

# Cristallographie à résolution ultra haute & Logiciel MoPro

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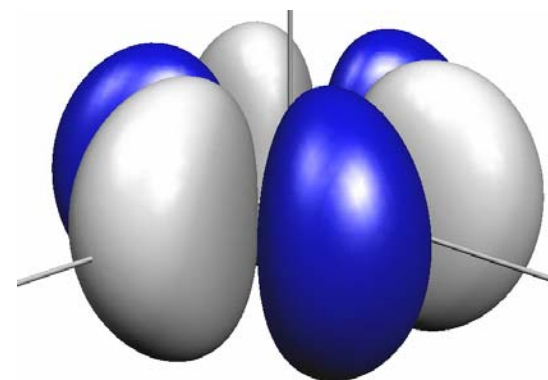
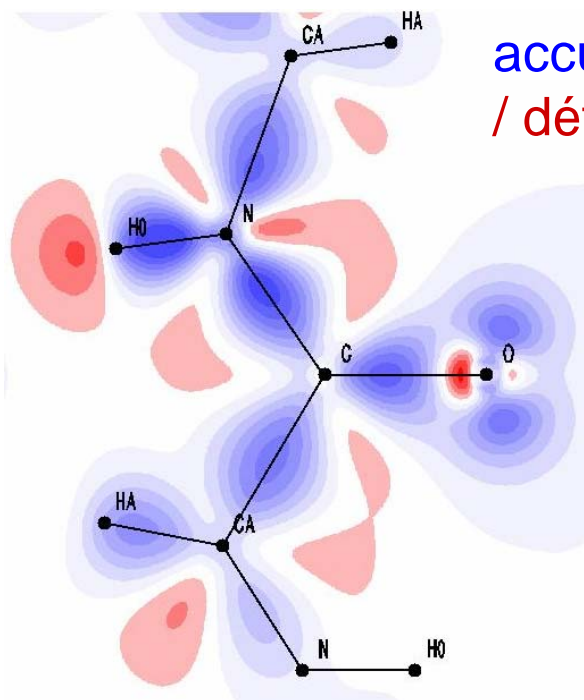


# Cristallographie des Rayons X à Résolution Ultra Haute

Observer la

Déformation de la Densité Electronique

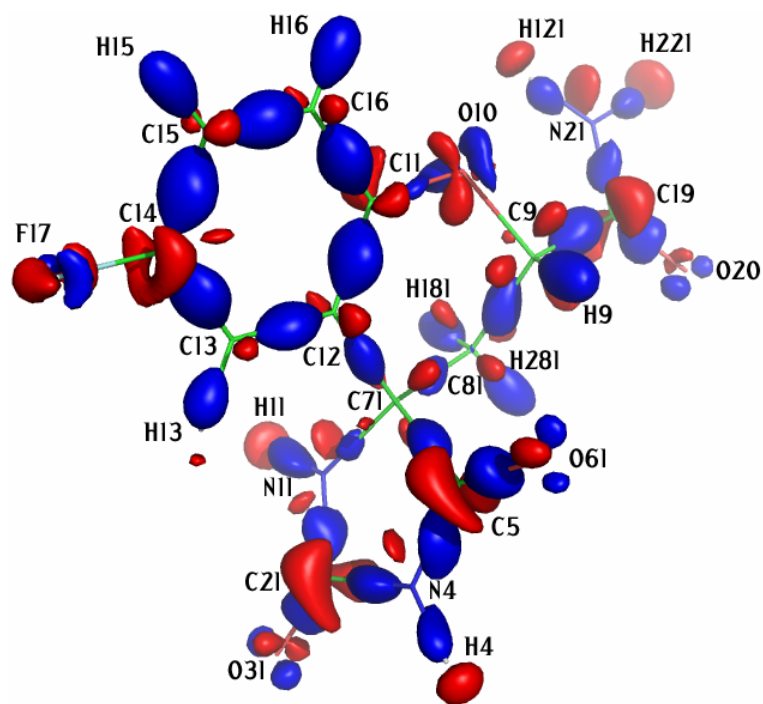
$$\Delta\rho = \rho_{\text{molécule}} - \rho_{\text{Atomes/Sphérique/Neutre}}$$



