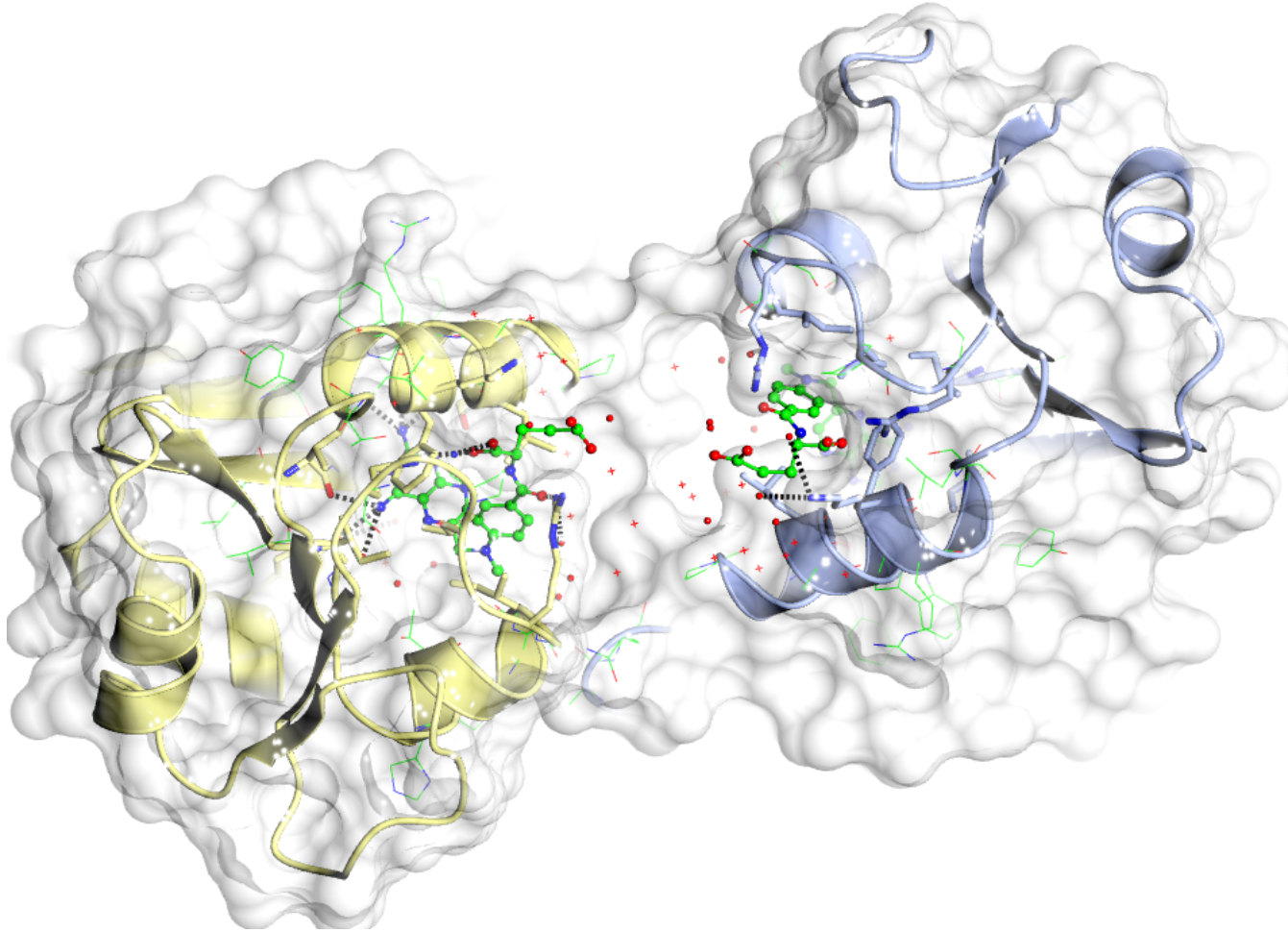


# CCP4MG



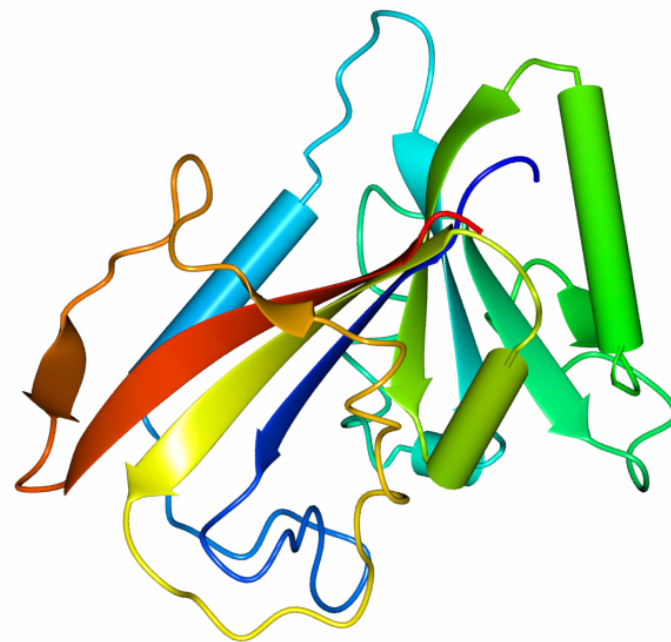
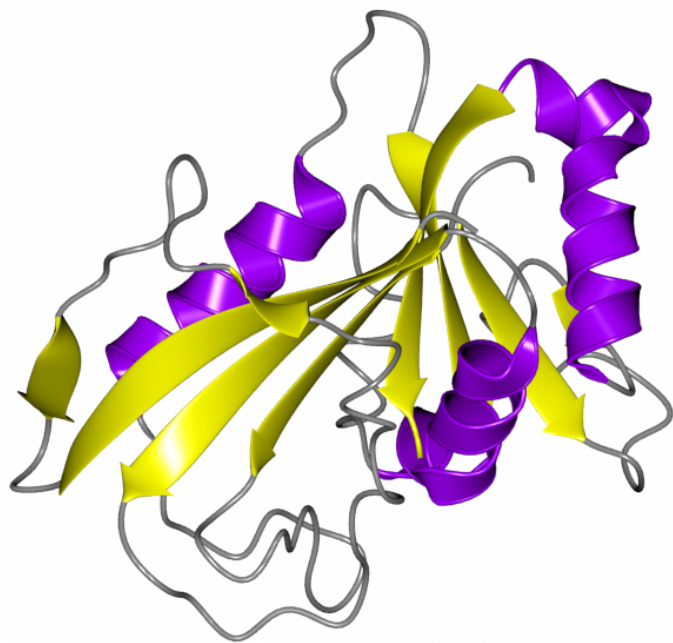
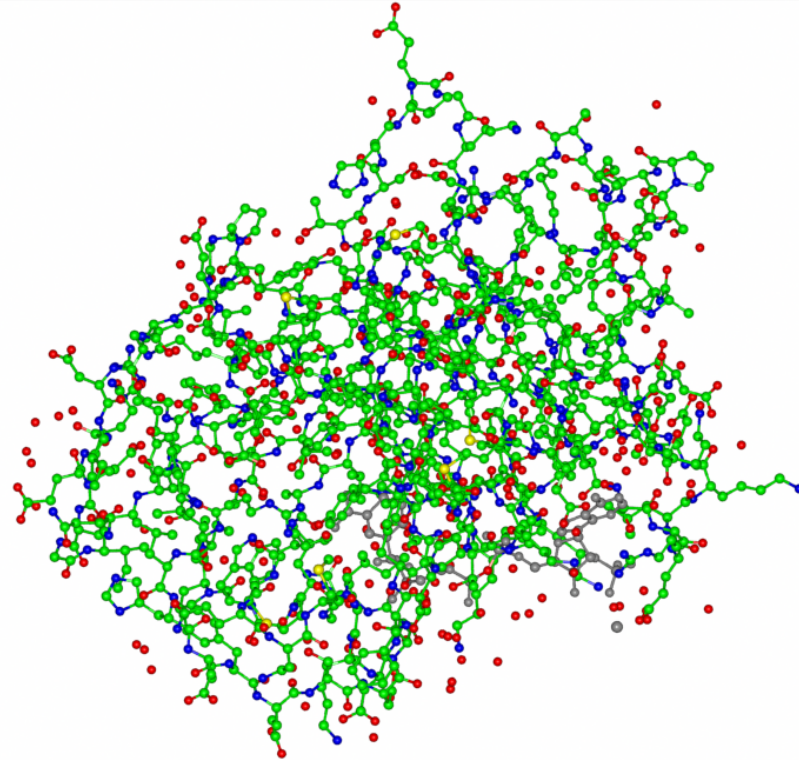
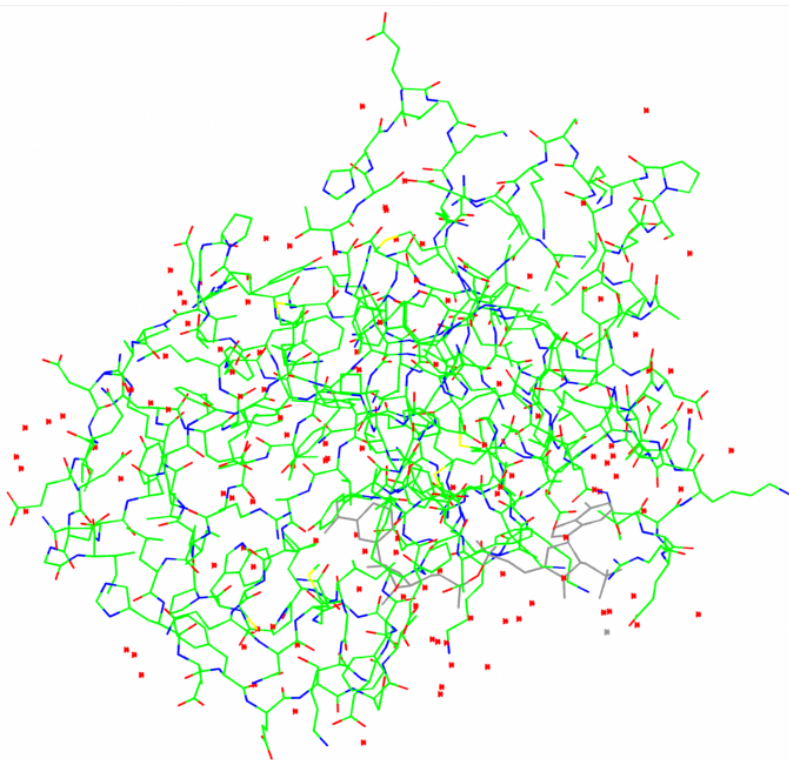
CCP4 Molecular Graphics Program

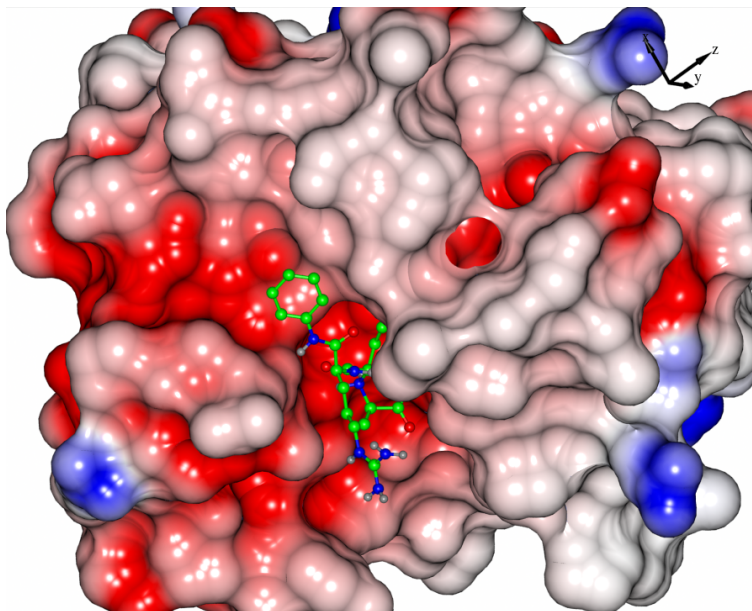
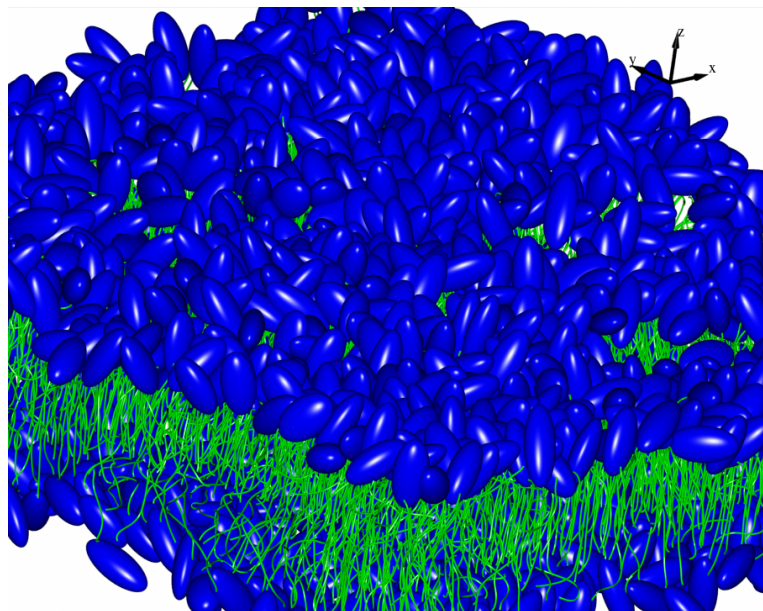
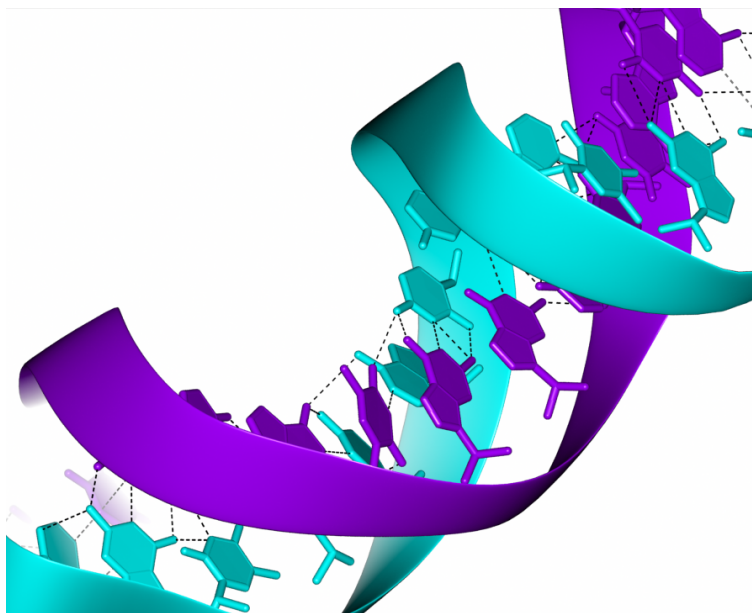
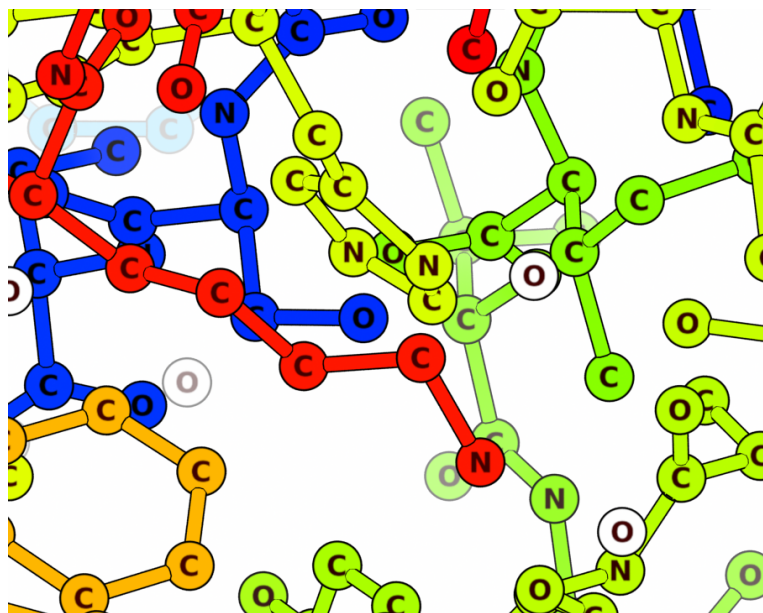
# Introduction

