Cristallographie à résolution ultra haute & Logiciel MoPro

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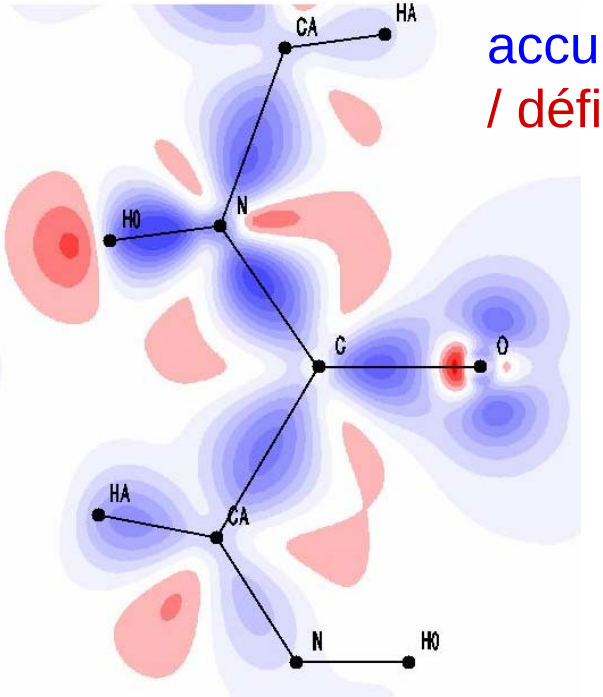
CRM^2
Cristallographie, Résonance Magnétique et Modélisations

cnrs
dépasser les frontières

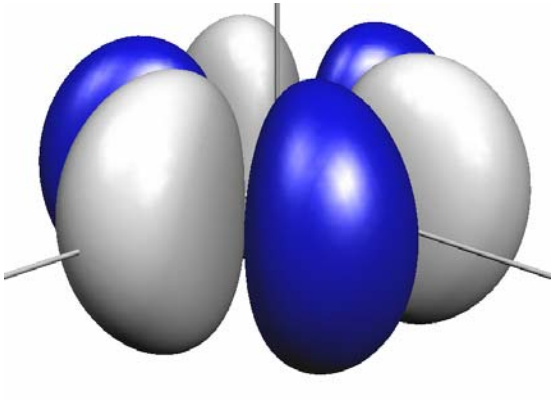
Cristallographie des Rayons X à Résolution Ultra Haute