Atomes Multipolaires

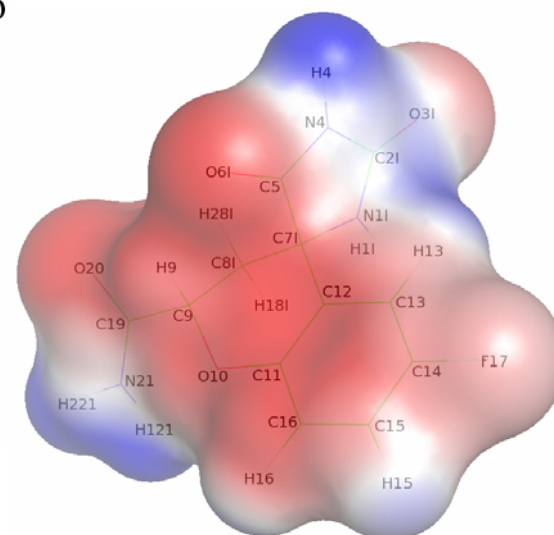
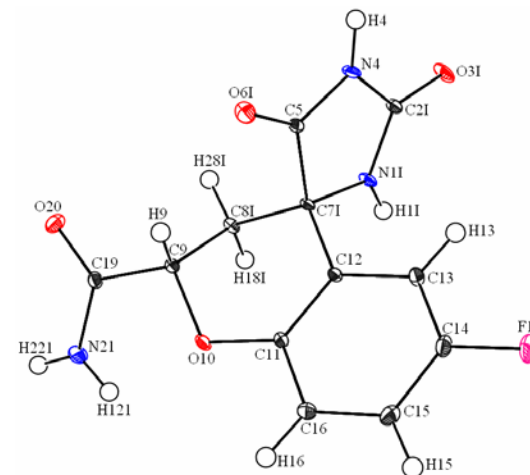
# Fidarestat : Inhibiteur Aldose Réductase Humaine

Déformation de la Densité Electronique  
Expérimentale



résolution = 0.50 Å

synchrotron Hambourg



Potentiel  
Electrostatique

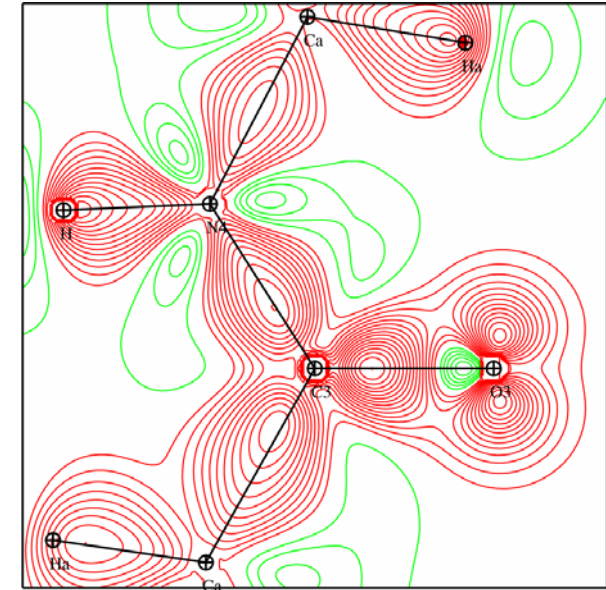
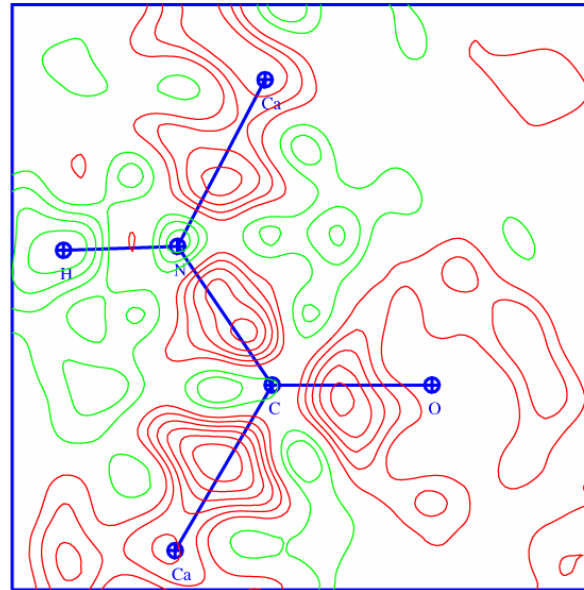
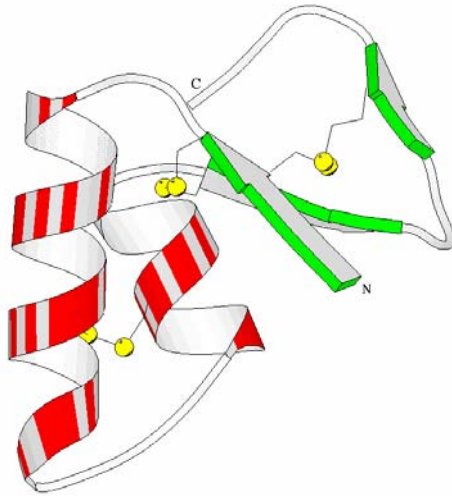