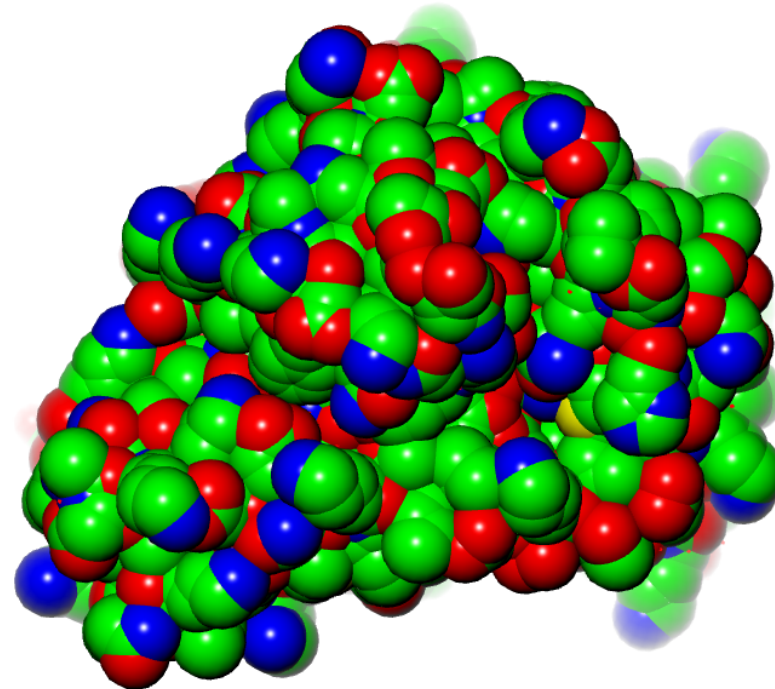
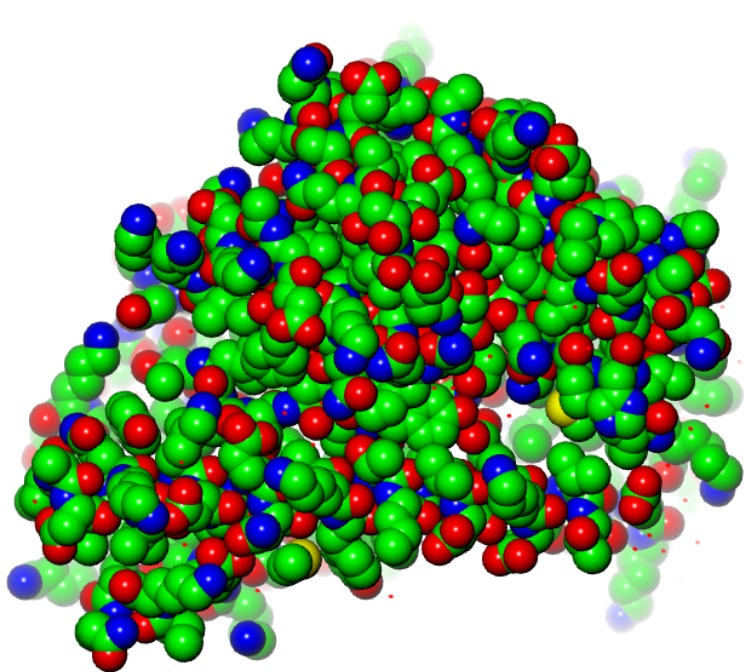
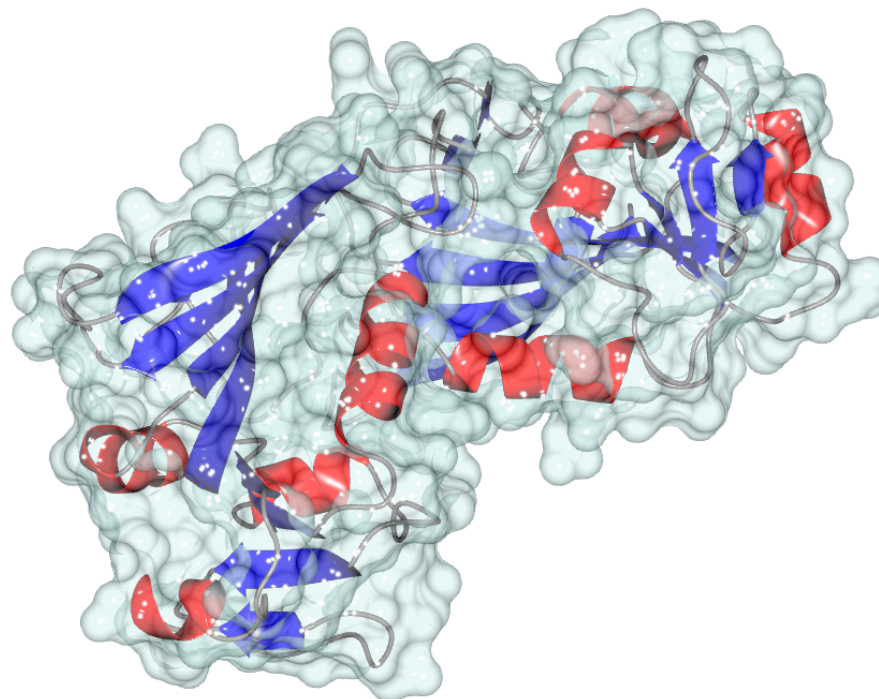
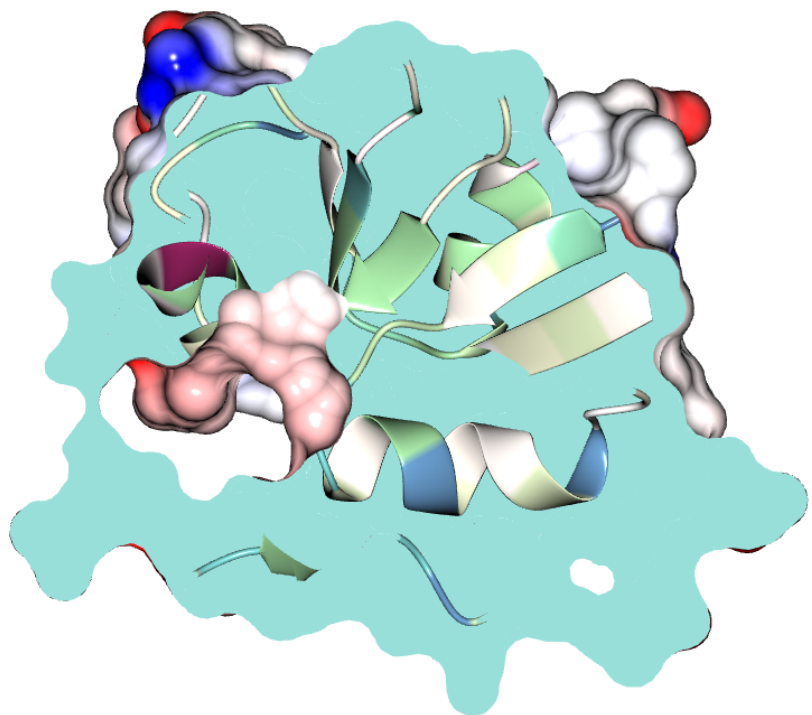
- CCP4MG is a molecular graphics program funded by CCP4.
- Its primary focus is the visualization and analysis of macromolecular structure.
- It produces high quality rendered images and movies.
- <http://www.ccp4.ac.uk/MG/>
  - Binaries for Windows, Mac and Linux.

# 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







CCP4MG version 2.7.1

Drawing style

Colour

Atom selection

Data object

Display object

Display Table

Create object Tools

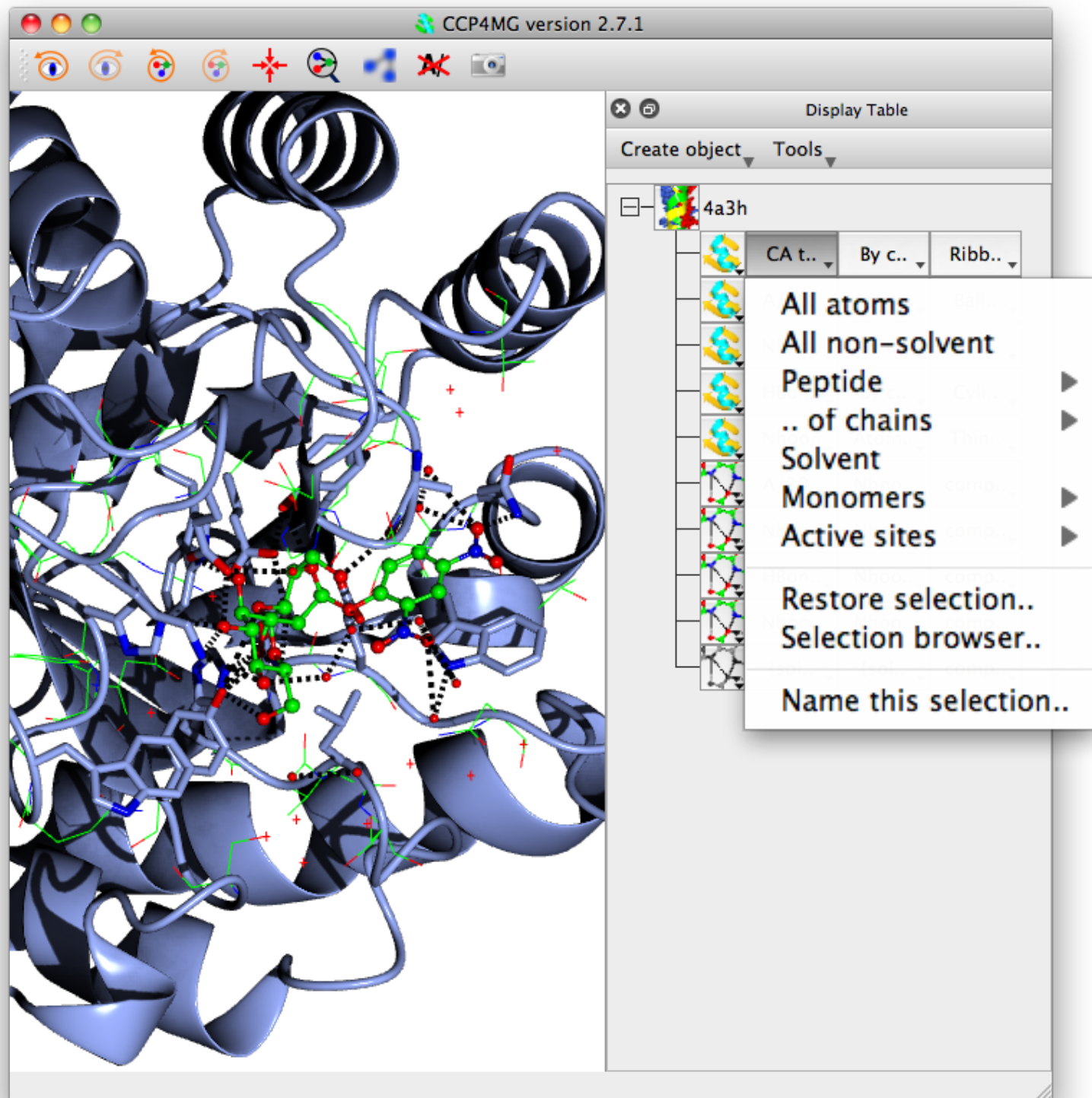
4a3h

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..

The image shows the CCP4MG version 2.7.1 software interface. The main window displays a 3D molecular model of a protein structure (blue ribbon) with a green stick model of a ligand (A/30..) bound to it. The 'Display Table' panel on the right lists various display options for the selected object (4a3h). Red arrows point from labels to specific UI elements: 'Drawing style' points to the 'Tools' dropdown; 'Colour' points to the 'CA t..' dropdown; 'Atom selection' points to the 'By c..' dropdown; 'Data object' points to the '4a3h' object name; and 'Display object' points to the 'A/30..' dropdown.

# 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



Select from 4a3h

Replace (NEW) current selection by neighbours

Select residues within 4.0 of selection..

4a3h

Include

☐ the central selection ☒ solvent

☒ non-Hbonding groups

Select neighbours

Show CA trace of..

