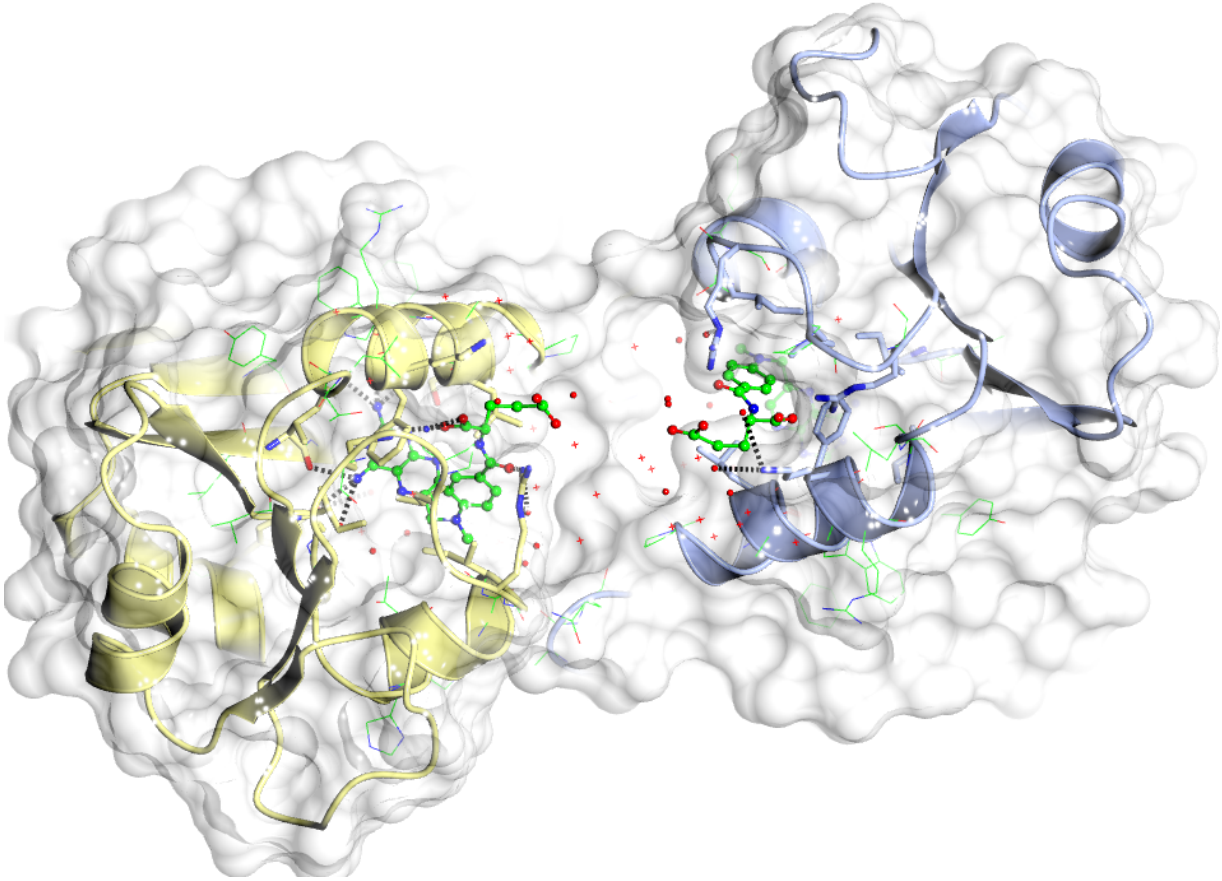
CCP4MG



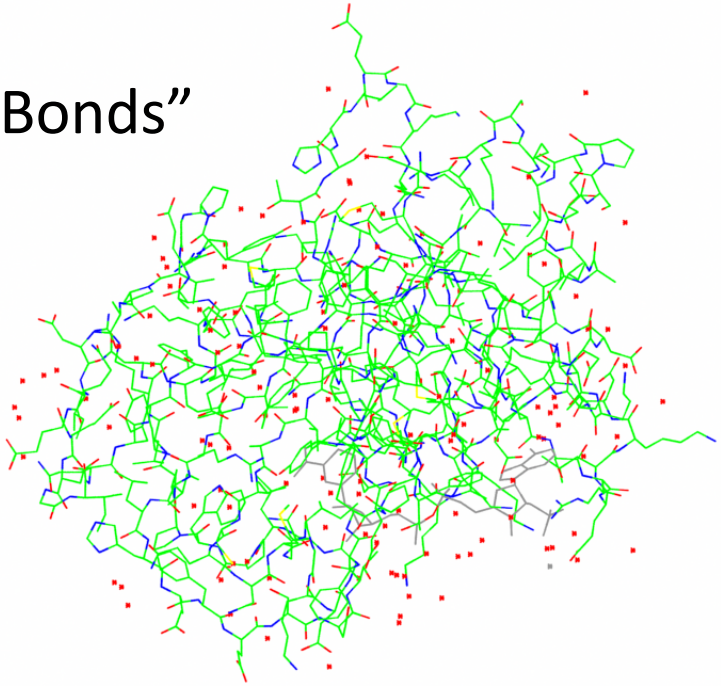
CCP4 Molecular Graphics Program

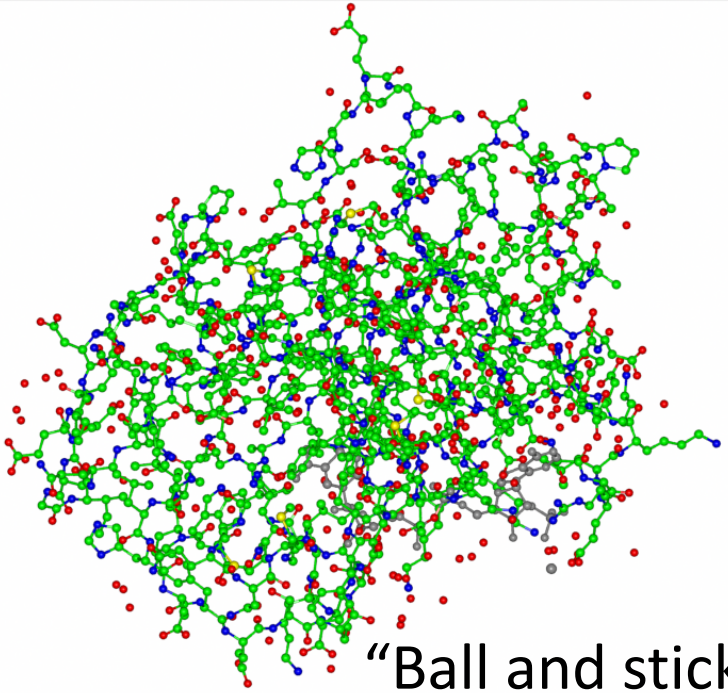
Introduction

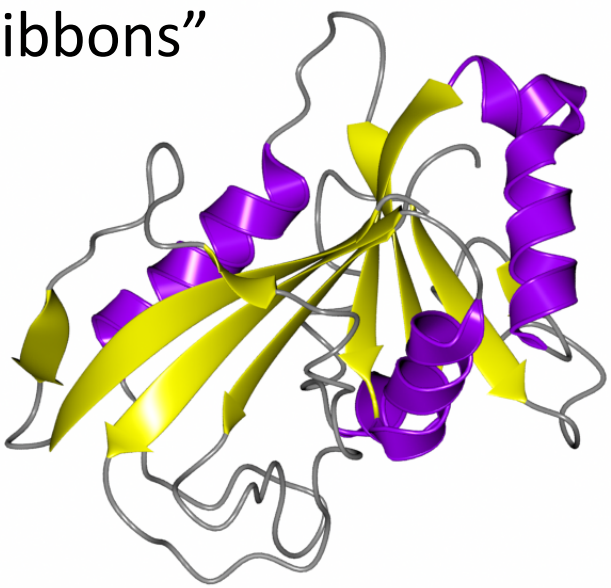
- CCP4MG is a molecular graphics program funded by CCP4.
- Its primary focus is the visualization and analysis of macromolecular structure.
- It produces high quality rendered images and movies.
- http://www.ccp4.ac.uk/MG/
  - Binaries for Windows, Mac and Linux.

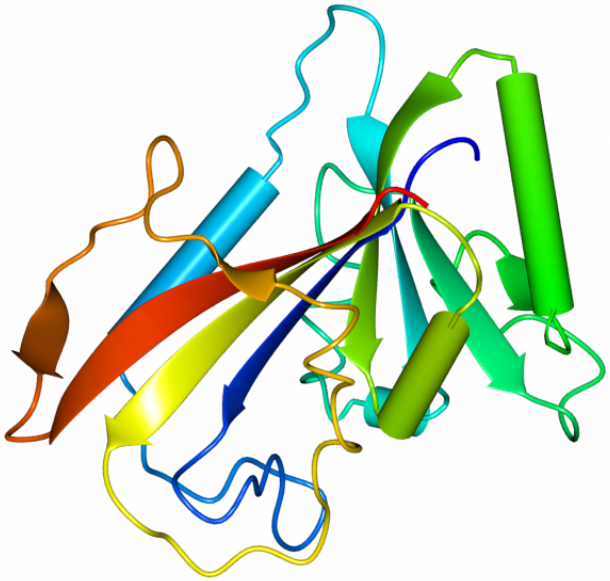
Displaying Molecules (styles)

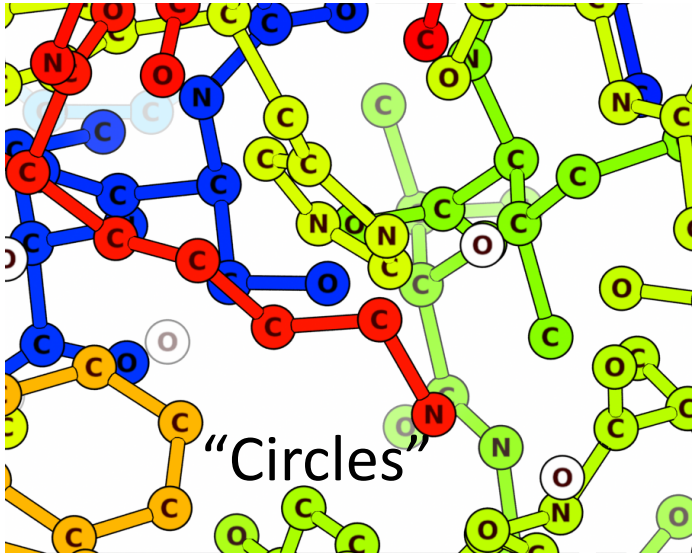
- CCP4MG can display molecules in many different ways:
  - Bonds, cylinders, ball and stick, spheres
  - CA traces
  - Thermal ellipsoids
  - Ribbons, worms, etc.
  - Base pair “sticks”, base blocks
  - Lipid cartoons
  - Surfaces

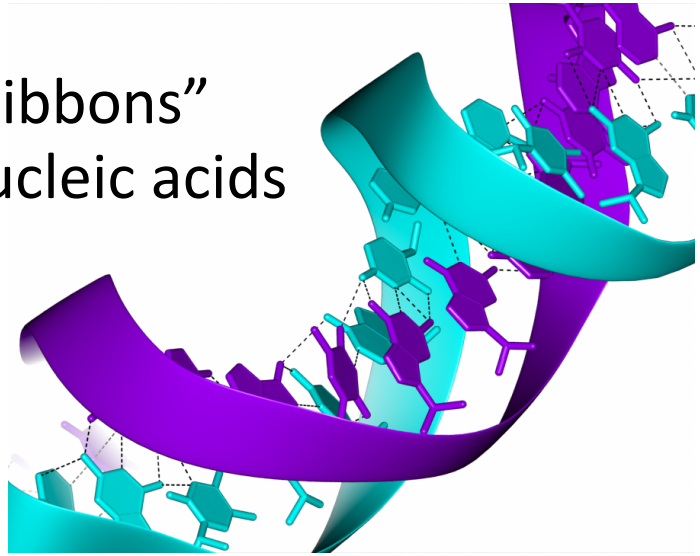

“Bonds”

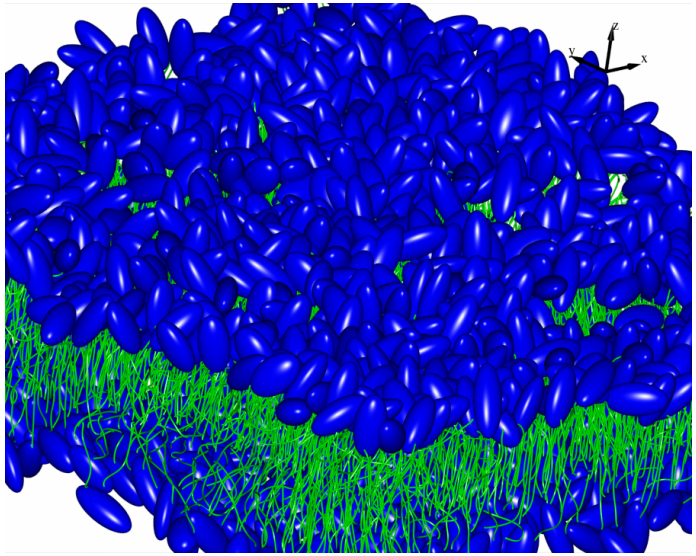

“Ball and stick”


“Ribbons”

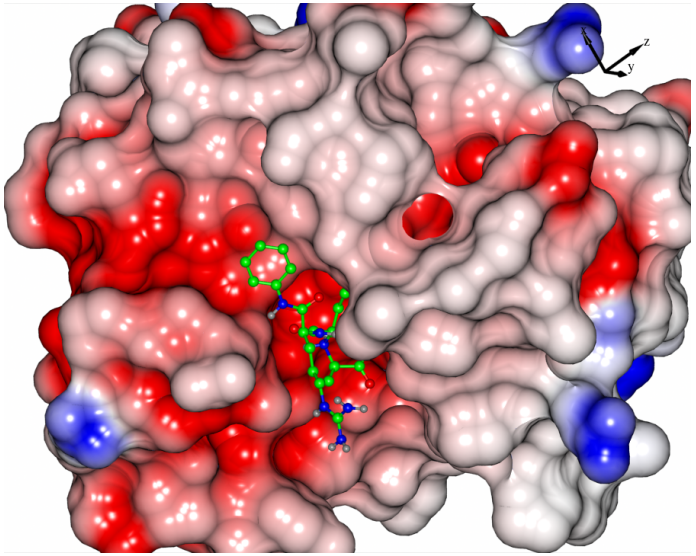

“Worms/tubes”



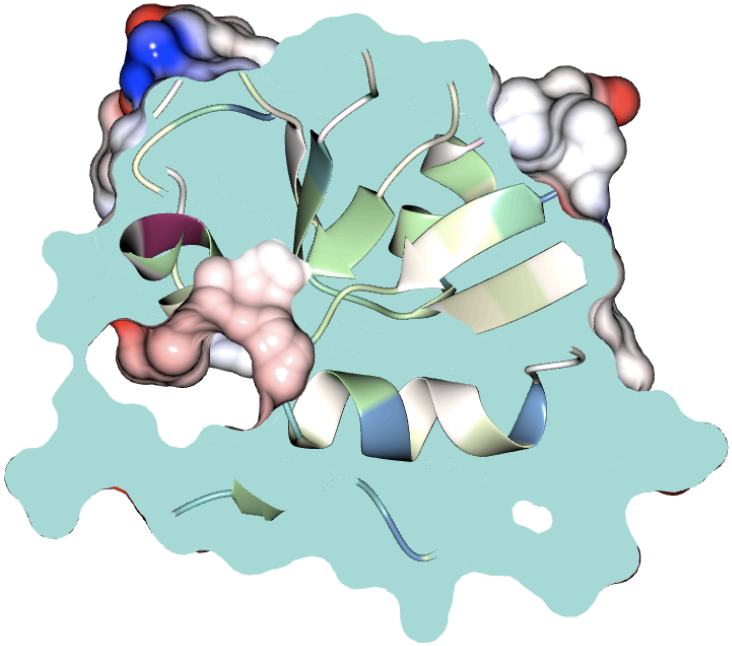


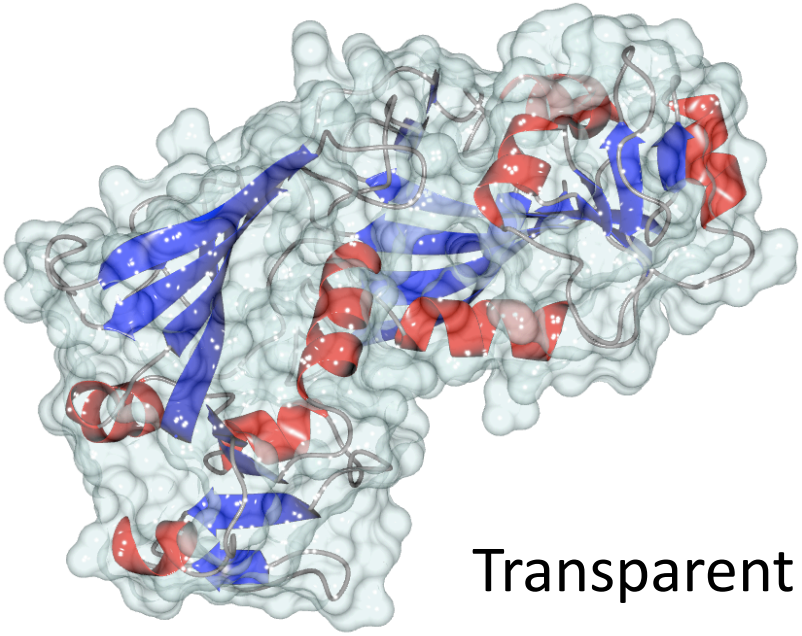


“Lipid Cartoon”

