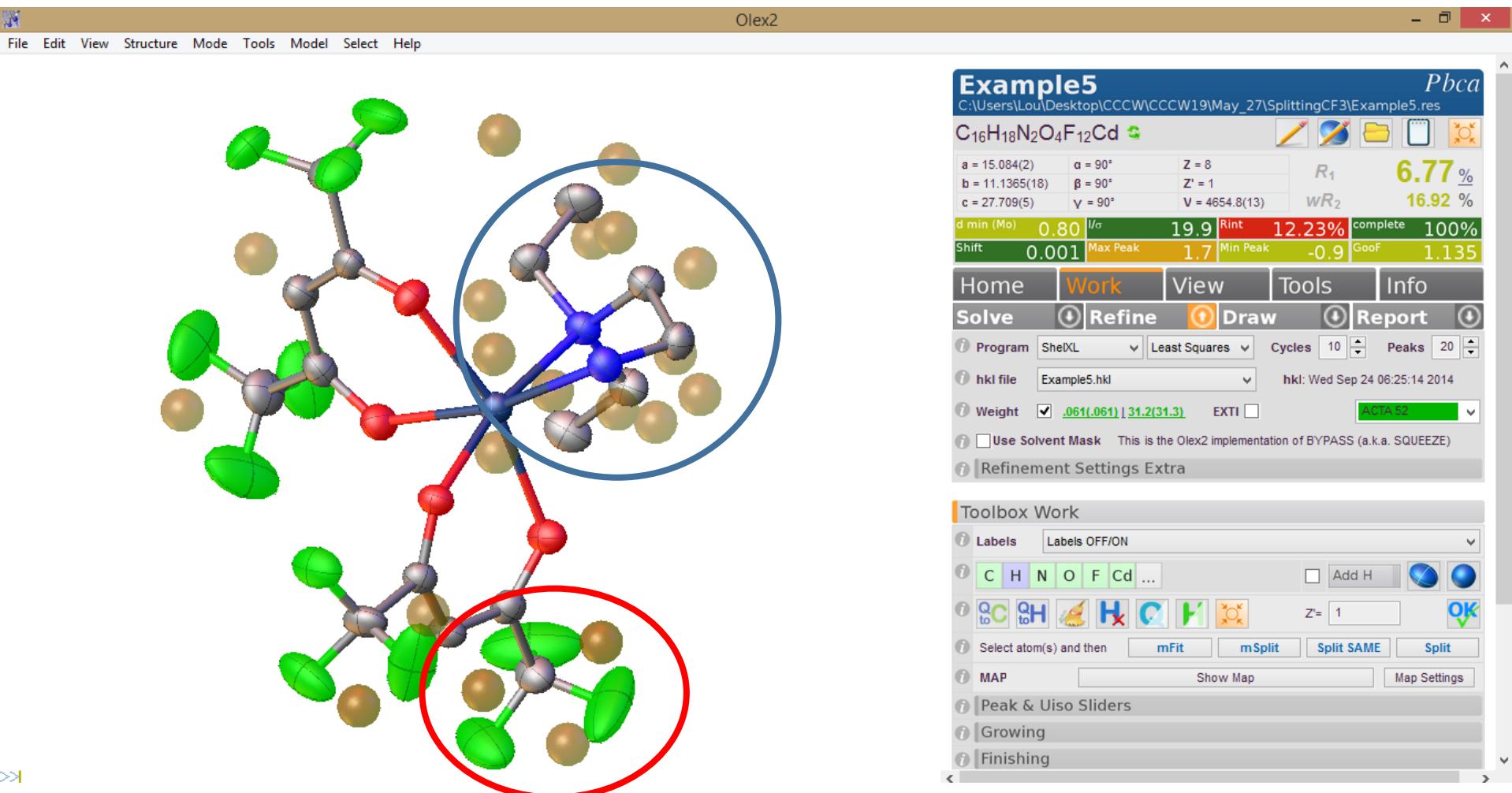
Refine dropdown

Refine with Shelxl



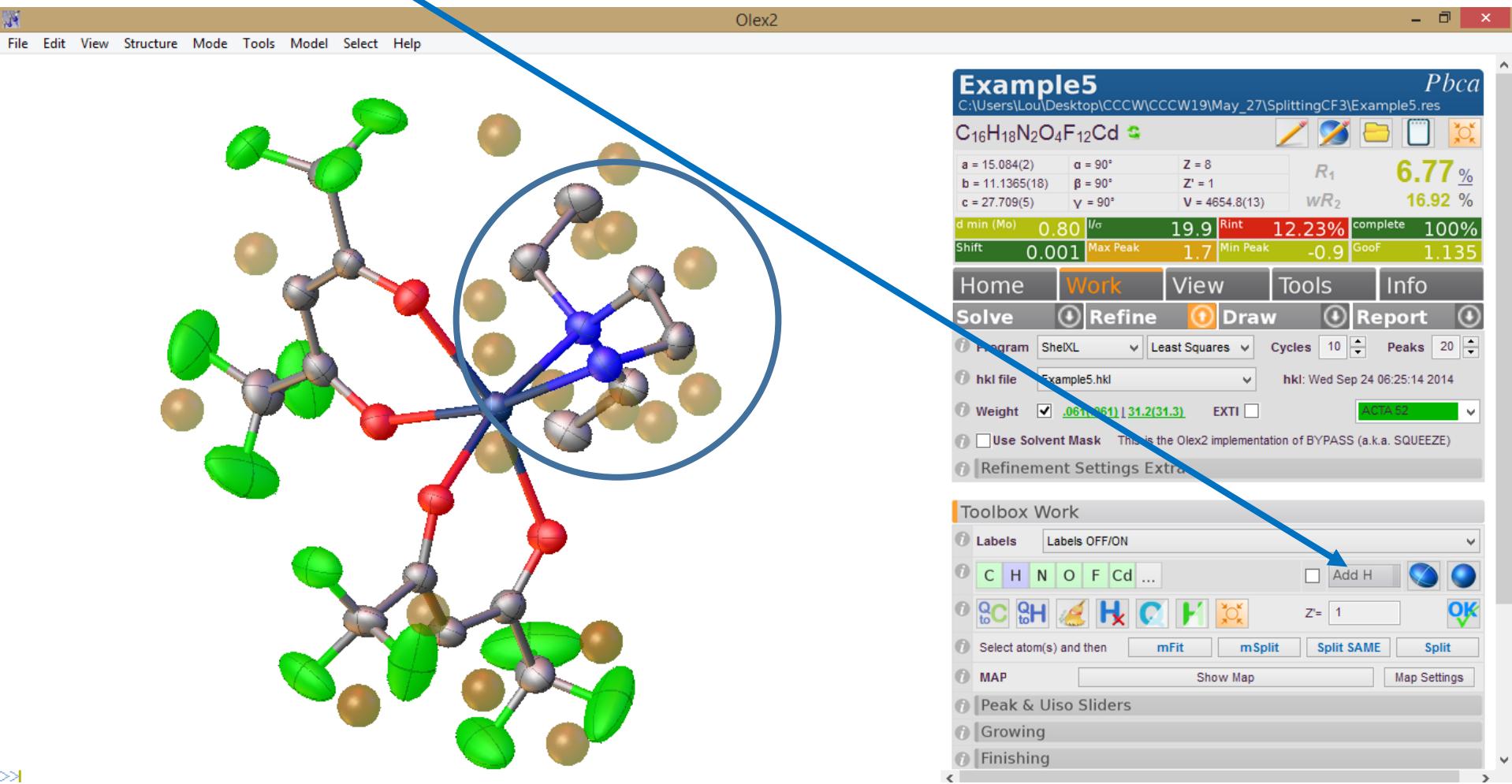
Notice two things here

1. Yes, we missed a bunch of hydrogens
2. There are three residual peaks directly between the F-atoms of this $-CF_3$ group

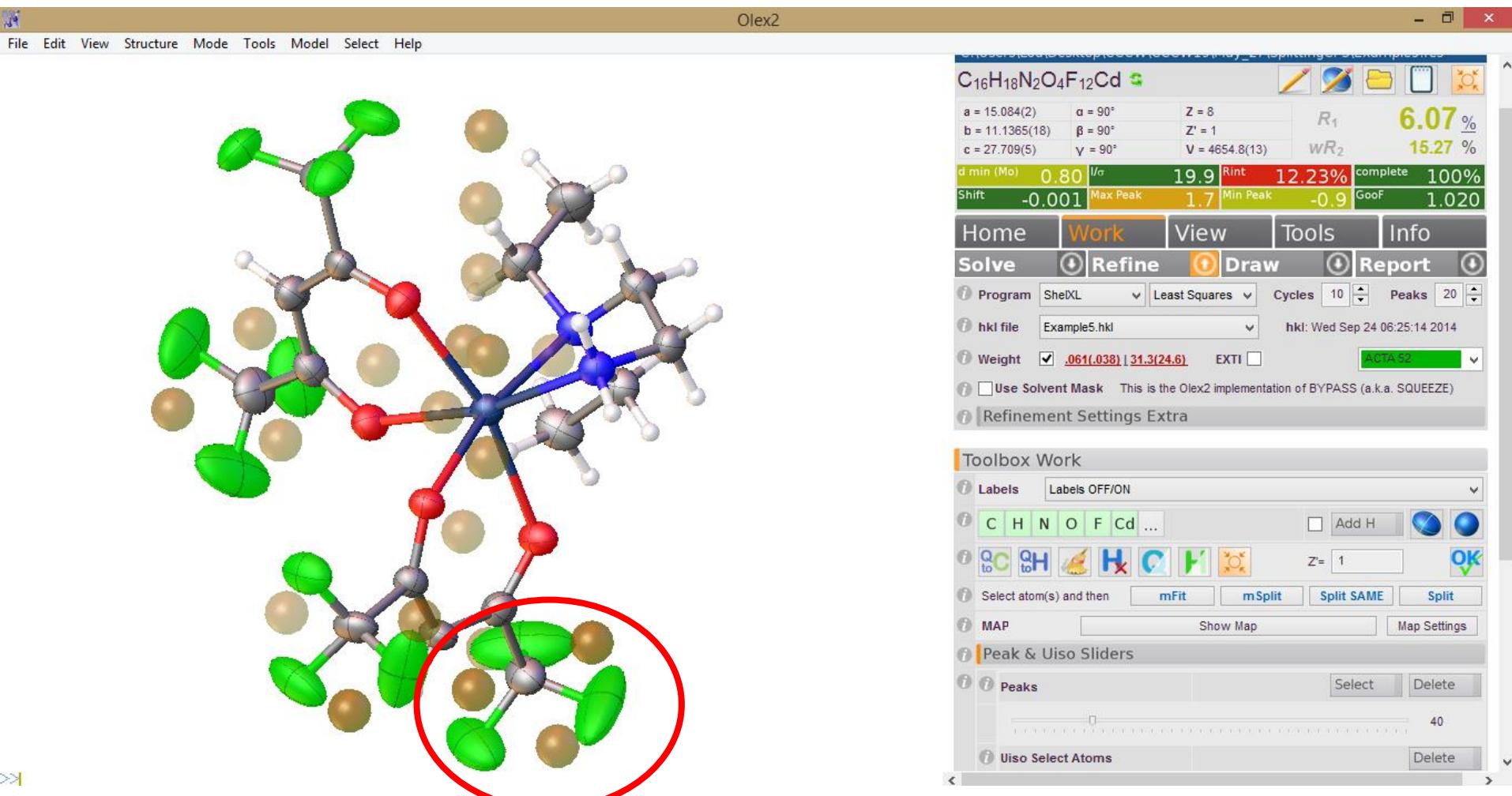


Now:

1. Add H; then Refine



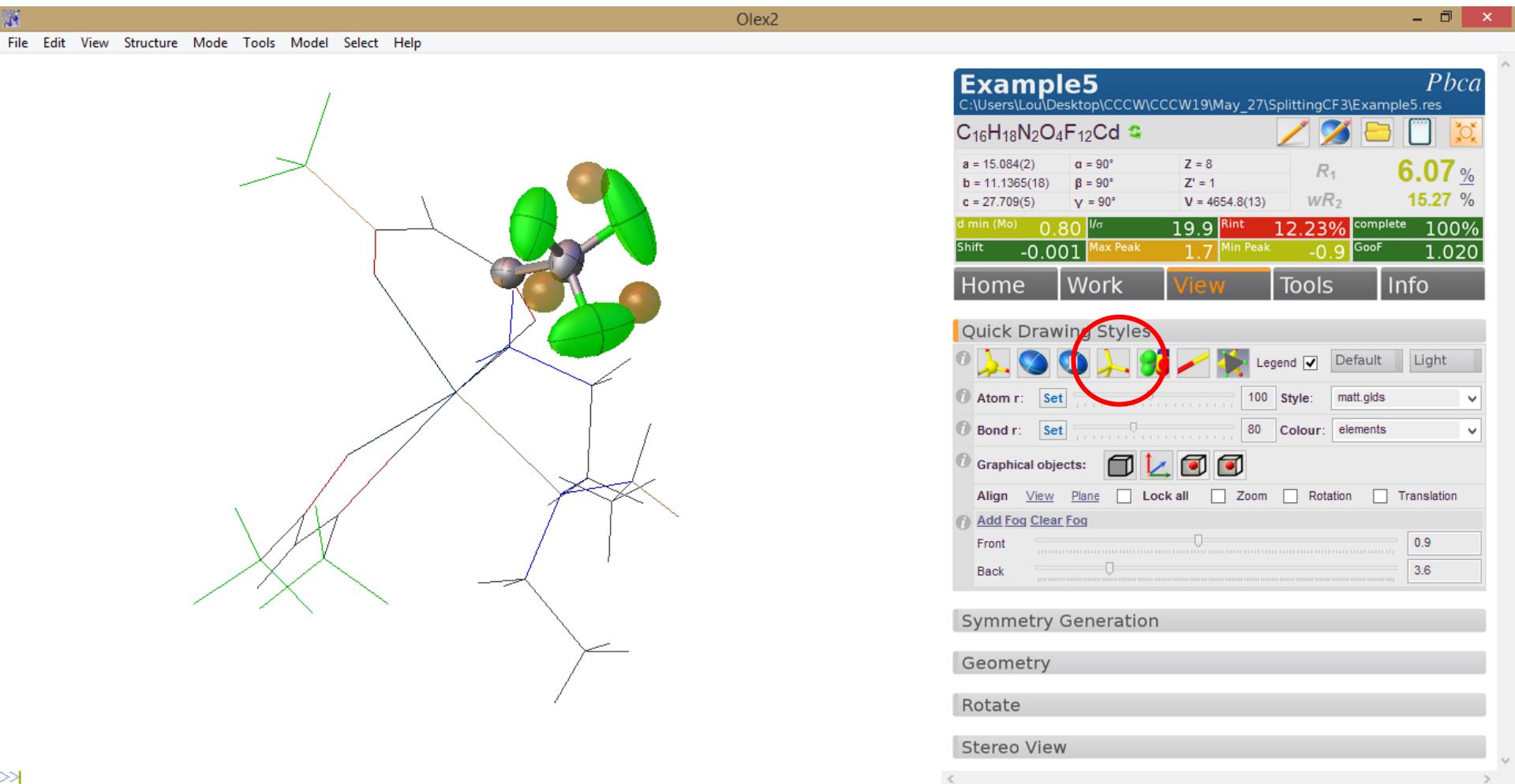
1. Looks good, but
 2. Now there are residual peaks between F-atoms in multiple $-CF_3$ groups!
- Let's deal with one of these groups; the highest residual peaks (Q1, Q2, Q4) are associated with the group comprised of C10, F10, F11, F12.



I'm going to tidy my display to work on this (mouse scroll down, or "Peak & Uiso Sliders" workbar, to show only the top four peaks and reorient my molecule to carefully inspect this group.)

Also, "Ctrl A", then select C8, C10, F10, F11, F12, then "View" and "Quick Drawing Styles" to convert everything else to a line

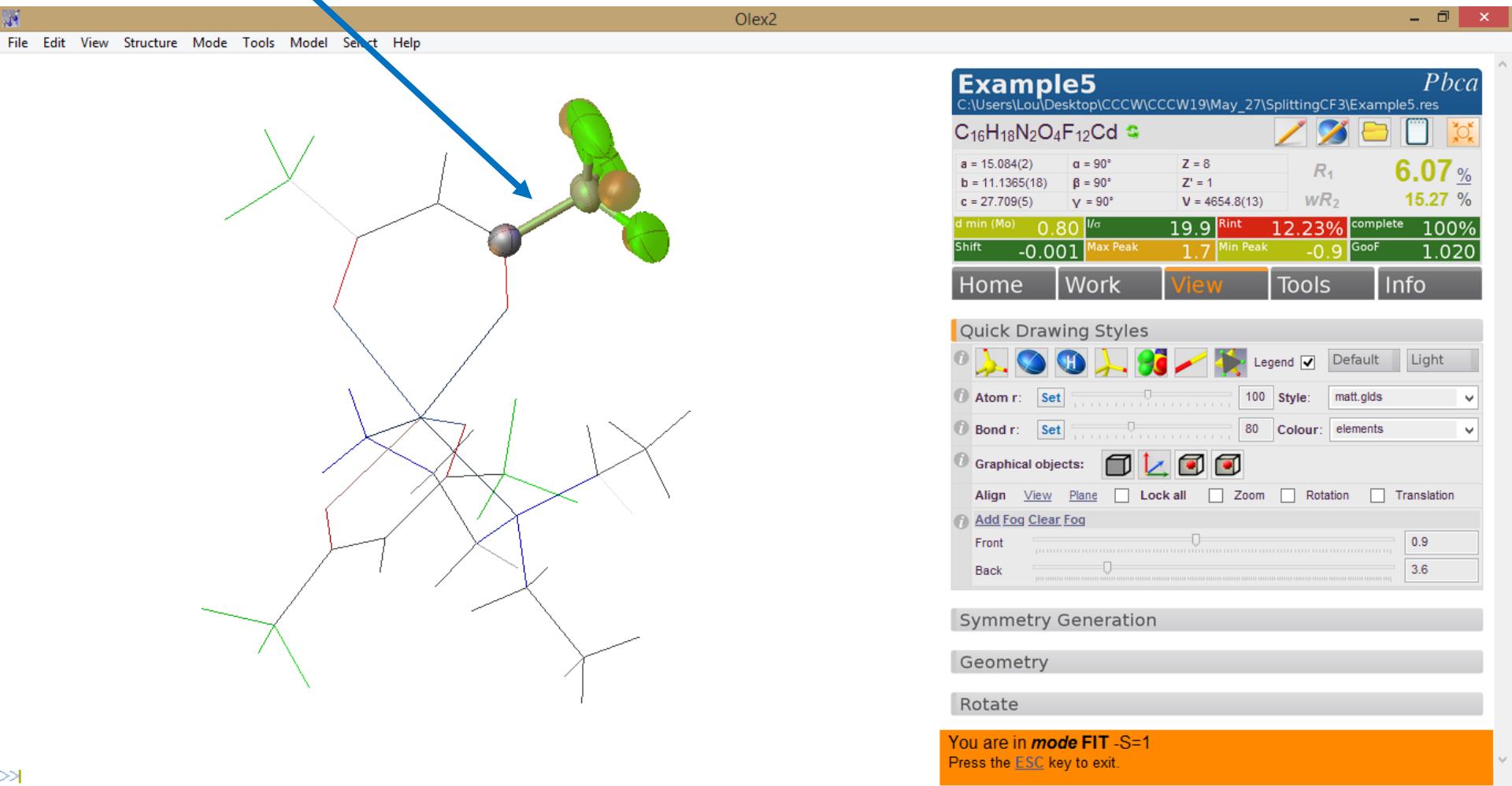
(You don't have to do this, but it makes my slide look better!)



Next, select C10, F10, F11, F12 in this order (or at least, C10 first, and then the three F atoms.) Then type:

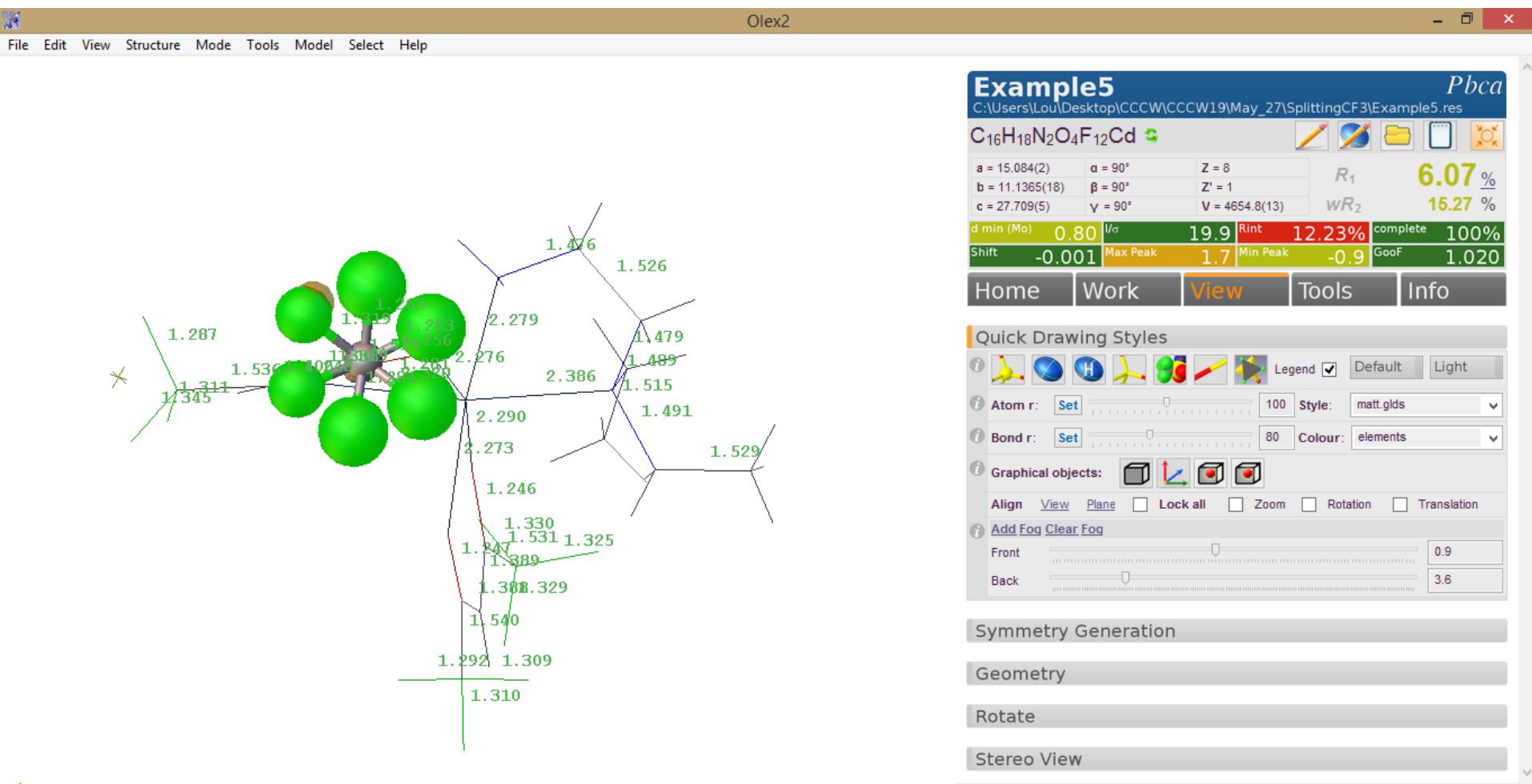
mode fit -s=1

Note that the C8-C10 bond is now selected as well (even though we didn't select C8.)



Right click on the C8-C10 bond once, and then use your left mouse key to rotate around this bond until the second set of F-atoms match up with your residual electron density peaks. Then hit esc

Only C8 has remained anisotropic. (You can use “Fn F3” to remove the distance labels.)



Go back to your Work menu and Sort your atoms.