Observer la **Déformation de la Densité Electronique**

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



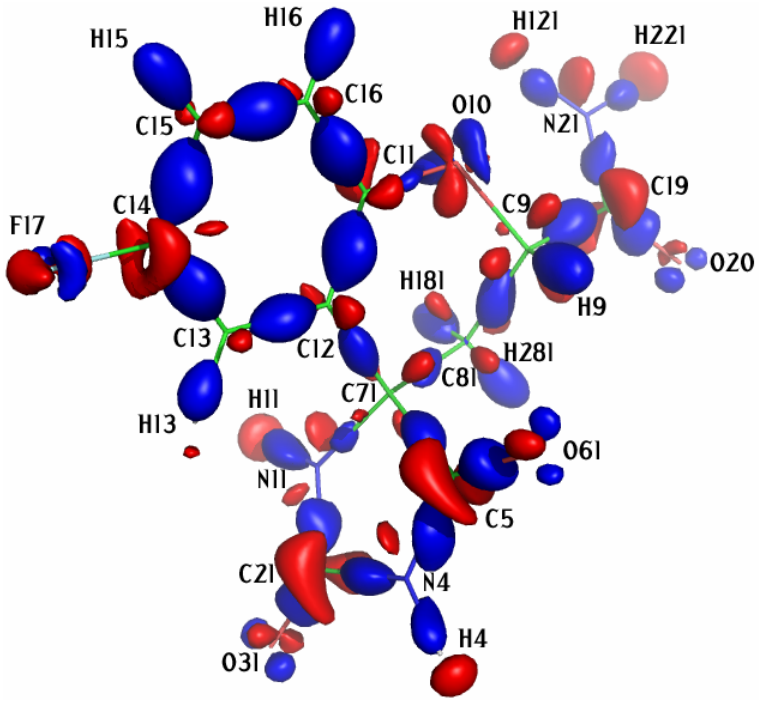
accumulation
/ déficit

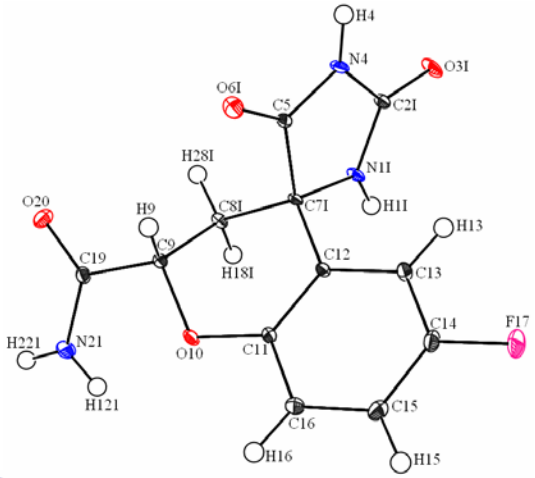


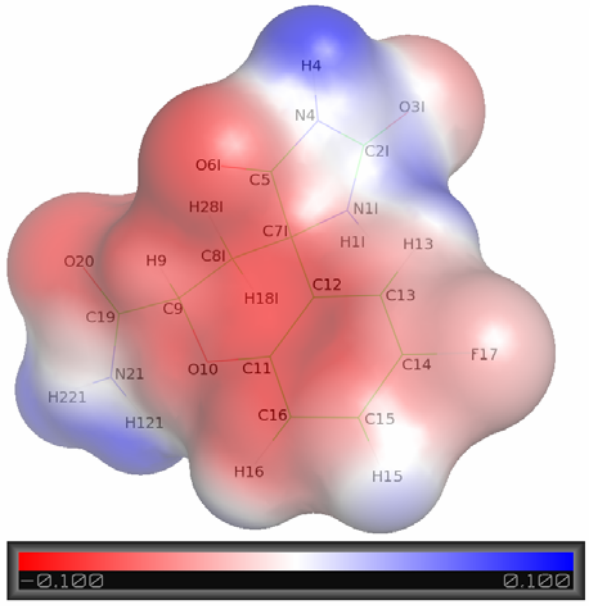
Atomes Multipolaires

Fidarestat : Inhibiteur Aldose Réductase Humaine

Déformation de la Densité Electronique Expérimentale







Potentiel Electrostatique

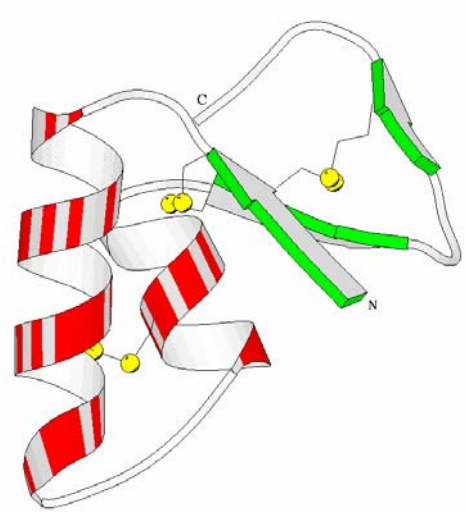
résolution = 0.50 Å

