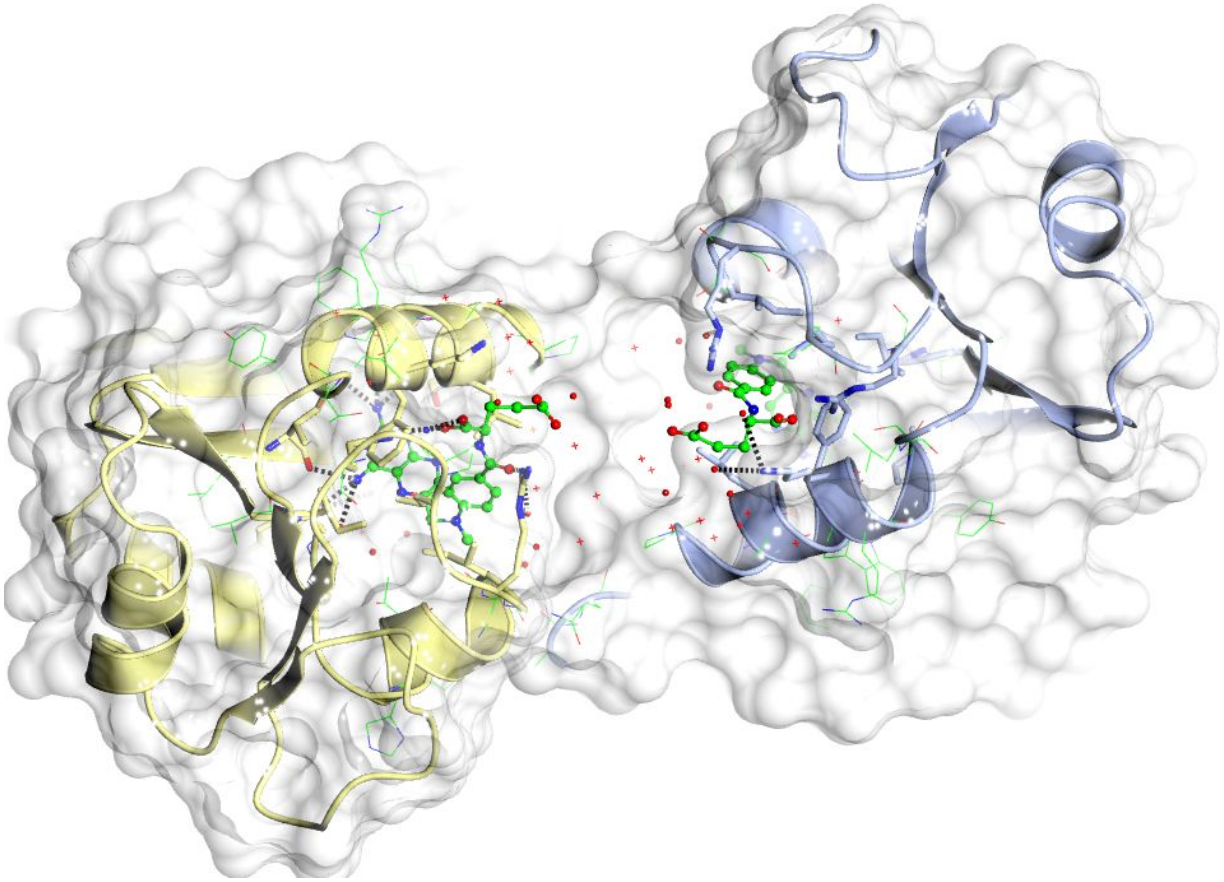
# CCP4MG



Diamond/CCP4 workshop 2023

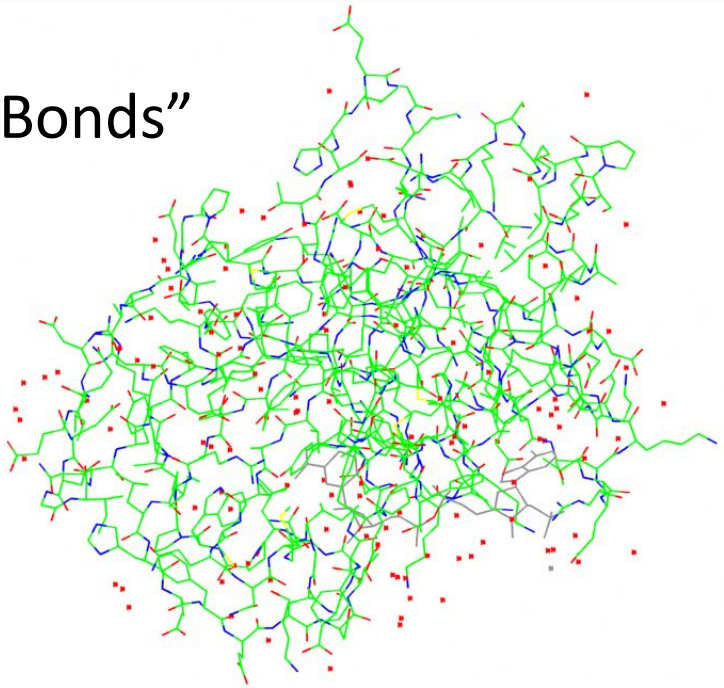
# Introduction

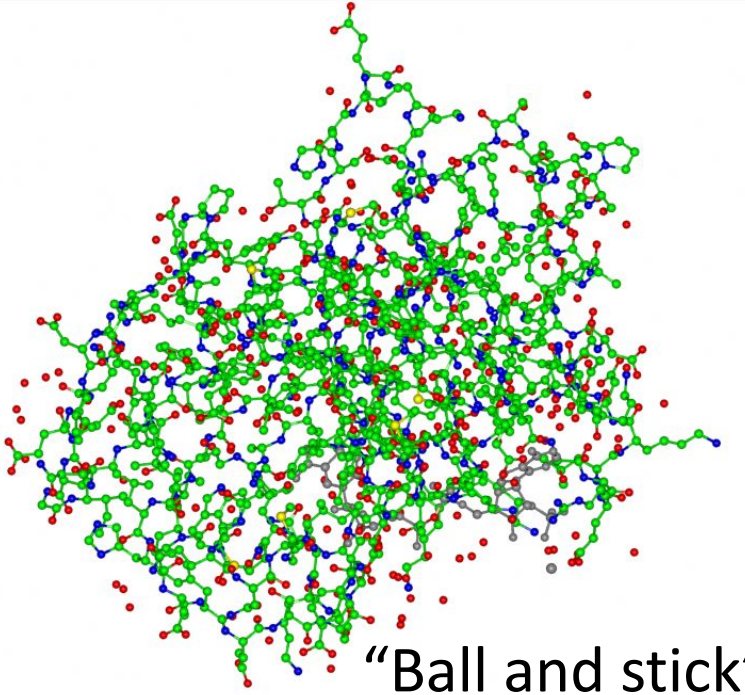
- CCP4MG is a molecular graphics program funded by CCP4.
- Its primary focus is the visualization and analysis of macromolecular structure.
- It produces high quality rendered images and movies.
- http://legacy.ccp4.ac.uk/MG/
  - Binaries for Windows, Mac and Linux.

# 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

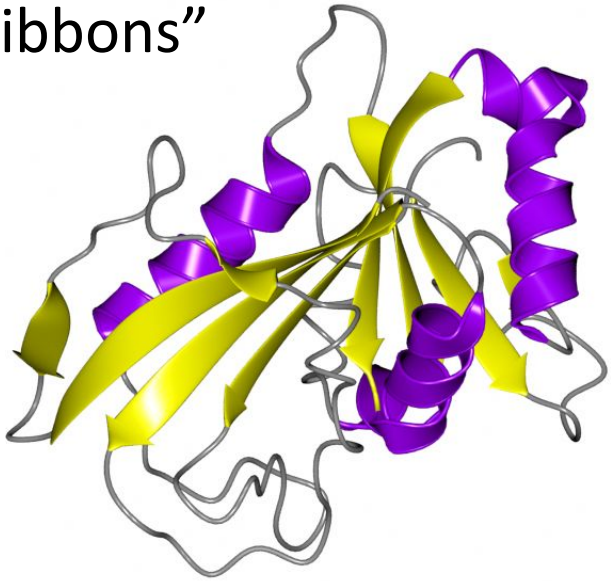
“Bonds”

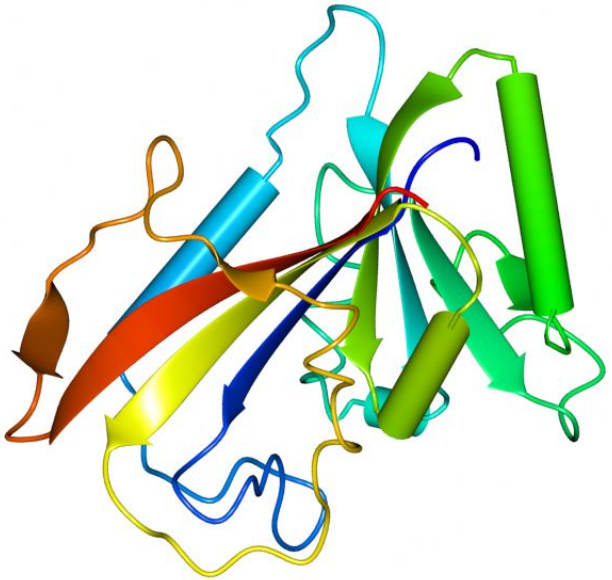




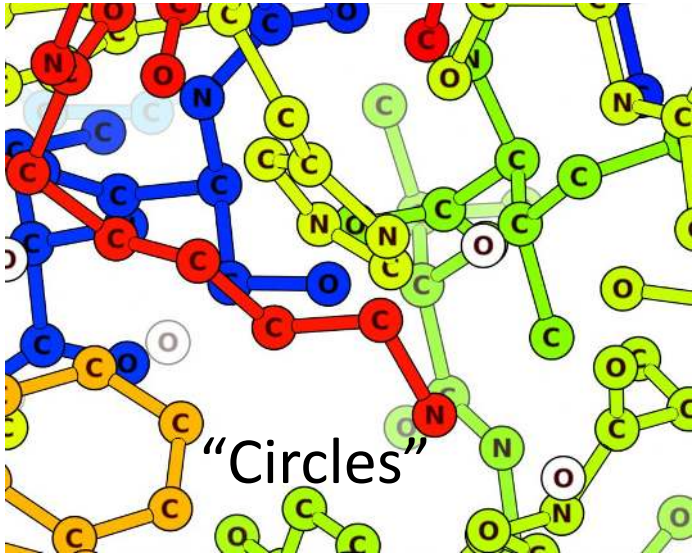
“Ball and stick”

“Ribbons”



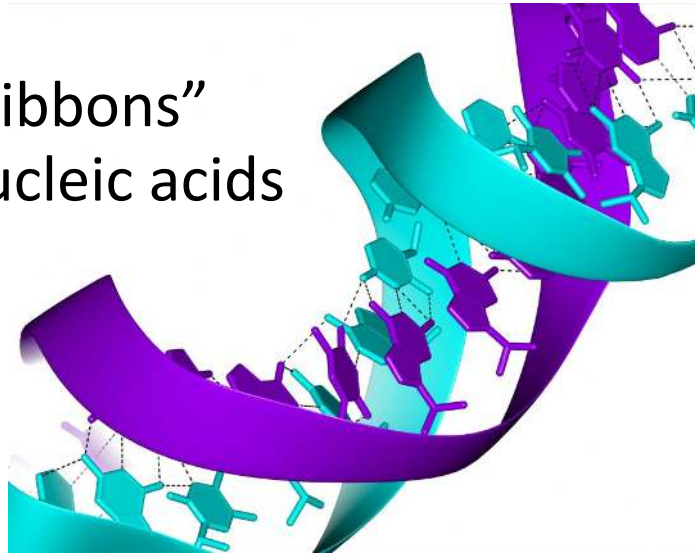


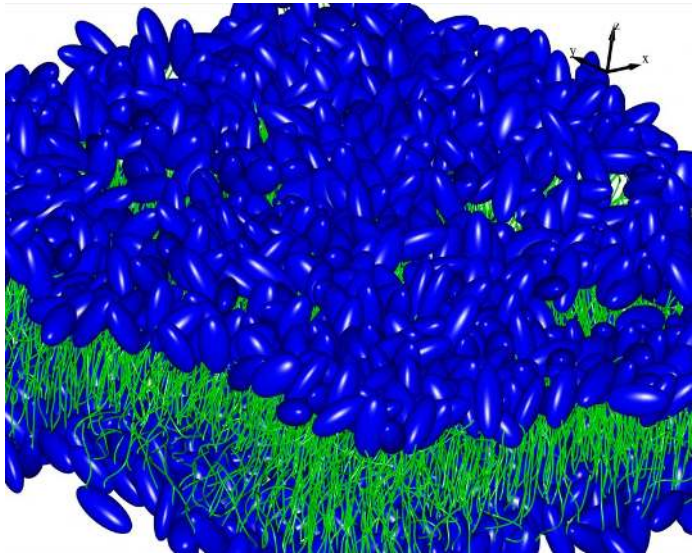
“Worms/tubes”



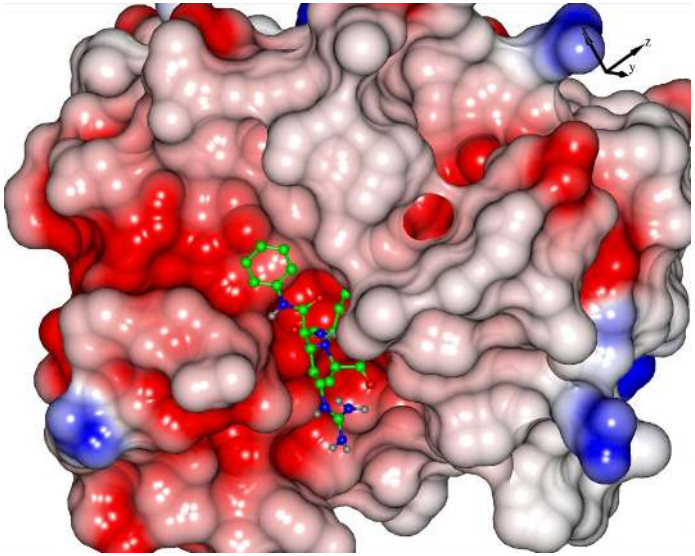
"Circles"

"Ribbons"
Nucleic acids

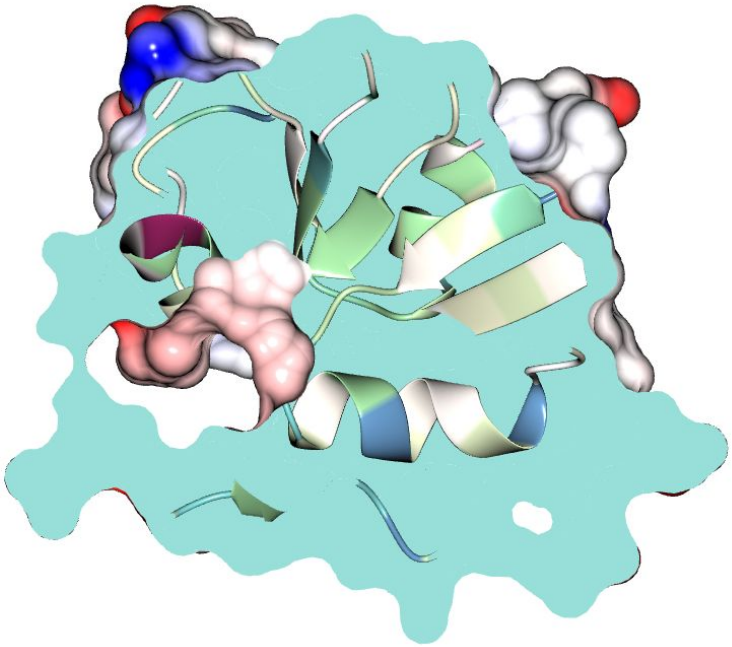


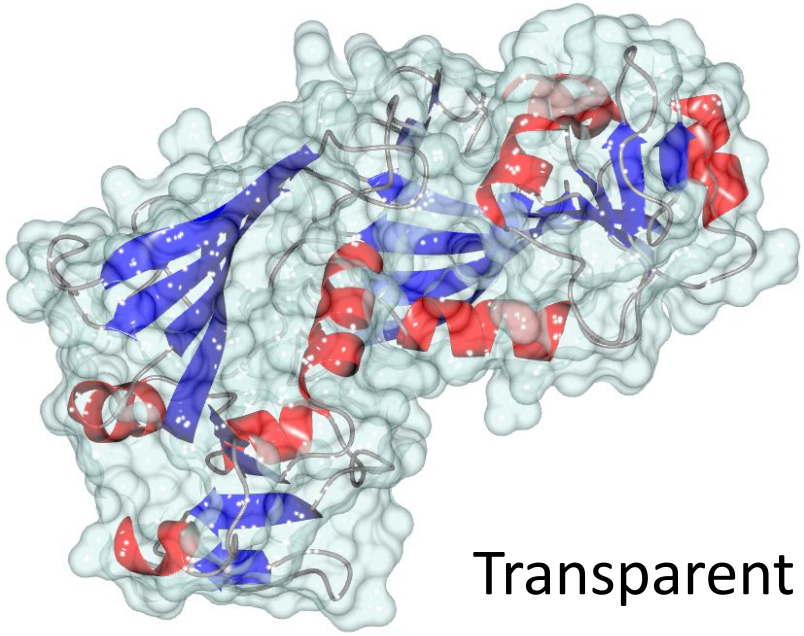


"Lipid Cartoon"