Then type “edit ins” at the prompt

Notes: Global RIGU (I'm deleting it), second free variable of 0.75, and two parts at bottom of the file with occupancies tied to the second free variable

Close your .ins

File Edit Format View Help

TITL disorder1 in Pbca
REM Solution 1 R1 0.144 Rweak 0.004, Alpha = 0.0755 in Pbca
CELL 0.71073 15.0844 11.1365 27.7091 90 90 90
ZERR 8 0.0024 0.0018 0.0045 0 0 0
LATT 1
SYMM 0.5-X,-Y,0.5+Z
SYMM -X,0.5+Y,0.5-Z
SYMM 0.5+X,0.5-Y,-Z
SFAC C H N O F Cd
UNIT 128 144 16 32 96 8
RIGU

L.S. 10
PLAN 20
TEMP -120|
BOND
LIST 6
MORE -1
CONF
fmap 2
acta 52
WGHT 0.0613 31.275499
FVAR 0.183 0.75

REM <olex2.extras>
REM <HklSrc "%.\Example5.hkl">
REM </olex2.extras>

H15A 2
H15B 2
AFIX 0
C16 1
0.00103
AFIX 23
H16A 2
H16B 2
AFIX 0
PART 1
F10 5
F11 5
F12 5
PART 0
PART 2
F10a 5
F11a 5
F12a 5
HKLF 4

END

Next, let's apply restraints

To Tools → Shelx Compatible Restraints → SADI

Select all C-F bonds in the group we are modelling and “GO”

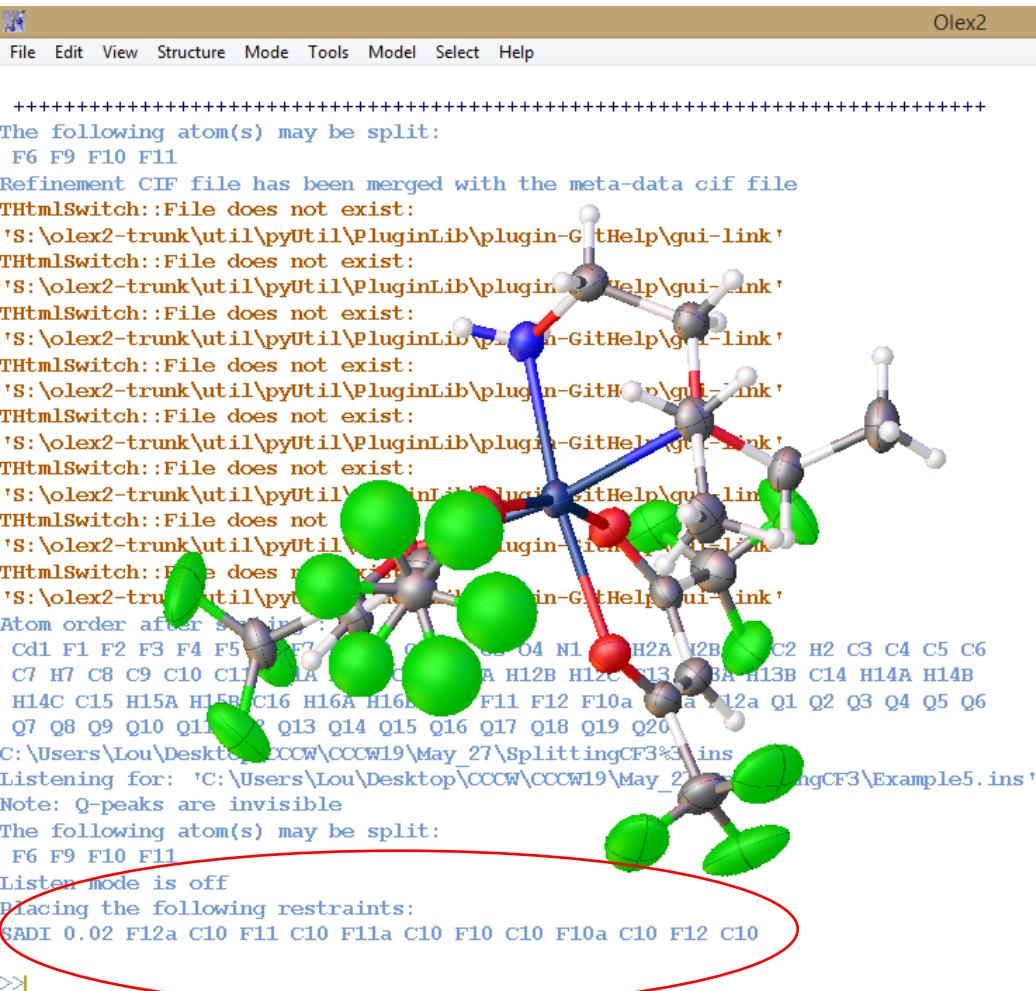
(I switched back to the default view with “Fn F2” for white background and “Ctrl T” to see text in background)

Note the formatting of the restraint; each sequential pair is restrained to have the same distance

Olex2

File Edit View Structure Mode Tools Model Select Help

```
+++++
The following atom(s) may be split:
F6 F9 F10 F11
Refinement CIF file has been merged with the meta-data cif file
THtmlSwitch::File does not exist:
'S:\olex2-trunk\util\pyUtil\PluginLib\plugin-GitHelp\gui-link'
Atom order after scaling:
Cd1 F1 F2 F3 F4 F5 F6 F7 F8 O4 N1 H2A I2B C2 H2 C3 C4 C5 C6
C7 H7 C8 C9 C10 C11 I1A I1B C12 A H12B H12C I13 H13A H13B C14 H14A H14B
H14C C15 H15A H15B C16 H16A H16B F11 F12 F10a F12a Q1 Q2 Q3 Q4 Q5 Q6
Q7 Q8 Q9 Q10 Q11 Q12 Q13 Q14 Q15 Q16 Q17 Q18 Q19 Q20
C:\Users\Lou\Desktop\CCCW\CCCW19\May_27\SplittingCF3\ins
Listening for: 'C:\Users\Lou\Desktop\CCCW\CCCW19\May_27\SplittingCF3\Example5.ins'
Note: Q-peaks are invisible
The following atom(s) may be split:
F6 F9 F10 F11
Listen mode is off
Placing the following restraints:
SADI 0.02 F12a C10 F11 C10 F11a C10 F10 C10 F10a C10 F12 C10
```



Example5
C:\Users\Lou\Desktop\CCCW\CCCW19\May_27\SplittingCF3\Example5.res

a = 15.084(2)	$\alpha = 90^\circ$	Z = 8
b = 11.1365(18)	$\beta = 90^\circ$	Z' = 1
c = 27.709(5)	$\gamma = 90^\circ$	V = 4654.8(13)

R₁ 6.07 %
wR₂ 15.27 %

d min (Mo)	0.80	I/I_0	19.9	Rint	12.23%	complete	100%
Shift	-0.001	Max Peak	1.7	Min Peak	-0.9	GooF	1.020

Home Work View Tools Info

HARt AutoChem 3.1 Images Maps Chemical Tools Olex2 Constraints Restraints Shelx Compatible Constraints Shelx Compatible Restraints

SADI 0.02 go

One Atom Selected. All 'outgoing' bonds will be restrained to be the same, all distances between these bound atoms will also be restrained - with double the e.s.d. This feature allows to 'regularise' entities like spherical counterions.

Note the formatting of the restraint; each sequential pair is restrained to have the same distance

We can select individual atoms in a pairwise manner and apply the same restraint. Let's do this with each of the 1,4 pairs in our disorder group.

If we want to do this with the 1,3 pairs we encounter a problem with using a GUI!

We can add these by editing our .ins (note that shelx doesn't "do" angle restraints, so we get around this with SADI)

```
File Edit Format View Help  
TITL disorder1 in Pbca  
REM Solution 1 R1 0.144 Rweak 0.004, Alpha = 0.0755 in Pbca  
CELL 0.71073 15.0844 11.1365 27.7091 90 90 90  
ZERR 8 0.0024 0.0018 0.0045 0 0 0  
LATT 1  
SYMM 0.5-X,-Y,0.5+Z  
SYMM -X,0.5+Y,0.5-Z  
SYMM 0.5+X,0.5-Y,-Z  
SFAC C H N O F Cd  
UNIT 128 144 16 32 96 8  
SADI F12a C10 F11 C10 F11a C10 F10 C10 F10a C10 F12 C10  
SADI F12 F11a F10a F11 F10 F12a ← CF distance restraints  
SADI F10 F11 F11 F12 F12 F10 F10a F11a F11a F12a F12a F10a| ← 1,4 distance restraints  
SADI F10 F11 F11 F12 F12 F10 F10a F11a F11a F12a F12a F10a| ← 1,3 distance restraints  
L.S. 10  
PLAN 20  
TEMP -120  
BOND  
LSTC
```

I'm still not ready to hit "Refine"

Let's think about how those 1,4 displacements should "look".

Select the 1,4 F-atoms, one pair at a time, and introduce "Shelx Compatible Constraints" EADP after each selection.

(WHOA! Just noticed that there is a LIST 6 instructions in this ins! This instructs the kind of structure factor output that is generated. LIST 6 is not compatible with many things; let's edit this to LIST 4)

Displacements, distances and effectively angles, are now managed. Let's hit "Refine".