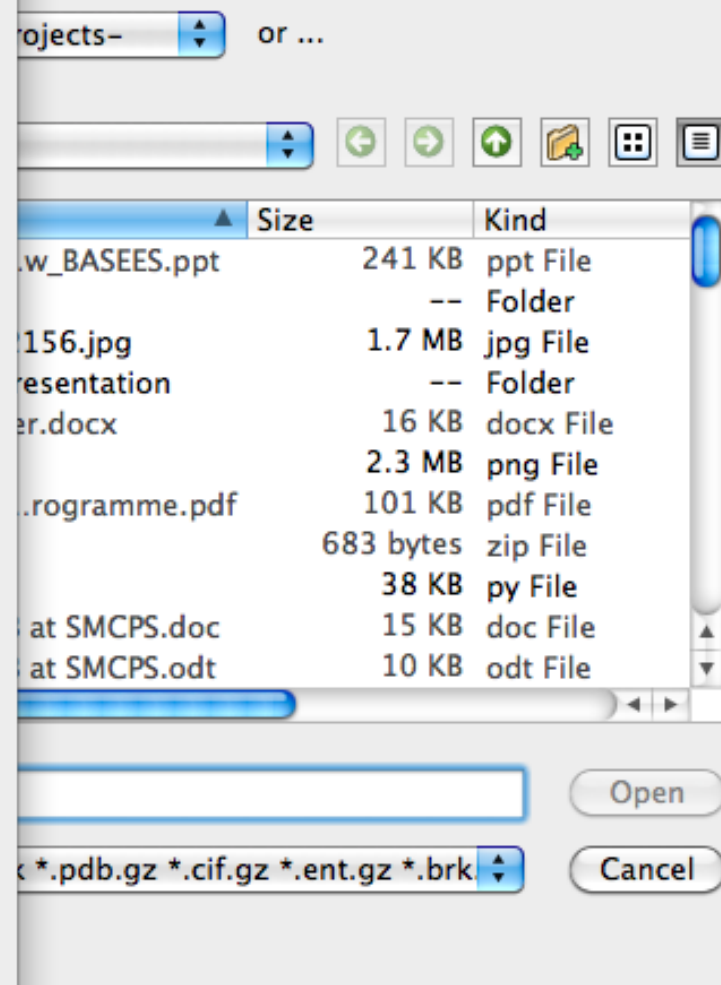
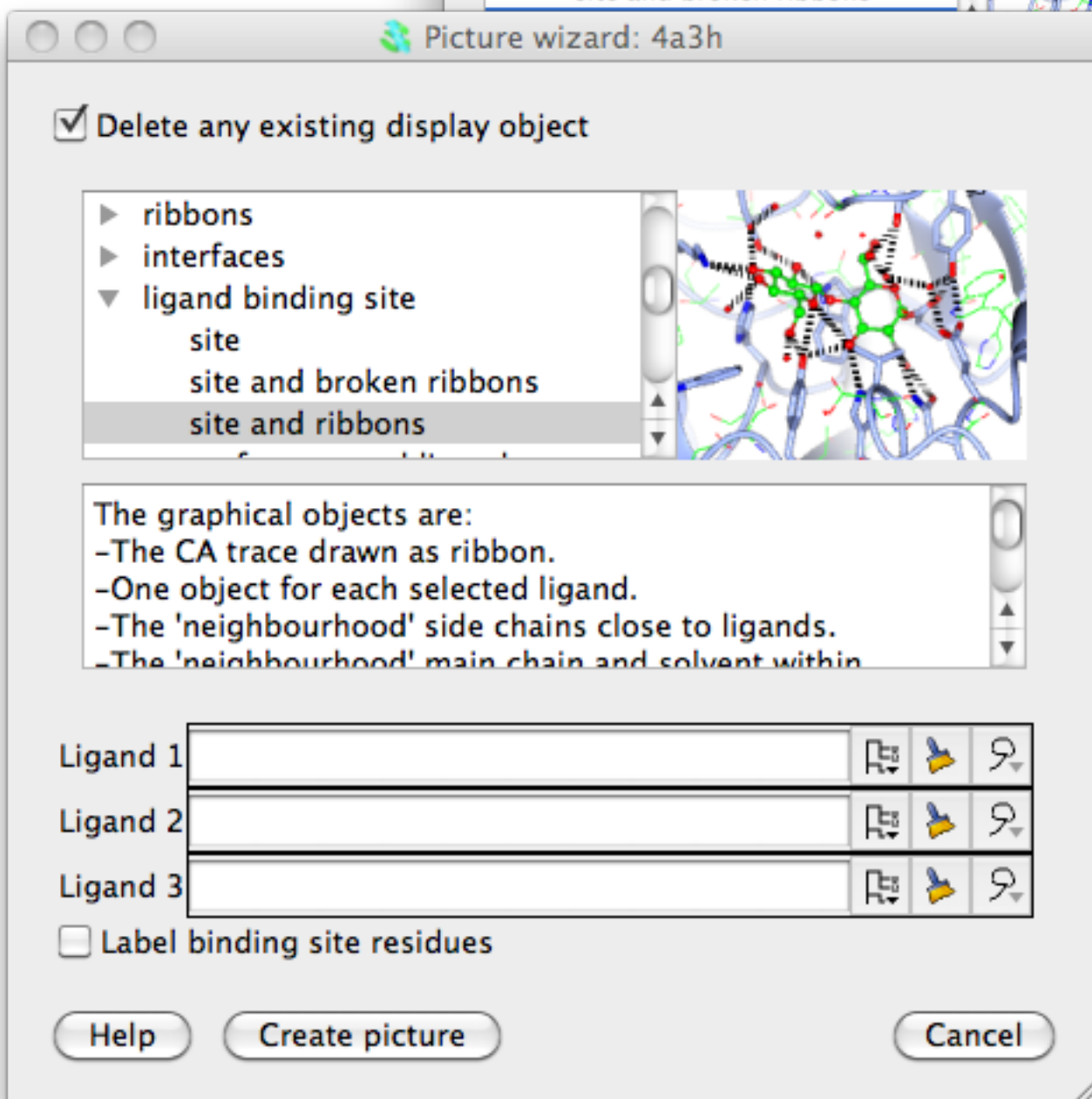
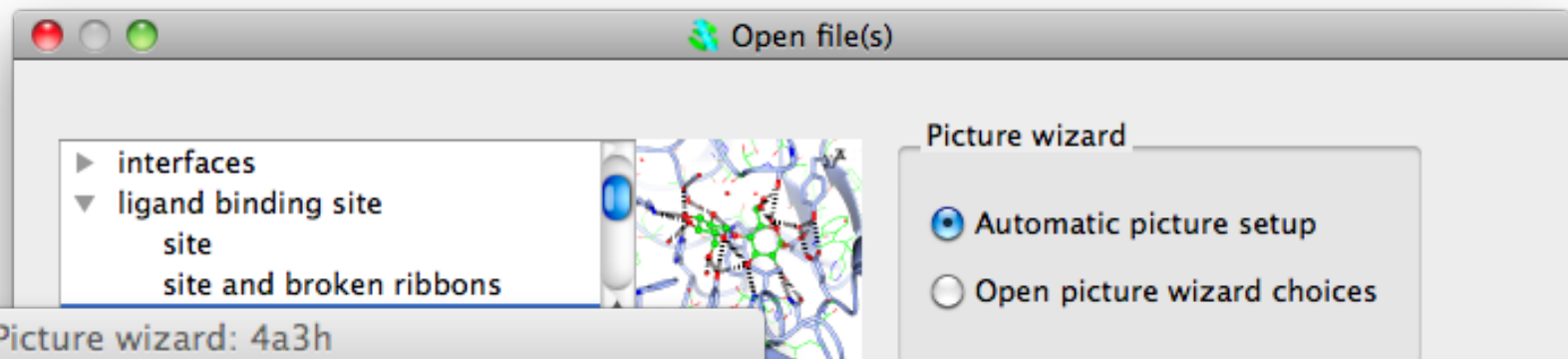
- ▶ Monomers
- ▶ Peptide
- ▶ Solvent

catrace

Help Clear Apply Save Close

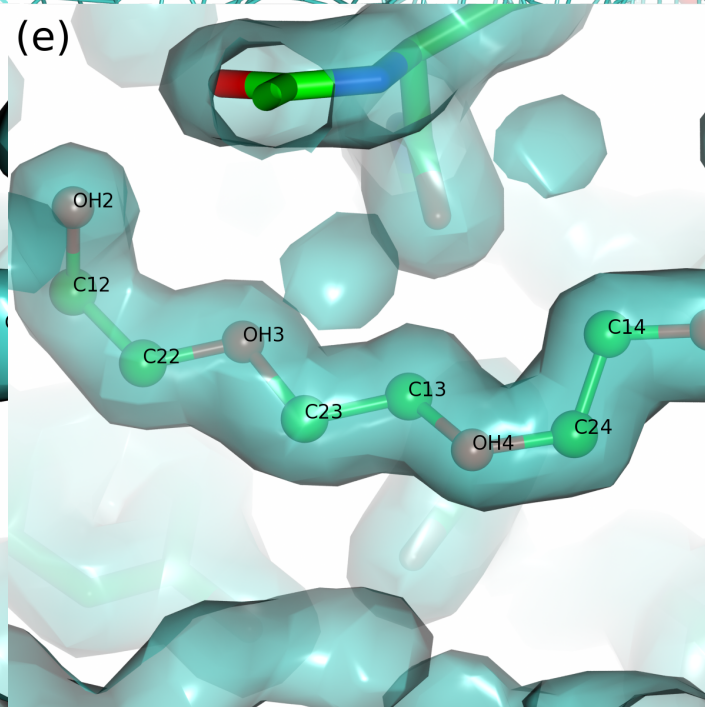
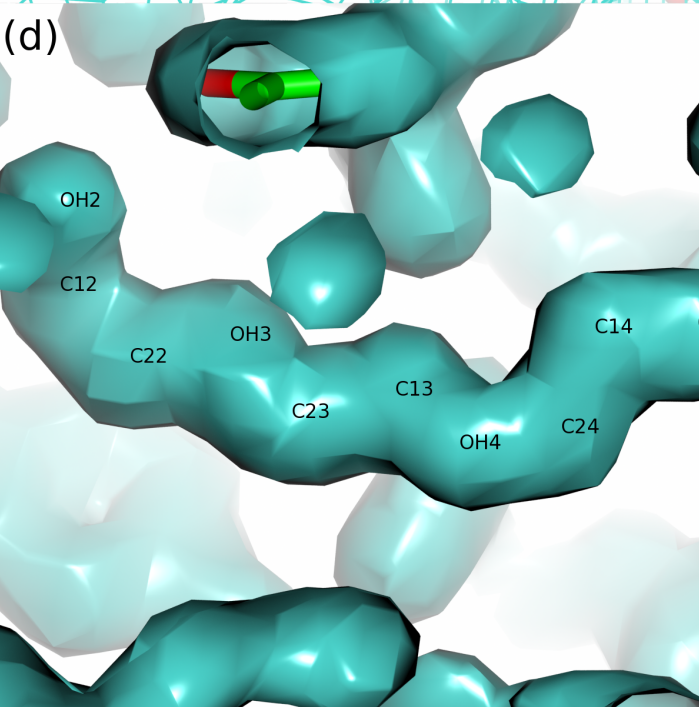
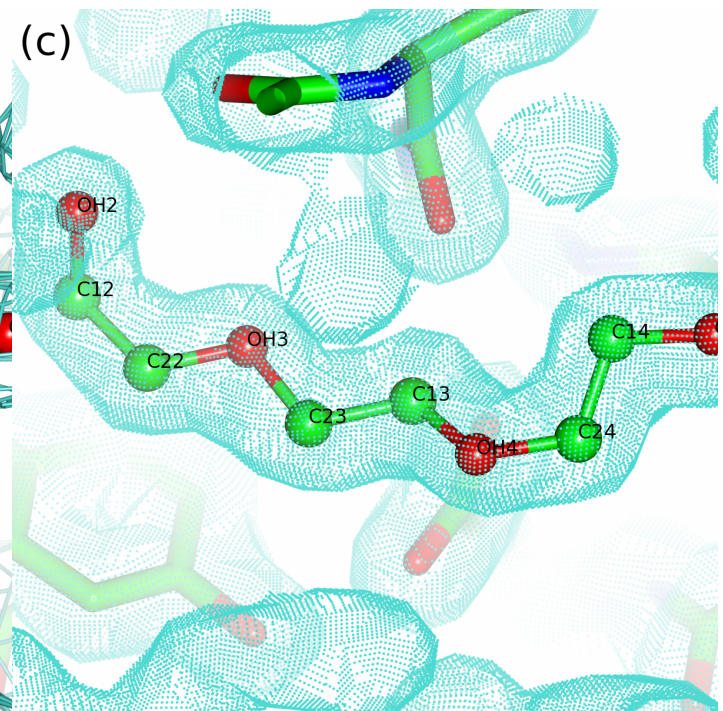
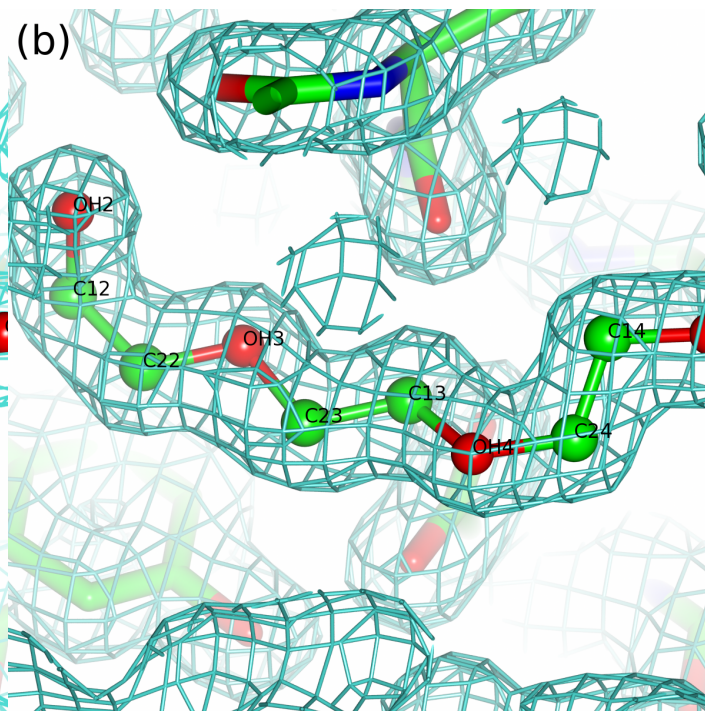
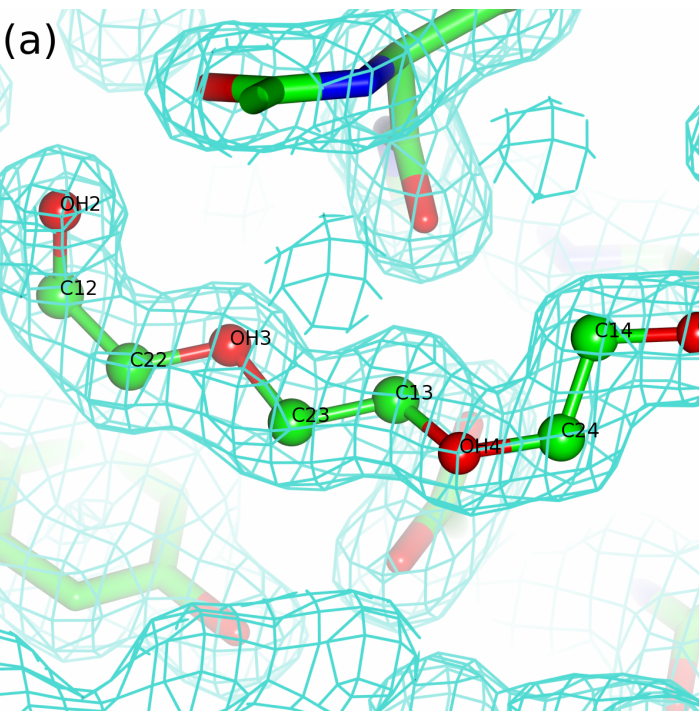
# Picture Wizard

- 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.



# Electron Density

- Electron density maps can be read/created from any CCP4 supported file format.
- Density can be represented as chickenwire lines, chickenwire cylinders, solid surface or dots.
- By default a 10Å cube 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.