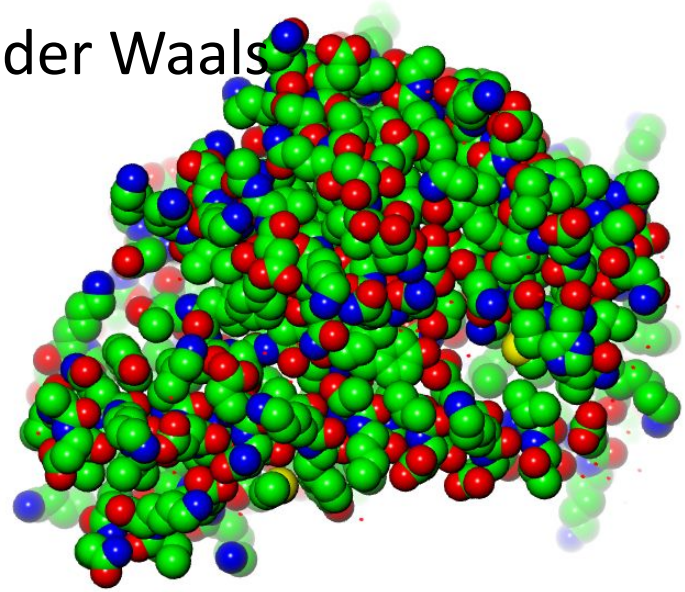
Electrostatic surface

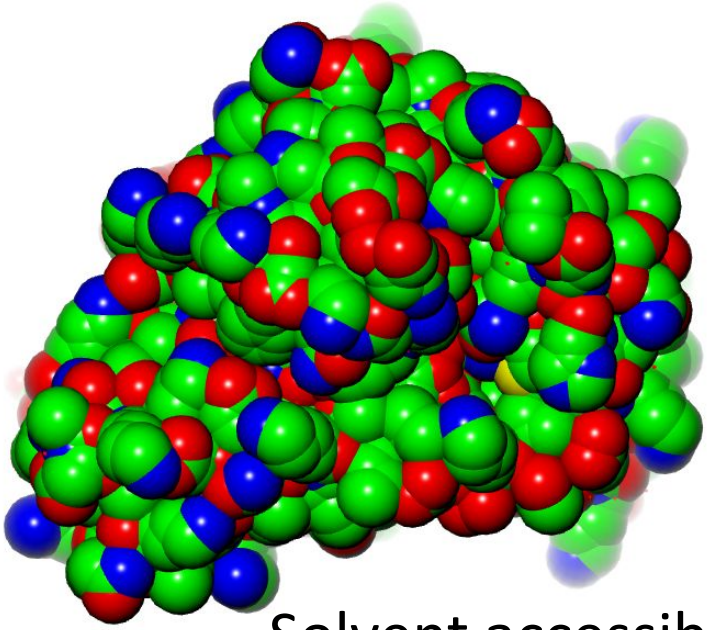




Transparent

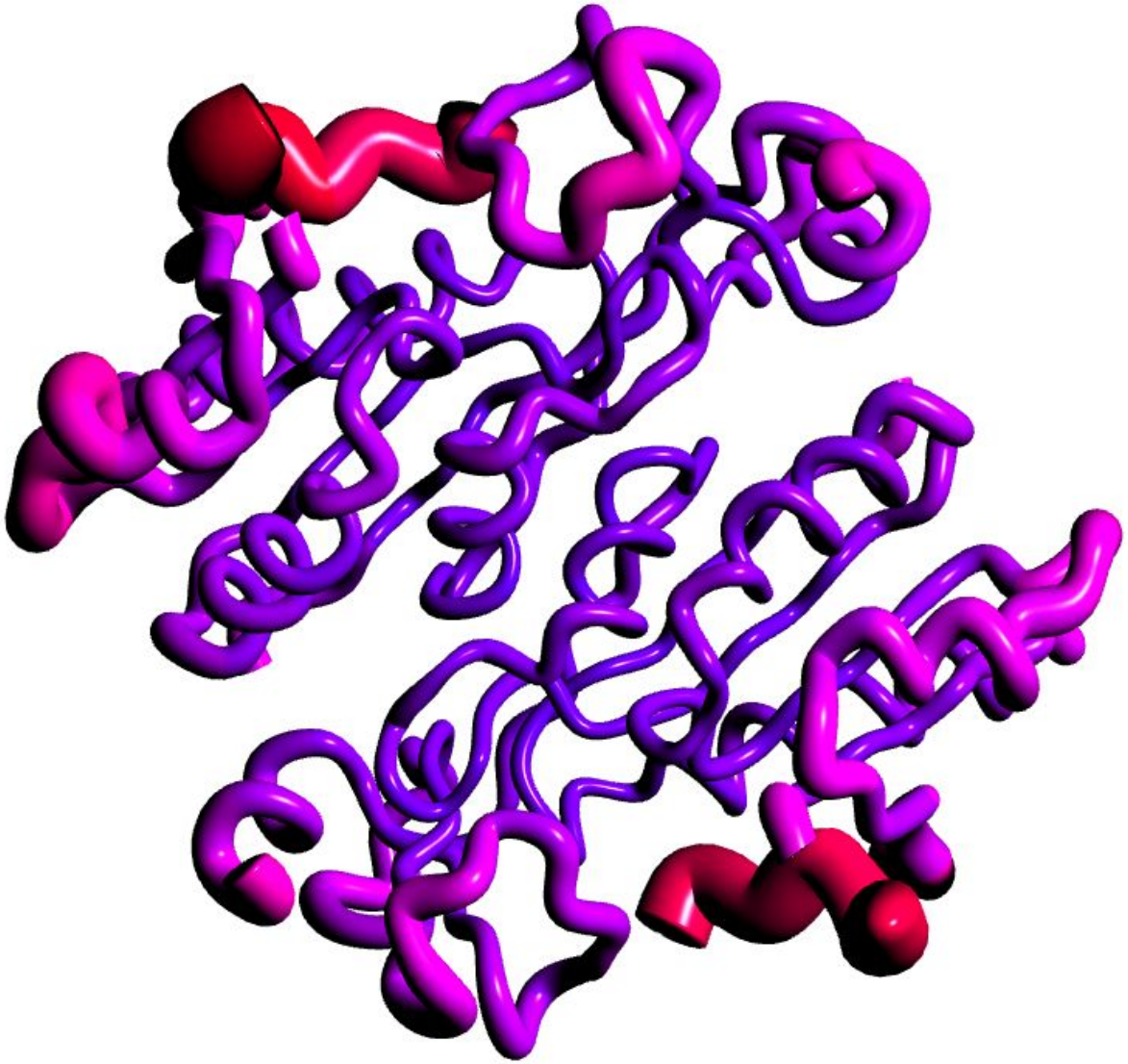
Van der Waals



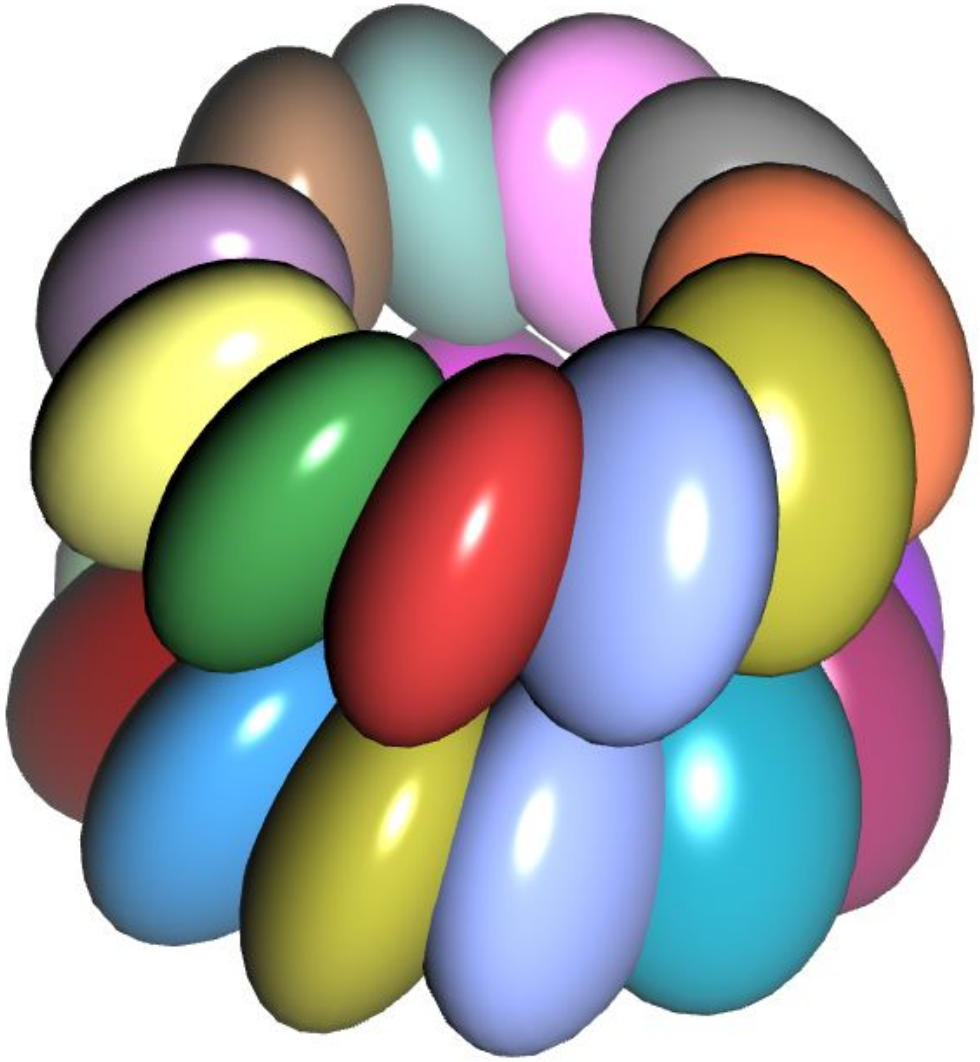


Solvent accessible

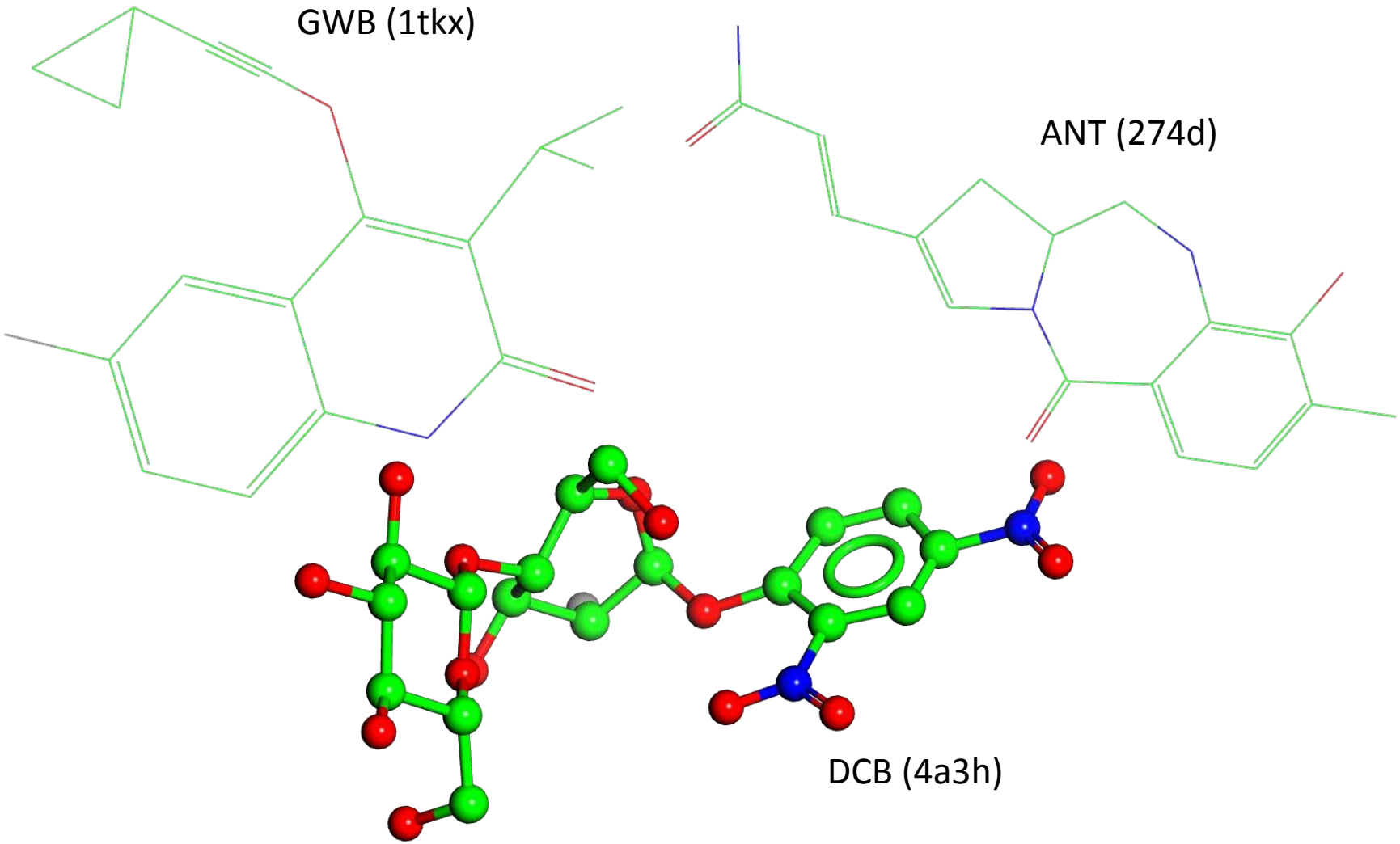
# Worm scaled by B-factor



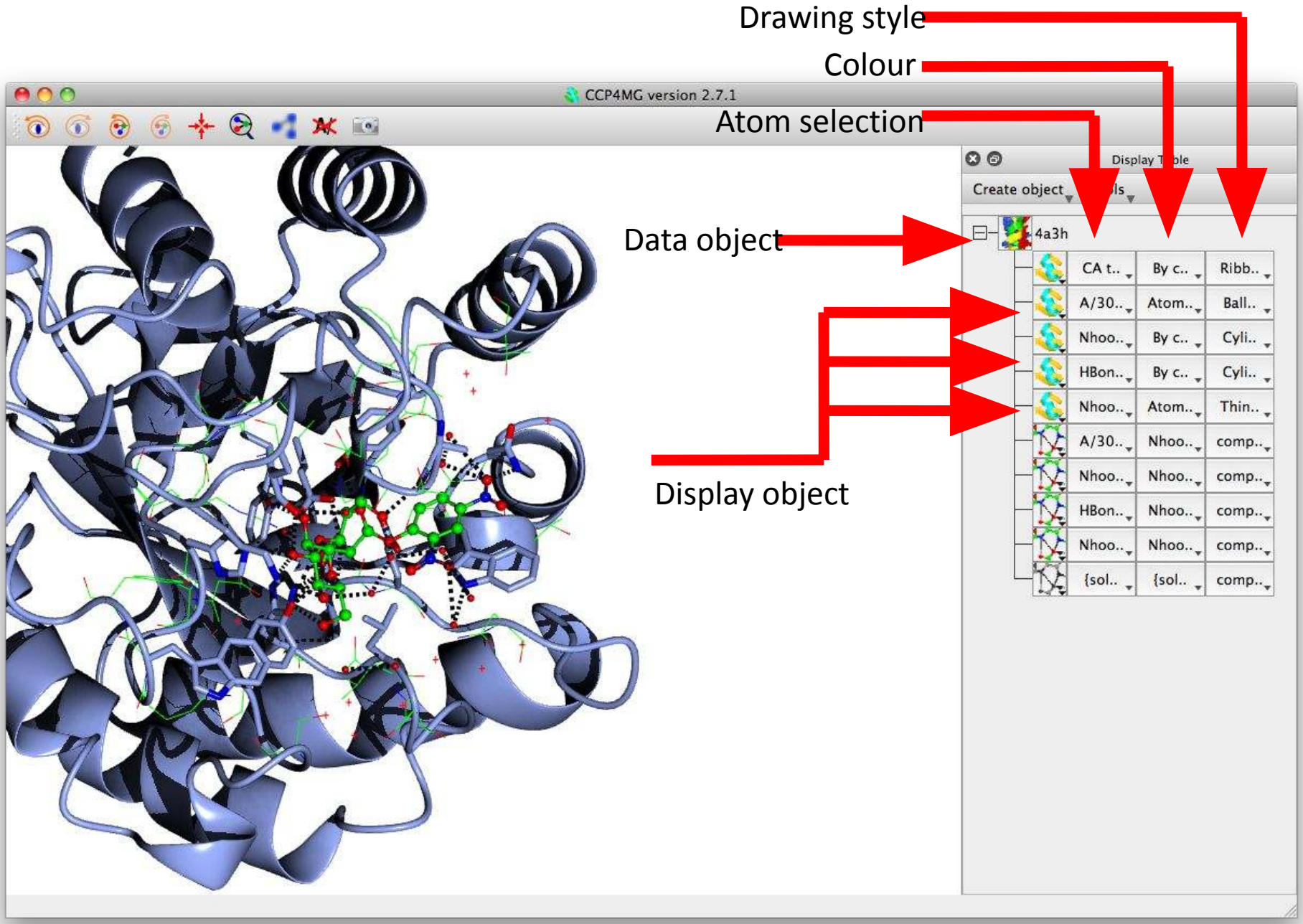
# Bloboids



# Multiple bonds

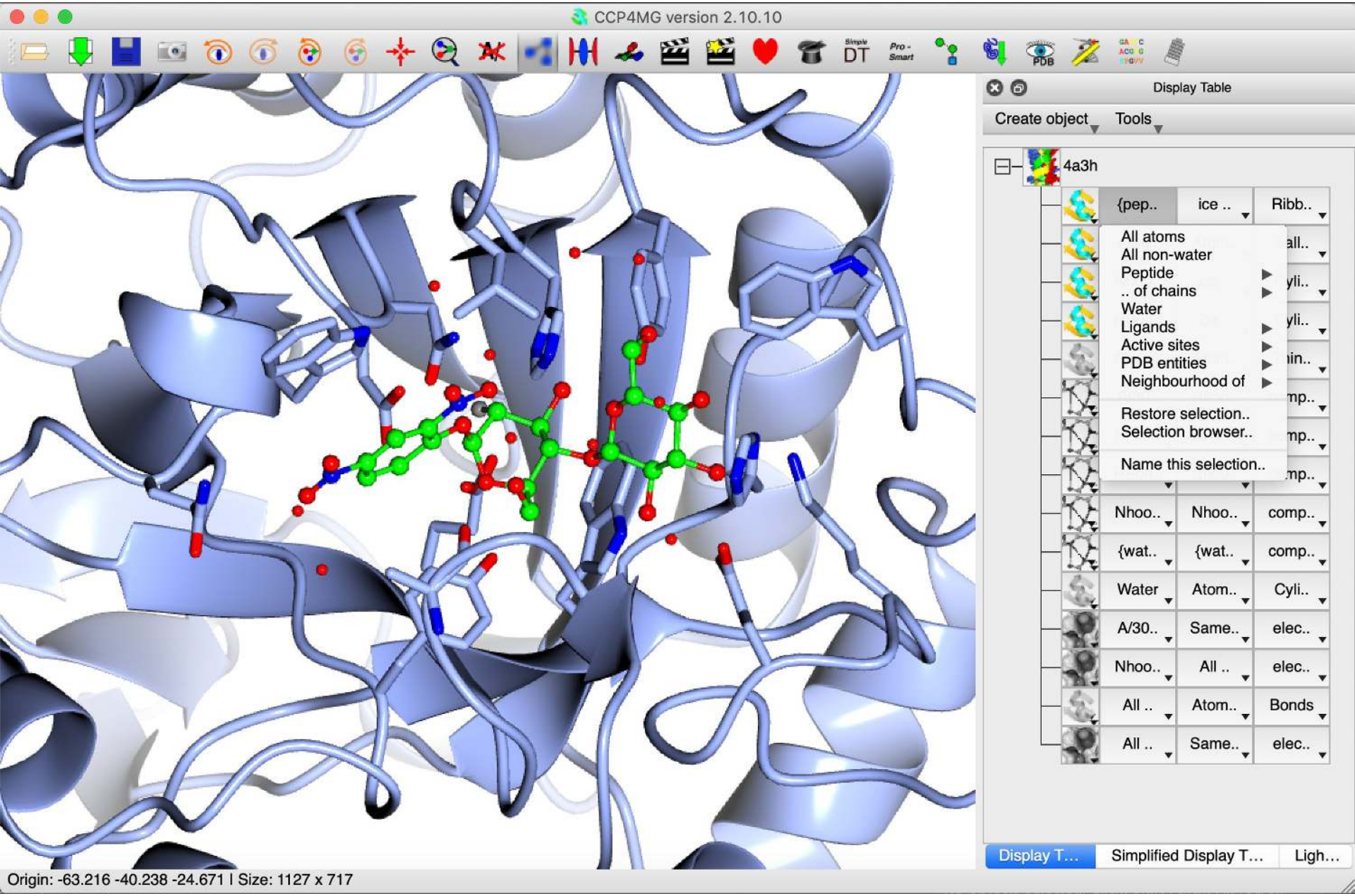


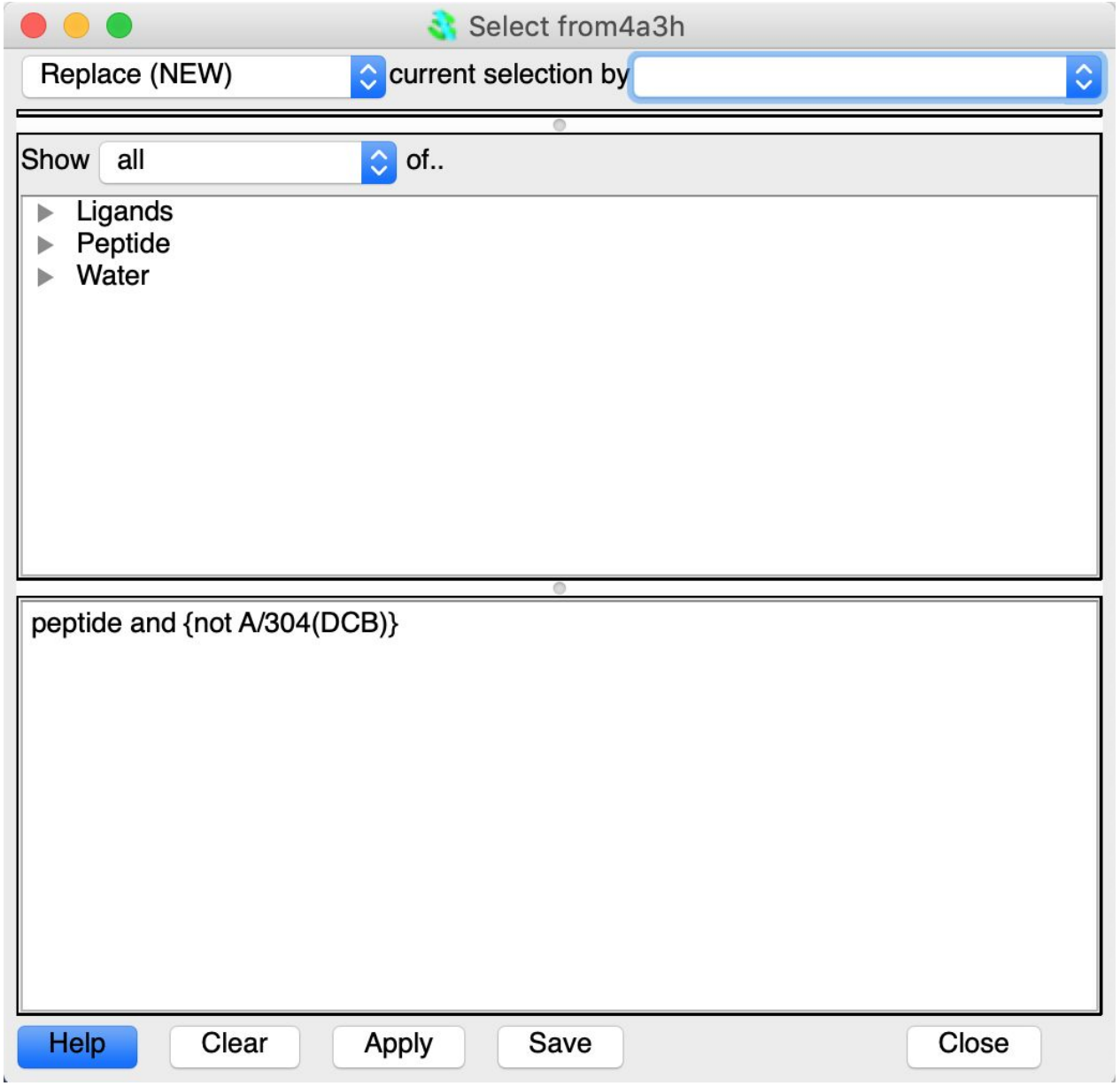
# The program interface (introduction)

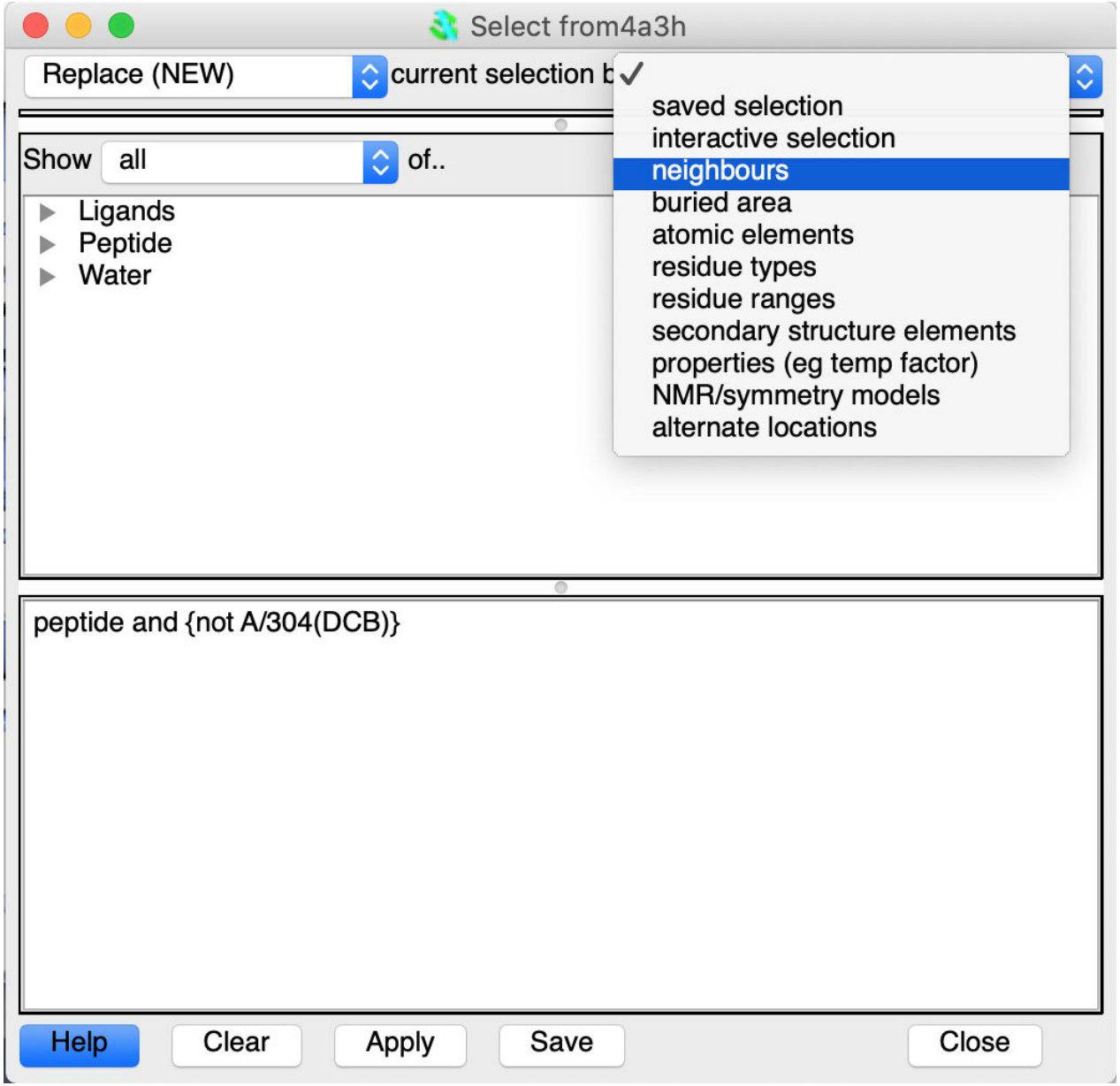

Drawing style
Colour
Atom selection
Data object
Display object
CCP4MG version 2.7.1
Create object
4a3h
CA t..
By c..
Ribb..
A/30..
Atom..
Ball..
Nhoo..
By c..
Cyli..
HBon..
By c..
Cyli..
Nhoo..
Atom..
Thin..
A/30..
Nhoo..
comp..
Nhoo..
Nhoo..
comp..
HBon..
Nhoo..
comp..
Nhoo..
Nhoo..
comp..
{sol..
{sol..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

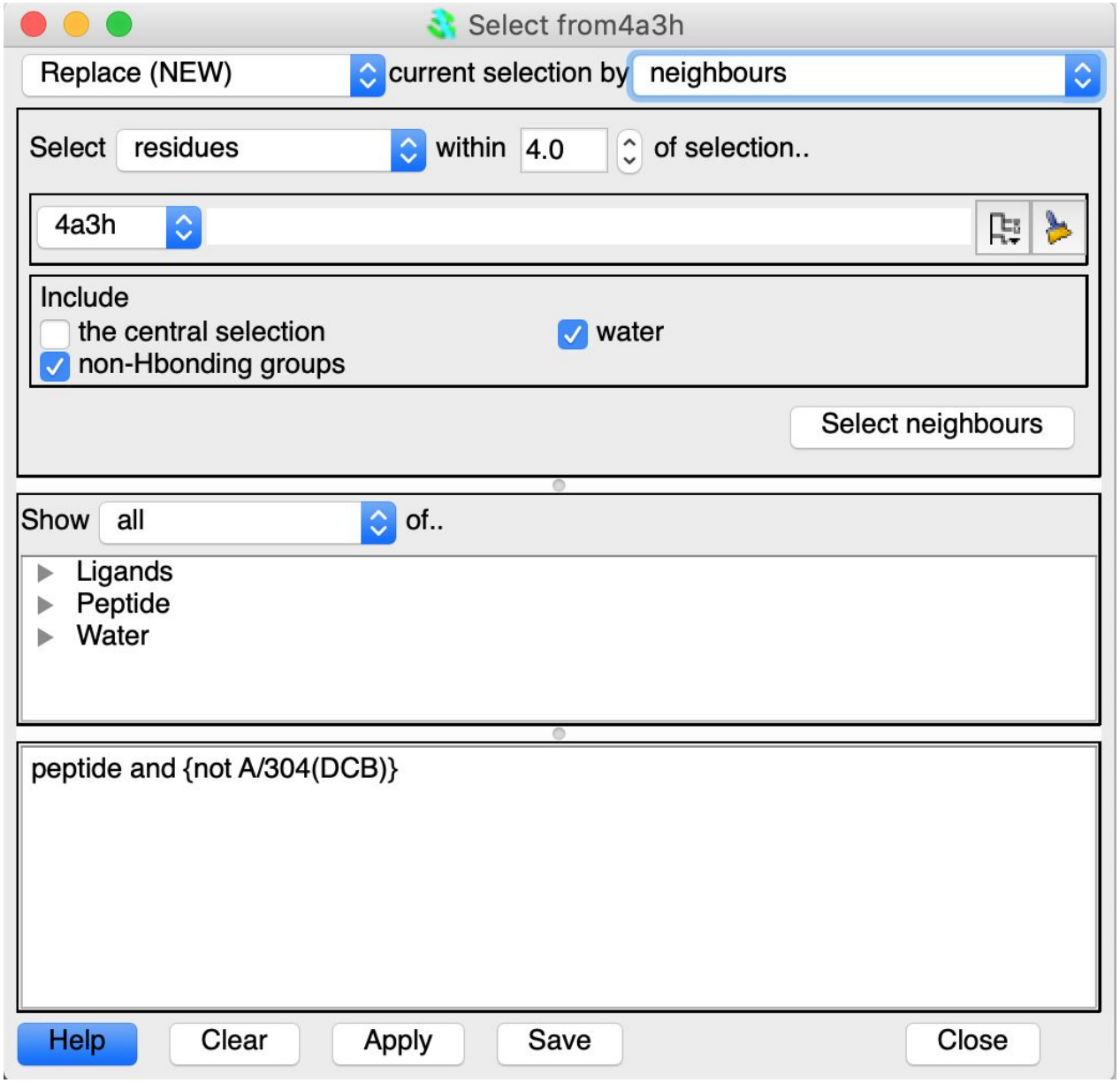
# Atom Selections

- Simple atom selections may be made with menu entries:
  - All atoms, all peptide, ligands, ligand neighbourhoods, 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

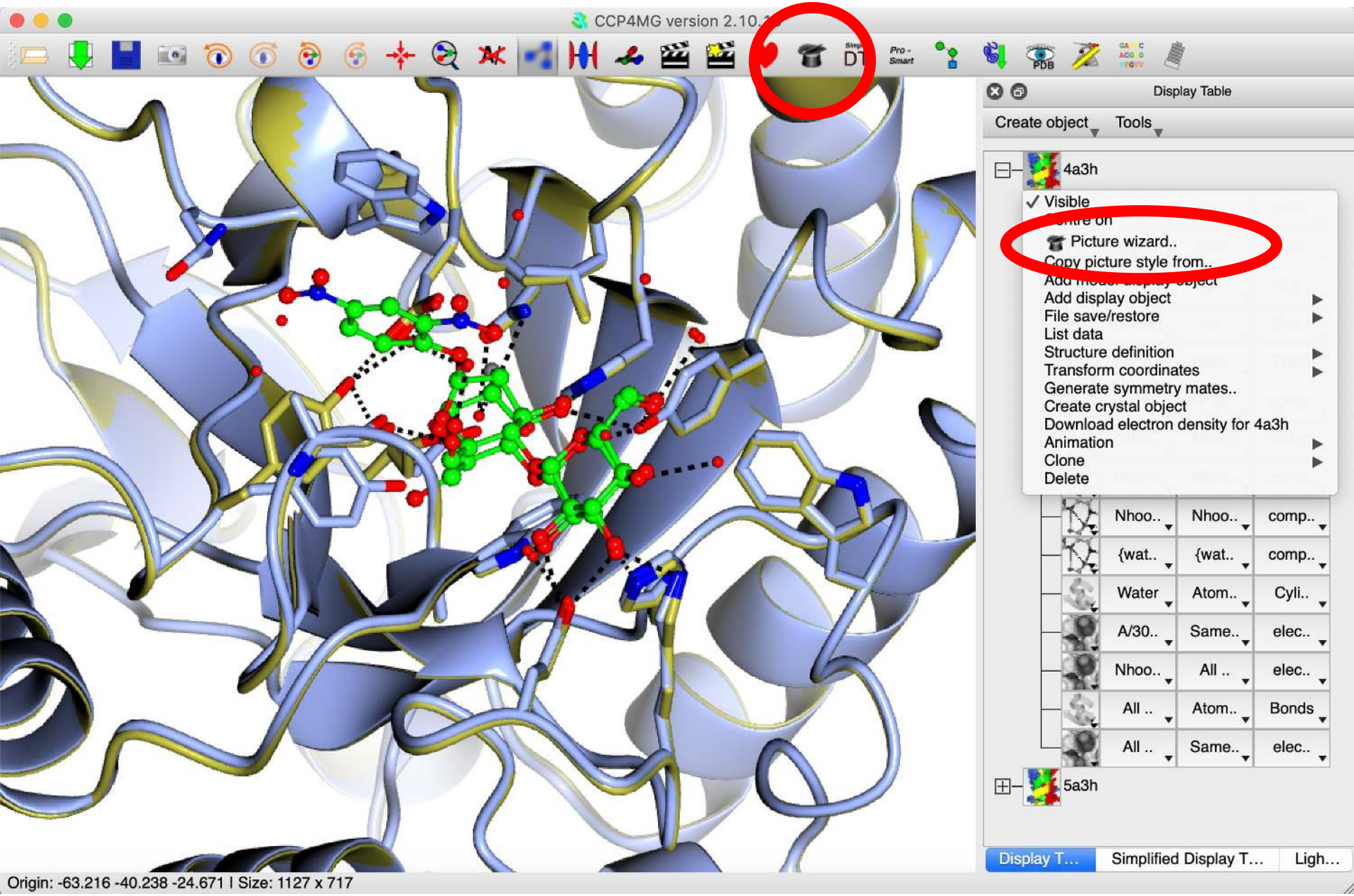

Select from4a3h
Replace (NEW)
current selection by
Show
all
of..
Ligands
Peptide
Water
peptide and {not A/304(DCB)}
Help
Clear
Apply
Save
Close


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
water
non-Hbonding groups
Select neighbours
Show
all
of..
Ligands
Peptide
Water
peptide and {not A/304(DCB)}
Help
Clear
Apply
Save
Close

# Picture Wizard

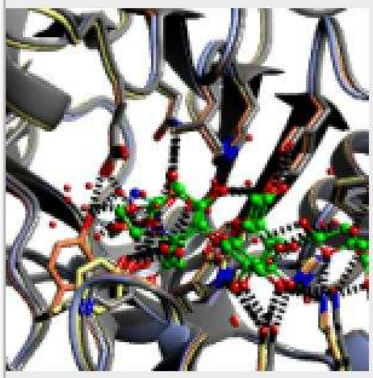
- The picture wizard is an automatic way of generating complex scenes with multiple selections, colouring, styles, etc.
- Representations are organised into various “styles”
- The picture wizard is shown at the top of the file browser window when a coordinate file is loaded, or can be accessed from the 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 I Size: 1127 x 717

Picture wizard to apply to ALL VISIBLE models

☑ Delete any existing display object ☑ Recentre

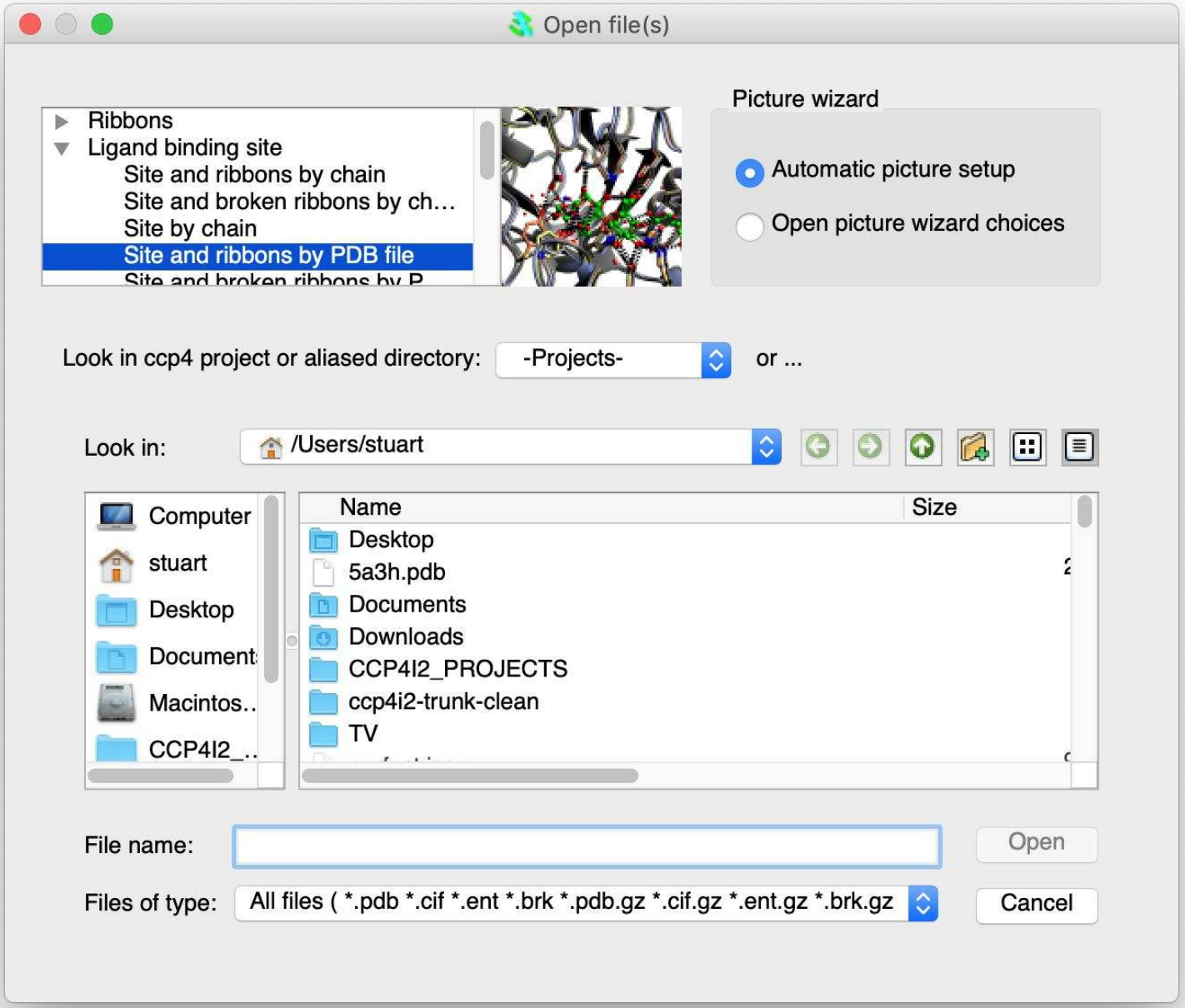
- ▶ Bonds
- ▶ Ribbons
- ▼ Ligand binding site
  - Site and ribbons by chain
  - Site and broken ribbons by ch…
  - Site by chain
  - **Site and ribbons by PDB file**
  - Site and broken ribbons by P…
  - Site by PDB file
  - surface by buried area
  - surface around ligand
  - surface electrostatics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

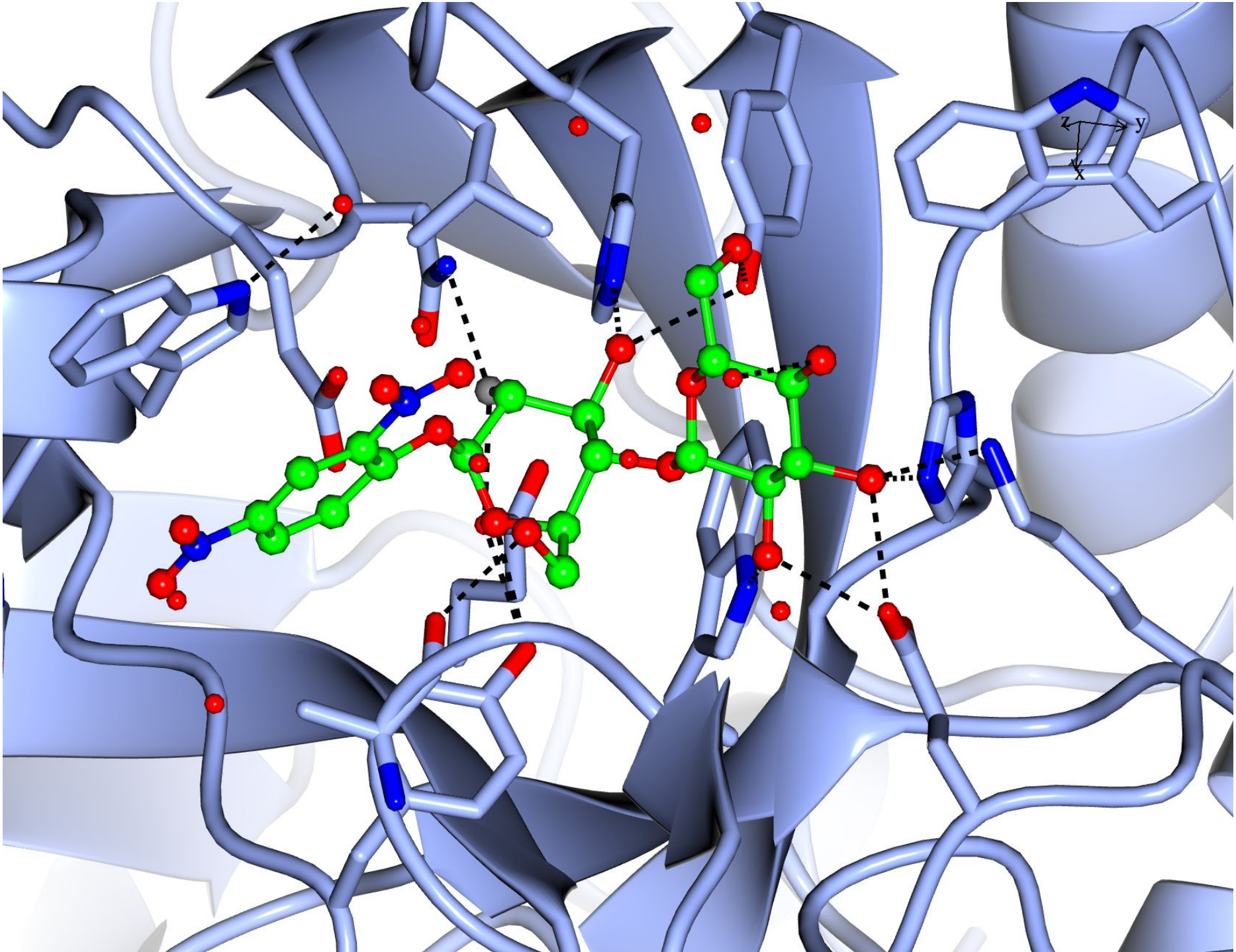


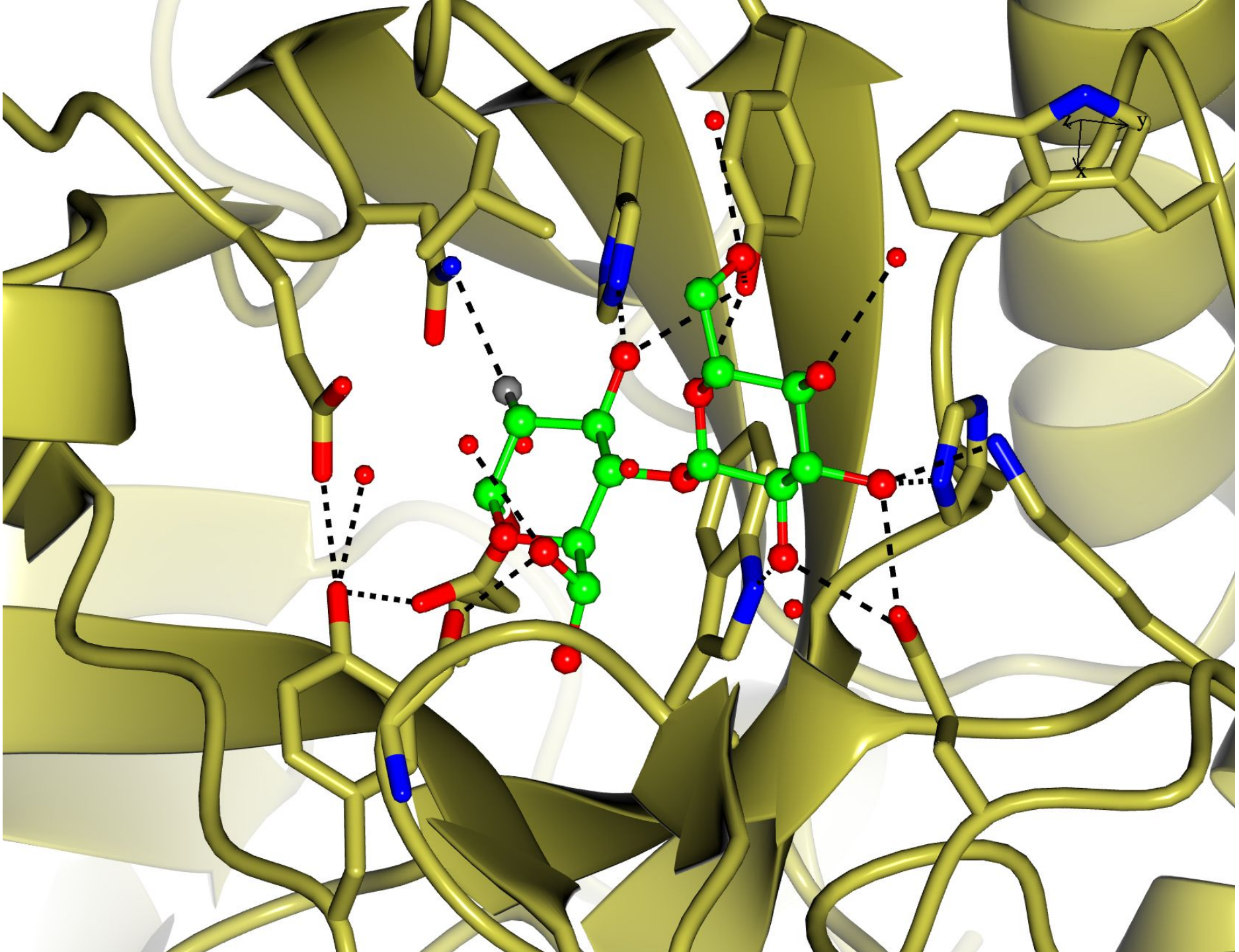
**Ligand binding site with peptide coloured by molecule.**
The graphical objects are:
-The CA trace drawn as ribbon.
-One object for each selected ligand.
-The 'neighbourhood' side chains close to ligands.
-The 'neighbourhood' main chain and water within hydrogen

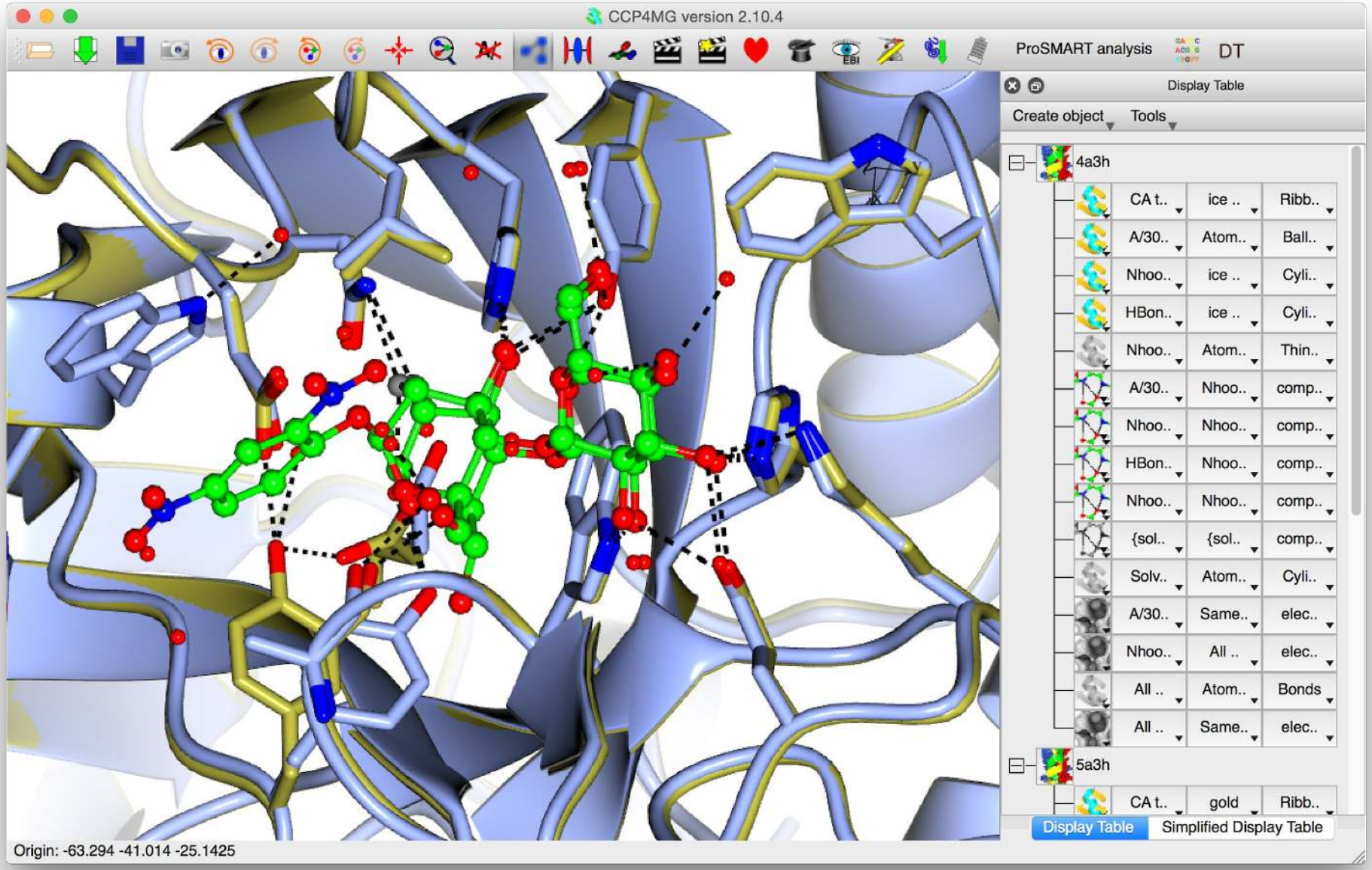
Only atoms in chain

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
Document
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