Fournier *et al.*, 2009. JACS

# Crambine : 1<sup>e</sup> Application aux Protéines

Cristallographie ultra haute résolution

Diffraction 0.54 Å



Densité  
Electronique

Fourier Résiduelle

$$F_{\text{obs}} - F_{\text{cal}}$$

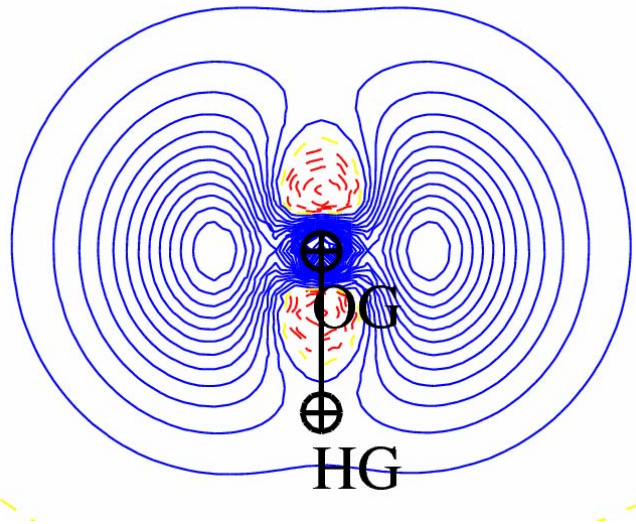
Déformation  
Affinement Crambine  
<Polypeptidide>

Jelsch *et al.* PNAS. 2000, 97.

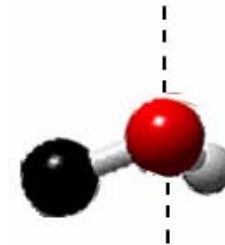
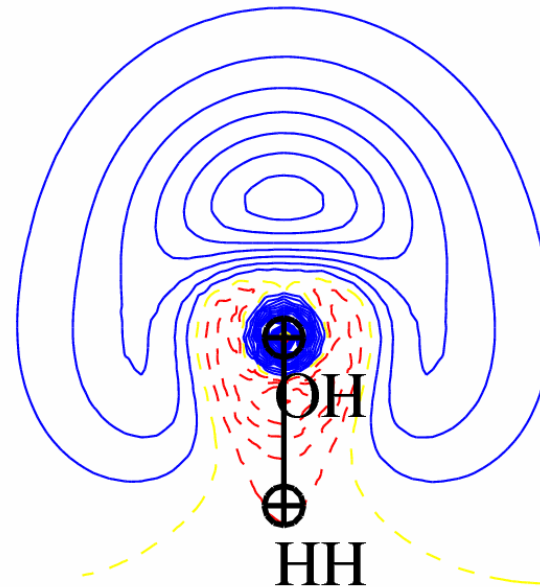
# Librairie Atomes Multipolaire

## Densité Electronique des Protéines

Serine  
Csp3-O-H



Tyrosine  
Csp2-O-H



Hydroxyle

Contours  
+/- 0.05 e/Å<sup>3</sup>,

Densité de Charge  
14 Cristaux Peptides

Pichon-Pesme *et al.* (2004) *Acta Cryst.* A60  
Zarychta *et al.* (2007) *Acta Cryst.* A38

# Logiciel Cristallographique *MoPro*



## Résolution

<b>Subatomique</b> <b>~0.5Å</b>	<b>Affinement</b> <b>Structure &amp; Densité Electronique</b>
<b>Atomique</b> <b>0.7 – 1.5 Å</b>	<b>Transfert Librairie Densité Electronique</b> <b>Affinement Structure</b>