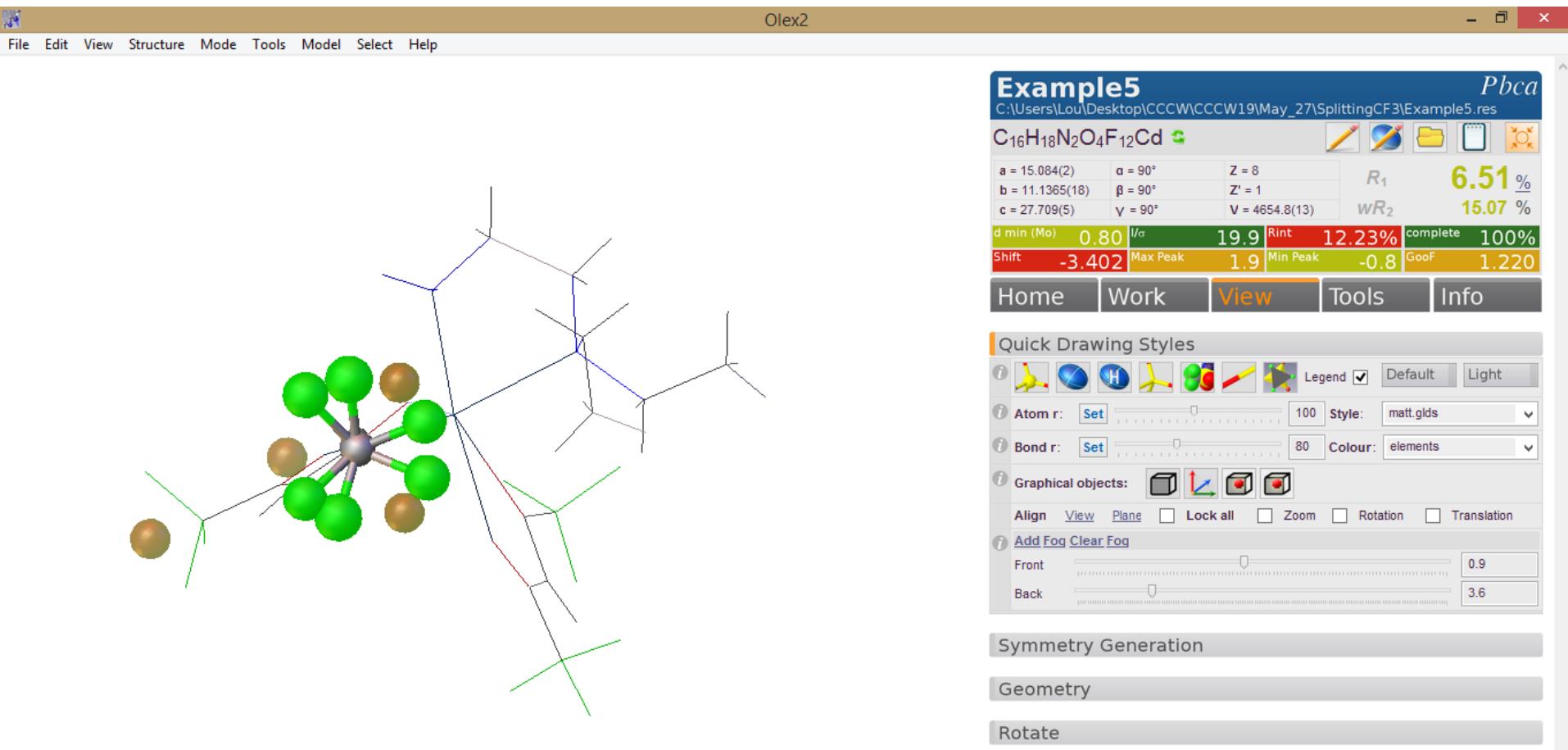
Example5.

```
File Edit Format View Help
TITL disorder1 in PbcA
REM Solution 1 R1 0.144 Rweak 0.004, Alpha = 0.0755 in PbcA
CELL 0.71073 15.0844 11.1365 27.7091 90 90 90
ZERR 8 0.0024 0.0018 0.0045 0 0 0
LATT 1
SYMM 0.5-X,-Y,0.5+Z
SYMM -X,0.5+Y,0.5-Z
SYMM 0.5+X,0.5-Y,-Z
SFAC C H N O F Cd
UNIT 128 144 16 32 96 8
SADI F12a C10 F11 C10 F11a C10 F10 C10 F10a C10 F12 C10
SADI F12 F11a F10a F11 F10 F12a
SADI F10 F11 F11 F12 F12 F10 F10a F11a F12a F12a F10a
EADP F10a F11
EADP F12 F11a
EADP F12a F10

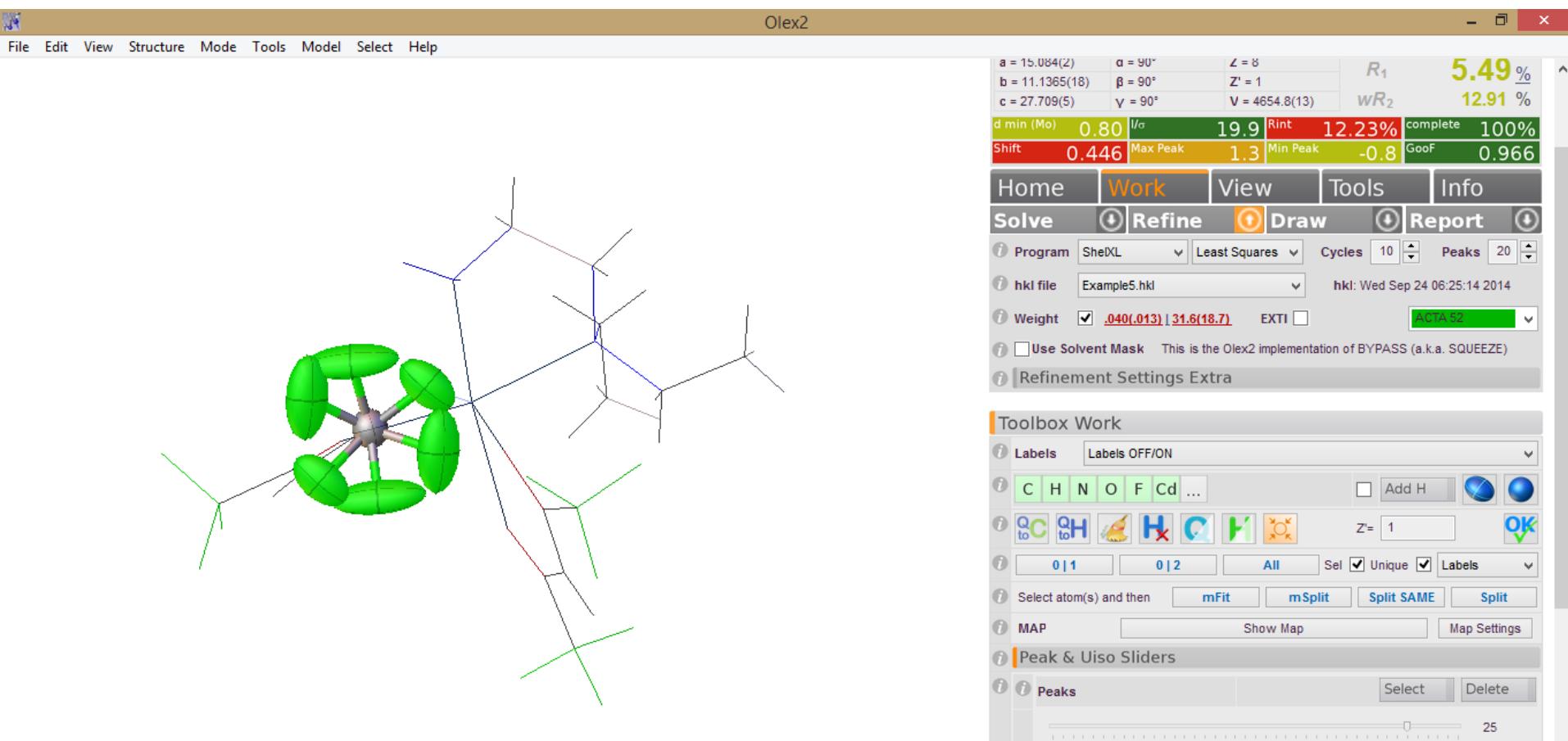
L.S. 10
PLAN 20
TEMP -120
BOND
LIST 6
MORE 1
CONF
fmap 2
```

Sigh...those 1,4 restraints...and those new residual density peaks...

In the meantime, change the isotropic atoms to anisotropic, and refine again.

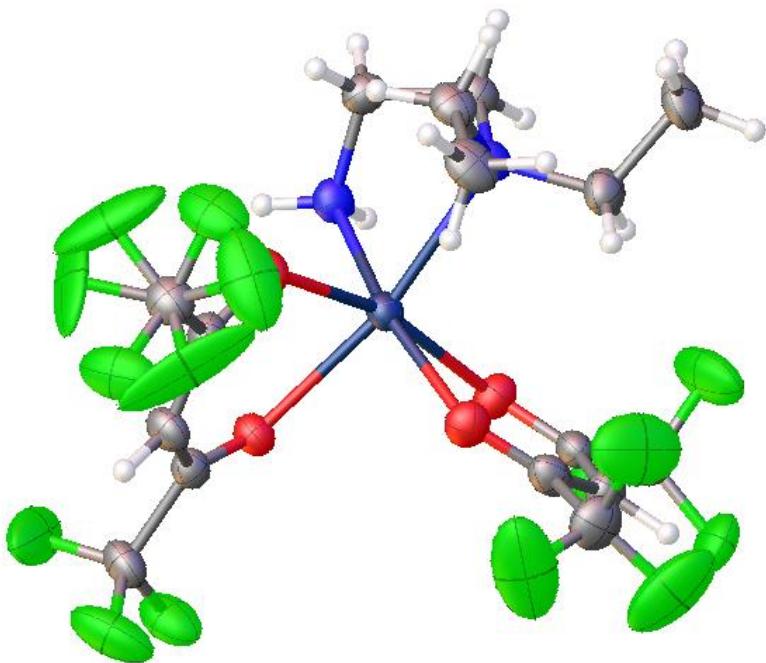


Well, anisotropic refinement dealt with those residual peaks, but is this a good model for what is taking place here?



We are done with this example, but here are a few things to consider:

1. I went in and manually changed the EADP constraints to RIGU restraints but this does not really improve the model.
2. You could go in and further model this with a third (and fourth, and fifth) orientation, tying the occupancies to a SUMP instruction (there is no convenient way to do this in OLEX2; you have to directly edit your ins.)
3. What about the other $-CF_3$ groups?
4. Everything would have been tidier if I had rotated my original second component by 180° instead of 60° .



Quick Drawing Styles

Atom r:	Set	100	Style: matt.gids
Bond r:	Set	80	Colour: elements
Graphical objects:	Set	80	Colour: elements

Align View Plane Lock all Zoom Rotation Translation

Add Fog Clear Fog

Front: 0.9
Back: 3.6

Symmetry Generation

Geometry

Rotate

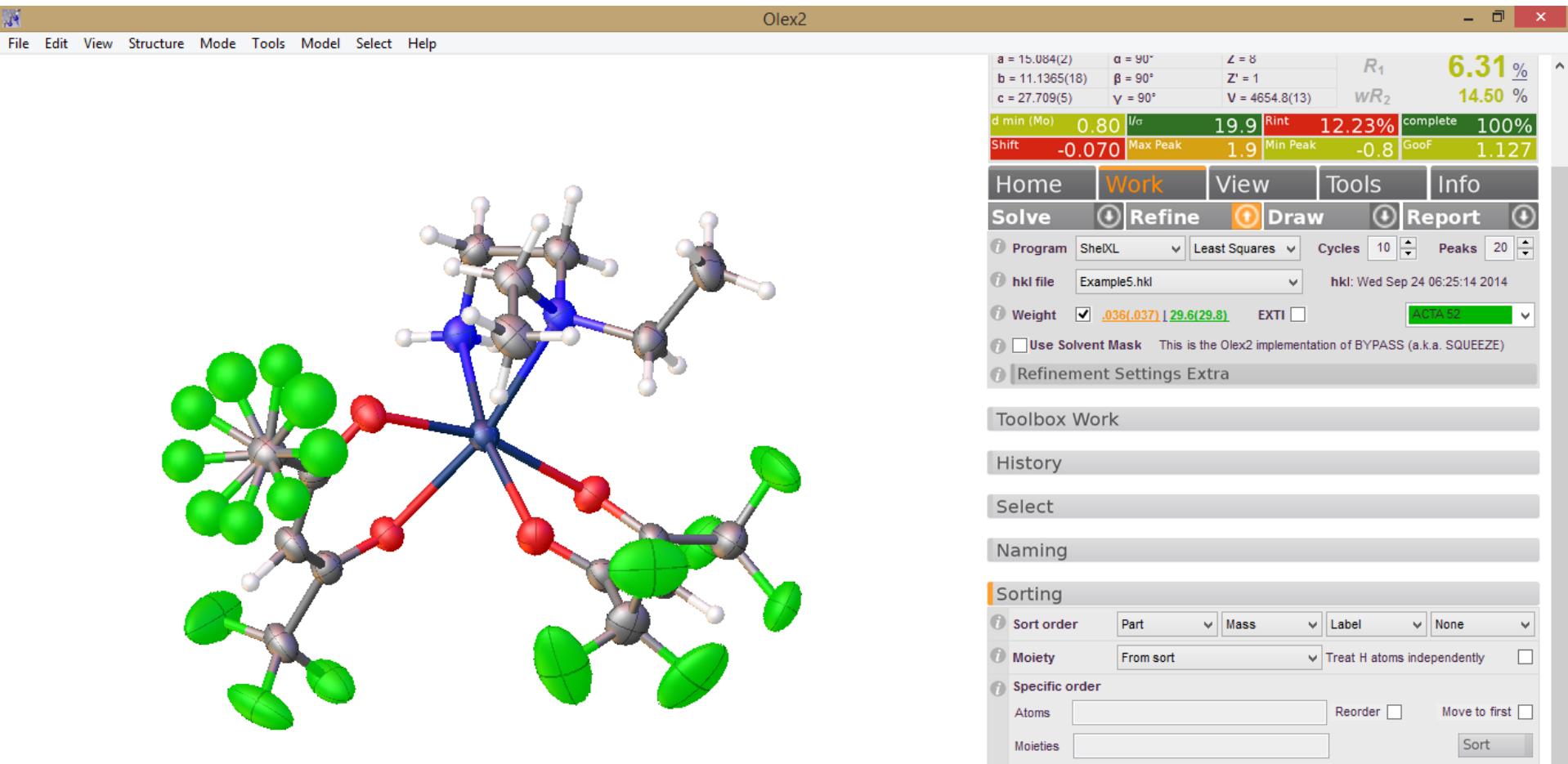
If I was going to split this into three components:

1. Go back to isotropic refinement. Run a round of least squares. Bring back those third component residual electron density peaks.
2. I introduced the next component by directly converting the three peaks to F atoms, and manually named them to F10B, F11B, F12B.
3. “Sort” and then edit ins.
4. Delete the 1,4 SADI restraints. Introduce a new set of C-F and 1,3 F-F SADI restraints for the B component (carry on to the next line using =). Combine all F atoms into a single RIGU line.
5. Find F10B, F11B, F12B, and move them to the bottom of the .cif, under a PART 3.
6. For PART 2, change all of the “-21.000” to “31.000”; for PART 3 change all of the “11.0000” to “41.000”
7. Go back to your FVAR line and change the second FVAR to 0.5, then add in a third with 0.3 and fourth with 0.2
8. Finally, add in the following line with your other instructions (this requires that the sum of the free variables add up to one.)