# 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.

# 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

z  
y

Crystals

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

00004

00005

00006

Record 4.00 secs

View rotate about

Details

Record 4.00 secs

View glid 000

Details

..glide through..  
for time proportio

1.00

Record 4.00 secs

View rock

Details

Save snapshot here

framerate: 15

Action

Edit

Help



# PISA

## The EBI website defines PISA:

PISA is an interactive tool for the exploration of macromolecular (protein, DNA/RNA and ligand) interfaces, prediction of probable quaternary structures (assemblies), database searches of structurally similar interfaces and assemblies, as well as searches on various assembly and PDB entry parameters

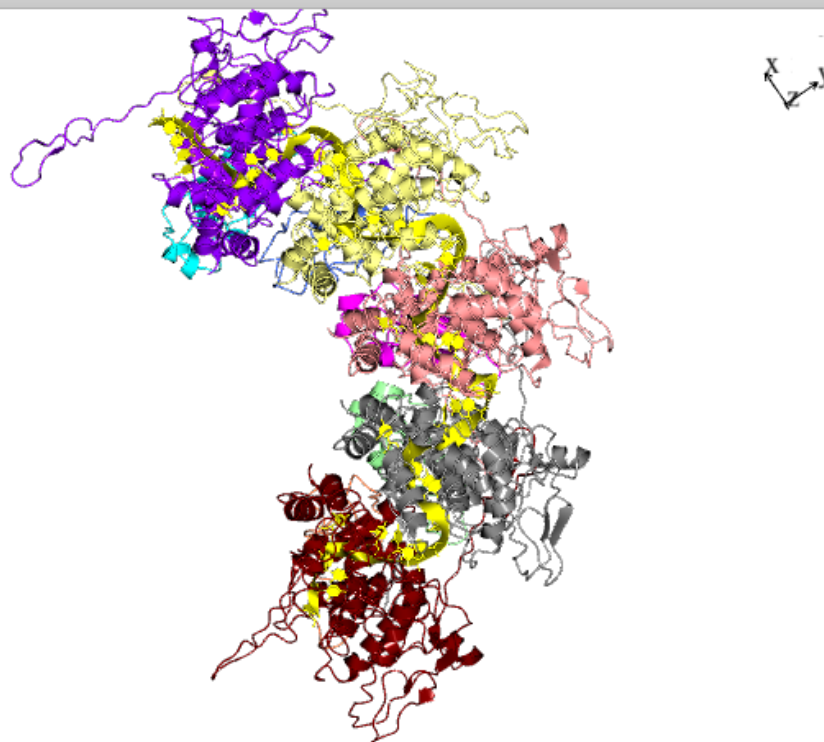
E. Krissinel and K. Henrick (2007). *Inference of macromolecular assemblies from crystalline state*. J. Mol. Biol. **372**, 774--797.

E. Krissinel and K. Henrick (2005). *Detection of Protein Assemblies in Crystals*. In: M.R. Berthold *et.al.* (Eds.): [CompLife 2005](#), LNBI 3695, pp. 163--174. Springer-Verlag Berlin Heidelberg.













E. Krissinel (2009). *Crystal contacts as nature's docking solutions*. J. Comp. Chem., in press; published on-line 6 May 2009; DOI 10.1002/jcc.21303}

# 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.



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

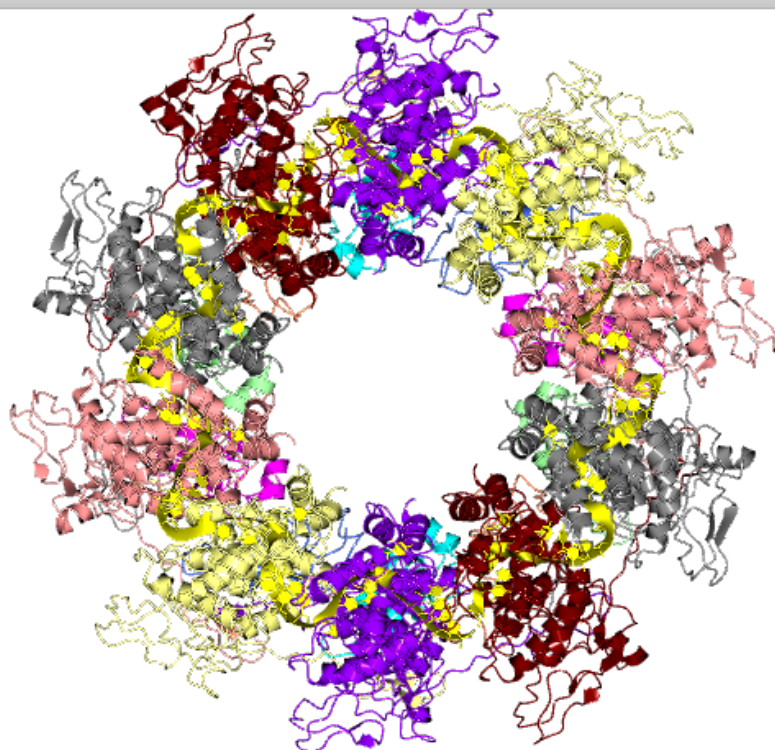
Close

Analyse structure













Show

Clear display

Help



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

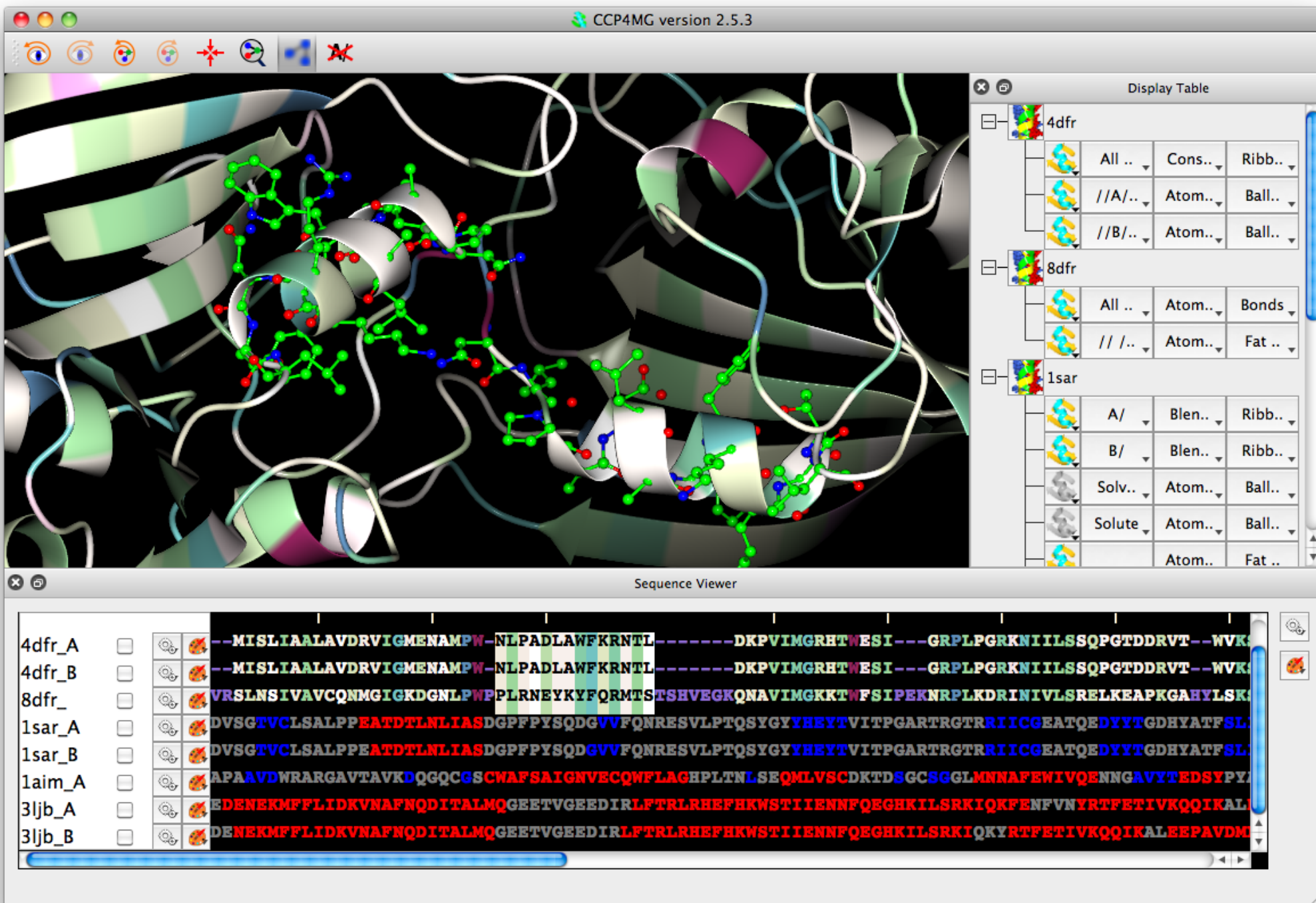
Help

# Structure Superposition

- CCP4MG has 3 (actually 4 – more on 4<sup>th</sup> later):
  - 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. (This will soon be replaced by *gesamt*.)
  - Close Residues. This method is useful for performing locally optimised superposition after a global superposition by SSM
  - User-defined. This is the most flexible: the user can specify in many ways the atoms to superpose.

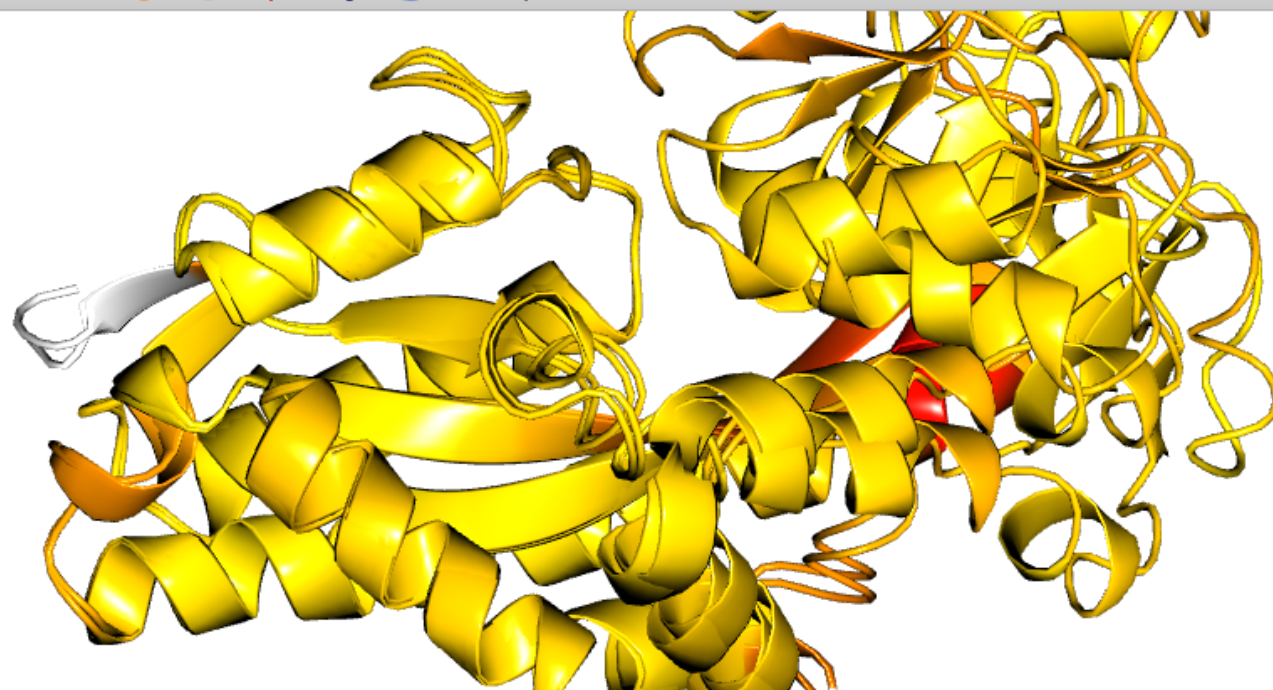
# Sequence Viewer

- Continuous colour by conservation.
- Colour by secondary structure.
- Blastn/blastp interface.
- Save as PDF/bitmap.
- Blast results cached.



# ProSMART

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



Display Table

Create object Tools

2CEX

All .. Atom.. Bonds

A/ ProS.. Ribb..

3B50

All .. Atom.. Bonds

A/ ProS.. Ribb..

ProSMART analysis

2CEX/D 3B50... 2CEX/A 3B50... 2CEX/A 2CEX/B 2CEX/C 3B50... 2CEX/B 3B50/A

Residue No. 1	Residue No. 2	Amino acid 1	Amino acid 2	Side RMS	Side AV	Min	Central	Rotate
2	2	ASP	ASP	4.505	3.758	0.5051	NA	NA
3	3	TYR	TYR	0.2811	0.2449	0.2347	NA	NA
4	4	ASP	ASP	0.4762	0.4326	0.2131	NA	NA
5	5	LEU	LEU	0.25	0.2355	0.1943	0.5051	0.0005425
6	6	LYS	LYS	0.8459	0.5697	0.1943	0.2347	0.003677
7	7	PHE	PHE	1.723	0.3356	0.1943	0.2131	0.003131
8	8	GLY	GLY	0.2454	0.2454	0.1943	0.1943	0.002141
9	9	MET	MET	0.2343	0.1728	0.1943	0.2113	0.003736

Show coloured by

Edit colours for

Superpose

Load ProSMART results

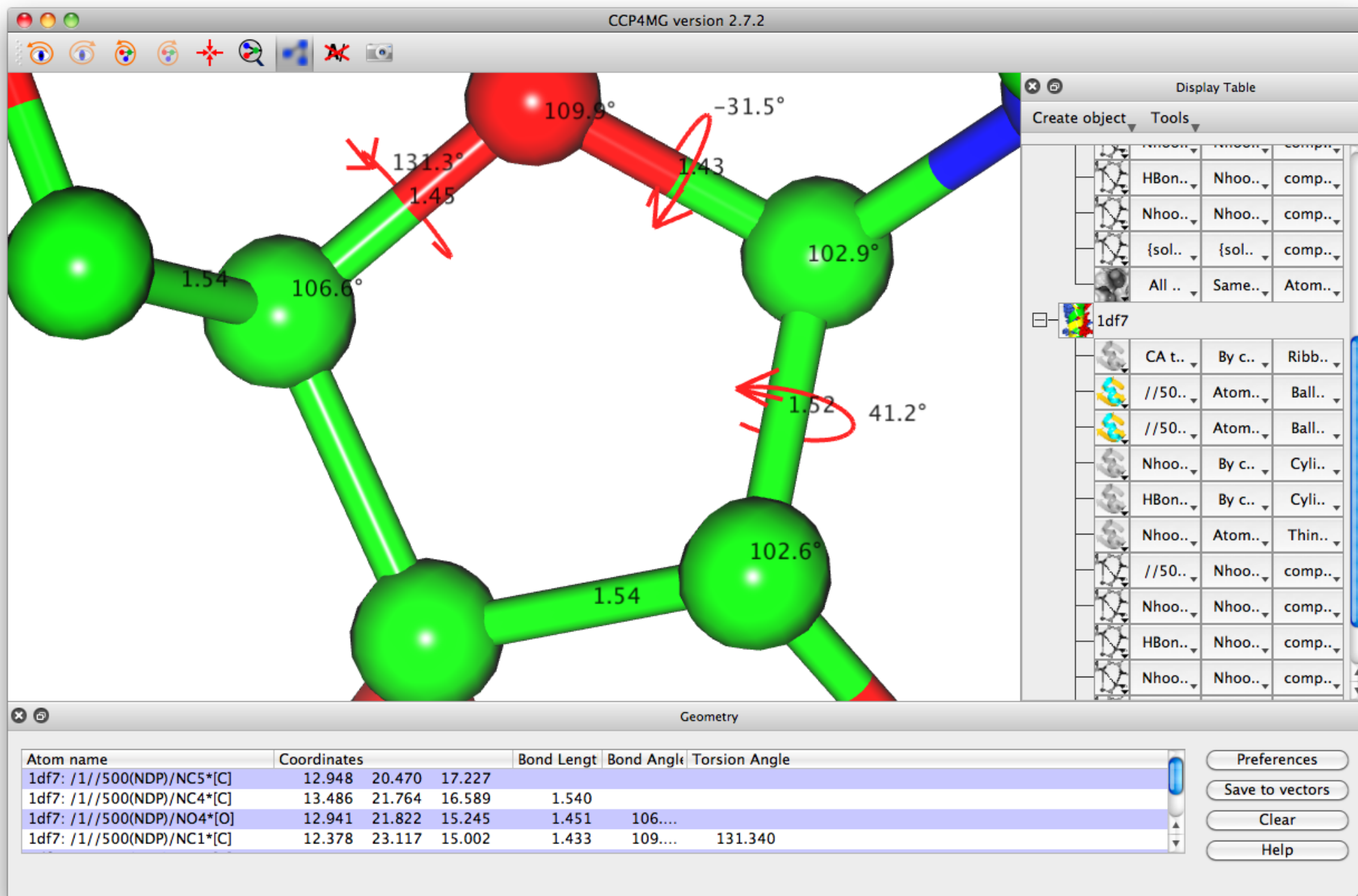
Run ProSMART

on:

2CEX A

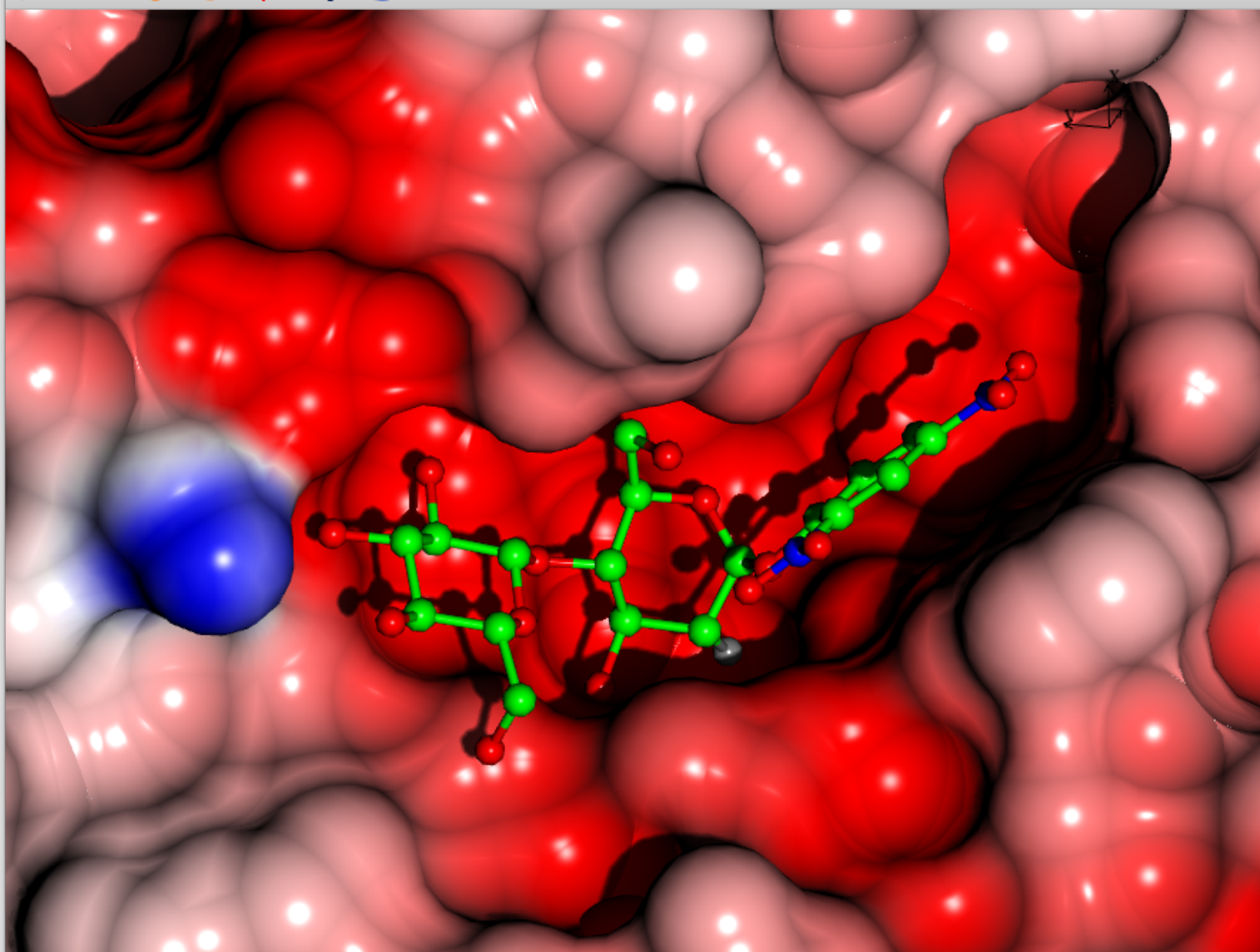
☒ 3B50 A

# Distances and angles



# 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.



Display Table

Create object Tools

4a3h

Atom Ball

Lighting

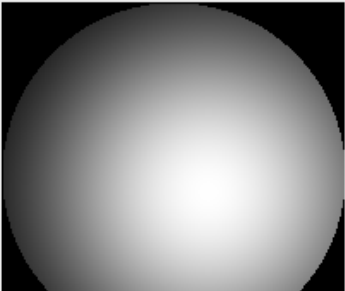
Light 0

☒ On

Diffuse  ☐

Specular  ☐

Ambient  ☐

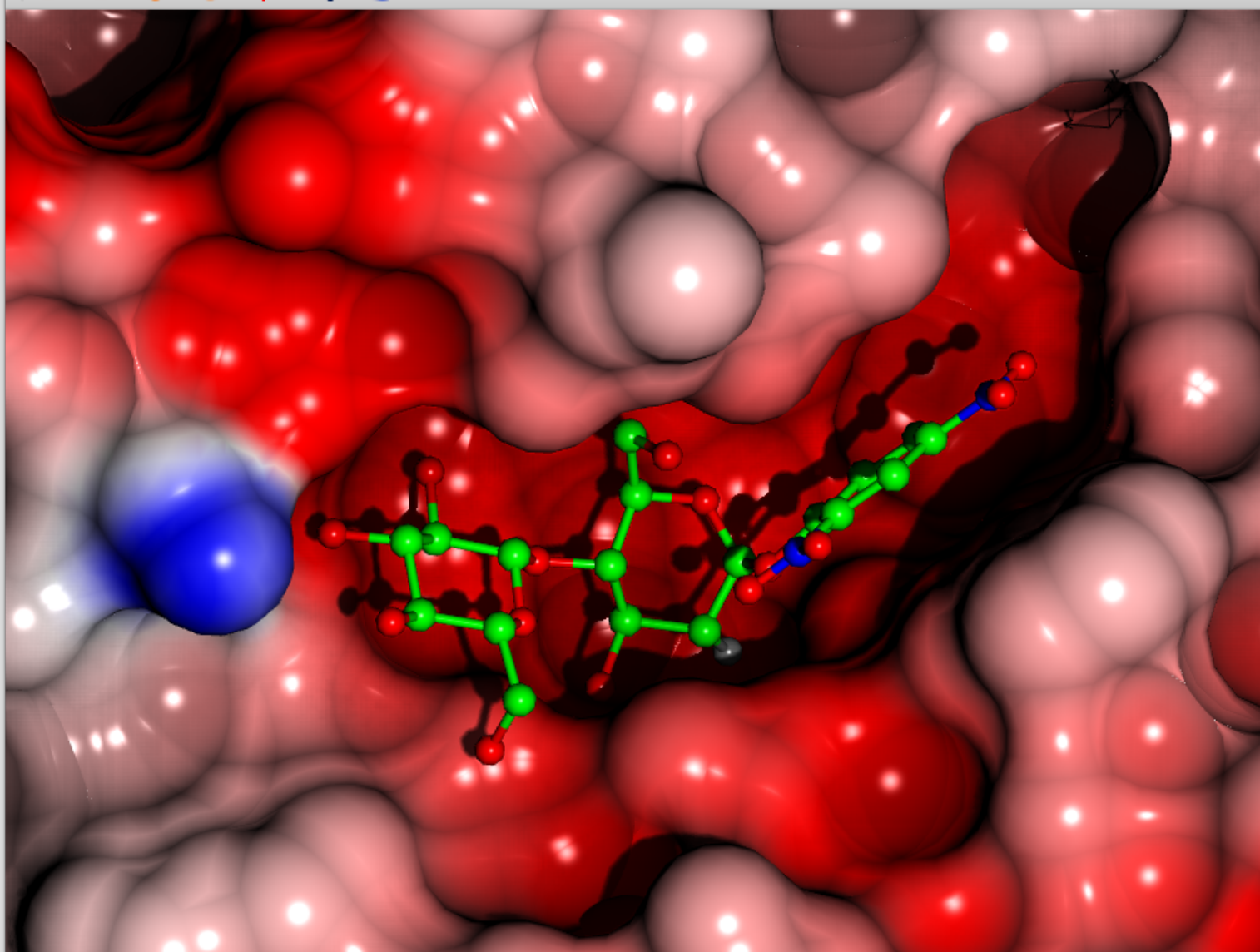


☒ Shadows (light 0 only)

☐ Occlusion

☐ Object outlines

Help



Display Table

Create object Tools

4a3h

Atom Ball

Lighting

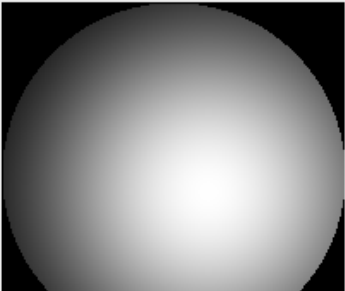
Light 0

☒ On

Diffuse  ☐

Specular  ☐

Ambient  ☐

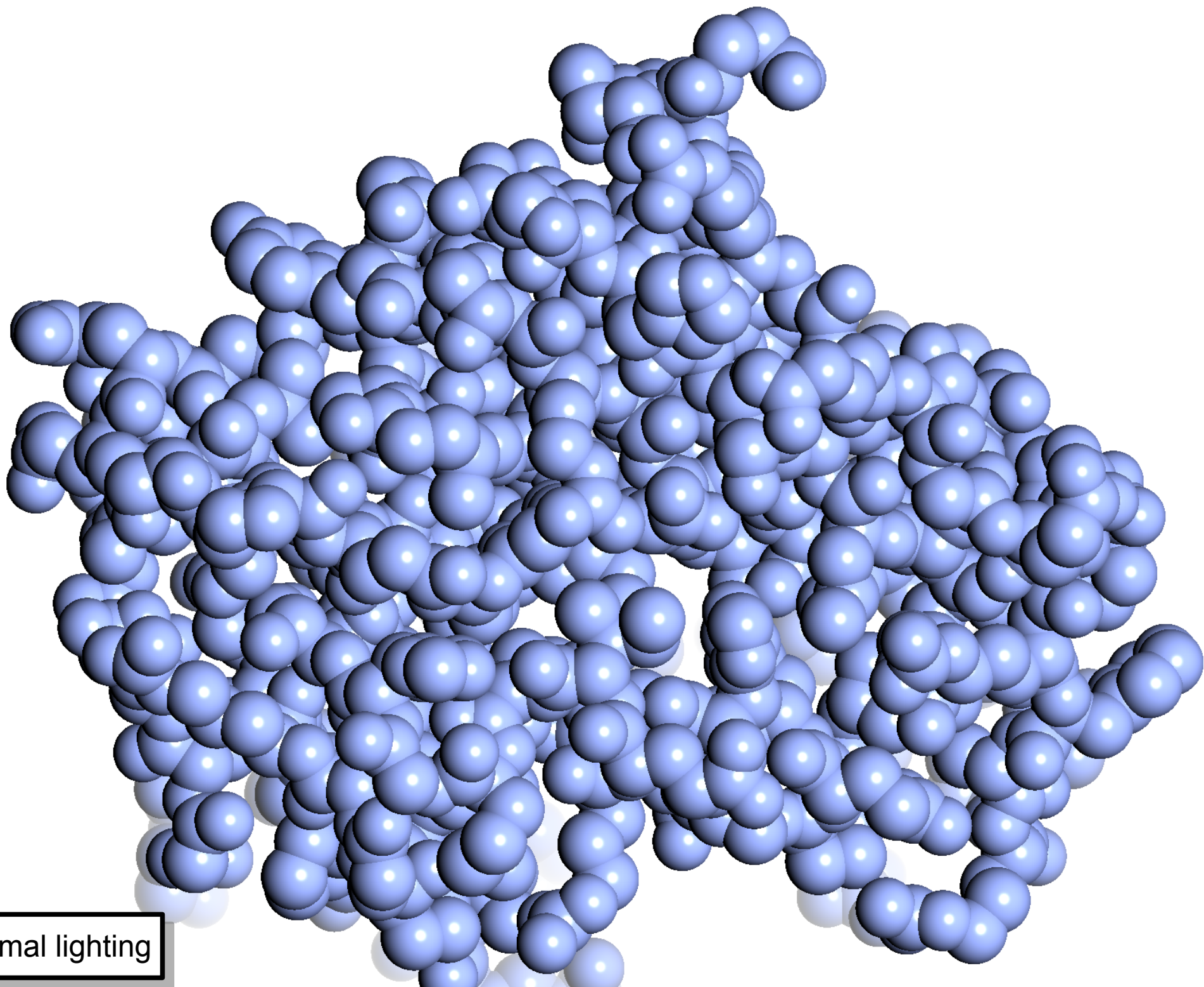


☒ Shadows (light 0 only)