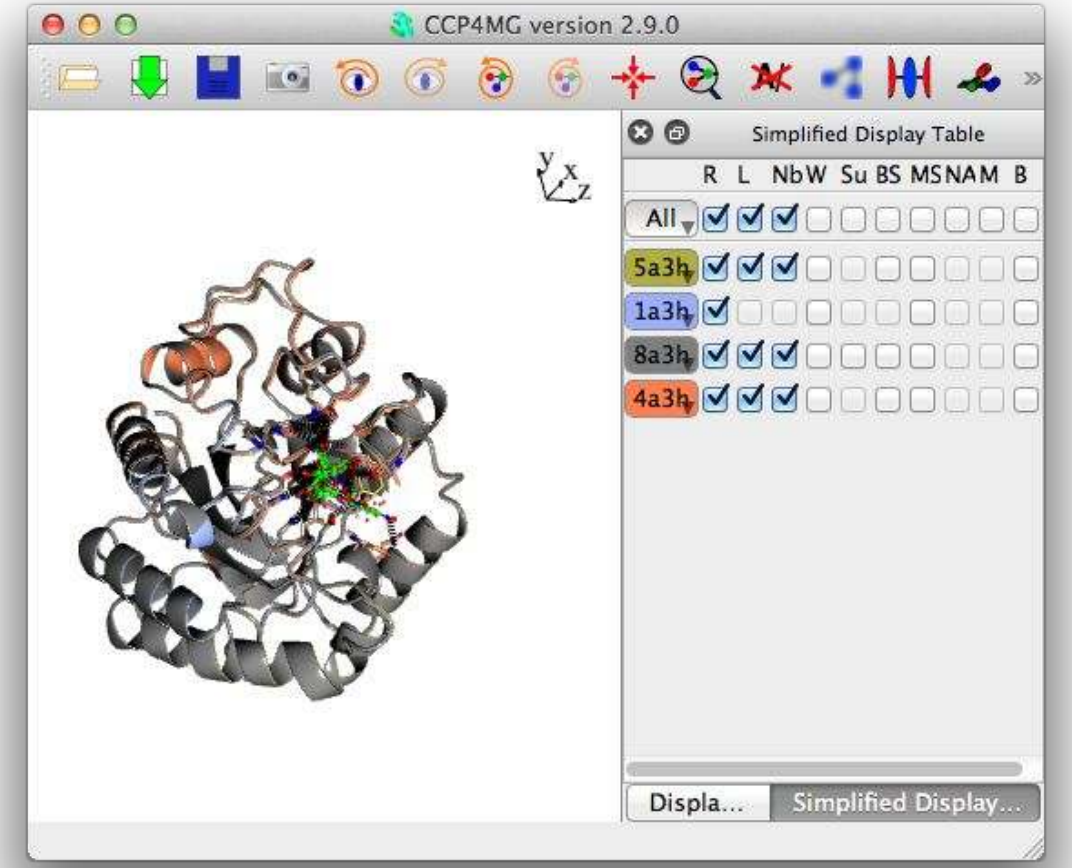

z
y
x


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

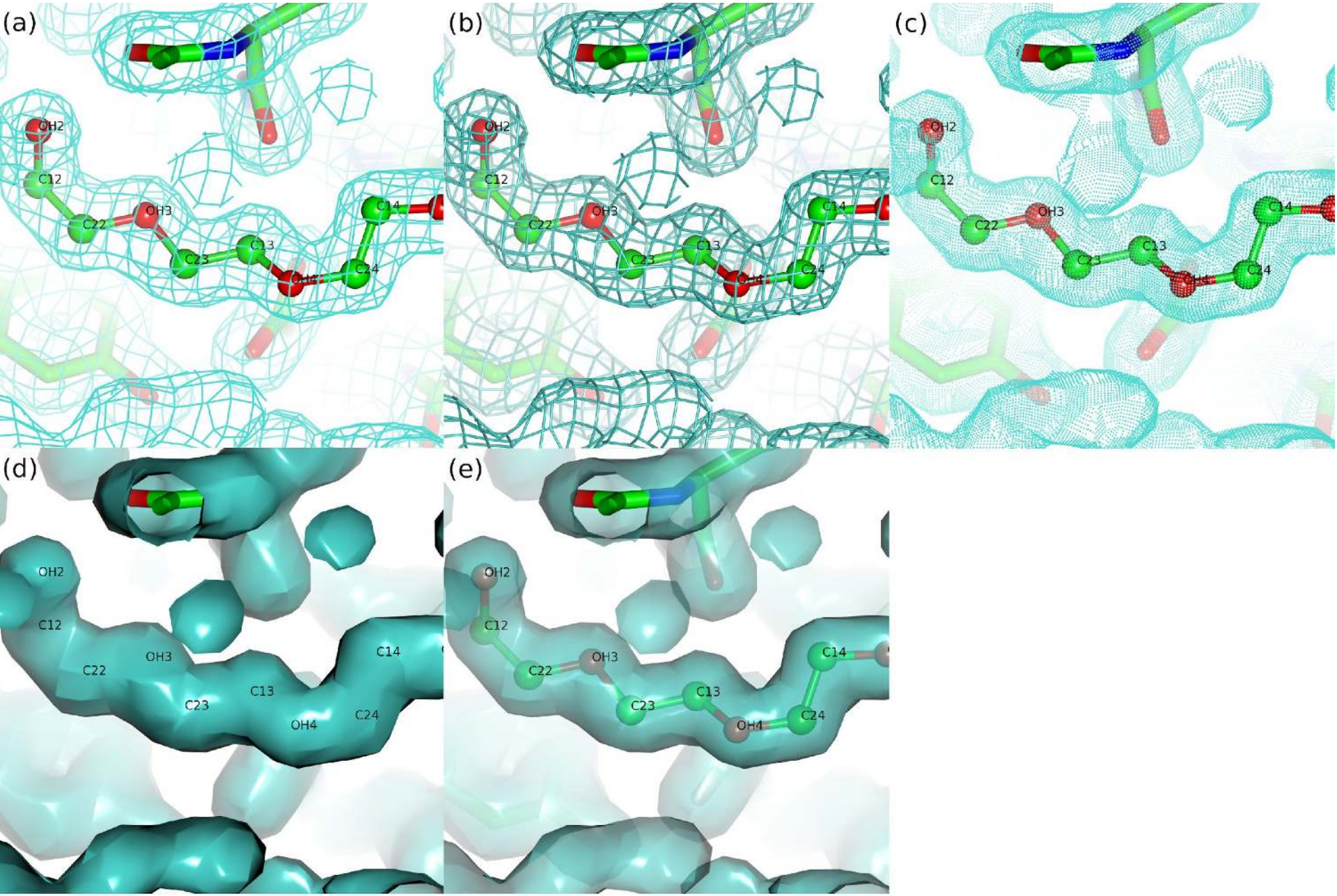
# Simplified Display Table

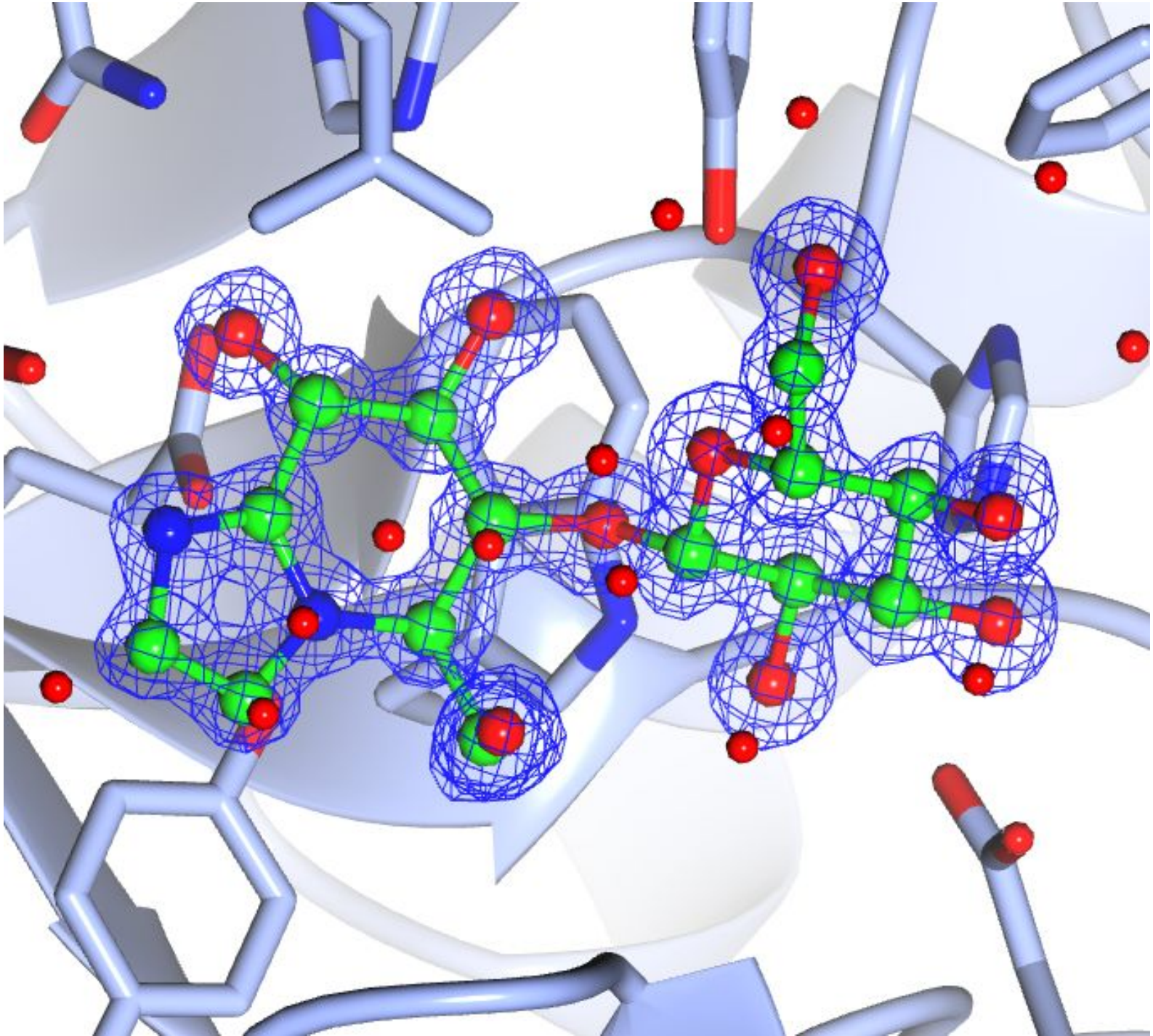
Tool for quickly turning on/off lots of related display objects. Particularly useful for looking at large numbers of similar files. (Not a replacement for "full" Display Table, but a useful alternative for some use cases).



# Electron Density

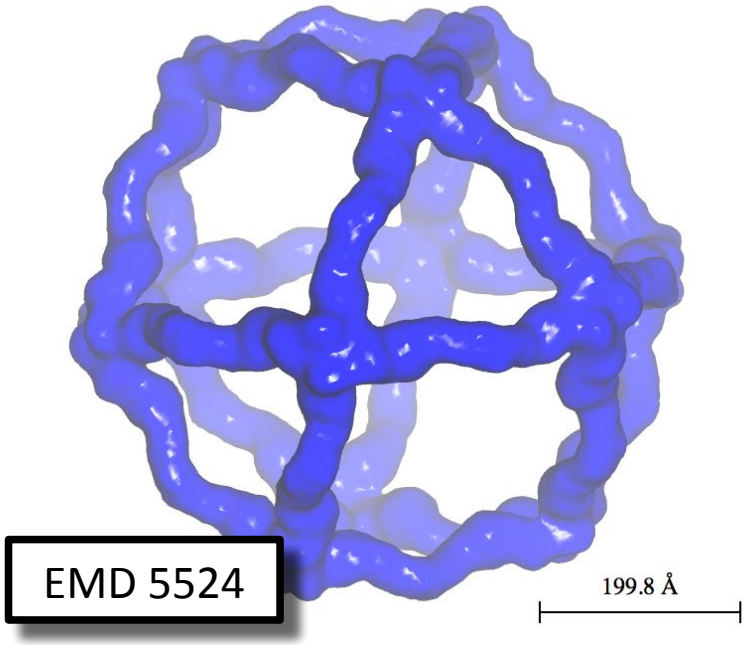
- Electron density maps can be read/created from any CCP4 supported file format, downloaded from PDB or generated from structure factors.
- Density can be represented as chickenwire lines, chickenwire cylinders, solid surface or dots.
- By default a 10Å parallelepiped of density at centre of screen is 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.

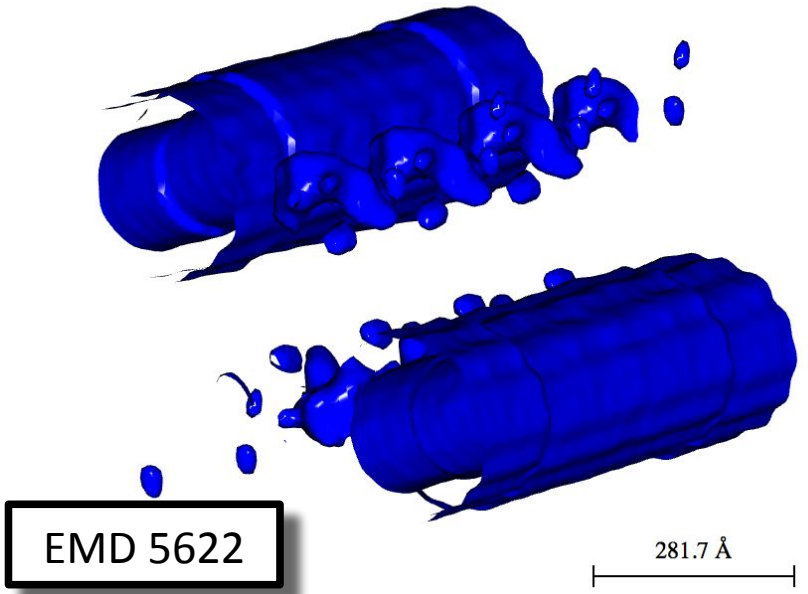

(a)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24
(b)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24
(c)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24
(d)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24
(e)
OH2
C12
C22
OH3
C23
C13
OH4
C14
C24

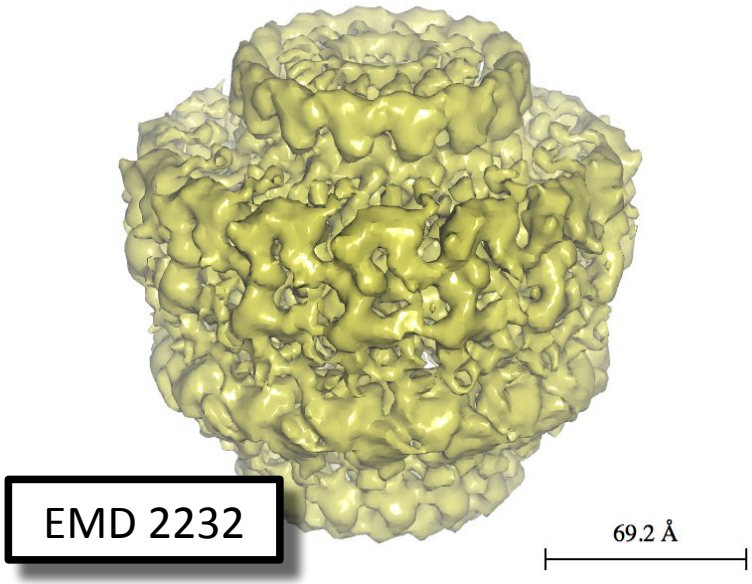


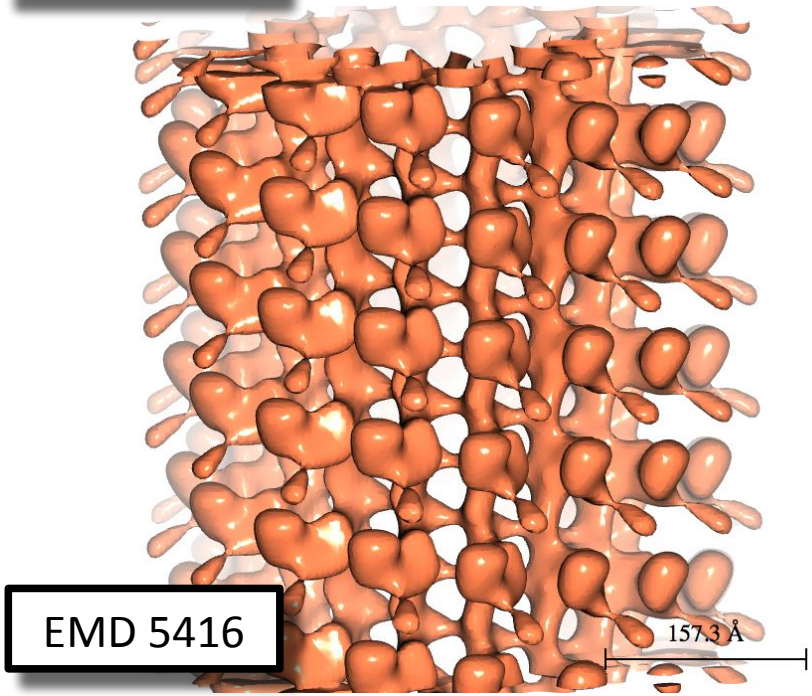
# Electron Microscopy Maps

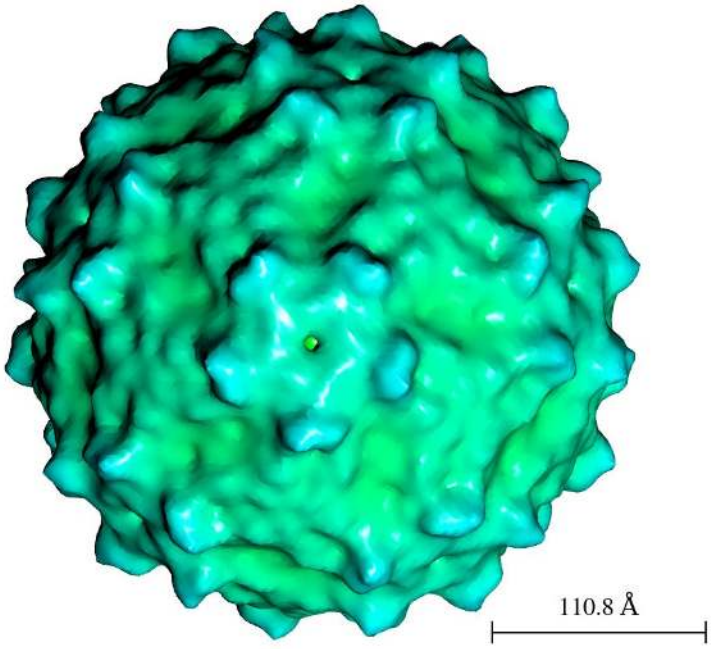
- CCP4MG can cope with 1000 angstrom sized maps.
- Maps from electron microscopy do not recalculate when moving view like X-ray maps. Massive speed improvement.
- Colour by distance from centre of map option – nice for virus maps.

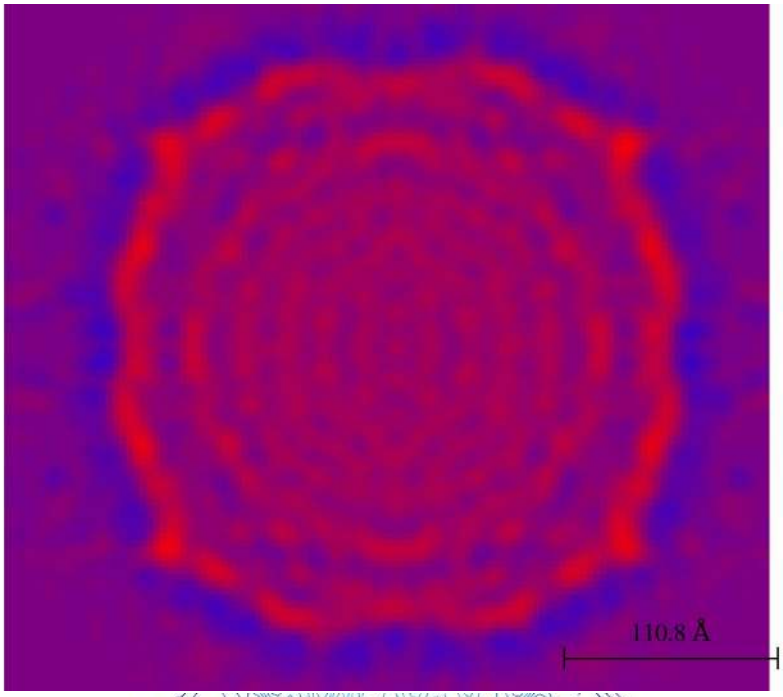

EMD 5524
199.8 Å

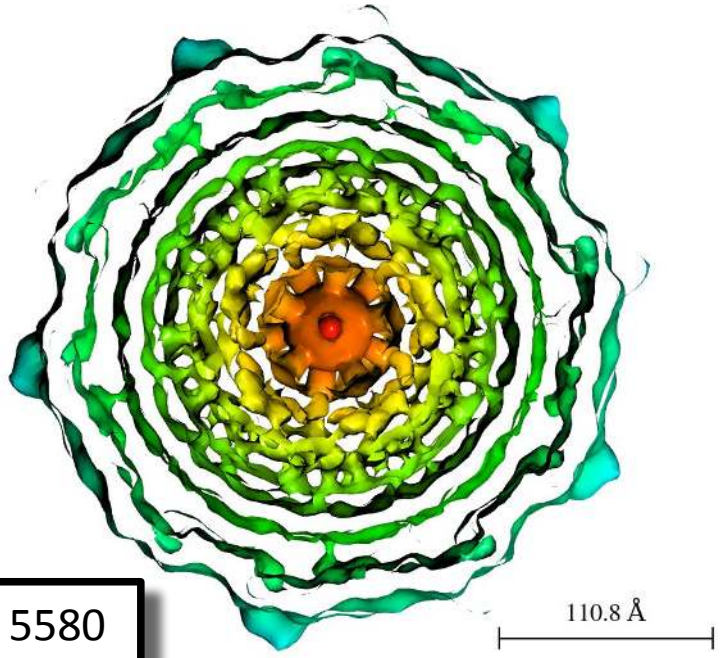

EMD 5622
281.7 Å

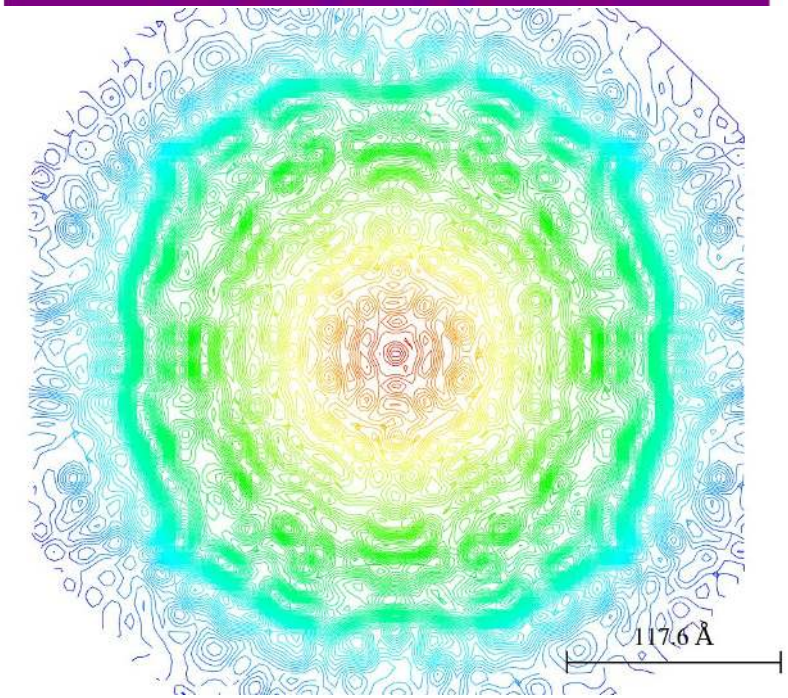

EMD 2232
69.2 Å


EMD 5416
157.3 Å

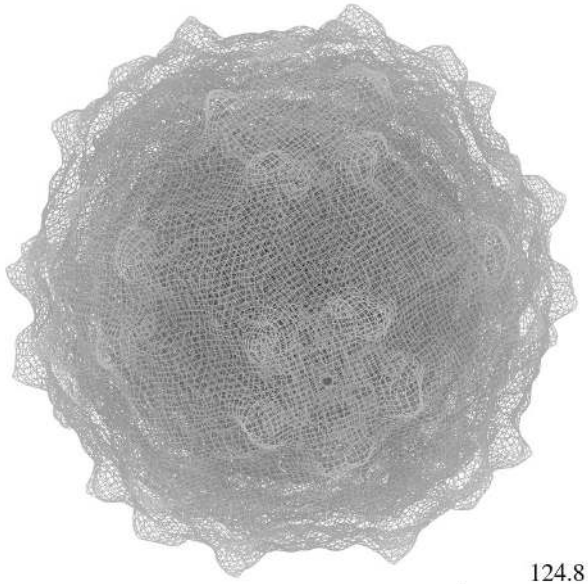


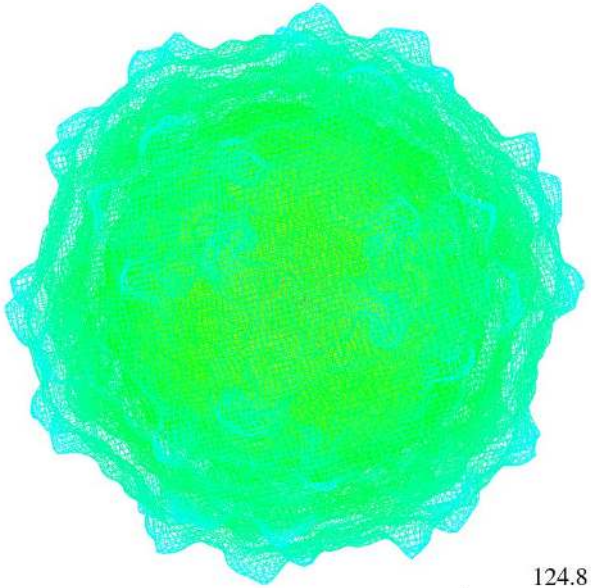



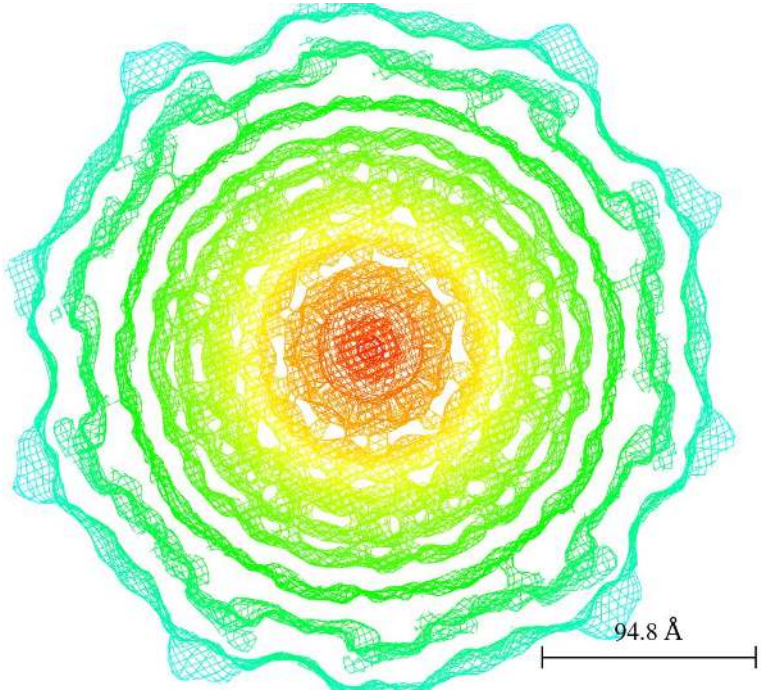

EMD 5580



124.8 Å



124.8 Å



94.8 Å

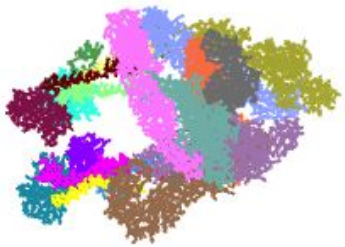
EMD 5580

# Symmetry

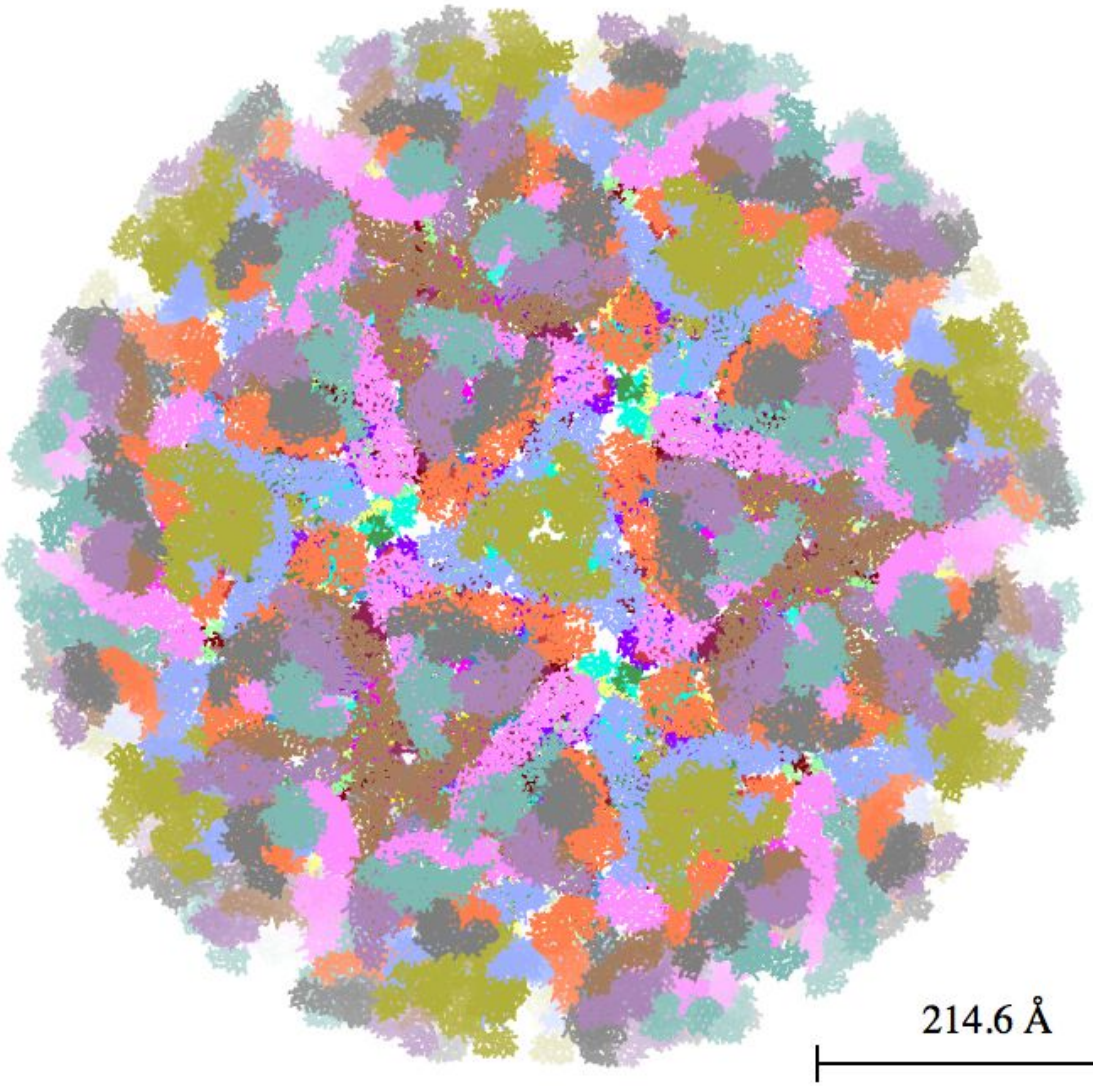
- Two ways:
  - Fast: Apply symmetry operations to objects which are drawn. “Continuous”, “About a point”, “unit cell”.
  - Not so fast: Create new display objects which can then have style, selections, etc. edited.