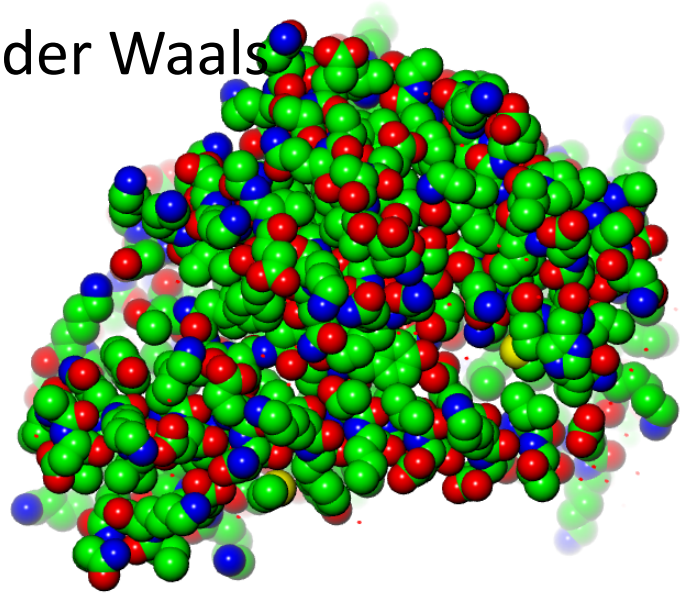


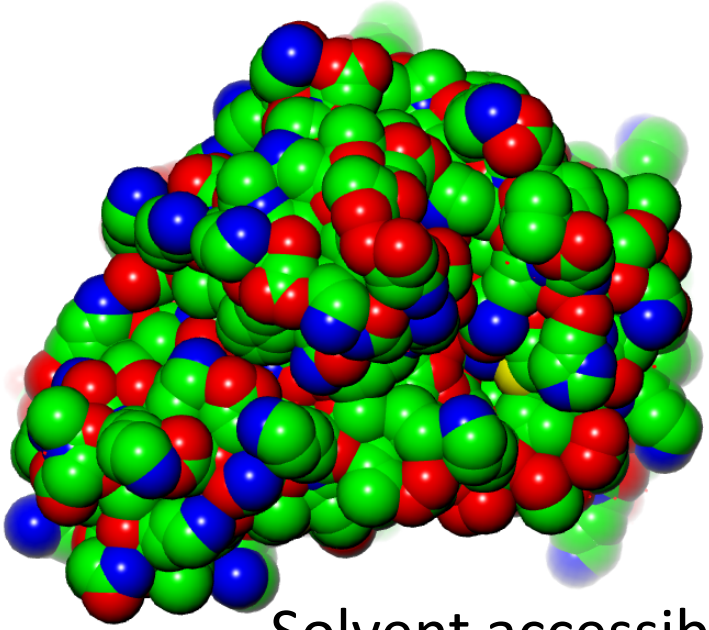
Electrostatic surface





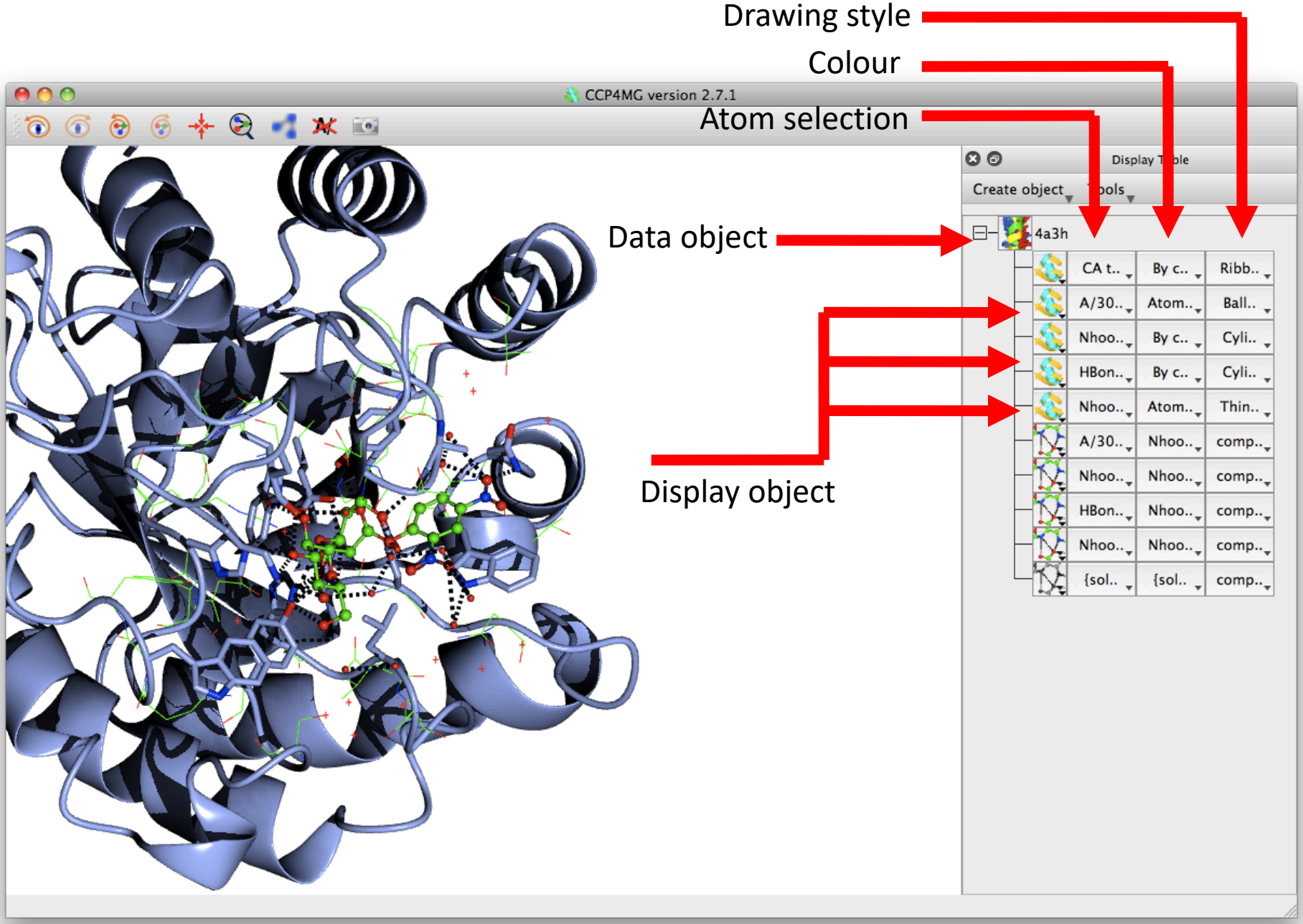
Van der Waals





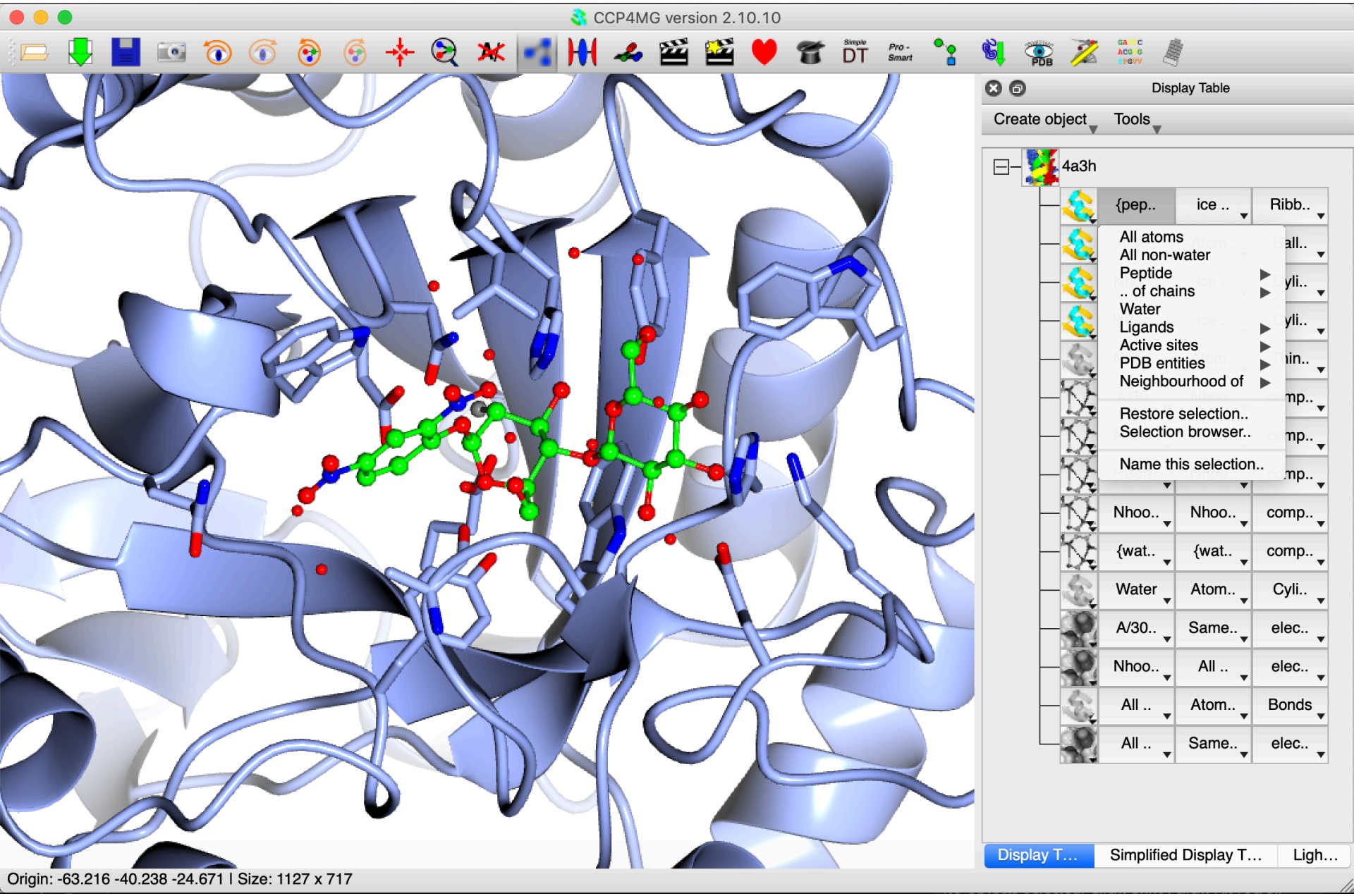
Solvent accessible

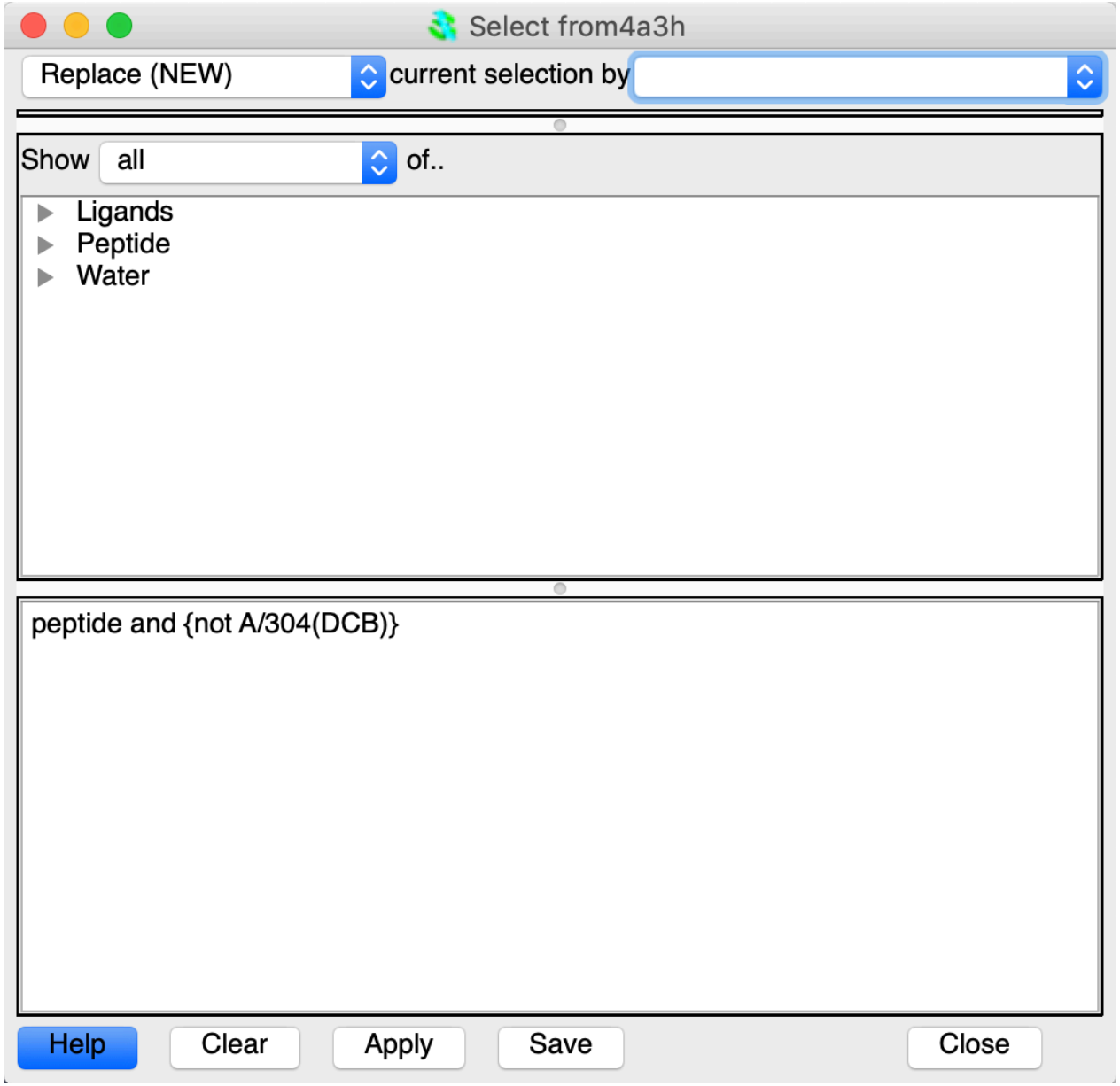
The program interface (introduction)

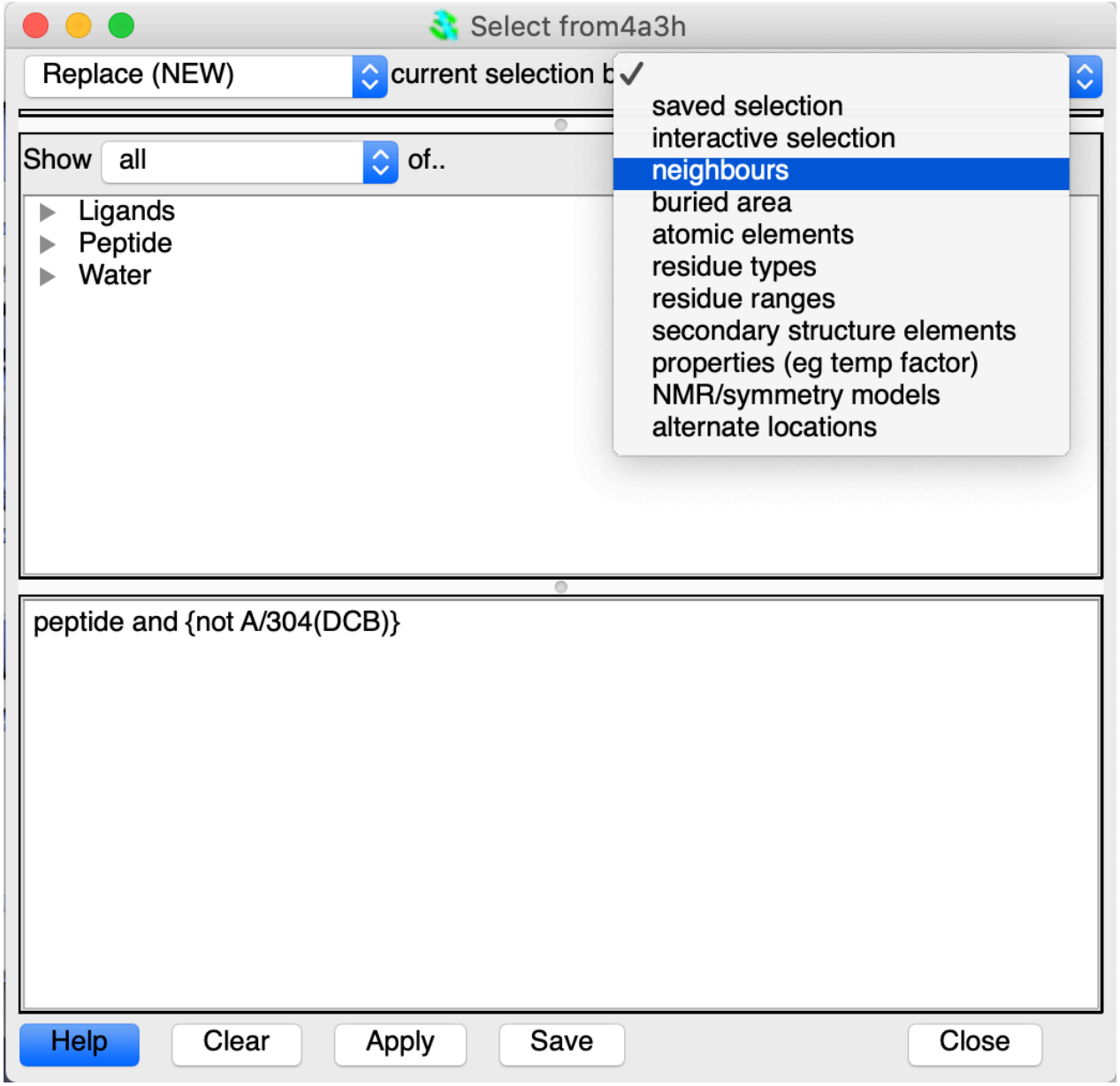

Drawing style
Colour
Atom selection
Data object
Display object
CCP4MG version 2.7.1
Display Table
Create object
Tools
4a3h
CA t..
By c..
Ribb..
A/30..
Atom..
Ball..
Nhoo..
By c..
Cyli..
HBon..
By c..
Cyli..
Nhoo..
Atom..
Thin..
A/30..
Nhoo..
comp..
Nhoo..
Nhoo..
comp..
HBon..
Nhoo..
comp..
Nhoo..
Nhoo..
comp..
{sol..
{sol..
comp..

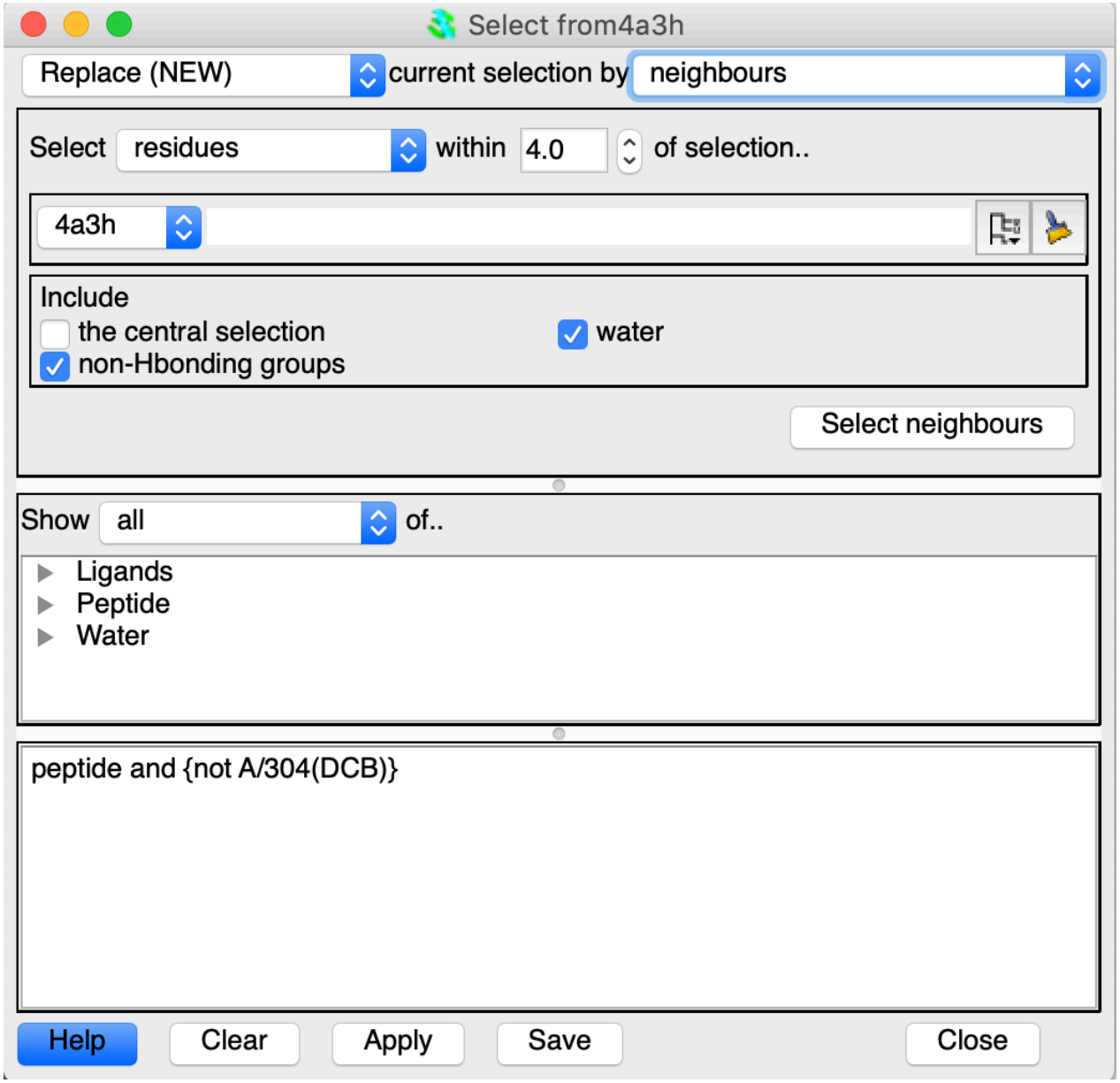
Atom Selections

- Simple atom selections may be made with menu entries:
  - All atoms, all peptide, monomers, etc.
- Arbitrarily complicated selections may be made using the “Selection browser”:
  - Neighbourhoods of various atoms
  - Atom types, residue types
  - Residue ranges
  - Secondary structure elements
  - Individual atoms
  - Logical and/or/not of all the above


CCP4MG version 2.10.10
Display Table
Create object
Tools
4a3h
{pep..
ice ..
Ribb..
All atoms
All non-water
Peptide
.. of chains
Water
Ligands
Active sites
PDB entities
Neighbourhood of
Restore selection..
Selection browser..
Name this selection..
Nhoo..
Nhoo..
comp..
{wat..
{wat..
comp..
Water
Atom..
Cyli..
A/30..
Same..
elec..
Nhoo..
All ..
elec..
All ..
Atom..
Bonds
All ..
Same..
elec..
Display T...
Simplified Display T...
Ligh...
Origin: -63.216 -40.238 -24.671 | Size: 1127 x 717

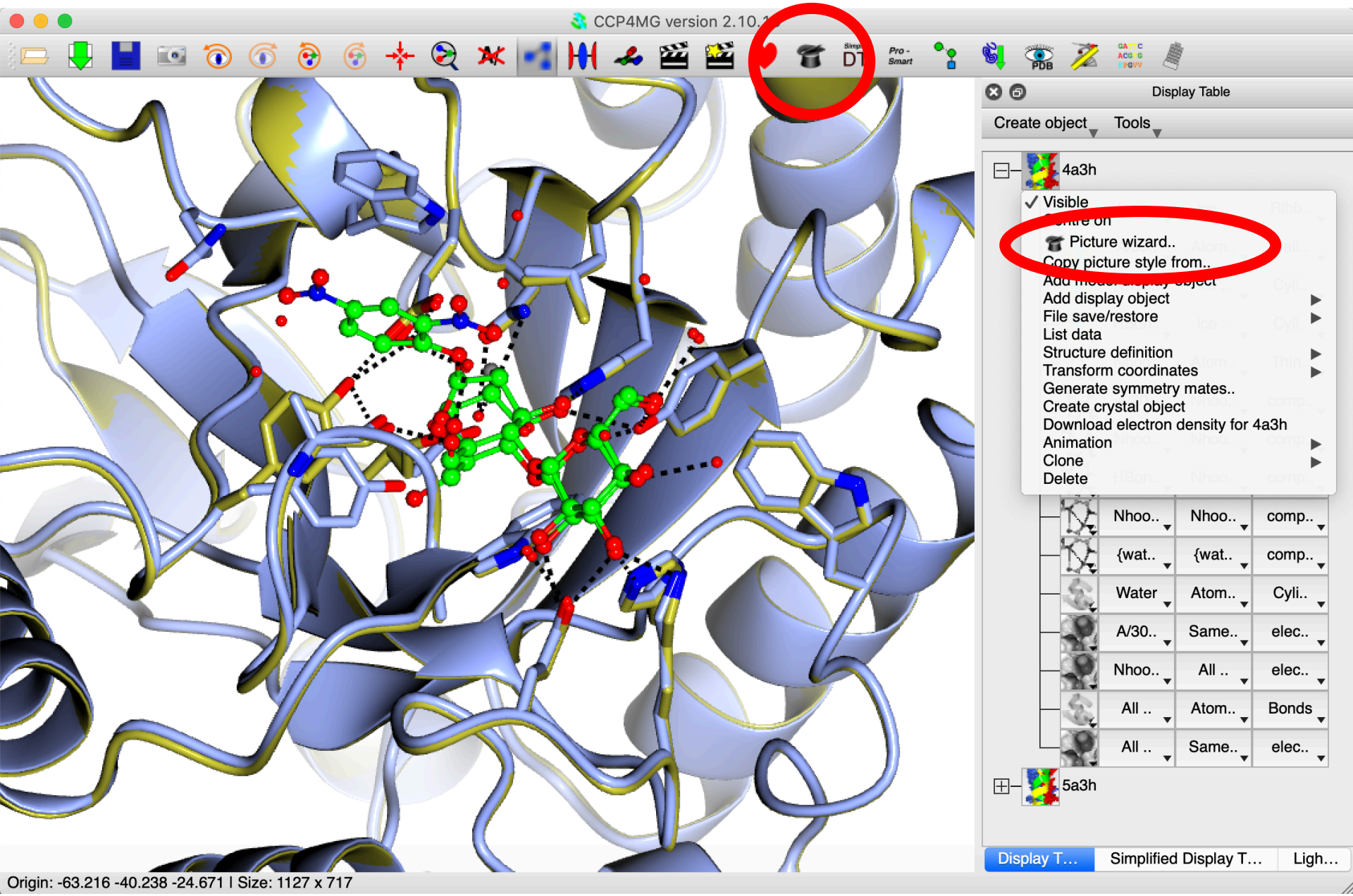

Select from4a3h
Replace (NEW)
current selection by
Show
all
of..
Ligands
Peptide
Water
peptide and {not A/304(DCB)}
Help
Clear
Apply
Save
Close


Select from4a3h
Replace (NEW)
current selection b
saved selection
interactive selection
neighbours
buried area
atomic elements
residue types
residue ranges
secondary structure elements
properties (eg temp factor)
NMR/symmetry models
alternate locations
Show
all
of..
Ligands
Peptide
Water
peptide and {not A/304(DCB)}
Help
Clear
Apply
Save
Close


Select from4a3h
Replace (NEW)
current selection by
neighbours
Select
residues
within
4.0
of selection..
4a3h
Include
the central selection
non-Hbonding groups
water
Select neighbours
Show
all
of..
Ligands
Peptide
Water
peptide and {not A/304(DCB)}
Help
Clear
Apply
Save
Close

Picture Wizard

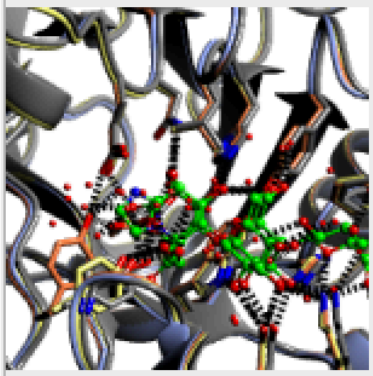
- The picture wizard is an automatic way of generating complex scenes with multiple selections, colouring, styles, etc.
- Representations are organised into various “styles”
- The picture wizard is shown at the top of the file browser window when a coordinate file is loaded, or can be accessed from the display table.


CCP4MG version 2.10.1
Display Table
Create object
Tools
4a3h
Visible
Picture wizard..
Copy picture style from..
Add display object
File save/restore
List data
Structure definition
Transform coordinates
Generate symmetry mates..
Create crystal object
Download electron density for 4a3h
Animation
Clone
Delete
Nhoo.. Nhoo.. comp..
{wat.. {wat.. comp..
Water Atom.. Cyli..
A/30.. Same.. elec..
Nhoo.. All .. elec..
All .. Atom.. Bonds
All .. Same.. elec..
5a3h
Display T...
Simplified Display T...
Ligh...
Origin: -63.216 -40.238 -24.671 | Size: 1127 x 717

Picture wizard to apply to ALL VISIBLE models

☑ Delete any existing display object ☑ Recentre

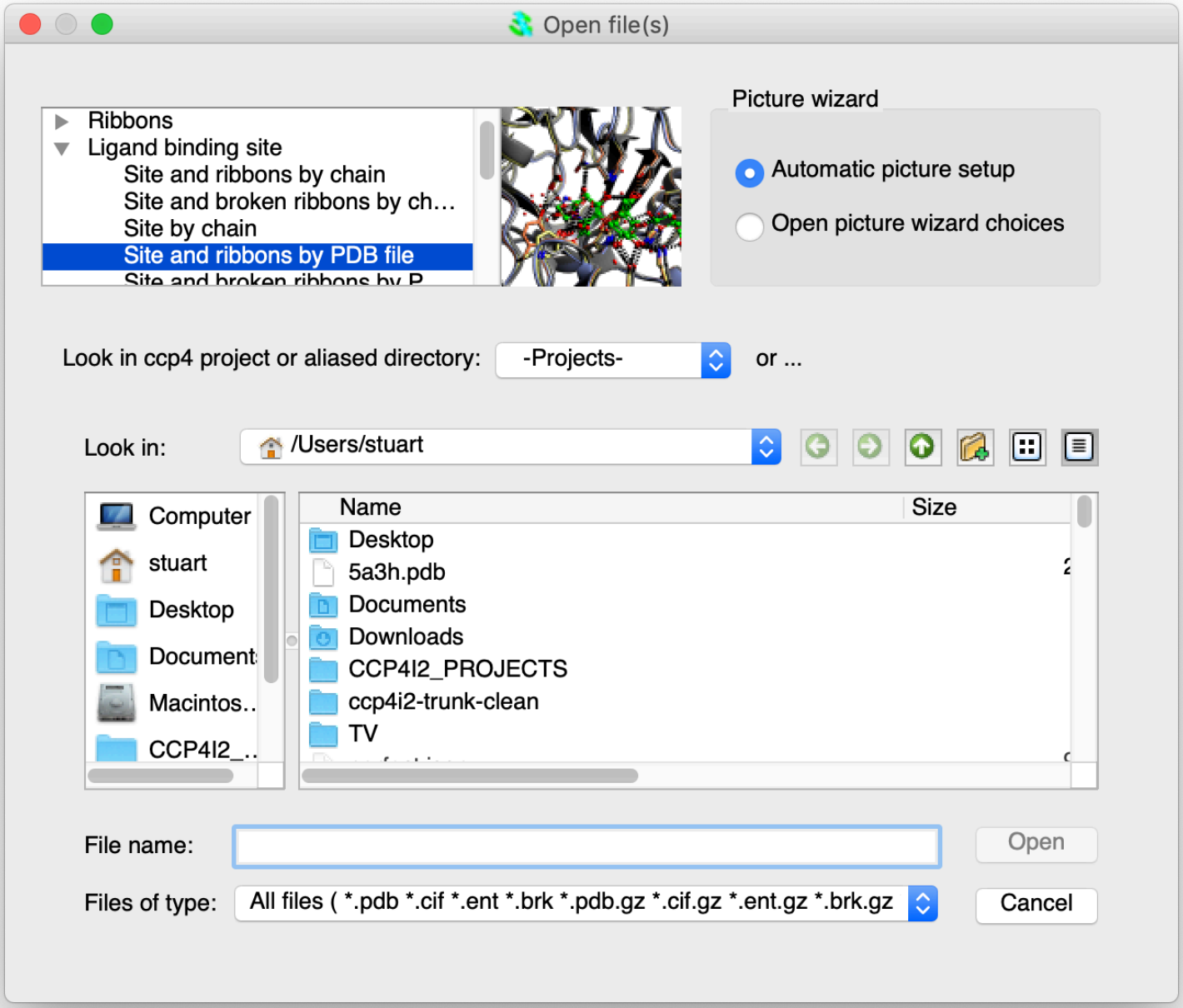
- ▶ Bonds
- ▶ Ribbons
- ▼ Ligand binding site
  - Site and ribbons by chain
  - Site and broken ribbons by ch…
  - Site by chain
  - Site and ribbons by PDB file
  - Site and broken ribbons by P…
  - Site by PDB file
  - surface by buried area
  - surface around ligand
  - surface electrostatics
- ▶ nucleic acid

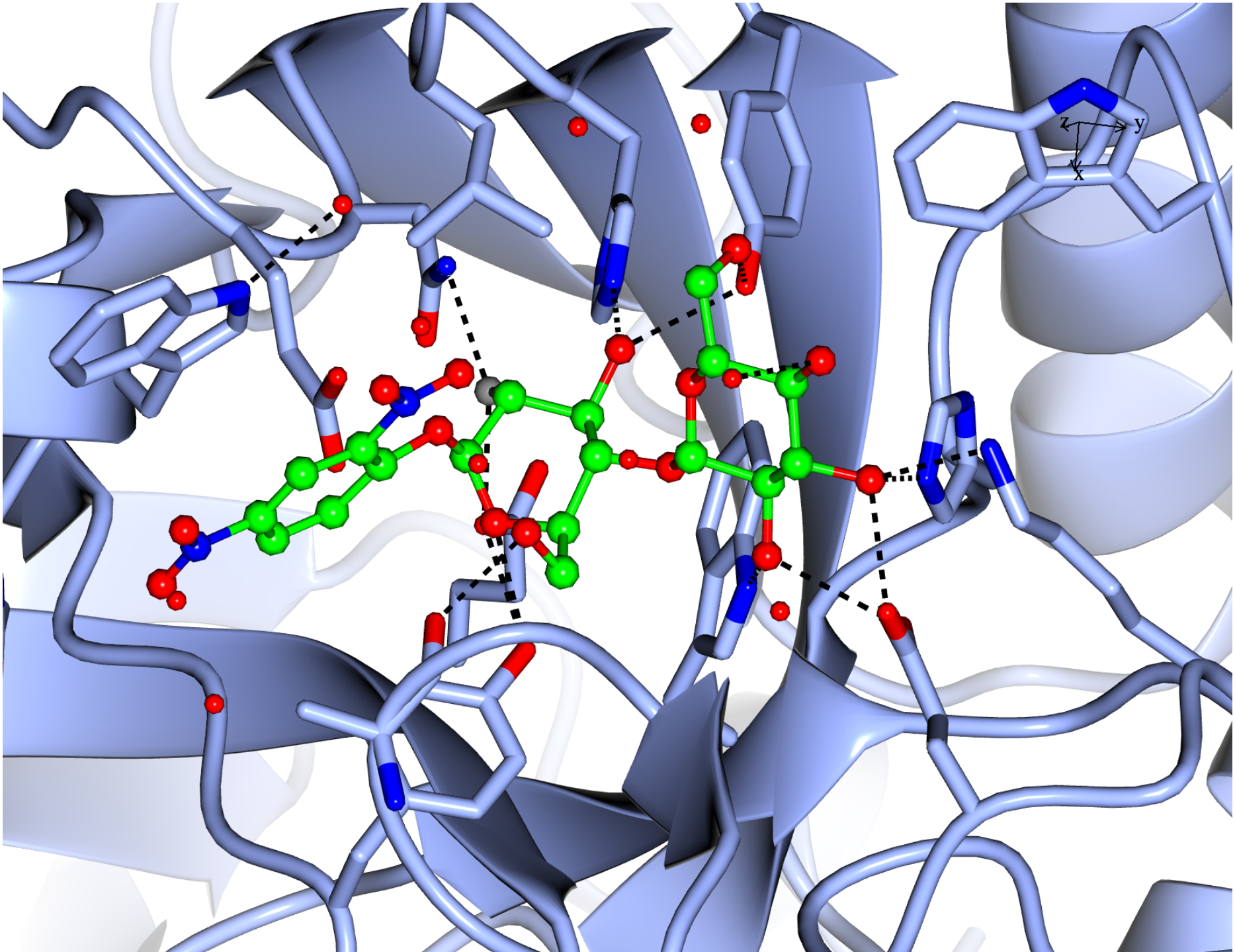


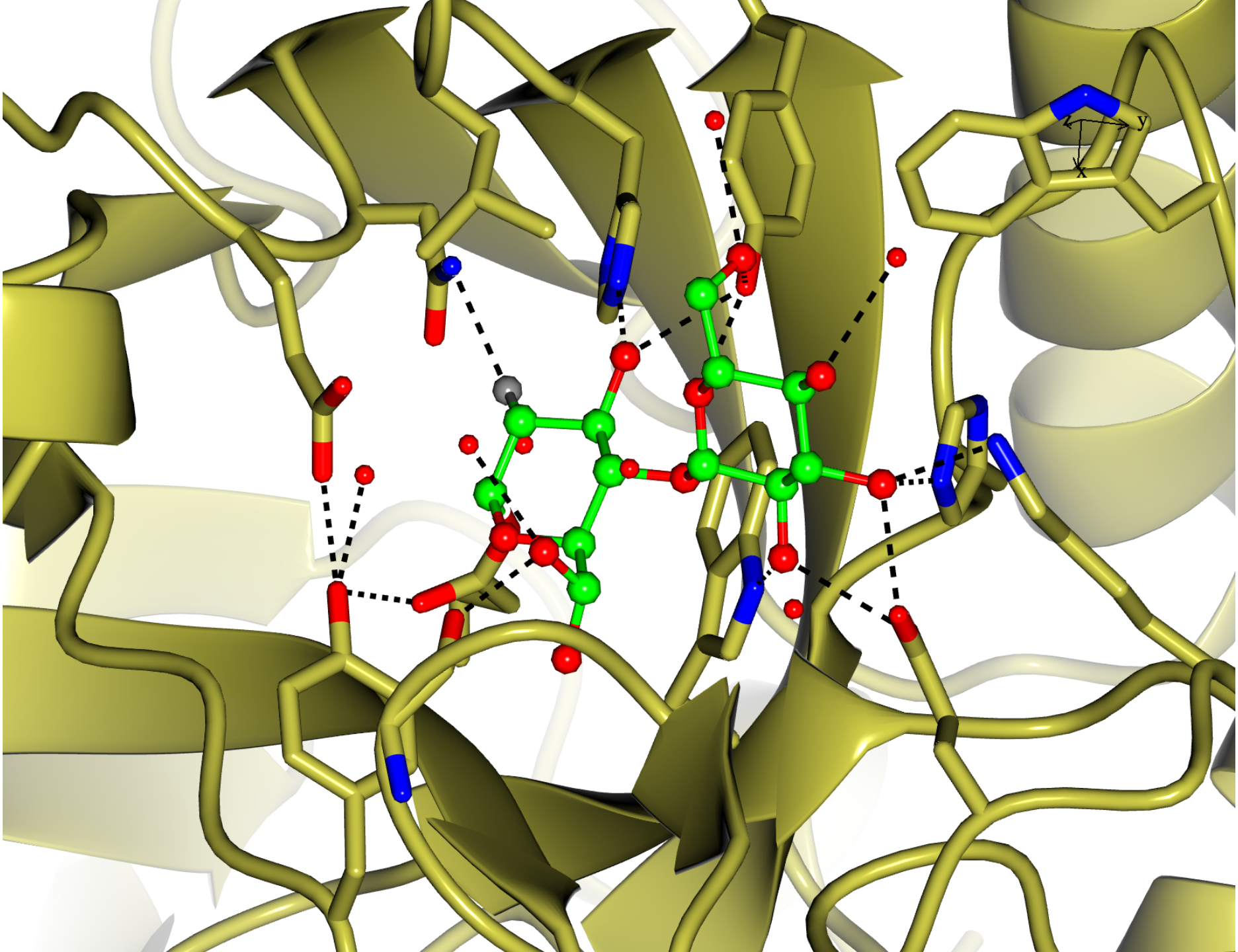
Ligand binding site with peptide coloured by molecule.
The graphical objects are:
-The CA trace drawn as ribbon.
-One object for each selected ligand.
-The 'neighbourhood' side chains close to ligands.
-The 'neighbourhood' main chain and water within hydrogen