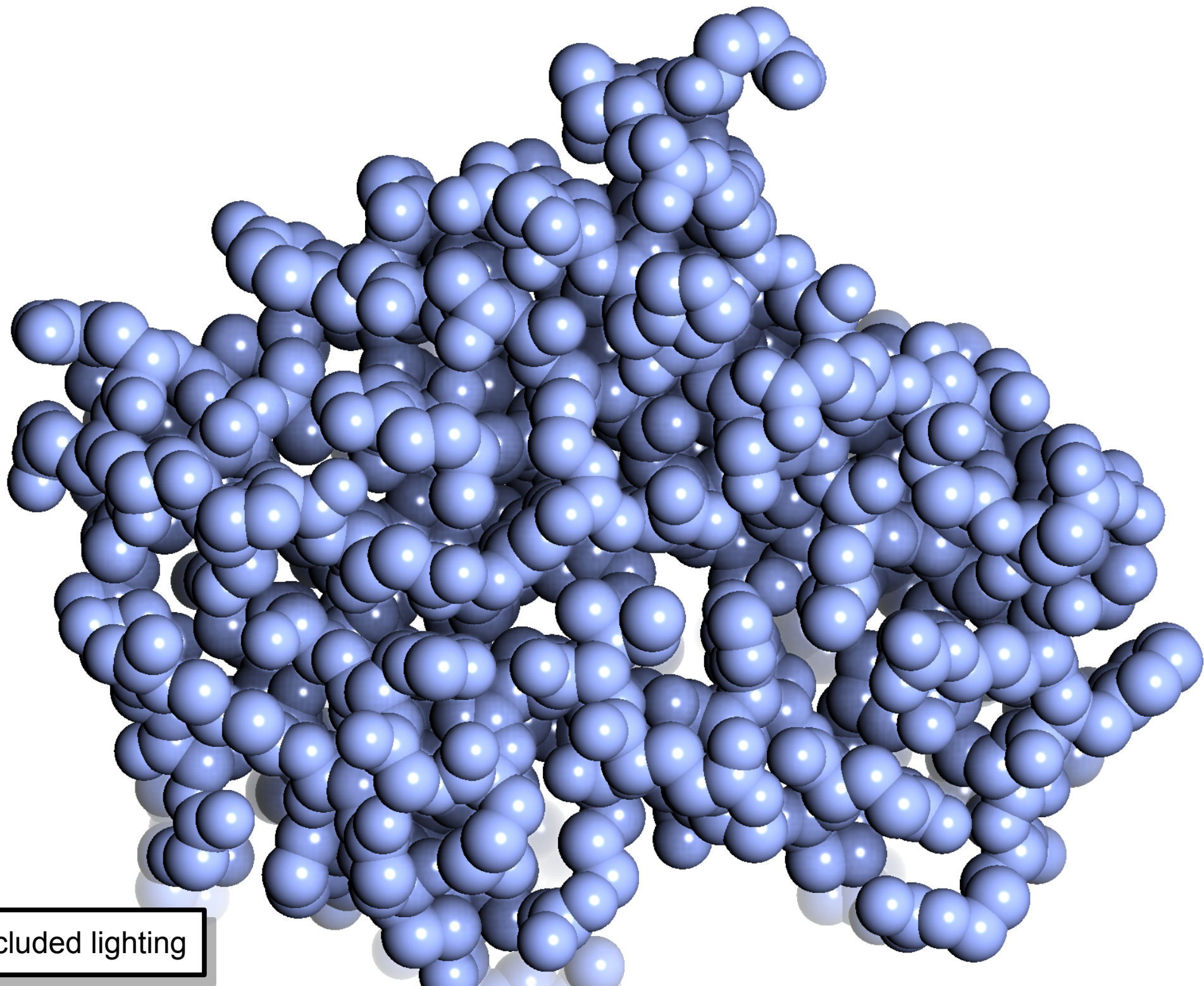
☒ Occlusion

☐ Object outlines

Help



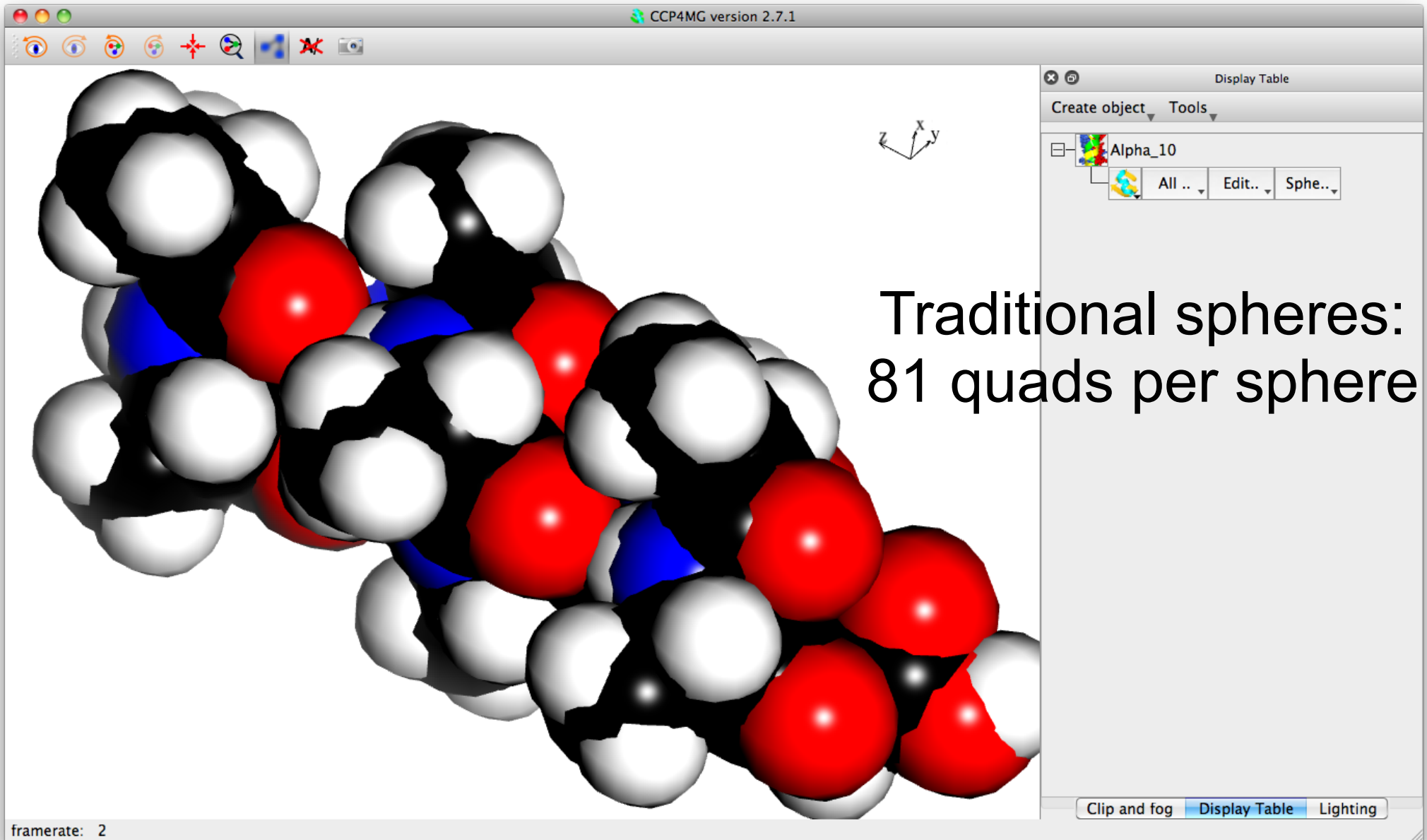
Normal lighting

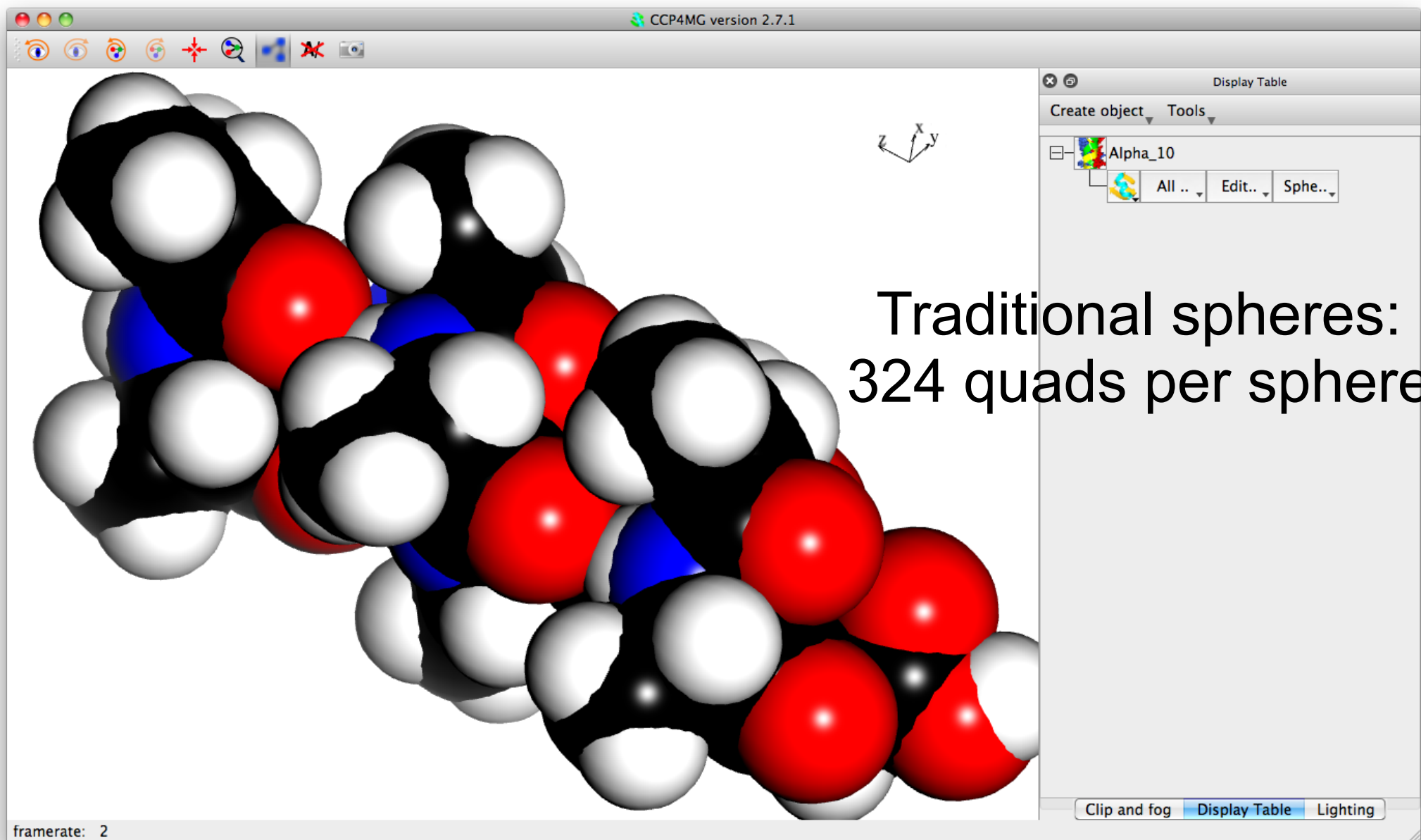


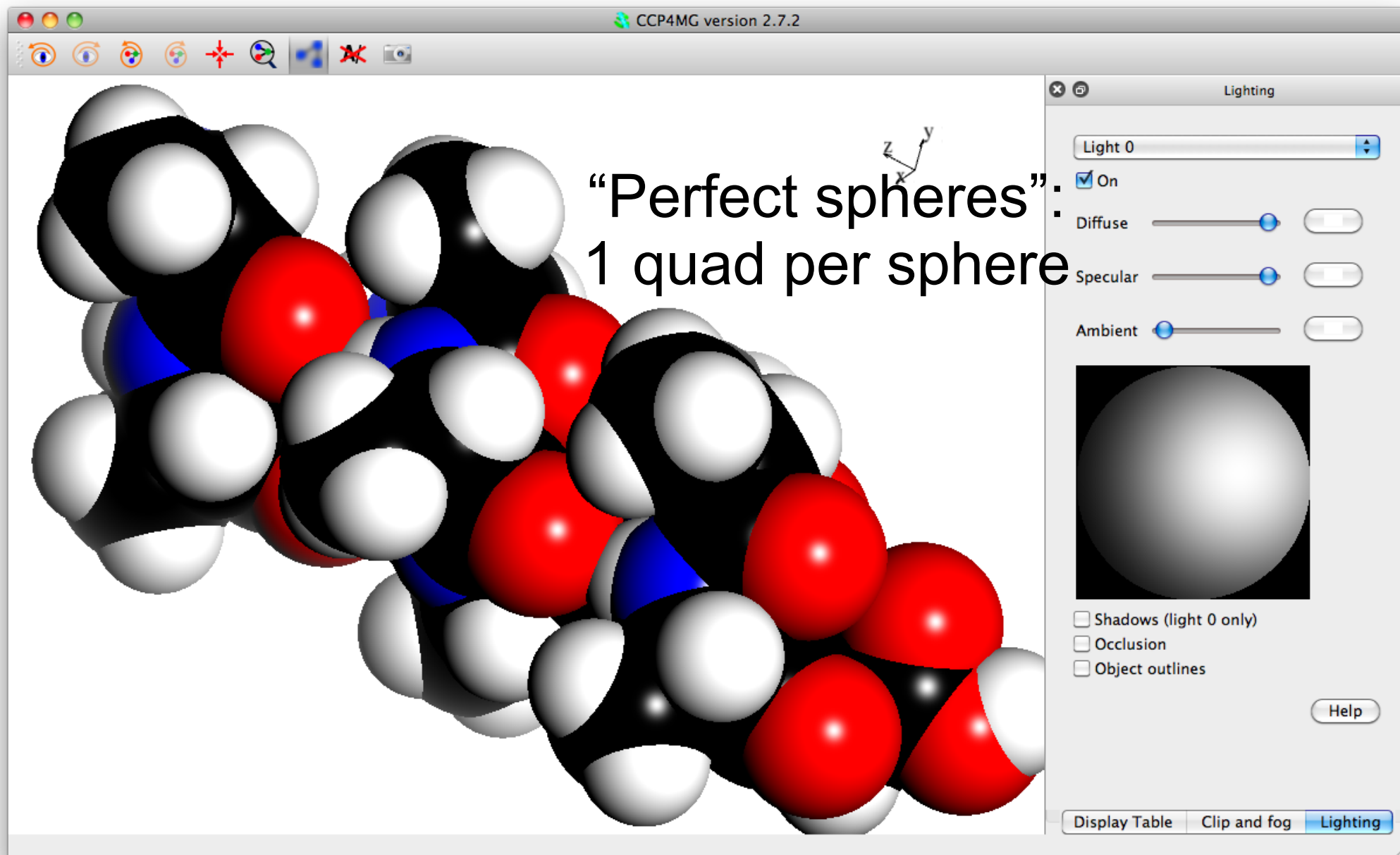
Occluded lighting

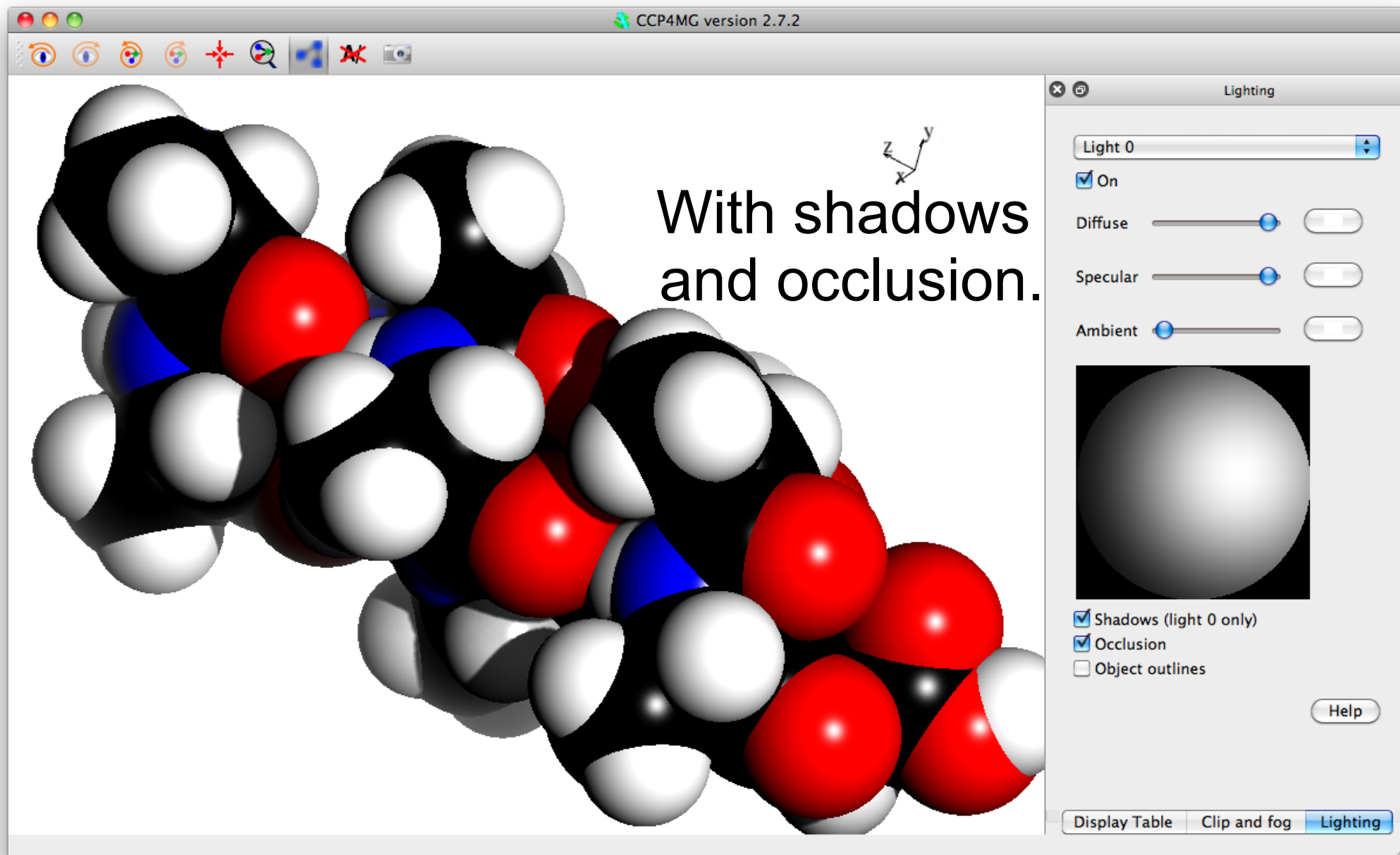
# “Perfect spheres”

- “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 Apple's drivers used more hardware features ....)









# To do (perfect spheres)

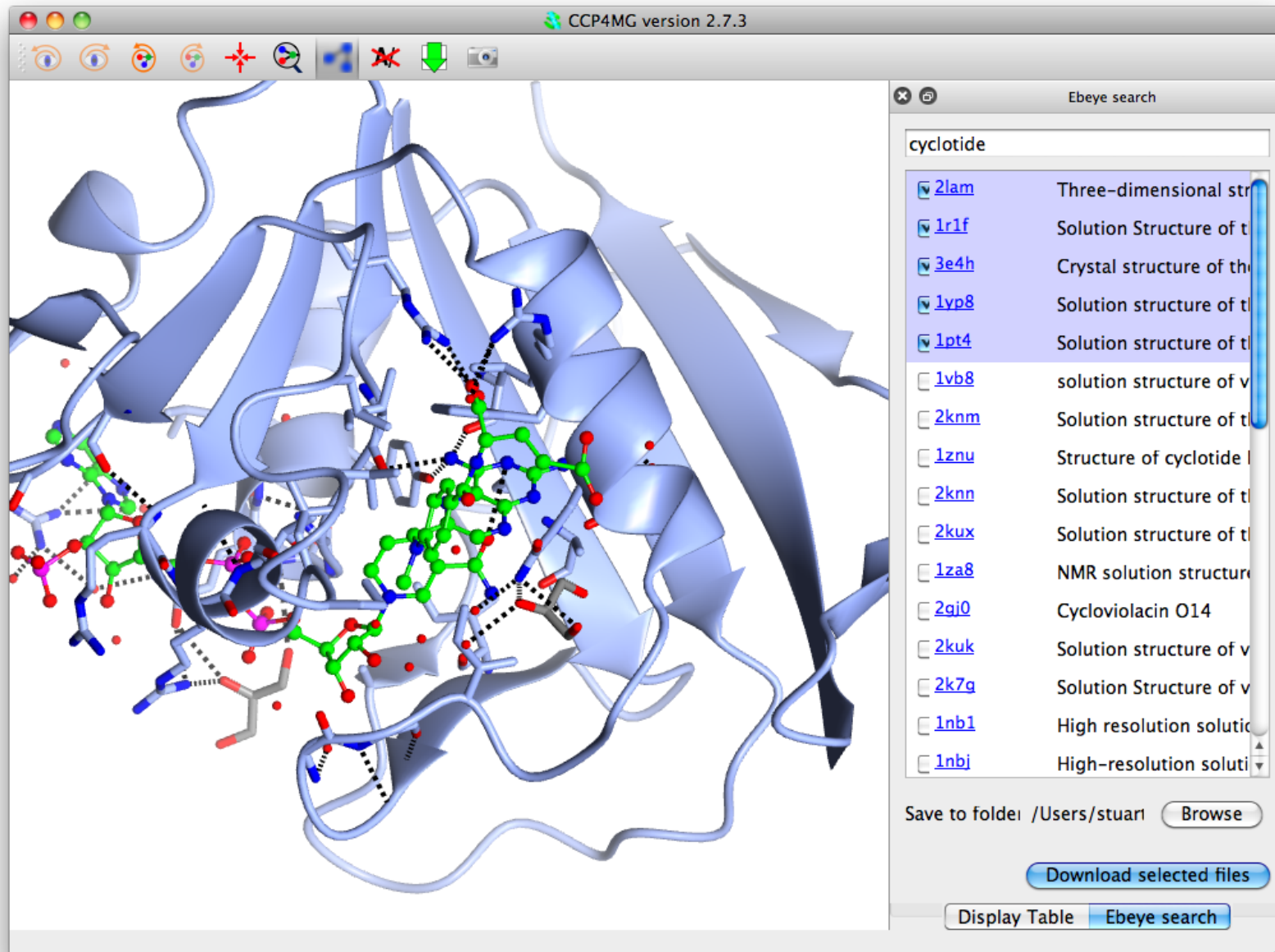
- Make faster.
- Same trick for cylinders, ball and stick representations.
- Cylinders by default look more rounded than spheres, so may not have to do anything with them for looks, but ray traced cylinders would also use less memory.

# Render vs. Screenshot

- These features mean that 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 antialiased. (So not so perfect!). This can be worked around (now) by taking screenshot at larger size (2x, 4x, etc.), though this should be automatic.
    - Render handles multiple transparent objects properly. This is a pain to sort out in OpenGL, but doable.

# Ebeye - search

CCP4MG version 2.7.3



**Ebeye search**

cyclotide

<input checked="" type="checkbox"/>	<a href="#">2lam</a>	Three-dimensional str
<input checked="" type="checkbox"/>	<a href="#">1r1f</a>	Solution Structure of t
<input checked="" type="checkbox"/>	<a href="#">3e4h</a>	Crystal structure of th
<input checked="" type="checkbox"/>	<a href="#">1yp8</a>	Solution structure of t
<input checked="" type="checkbox"/>	<a href="#">1pt4</a>	Solution structure of t
<input type="checkbox"/>	<a href="#">1vb8</a>	solution structure of v
<input type="checkbox"/>	<a href="#">2knm</a>	Solution structure of t