SUMP 1.0 0.001 1.0 2 1.0 3 1.0 4

9. Hit save. Close the .ins. Hit Refine. Good luck to you. History is still there in case of disaster!

This is before I hit refine. The next slide is what my .ins looks like, just before I hit refine.



```
SYMM -X,0.5+Y,0.5-Z
SYMM 0.5+X,0.5-Y,-Z
SFAC C H N O F Cd
UNIT 128 144 16 32 96 8
SADI F12A C10 F11 C10 F11A C10 F10 C10 F10A C10 F12 C10 =
F10B C10 F11B C10 F12B C10
SADI F10 F11 F11 F12 F12 F10 F10A F11A F11A F12A F12A F10A =
F10B F11B F11B F12B F12B F10B
RIGU F10 F10A F10B F11 F11A F11B F12 F12A F12B
SUMP 1.0 0.001 1.0 2 1.0 3 1.0 4
```

L.S. 10

PLAN 20

TEMP -120

BOND

LIST 4

MORE -1

CONF

fmap 2

acta 52

WGHT 0.0359 29.634201

FVAR 0.18368 0.5 0.3 0.2

REM <olex2.extras>

REM <HklSrc "%.\Example5.hkl">

REM </olex2.extras>

	AFIX	23					
H16A	2	0.72559	0.46002	0.41364	11.00000	-1.20000	
H16B	2	0.74317	0.57743	0.44573	11.00000	-1.20000	

	AFIX	0					
	PART	1					

F10	5	0.52945	0.10426	0.30518	21.00000	0.06323
F11	5	0.63609	0.05060	0.34907	21.00000	0.06735
F12	5	0.50936	-0.03925	0.35458	21.00000	0.05607

	PART	2					
F10A	5	0.48861	-0.01254	0.33930	31.00000	0.05231	
F11A	5	0.58560	0.11146	0.30990	31.00000	0.08463	
F12A	5	0.61935	0.00110	0.36795	31.00000	0.05323	

	PART	3					
F10B	5	0.49590	0.04800	0.32080	41.00000	0.05000	
F11B	5	0.63050	0.10340	0.32540	41.00000	0.05000	
F12B	5	0.56990	-0.03840	0.36780	41.00000	0.05000	

	PART	0					
--	------	---	--	--	--	--	--

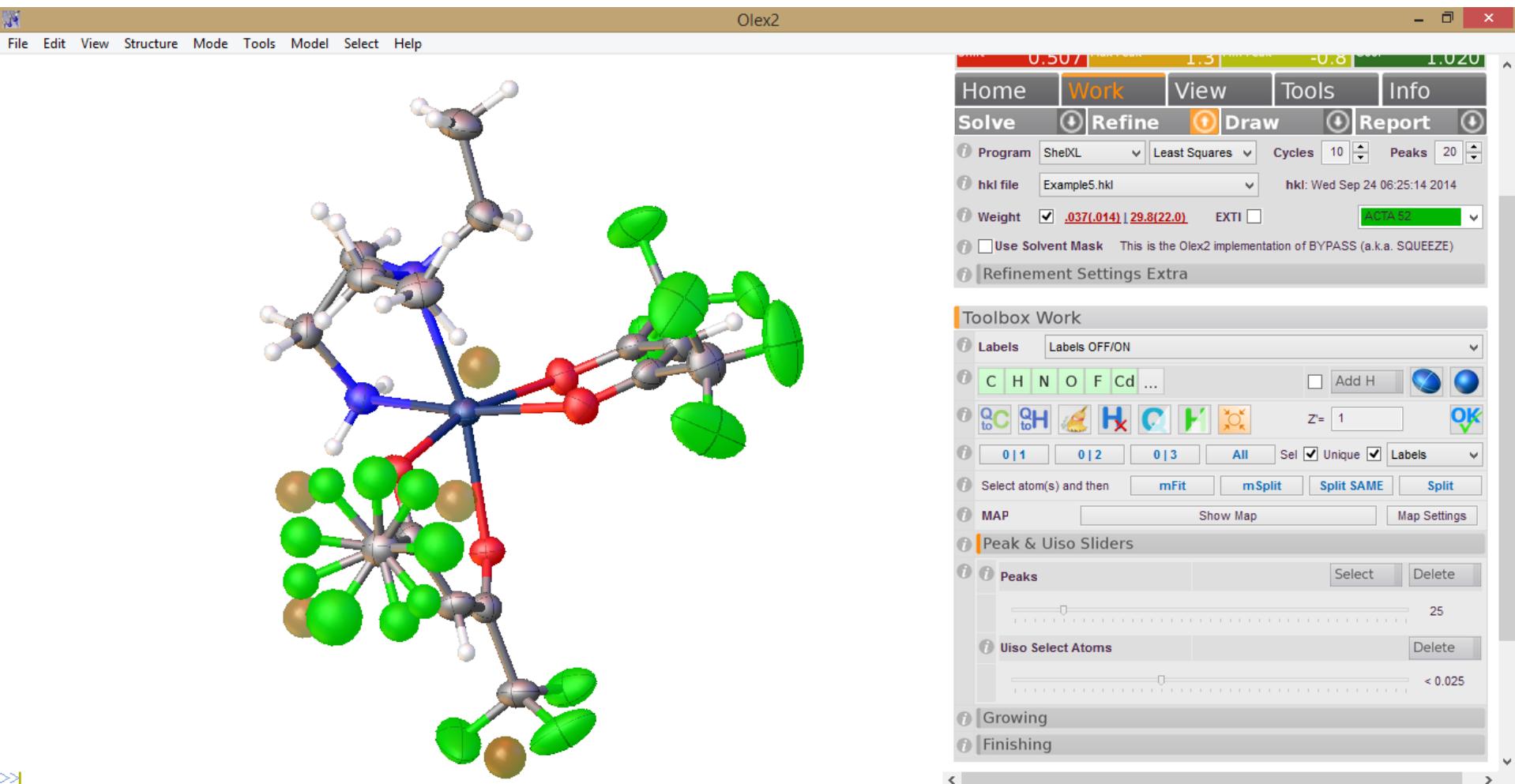
	HKLF	4					
--	------	---	--	--	--	--	--

END

Post refine. Still some peaks.

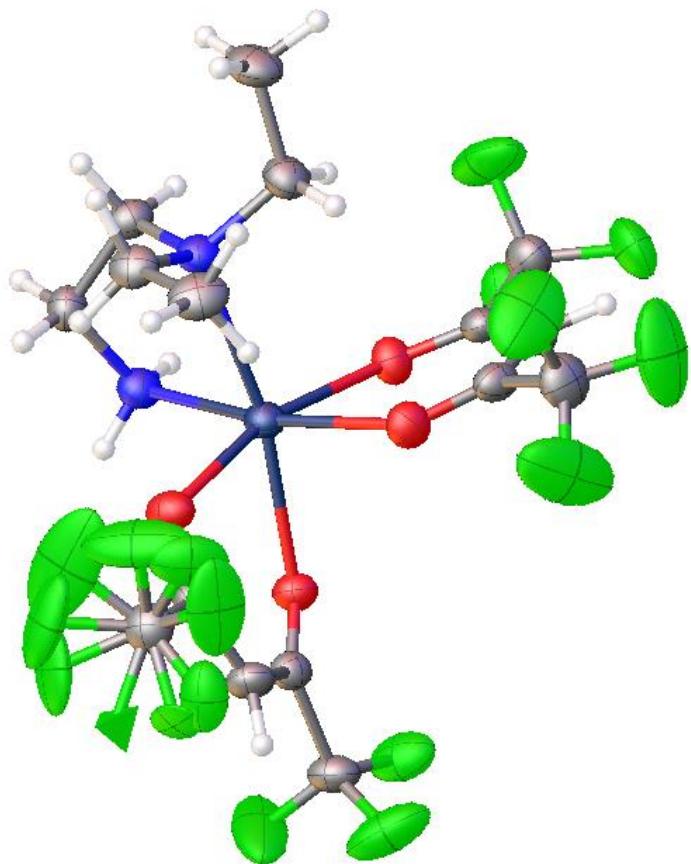
Hover over the atoms to see their occupancies.

Let's go anisotropic.



Ugh. Let's go home.

(No, seriously, I could probably "fix" this with some ISOR restraints, or EADP constraints, or changing the default RIGU esd to something much smaller. But that doesn't make it "right".)



o min (Mo)	0.80	1/ σ	19.9	Rint	12.23%	complete	100%
Shift	-0.092	Max Peak	1.3	Min Peak	-0.8	GooF	1.095

Home Work View Tools Info

HARt

AutoChem 3.1

Images

Maps

Chemical Tools

Olex2 Constraints Restraints

Shelx Compatible Constraints

Shelx Compatible Restraints

SADI 0.02 go

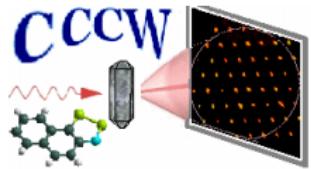
One Atom Selected All 'outgoing' bonds will be restrained to be the same, all distances between these bound atoms will also be restrained - with double the e.s.d. This feature allows to 'regularise' entities like spherical counterions.

Two or more Bonds Selected The selected bonds will be restrained to be the same.

Three Atoms in a row The bonds between the two atoms bound to the central atoms will be restrained to be the same.

Pairwise atom selection If an even number of atoms is selected, the distances between pairs of atoms will be restrained to be the same, depending on the order of selection.

Hydrogen Atoms



Canadian National Committee
for Crystallography
<http://xtallography.ca/>

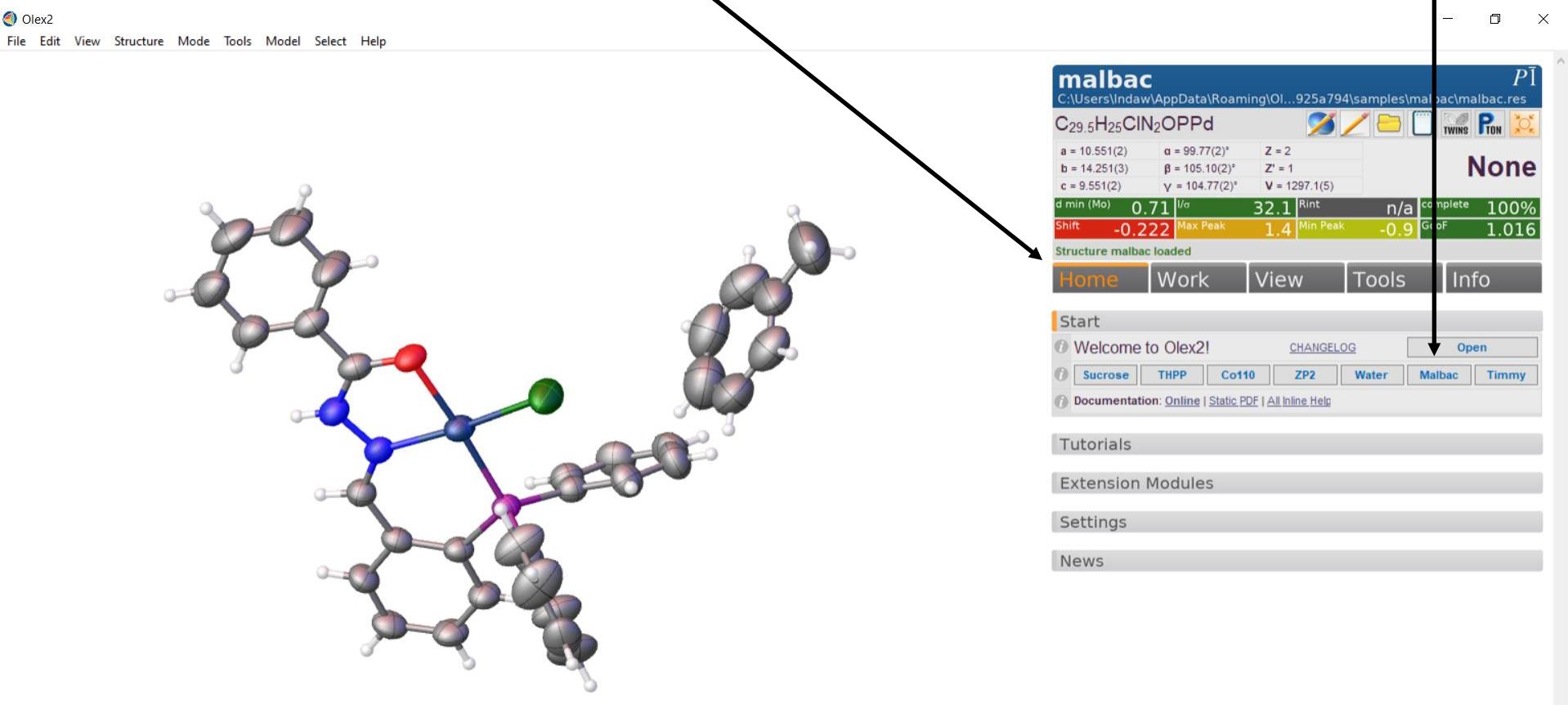
Solvent or Anion Disorder: Fixed Positions

Check out the OLEX2 youtube channel for a similar example:

<https://www.youtube.com/watch?v=hCI4VdQ8iBg&list=PLJgQksgBlpeAMDW5PVOI0r9EqFZ8p-Y4 &index=7&t=0s>

Navigate to Home.