# 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.



214.6 Å

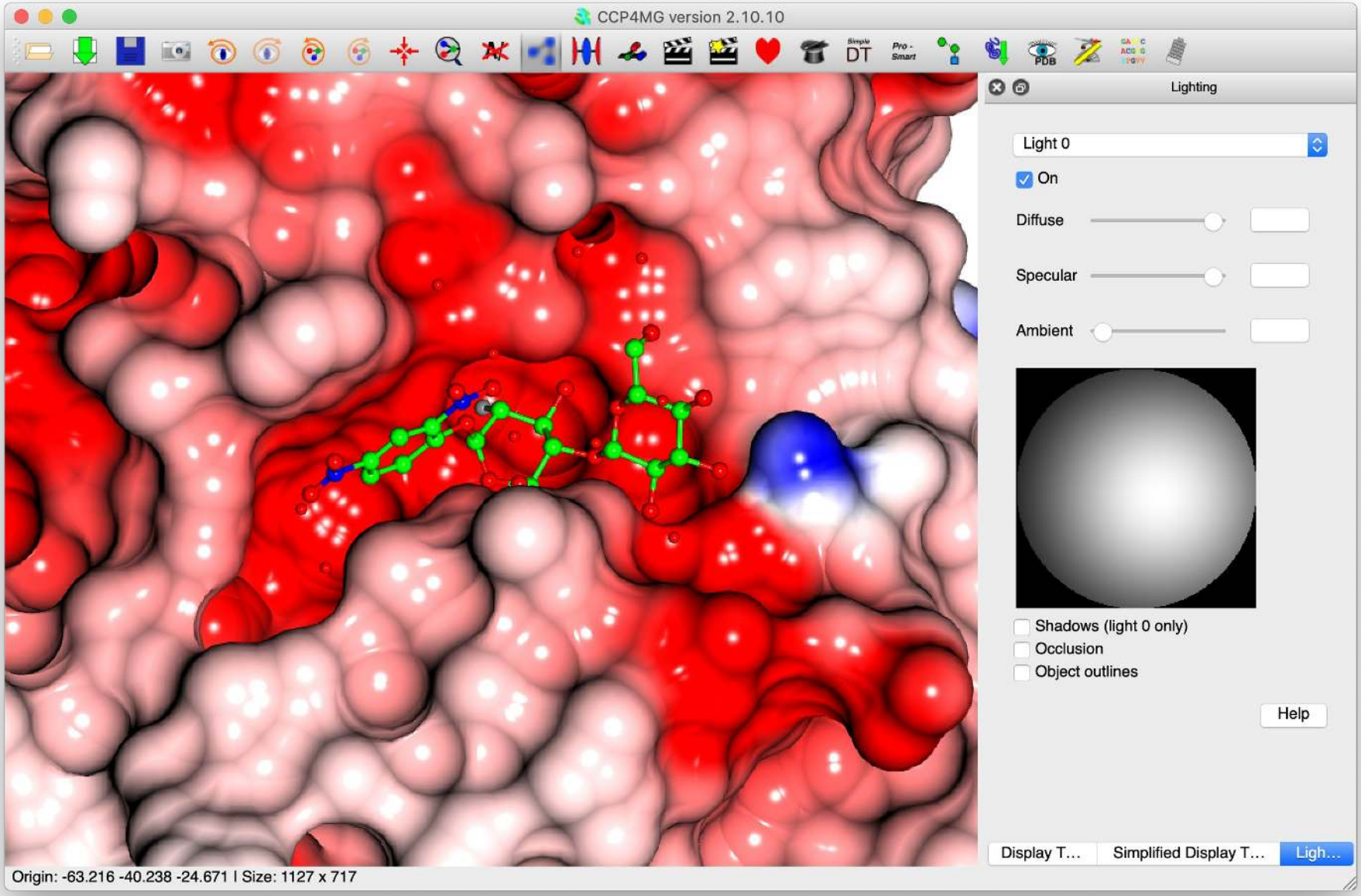


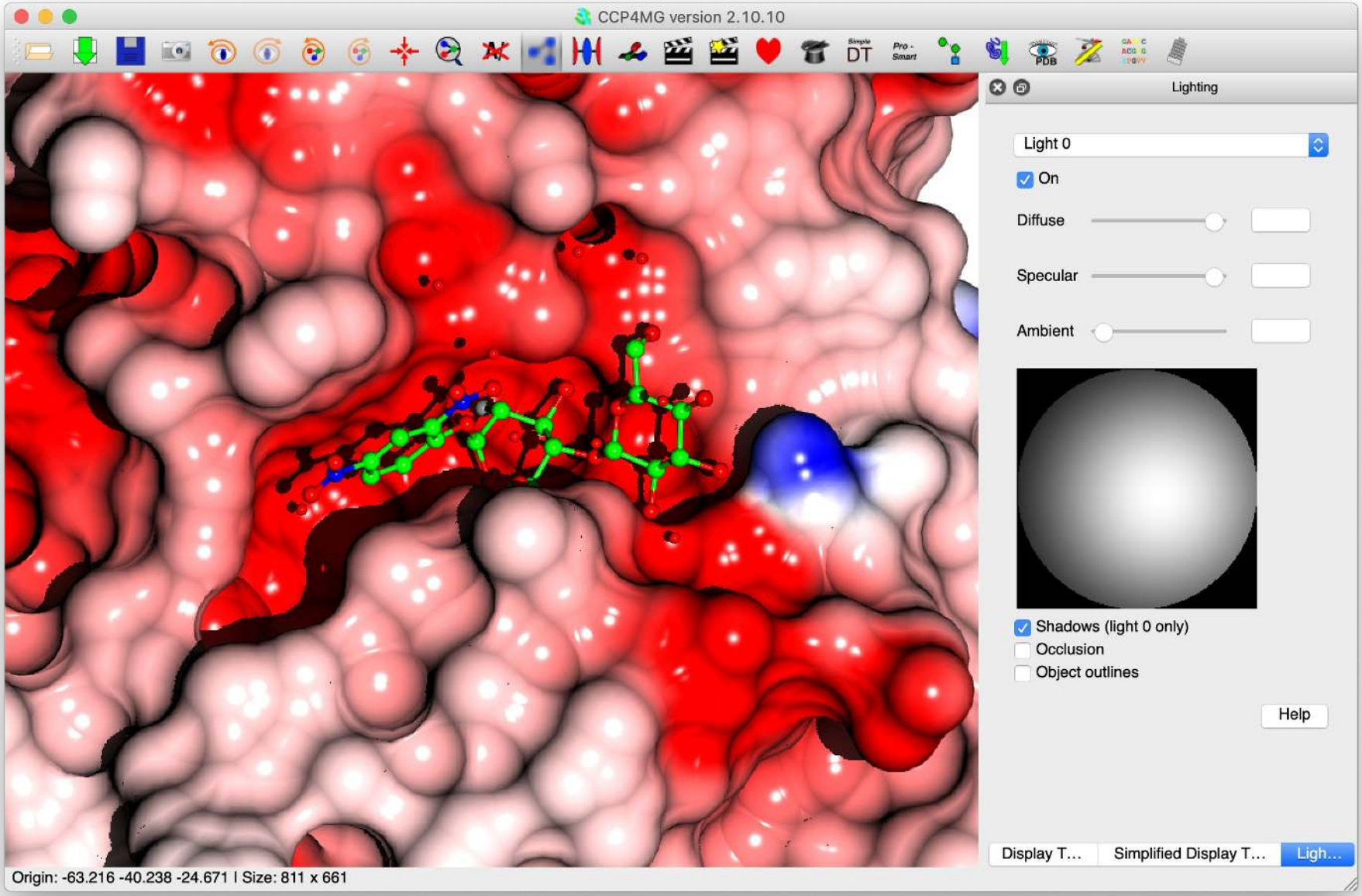
214.6 Å

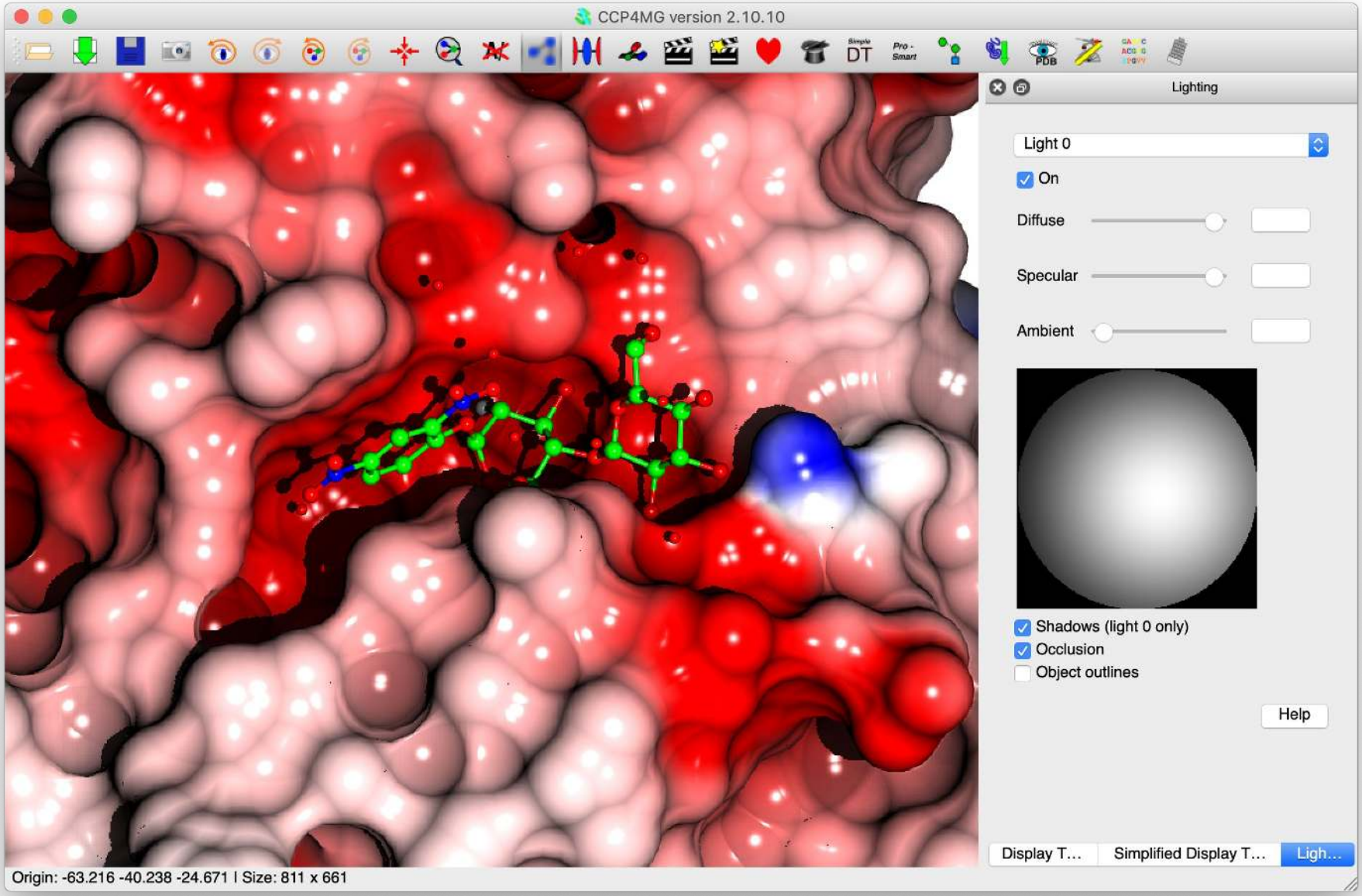
PDB 3j2w

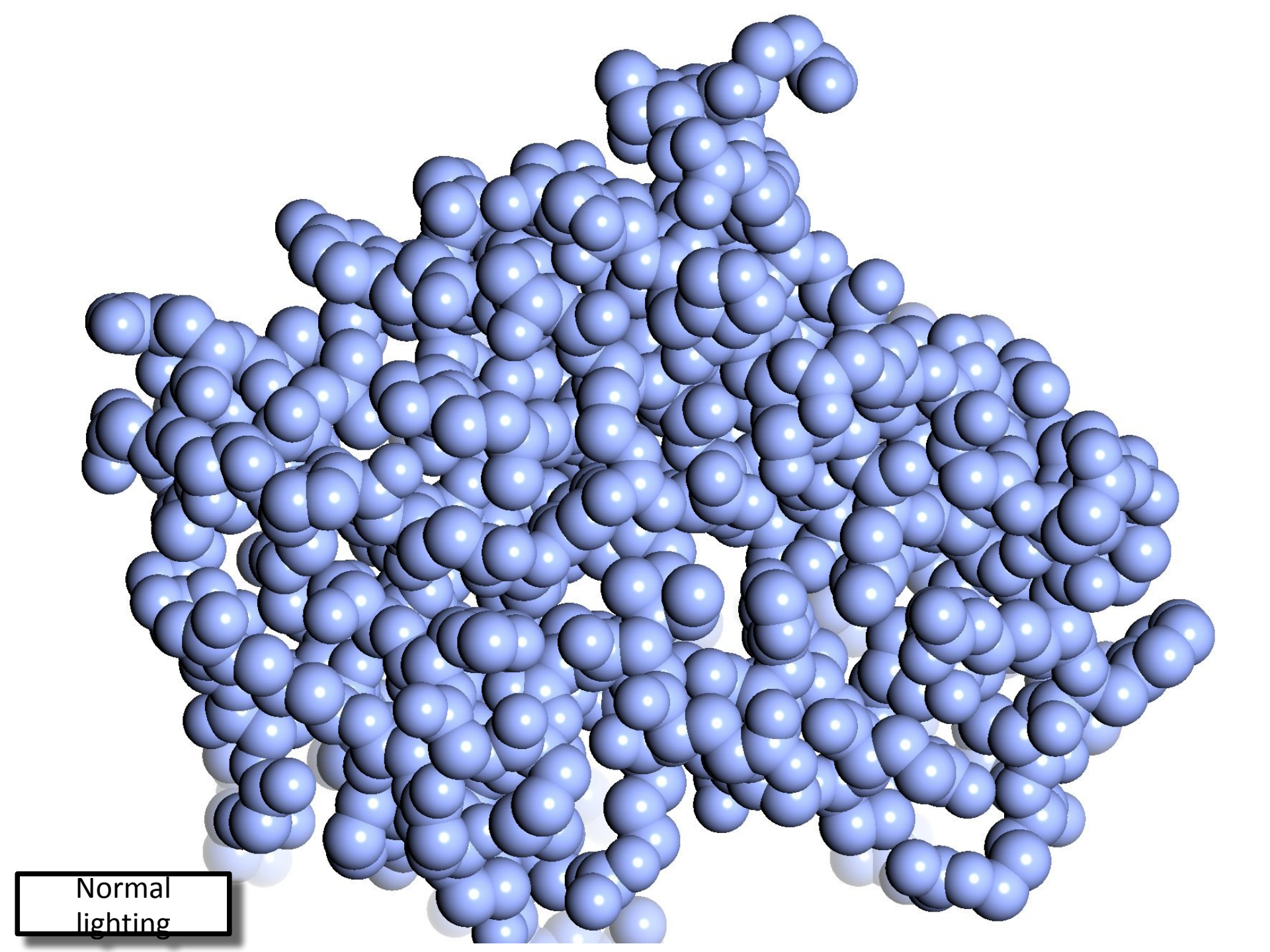
# Shadows and Occlusion

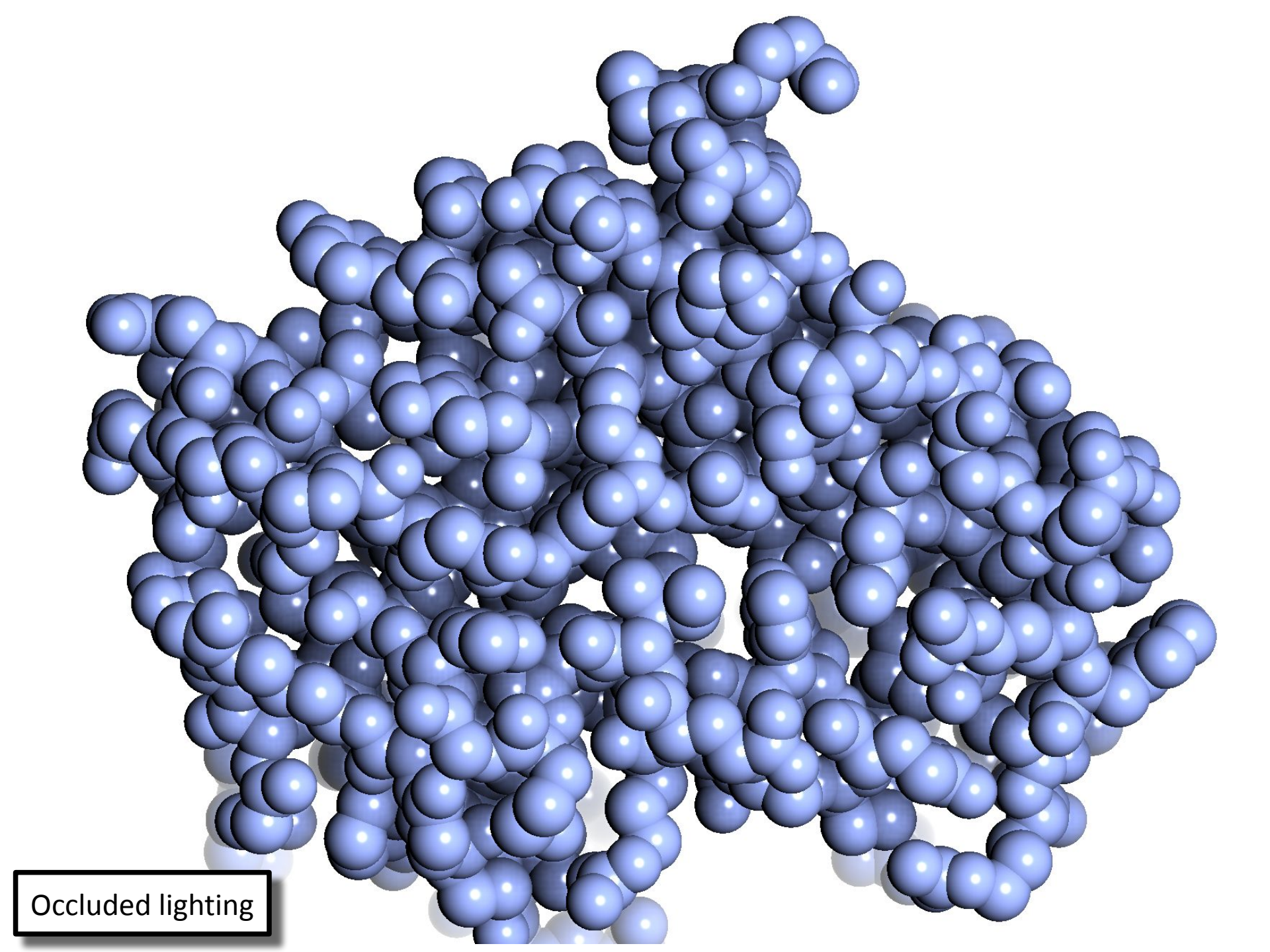
- “Real-time” shadows, i.e. active all time in graphics window, not just when you “Render”.
- Occlusion is darkening of buried bits which are not exposed to as much light as exterior parts of macromolecules. Also a “real-time” effect.


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

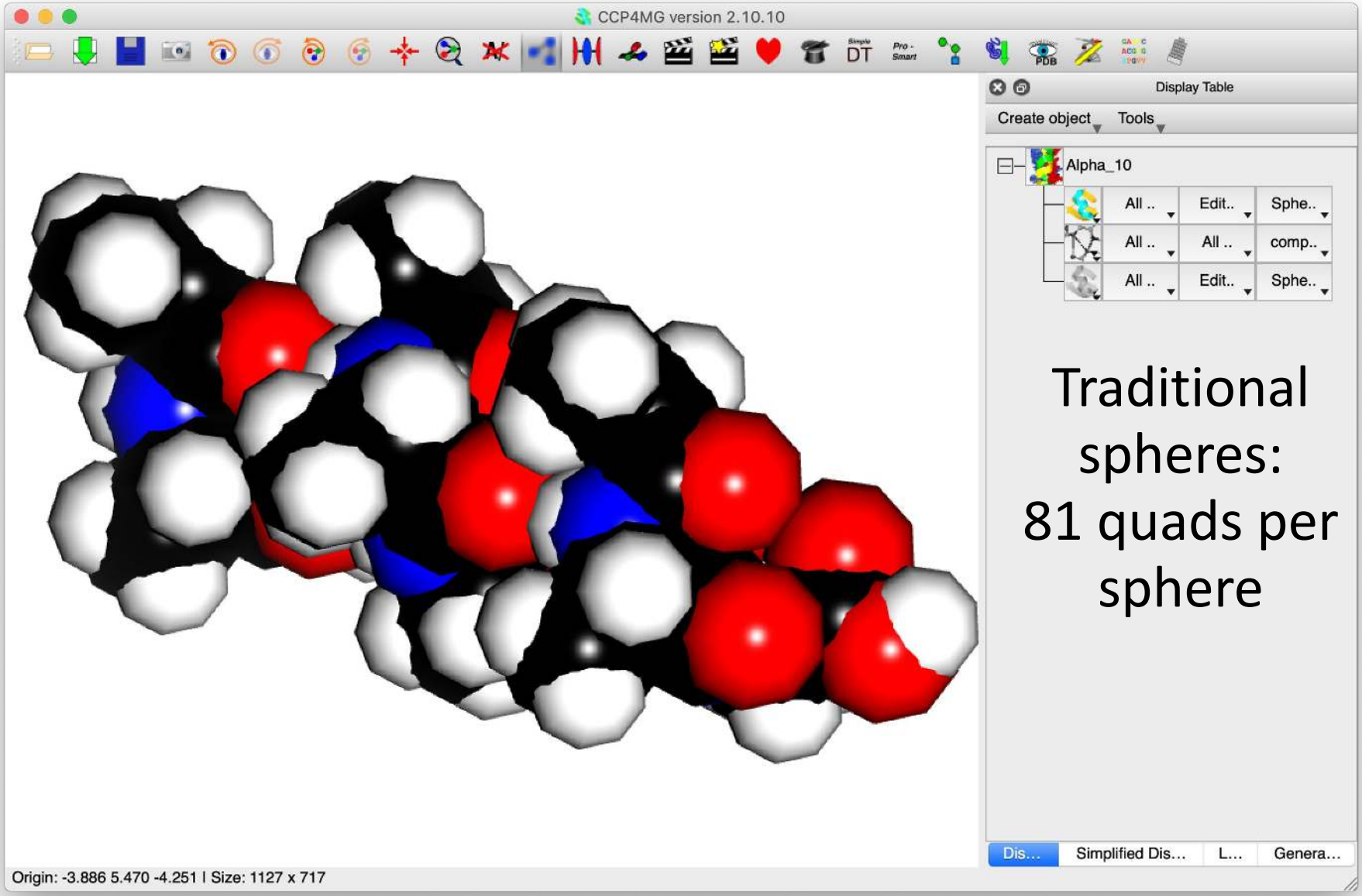

CCP4MG version 2.10.10
Lighting
Light 0
On
Diffuse
Specular
Ambient
Shadows (light 0 only)
Occlusion
Object outlines
Help
Display T…
Simplified Display T…
Ligh…
Origin: -63.216 -40.238 -24.671 | Size: 811 x 661

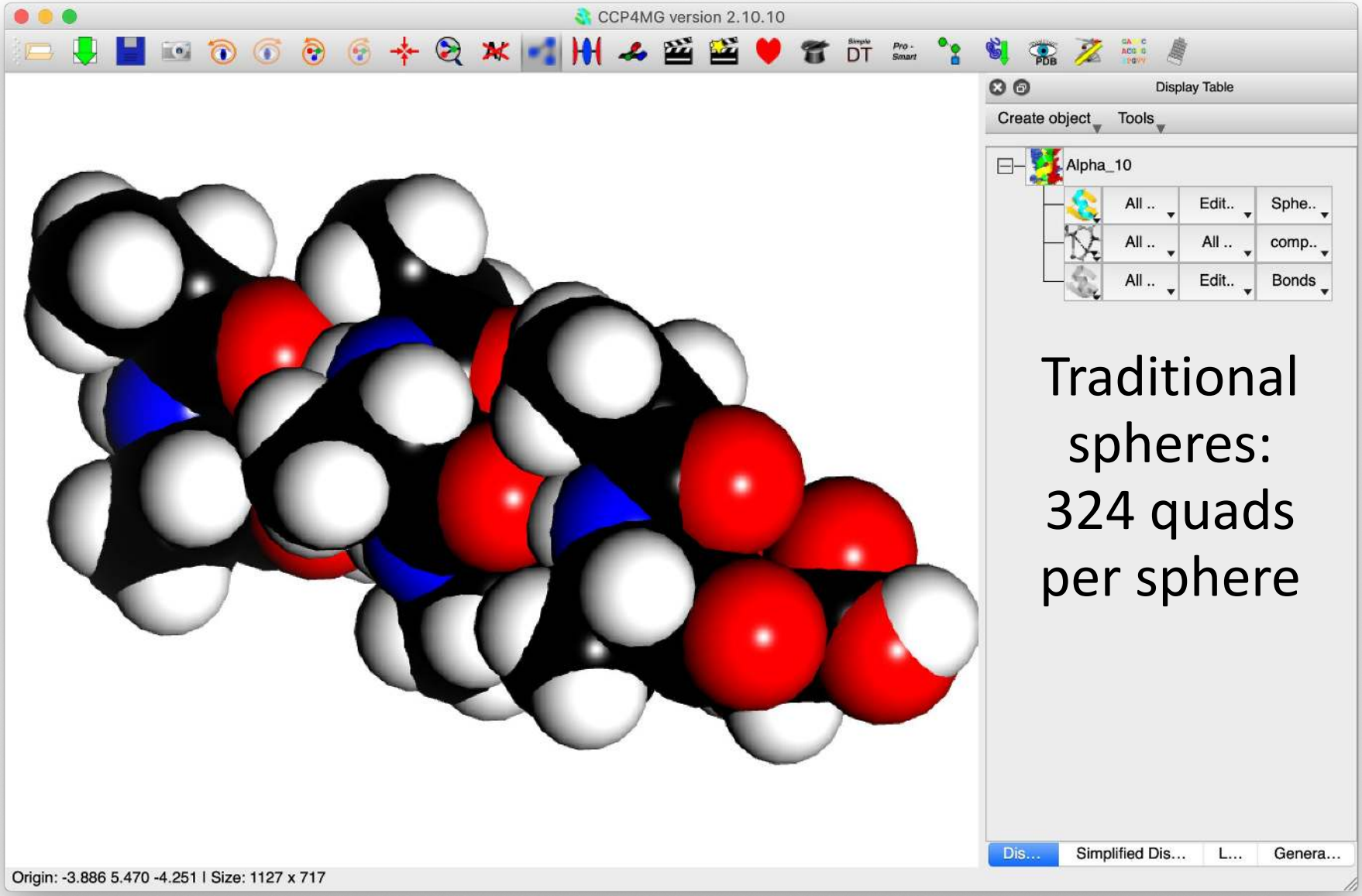

Normal
lighting

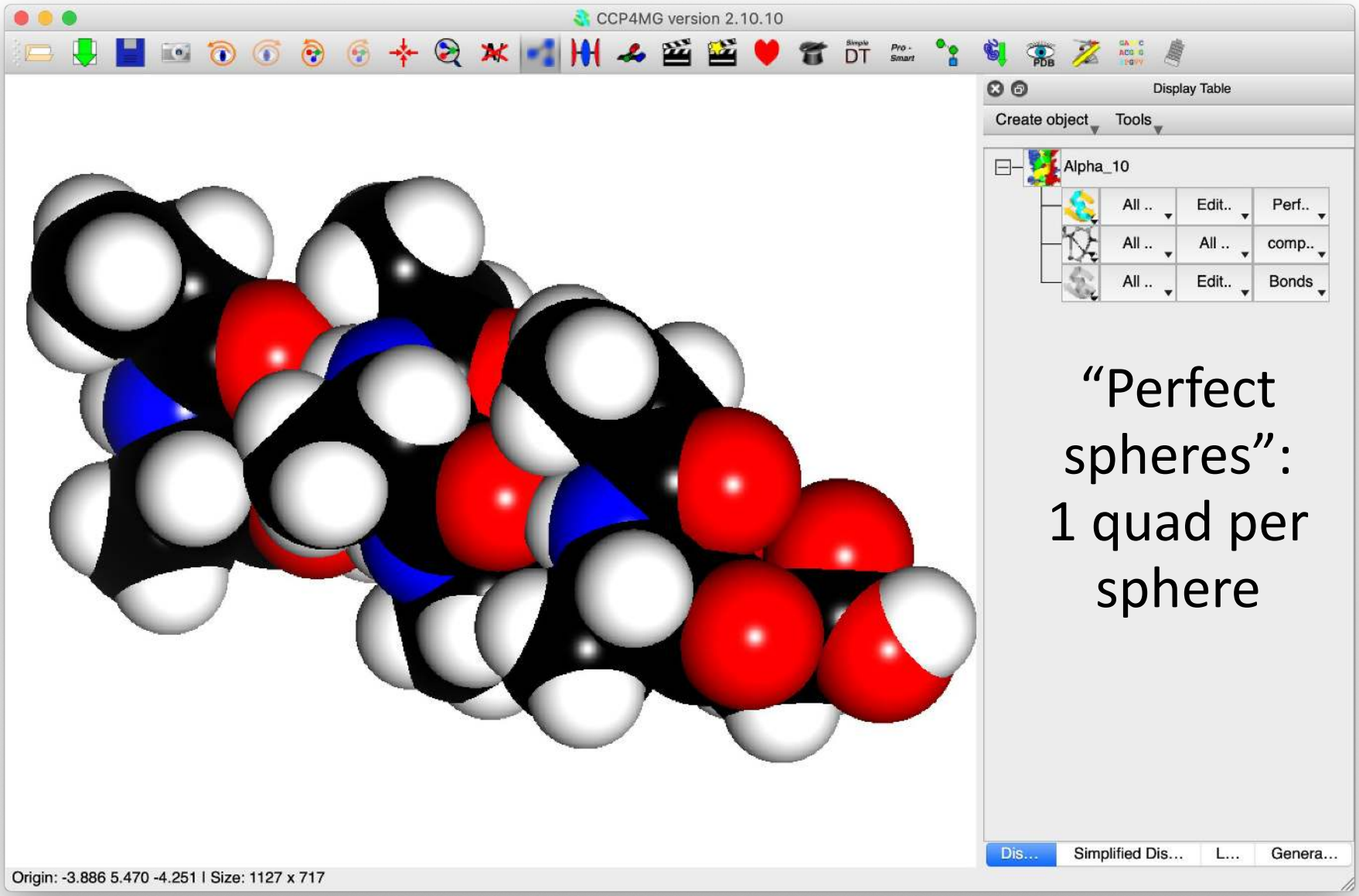

Occluded lighting

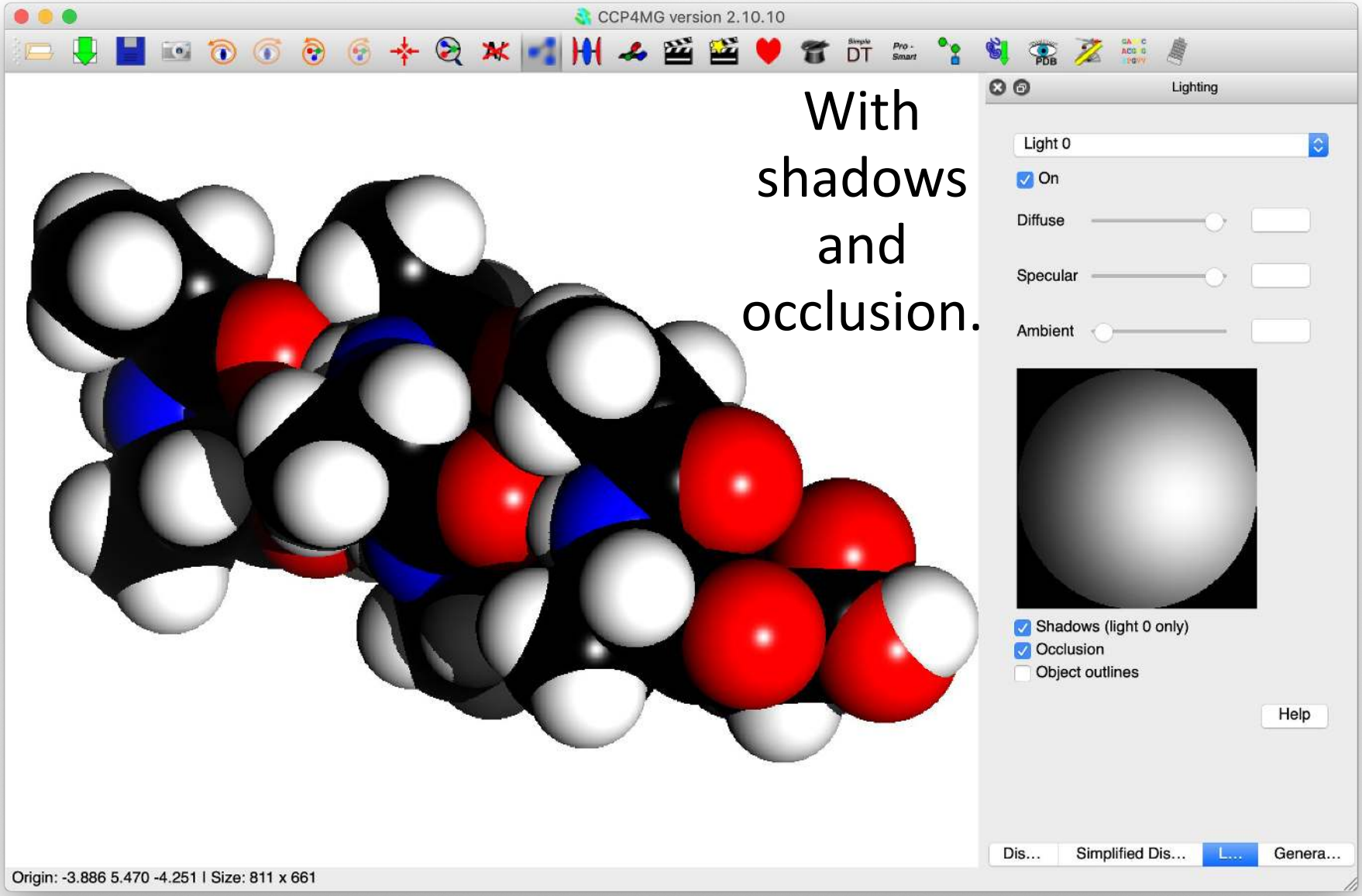
# “Perfect spheres”

- “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 I 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 I Size: 1127 x 717


CCP4MG version 2.10.10
Display Table
Create object
Tools
Alpha_10
All ..
Edit..
Perf..
All ..
All ..
comp..
All ..
Edit..
Bonds
"Perfect spheres": 1 quad per sphere
Dis...
Simplified Dis...
L...
Genera...
Origin: -3.886 5.470 -4.251 I Size: 1127 x 717


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

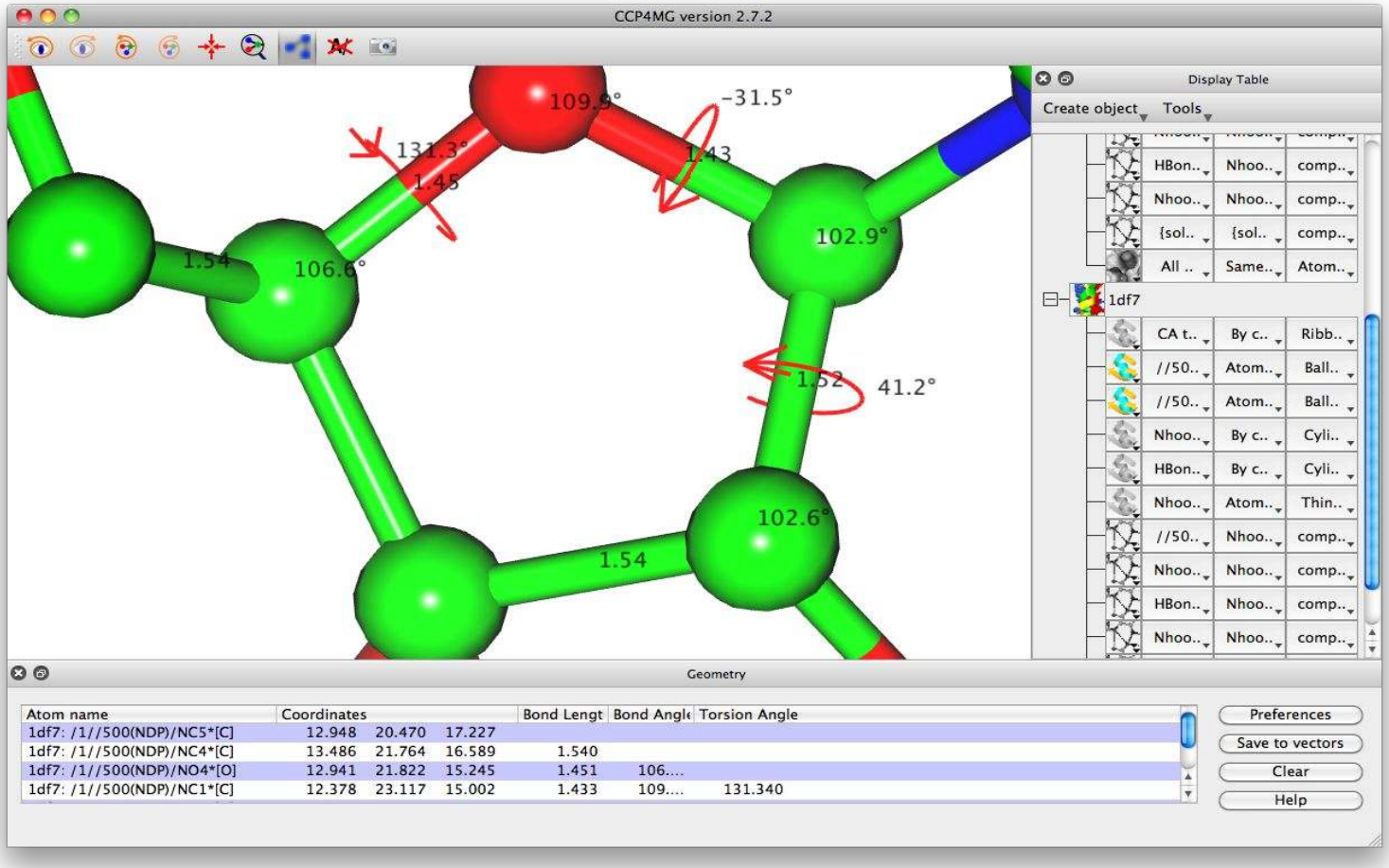
- Real-time shadows and occlusion and “perfect spheres” mean OpenGL is now arguably a better choice for rendering than “Render” module.
- Screenshot pros:
  - Shadows make “Render” slow, but bearable.
  - Ambient occlusion makes “Render” really, really slow.
  - Darkness of OpenGL shadows could be changeable, “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.
  - “Perfect spheres” are not anti-aliased (smoothed) - 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.)
  - Screenshots do not work with all graphics drivers