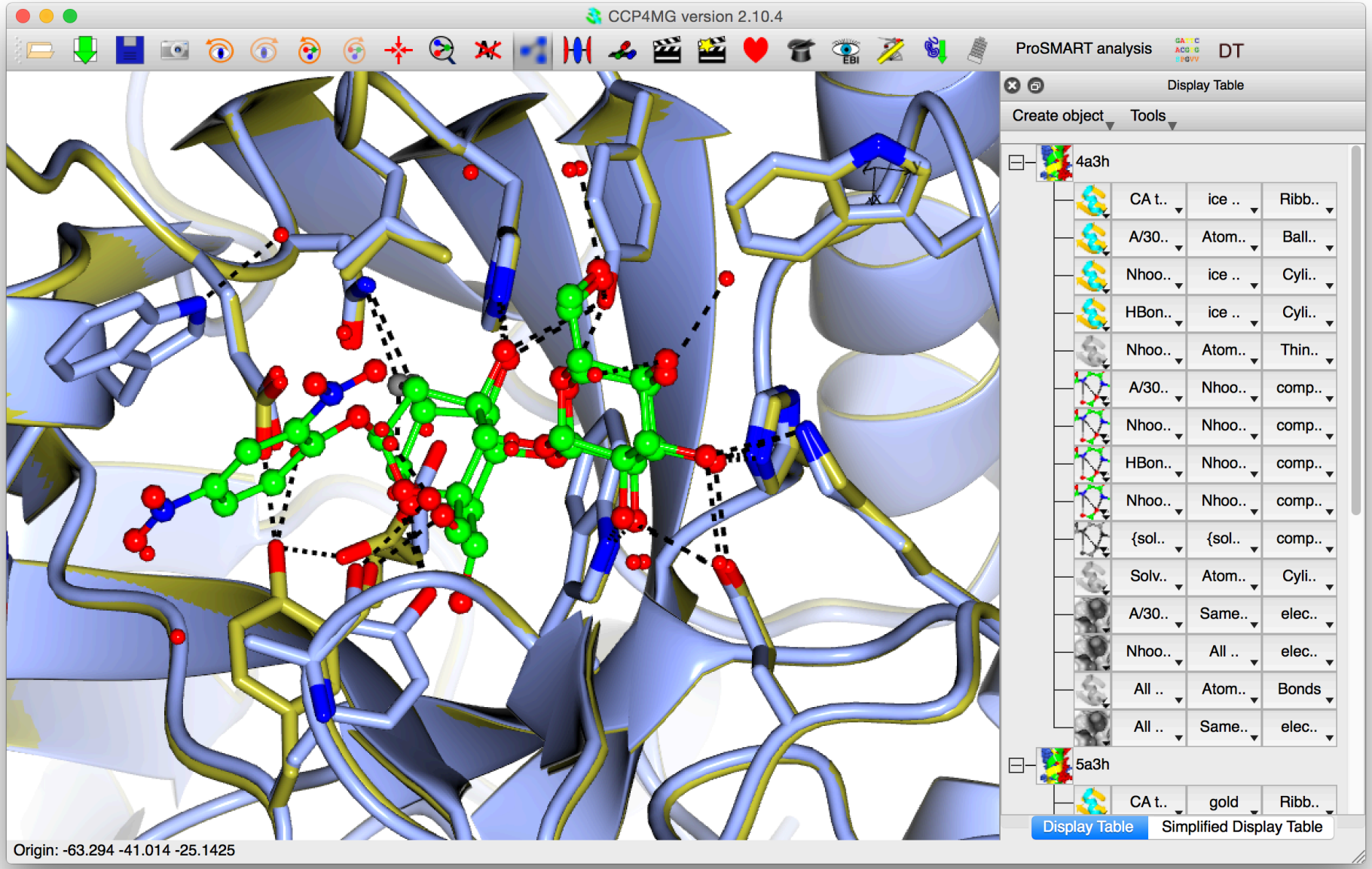
Only atoms in chain

Help | Create picture | Cancel


Open file(s)
Ribbons
Ligand binding site
Site and ribbons by chain
Site and broken ribbons by ch…
Site by chain
Site and ribbons by PDB file
Picture wizard
Automatic picture setup
Open picture wizard choices
Look in ccp4 project or aliased directory:
-Projects-
or ...
Look in:
/Users/stuart
Computer
stuart
Desktop
Documents
Macintos…
CCP4I2_…
Name
Size
Desktop
5a3h.pdb
Documents
Downloads
CCP4I2_PROJECTS
ccp4i2-trunk-clean
TV
File name:
Open
Files of type:
All files (*.pdb *.cif *.ent *.brk *.pdb.gz *.cif.gz *.ent.gz *.brk.gz
Cancel

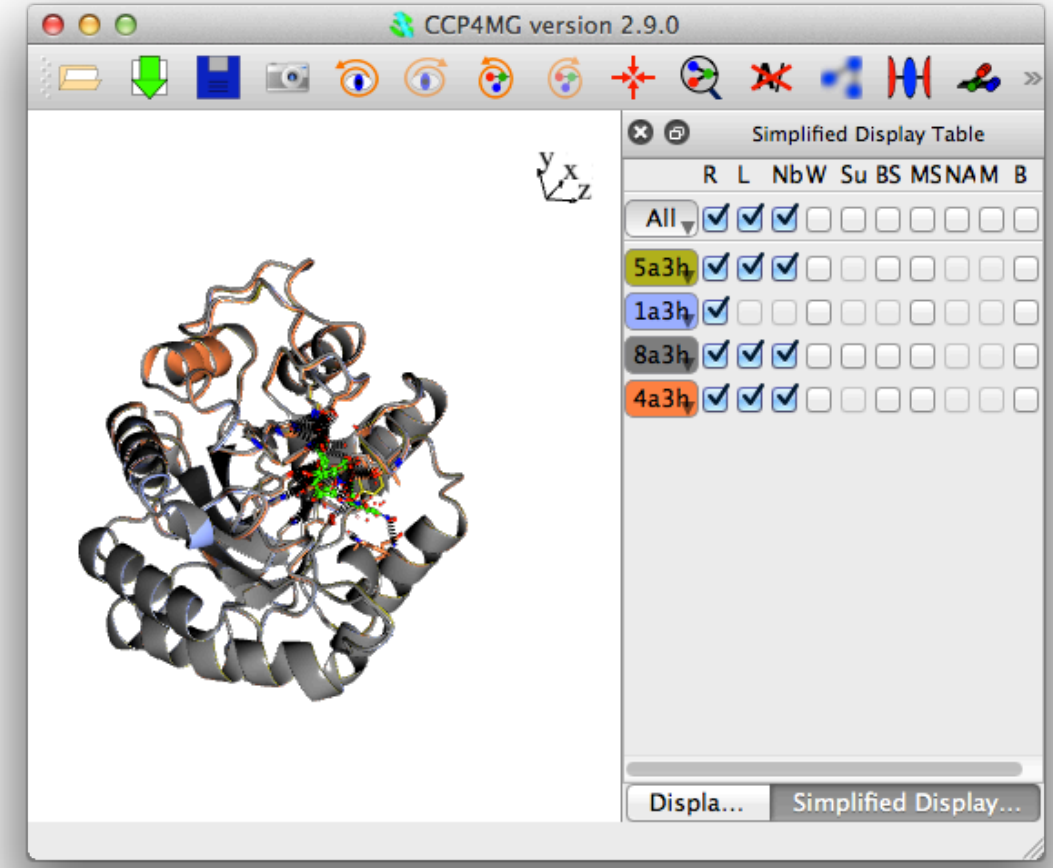

z
y
x


z
y
x


CCP4MG version 2.10.4
ProSMART analysis
DT
Display Table
Create object
Tools
4a3h
CA t.. ice .. Ribb..
A/30.. Atom.. Ball..
Nhoo.. ice .. Cyli..
HBon.. ice .. Cyli..
Nhoo.. Atom.. Thin..
A/30.. Nhoo.. comp..
Nhoo.. Nhoo.. comp..
HBon.. Nhoo.. comp..
Nhoo.. Nhoo.. comp..
{sol.. {sol.. comp..
Solv.. Atom.. Cyli..
A/30.. Same.. elec..
Nhoo.. All .. elec..
All .. Atom.. Bonds
All .. Same.. elec..
5a3h
CA t.. gold Ribb..
Display Table
Simplified Display Table
Origin: -63.294 -41.014 -25.1425

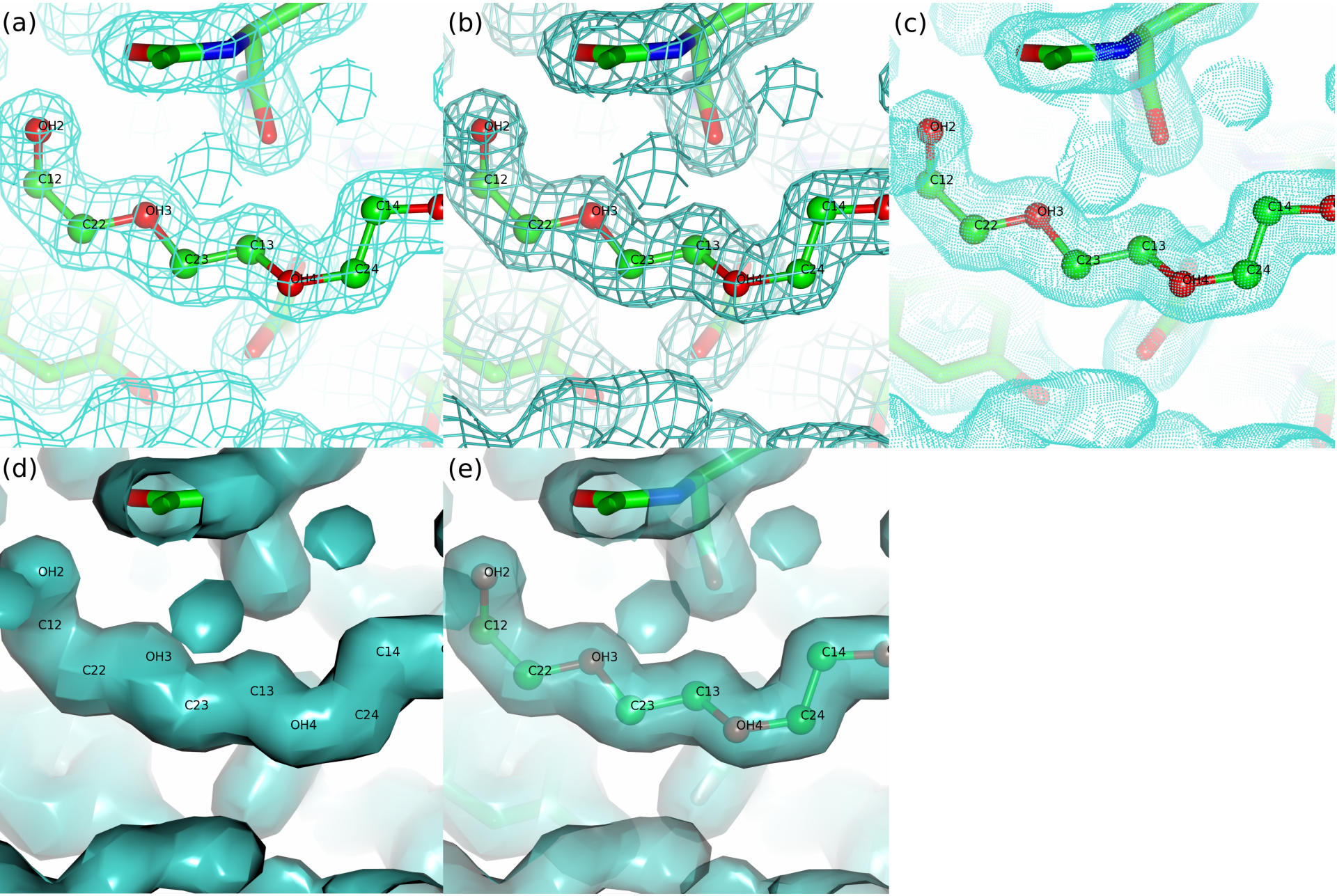
Simplified Display Table

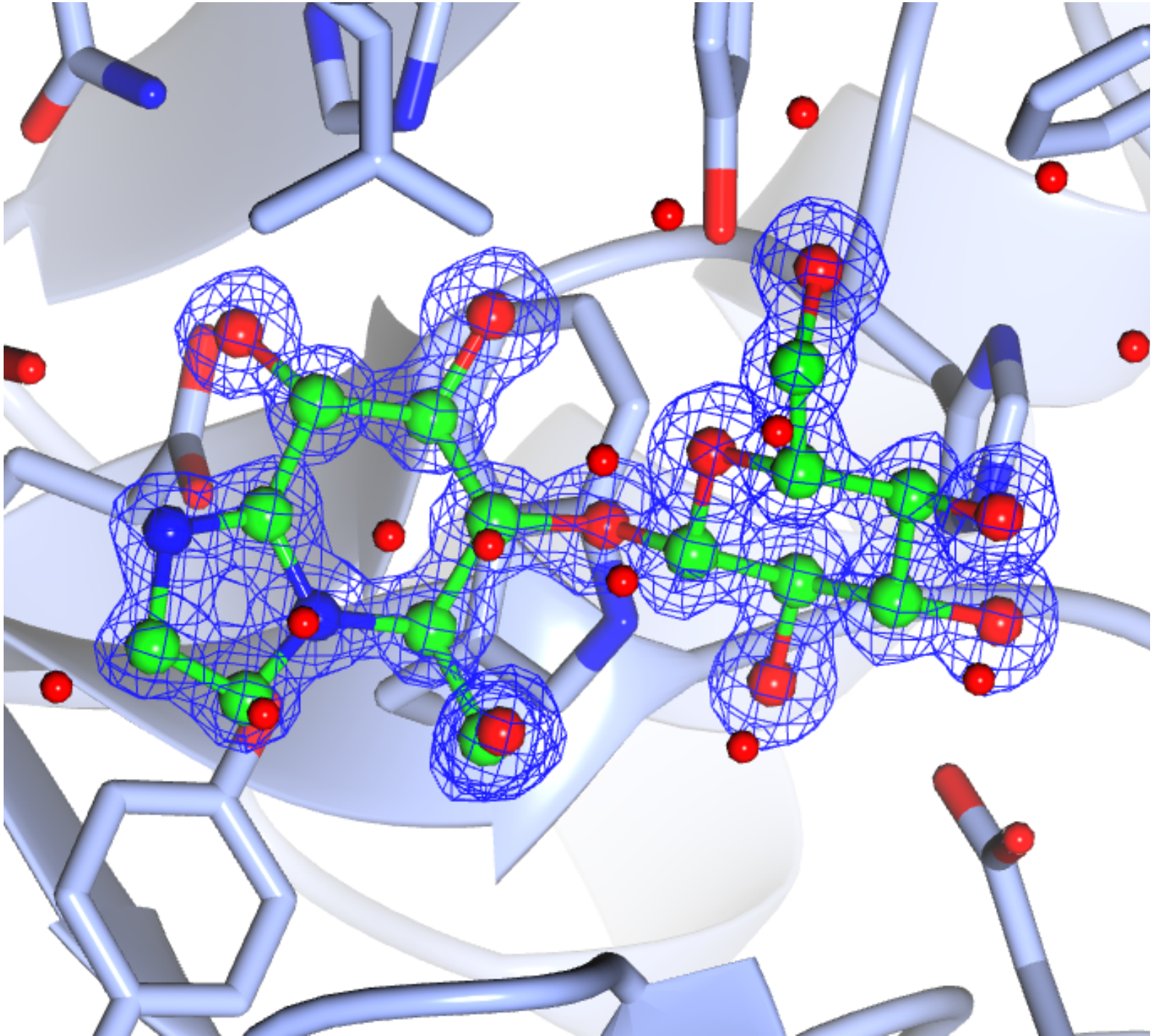
Tool for quickly turning on/off lots of related display objects. Particularly useful for looking at large numbers of similar files. (Not a replacement for "full" Display Table, but a useful alternative for some use cases).



Electron Density

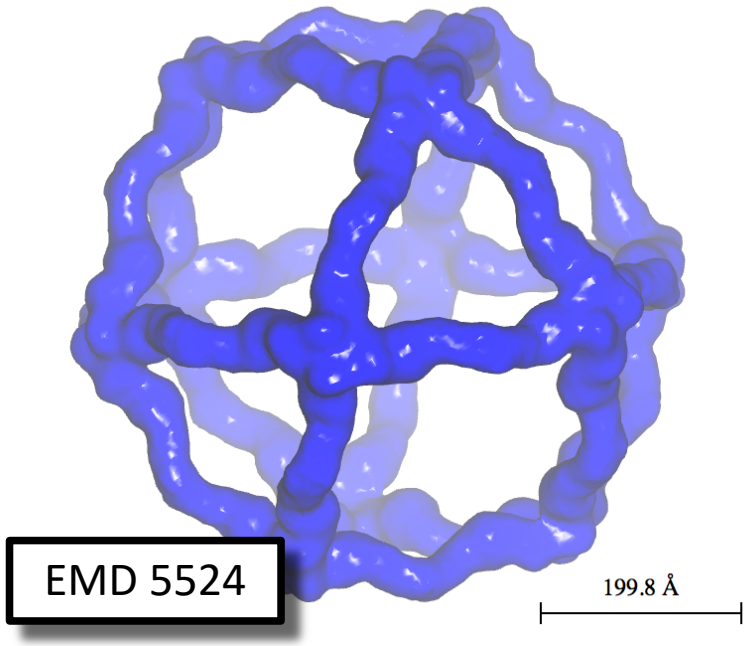
- Electron density maps can be read/created from any CCP4 supported file format, downloaded from PDB or generated from structure factors.
- Density can be represented as chickenwire lines, chickenwire cylinders, solid surface or dots.
- By default a 10Å parallelepiped of density at centre of screen is drawn, this size may be changed by user. The density is recalculated and redrawn when the viewpoint changes
- The density can be clipped to a set of atoms.

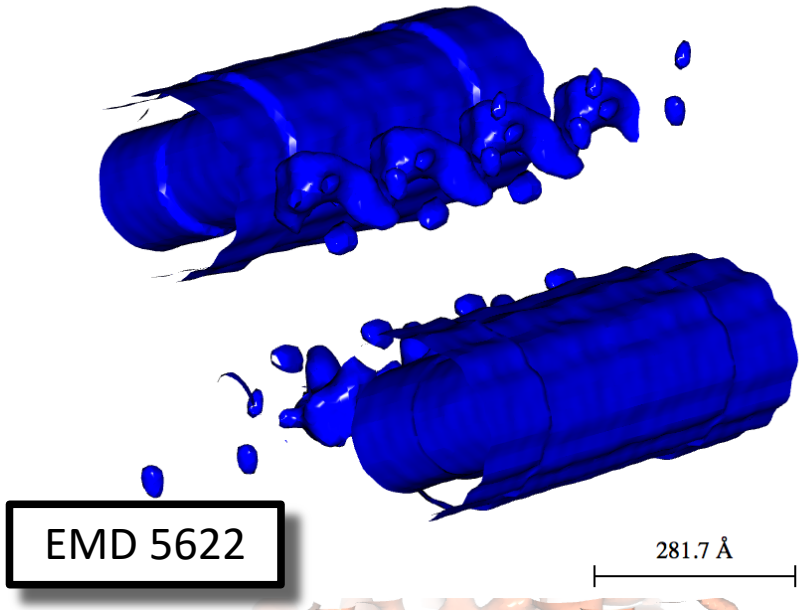

(a)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24
(b)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24
(c)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24
(d)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24
(e)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24

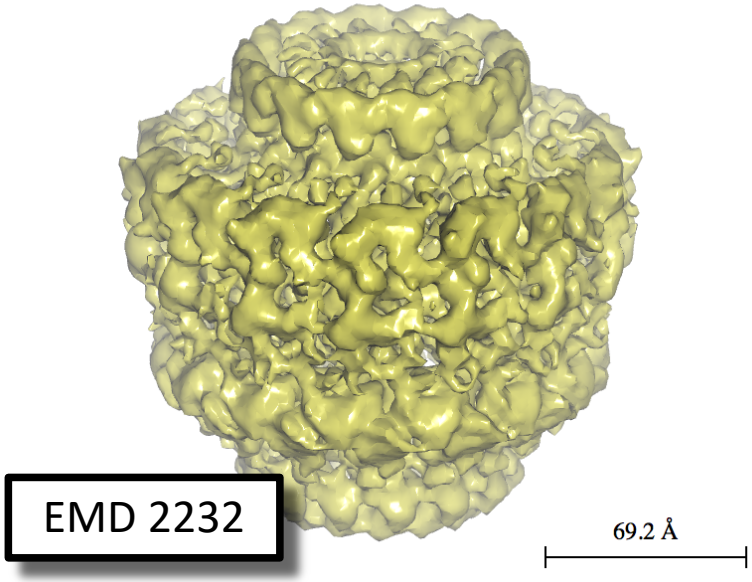


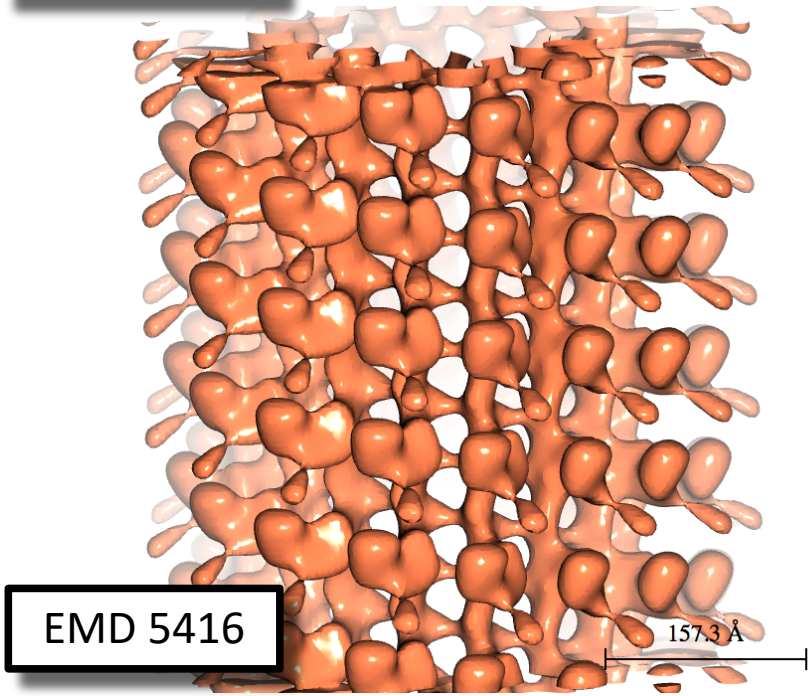
Electron Microscopy Maps

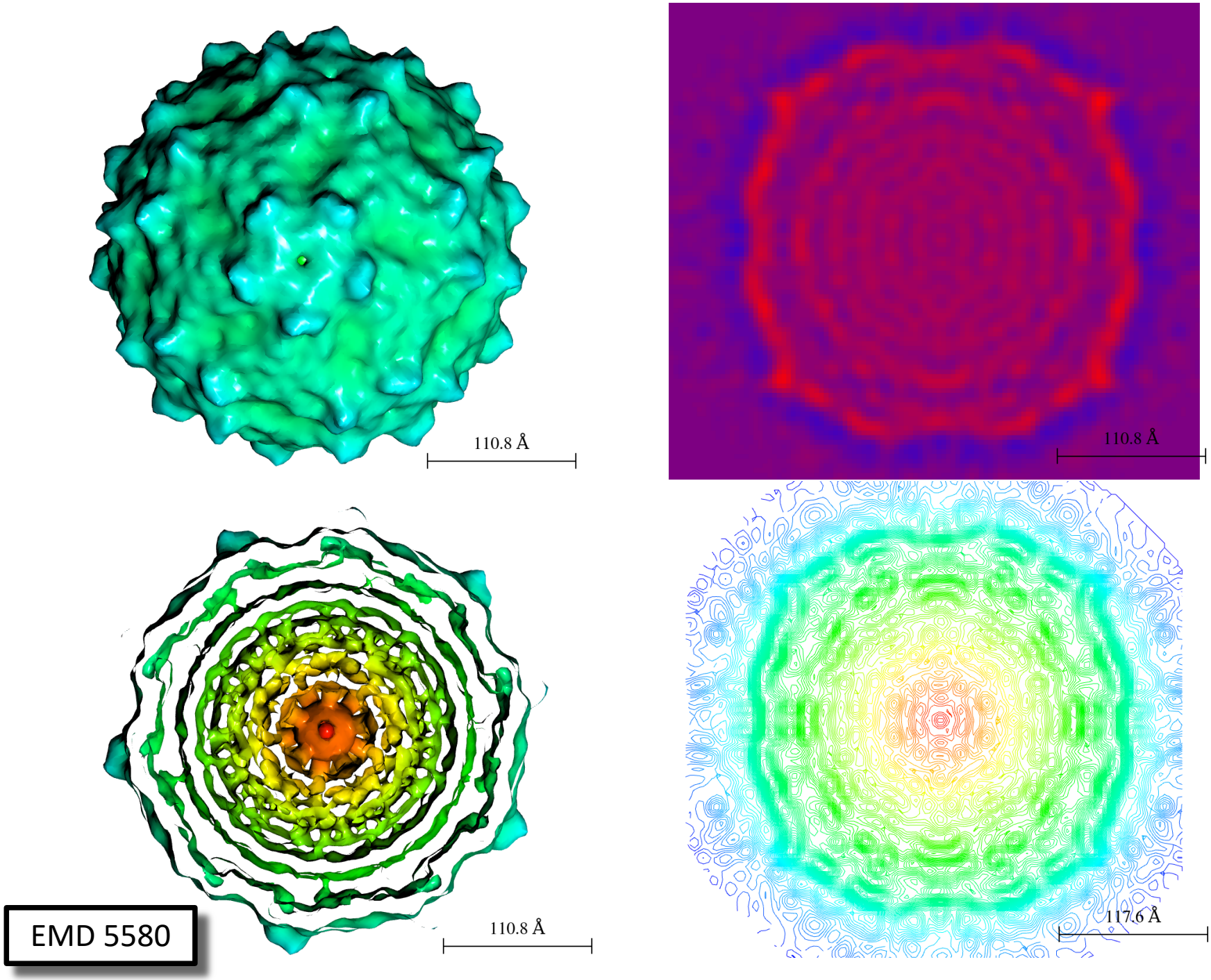
- CCP4MG can cope with 1000 angstrom sized maps.
- Maps from electron microscopy do not recalculate when moving view like X-ray maps. Massive speed improvement.
- Colour by distance from centre of map option – nice for virus maps.