Under Start, select “Malbec”

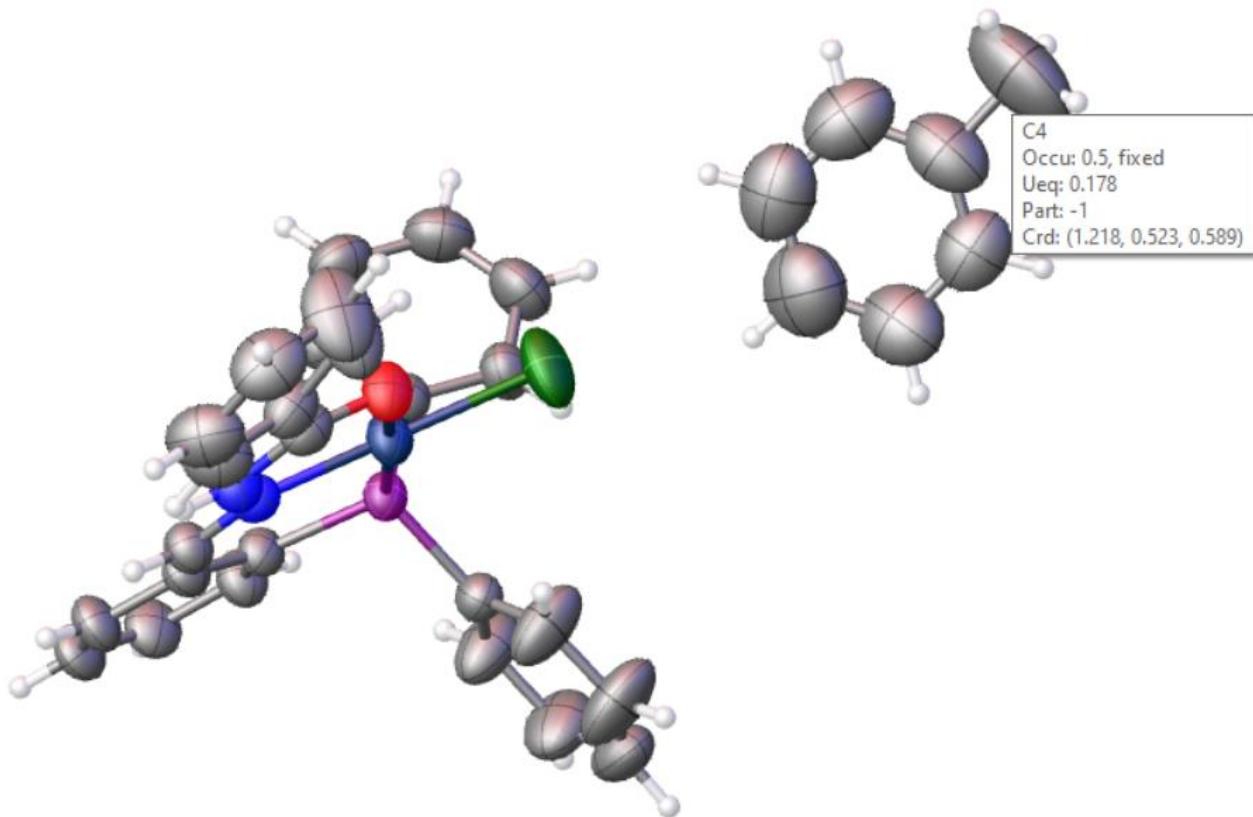


This is the finished structure.

Toluene looks disordered.

Hover over any atom; occupancy is 0.5, and it is PART -1

Why?

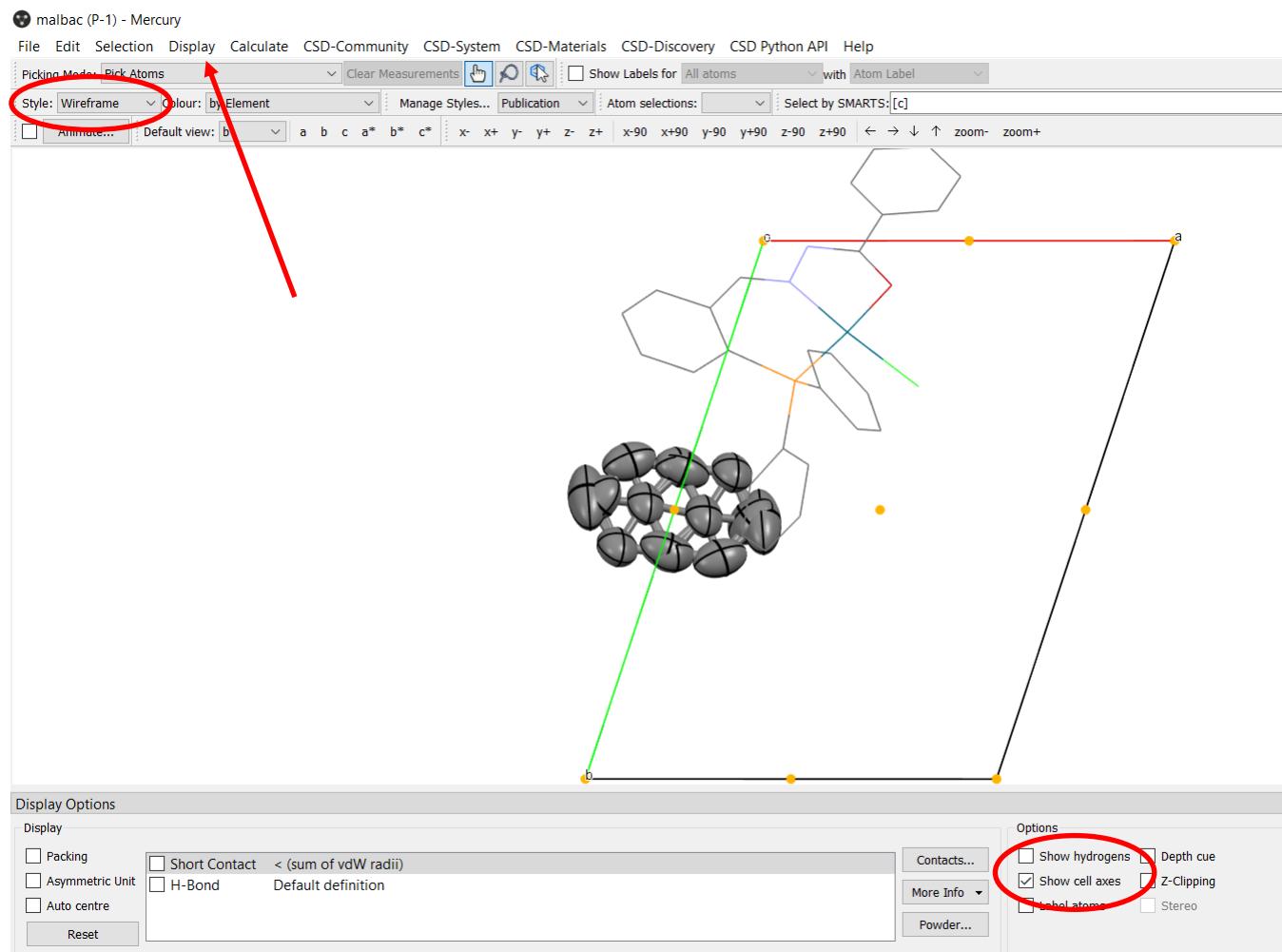


Open the .cif in Mercury; I got my file path by looking here:

malbac
C:\Users\Indaw\AppData\Roaming\O...925a794\samples\malbac\malbac.res
C₂₉.5H₂₅CIN₂OPPd

Right click on the main molecule (not toluene): Selection → Select Molecule

I then changed my style to “Wireframe”, deselected “Show hydrogen”, selected “Show cell axes”, and then went to: Display → Symmetry Elements... → OK



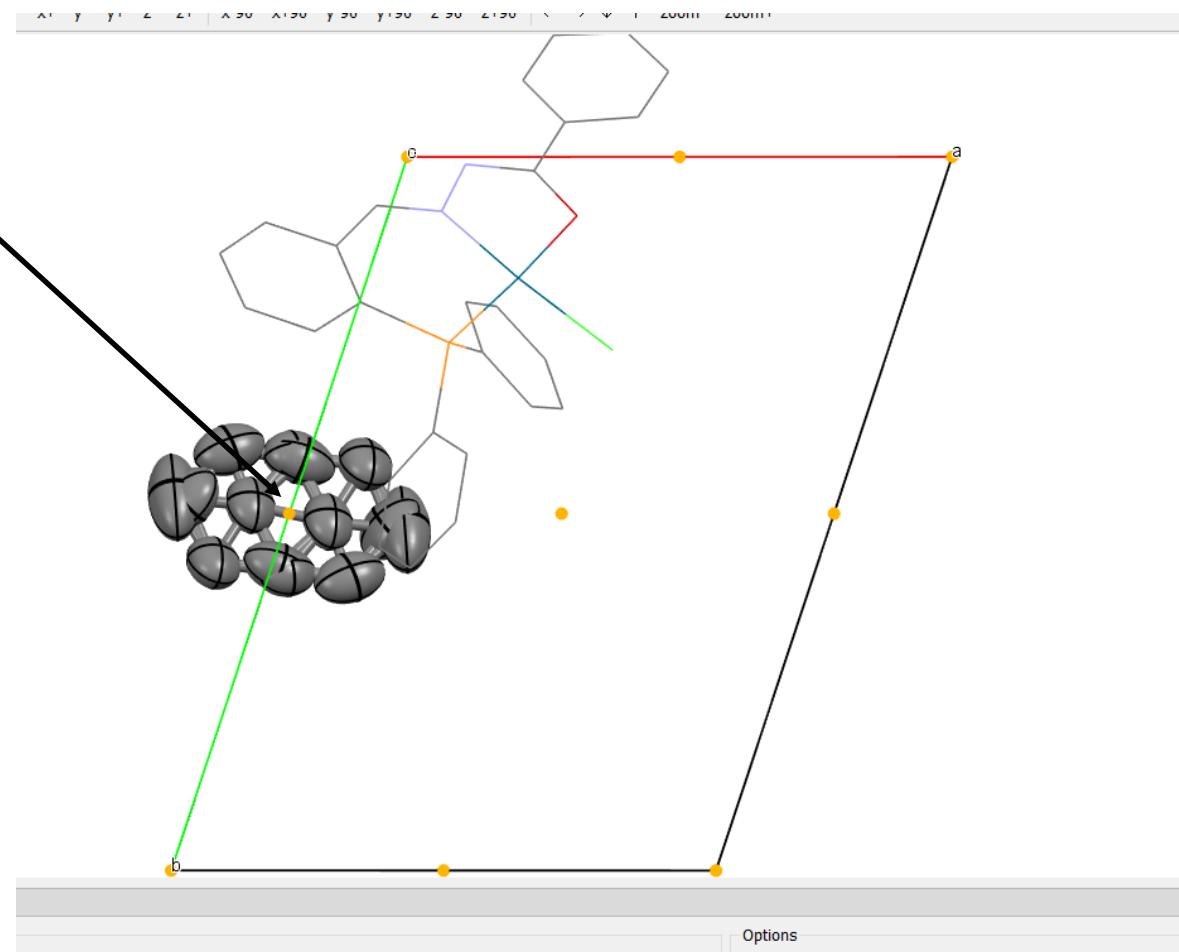
Looking at this structure in Mercury:

Space group is P-1

The only symmetry is inversion

Toluene is “sitting on” an inversion centre, yet its molecular symmetry does not exhibit inversion.