<input type="checkbox"/>	<a href="#">1znu</a>	Structure of cyclotide l
<input type="checkbox"/>	<a href="#">2knn</a>	Solution structure of t
<input type="checkbox"/>	<a href="#">2kux</a>	Solution structure of t
<input type="checkbox"/>	<a href="#">1za8</a>	NMR solution structure
<input type="checkbox"/>	<a href="#">2qj0</a>	Cycloviolacin O14
<input type="checkbox"/>	<a href="#">2kuk</a>	Solution structure of v
<input type="checkbox"/>	<a href="#">2k7g</a>	Solution Structure of v
<input type="checkbox"/>	<a href="#">1nb1</a>	High resolution soluti
<input type="checkbox"/>	<a href="#">1nbj</a>	High-resolution soluti

Save to folder: /Users/stuart

# Normal Modes

- Simple approximate elastic network model.

The screenshot displays the CCP4MG version 2.7.3 software interface. The main window shows a green wireframe model of a protein structure. On the right side, there are three panels:

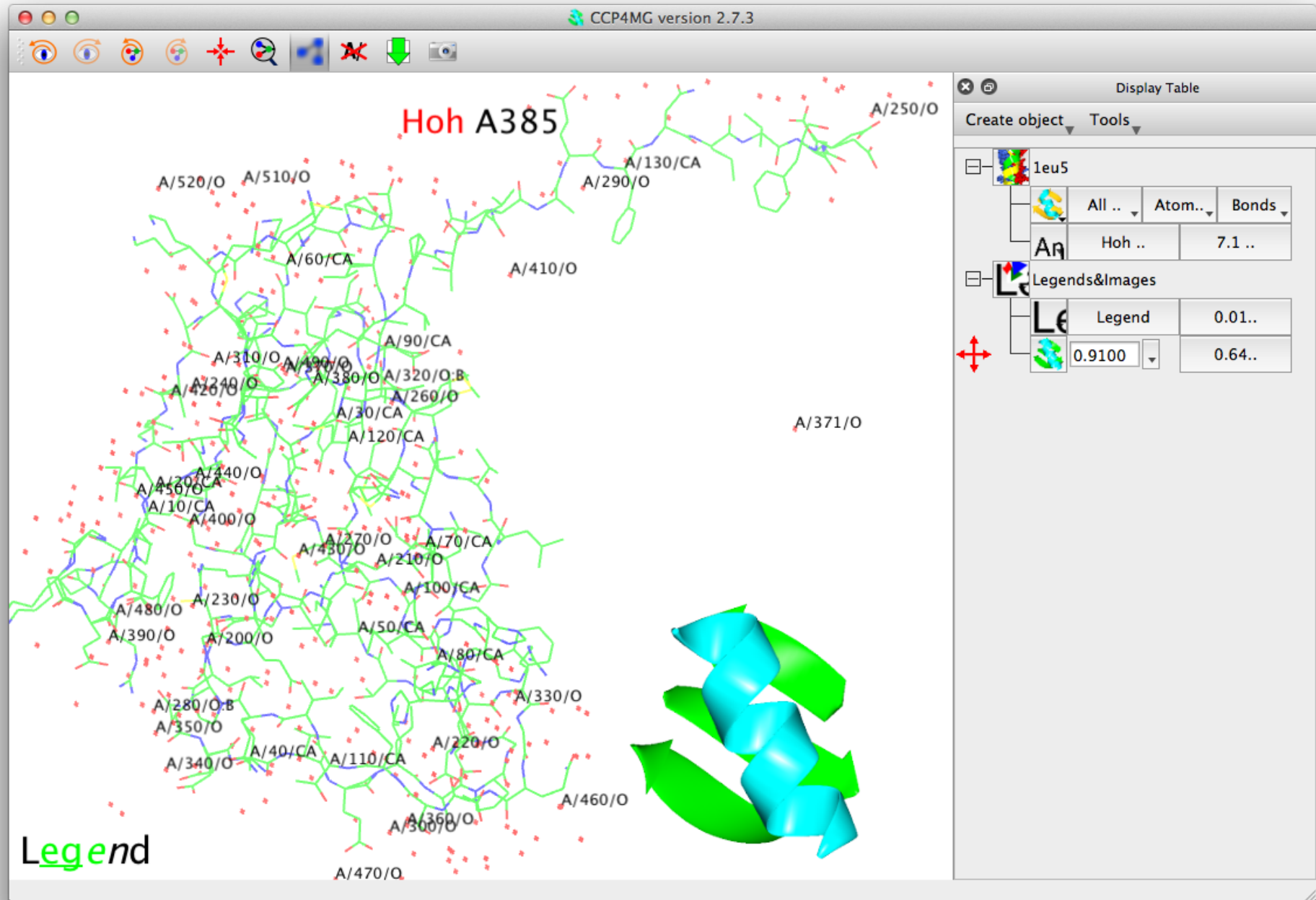
- Display Table**: Contains a 'Create object' dropdown and a 'Tools' dropdown. A list shows '1qb0' with a corresponding icon.
- Vibrations**: Contains a 'Model to analyse' dropdown set to '1qb0'. Below it are three buttons: 'Show Theoretical B-Values', 'Show Cross-correlation', and 'Calculate Normal Modes'. A table lists the first seven normal modes:

Mode	Frequency (Å <sup>-1</sup> )
1	0.30458
2	0.39822
3	0.57978
4	0.66291
5	0.72548
6	0.77825
7	0.86527

Below the table is a 'Show motion' button.

- Animation of 1qb0**: Contains an 'Animation frame (2-11):' slider set to 6. Below it are 'Run in direction' checkboxes for 'forward' (checked) and 'backward'. At the bottom is an 'Animation time interval (ms):' slider set to 100, followed by play and stop buttons.