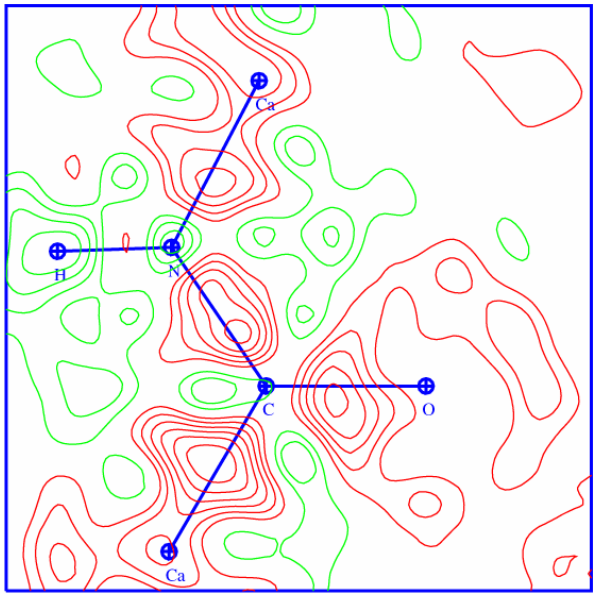
synchrotron Hambourg

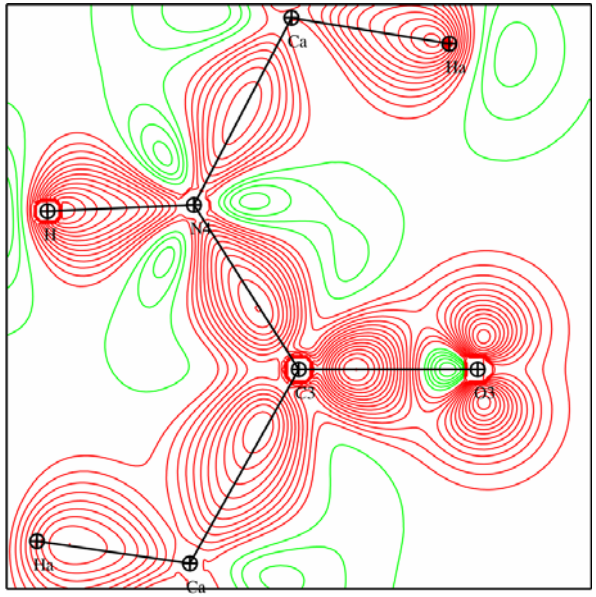
Fournier *et al.*, 2009. JACS

Crambine : 1^{e} Application aux Protéines

Cristallographie ultra haute résolution **Diffraction 0.54 Å**







Densité Electronique

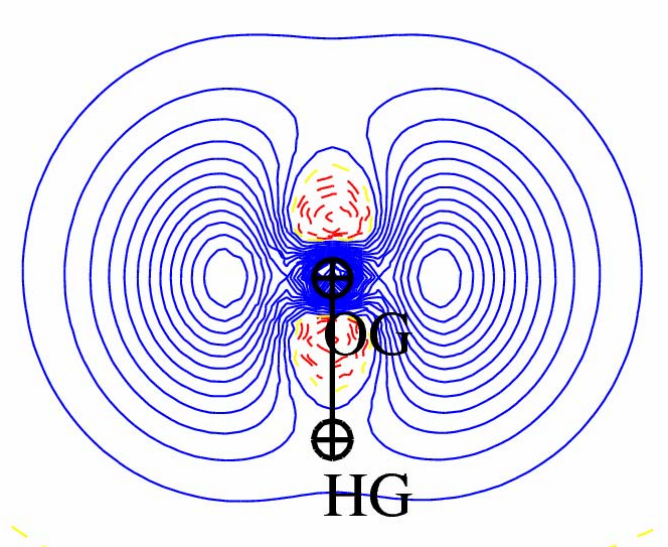
Fourier Résiduelle
$F_{obs} - F_{cal}$

Déformation Affinement Crambine <Polypeptidide>

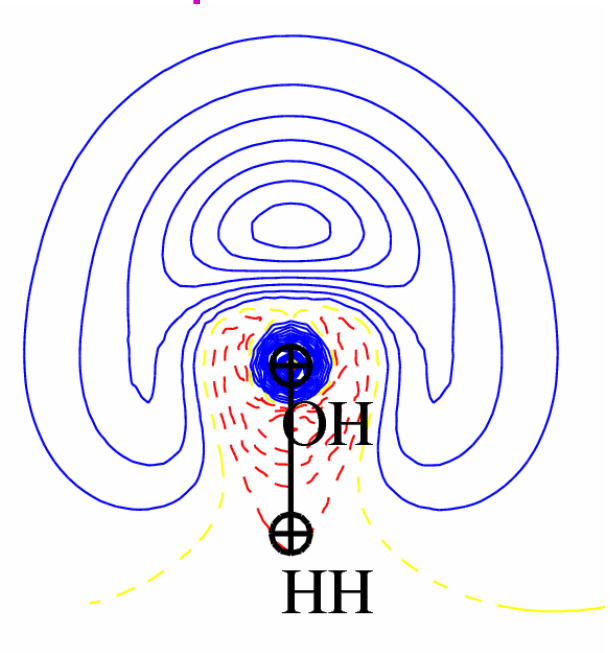
Jelsch *et al*. PNAS. 2000, 97.