# “Batch” rendering

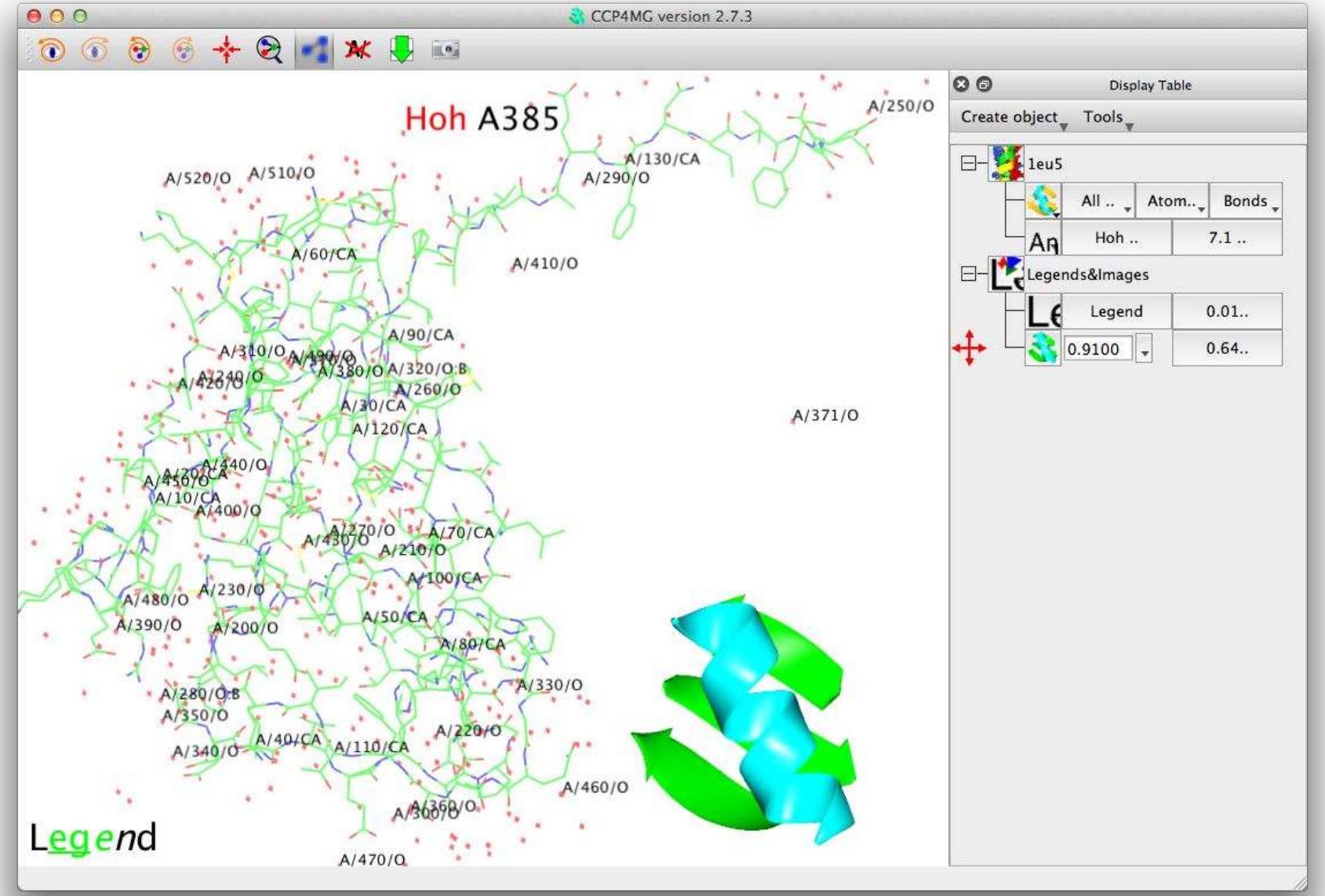
- Images may be rendered from command line or from scripts without starting up the main program.
- `ccp4mg -norestore -picture mypic.mgpic.py -R test.png -RO '{"size":"1600x1600","smoothribbons":"1", "raytrace":"1"}' -quit`
- The file mypic.mpic.py is a file containing a scene description: lists of data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

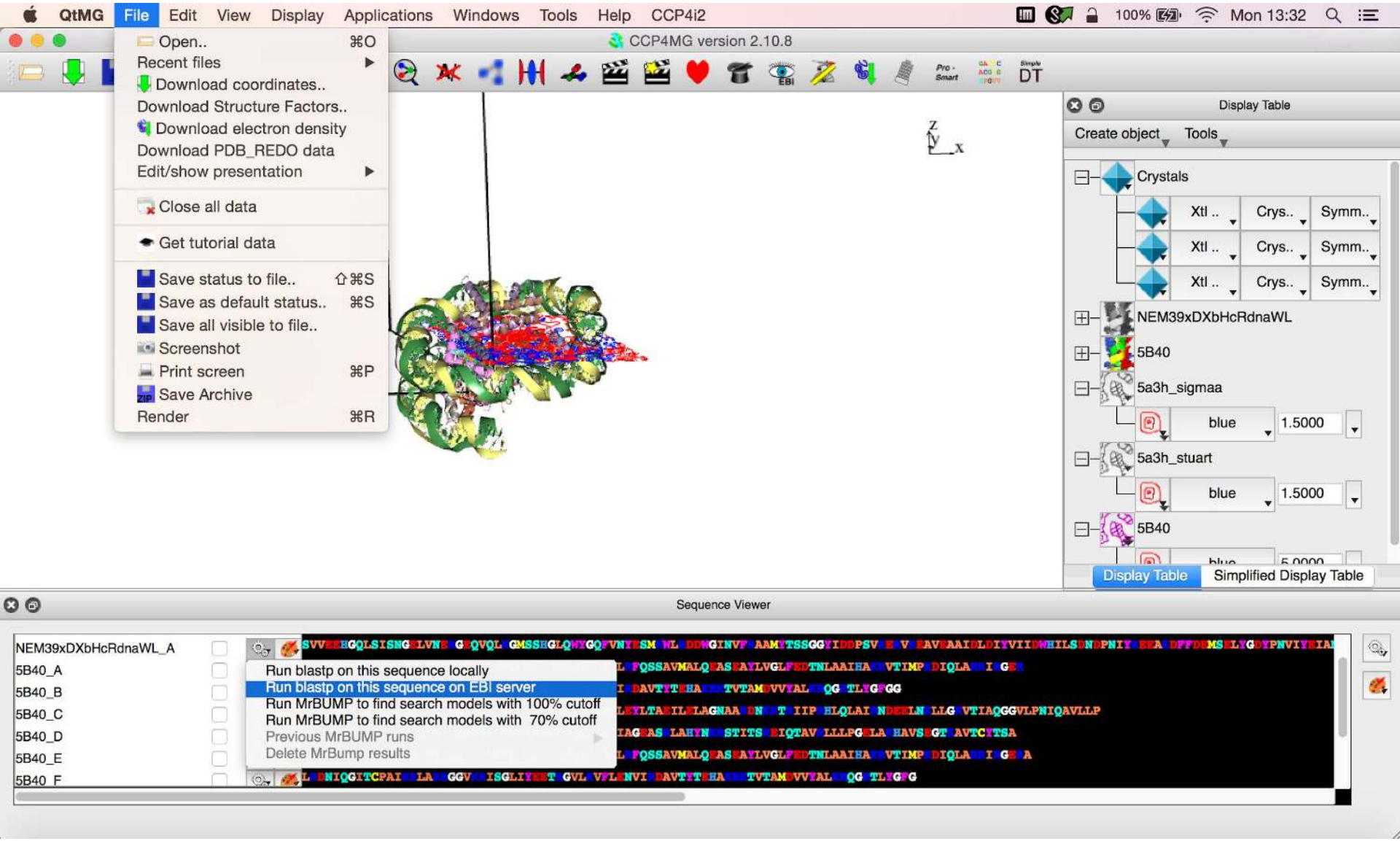


# On screen text and images



# 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
- Blast searches (EBI)

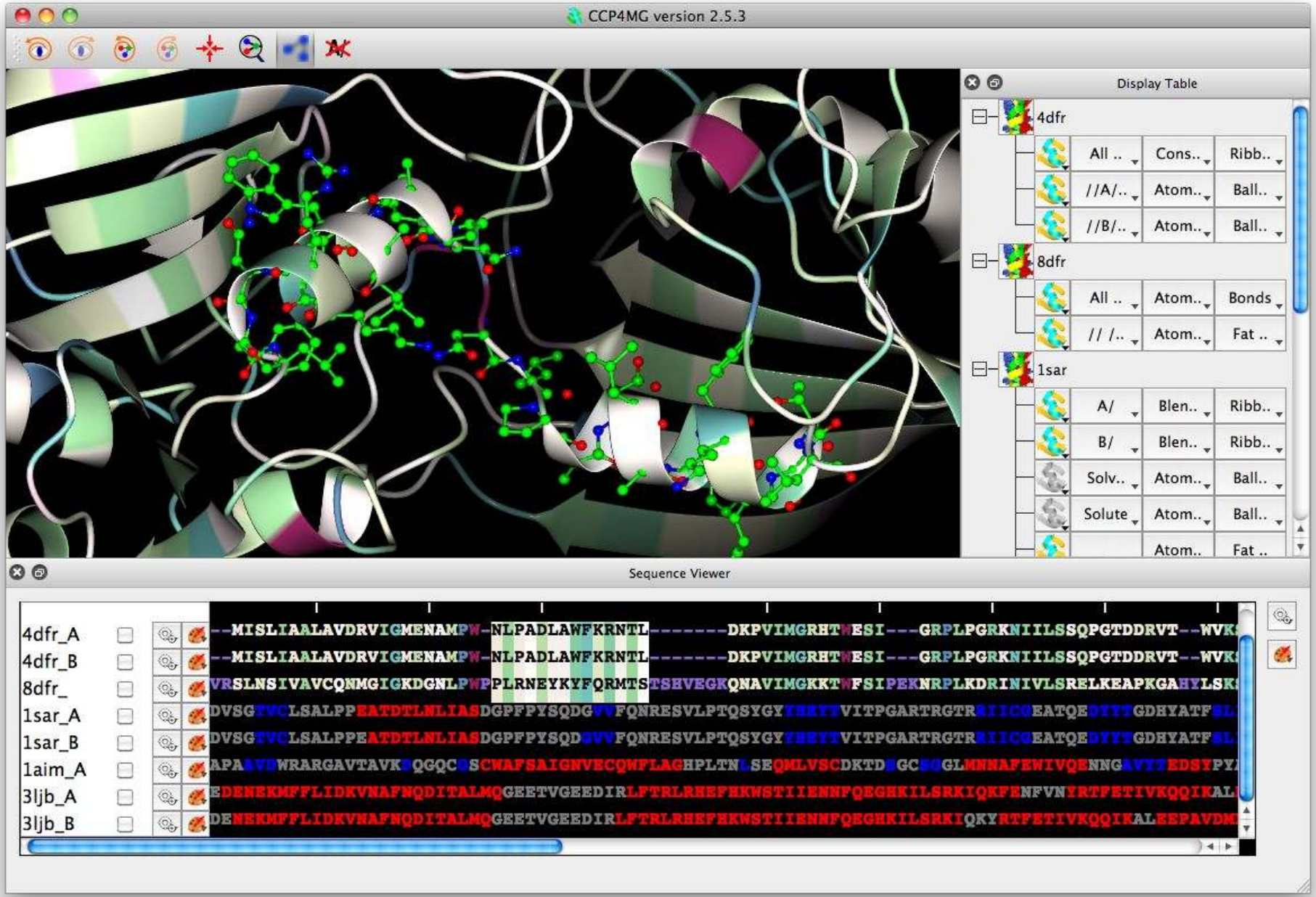

QtMG
File
Edit
View
Display
Applications
Windows
Tools
Help
CCP4i2
Mon 13:32
CCP4MG version 2.10.8
Open..
Recent files
Download coordinates..
Download Structure Factors..
Download electron density
Download PDB_REDO data
Edit/show presentation
Close all data
Get tutorial data
Save status to file..
Save as default status..
Save all visible to file..
Screenshot
Print screen
Save Archive
Render
Display Table
Create object
Tools
Crystals
Xtl ..
Crys..
Symm..
NEM39xDXbHcRdnaWL
5B40
5a3h_sigmaa
blue
1.5000
5a3h_stuart
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

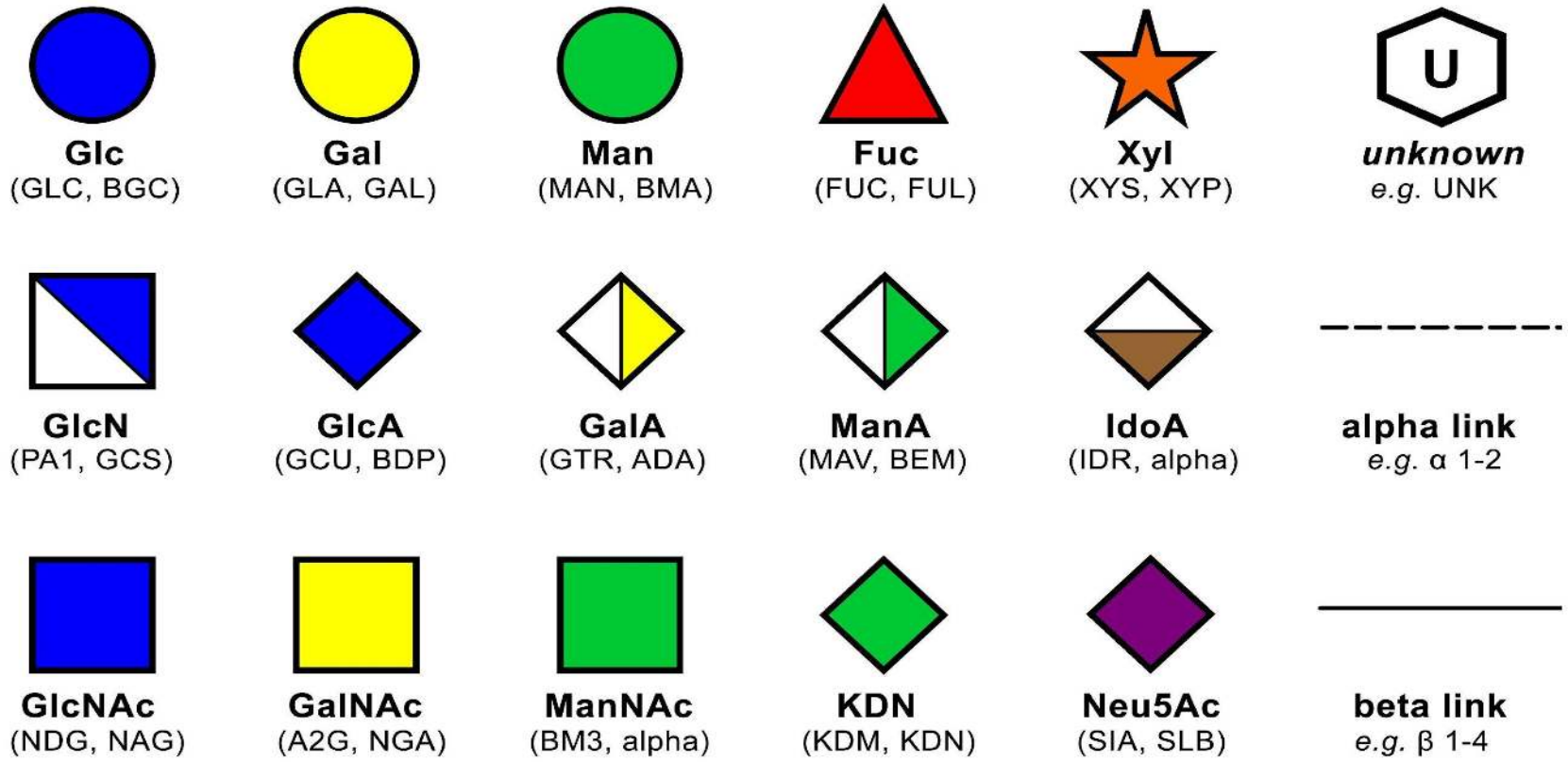
- Align sequences using muscle (a free multiple-alignment program) or ClustalW.
- Continuous (consurf style) or discrete traffic-light colour by conservation.
- Colour by secondary structure.
- Blastn/blastp interface. Blast results cached between sessions. Blast normally run remotely (EBI) with explicit 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 | $ASN_{A/62}$

N-linked glycosylation

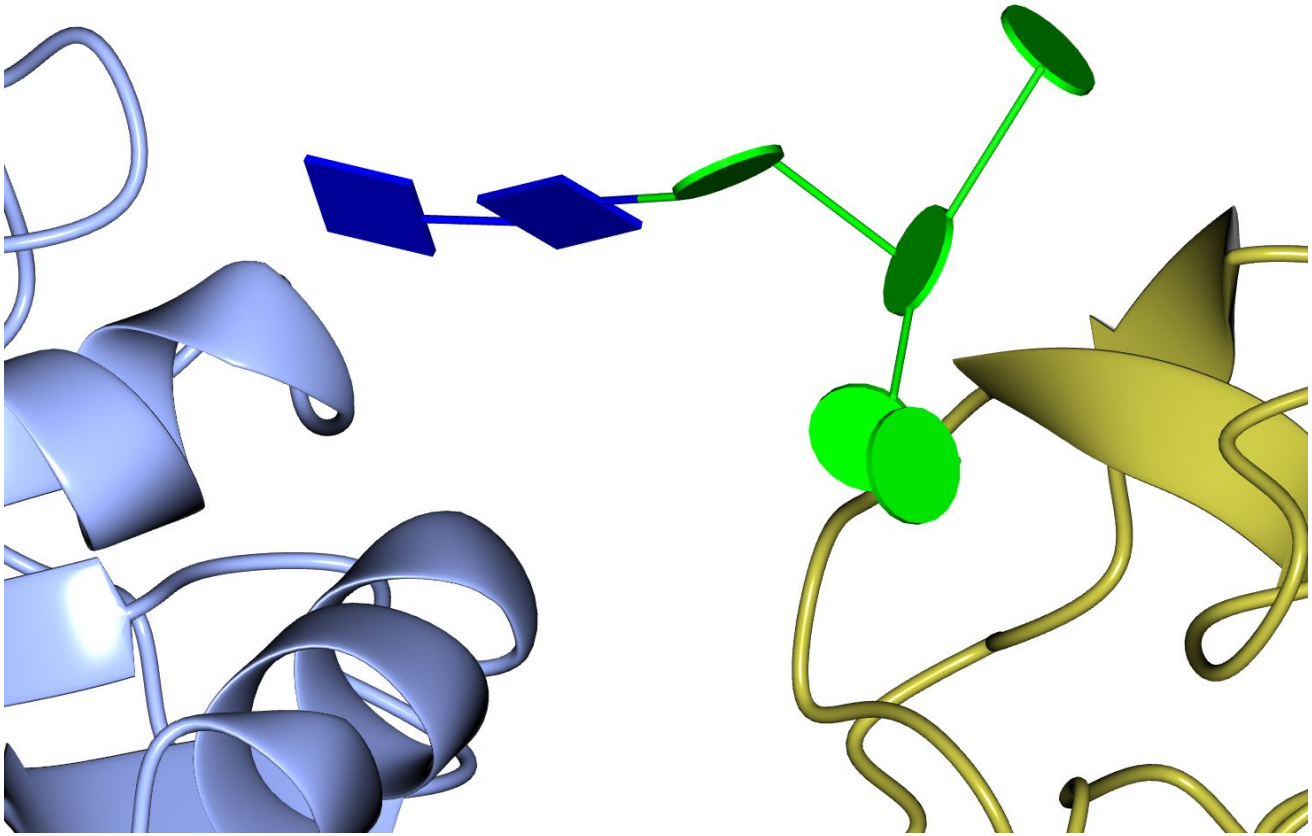
o | $THR_{T/1000}$

O-linked glycosylation

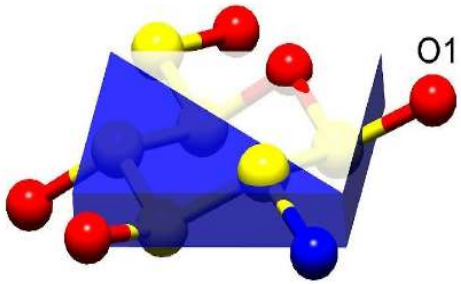
s | $CYS_{C/4}$

S-linked glycosylation

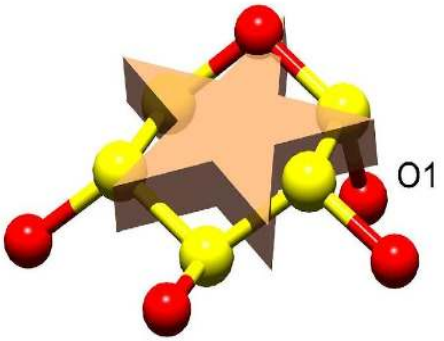
# Saccharide display



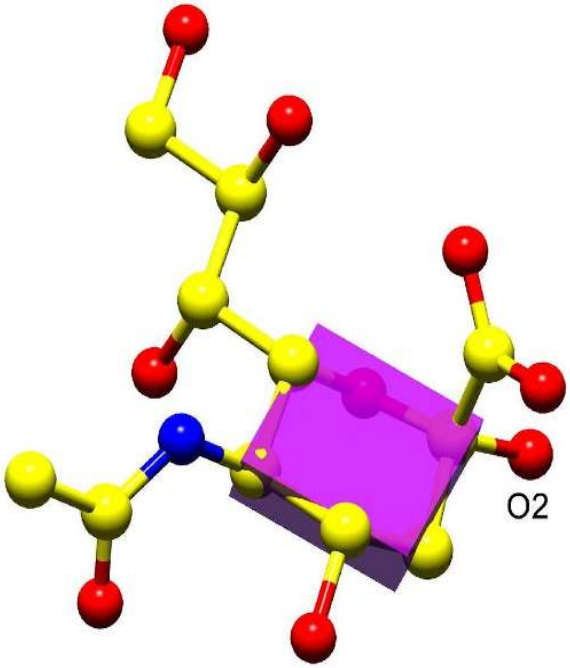
# Saccharide display



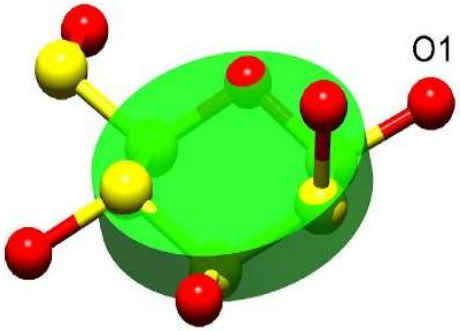

**β-D-Glucosamine**
(GCS)



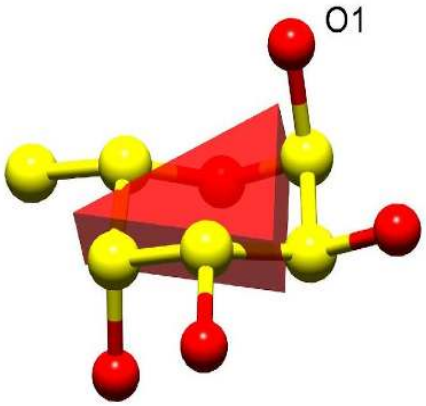

**α-D-Xylopyranose**
(XYS)




**N-acetyl α-L-Neuraminic Acid**
(SIA)

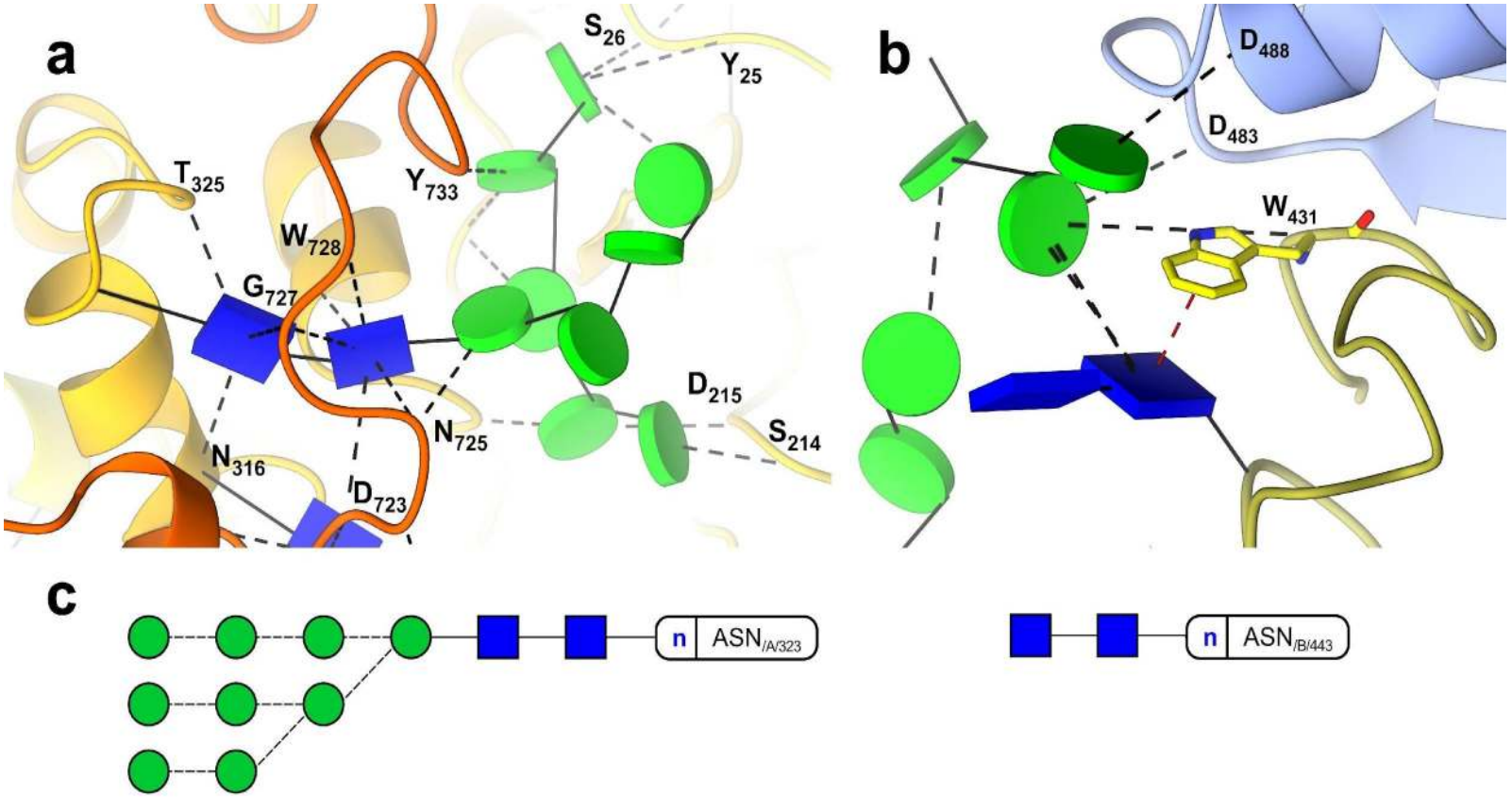



**β-D-Mannose**
(BMA)




**α-L-Fucose**
(FUC)

# Saccharide display

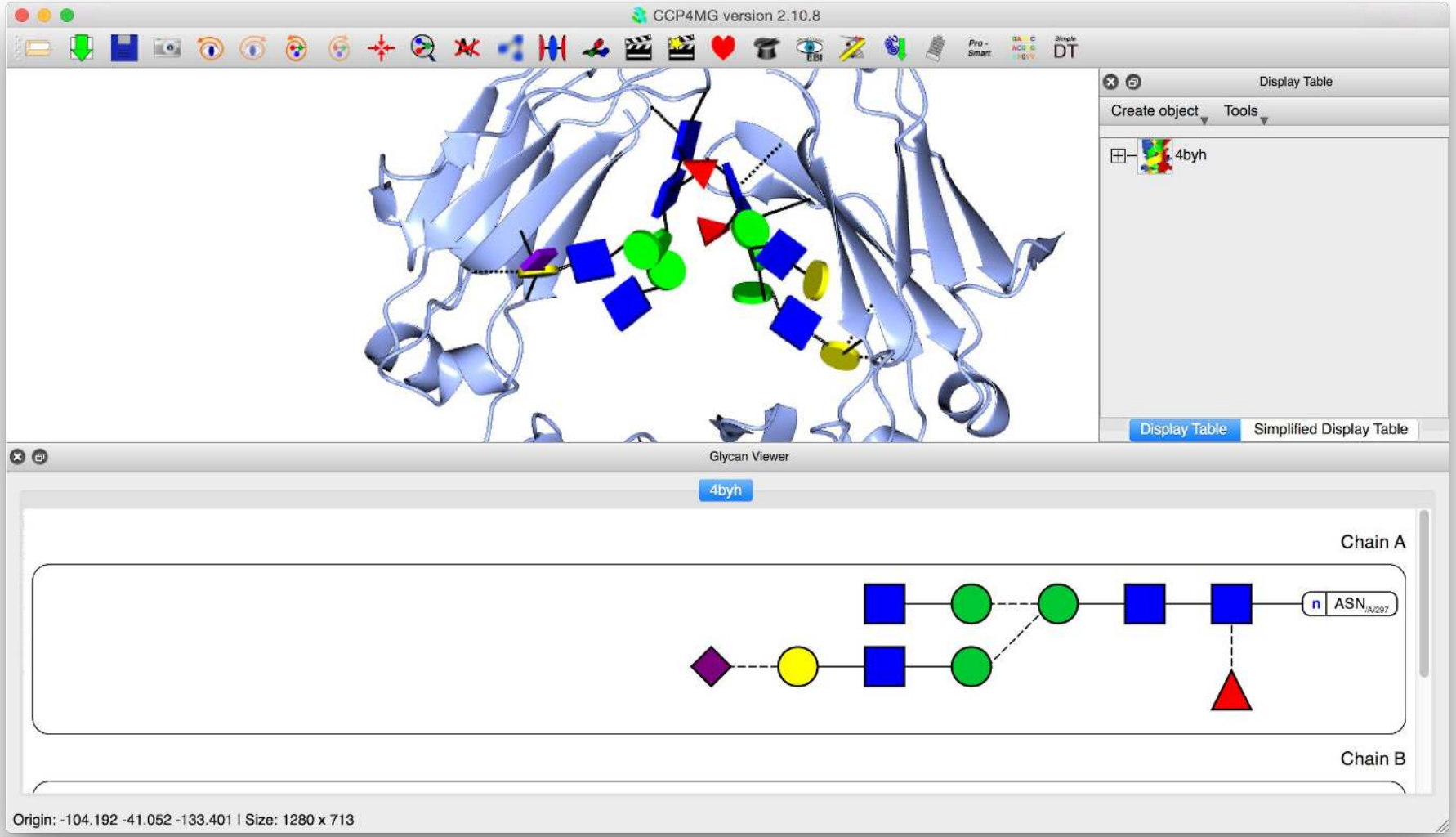



Hydrogen bonds to multiple domains.

GlcNAc to TRP stacking interaction.