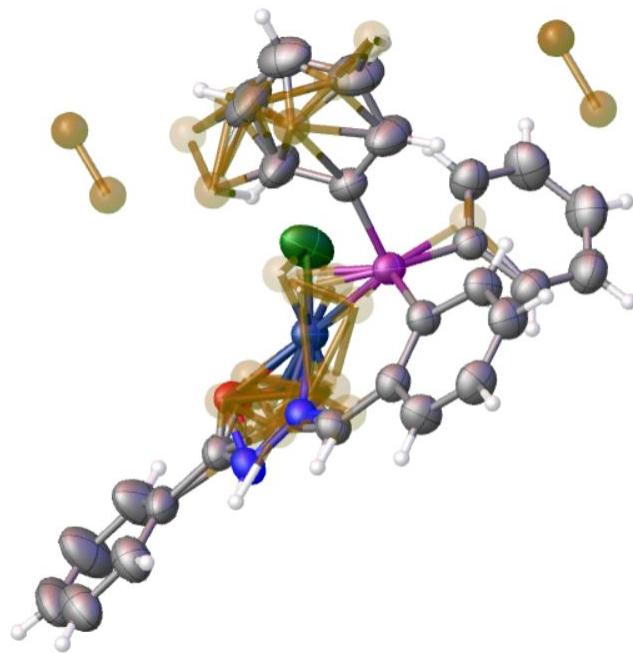
How do we model this?



Back in OLEX2

1. Delete toluene, set your rounds of least squares to five, set your peaks to 25, and refine.
2. Assemble your fragments.
3. Display only your top four peaks, and type “grow”.

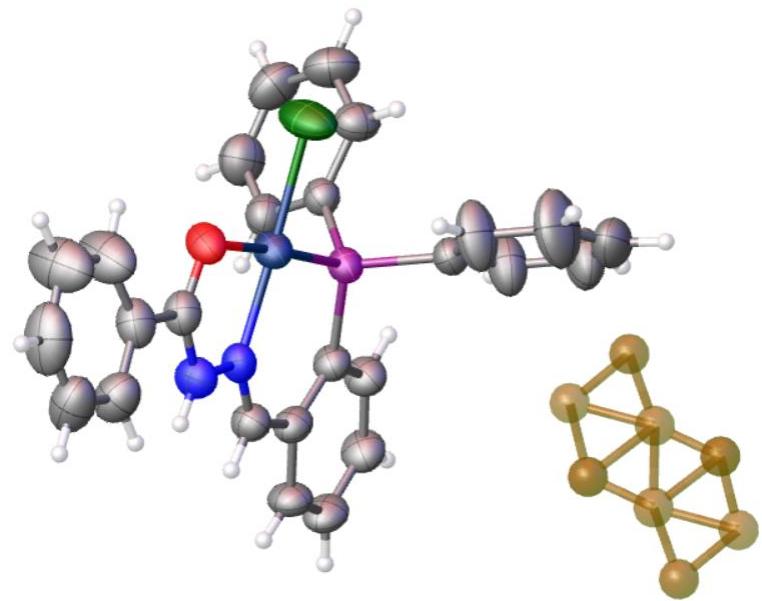
1.



2.



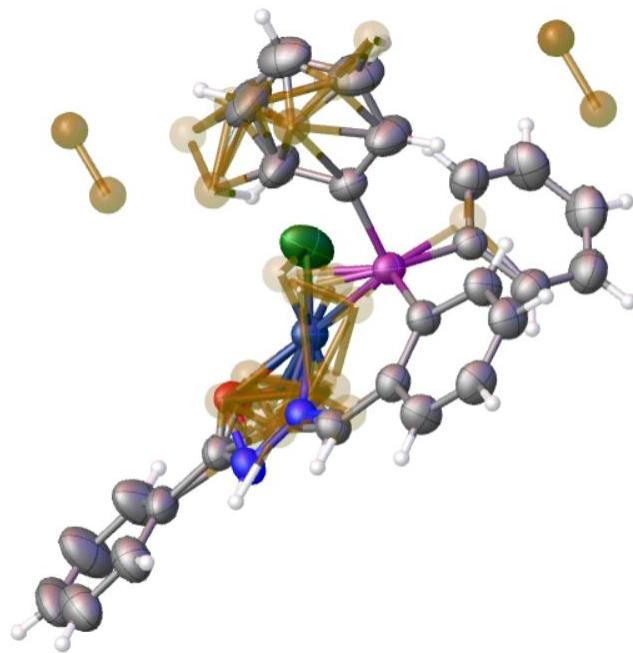
3.



Back in OLEX2

1. Delete toluene, set your rounds of least squares to five, set your peaks to 25, and refine.
2. Assemble your fragments.
3. Display only your top four peaks, and type “grow”.
4. Imagination!

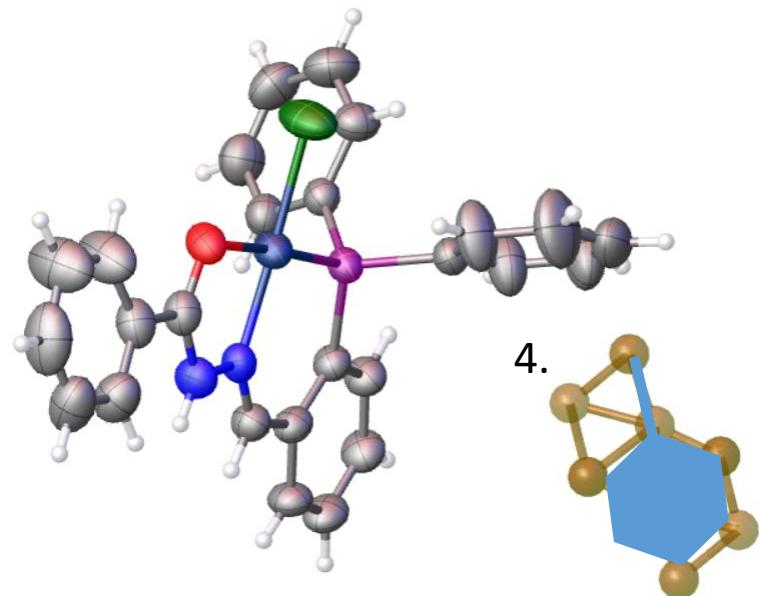
1.



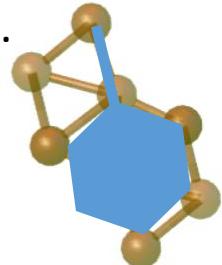
2.



3.



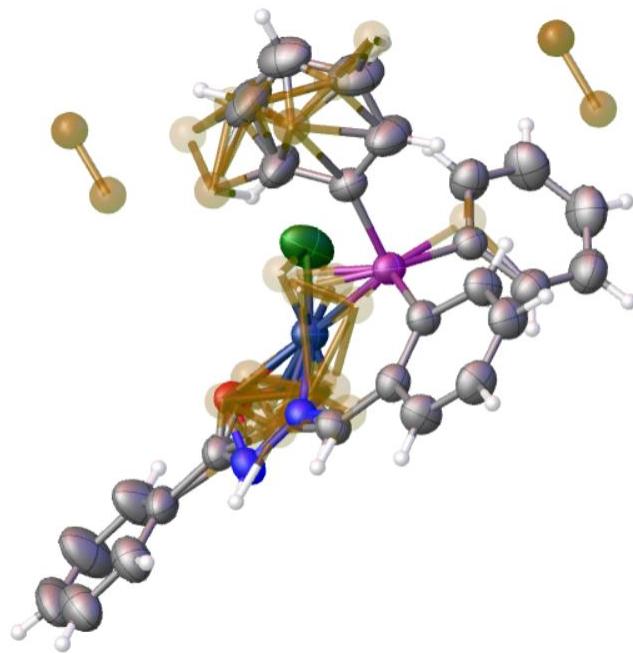
4.



Back in OLEX2

1. Delete toluene, set your rounds of least squares to five, set your peaks to 25, and refine.
2. Assemble your fragments.
3. Display only your top four peaks, and type “grow”.
4. Imagination! (No seriously now, how do I make it do that?)

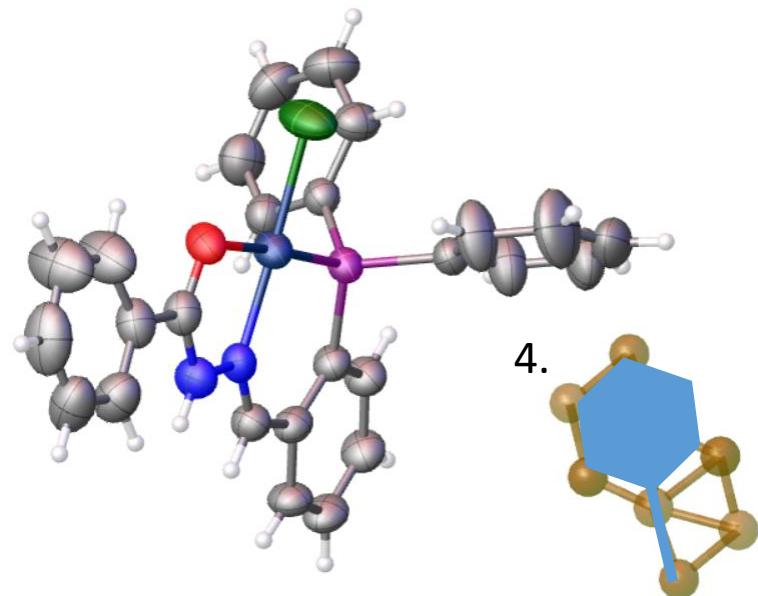
1.



2.



3.



OLEX2 makes FRAG/FEND “simple”

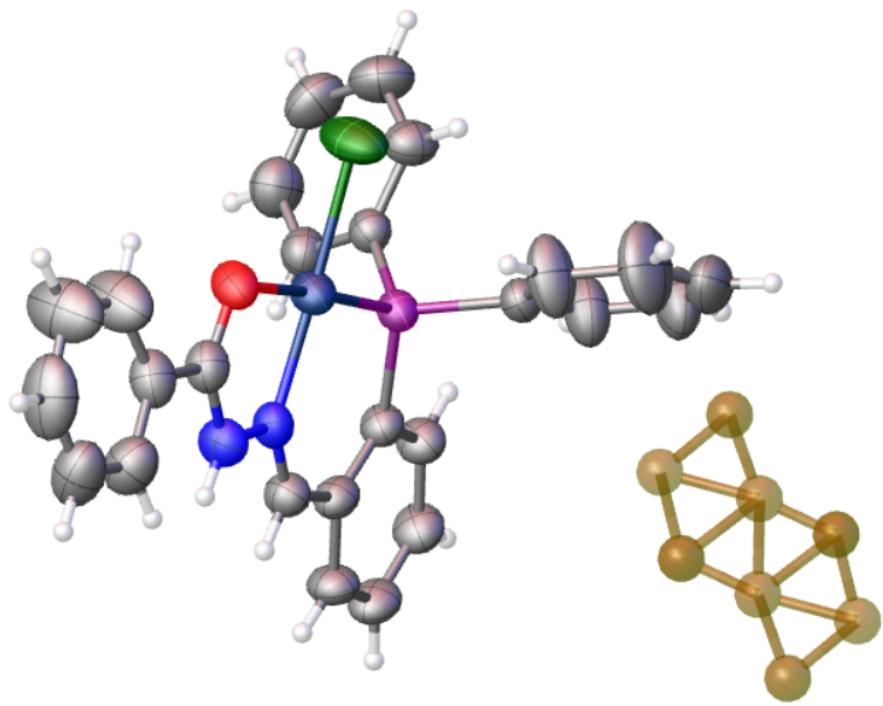
From the shelx manual:

FRAG code[17] a[1] b[1] c[1] α [90] β [90] γ [90] Enables a fragment to be input using a cell and coordinates taken from the literature. Orthogonal coordinates may also be input in this way. Such a fragment may be fitted to the set of atoms following an AFIX instruction with m=code (code must be greater than 16); there must be the same number of atoms in this set as there are following FRAG, and they must be in the same order. Atoms with zero coordinates are not fitted, but new coordinates are generated for these atoms. The atom names, sfac numbers, sof and Uij of the FRAG fragment are ignored, only the coordinates are used. A FRAG fragment may be given anywhere between UNIT and HKLF or END or in an 'include' file, and must be terminated by a FEND instruction, but must precede any AFIX instruction which refers to it. This rigid fit is often a preliminary to a rigid group refinement (AFIX 6).