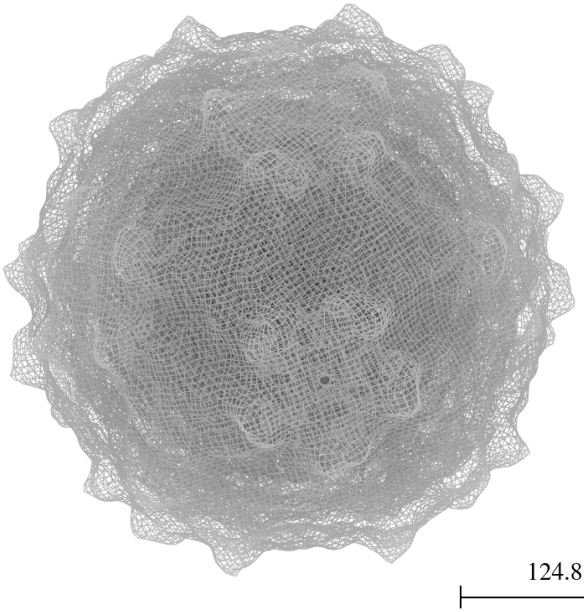

EMD 5524
199.8 Å

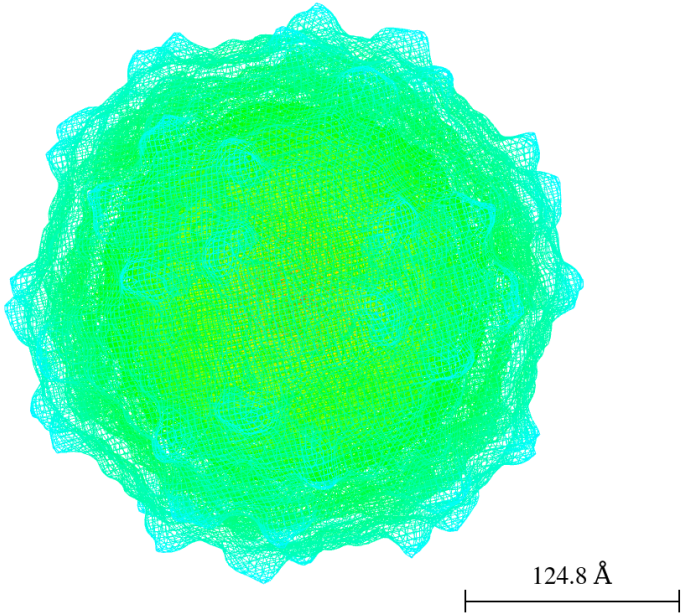

EMD 5622
281.7 Å

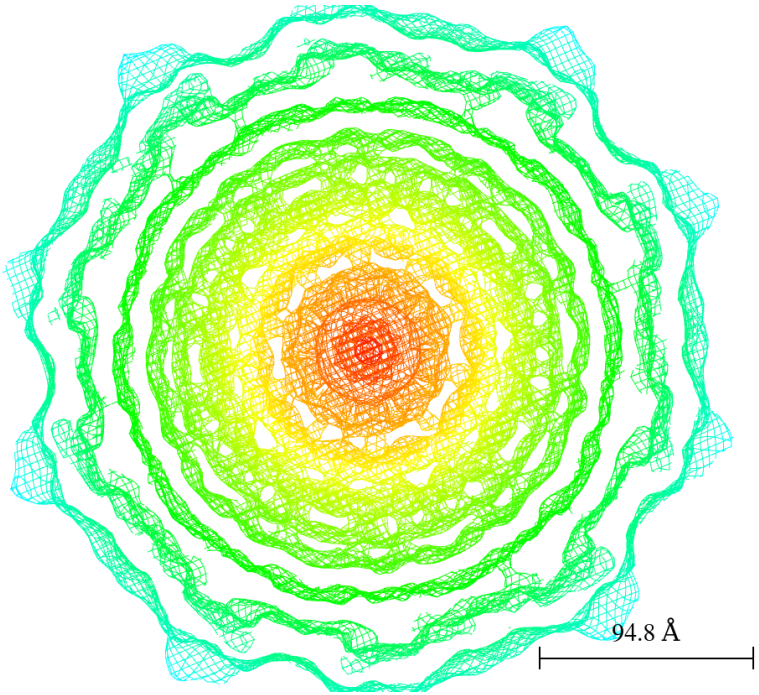

EMD 2232
69.2 Å


EMD 5416
157.3 Å


110.8 Å
110.8 Å
110.8 Å
117.6 Å
EMD 5580







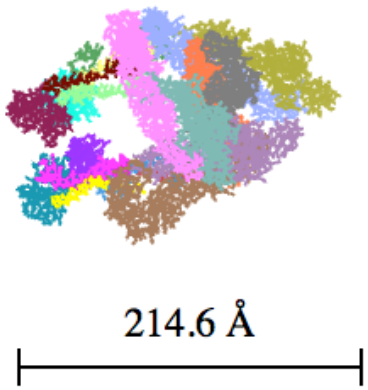
EMD 5580

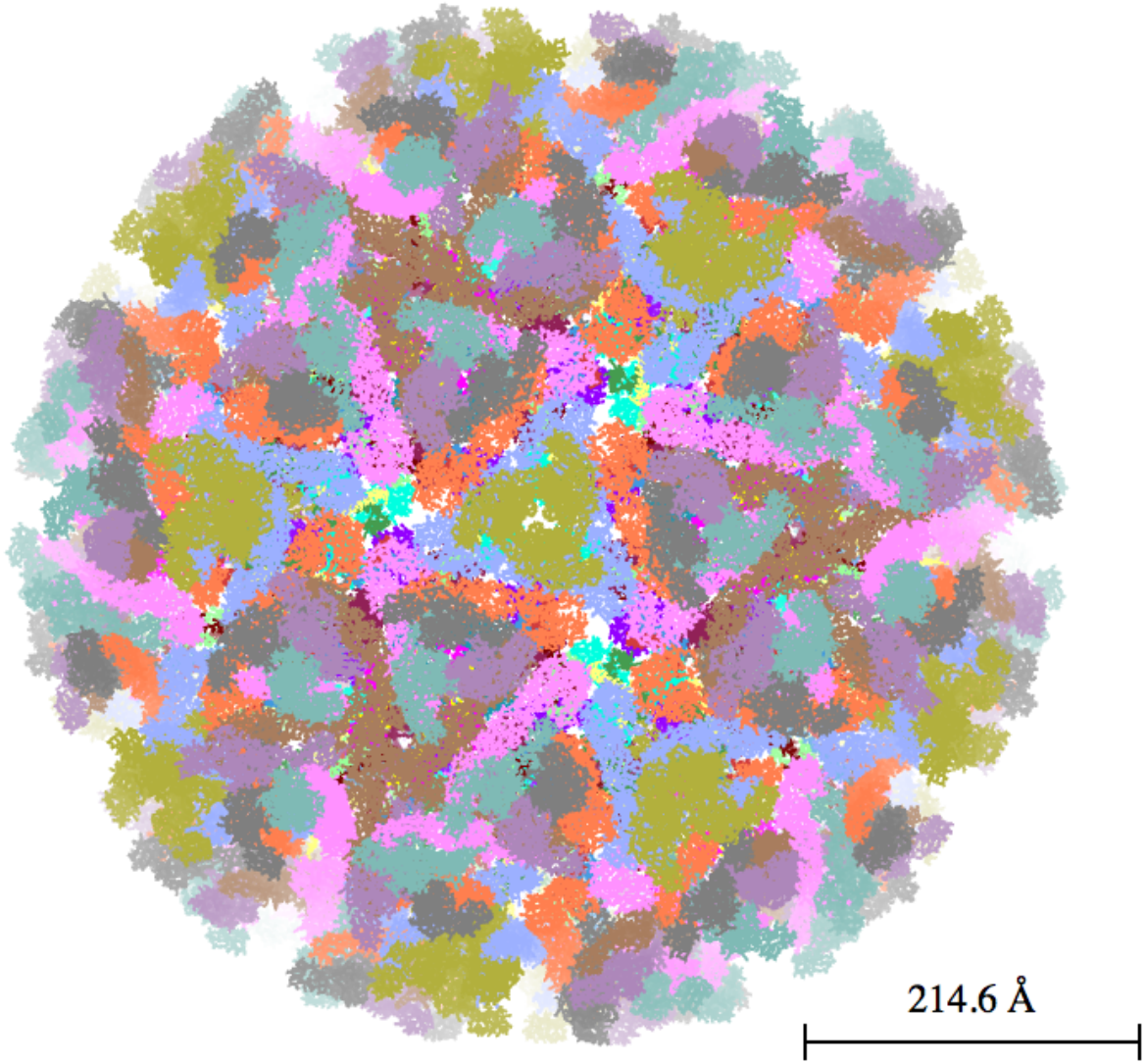
Symmetry

- Two ways:
  - Fast: Apply symmetry operations to objects which are drawn. “Continuous”, “About a point”, “unit cell”.
  - Not so fast: Create new display objects which can then have style, selections, etc. edited.
  - Will demonstrate on Monday.

Biological Assemblies

- CCP4MG can parse the biological assembly information contained in PDB files.
  - Set of transformation matrices that create symmetry mates of model information to create a complete assembly.