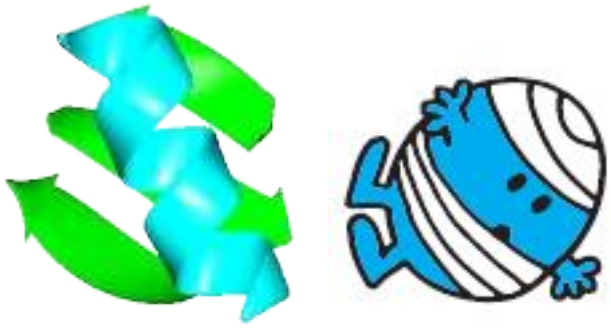
5FJJ, Agirre et. al., *Acta Crystallogr D Struct Biol* **72**, 254-265 (2016)

# 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

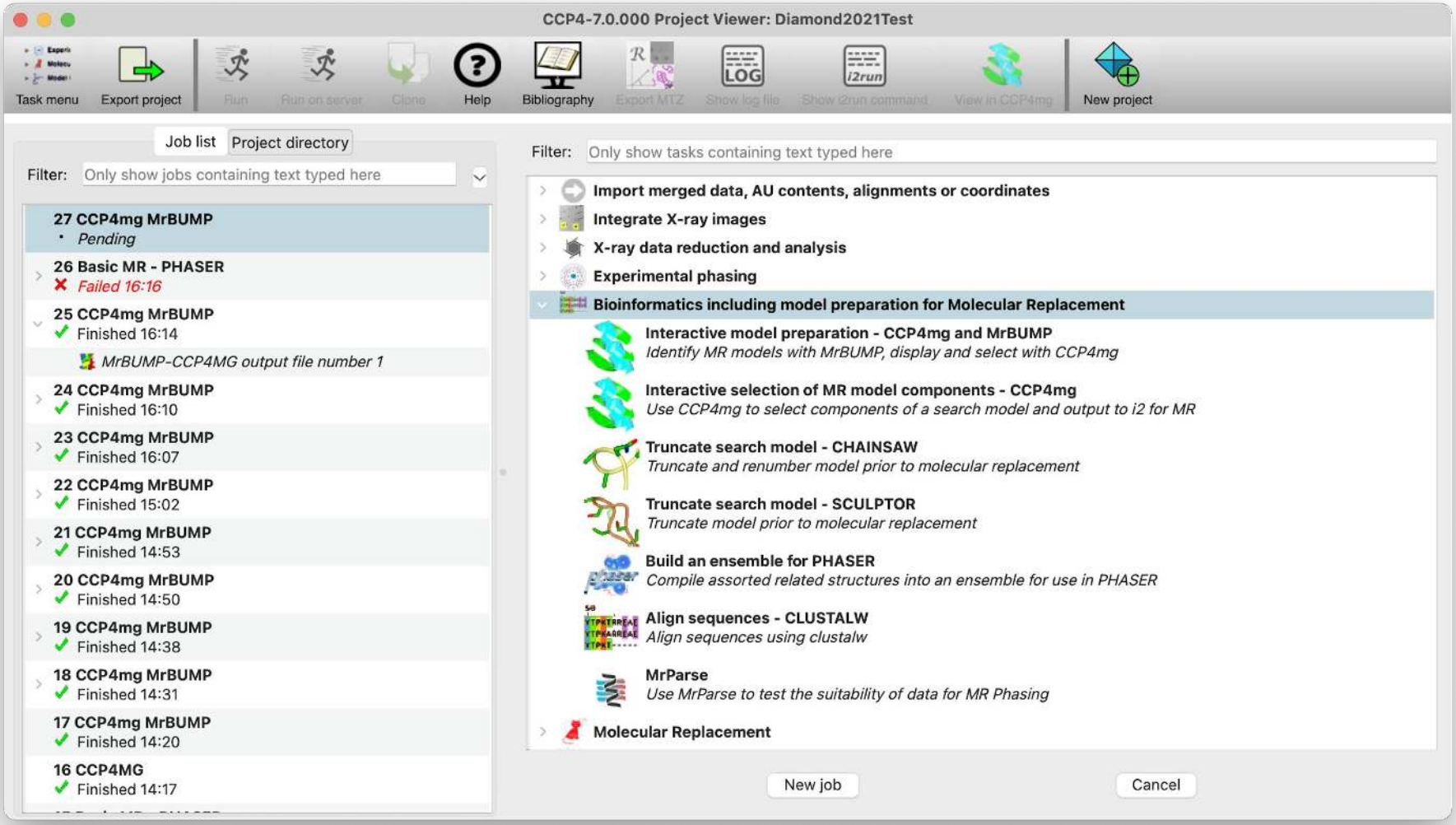
- Goal is to provide i2 users with a graphical driven interface to the model search and preparation steps for molecular replacement in MrBUMP. The intention is to derive a graphically-informed single “best” search model for passing back to i2 and the Phaser/Molrep interfaces

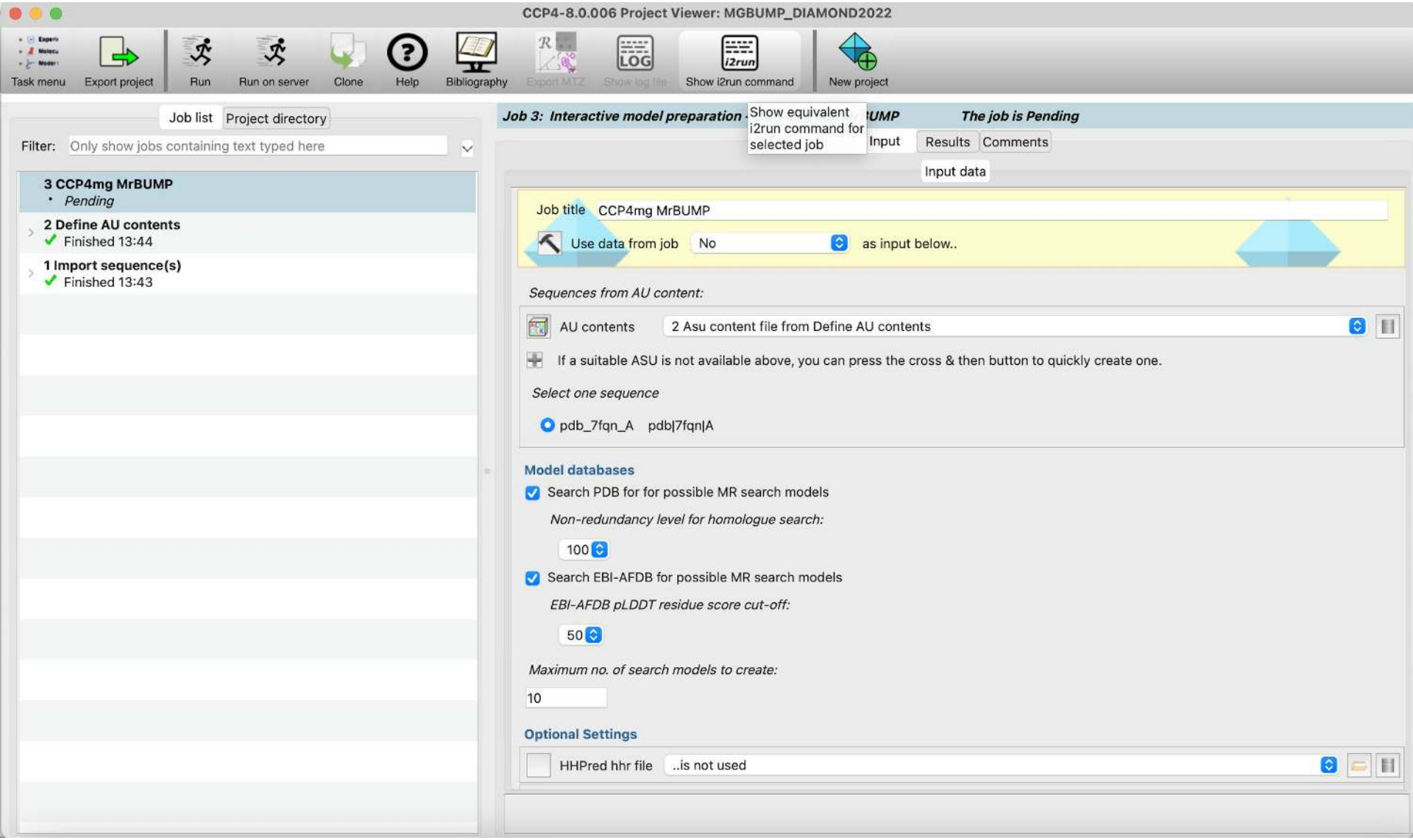
# CCP4MG and MrBUMP

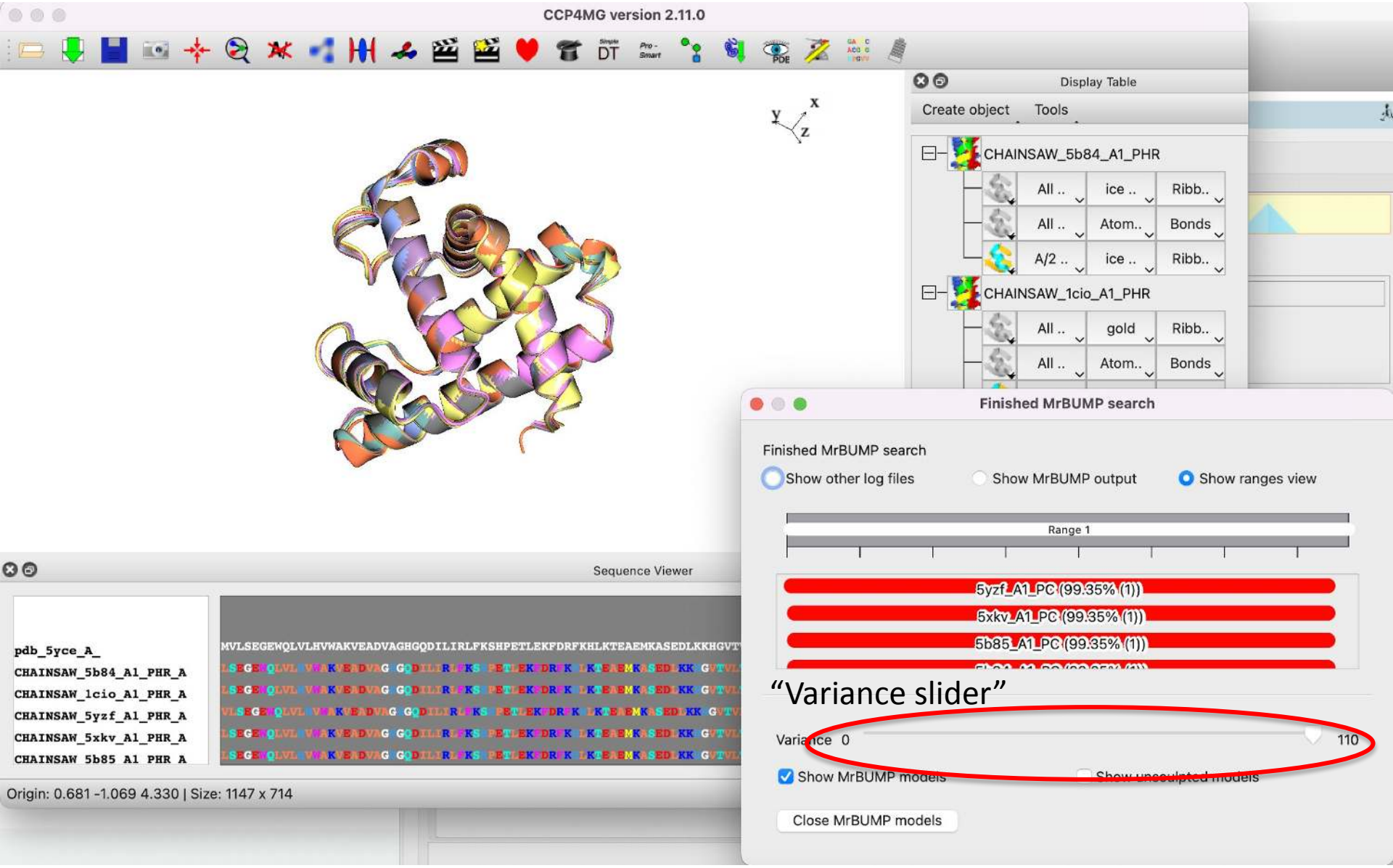
- CCP4MG uses initial steps of the MrBUMP to interactively edit molecular replacement models.
- Scheme:
  - MrBUMP is sent a sequence from CCP4MG
  - uses the phmmer tool to search for homologous structures with a maximum similarity between them of 100%, 95%, 90%, 70% or 50%.
  - select just the relevant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

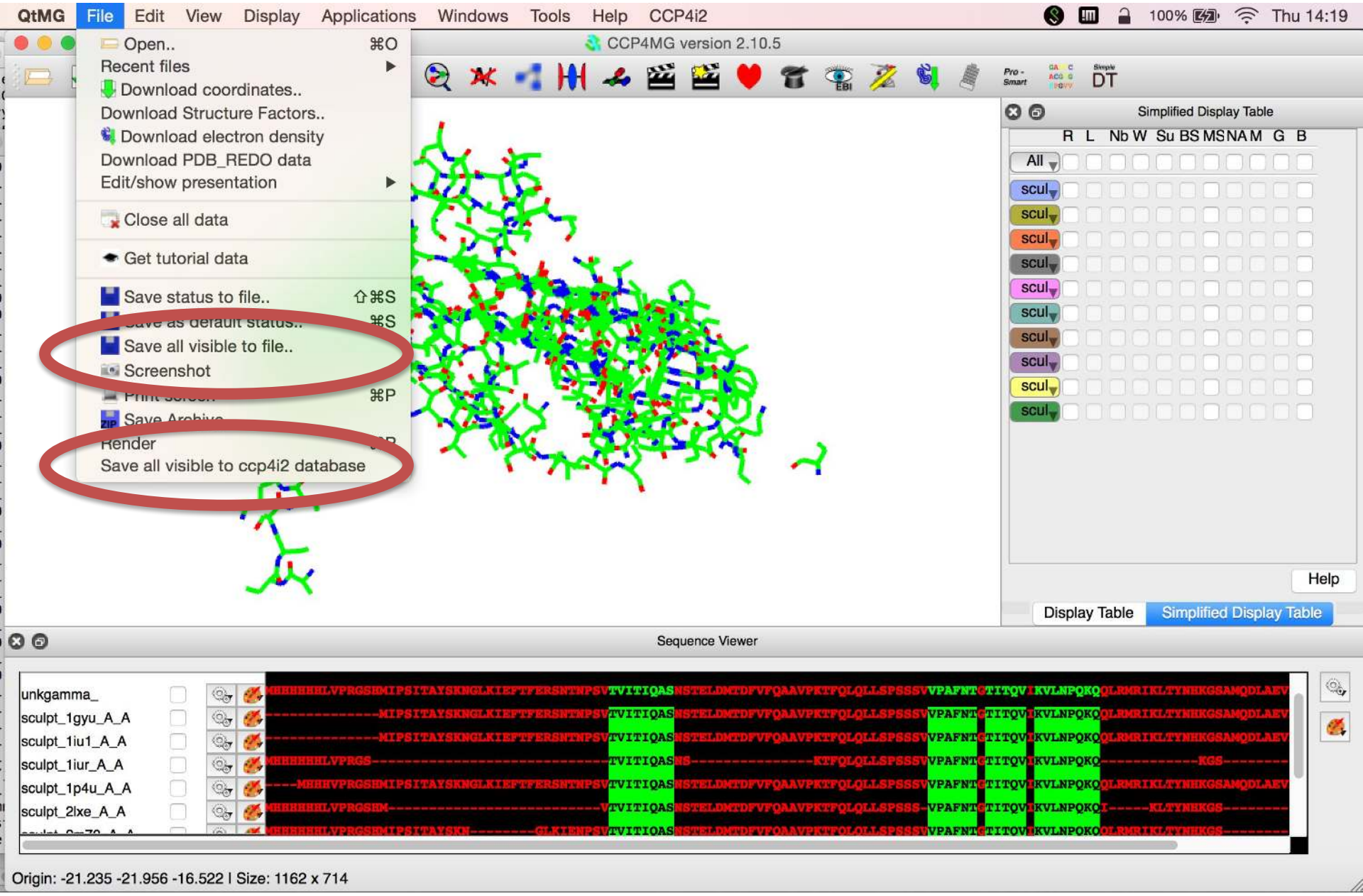
# CCP4MG and MrBUMP

- 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.


CCP4-7.0.000 Project Viewer: Diamond2021Test
Task menu
Export project
Run
Run on server
Clone
Help
Bibliography
Export MTZ
Show log file
Show i2run command
View in CCP4mg
New project
Job list
Project directory
Filter:
Only show jobs containing text typed here
27 CCP4mg MrBUMP
Pending
26 Basic MR - PHASER
Failed 16:16
25 CCP4mg MrBUMP
Finished 16:14
MrBUMP-CCP4MG output file number 1
24 CCP4mg MrBUMP
Finished 16:10
23 CCP4mg MrBUMP
Finished 16:07
22 CCP4mg MrBUMP
Finished 15:02
21 CCP4mg MrBUMP
Finished 14:53
20 CCP4mg MrBUMP
Finished 14:50
19 CCP4mg MrBUMP
Finished 14:38
18 CCP4mg MrBUMP
Finished 14:31
17 CCP4mg MrBUMP
Finished 14:20
16 CCP4MG
Finished 14:17
Filter:
Only show tasks containing text typed here
Import merged data, AU 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
MrParse
Use MrParse to test the suitability of data for MR Phasing
Molecular Replacement
New job
Cancel


CCP4-8.0.006 Project Viewer: MGBUMP_DIAMOND2022
Task menu
Export project
Run
Run on server
Clone
Help
Bibliography
Export MTZ
Show log file
Show i2run command
New project
Job list
Project directory
Filter:
Only show jobs containing text typed here
3 CCP4mg MrBUMP
Pending
2 Define AU contents
Finished 13:44
1 Import sequence(s)
Finished 13:43
Job 3: Interactive model preparation
The job is Pending
Show equivalent i2run command for selected job
Input
Results
Comments
Input data
Job title
CCP4mg MrBUMP
Use data from job
No
as input below..
Sequences from AU content:
AU contents
2 Asu content file from Define AU contents
If a suitable ASU is not available above, you can press the cross & then button to quickly create one.
Select one sequence
pdb_7fqn_A
pdb|7fqn|A
Model databases
Search PDB for for possible MR search models
Non-redundancy level for homologue search:
100
Search EBI-AFDB for possible MR search models
EBI-AFDB pLDDT residue score cut-off:
50
Maximum no. of search models to create:
10
Optional Settings
HHPred hhr file
..is not used


CCP4MG version 2.11.0
Display Table
Create object
Tools
CHAINSAW_5b84_A1_PHR
All ..
ice ..
Ribb..
All ..
Atom..
Bonds
A/2 ..
ice ..
Ribb..
CHAINSAW_1cio_A1_PHR
All ..
gold
Ribb..
All ..
Atom..
Bonds
Finished MrBUMP search
Finished MrBUMP search
Show other log files
Show MrBUMP output
Show ranges view
Range 1
5yzf_A1_PC (99.35% (1))
5xkv_A1_PC (99.35% (1))
5b85_A1_PC (99.35% (1))
"Variance slider"
Variance 0
110
Show MrBUMP models
Close MrBUMP models
Sequence Viewer
pdb_5yce_A_
CHAINSAW_5b84_A1_PHR_A
CHAINSAW_1cio_A1_PHR_A
CHAINSAW_5yzf_A1_PHR_A
CHAINSAW_5xkv_A1_PHR_A
CHAINSAW_5b85_A1_PHR_A
MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHPETLEKFDRFKHLKTEAEMKASEDLKKHGVT
Origin: 0.681 -1.069 4.330 | Size: 1147 x 714


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
⌘S
Save all visible to file..
Screenshot
⌘P
Render
Save all visible to ccp4i2 database
Simplified Display Table
R L Nb W Su BS MS NA M G B
All
Help
Display Table
Simplified Display Table
Sequence Viewer
unkgamma_
sculpt_1gyu_A_A
sculpt_1iu1_A_A
sculpt_1iur_A_A
sculpt_1p4u_A_A
sculpt_2lxe_A_A
Origin: -21.235 -21.956 -16.522 | Size: 1162 x 714

# Other details

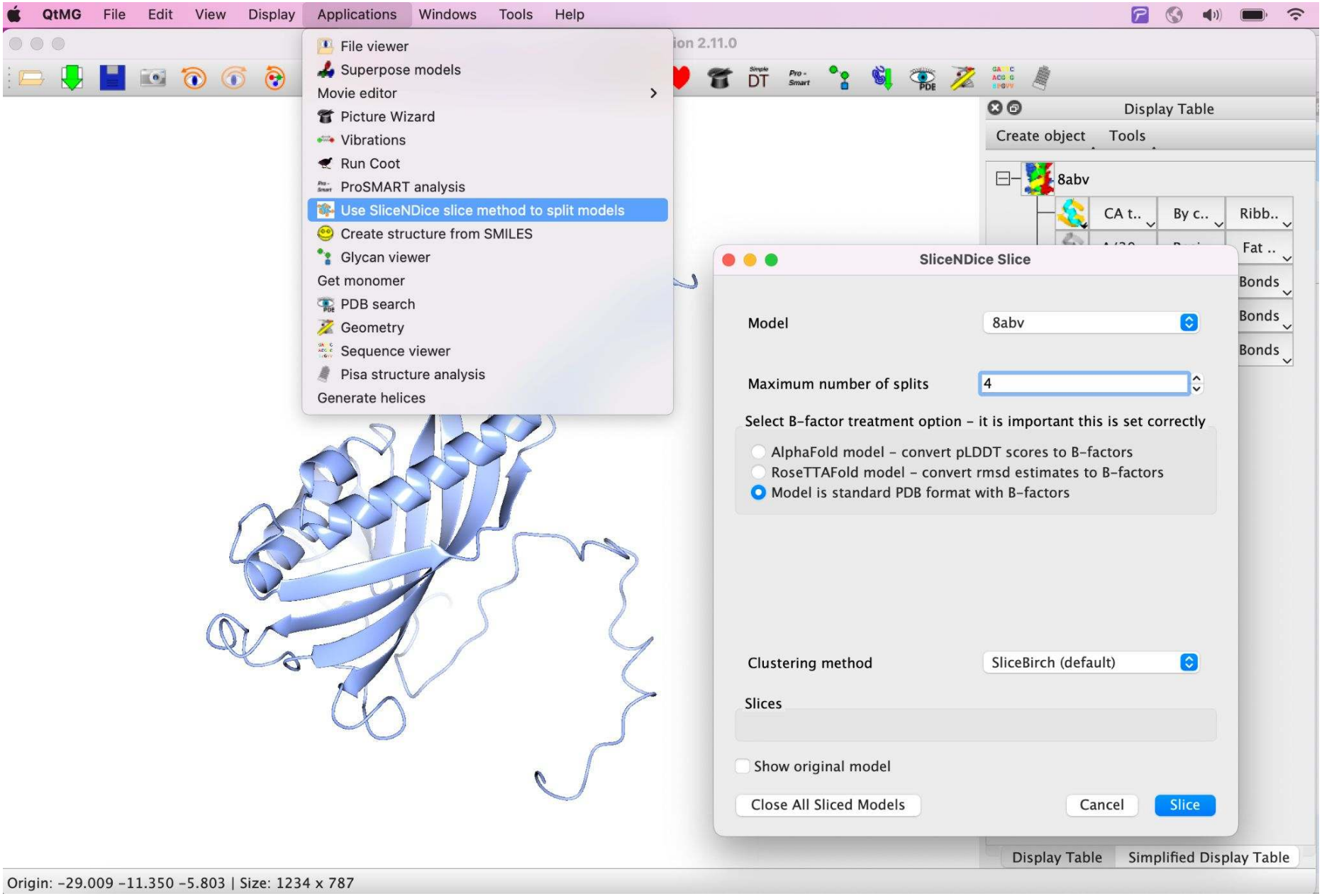
- Only final ensemble (or individual structures) are saved to i2 database. All MrBUMP results and model are save in ~/.CCP4MG/mrbump_results.
- Results from previous jobs can be loaded in later sessions without having to rerun the MrBUMP search.
- Results can be deleted when no longer of interest.

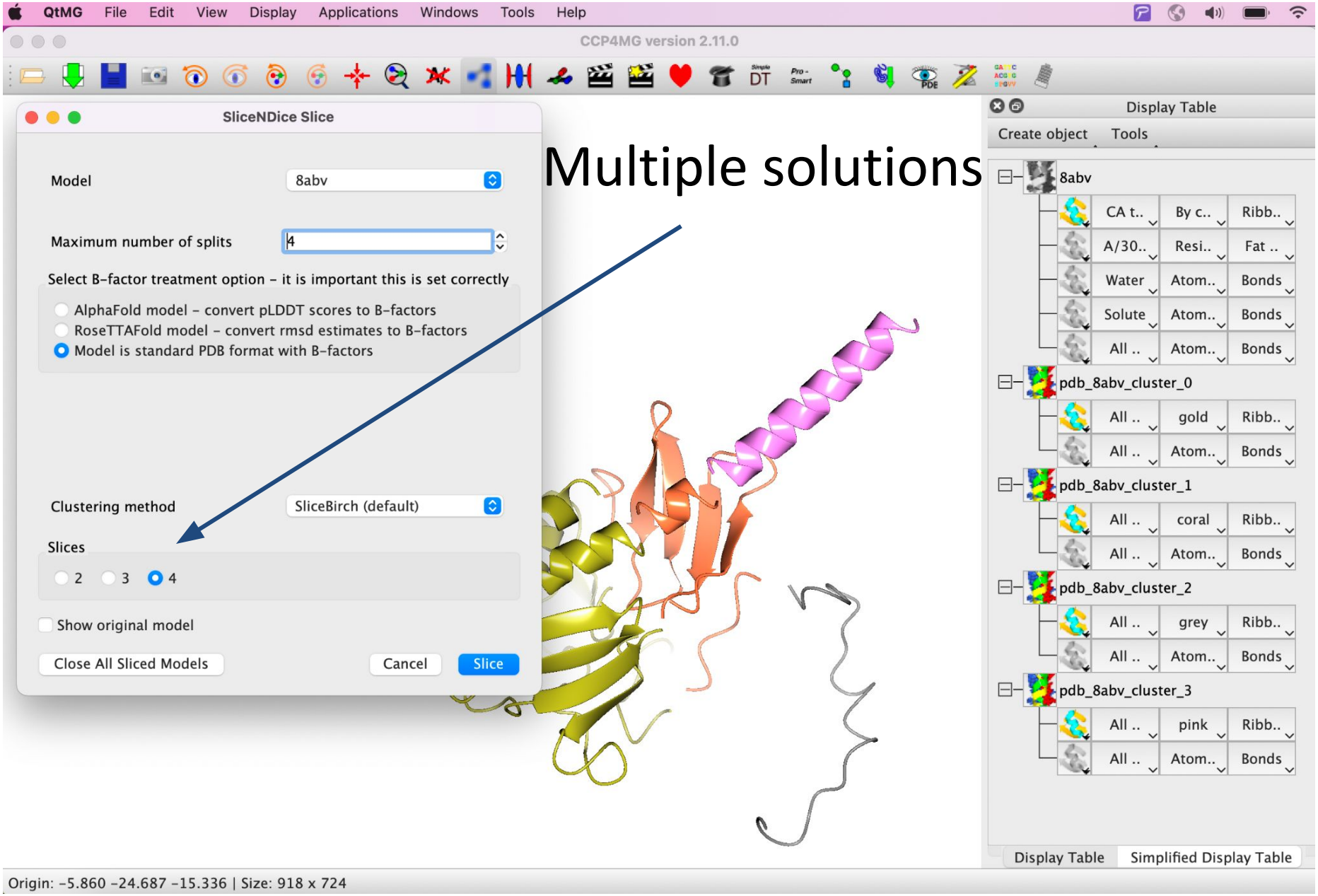
# Model Slicing

Often it is convenient to split a coordinate file into smaller sections which may be more useful models for molecular replacement. e.g. Your input model and the final model you desire may be homologues in different conformations. By splitting the model the different parts are able to adopt different arrangements in MR.

# Slice(NDice)

- CCP4MG uses the “slice” part of the SliceNDice program (Simkin et al.) to do this. *Acta Cryst.* (2023). D**79**, 806-819
- In addition to a coordinate file you have to provide some options:
  - The maximum number of splits
  - What type of coordinate file you are supplying (standard PDB format, AlphaFold, or RosettaFold model).
  - The clustering method to use. There are several - I don’t know the differences between them, but you can try different ones if the default does not help your structure solution.


QtMG
File
Edit
View
Display
Applications
Windows
Tools
Help
File viewer
Superpose models
Movie editor
Picture Wizard
Vibrations
Run Coot
ProSMART analysis
Use SliceNDice slice method to split models
Create structure from SMILES
Glycan viewer
Get monomer
PDB search
Geometry
Sequence viewer
Pisa structure analysis
Generate helices
Display Table
Create object
Tools
8abv
CA t..
By c..
Ribb..
Fat ..
Bonds
Bonds
Bonds
SliceNDice Slice
Model
8abv
Maximum number of splits
4
Select B-factor treatment option - it is important this is set correctly
AlphaFold model - convert pLDDT scores to B-factors
RoseTTAFold model - convert rmsd estimates to B-factors
Model is standard PDB format with B-factors
Clustering method
SliceBirch (default)
Slices
Show original model
Close All Sliced Models
Cancel
Slice
Display Table
Simplified Display Table
Origin: -29.009 -11.350 -5.803 | Size: 1234 x 787


QtMG File Edit View Display Applications Windows Tools Help
CCP4MG version 2.11.0
SliceNDice Slice
Model
8abv
Maximum number of splits
4
Select B-factor treatment option - it is important this is set correctly
AlphaFold model - convert pLDDT scores to B-factors
RoseTTAFold model - convert rmsd estimates to B-factors
Model is standard PDB format with B-factors
Clustering method
SliceBirch (default)
Slices
2
3
4
Show original model
Close All Sliced Models
Cancel
Slice
Multiple solutions
Display Table
Create object
Tools
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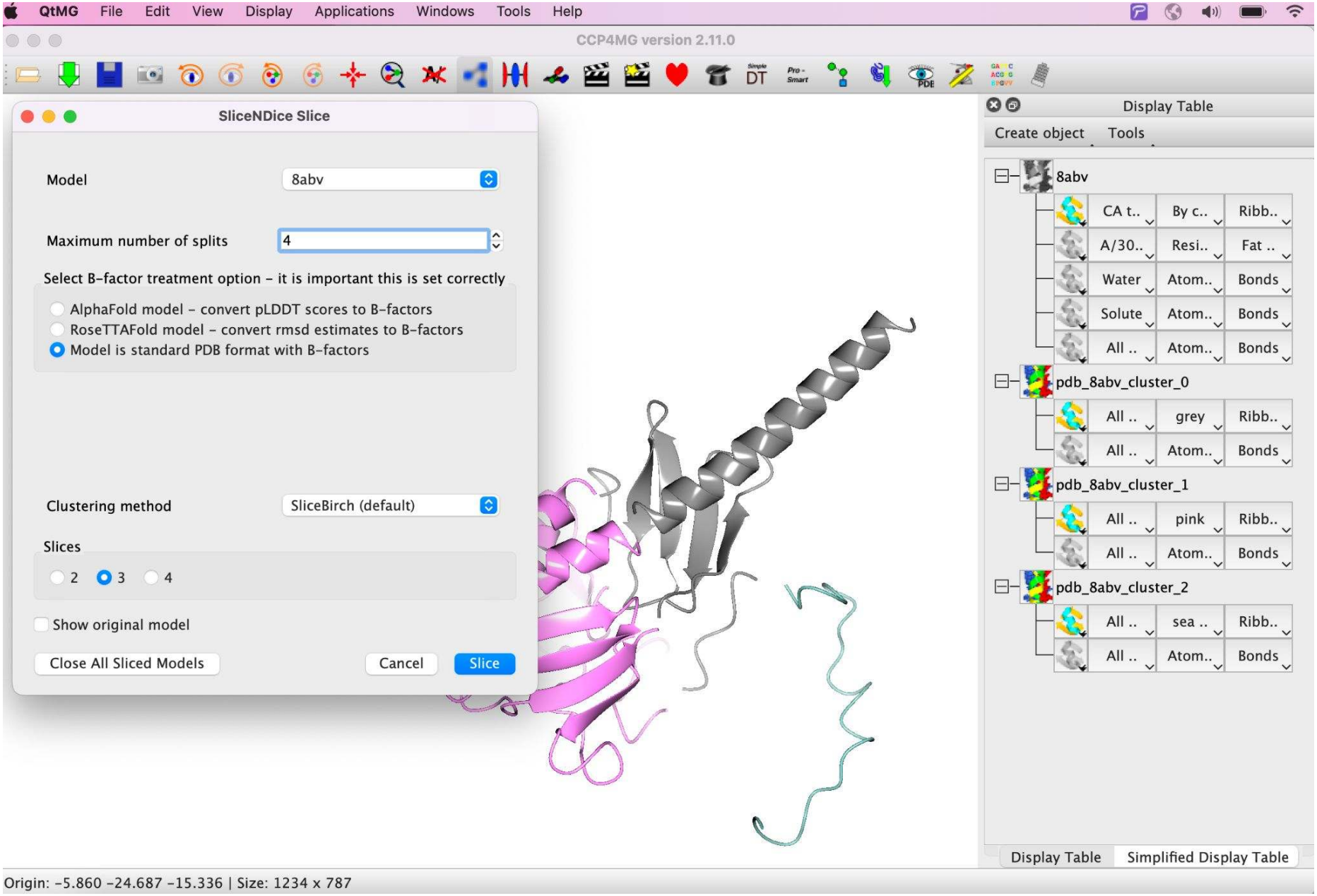
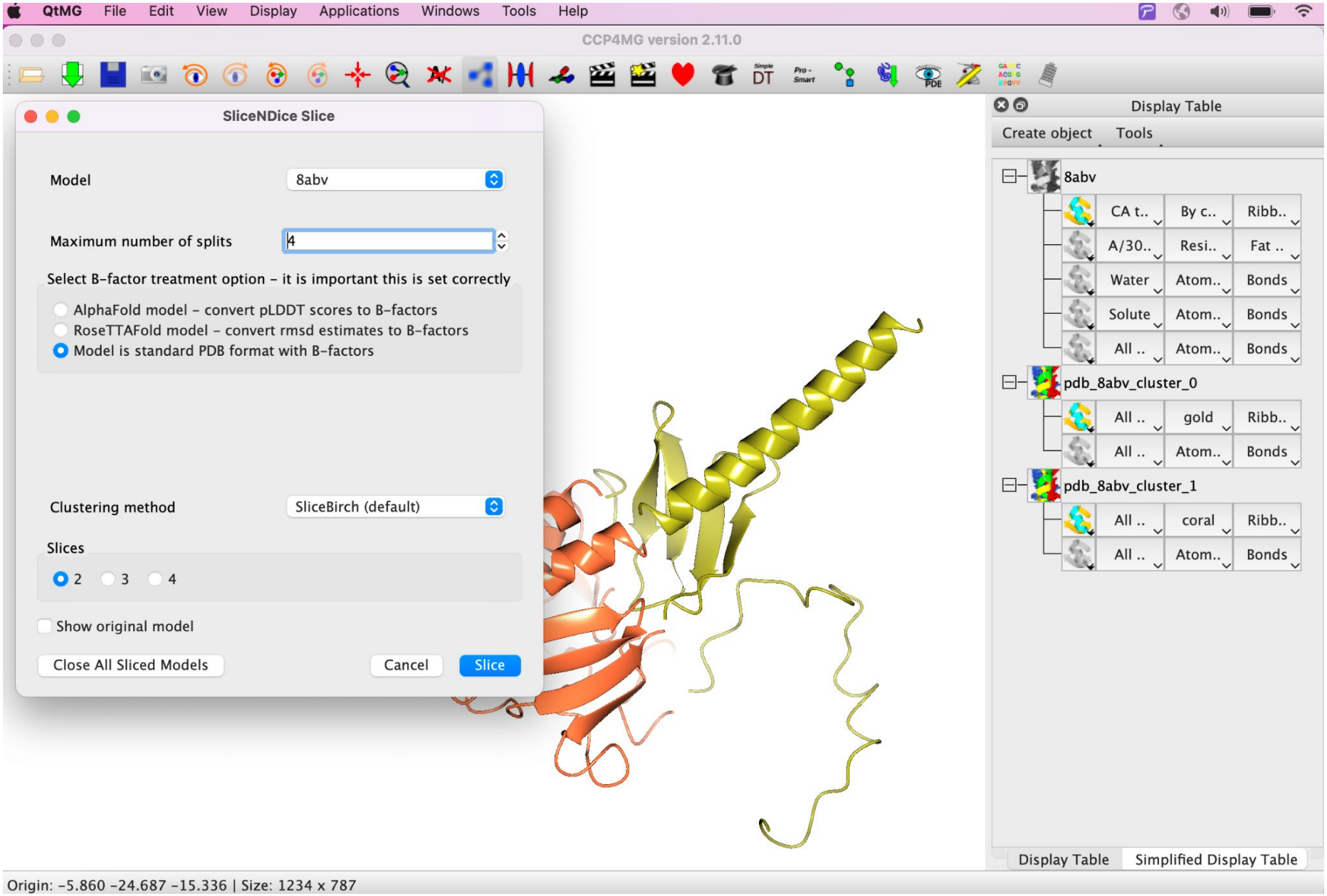
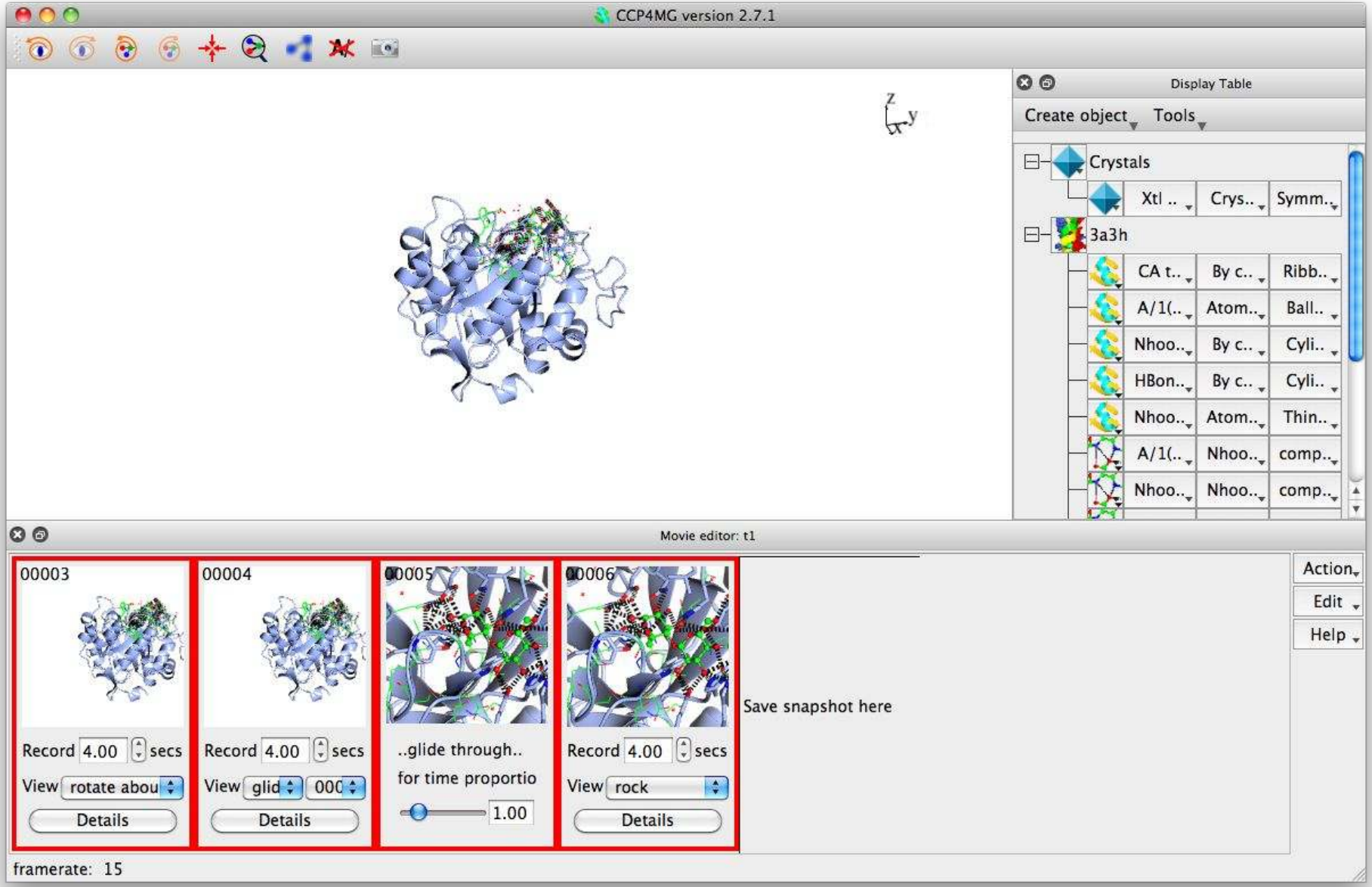
By c..
Ribb..
A/30..
Resi..
Fat ..
Water
Atom..
Bonds
Solute
Atom..
Bonds
All ..
Atom..
Bonds
pdb_8abv_cluster_0
All ..
gold
Ribb..
All ..
Atom..
Bonds
pdb_8abv_cluster_1
All ..
coral
Ribb..
All ..
Atom..
Bonds
pdb_8abv_cluster_2
All ..
grey
Ribb..
All ..
Atom..
Bonds
pdb_8abv_cluster_3
All ..
pink
Ribb..
All ..
Atom..
Bonds
Display Table
Simplified Display Table
Origin: -5.860 -24.687 -15.336 | Size: 918 x 724