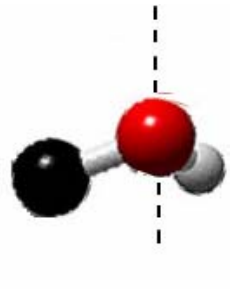
Librairie Atomes Multipolaire
Densité Electronique des Protéines

Serine
Csp3-O-H



Tyrosine
Csp2-O-H





Hydroxyle

Contours
+/- 0.05 e/Å^3 ,

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

Subatomique ~0.5Å	**Affinement** **Structure & Densité Electronique**
Atomique ***0.7 – 1.5 Å***	**Transfert Librairie Densité Electronique** **Affinement Structure**

minéraux, petites & macro-molécules

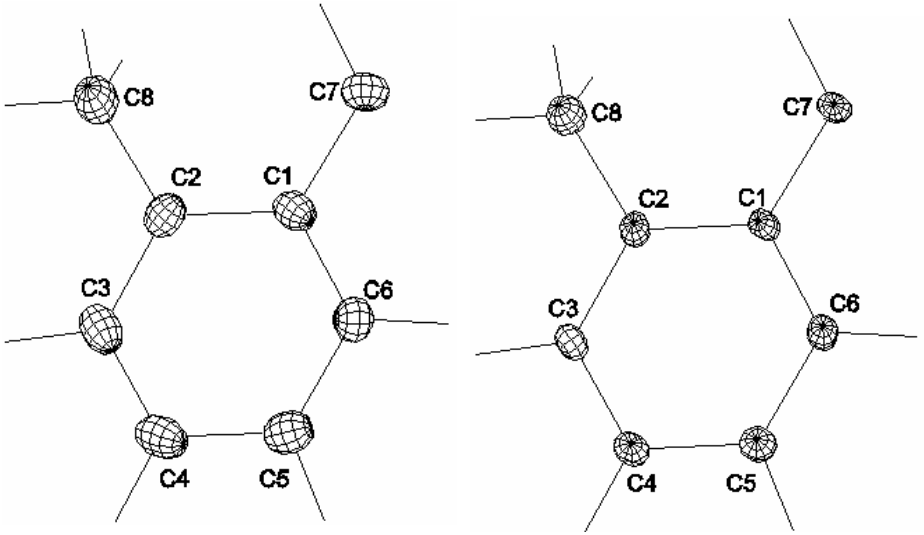
affinement automatique

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

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

Transfert Librairie Multipolaire à Structures de Résolution Moindre

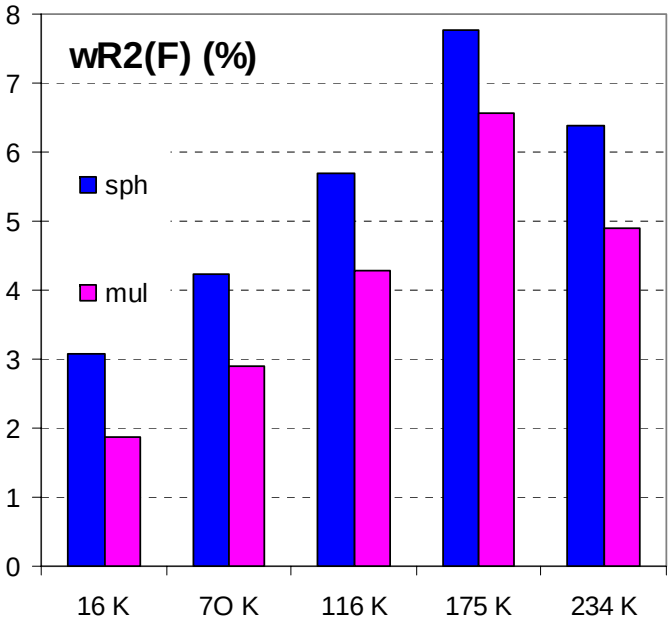
Ellipsoides Agitation Thermique plus justes