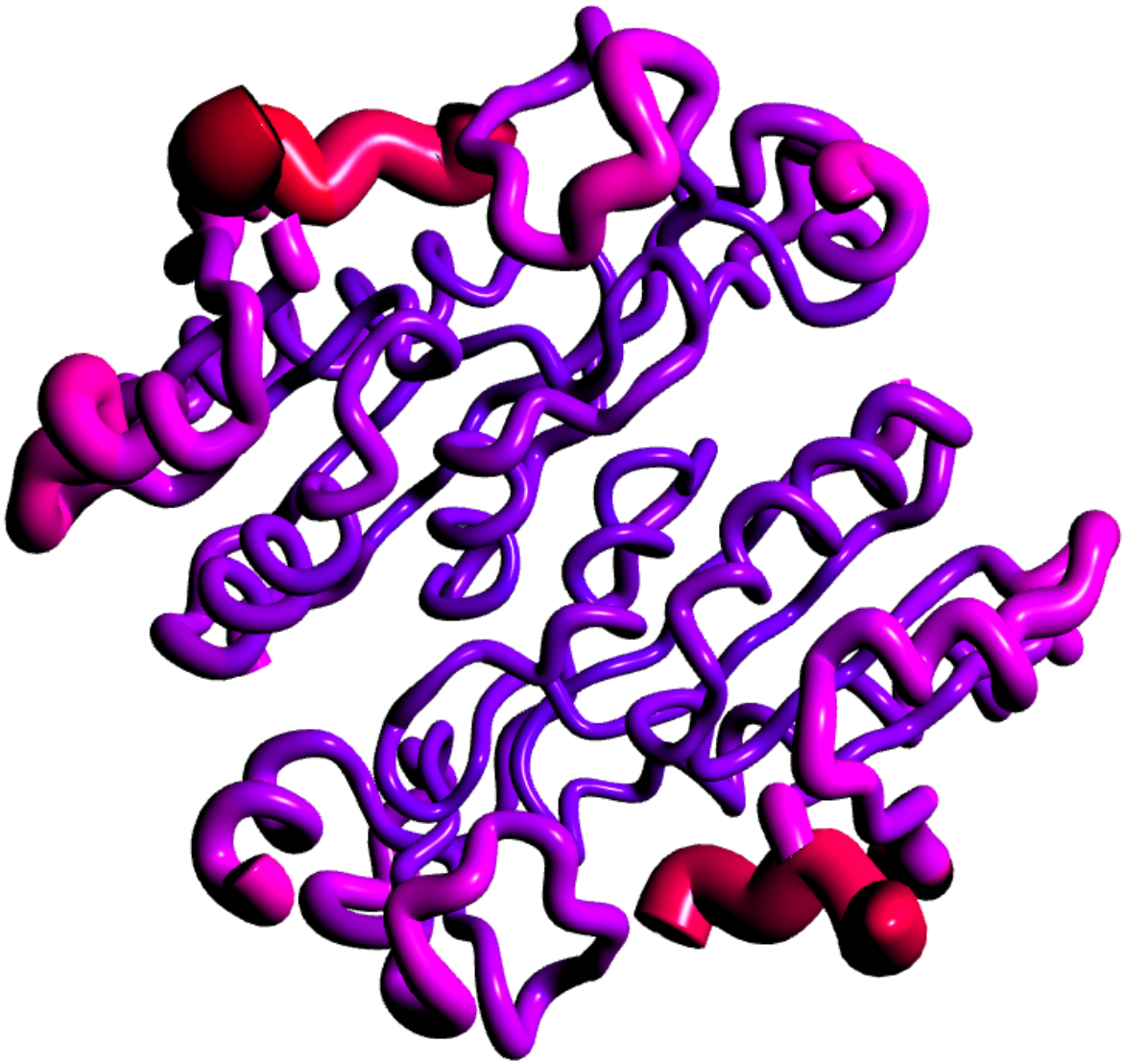




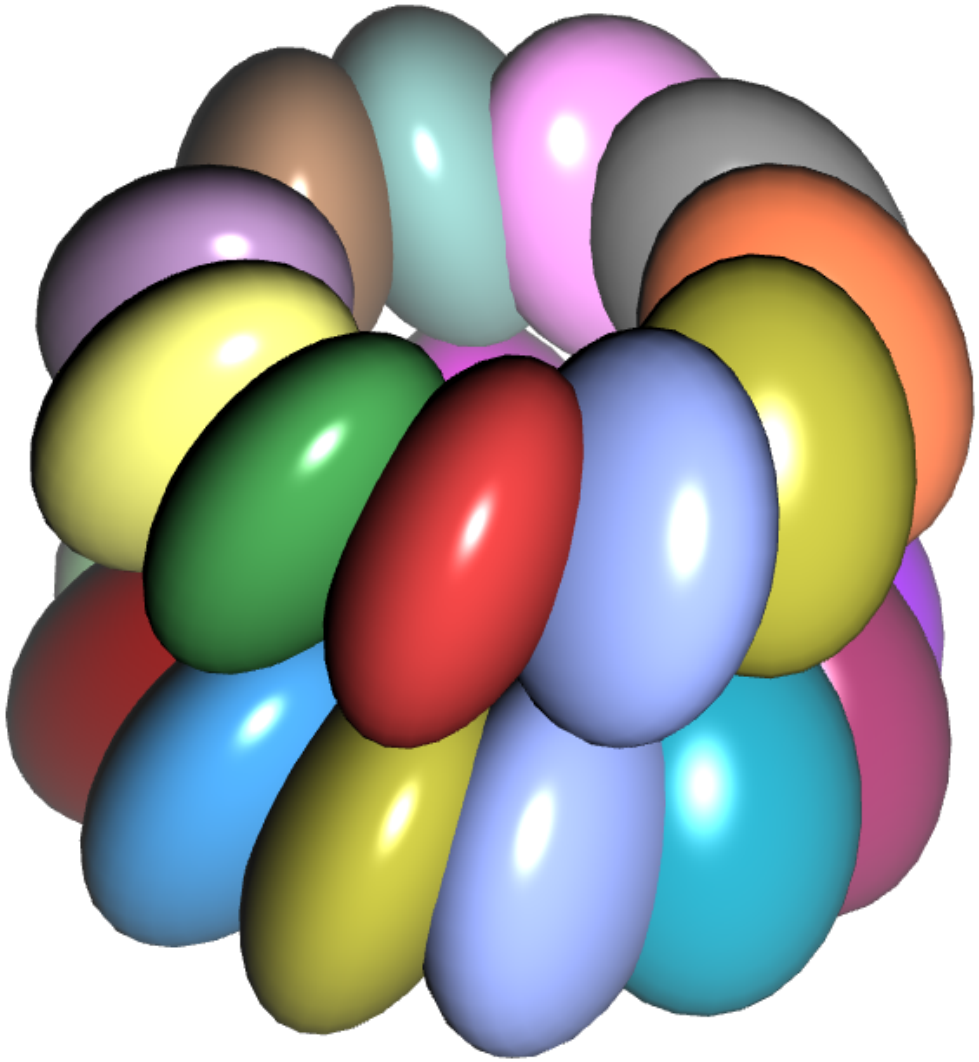
PDB 3j2w

Some other drawing styles

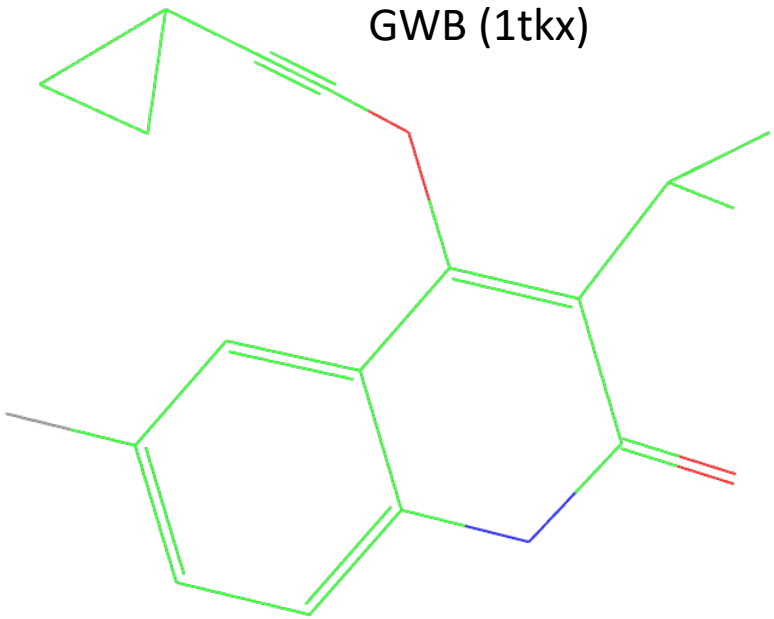
Worm scaled by B-factor

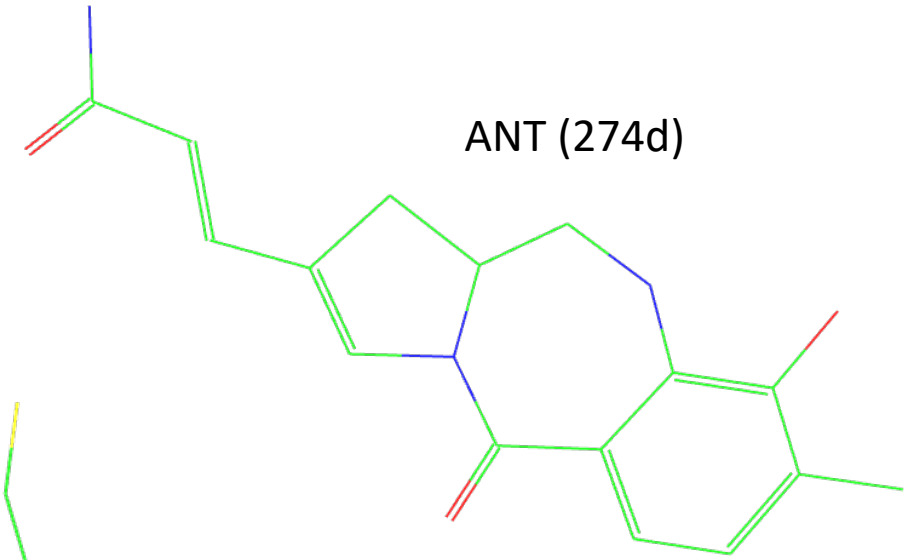


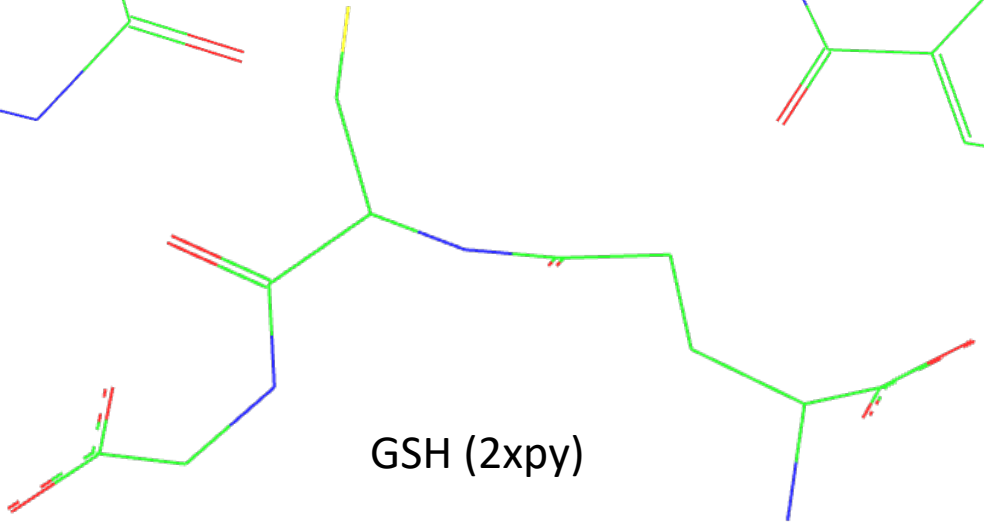
Bloboids



Multiple bonds

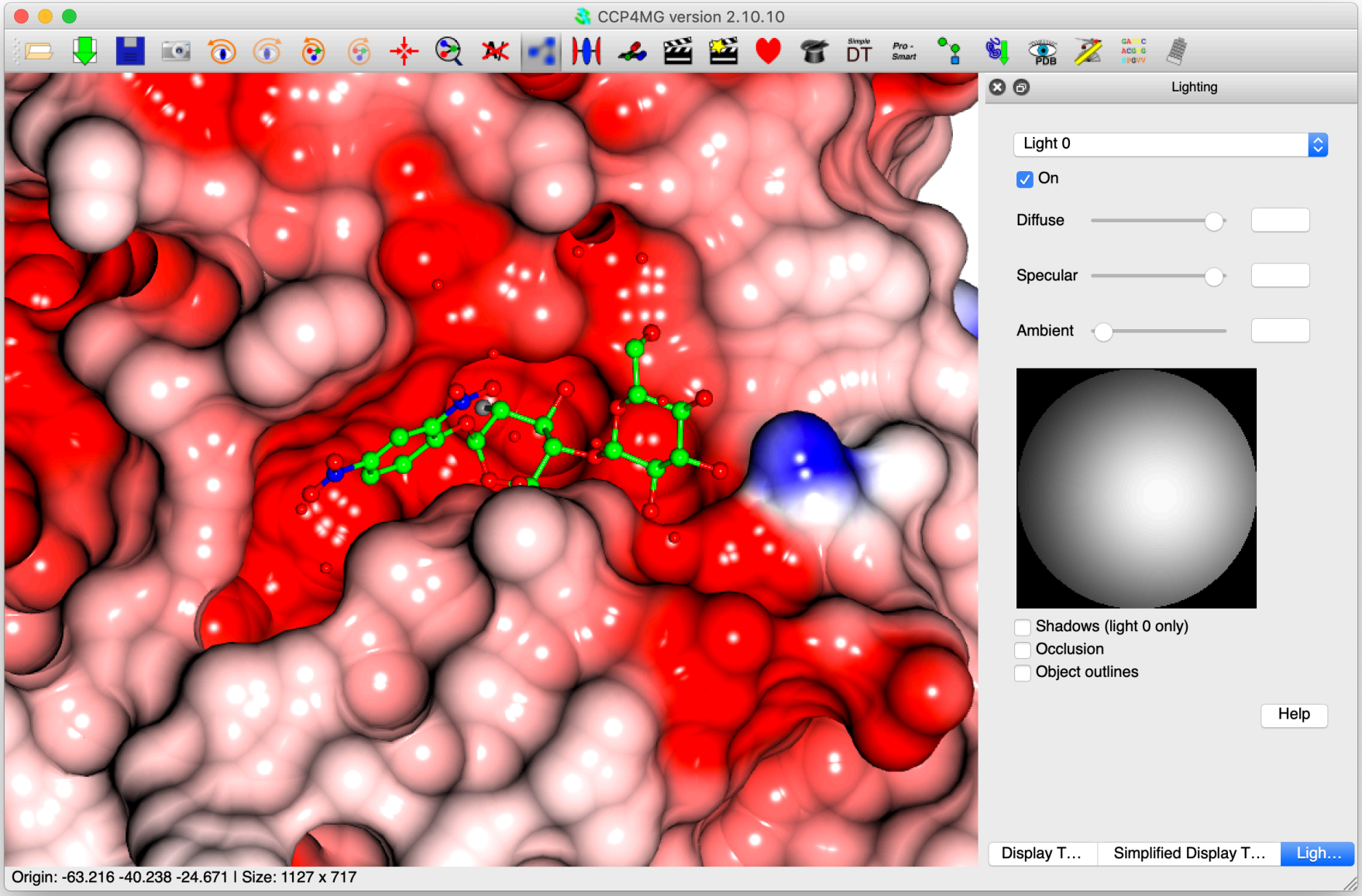


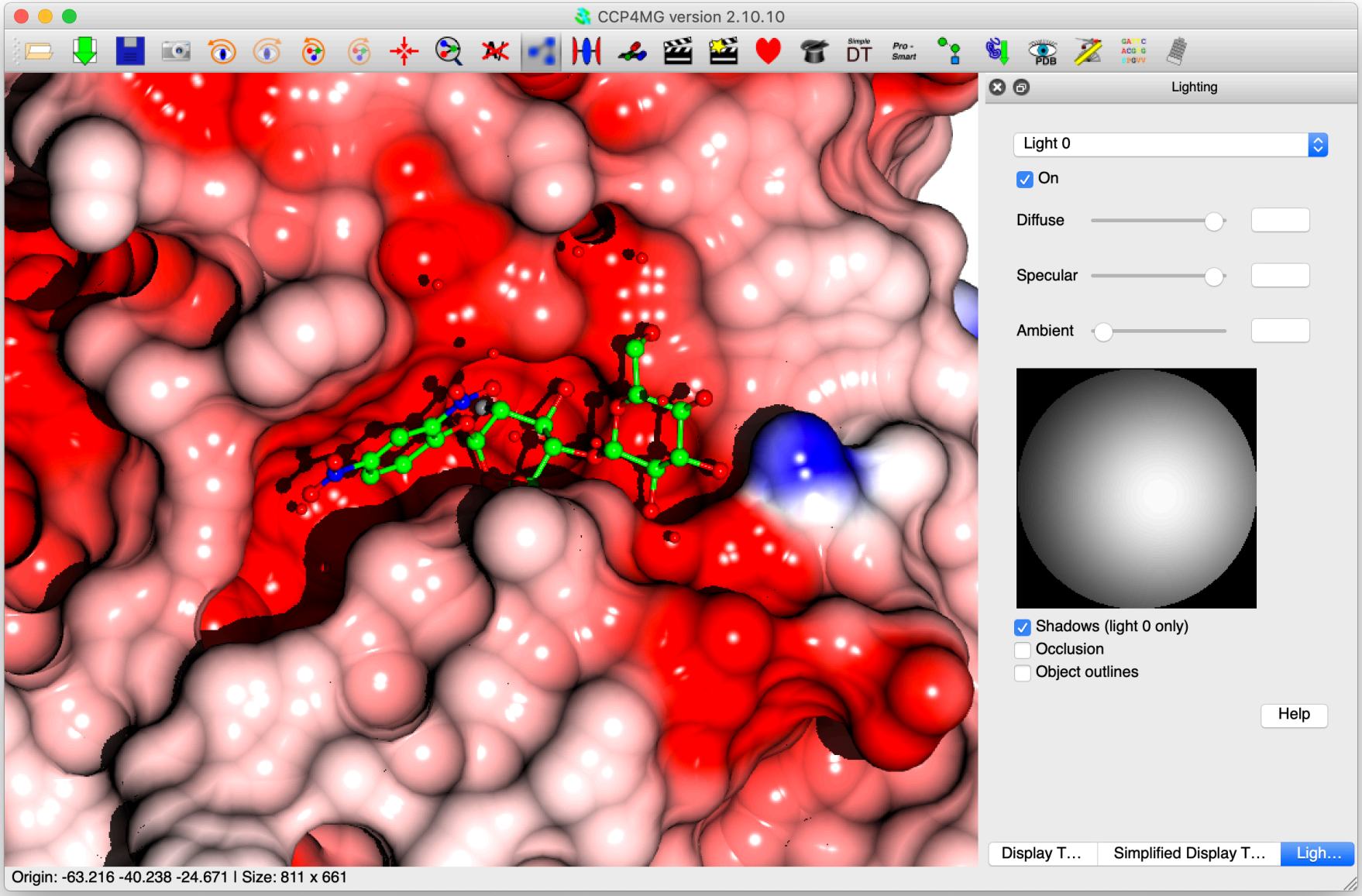


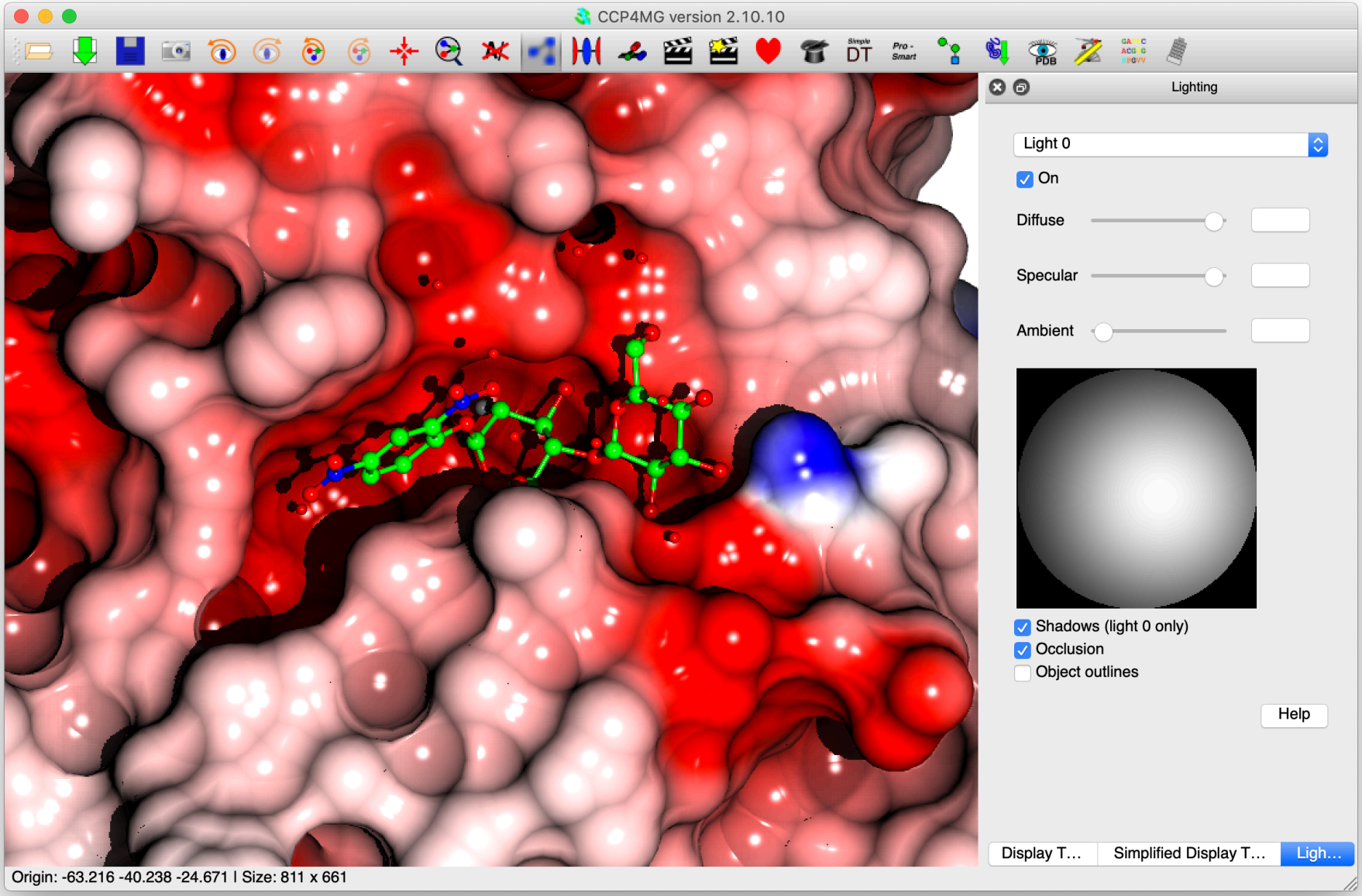


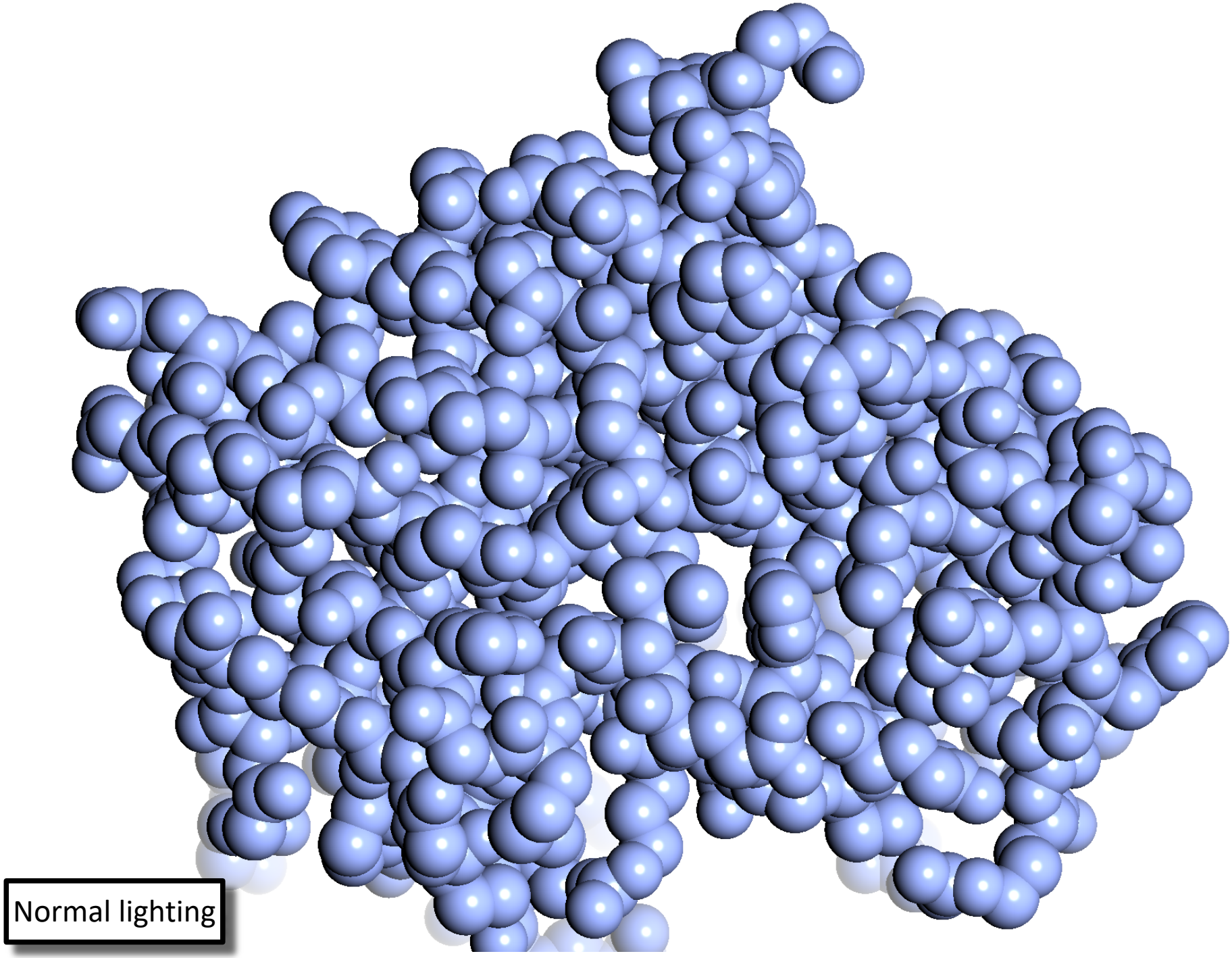
Shadows and Occlusion

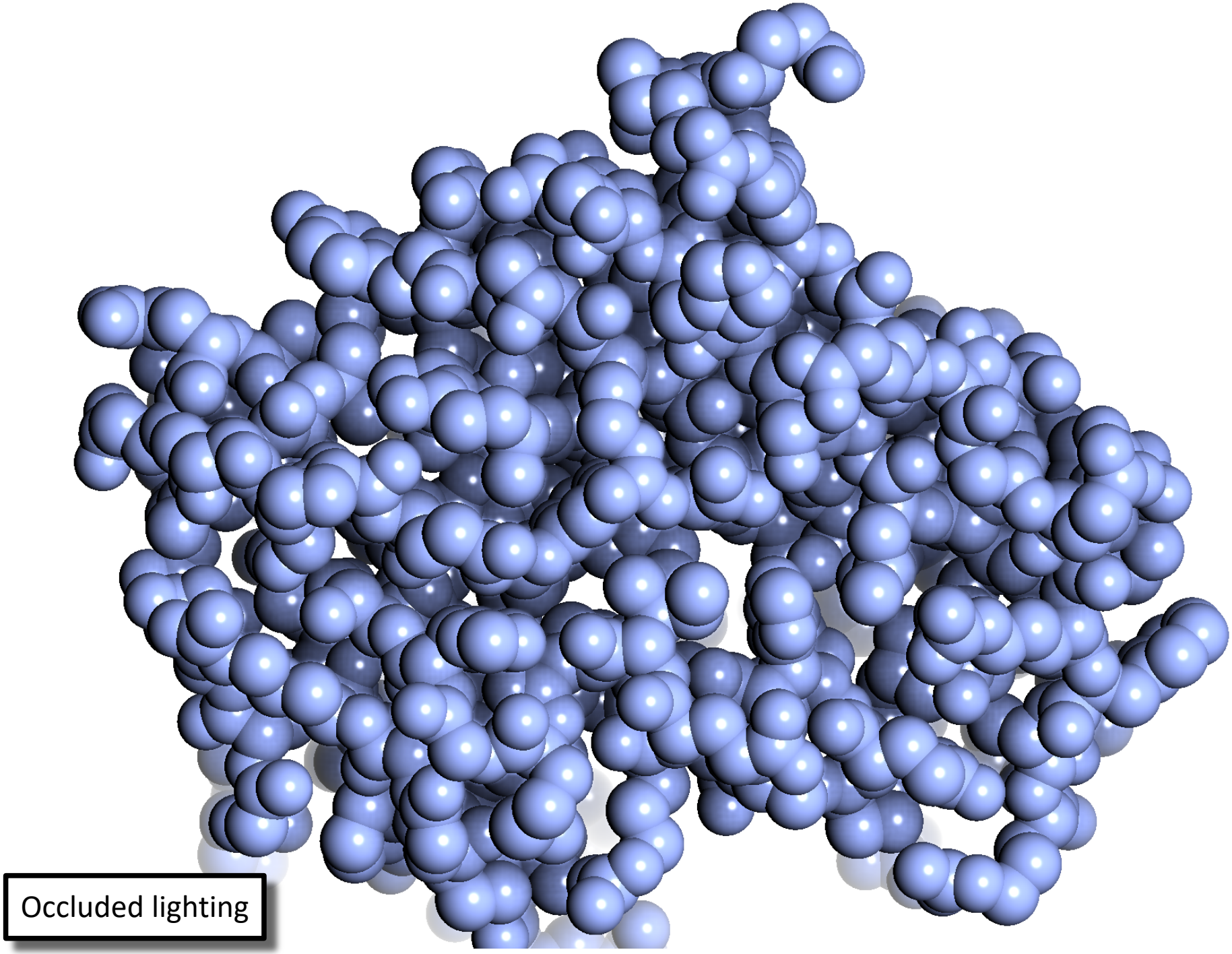
- “Real-time” shadows, i.e. active all time in graphics window, not just when you “Render”.
- Occlusion is darkening of buried bits which are not exposed to as much light as exterior parts of macromolecules. Also a “real-time” effect.


CCP4MG version 2.10.10
Lighting
Light 0
On
Diffuse
Specular
Ambient
Shadows (light 0 only)
Occlusion
Object outlines
Help
Display T…
Simplified Display T…
Ligh…
Origin: -63.216 -40.238 -24.671 | Size: 1127 x 717


CCP4MG version 2.10.10
Lighting
Light 0
On
Diffuse
Specular
Ambient
Shadows (light 0 only)
Occlusion
Object outlines
Help
Display T…
Simplified Display T…
Ligh…
Origin: -63.216 -40.238 -24.671 | Size: 811 x 661

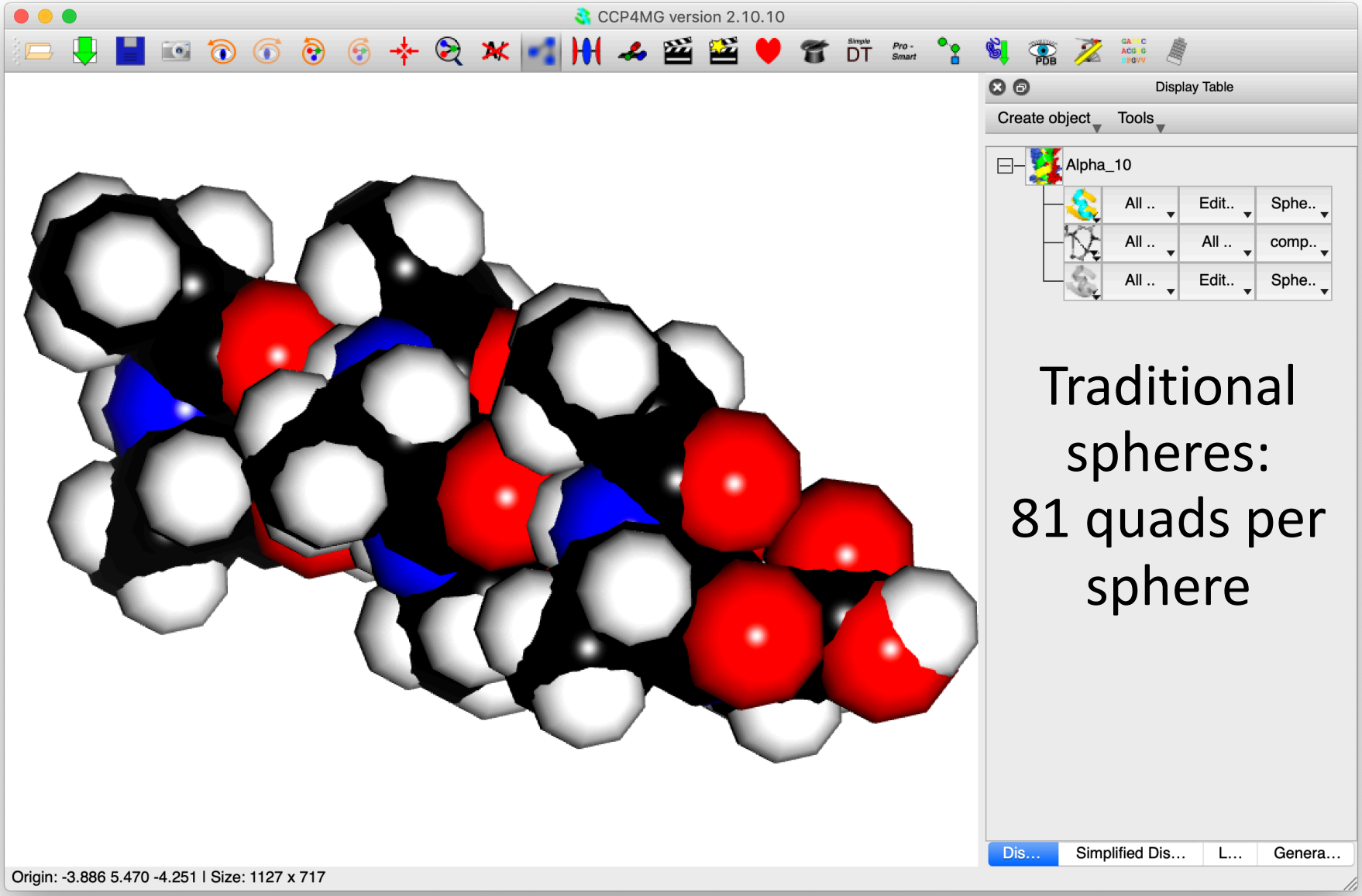

CCP4MG version 2.10.10
Lighting
Light 0
On
Diffuse
Specular
Ambient
Shadows (light 0 only)
Occlusion
Object outlines
Help
Display T…
Simplified Display T…
Ligh…
Origin: -63.216 -40.238 -24.671 | Size: 811 x 661

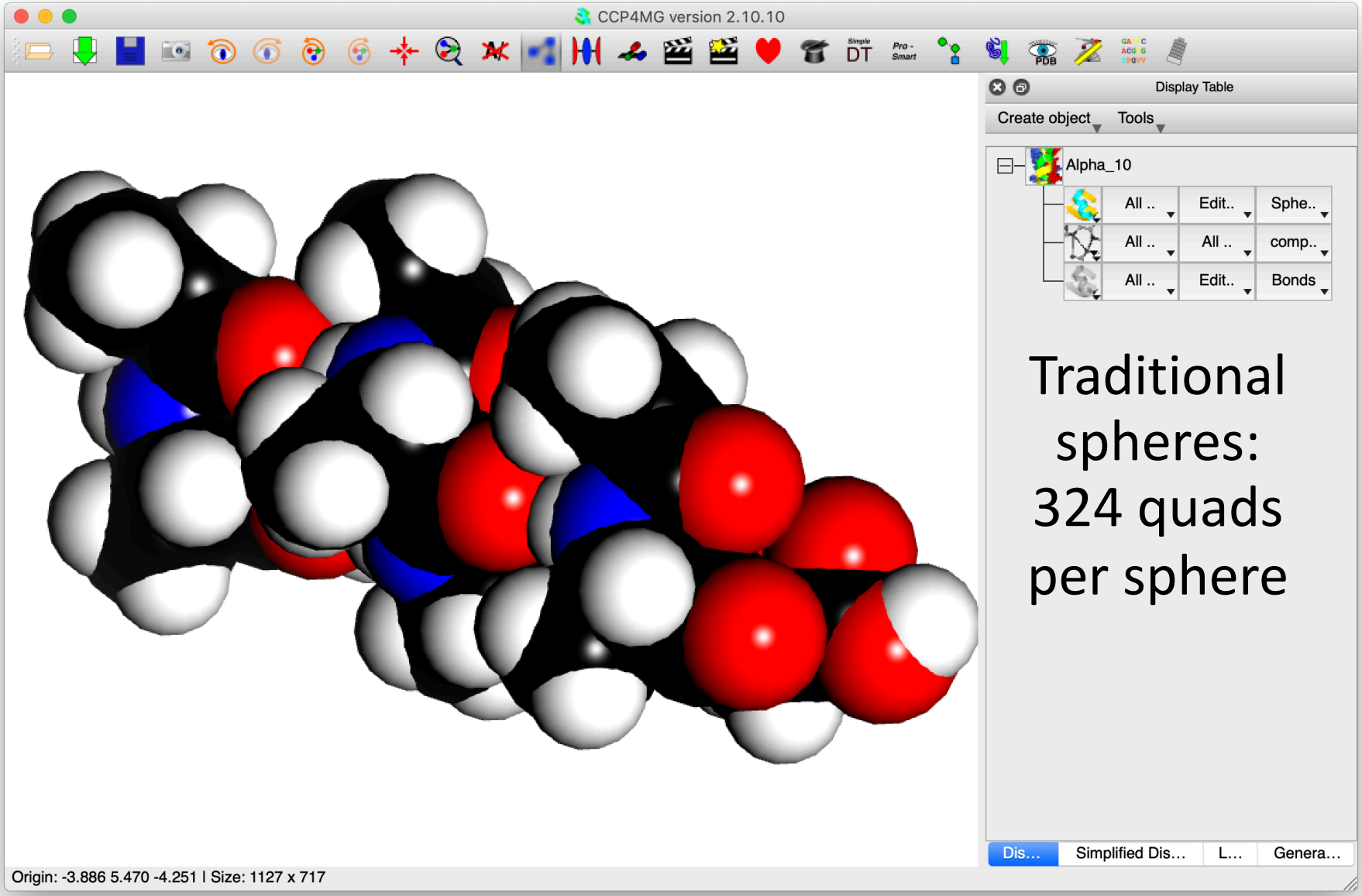

Normal lighting

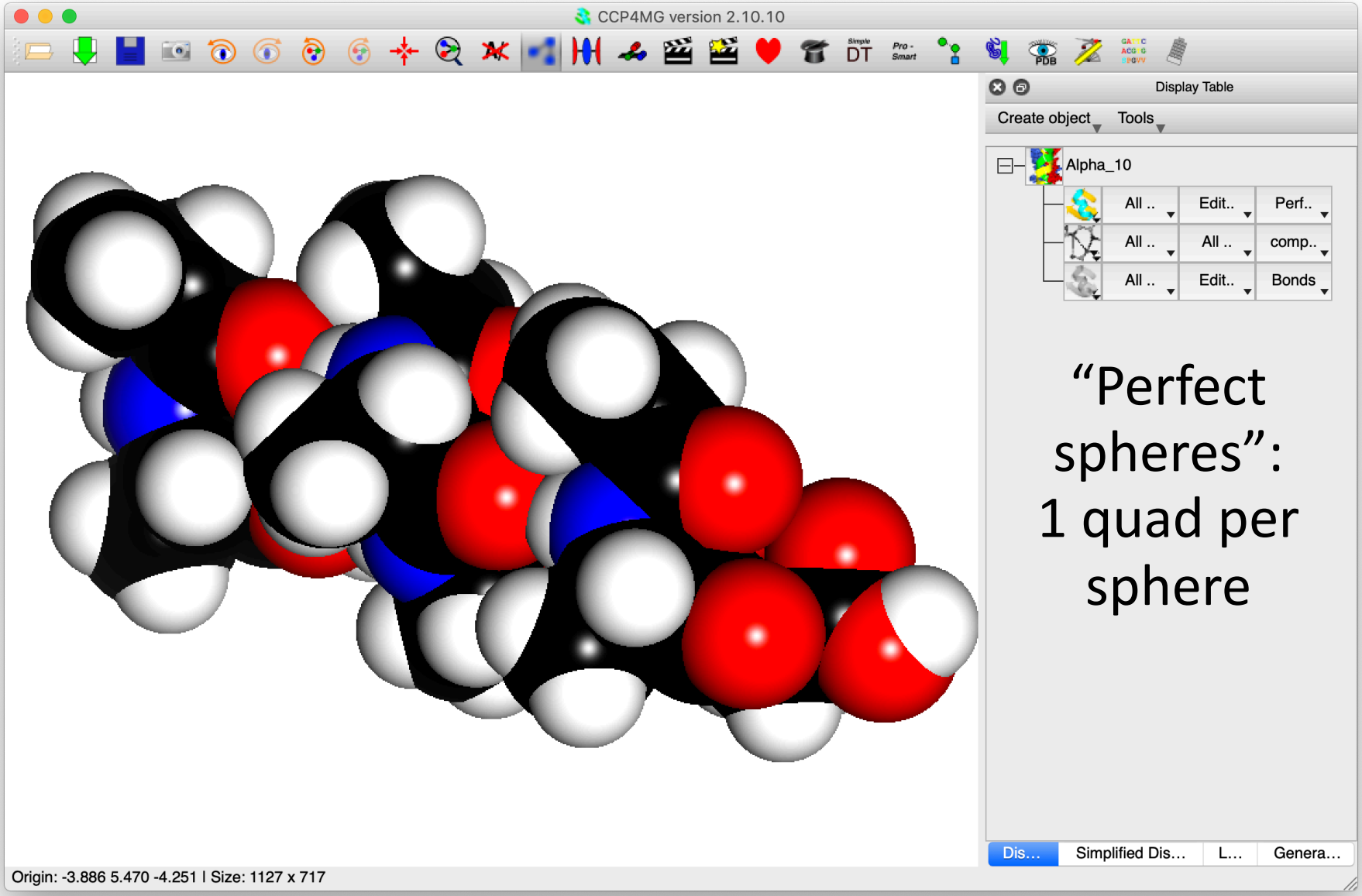

Occluded lighting

“Perfect spheres”