**minéraux, petites & macro-molécules**

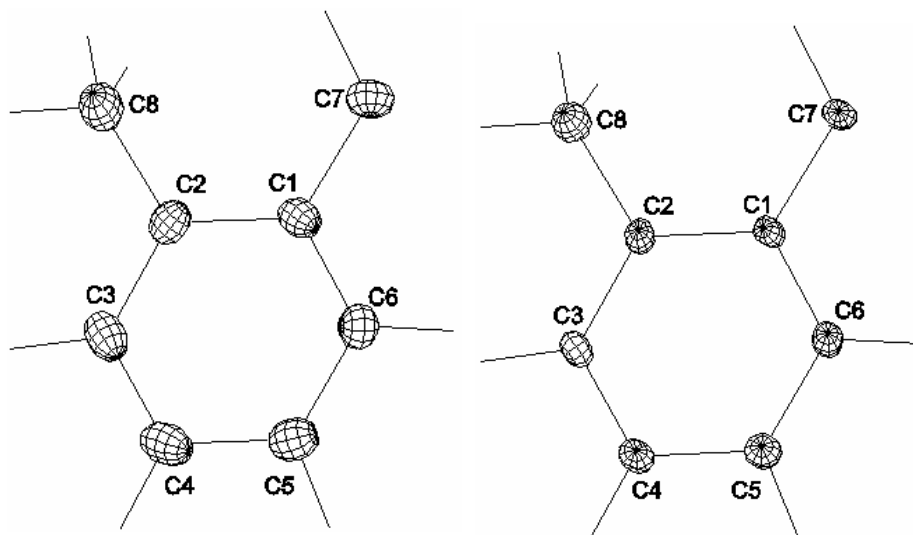
**affinement automatique**

Guillot *et al.*, J. Appl. Cryst. (2001) 34

Jelsch *et al.*, J. Appl. Cryst. (2005) 38

# Transfert Librairie Multipolaire à Structures de Résolution Moindre

**Ellipsoïdes Agitation  
Thermique plus justes**

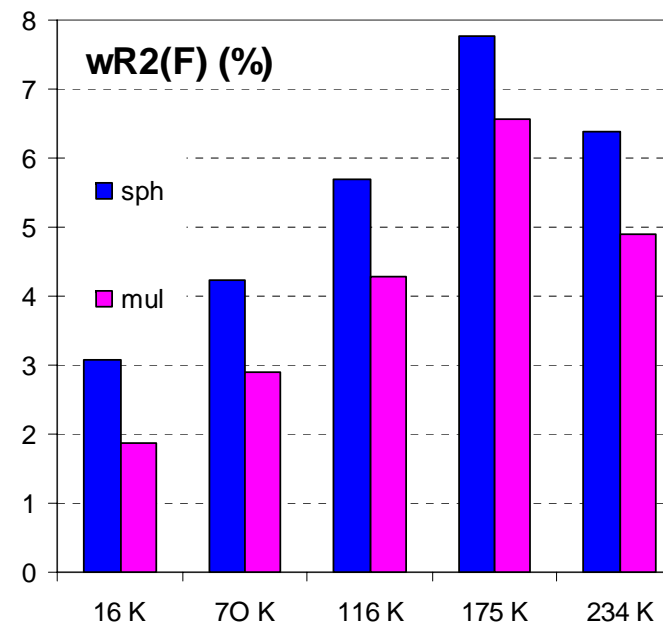


SPH

MUL

*dimethyl-stilbene*  $T=16K$

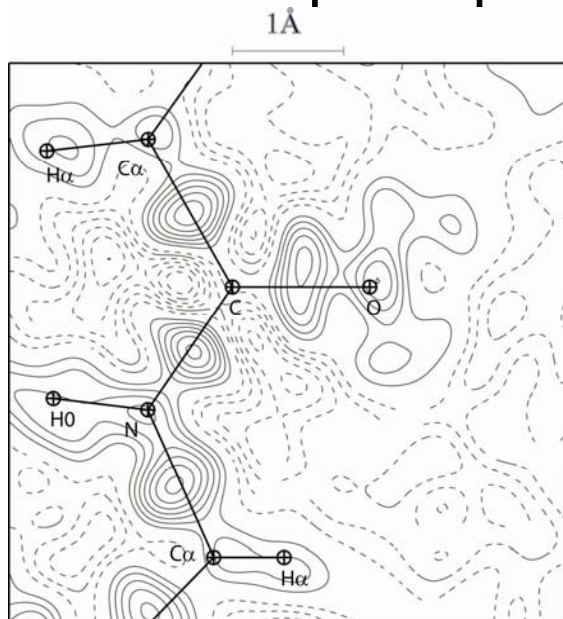
**Meilleur facteur  
d'accord  
cristallographique**