SPH MUL

dimethyl-stilbene T=16K

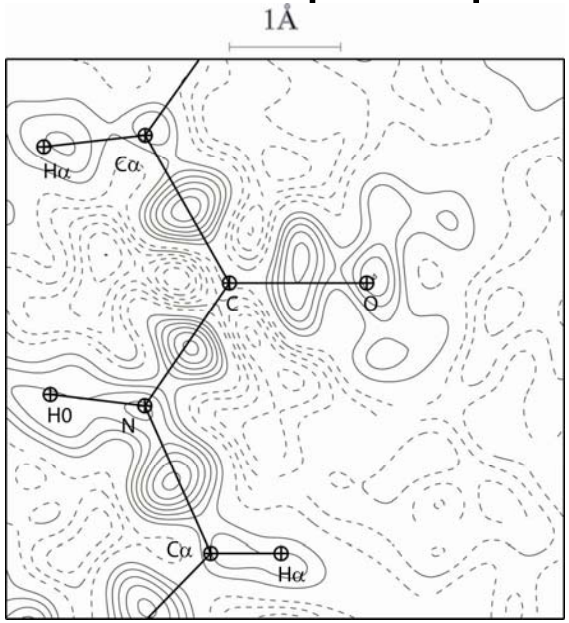
Meilleur facteur d'accord cristallographique



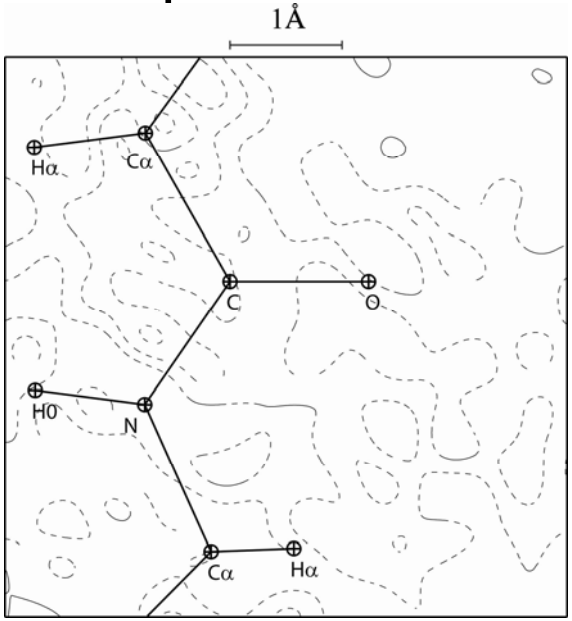
Transfert Librairie Multipolaire & Affinement Cristallographique