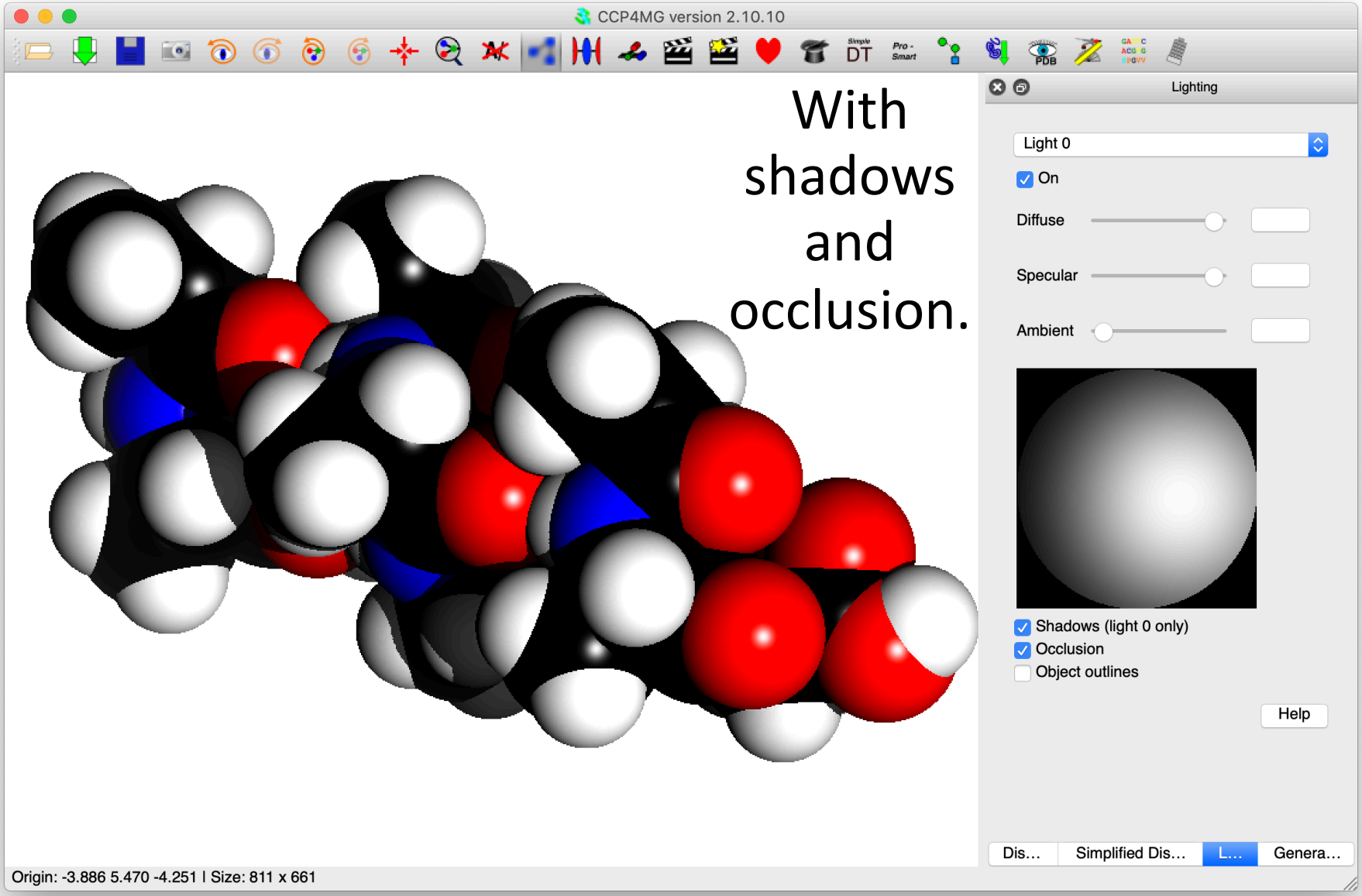
- “Ray-traced”, perfectly spherical spheres in main graphics window.
- 1 quadrilateral per sphere compared with traditional method with 81 (smooth) or 324 (deluxe) quads. So use much less memory. Further memory reductions are also possible with newer graphics cards, but this is not yet done.
- Faster when zoomed out, same speed (possibly slower) when zoomed in. Work needed to claw back some optimisations. (Could be less of a problem if e.g. Apple's drivers used more hardware features ….)


CCP4MG version 2.10.10
Display Table
Create object
Tools
Alpha_10
All ..
Edit..
Sphe..
All ..
All ..
comp..
All ..
Edit..
Sphe..
Traditional spheres: 81 quads per sphere
Dis...
Simplified Dis...
L...
Genera...
Origin: -3.886 5.470 -4.251 | Size: 1127 x 717


CCP4MG version 2.10.10
Display Table
Create object
Tools
Alpha_10
All ..
Edit..
Sphe..
All ..
All ..
comp..
All ..
Edit..
Bonds
Traditional spheres: 324 quads per sphere
Dis...
Simplified Dis...
L...
Genera...
Origin: -3.886 5.470 -4.251 | Size: 1127 x 717



"Perfect spheres": 1 quad per sphere


CCP4MG version 2.10.10
With shadows and occlusion.
Lighting
Light 0
On
Diffuse
Specular
Ambient
Shadows (light 0 only)
Occlusion
Object outlines
Help
Dis...
Simplified Dis...
L...
Genera...
Origin: -3.886 5.470 -4.251 | Size: 811 x 661

Other Display Details

- All objects
  - May be visible/invisible
  - “Flash”
  - Be transparent with arbitrary opacity
- One can have multiple views (e.g. side-by-side stereo)
- Hardware/Zalman stereo.
- Depth-cueing fog, clipping, background colour and lighting are all user definable
- Lots of stuff is highly customizable (Edit->Preferences (Windows/Linux), QtMG->Preferences (Mac))

“Rendering”

- CCP4MG has two methods of producing final images:
  - Screenshot. A simple dump of the screen pixels is performed. Images may be up to ca. 8000x8000 pixels. *On most systems.*
  - “Rendering”. This uses a Renderman compatible renderer “Pixie”. Some aspects of these images are of much higher quality than the simple screen dump (spheres particularly). Better transparency with more than one transparent object is possible.

Render vs. Screenshot

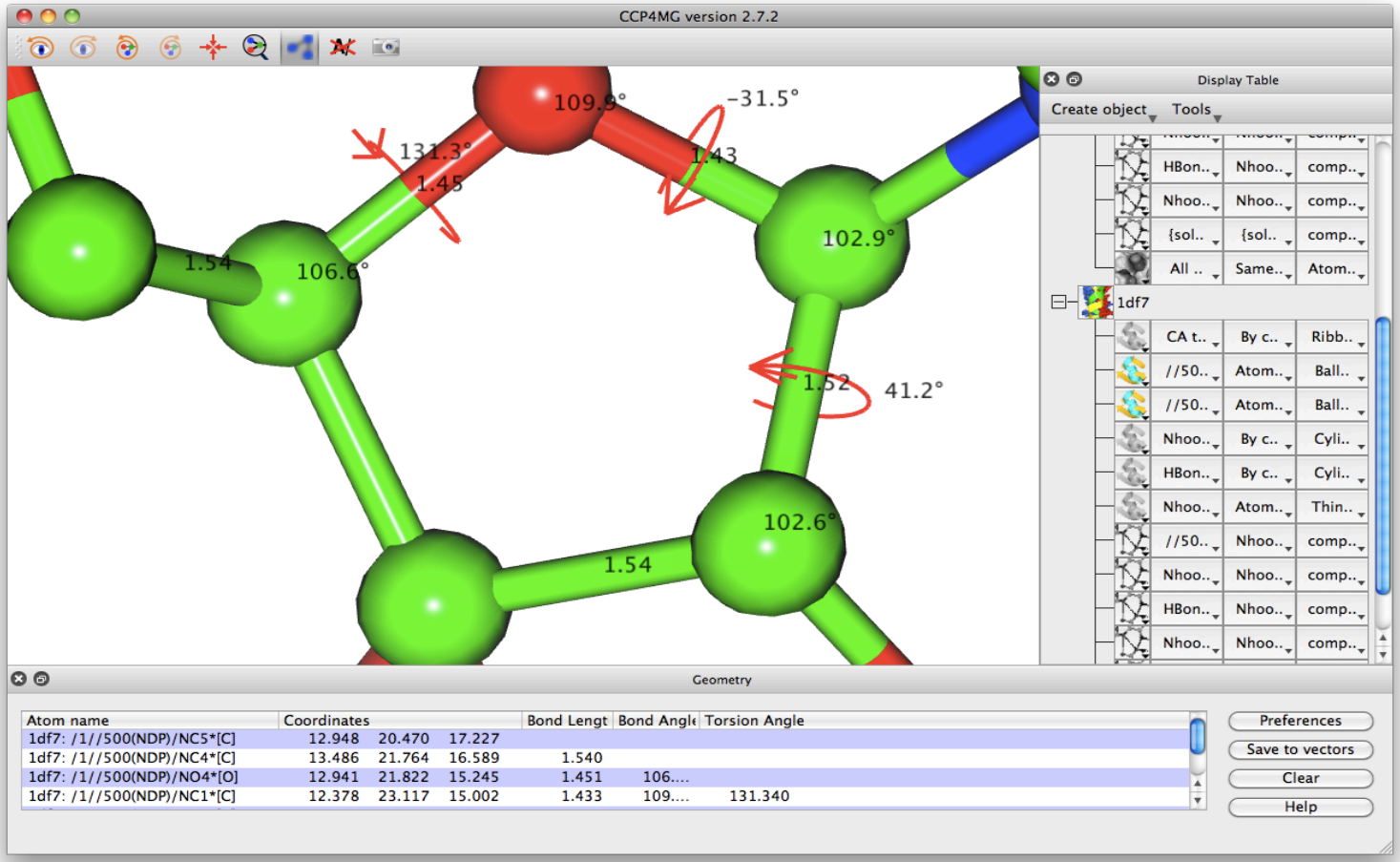
- Real-time shadows and occlusion and “perfect spheres” mean OpenGL is now arguably a better choice for rendering than “Render” module.
- Screenshot pros:
  - Shadows make “Render” slow, but bearable.
  - Ambient occlusion makes “Render” really, really slow.
  - Darkness of OpenGL shadows could be changeable, “Render” ones are simply very black.
  - Much faster. 1DF7 ribbon + sphere ligand + shadow + 2x supersampling: 84s “Render”, 3s screenshot.
- Screenshot cons:
  - OpenGL shadows can be too soft and fuzzy with large structure. This can be improved by more intelligent use of depth buffer.
  - “Perfect spheres” are not anti-aliased. (So not so perfect!). This can be worked around (now) by taking screenshot at larger size (2x, 4x, etc.), though this ought to be automatic.
  - Render handles multiple transparent objects properly. (Work in progress to make OpenGL renderer cope with multiple objects.)

“Batch” rendering

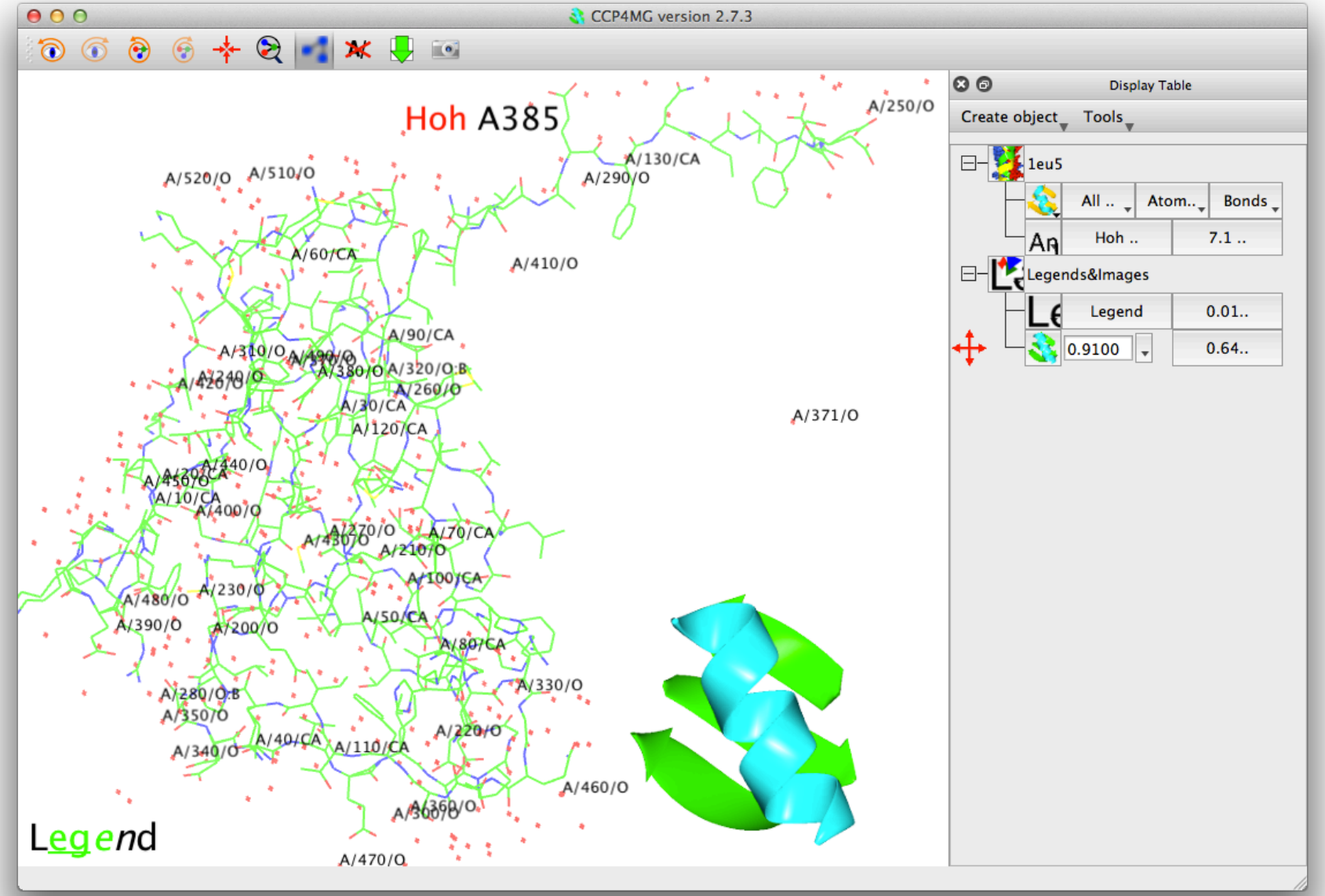
- Images may be rendered from command line or from scripts without starting up the main program.
- `ccp4mg -norestore -picture mypic.mgpic.py -R test.png -RO '{"size":"1600x1600","smoothribbons":"1", "raytrace":"1"}' -quit`
- The file mypic.mpic.py is a file containing a scene description: lists of data files, representations, view, etc.

Distances and angles

- Double-click on one atom then another to measure bonds.
- Shift-double click on other atoms will measure angles.
- Results appear in table below and in graphics window.



On screen text and images



Online data access

- Download PDB files (PDB)
- Download MTZ files (PDB)
- Download Structure Factors (PDB)
- Download EM map files (EMDB)
- Download PDB-REDO PDB/MTZ (Broken in current CCP4 release, fixed in next release CCP4 7.1 / CCP4MG 2.10.11)
- Blast searches (EBI)

QtMG File Edit View Display Applications Windows Tools Help CCP4i2 100% Mon 13:32

CCP4MG version 2.10.8

- Open.. ⌘O
- Recent files ▶
- Download coordinates..
- Download Structure Factors..
- Download electron density
- Download PDB_REDO data
- Edit/show presentation ▶
- Close all data
- Get tutorial data
- Save status to file.. ⇧⌘S
- Save as default status.. ⌘S
- Save all visible to file..
- Screenshot
- Print screen ⌘P
- Save Archive
- Render ⌘R

Display Table

Create object | Tools

- Crystals
  - Xtl .. | Crys.. | Symm..
  - Xtl .. | Crys.. | Symm..
  - Xtl .. | Crys.. | Symm..
- NEM39xDXbHcRdnaWL
- 5B40
- 5a3h_sigmaa
  - blue | 1.5000
- 5a3h_stuart
  - blue | 1.5000
- 5B40
  - blue | 5.0000

Display Table | Simplified Display Table

Sequence Viewer

NEM39xDXbHcRdnaWL_A
5B40_A
5B40_B
5B40_C
5B40_D
5B40_E
5B40_F

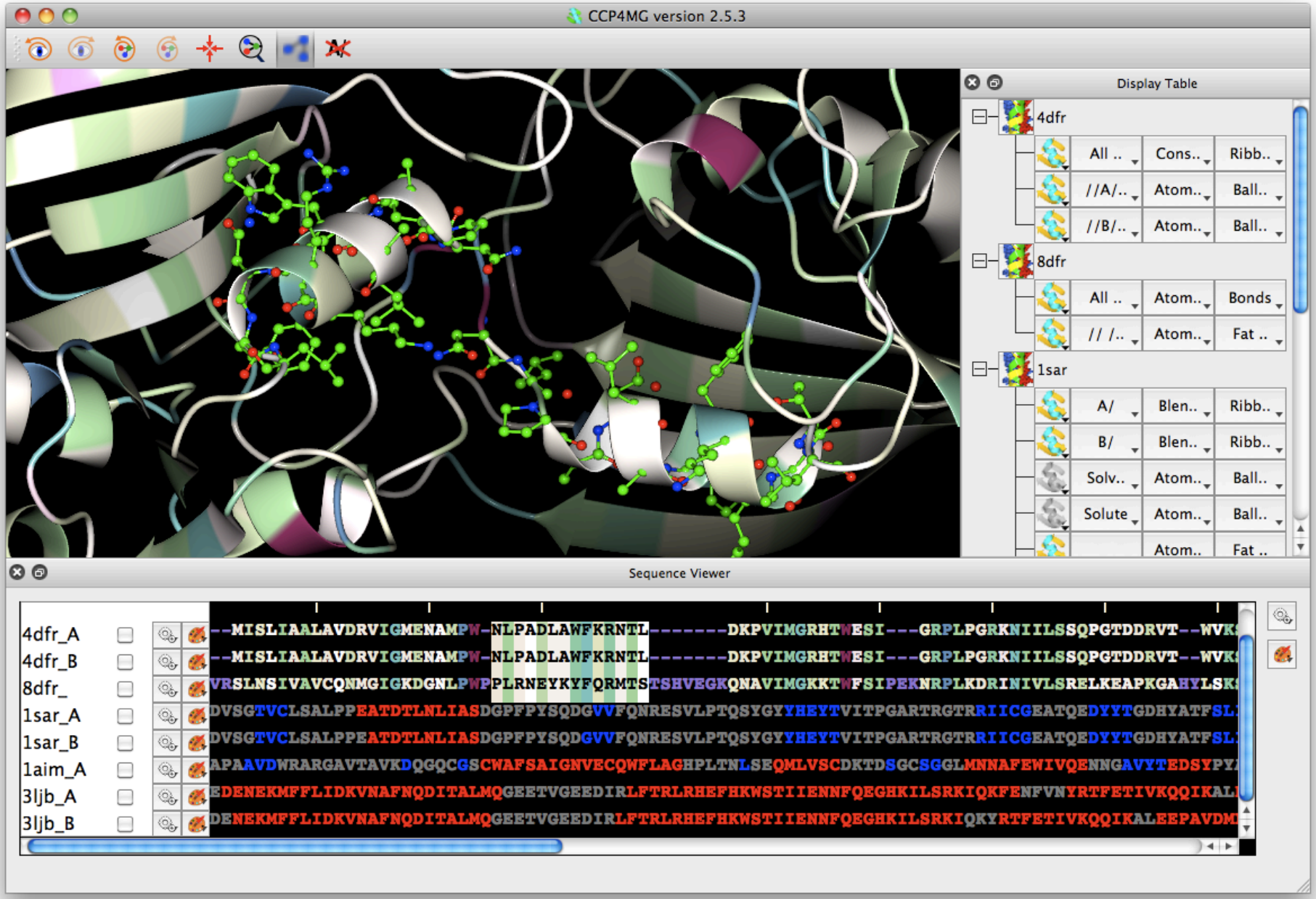
- Run blastp on this sequence locally
- Run blastp on this sequence on EBI server
- Run MrBUMP to find search models with 100% cutoff
- Run MrBUMP to find search models with 70% cutoff
- Previous MrBUMP runs
- Delete MrBump results

Structure Superposition

- CCP4MG has several methods of structure superposition:
  - SSM - This is the default method. It is the simplest to use and usually gives excellent results. The method attempts to match secondary structure elements in different coordinate sets.
  - Gesamt – a more general method which matches fragments which need not be defined by secondary structure elements.
  - Close Residues -This method is useful for performing locally optimised superposition after a global superposition by SSM/gesamt.
  - User-defined. This is the most flexible, but least easy to use: the user can specify in many ways the atoms to superpose.

Sequence Viewer

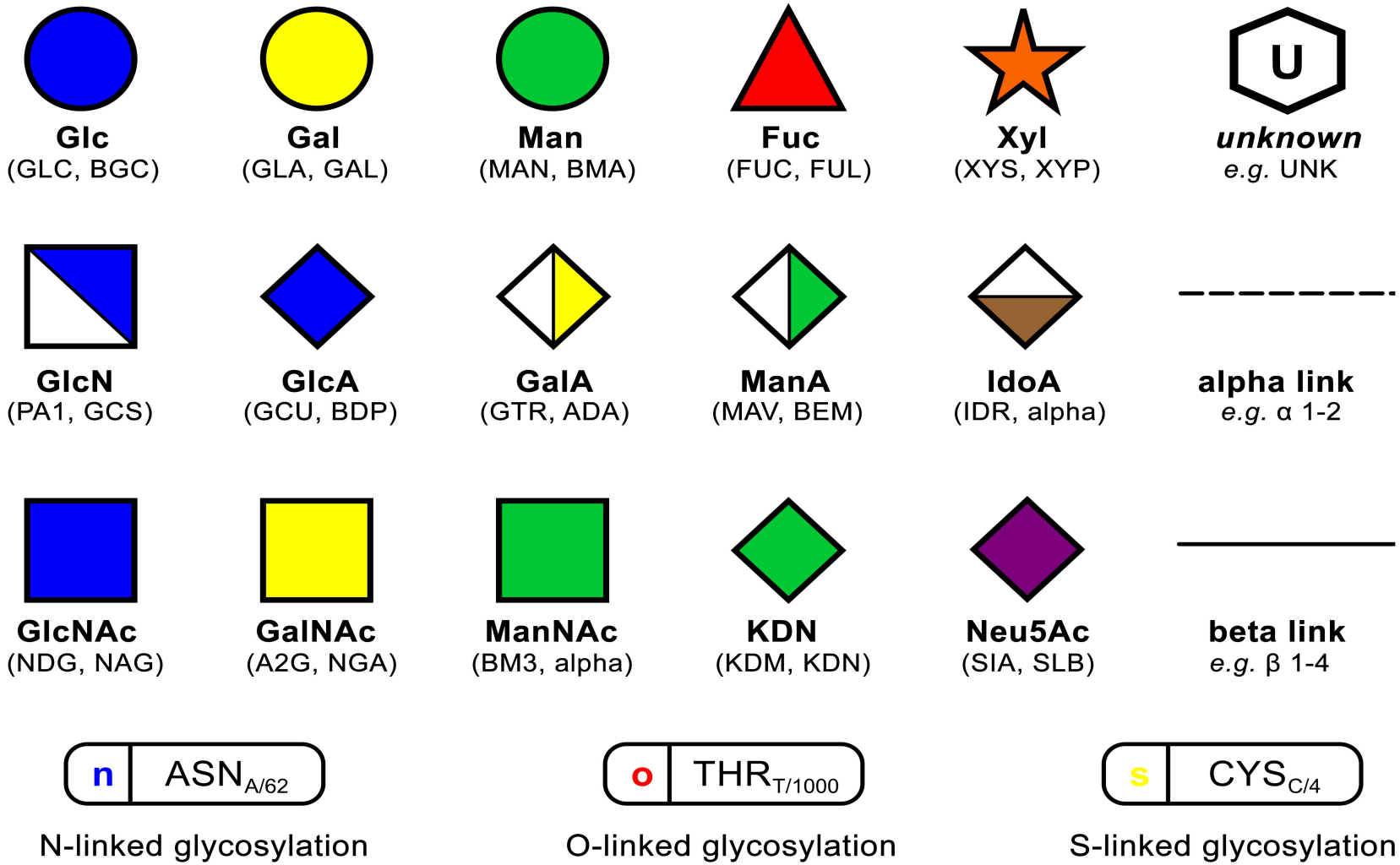
- Align sequences using muscle (a free multiple-alignment program) or ClustalW.
- Continuous (consurf style) or discrete traffic-light colour by conservation.
- Colour by secondary structure.
- Blastn/blastp interface. Blast results cached between sessions. Blast normally run remotely (EBI) with explicit user permission, but can also use local blast installation.
- Save sequence as PDF/bitmap/plain text.
- Click, shift-click, ctrl-click, etc. on residues in sequence to display atoms in the mail window.


CCP4MG version 2.5.3
Display Table
4dfr
All ..
Cons..
Ribb..
//A/..
Atom..
Ball..
//B/..
Atom..
Ball..
8dfr
All ..
Atom..
Bonds
// /..
Atom..
Fat ..
1sar
A/
Blen..
Ribb..
B/
Blen..
Ribb..
Solv..
Atom..
Ball..
Solute
Atom..
Ball..
Atom..
Fat ..
Sequence Viewer
4dfr_A
4dfr_B
8dfr_
1sar_A
1sar_B
1aim_A
3ljb_A
3ljb_B

Saccharide display (Glycoblocks)

- Visual style useful for comparing positions/orientations of (poly-)sacchardides in multiple coordinate files in a way which is easy to visualize.
- 3D equivalent of conventional 2D glycosolation trees with “standard” symbols and colours representing the different sugar types.
- Would be nice to do the same in 3D using same symbols.
- Work done with Jon Agirre, University of York.