# Transfert Librairie Multipolaire & Affinement Cristallographique

densité électronique Fourier résiduelle

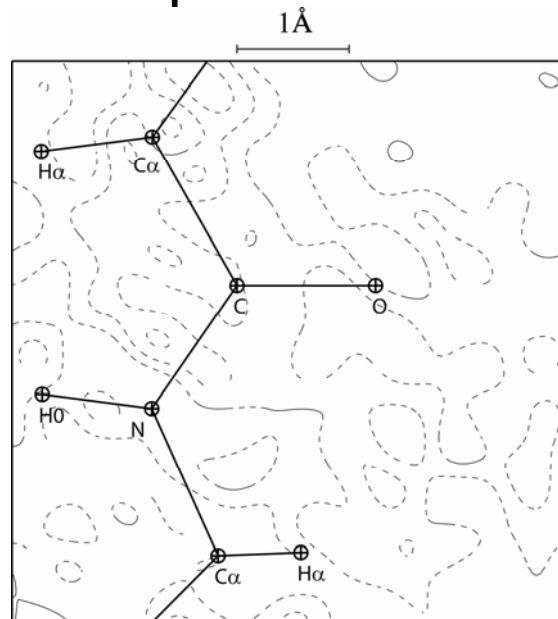
Atomes Sphériques



3.4 %

3.8%

Multipolaires



$wR2(F)$

$wR2_{free}(F)$

1.6 %

1.8 %

L-alanyl  
-L-threonine

Résolution  
0.62 Å

Contours  
 $\pm 0.05 \text{ e}\text{\AA}^{-3}$ ,

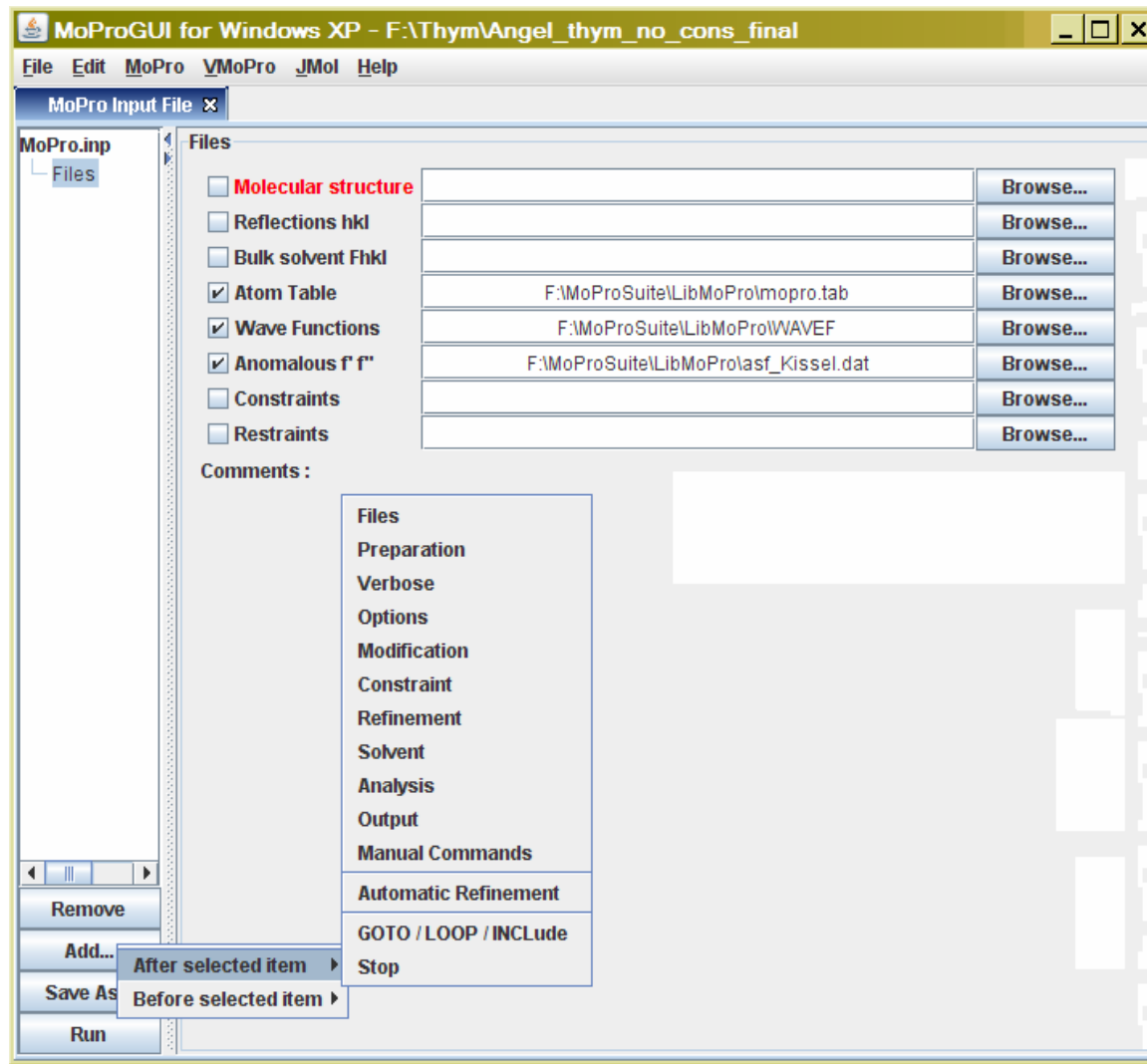


Logiciel MoPro

Interface  
Graphique

Téléchargement :

[www.crm2.uhp-nancy.fr/emqc/](http://www.crm2.uhp-nancy.fr/emqc/)



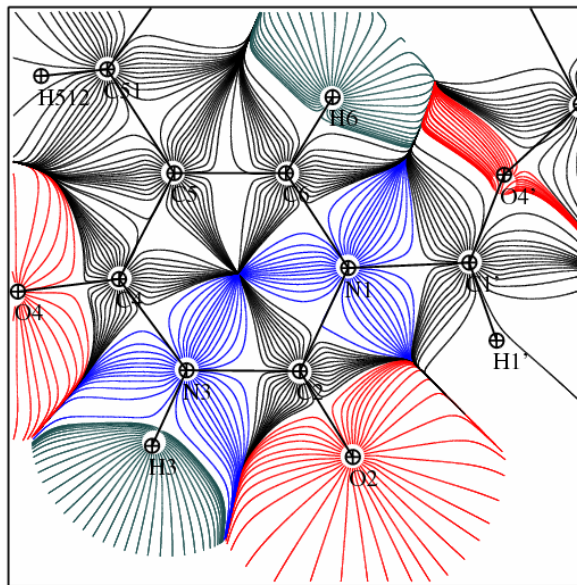
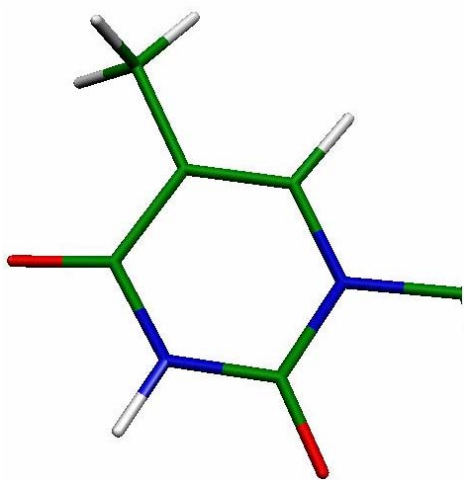
# Logiciel VMoPro Visualisation Propriétés

Densité Electronique  $\rho$  Statique & Fourier

Potentiel Electrostatique

Gradient Densité ou Champ Electrique

Laplacien  $\Delta\rho$ , points critiques  $\nabla\rho=0$



Lignes  
de gradient  
 $\rho(\mathbf{r})$

The screenshot displays the MoPro Viewer software interface. The main window shows a molecular model with a green isosurface. The interface includes several panels:

- Molecular tree:** Lists 'DefaultMolecule' with sub-items 'ALA 1' and 'MET 2'.
- Log console:** Shows the output of the VMoPro process, including the command path and the message 'VMoPro has finished its task'.
- Map Manager:** Contains a tabbed interface for managing maps (Map 1 to Map 10). The current map shows parameters for 'Isosurface 1' and 'Isosurface 2', including 'Maximum', 'Minimum', 'Average', and 'Std. deviation' values, along with 'Isovalue' and 'Filled surface' options.
- VMoPro 2D map:** A configuration panel for the 2D map, including options for 'Map type' (Deformation, Total, Multipolar, Valence, Neutral, Spherical), 'Critical Points' (None, Bond, Inter, Hydrogen bond), 'Fourier Map' (Unmerged, Merged, Except Friedels), and 'Contributing Symetries' (55501). It also includes a 'Plane' section with origin and axis coordinates, and a 'Sampling' section with a value of 0.050 Å.

MOPro Viewer Benoit Guillot CRM2