densité électronique Fourier résiduelle

Atomes Sphériques



Multipolaires



L-alanyl -L-threonine

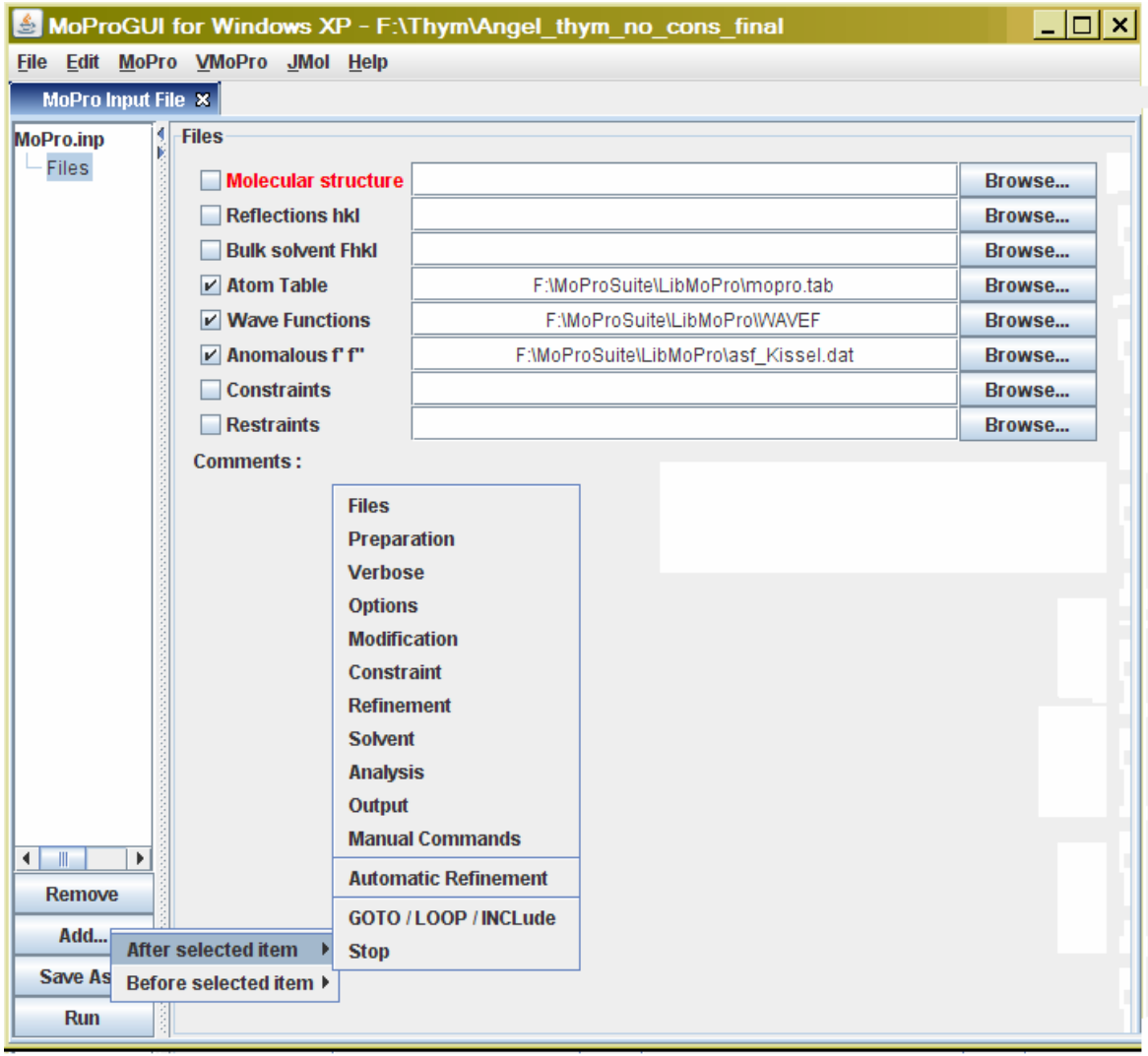
Résolution 0.62 Å

Contours ±0.05 eÅ^{-3} ,

3.4 %	*wR2*(*F*)	1.6 %
3.8%	*wR2*_free(F)	1.8 %

Logiciel MoPro

Interface Graphique



Téléchargement :

www.crm2.uhp-nancy.fr/emqc/

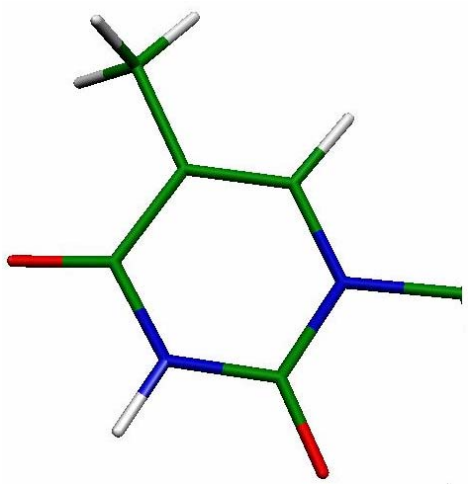
Logiciel VMoPro Visualisation Propriétés

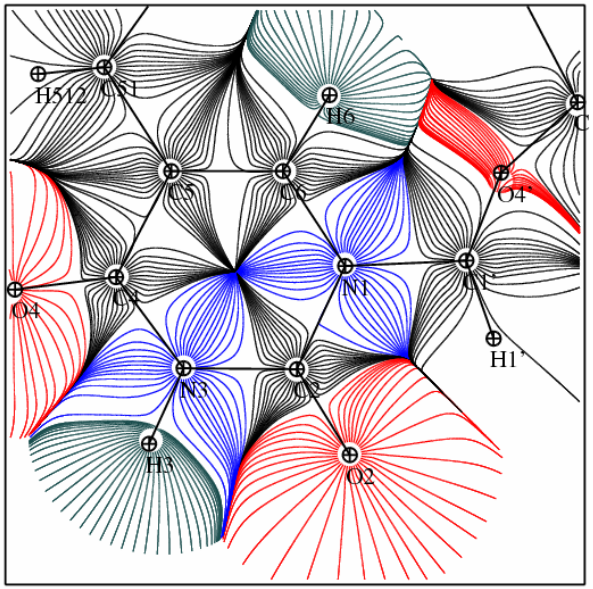
Densité Electronique ρ Statique & Fourier