Saccharide display

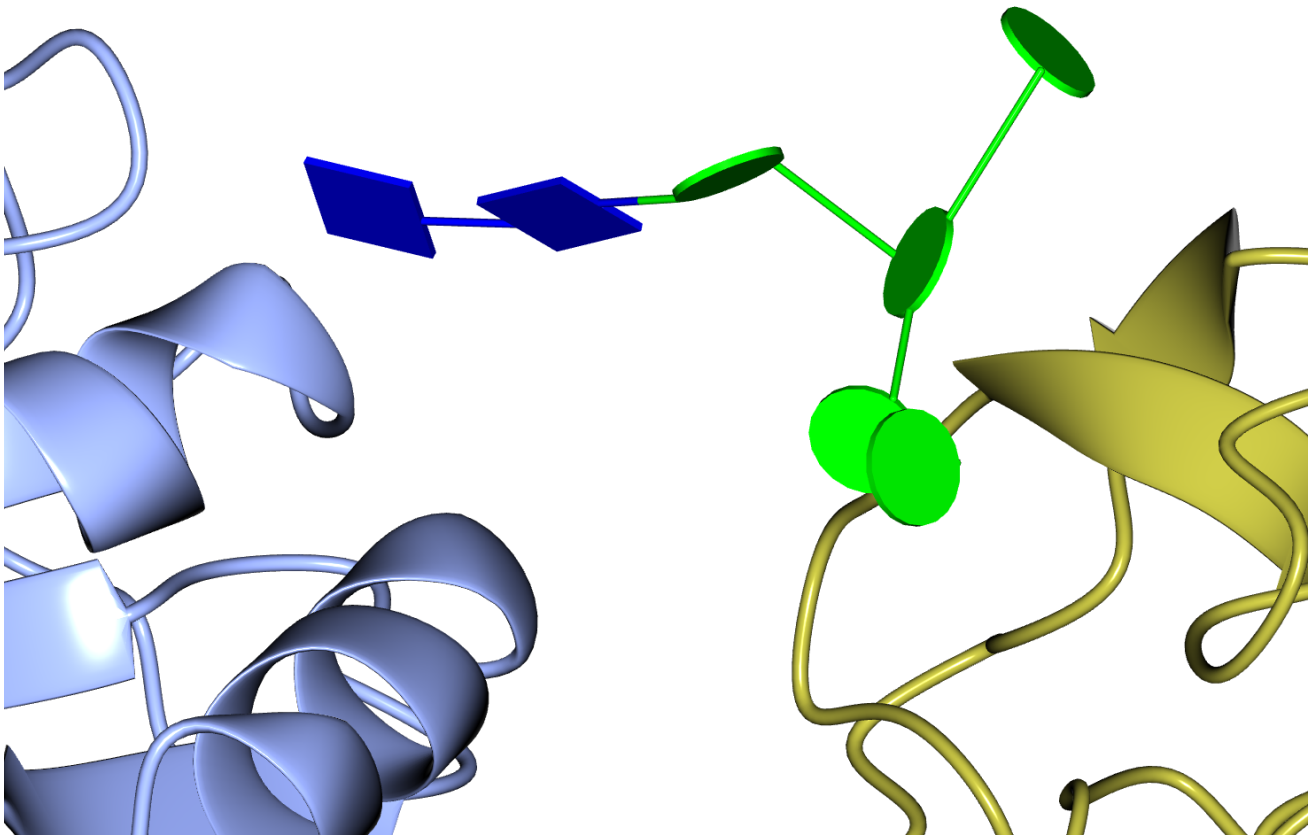


N-linked glycosylation

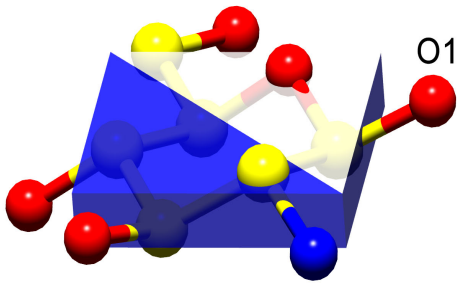
O-linked glycosylation

S-linked glycosylation

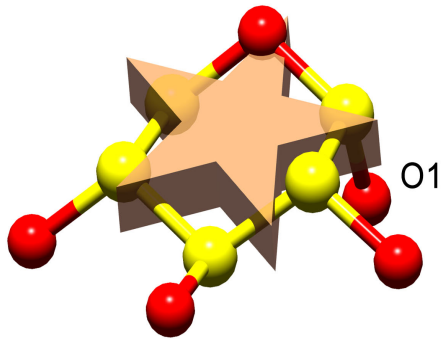
Saccharide display



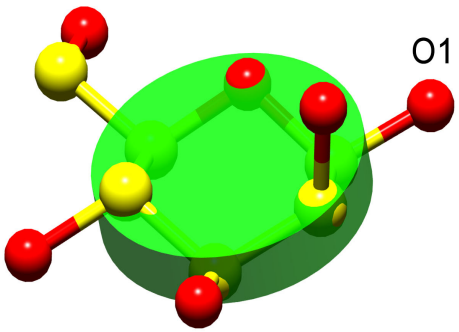
Saccharide display



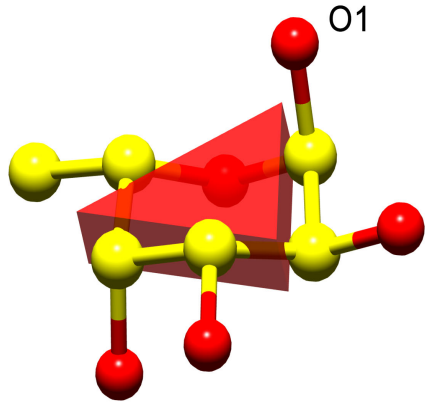
β-D-Glucosamine
(GCS)



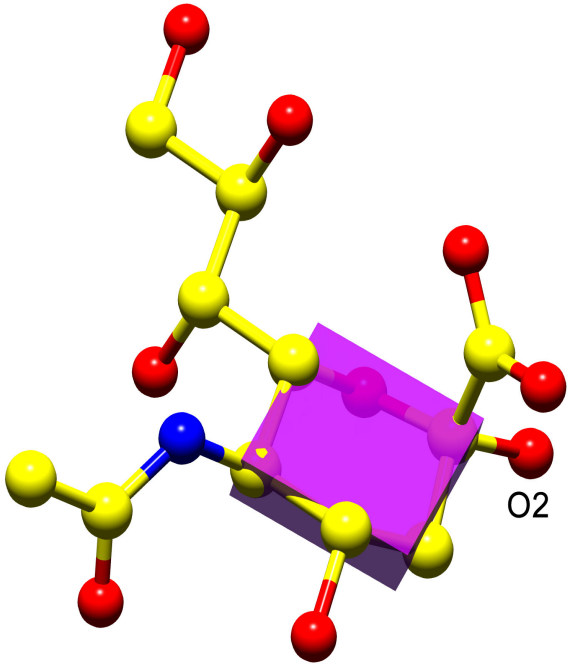
α-D-Xylopyranose
(XYS)



β-D-Mannose
(BMA)

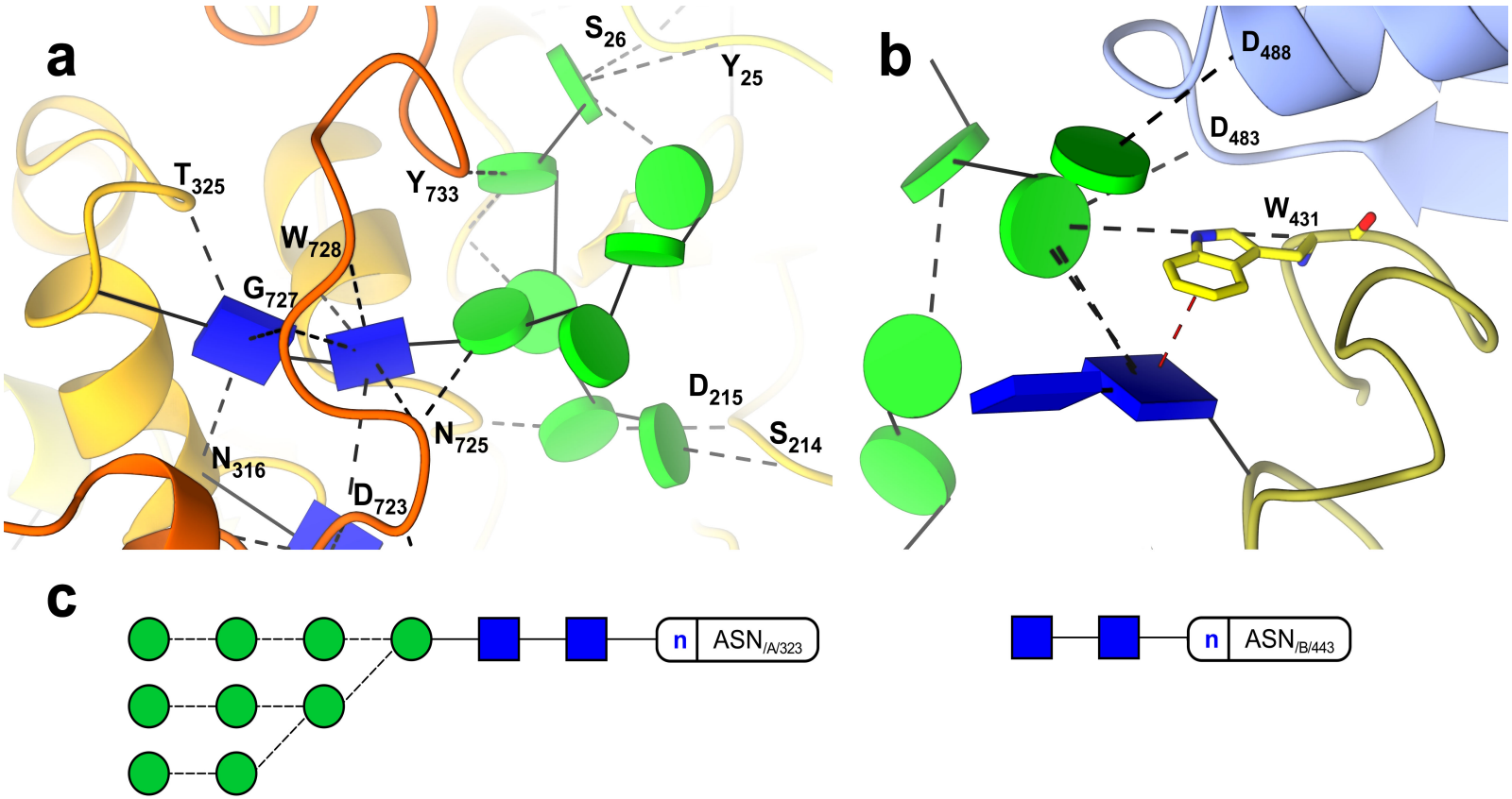


α-L-Fucose
(FUC)



N-acetyl α-L-Neuraminic Acid
(SIA)

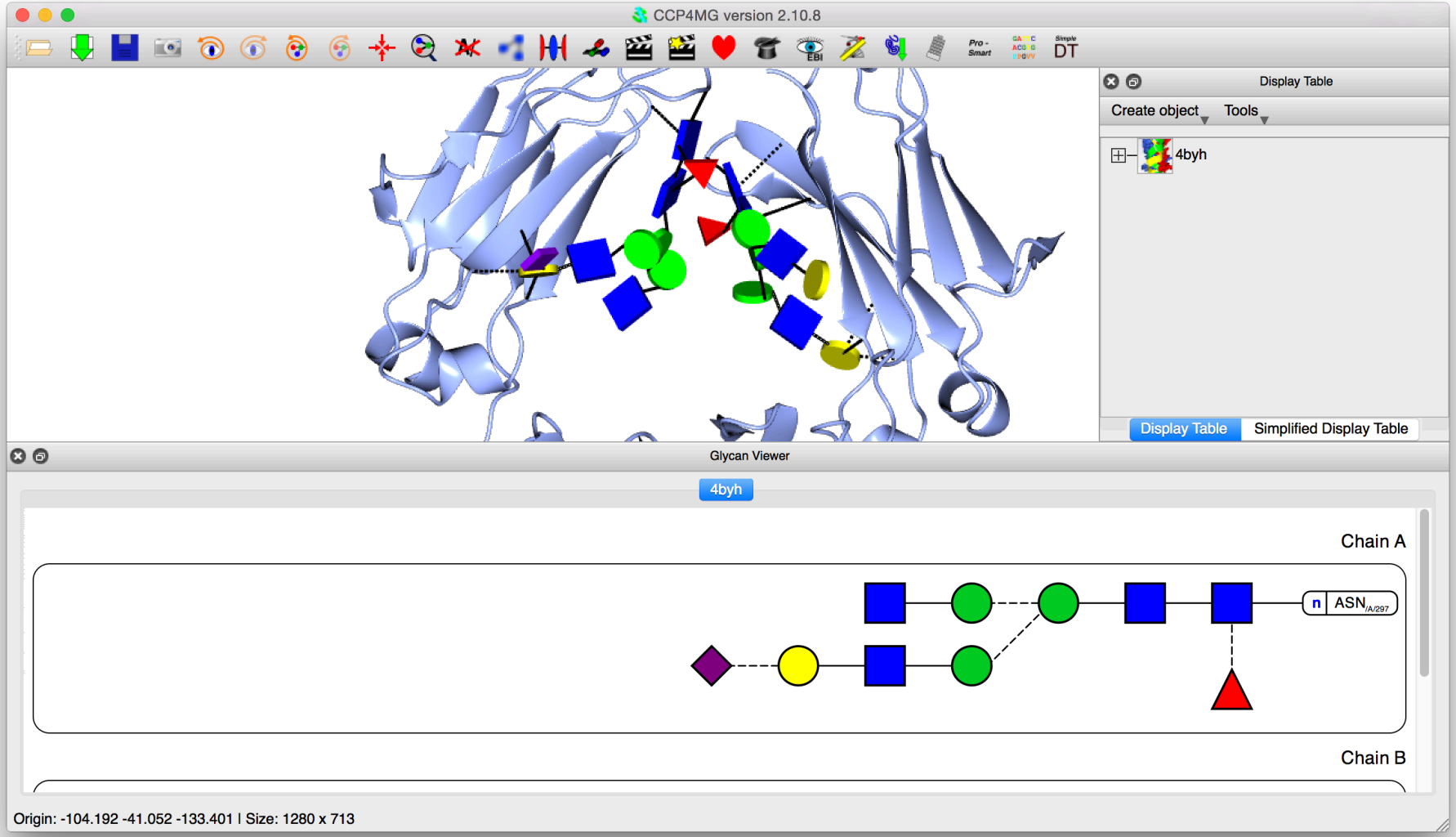
Saccharide display



Hydrogen bonds to multiple domains. GlcNAc to TRP stacking interaction.

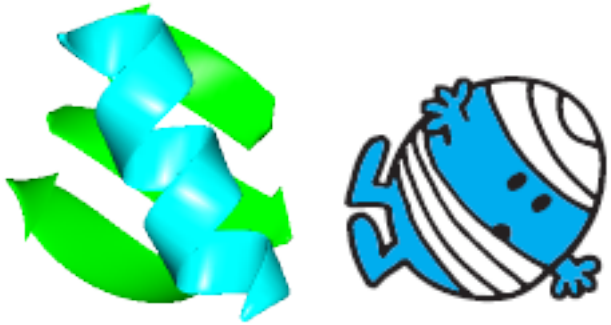
5FJJ, Agirre et. al., *Acta Crystallogr D Struct Biol* **72**, 254-265 (2016)

Glycan Viewer



2D representations generated by Privateer, Jon Agirre and Kevin Cowtan.

CCP4MG / MrBUMP



MrBUMP

- MrBUMP is an automated scheme for Molecular Replacement. Given a target sequence and experimental structure factors, it will search for homologous structures, create a set of suitable search models from the template structures, do molecular replacement, and test the solutions with some rounds of restrained refinement.
- A component of the CCP4 suite of programs.
- **MrBUMP: an automated pipeline for molecular replacement**, Keegan, RM and Winn, MD, *Acta Crystallogr. D Biol Crystallogr. 2008; 64, pp 119-124*

CCP4MG and MrBUMP

- Goal is to provide i2 users with a graphical driven interface to the model search and preparation steps for molecular replacement in MrBUMP. The intention is to derive a graphically-informed single “best” search model for passing back to i2 and the Phaser/Molrep interfaces

CCP4MG and MrBUMP

- CCP4MG uses initial steps of the MrBUMP to interactively edit molecular replacement models.
- Scheme:
  - MrBUMP is sent a sequence from CCP4MG
  - uses the phmmer tool to search for homologous structures with a maximum similarity between them of 100%, 95%, 90%, 70% or 50%.
  - select just the relevant chains from the structures.
  - prune side chains.
  - structurally align the pruned structures (gesamt).
  - CCP4MG loads the structures and shows a MrBump results window.

CCP4MG and MrBUMP

- Then CCP4MG can be used to select subsets of atoms from the newly loaded structures:
  - Completely hide some structures.
  - Select e.g. just alpha-helices
  - Prune terminating loops.
  - Whatever … (including “gesamt variance slider”).
- And then everything visible can be saved into one ensemble coordinate file for use in a molecular replacement calculation.

CCP4-7.1.000 Project Viewer: NewMenuTest

Task menu | Export project | Run | Run on server | Clone | Help | Bibliography | Export MTZ | Show log file

Job list | Project directory

Filter: Only show jobs containing text typed here

Job/File	Evaluation
10 CCP4mg MrBUMP	
9 CCP4mg MrBUMP	
8 BUCCANEER	R=0.25 %=
7 REFMAC5	
6 REFMAC5	R=0.23 RF
5 Define crystal contents	
4 MOLREP	R=0.24 RF
3 Data reduction	Sgp=P 21
2 Data reduction	Sgp=P 21
1 Data reduction	Sgp=P 21

Filter: Only show tasks containing text typed here

- **Import merged data, crystal contents, alignments or coordinates**
- **Integrate X-ray images**
- **X-ray data reduction and analysis**
- **Experimental phasing**
- **Bioinformatics including model preparation for Molecular Replacement**
  - **Interactive model preparation - CCP4mg and MrBUMP**
    Identify MR models with MrBUMP, display and select with CCP4mg
  - **Interactive selection of MR model components - CCP4mg**
    Use CCP4mg to select components of a search model and output to i2 for MR
  - **Truncate search model - CHAINSAW**
    Truncate and renumber model prior to molecular replacement
  - **Truncate search model - SCULPTOR**
    Truncate model prior to molecular replacement
  - **Build an ensemble for PHASER**
    Compile assorted related structures into an ensemble for use in PHASER
  - **Align sequences - CLUSTALW**
    Align sequences using clustalw
- **Molecular Replacement**
- **Density modification**
- **Model building and Graphics**
- **Refinement**

New job | Cancel

CCP4-7.1.000 Project Viewer: NewMenuTest

Task menu | Export project | Run | Run on server | Clone | Help | Bibliography | Export MTZ | Show log file

Job list | Project directory

Filter: Only show jobs containing text typed here

Job/File	Evaluation
10 CCP4mg MrBUMP	
9 CCP4mg MrBUMP	
8 BUCCANEER	R=0.25 %=
7 REFMAC5	
6 REFMAC5	R=0.23 RF
5 Define crystal contents	
4 MOLREP	R=0.24 RF
3 Data reduction	Sgp=P 21
2 Data reduction	Sgp=P 21
1 Data reduction	Sgp=P 21

Job 10: Interactive model preparation - CCP4mg and MrBUMP The job is Pending

Input | Results | Comments

Input data

Job title: CCP4mg MrBUMP

Use data from job: 1 Data reduction - AIMLESS as inpu

Sequences from crystal content:

Crystal contents: 5 Asu content file from Define crystal contents

Specify crystal contents

Select one sequence

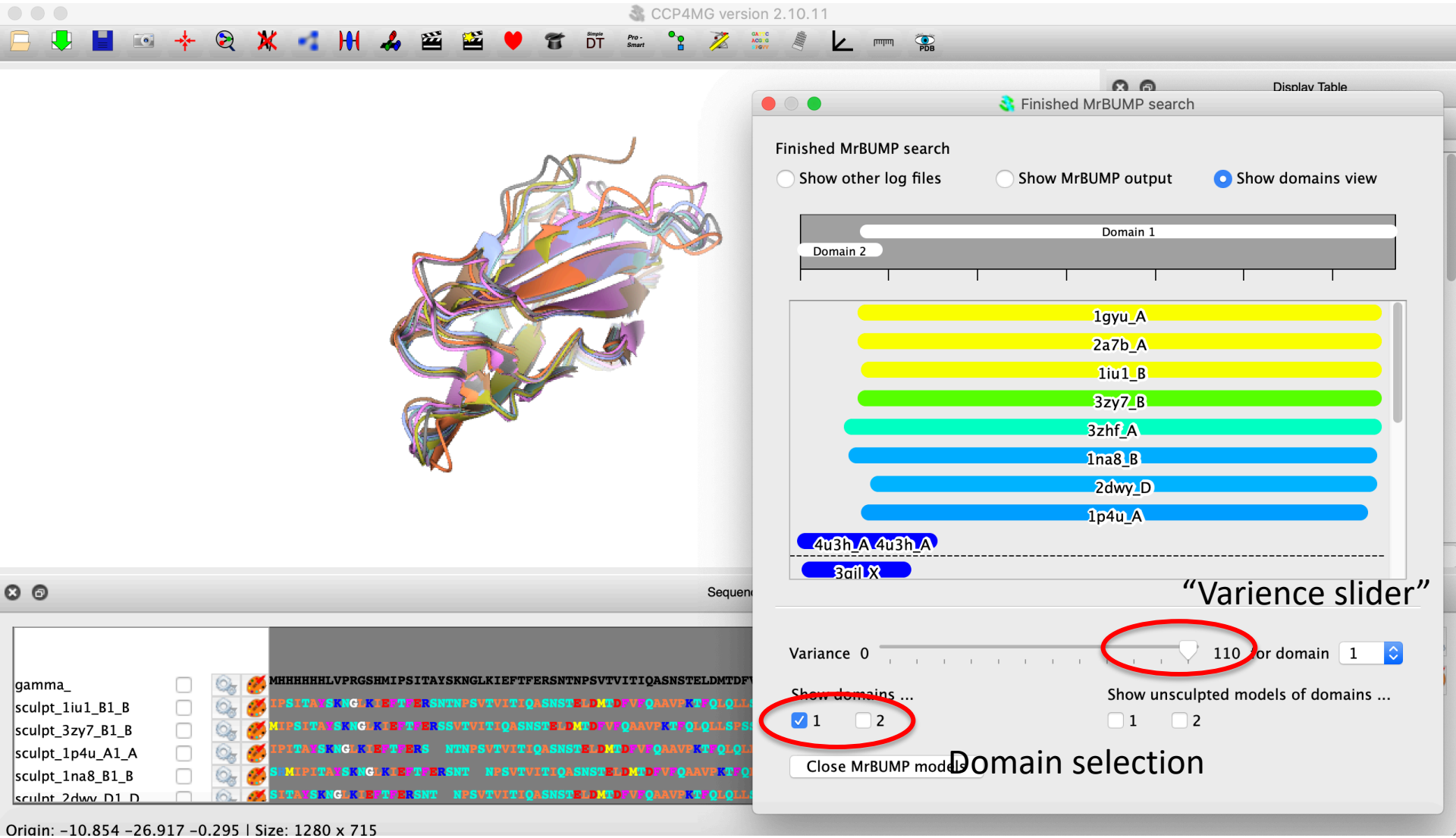
gamma

Non-redundancy level for homologue search:

95

Cutoff threshold for phmmer results:

20


CCP4MG version 2.10.11
Finished MrBUMP search
Finished MrBUMP search
Show other log files
Show MrBUMP output
Show domains view
Domain 1
Domain 2
1gyu_A
2a7b_A
1iu1_B
3zy7_B
3zhf_A
1na8_B
2dwy_D
1p4u_A
4u3h_A 4u3h_A
3qil_X
"Varience slider"
Variance 0
110
or domain
1
Show domains ...
1
2
Show unsculpted models of domains ...
1
2
Close MrBUMP models
Domain selection
gamma_
sculpt_1iu1_B1_B
sculpt_3zy7_B1_B
sculpt_1p4u_A1_A
sculpt_1na8_B1_B
Origin: -10.854 -26.917 -0.295 | Size: 1280 x 715

QtMG File Edit View Display Applications Windows Tools Help CCP4i2 100% Thu 14:19

CCP4MG version 2.10.5

- Open.. ⌘O
- Recent files ▶
- Download coordinates..
- Download Structure Factors..
- Download electron density
- Download PDB_REDO data
- Edit/show presentation ▶
- Close all data
- Get tutorial data
- Save status to file.. ⇧⌘S
- Save as default status.. ⌘S
- Save all visible to file..
- Screenshot
- Print screen.. ⌘P
- Save Archive
- Render
- Save all visible to ccp4i2 database

Simplified Display Table

	R	L	Nb	W	Su	BS	MS	NA	M	G	B
All											
scul											
scul											
scul											
scul											
scul											
scul											
scul											
scul											
scul											
scul											

Help

Display Table | Simplified Display Table

Sequence Viewer

```
unkgamma_        MHHHHHHLVPRGSHMIPSITAYSKNGLKIEFTFERSNTNPSVTVITIQASNSTELDMTDFVFQAAVPKTFQLQLLSPSSSVVPAFNTGTITQVIKVLNPQKQQLRMRIKLTYNHKGSAMQDLAEV
sculpt_1gyu_A_A  -------------MIPSITAYSKNGLKIEFTFERSNTNPSVTVITIQASNSTELDMTDFVFQAAVPKTFQLQLLSPSSSVVPAFNTGTITQVIKVLNPQKQQLRMRIKLTYNHKGSAMQDLAEV
sculpt_1iu1_A_A  -------------MIPSITAYSKNGLKIEFTFERSNTNPSVTVITIQASNSTELDMTDFVFQAAVPKTFQLQLLSPSSSVVPAFNTGTITQVIKVLNPQKQQLRMRIKLTYNHKGSAMQDLAEV
sculpt_1iur_A_A  MHHHHHHLVPRGS----------------------------TVITIQASNS---------------KTFQLQLLSPSSSVVPAFNTGTITQVIKVLNPQKQ------------KGS--------
sculpt_1p4u_A_A  ----MHHHVPRGSHMIPSITAYSKNGLKIEFTFERSNTNPSVTVITIQASNSTELDMTDFVFQAAVPKTFQLQLLSPSSSVVPAFNTGTITQVIKVLNPQKQQLRMRIKLTYNHKGSAMQDLAEV
sculpt_2lxe_A_A  MHHHHHHLVPRGSHM--------------------------VTVITIQASNSTELDMTDFVFQAAVPKTFQLQLLSPSSS-VPAFNTGTITQVIKVLNPQKQI-----KLTYNHKGS--------
```

Origin: -21.235 -21.956 -16.522 | Size: 1162 x 714

Other details

- Only final ensemble (or individual structures) are saved to i2 database. All MrBUMP results and model are save in ~/.CCP4MG/mrbump_results.
- Results from previous jobs can be loaded in later sessions without having to rerun the MrBUMP search.
- Results can be deleted when no longer of interest.