QtMG File Edit View Display Applications Windows Tools Help
CCP4MG version 2.11.0
SliceNDice Slice
Model
8abv
Maximum number of splits
4
Select B-factor treatment option – it is important this is set correctly
AlphaFold model – convert pLDDT scores to B-factors
RoseTTAFold model – convert rmsd estimates to B-factors
Model is standard PDB format with B-factors
Clustering method
SliceBirch (default)
Slices
2
3
4
Show original model
Close All Sliced Models
Cancel
Slice
Display Table
Create object
Tools
8abv
CA t..
By c..
Ribb..
A/30..
Resi..
Fat ..
Water
Atom..
Bonds
Solute
Atom..
Bonds
All ..
Atom..
Bonds
pdb_8abv_cluster_0
All ..
grey
Ribb..
All ..
Atom..
Bonds
pdb_8abv_cluster_1
All ..
pink
Ribb..
All ..
Atom..
Bonds
pdb_8abv_cluster_2
All ..
sea ..
Ribb..
All ..
Atom..
Bonds
Display Table
Simplified Display Table
Origin: -5.860 -24.687 -15.336 | Size: 1234 x 787


QtMG File Edit View Display Applications Windows Tools Help
CCP4MG version 2.11.0
SliceNDice Slice
Model
8abv
Maximum number of splits
4
Select B-factor treatment option - it is important this is set correctly
AlphaFold model - convert pLDDT scores to B-factors
RoseTTAFold model - convert rmsd estimates to B-factors
Model is standard PDB format with B-factors
Clustering method
SliceBirch (default)
Slices
2 3 4
Show original model
Close All Sliced Models
Cancel
Slice
Display Table
Create object
Tools
8abv
CA t..
By c..
Ribb..
A/30..
Resi..
Fat ..
Water
Atom..
Bonds
Solute
Atom..
Bonds
All ..
Atom..
Bonds
pdb_8abv_cluster_0
All ..
gold
Ribb..
All ..
Atom..
Bonds
pdb_8abv_cluster_1
All ..
coral
Ribb..
All ..
Atom..
Bonds
Display Table
Simplified Display Table
Origin: -5.860 -24.687 -15.336 | Size: 1234 x 787

# Movies

- Movies are created 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..
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Nhoo..
comp..
Nhoo..
Nhoo..
comp..
Movie editor: t1
00003
Record 4.00 secs
View rotate abou
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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

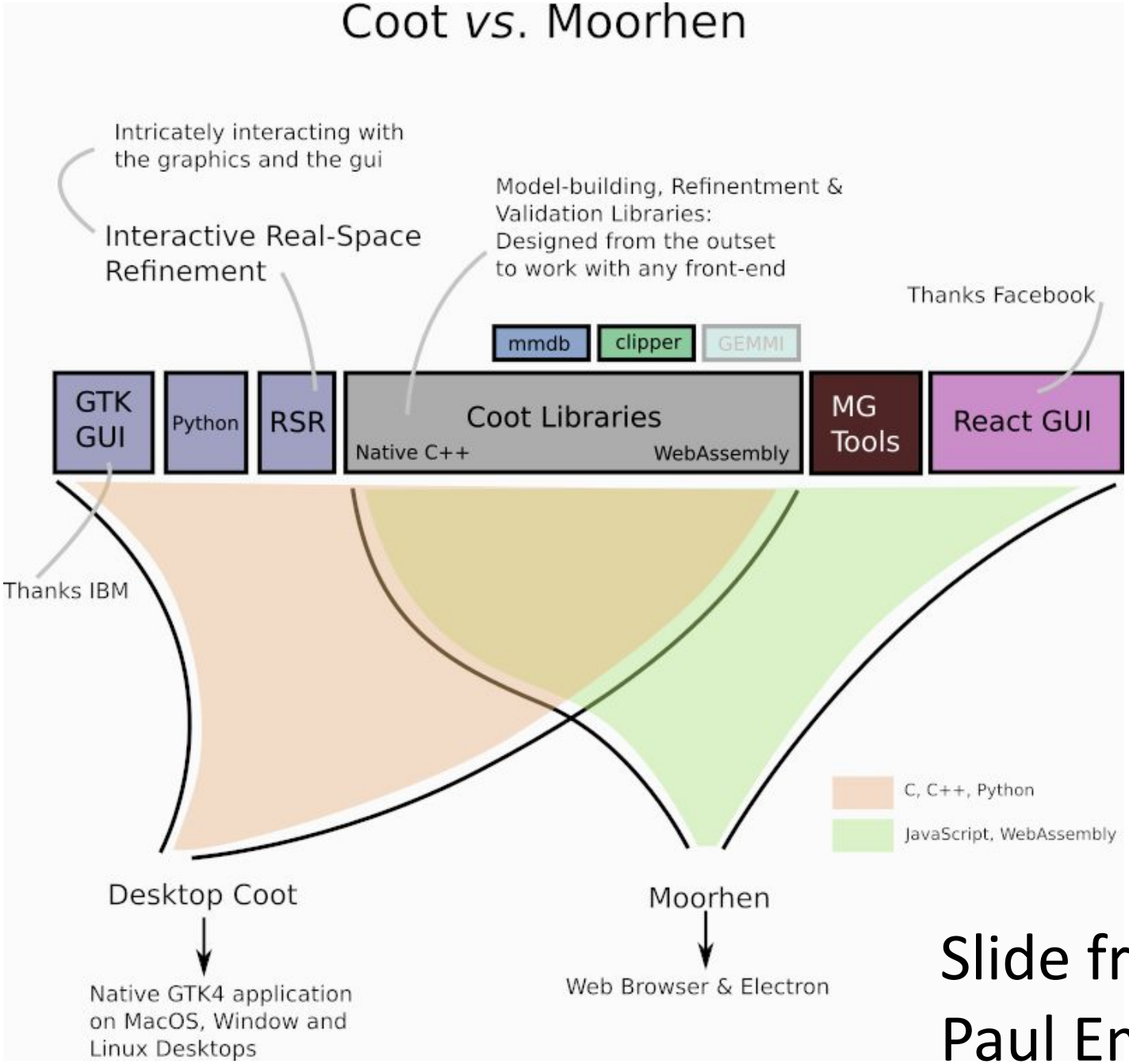
- Distributed with the CCP4 Suite (except for software to compile movies) : http://www.ccp4.ac.uk

# Tutorials

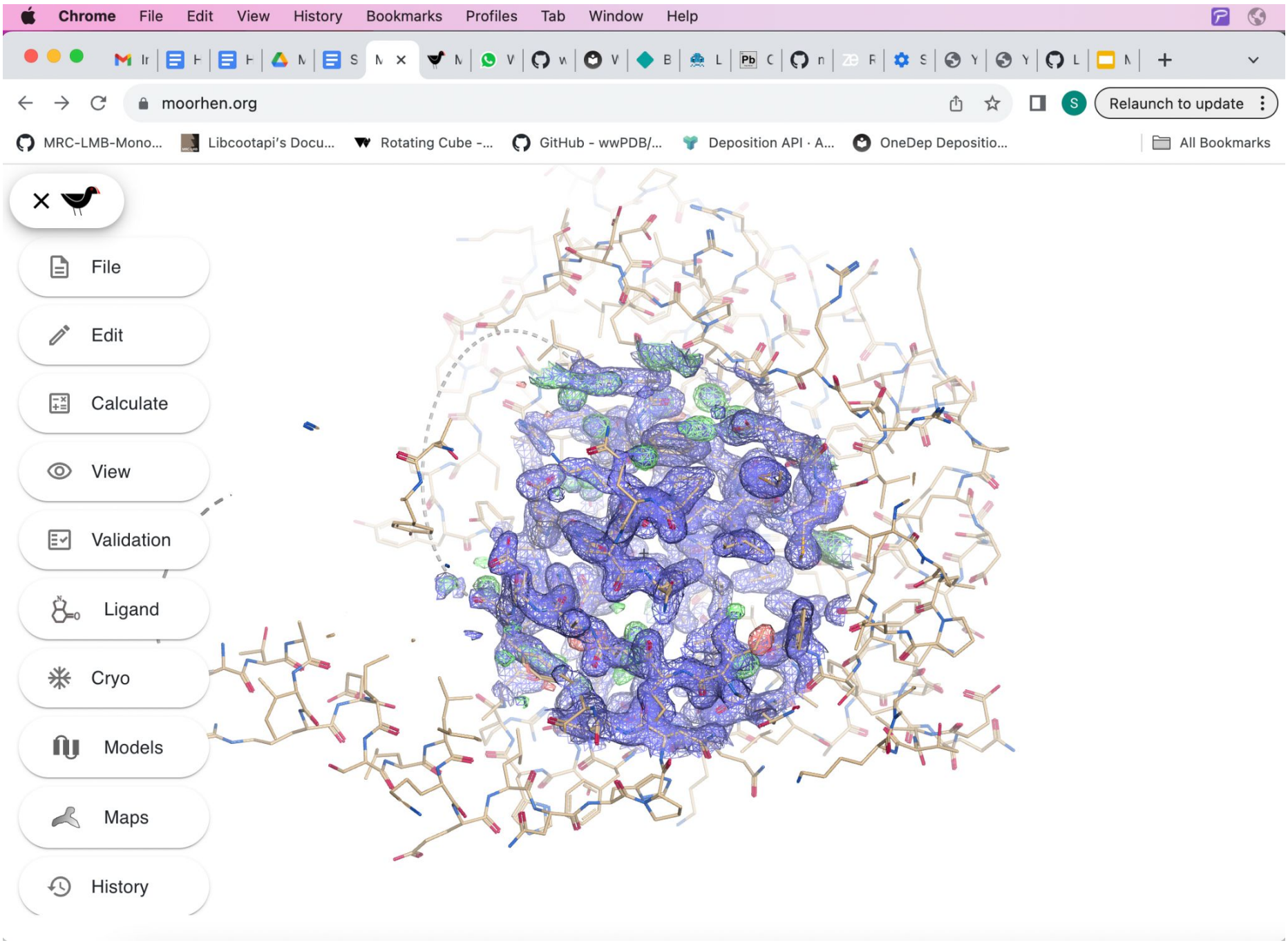
- Various tutorials at https://www.ccp4.ac.uk/MG/ccp4mg_help/tutorial/index.html
- Paul Bond has recently been revising the "main tutorial" (first of the ones in link above): https://paulsbond.co.uk/ccp4mg-tutorial/ I would recommend this.

# The future - Moorhen?

- The intention is that Moorhen(WebCoot) - described last week by Filo - will be able to do everything that CCP4MG can, and thus succeed it.
- This will be both as the https://moorhen.org web site and a desktop “Electron” application.




Slide from Paul Emsley

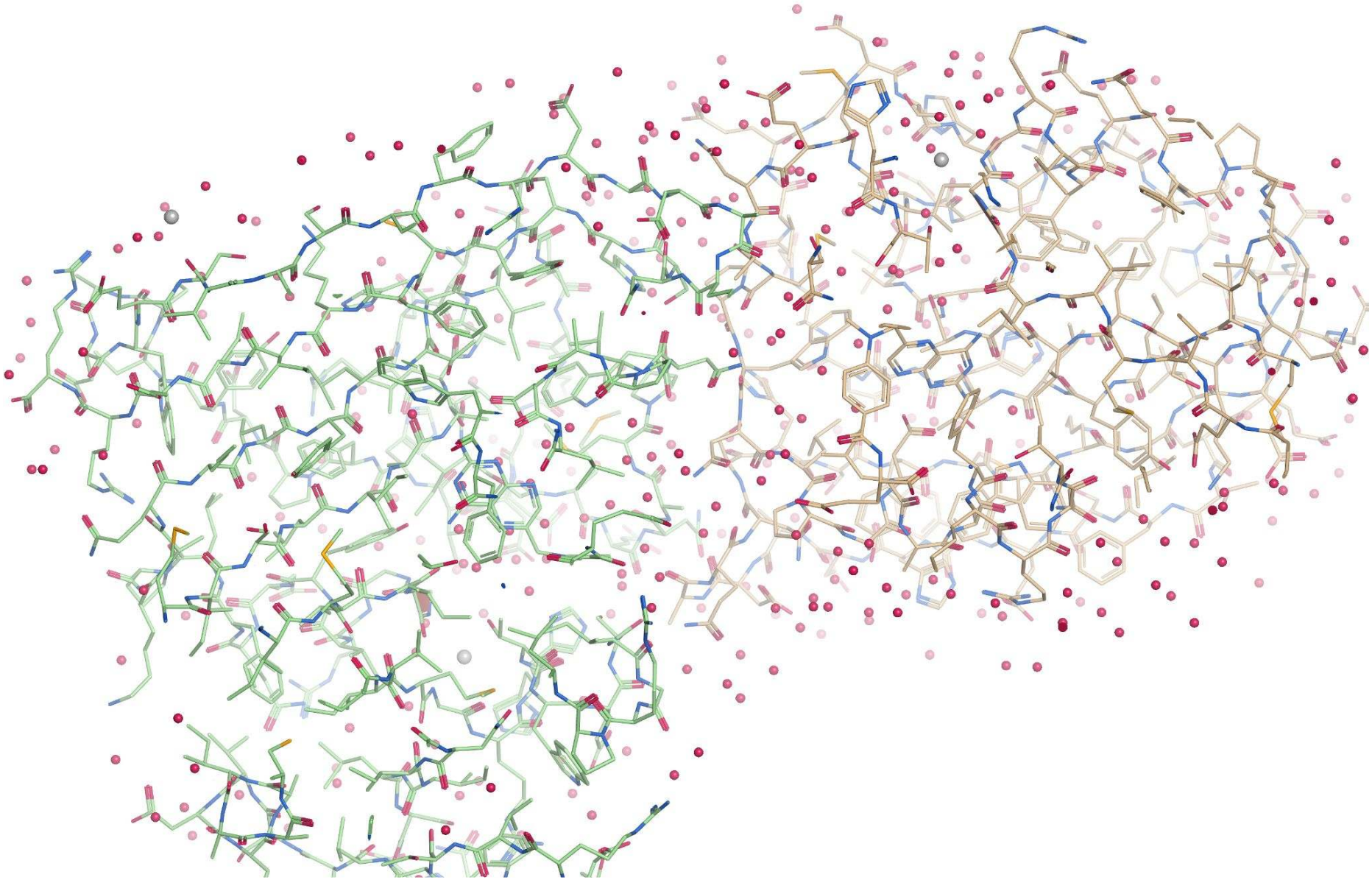

Chrome File Edit View History Bookmarks Profiles Tab Window Help
moorhen.org
Relaunch to update
MRC-LMB-Mono...
Libcootapi's Docu...
Rotating Cube -...
GitHub - wwPDB/...
Deposition API · A...
OneDep Depositio...
All Bookmarks
File
Edit
Calculate
View
Validation
Ligand
Cryo
Models
Maps
History

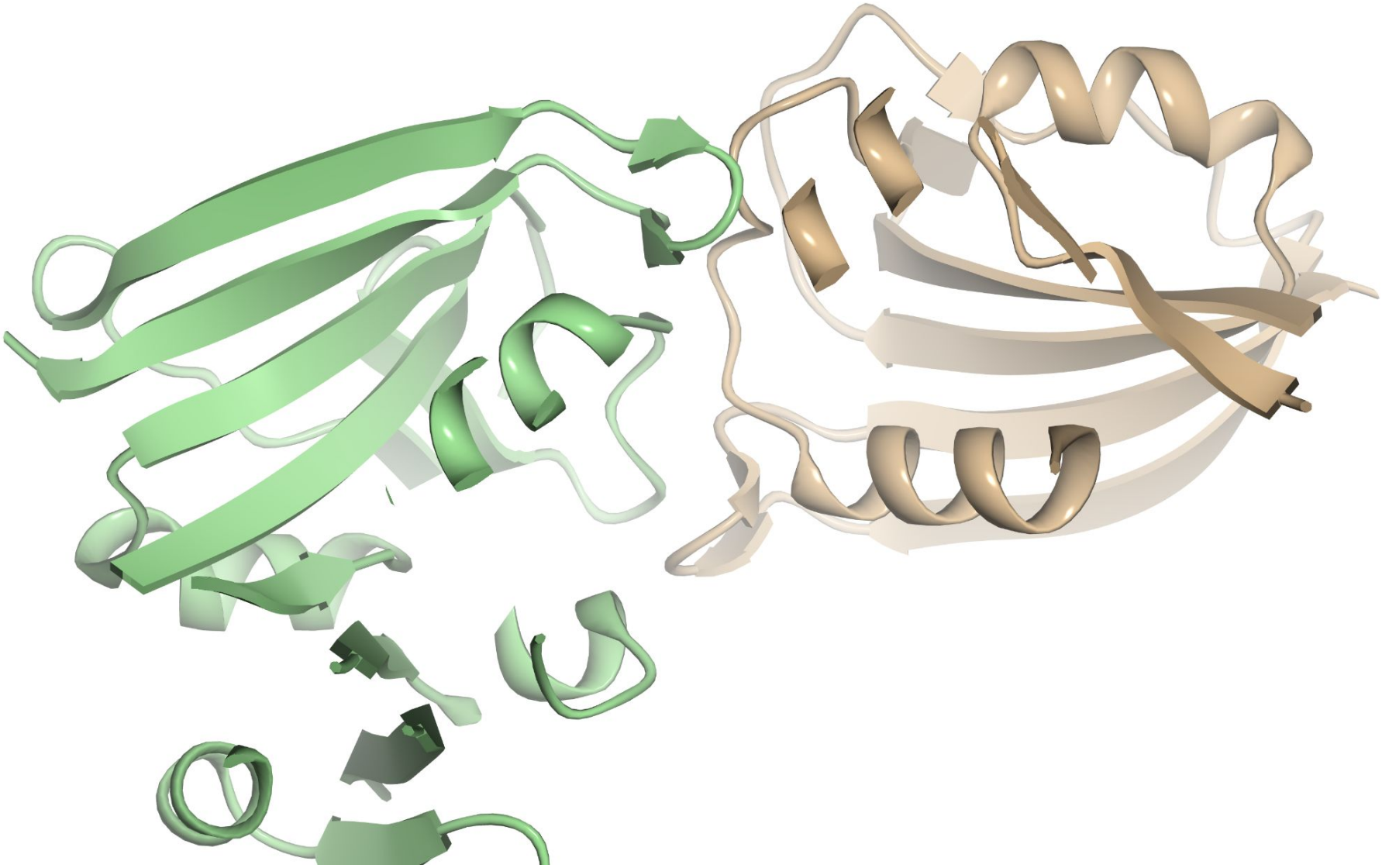
# Current status of Moorhen's figure-making capabilities

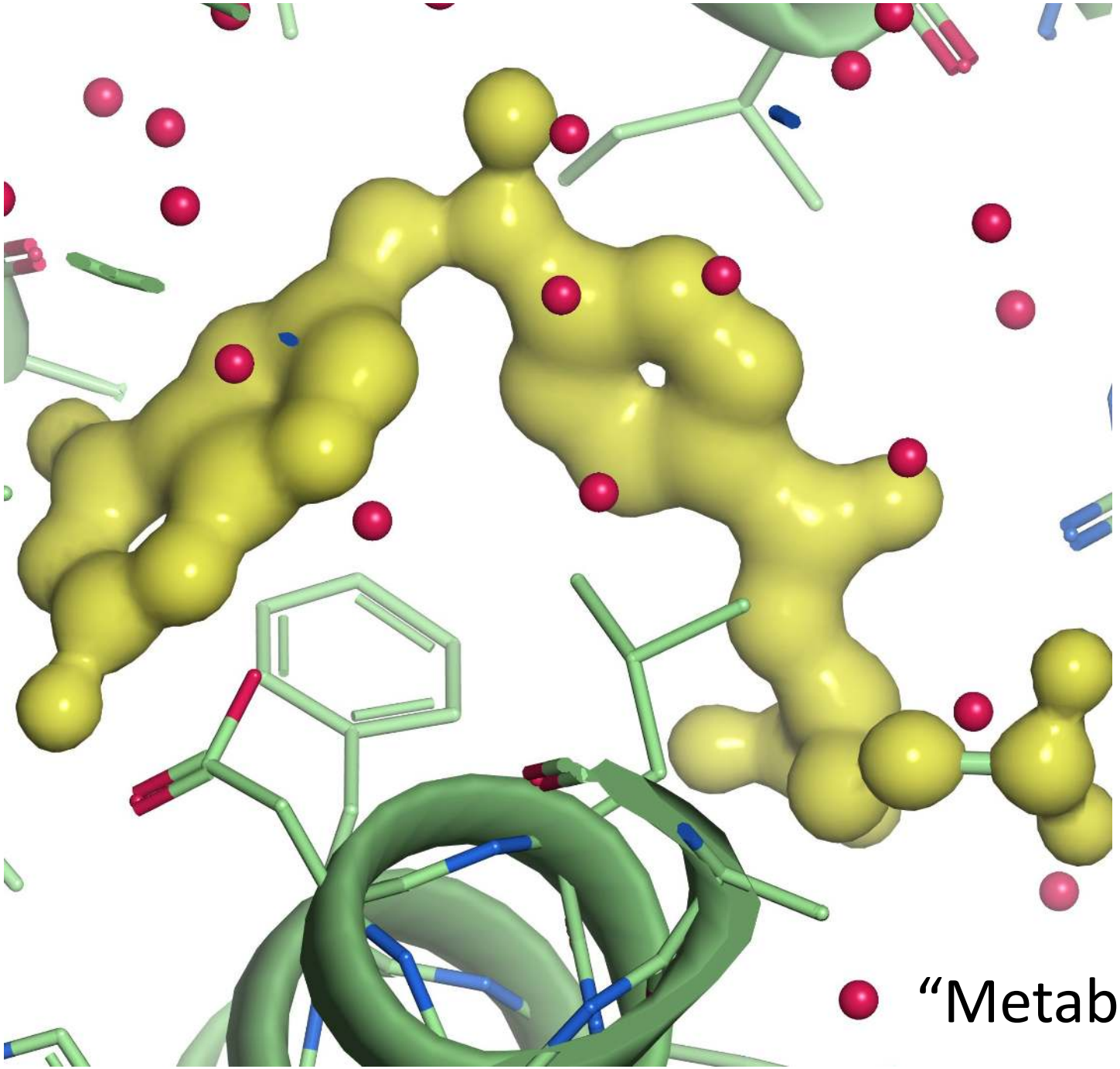
- Multiple representation styles: bonds (cylinders, ball + stick), ribbons, surfaces, CA-traces, spheres, hydrogen bonds, glycoblocks.
- As well as some that CCP4MG does not have (Coot representations): Gaussian surface, Ramachandran and rotamer quality visualization, contact dots, restraints.
- And metaballs.

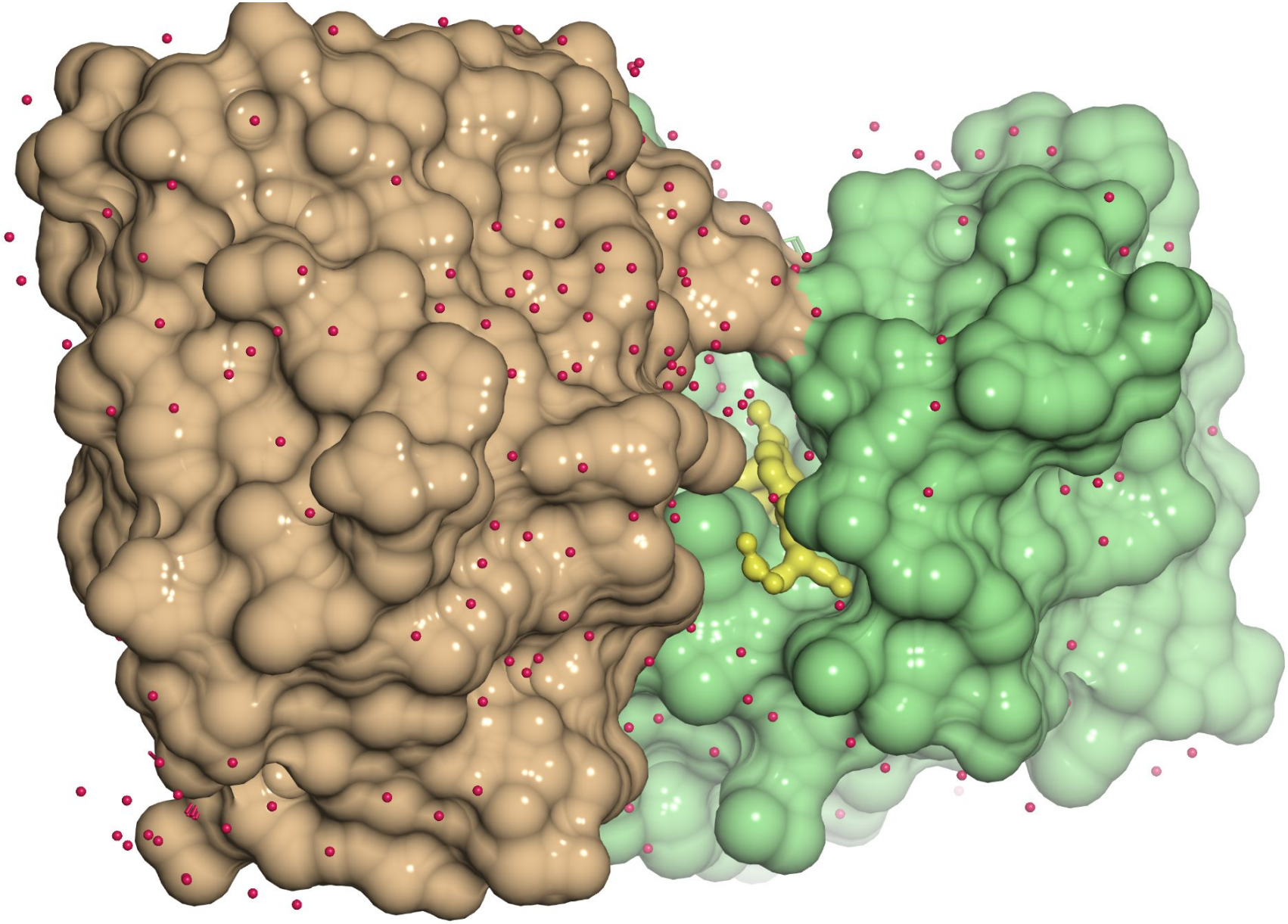
# Current status of Moorhen's figure-making capabilities

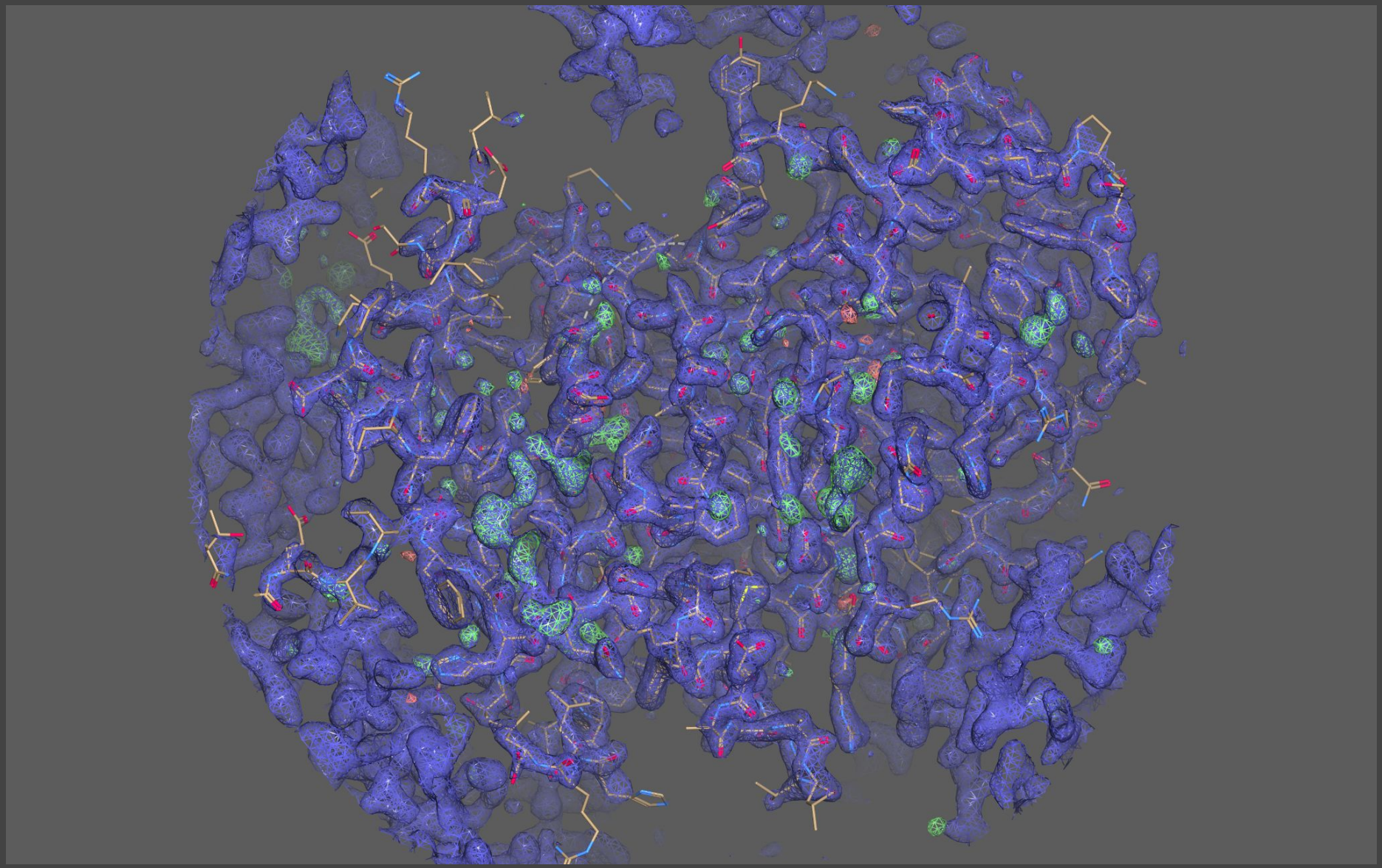
- Most of these representation can also be done with arbitrary atom selections and custom colouring.
- Sequence viewer / selection tool.
- Extensive online data resource access.
- Structure superposition.
- Shadows, occlusion, depth blur.
- Rudimentary movie making.
- Perspective projection.
- Distance and angle measurements.