Tools → FragmentDB → Find toluene from the list

Next: PART = -1; Occupancy = 0.5 (Why?)

Tools Model Select Help



malbac

C_{29.5}H₂₅CIN₂OPPd

$a = 10.551(2)$ $\alpha = 99.77(2)^\circ$ $Z = 2$
 $b = 14.251(3)$ $\beta = 105.10(2)^\circ$ $Z' = 1$
 $c = 9.551(2)$ $\gamma = 104.77(2)^\circ$ $V = 1297.1(5)$

$d_{\min}(\text{Mo})$ 0.71 l/σ 32.1 R_{int} n/a complete 100%
Shift 0.224 Max Peak 3.3 Min Peak -0.8 GooF 1.834

WARNING: Input data appear to be merged: CIF file will be incomplete

Home Work View Tools Info

HART

ReportPlus

FragmentDB

Toluene, C₇H₈

Fit! Edit

PART: -1 Free Variable: 1 Occupancy: 0.5 = 10.5

Use a residue: Residue Class: TOL Invert: Calculate DFIX:

Replace Mode: No Restraints: Rigid Group: Revert Fit

List of most disagreeable restraints:

Observed	Target	Error	Sigma	Restraint
-	-	-	-	-

Tools → FragmentDB → Find toluene from the list

Next: PART = -1; Occupancy = 0.5 (Why?)

Directly from Peter Mueller: <http://web.mit.edu/pmueller/www/ACA2007/WK01/Disorder.pdf>

Disorder Involving Special Positions

Imagine a molecule sitting on or near a special position without fulfilling the geometry of that symmetry element (e.g. toluene on inversion center).

Two possible ways of describing: either use different space group without the symmetry element(s) in question or refine a disorder about the special position.

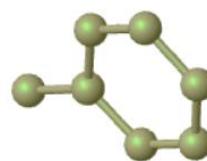
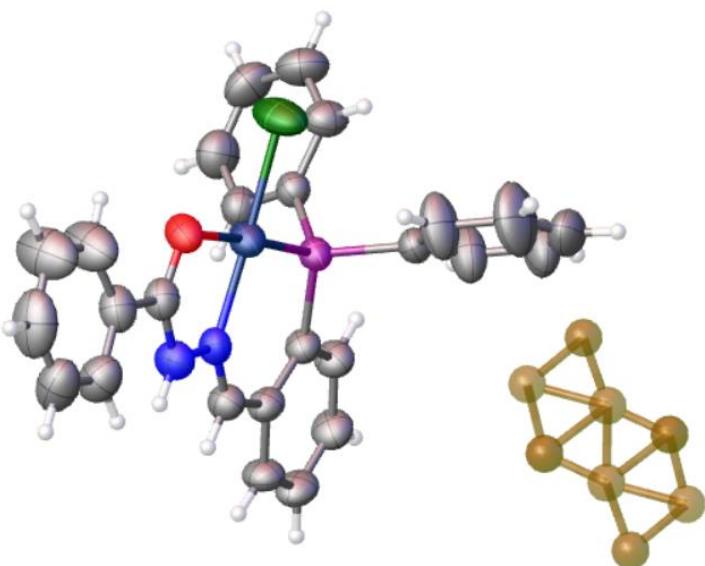
Refinement is easy: you need only one set of coordinates, as the second one can be generated from the first by means of the symmetry operator(s) corresponding to the special position in question. Therefore instead of **PART 1** and **PART 2** you only need one component, which has to be placed in **PART -1**.

The ratio does not need to be refined as it corresponds to the multiplicity of the symmetry operator (0.5 for an inversion center, mirror and twofold axis; 0.3333 for a threefold, 0.25 for a fourfold and 0.1667 for a sixfold). Combinations of symmetry operators are possible, of course.

Once you have selected toluene from the list, hit “Fit”

A “shadow” toluene will appear.

Click on one atom in the shadow, and then click on one of your electron density peaks that you want to line up with the shadow.



Home Work View Tools Info

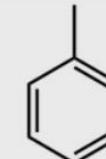
HART

ReportPlus

FragmentDB

Toluene, C₇H₈

Fit!



PART: -1 Free Variable: 1 Occupancy: 0.5 => 10.5

Use a residue: Residue Class: TOL Invert: Calculate DFIX:

Replace Mode: No Restraints: Rigid Group:

List of most disagreeable restraints:

Observed	Target	Error	Sigma	Restraint
--	--	--	--	--

AC4

Twinning

You are in mode MODE_DISP

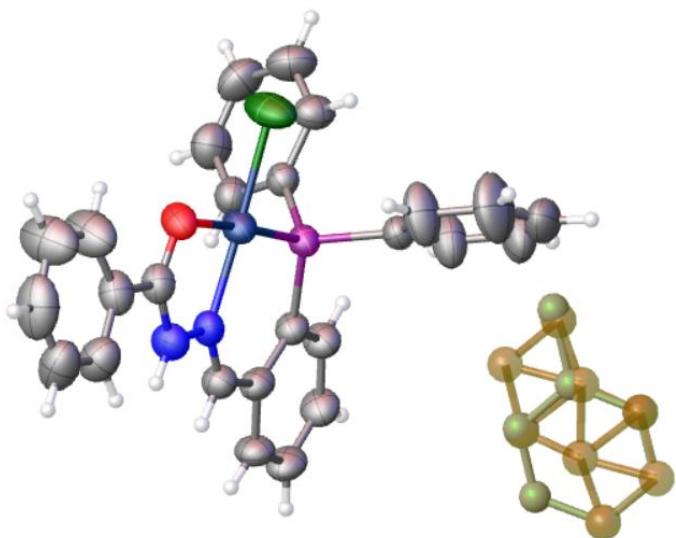
Press the ESC key to exit.

Once you have selected toluene from the list, hit “Fit”

A “shadow” toluene will appear.

Click on one atom in the shadow, and then click on one of your electron density peaks that you want to line up with the shadow.

Keep selecting one shadow peak (green) and one electron density peak (orange) until you get a reasonable fit. This took me three clicks.



c = 9.551(2) V = 104.77(2)^o V = 1297.1(5) WTK2 21.00 %

d min (Mo)	0.71	I/o	32.1	Rint	n/a	complete	100%
Shift	0.224	Max Peak	3.3	Min Peak	-0.8	GooF	1.834

WARNING: Input data appear to be merged: CIF file will be incomplete

Home Work View Tools Info

HART

ReportPlus

FragmentDB

Toluene, C7H8

PART: -1 Free Variable: 1 Occupancy: 0.5 => 10.5

Use a residue: Residue Class: Invert: Calculate DFIX:

Replace Mode: No Restraints: Rigid Group:

List of most disagreeable restraints:

Observed	Target	Error	Sigma	Restraint
--	--	--	--	--

AC4

Twining

You are in mode MODE_DISP
Press the ESC key to exit

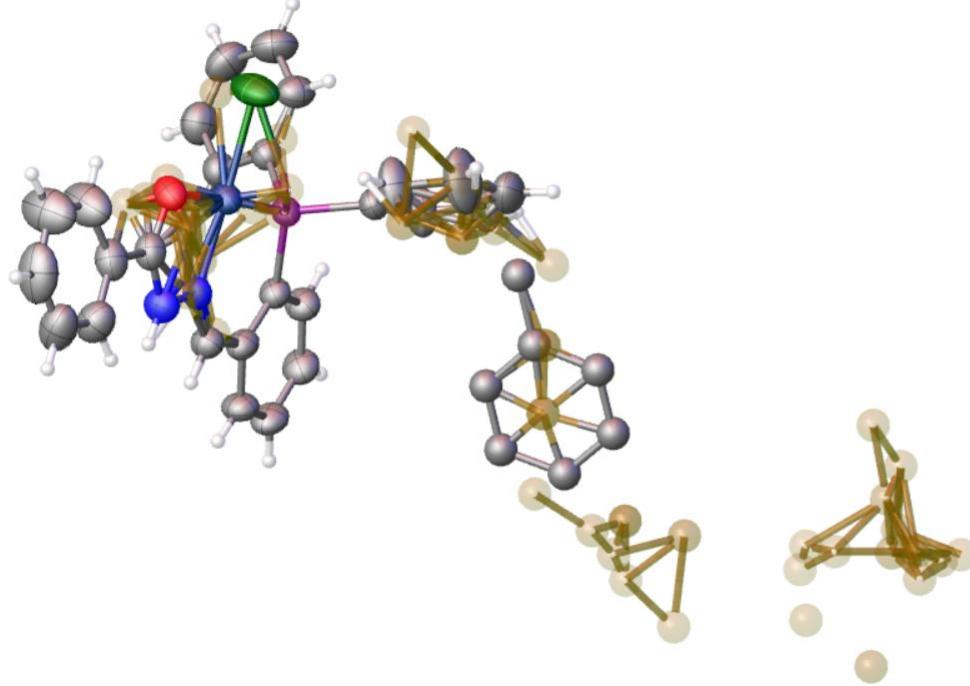
Once you have selected toluene from the list, hit “Fit”

A “shadow” toluene will appear.

Click on one atom in the shadow, and then click on one of your electron density peaks that you want to line up with the shadow.

Keep selecting one shadow peak (green) and one electron density peak (orange) until you get a reasonable fit. This took me three clicks.

Then hit “Esc”



C = 9.551(2) V = 104.77(2)^a V = 1297.1(5) W/F₂ Z = 1.00 70

d min (Mo)	0.71	I/σ	32.1	Rint	n/a	complete	100%
Shift	0.224	Max Peak	3.3	Min Peak	-0.8	GooF	1.834

WARNING: Input data appear to be merged: CIF file will be incomplete

Home Work View Tools Info

HARt

ReportPlus

FragmentDB

Toluene, C₇H₈

PART: -1 Free Variable: 1 Occupancy: 0.5 => 10.5

Use a residue: Residue Class: TOL Invert: Calculate DFIX:

Replace Mode: No Restraints: Rigid Group:

List of most disagreeable restraints:

Observed	Target	Error	Sigma	Restraint
--	--	--	--	--

AC4

Twinning

To keep things ordered, I then named the tolune C50 – C56, and sorted my atoms, so that I could see what all this clicking did in my instruction file.

malbac.ins - Notepad

File Edit Format View Help

```
TITL r26
REM r26
REM 384 parameters refined using 6 restraints
CELL 0.71078 10.551 14.251 9.551 99.77 105.1 104.77
ZERR 2 0.002 0.003 0.002 0.02 0.02 0.02
LATT 1
SFAC C H Cl N O P Pd
UNIT 59 50 2 4 2 2 2
DFIX 1.51 C50 C51
DANG 2.42 C51 C53
FLAT C50 C51 C52 C53 C54 C55 C56
DFIX 1.39 C51 C52 C51 C56 C53 C54
DANG 2.39 C52 C54
DFIX 1.38 C52 C53 C54 C55 C55 C56
RIGU C50 > C56
SADI C51 C52 C52 C53 C53 C54 C54 C55 C55 C56 C56 C51
DANG 2.41 C51 C55
SADI 0.04 C51 C55 C51 C53 C56 C54 C52 C56 C53 C55 C52 C54
DANG 2.4 C53 C55 C54 C56
SIMU C50 > C56
SADI 0.04 C50 C56 C50 C52
DANG 2.52 C50 C52 C50 C56
```

	PART	-1						
C50	1	0.22881	0.51794	-0.40920	10.50000	0.05000		
C51	1	0.07692	0.50459	-0.47142	10.50000	0.05000		
C52	1	0.03148	0.57907	-0.52536	10.50000	0.05000		
C53	1	-0.10717	0.56792	-0.58177	10.50000	0.05000		
C54	1	-0.20480	0.48040	-0.58520	10.50000	0.05000		
C55	1	-0.16180	0.40549	-0.53257	10.50000	0.05000		
C56	1	-0.02268	0.41731	-0.47593	10.50000	0.05000		
	HKLF	4						

END

Close your .ins and Refine.

Make your toluene anisotropic, and Refine.

Add your hydrogen atoms, and Refine.

If you “grow”, OLEX2 does not show you the other “half”, but if you open your structure in Mercury, or if you go to “View → Symmetry Generation → Packing → Pack to limits” (for example), your full disorder model will be visible.