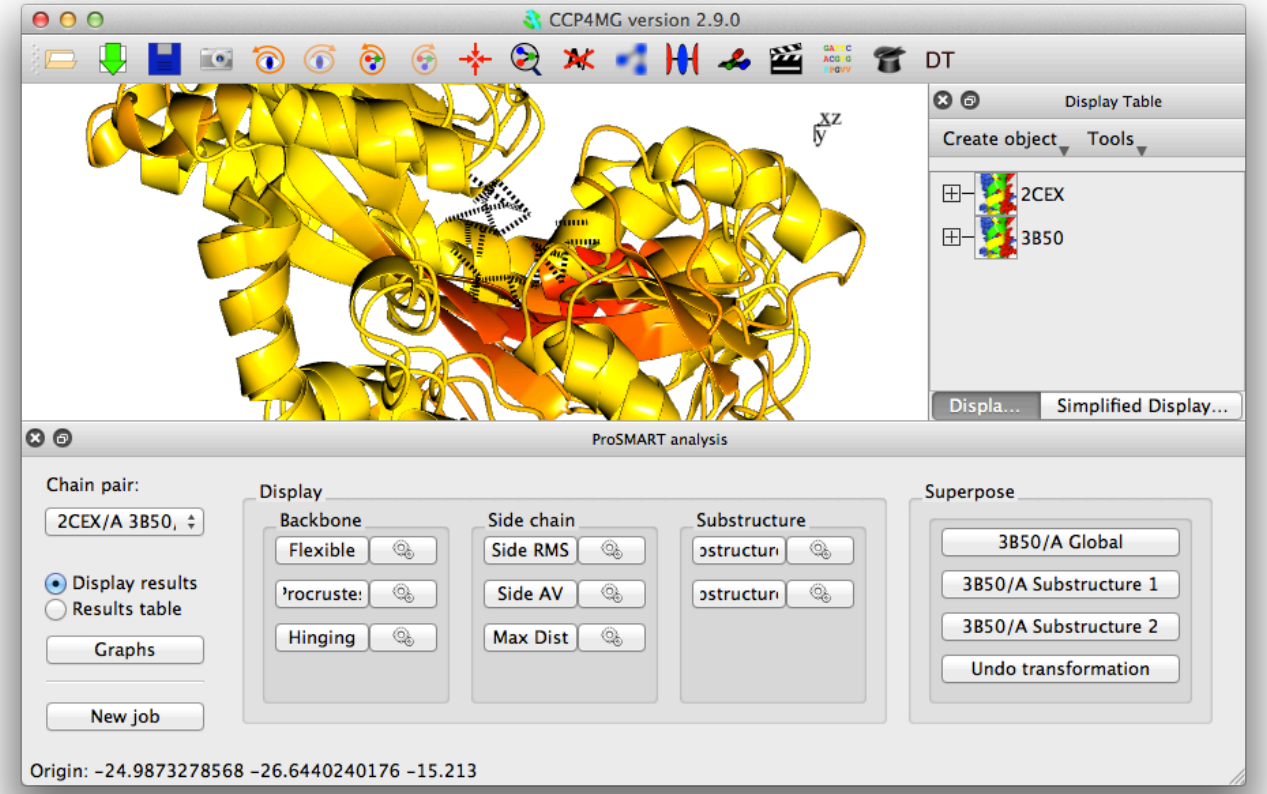
ProSMART

- ProSMART (Procrustes Structural Matching Alignment and Restraint Tool) is a software tool designed for the conformation-independent structural comparison of protein chains. At current, ProSMART has two components:
- ProSMART ALIGN - for the alignment, superposition, and scoring of protein chains;
- ProSMART RESTRAIN - for the generation of external restraints for use in the crystallographic refinement of protein structures.
- http://www2.mrc-lmb.cam.ac.uk/groups/murshudov/content/prosmart/documentation.html#summary

  http://www2.mrc-lmb.cam.ac.uk/groups/murshudov/content/prosmart/docs/rob_nicholls_thesis.pdf

ProSMART interface

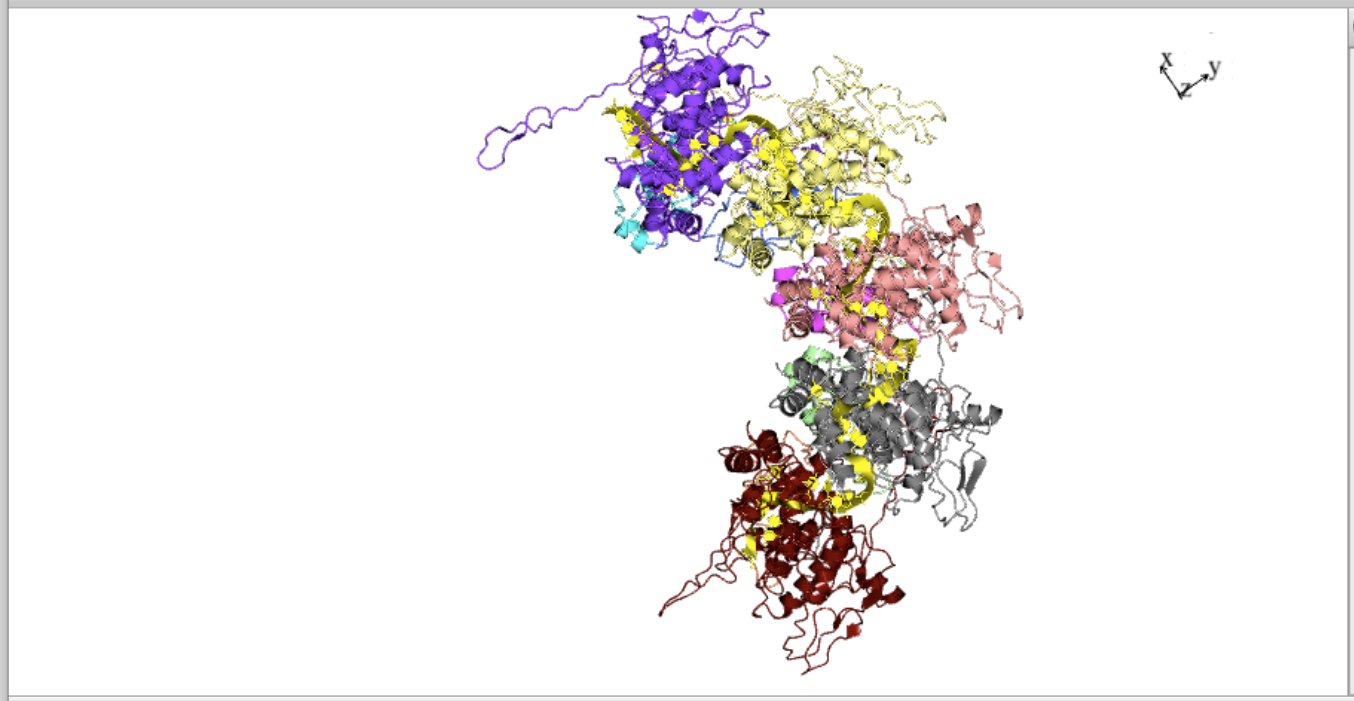
- ProSMART interface is a simple “push button to see stuff”.



PISA

- There is a command line version of PISA to which CCP4MG has an interface.
- One can simply ask PISA to analyse a structure
- Interfaces and assemblies may be visualized from the results.

CCP4MG version 2.5.2



Display Table

3lel_10

A/ o..	By c..	Ribb..
All ..	By c..	Ribb..
Bases	By c..	Cyli..
All ..	By c..	Nucl..
Metals	Atom..	Sphe..

3hhz

A/ o..	By c..	Ribb..
All ..	By c..	Ribb..
Bases	By c..	Cyli..
All ..	By c..	Nucl..
All ..	Atom..	Bonds

Pisa structure analysis 3hhz

Analyse model: 3hhz

monomers | interfaces | assemblies

Set	No	Size	Id	ASA	BSA	DGdiss	Formula
1	1	22	0	216014.0	104815.0	195.7	A(10)B(10)C(2)
2	2	12	1	190285.0	78373.0	193.6	A(10)B(2)
	3	1	2	5747.5	0.0	-0.0	A
	4	1	2	4956.9	0.0	-0.0	A

Close

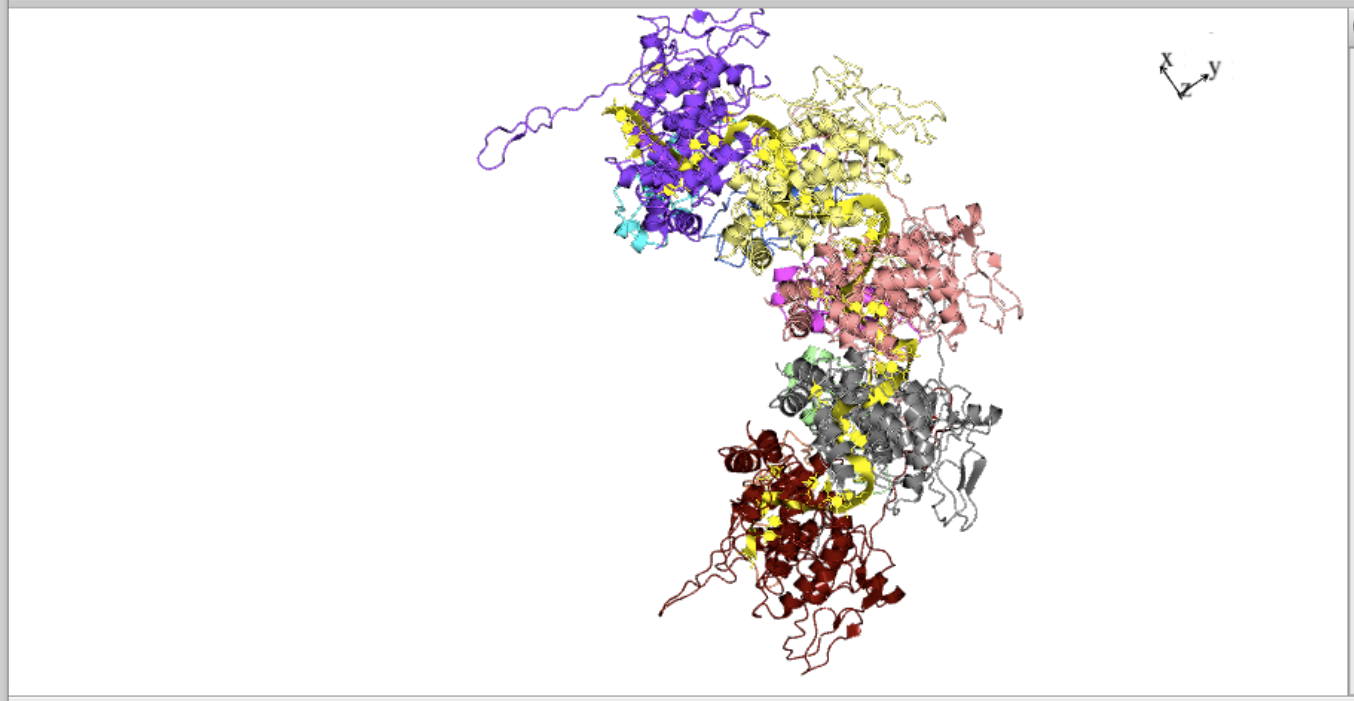
Analyse structure

Show

Clear display

Help

CCP4MG version 2.5.2



Display Table

3lel_10

A/ o..	By c..	Ribb..
All ..	By c..	Ribb..
Bases	By c..	Cyli..
All ..	By c..	Nucl..
Metals	Atom..	Sphe..

3hhz

A/ o..	By c..	Ribb..
All ..	By c..	Ribb..
Bases	By c..	Cyli..
All ..	By c..	Nucl..
All ..	Atom..	Bonds

Pisa structure analysis 3hhz

Analyse model: 3hhz

monomers | interfaces | assemblies

Set	No	Size	Id	ASA	BSA	DGdiss	Formula
1	1	22	0	216014.0	104815.0	195.7	A(10)B(10)C(2)
2	2	12	1	190285.0	78373.0	193.6	A(10)B(2)
	3	1	2	5747.5	0.0	-0.0	A
	4	1	2	4956.9	0.0	-0.0	A

Close

Analyse structure

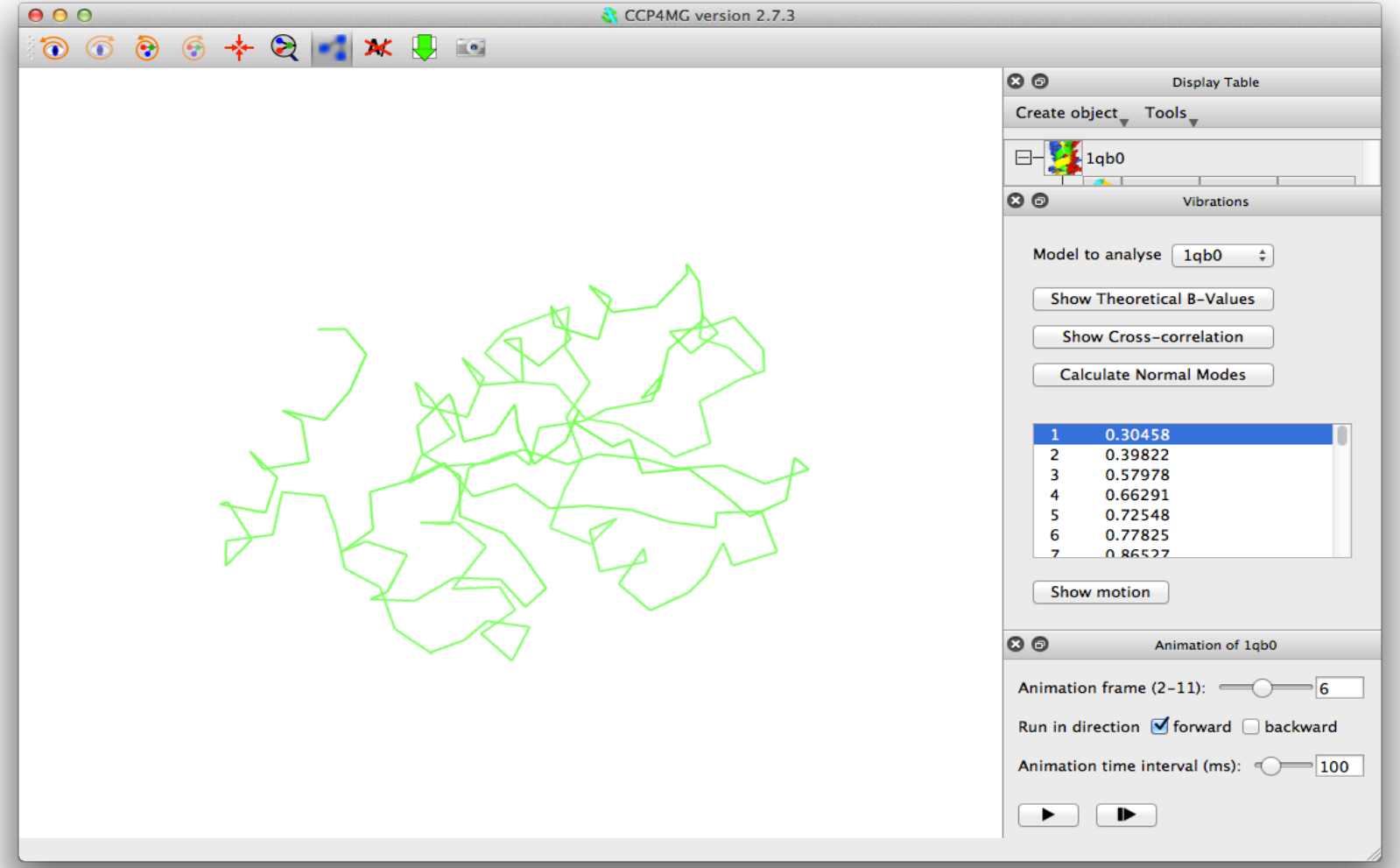
Show

Clear display

Help

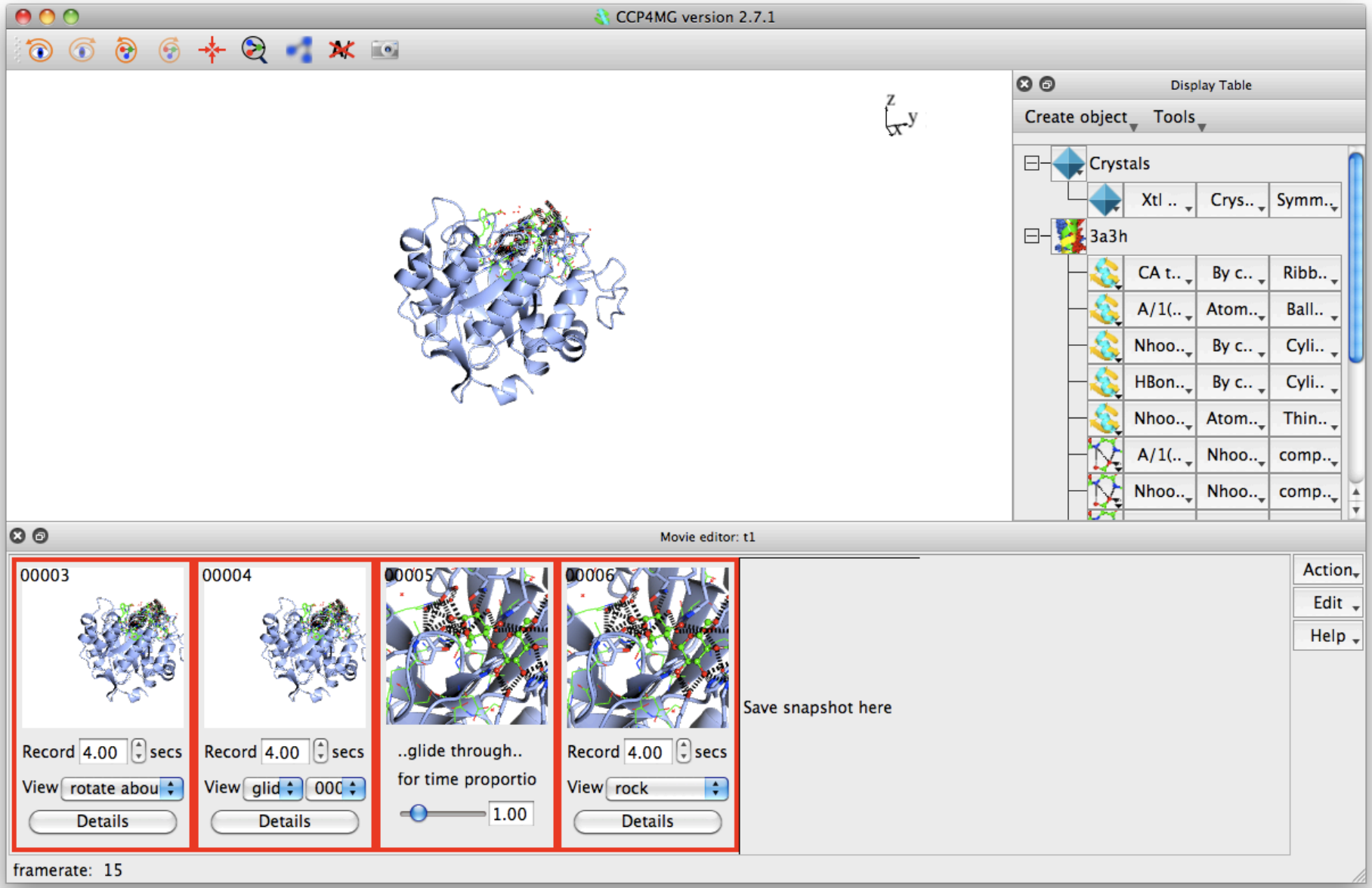
Normal Modes

- Simple approximate elastic network model.



Movies

- Movies are creates by defining a series of “key frames” and then (optionally) interpolating between them.
- Key frames may also define simple transformations (rock, roll, etc.)
- Movies can be created either as animated gifs or as MPEG streams.


CCP4MG version 2.7.1
Display Table
Create object
Tools
Crystals
Xtl ..
Crys..
Symm..
3a3h
CA t..
By c..
Ribb..
A/1(..
Atom..
Ball..
Nhoo..
By c..
Cyli..
HBon..
By c..
Cyli..
Nhoo..
Atom..
Thin..
A/1(..
Nhoo..
comp..
Nhoo..
Nhoo..
comp..
Movie editor: t1
00003
Record 4.00 secs
View rotate abou
Details
00004
Record 4.00 secs
View glid 000
Details
00005
..glide through..
for time proportio
1.00
00006
Record 4.00 secs
View rock
Details
Save snapshot here
Action
Edit
Help
framerate: 15

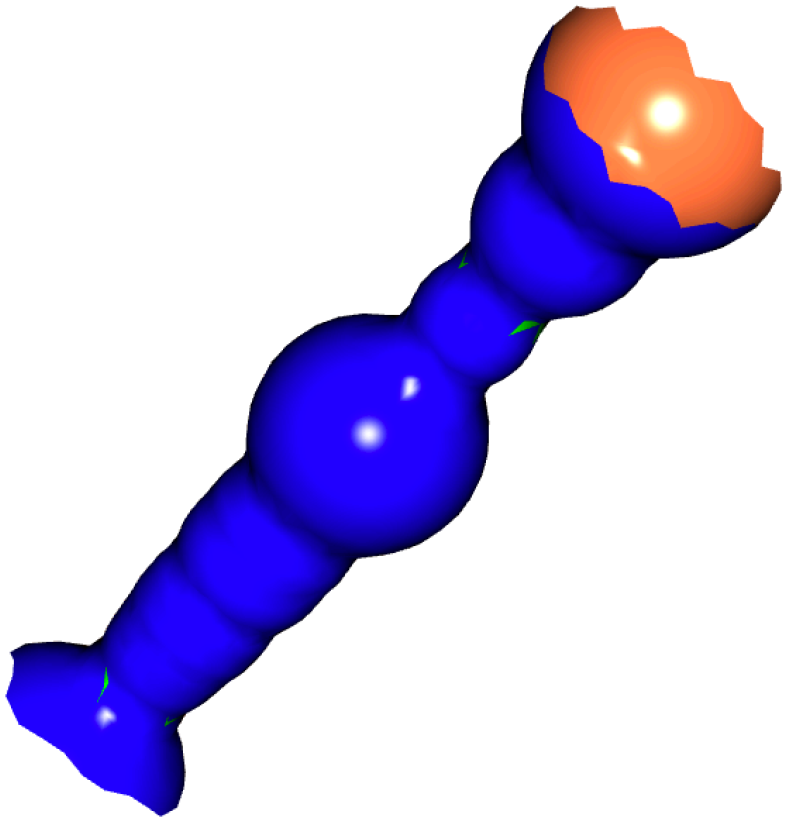
Getting CCP4MG

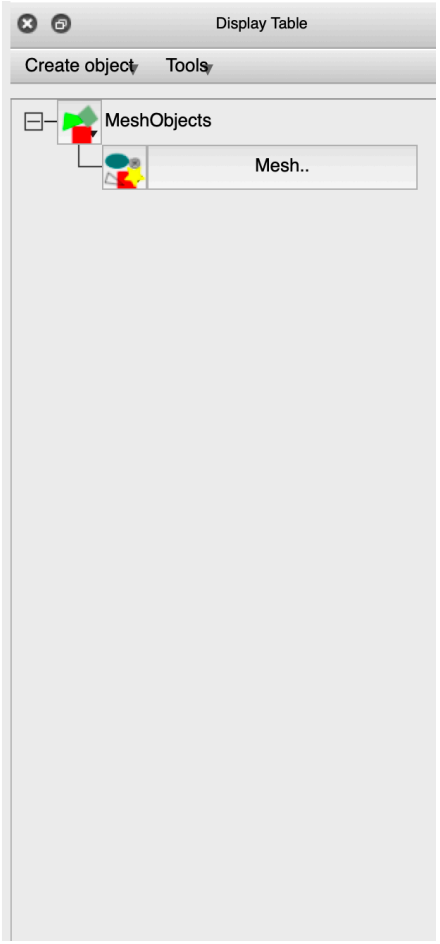
- Distributed with the CCP4 Suite (except for software to compile movies) : http://www.ccp4.ac.uk
- “Standalone” versions (including movie software *ffmpeg*): http://www.ccp4.ac.uk/MG
- Current version 2.10.11 (Nov 2019).

New in 2.10.11 (Nov 2019)

- Shadows work on most Linux and Windows computers now.
- Perfect spheres work on most Linux and Windows computers now.
- Can download multiple comma-separated PDB ids at once.
- Updates to make multiple domains easier to view in MrBUMP module.
- Workaround crash with some PDB files.
- HOLE surface visualisation.
- Download from PDB-REDO server fixed.
- Various bug fixes.

Hole





Display the “VMD format” meshes produced by the HOLE program (Oliver Smart) for visualising ion channels in molecular structure.

www.holeprogram.org

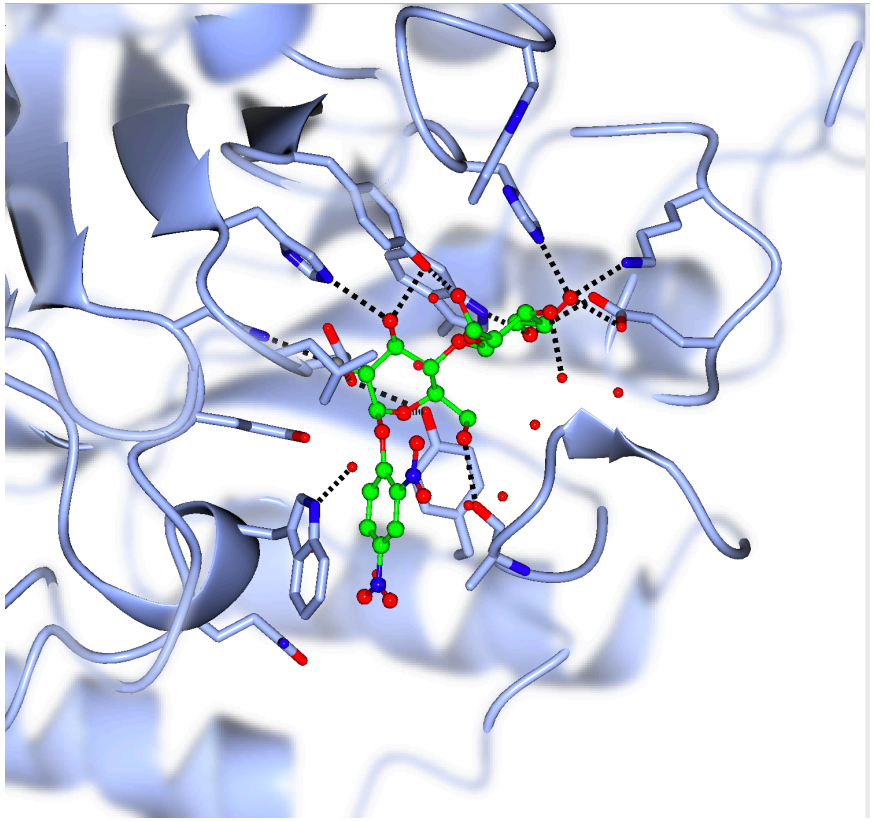
Not in current CCP4 release – will be in CCP4 7.1/CCP4MG 2.10.11

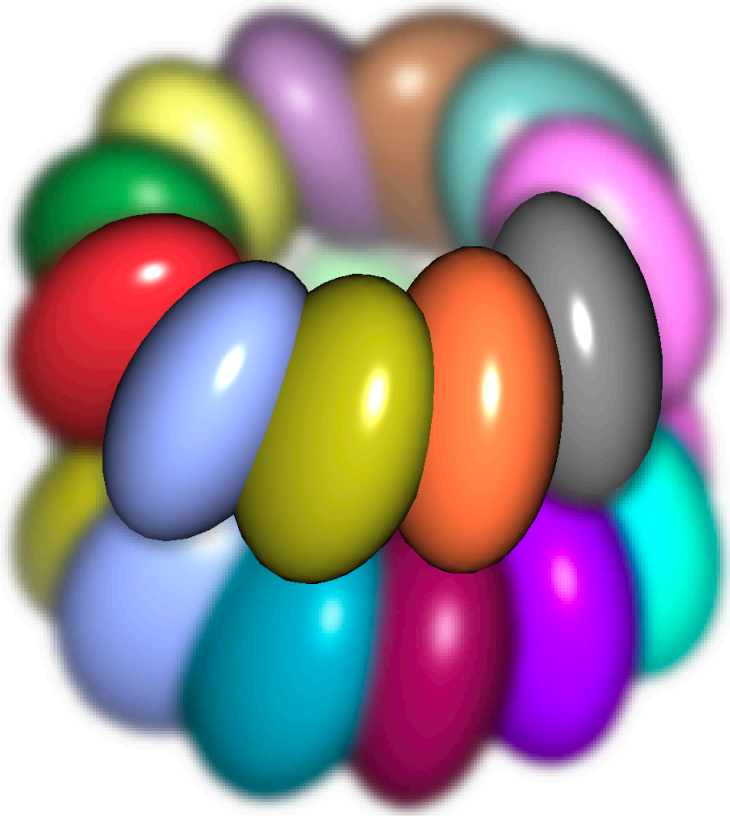
Coming soon

Coming soon

- Python 3/Qt5/OpenGL3 (technical), but will enable
  - Better transparency
  - Depth blurring
  - Glassy objects

Depth blur





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