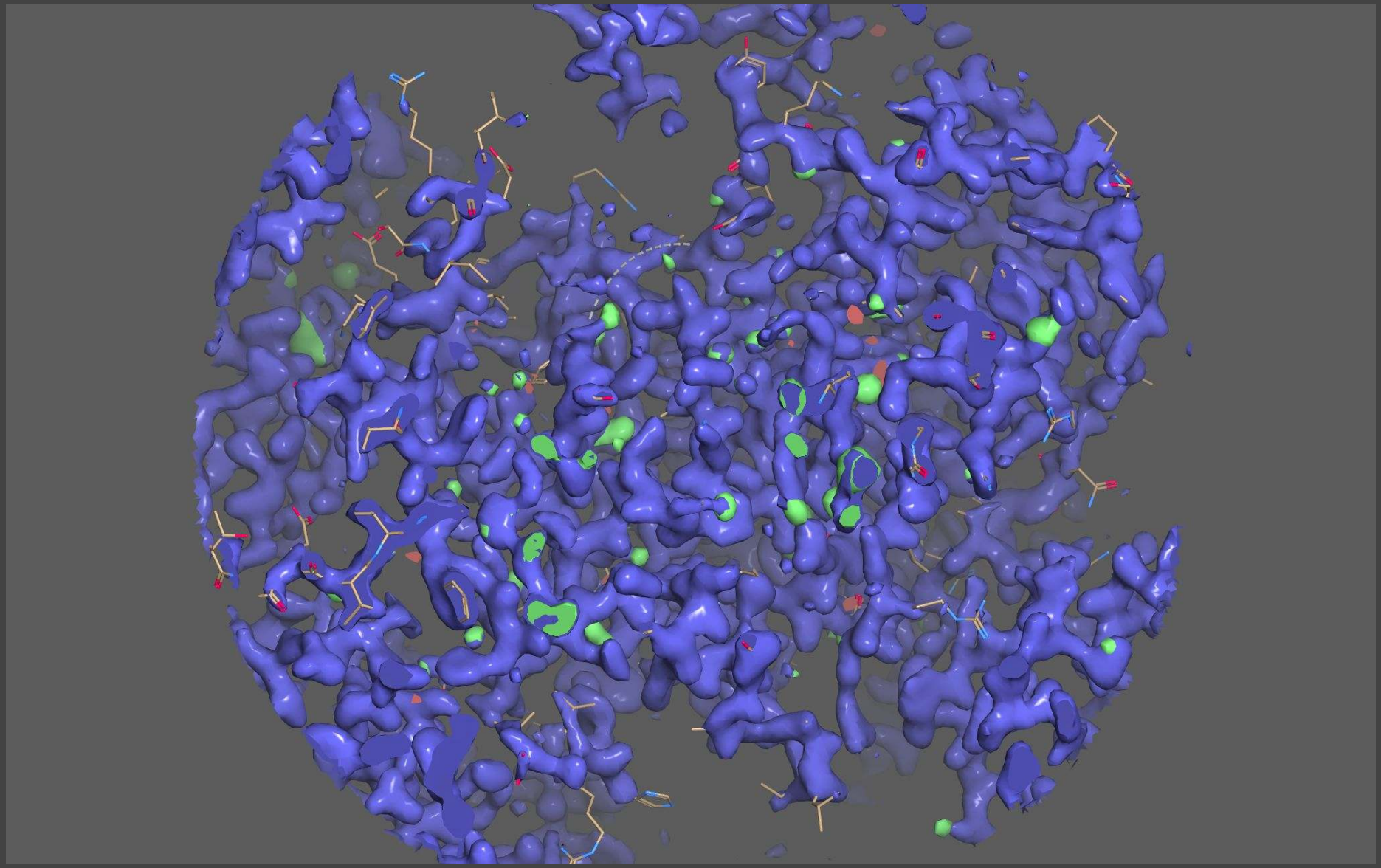


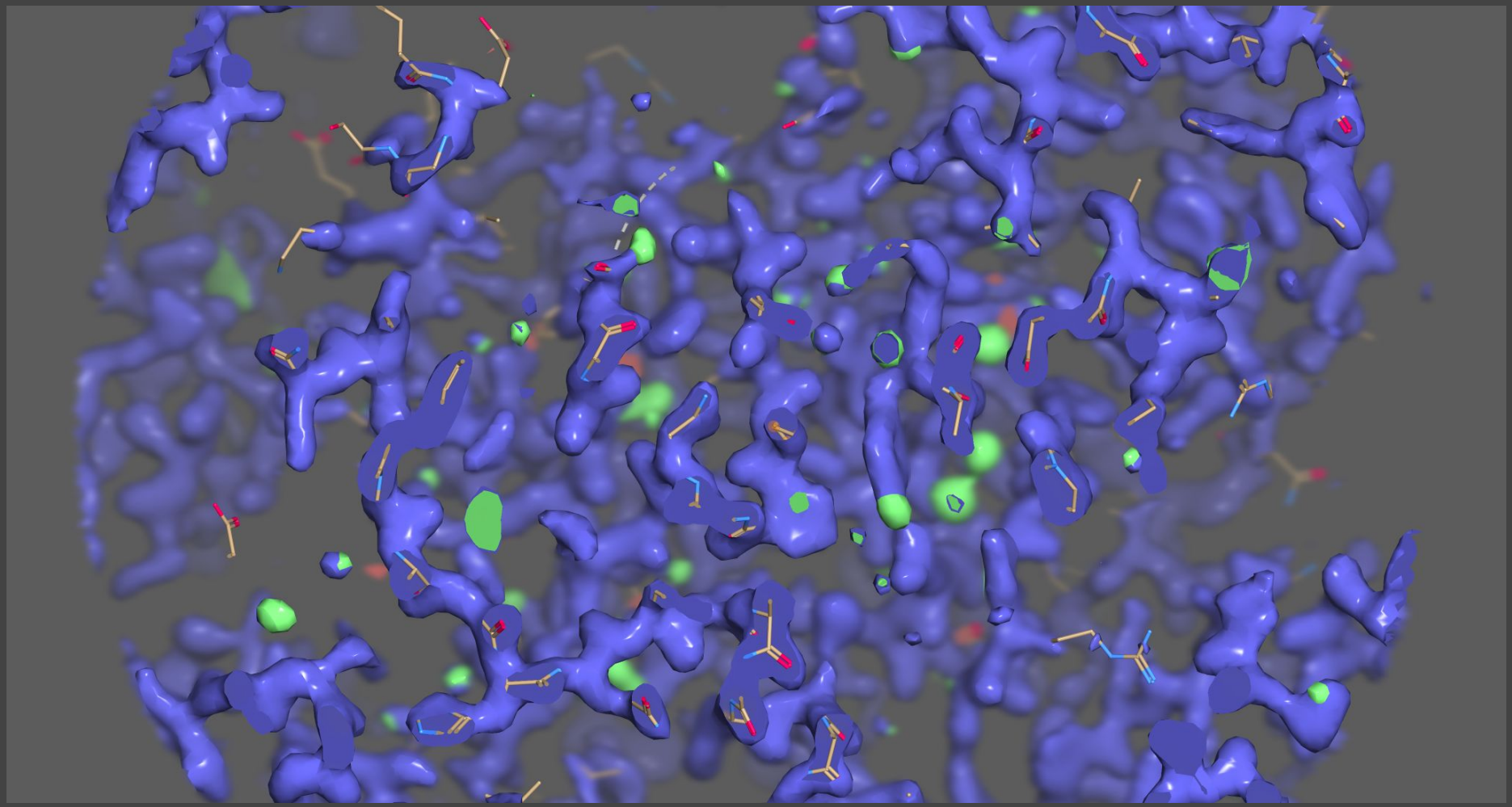

“Metaballs”



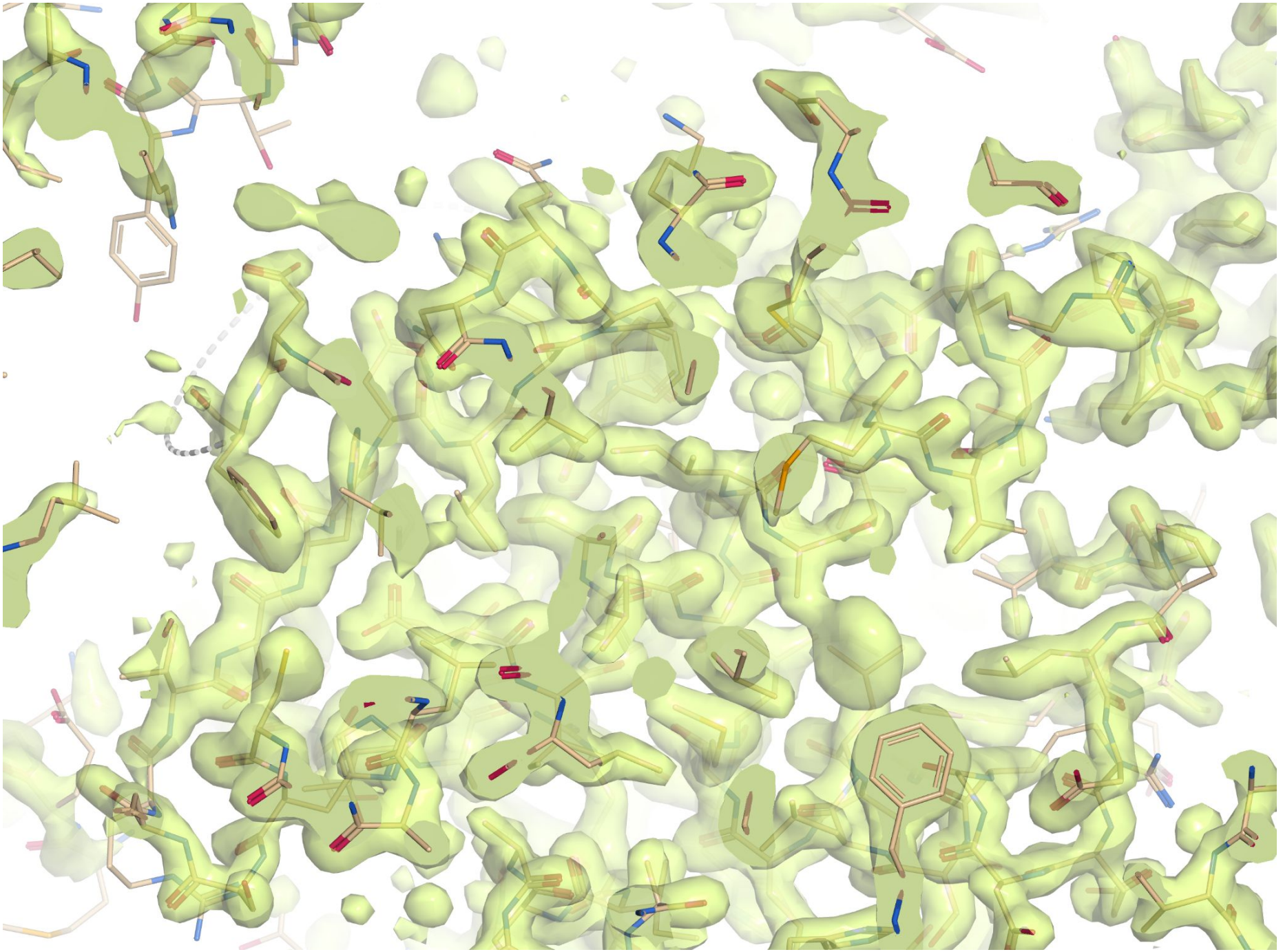


“Lit” lines

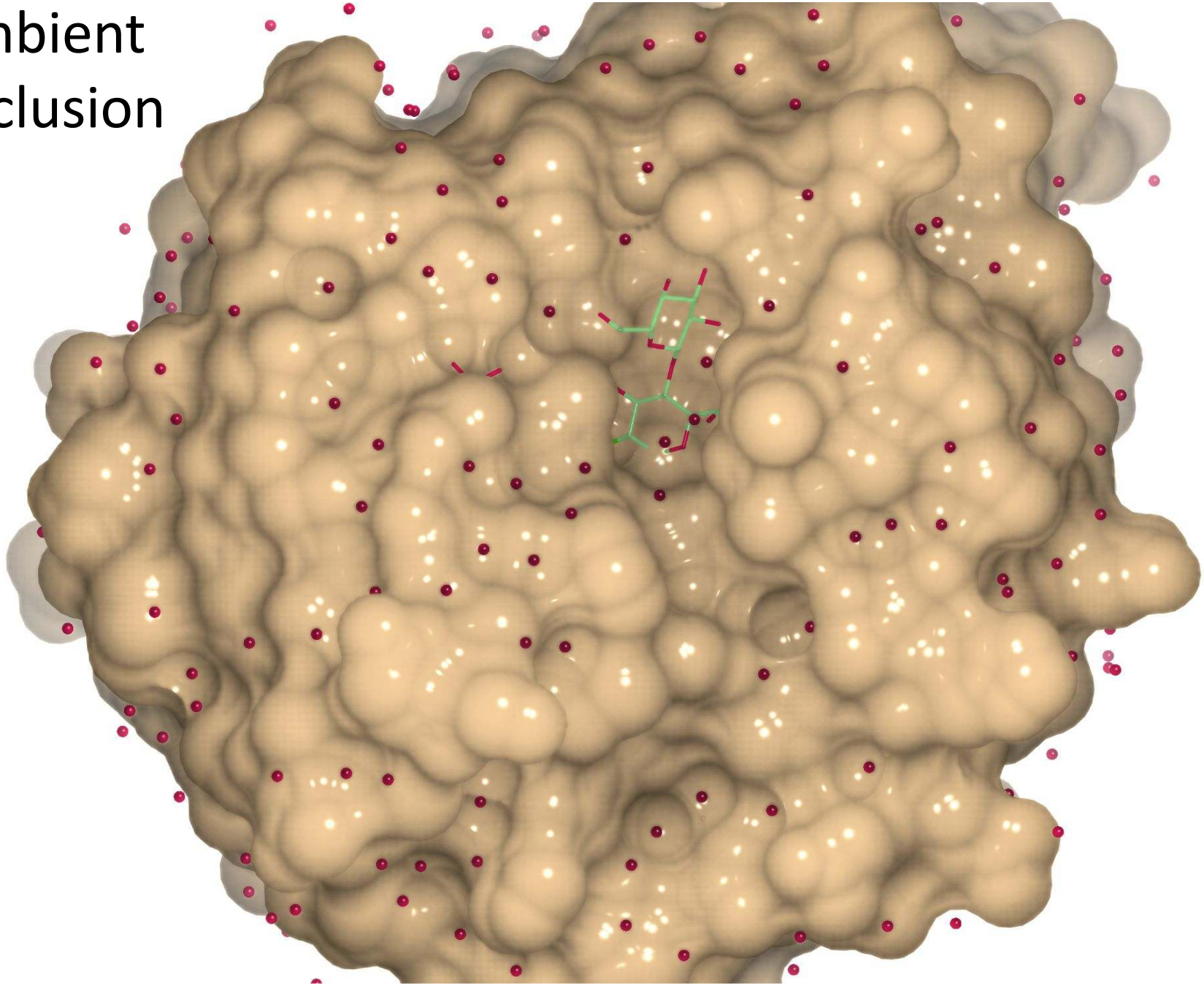


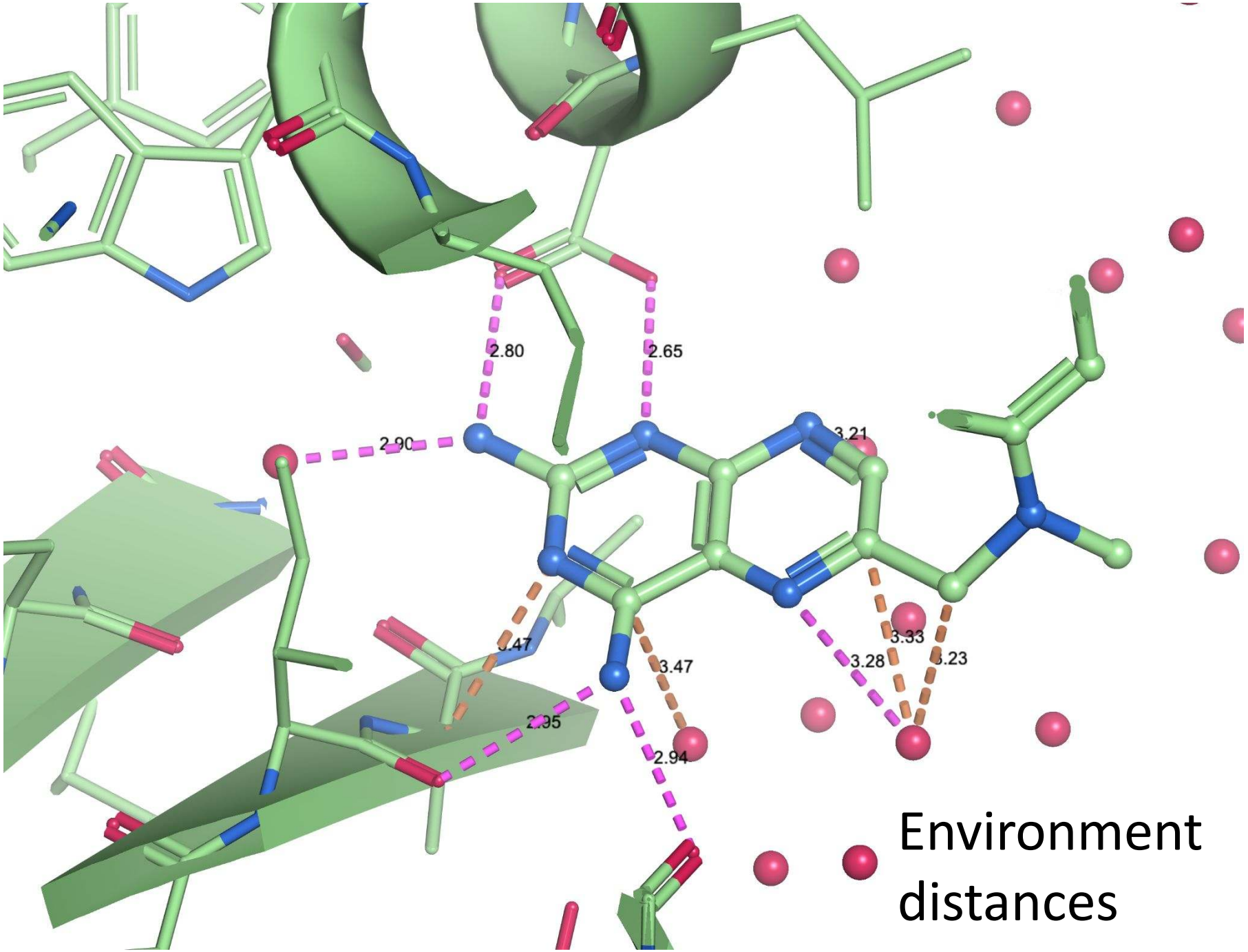


Depth blurring

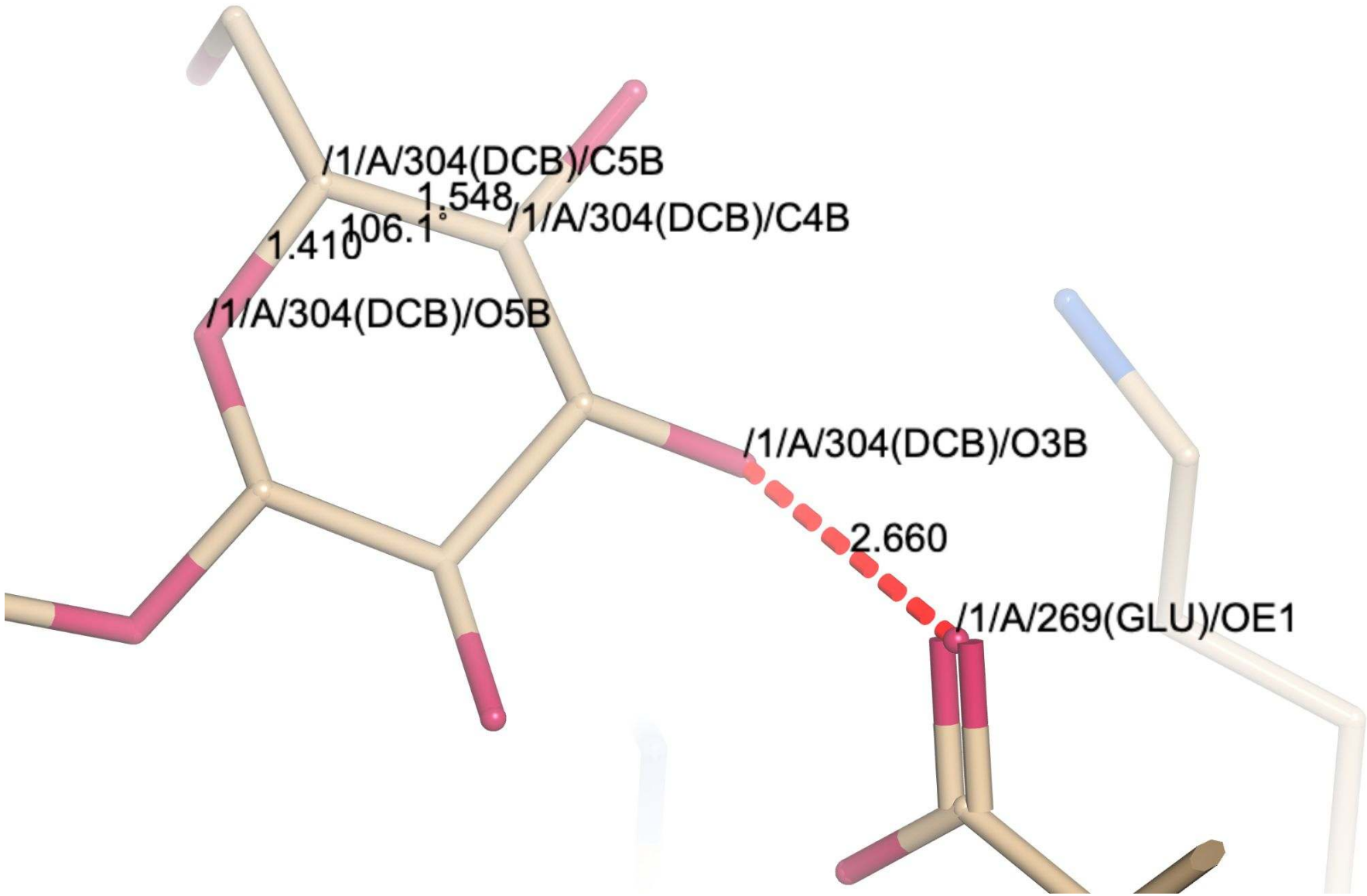


Ambient occlusion

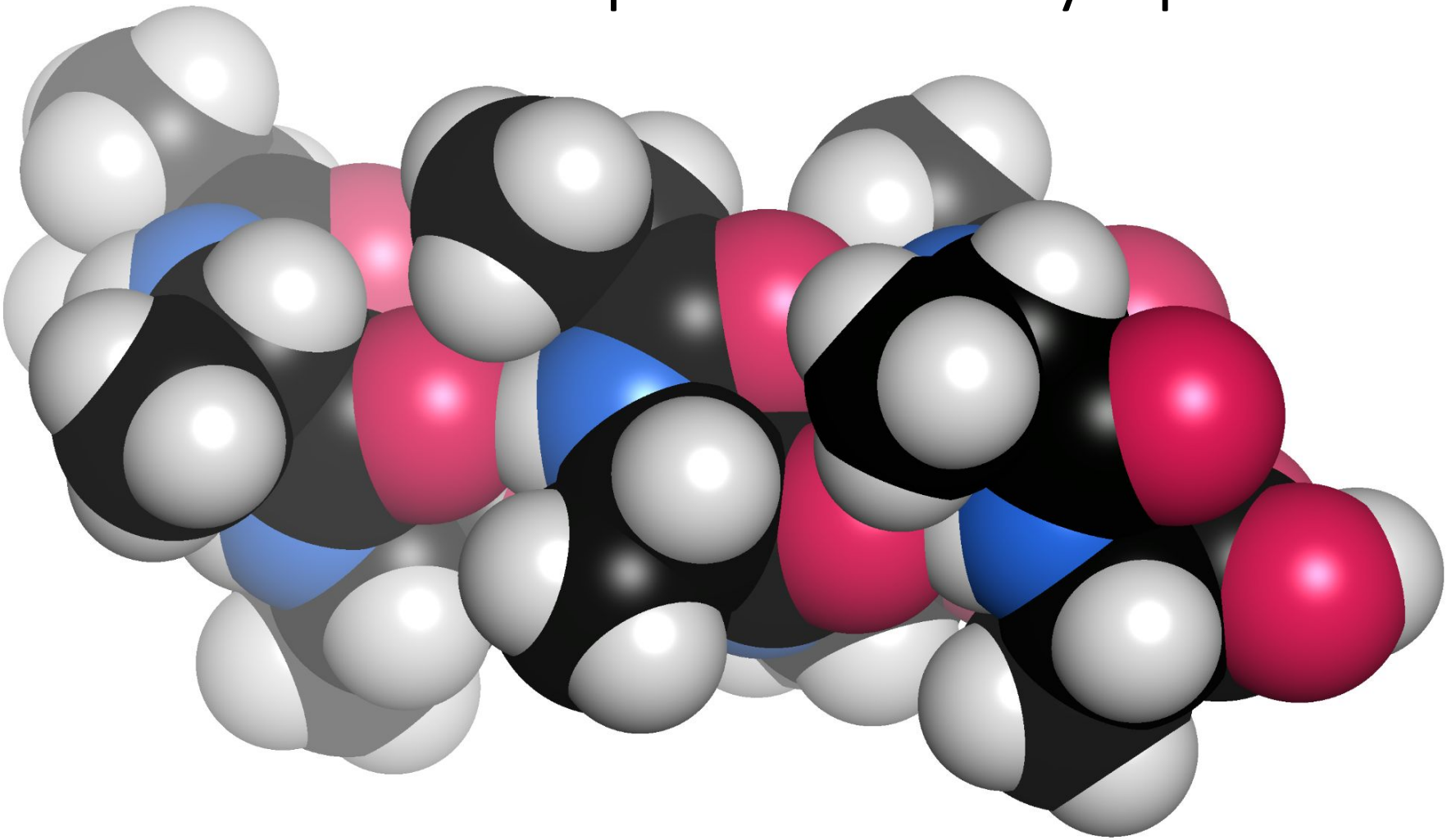


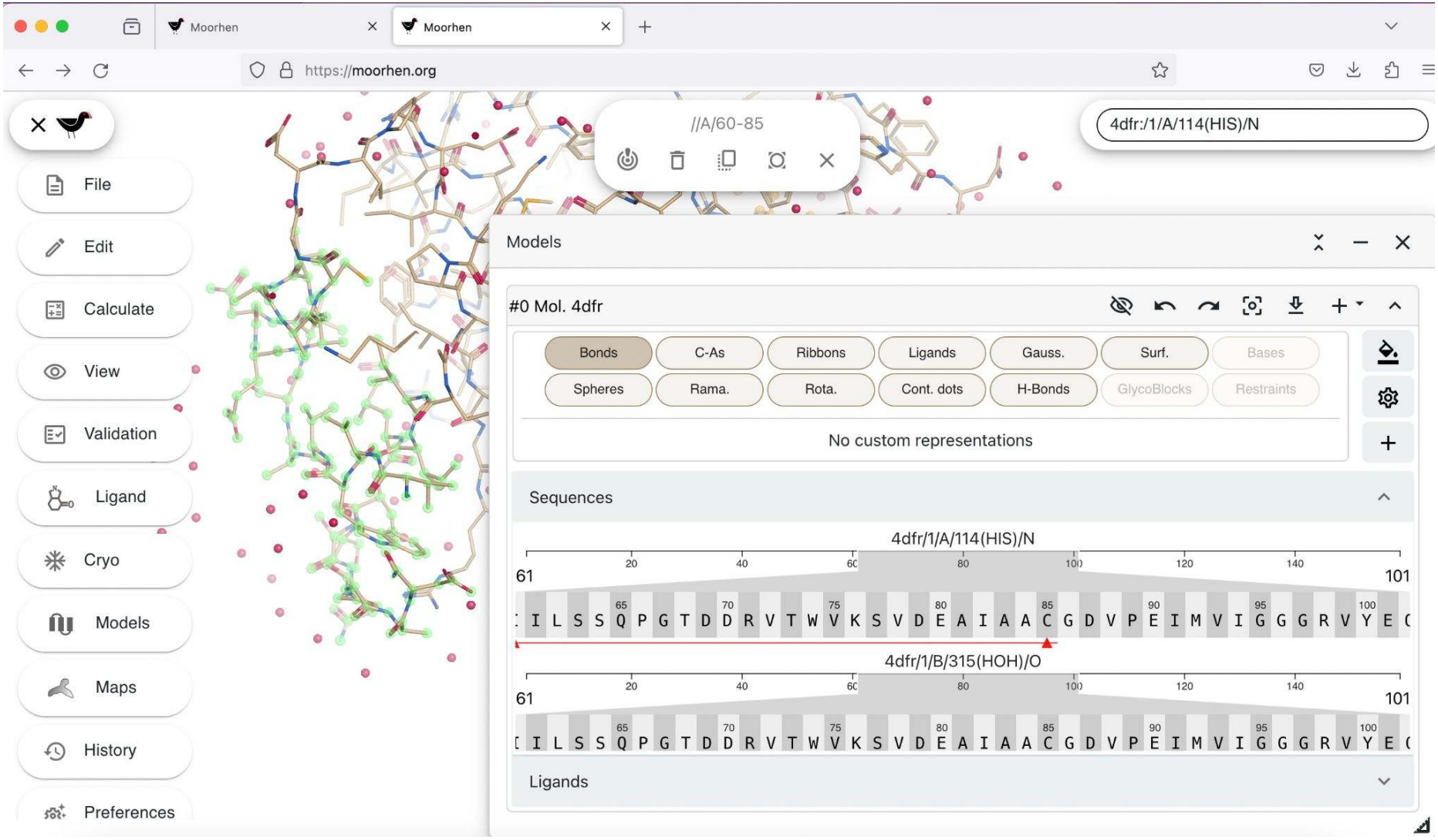

2.80
2.65
2.90
3.21
3.47
3.47
3.33
3.28
2.94
Environment
distances

# “Click+m” measuring



Spheres are always “perfect”




Moorhen
Moorhen
https://moorhen.org
//A/60-85
4dfr:/1/A/114(HIS)/N
File
Edit
Calculate
View
Validation
Ligand
Cryo
Models
Maps
History
Preferences
Models
#0 Mol. 4dfr
Bonds
C-As
Ribbons
Ligands
Gauss.
Surf.
Bases
Spheres
Rama.
Rota.
Cont. dots
H-Bonds
GlycoBlocks
Restraints
No custom representations
Sequences
4dfr/1/A/114(HIS)/N
61
101
I L S S Q P G T D D R V T W V K S V D E A I A A C G D V P E I M V I G G G R V Y E
4dfr/1/B/315(HOH)/O
61
101
I L S S Q P G T D D R V T W V K S V D E A I A A C G D V P E I M V I G G G R V Y E
Ligands

# What's missing from Moorhen figure-making capabilities?

- Neighbourhood selections - coming real soon now. (I might be wrong we might have it already).
- Complex selection tools like CCP4MG.
- Electrostatic colouring of surfaces.
- Thermal ellipsoids, worms scaled by B-Factor, lipid cartoons, bloboids.
- Wizards.
- MR tools (MrBUMP, Slice) - work will begin on this in New Year.
- Complex movie making.
- Assembly generation (from `BIOMT` info).
- Transparency of any object.
- Perspective does not play nicely with occlusion.
- Scale bar
- Arbitrary text (and image) annotations.
- User-defined atoms for superposition.

# Getting Moorhen

- Web services:
  - CCP4 - Cloud: https://cloud.ccp4.ac.uk/
  - Standalone service: https://moorhen.org
  - Privateer: https://privateer.york.ac.uk/
- Source code:
  - https://github.com/moorhen-coot/Moorhen
- Desktop:
  - "Electron" app: https://github.com/moorhen-coot/MoorhenElectron
  - ccp4i2 *hopefully* in near future.
- Integrate into your own project:
  - https://github.com/moorhen-coot/Moorhen/releases/download/v0.6.5/moorhen-0.6.5.tgz
    (Please ask Filo, not me). This is being done for CCP-EM.

Validate your carbohydrates online with

# Privateer

The Swiss Army knife for carbohydrate structure validation, refinement and analysis

← Back To Table

## Glycan Details

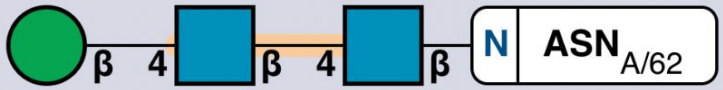
### Validation Report

Glycan ID: **NAG-1/E_ASN-62/A**

Number of conformation issues: **0**
Number of anomer issues: **0**
Number of torsion issues: **1**
Number of pucker issues: **0**
Number of chirality issues: **0**

Glytoucan ID: **G15407YE**

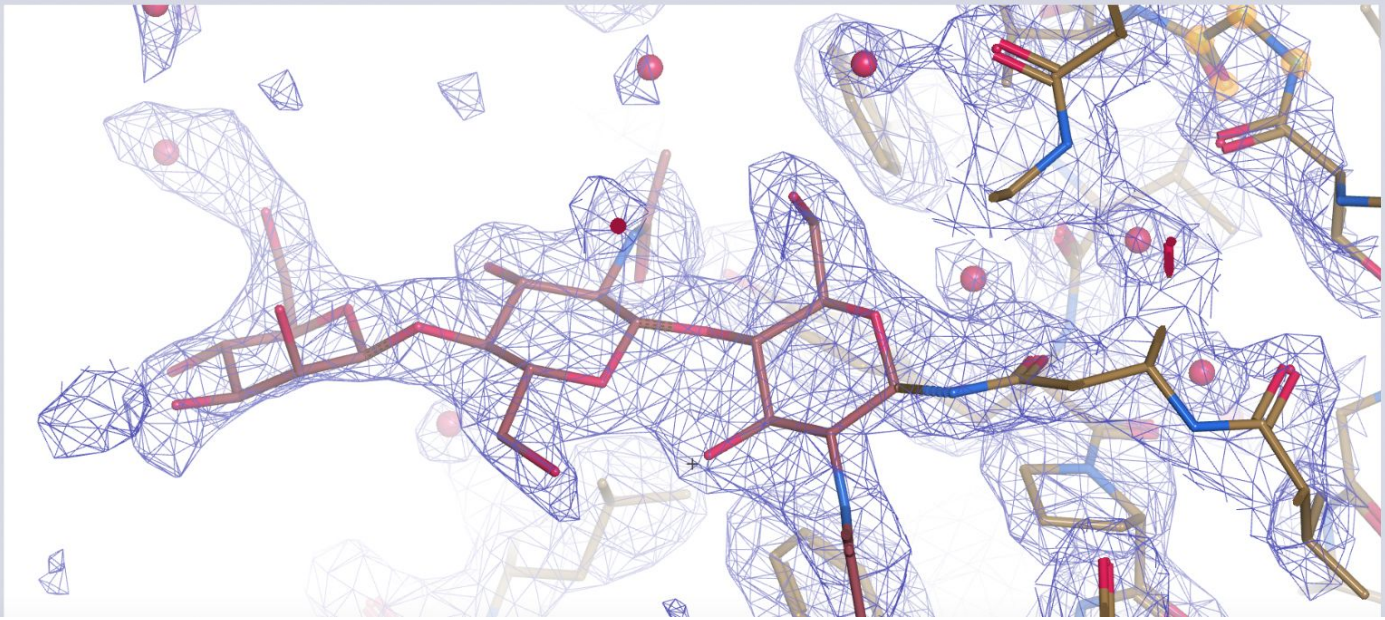
### SNFG




Hover over a linkage to see a summary

## Visualise

Map Contour



# Acknowledgements


- Liz Potterton
- Eugene Krissenel
- Kevin Cowtan
- Paul Emsley
- Martin Noble
- Jan Gruber
- Bernhard Lohkamp
- Rob Nicholls
- Jon Agirre
- Paul Bond
- Marcin Wojdyr
- Ronan Keegan
- Filomeno Sanchez Rodriguez
- Lucrezia Catapano
- Jakub Smulski
- Adam Simkin

- Funding: CCP4