Potentiel Electrostatique

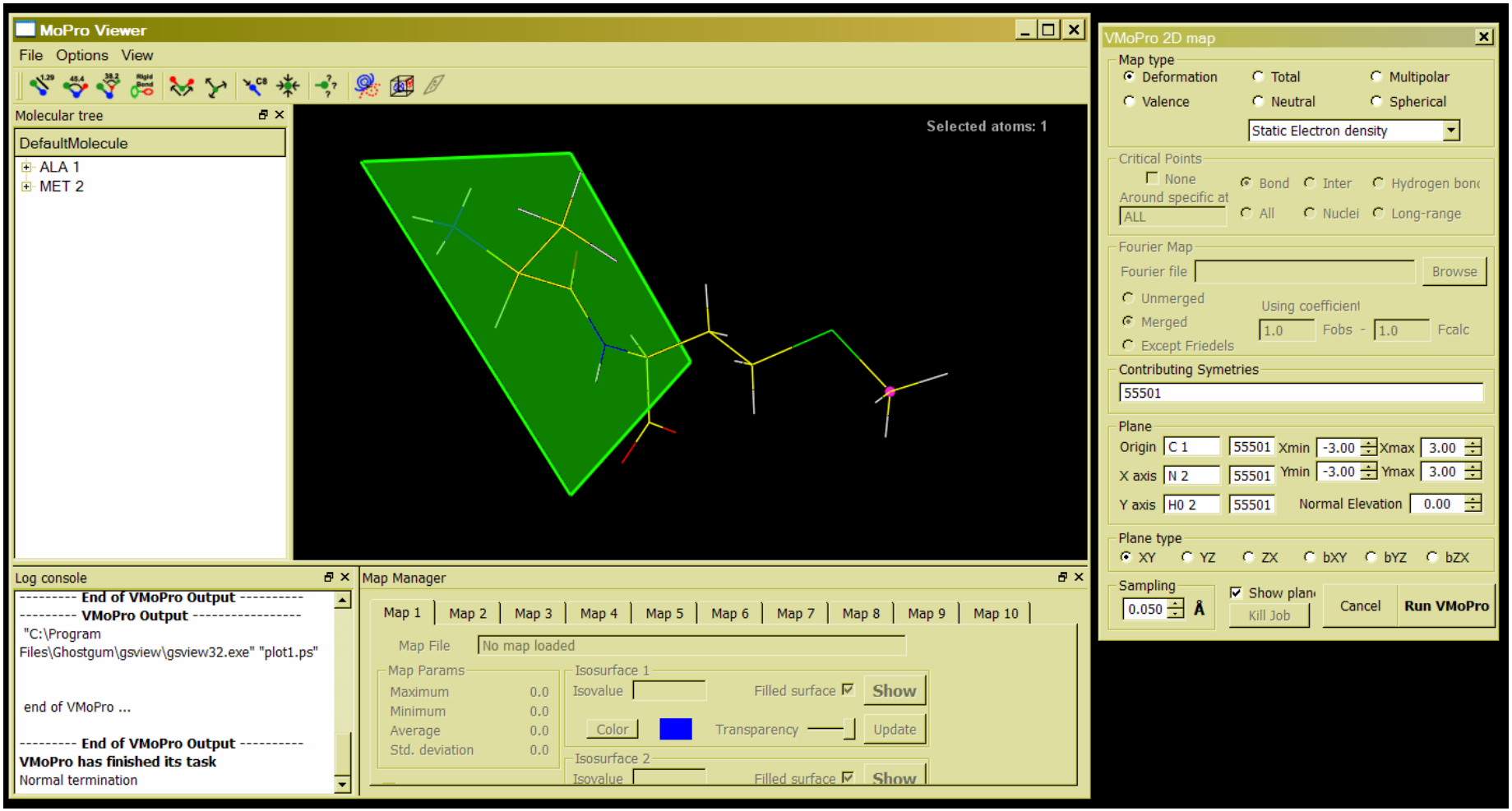
Gradient Densité ou Champ Electrique

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





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



MOPro Viewer Benoit Guillot CRM2