# On screen text and images



# “Batch” rendering

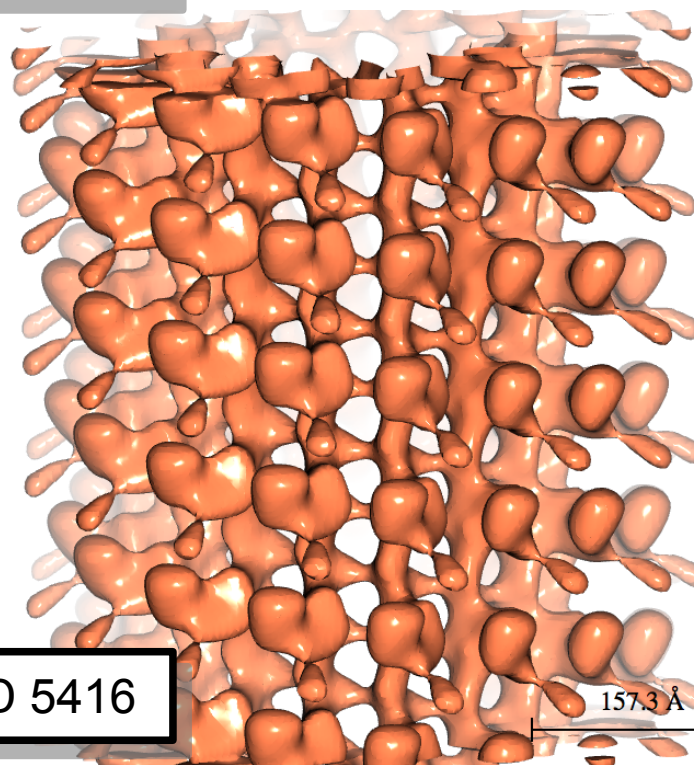
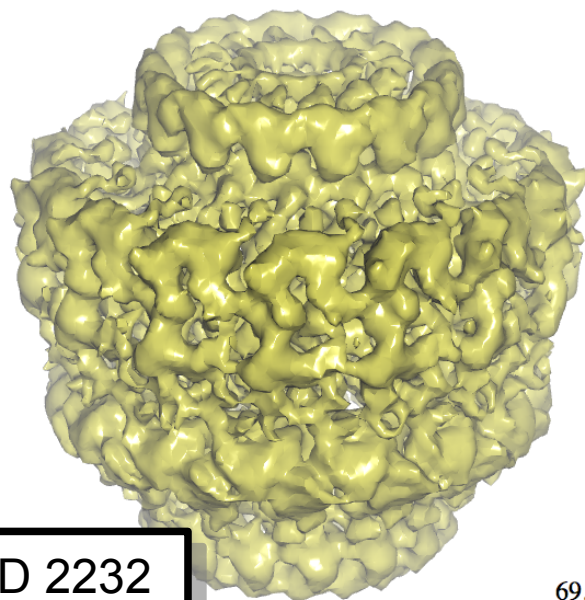
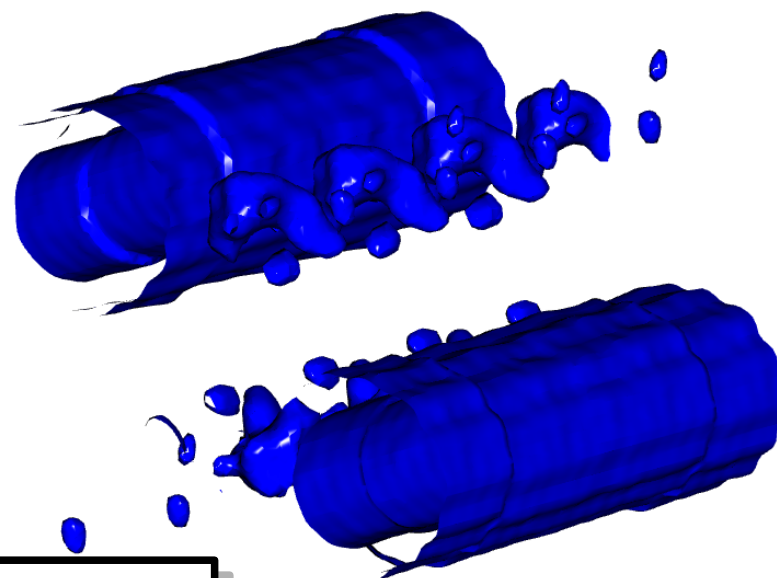
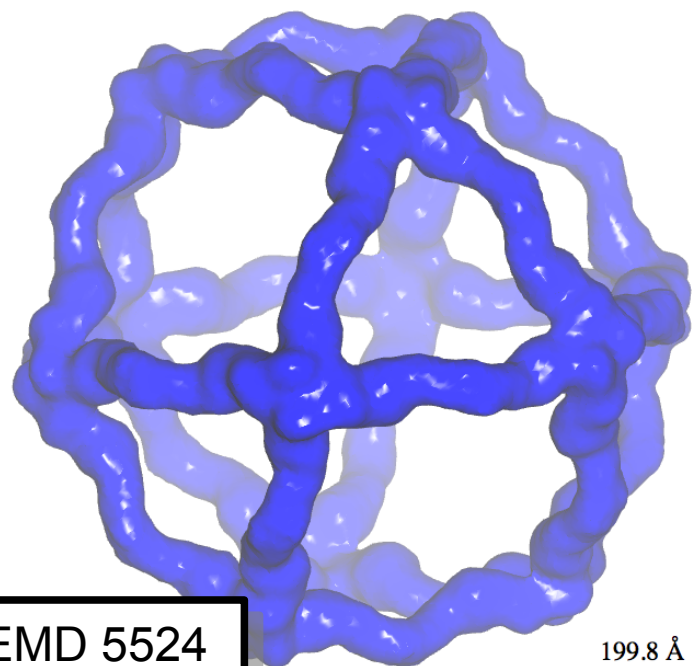
- Images may be rendered from command line or from scripts without starting up the main program.
- `ccp4mg -norestore -picture  
mypic.mgp.py -R test.png -RO  
'{"size":"1600x1600","smoothribbons  
":"1", "raytrace":"1"}' -quit`
- The file `mypic.mpic.py` is a file containing a scene description: lists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

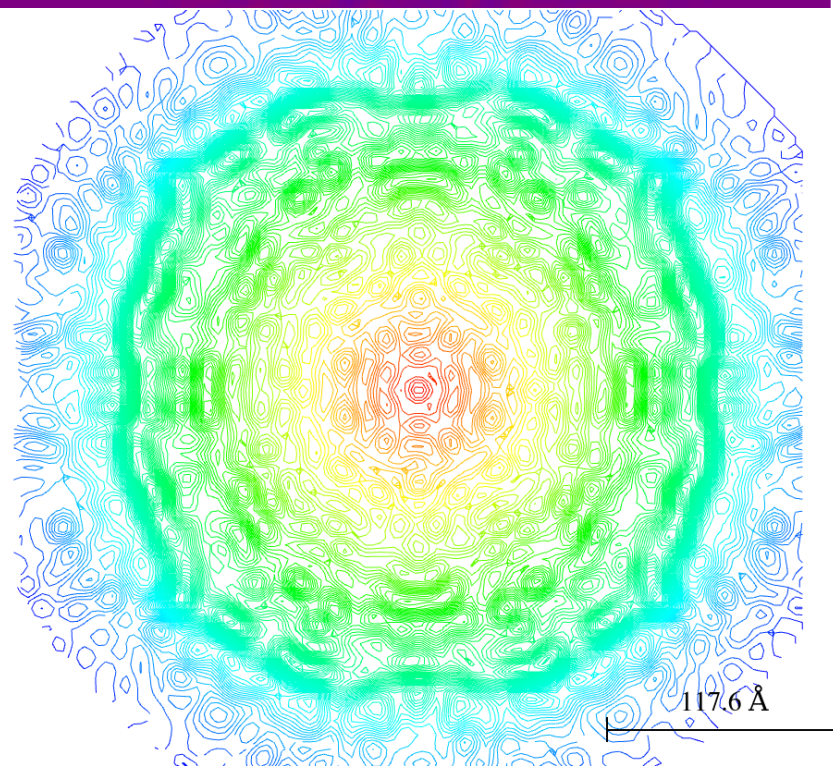
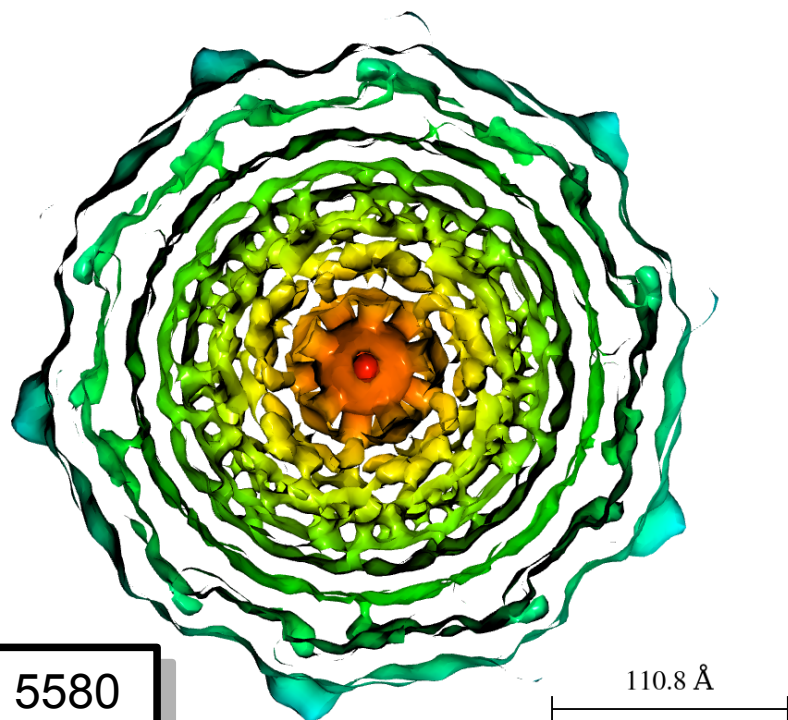
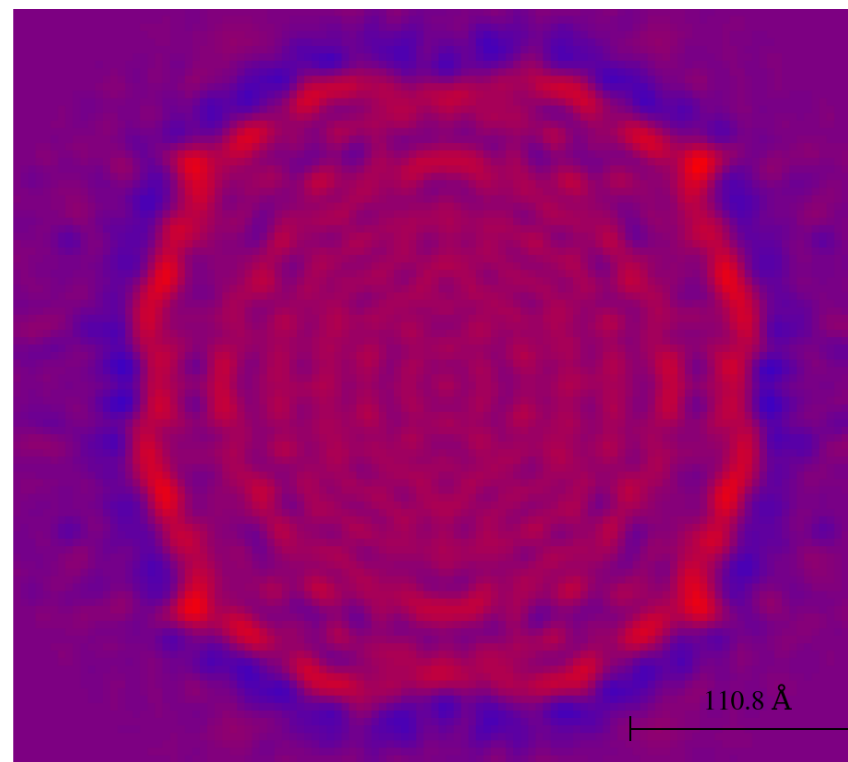
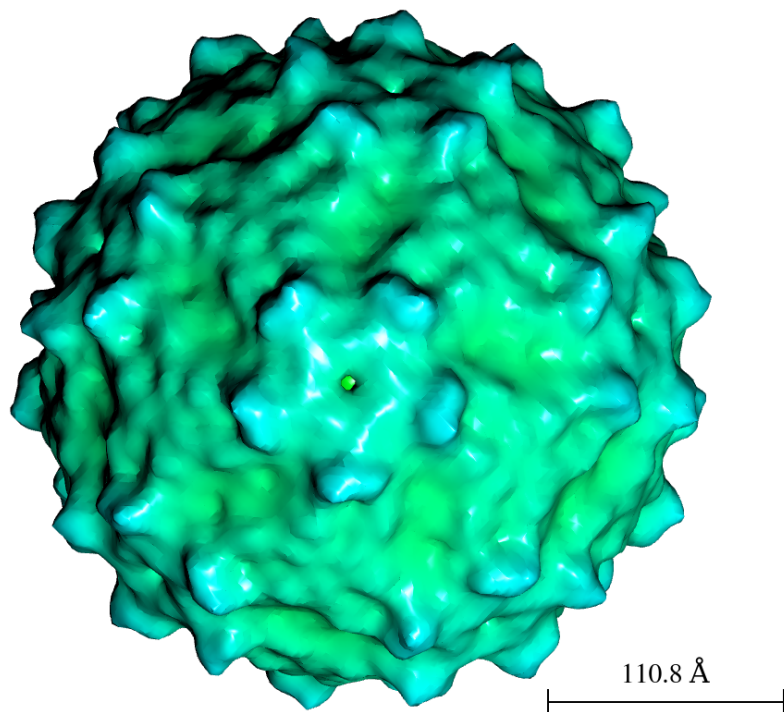
# Recent developments

- Bleeding edge :
  - Electron microscopy maps.
  - Biological assemblies.
  - Structure factor files (from PDB-E) can be downloaded and use to calculate electron density (with an appropriate model).
  - Worm width scaled by B-factor or average position of NMR models.
  - <http://www.ysbl.york.ac.uk/~ccp4mg/nightly/>

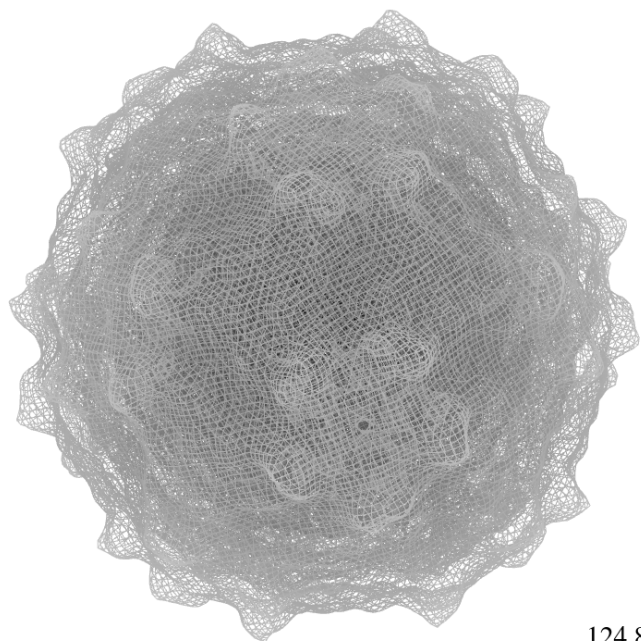
# Electron Microscopy Maps

- Changes made to CCP4MG to handle electron density maps larger than about 200 angstroms.
- 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.
- Scale bar to show size of maps. Do not always have close up view of atoms with EM maps.

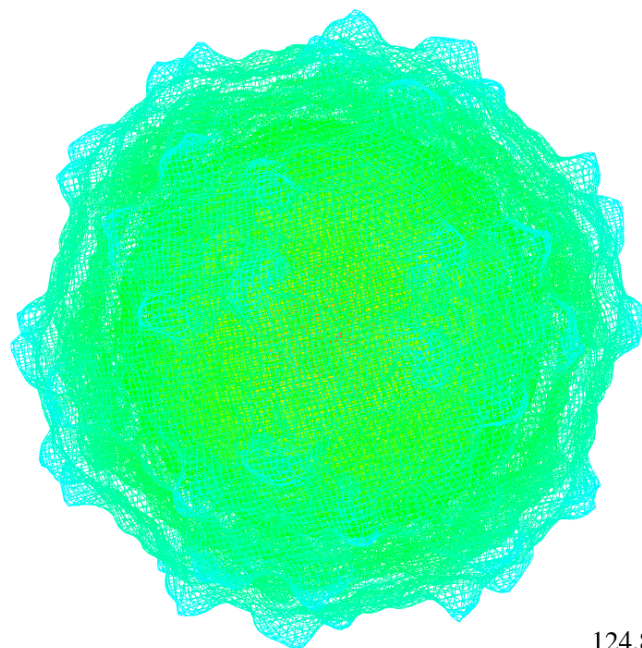




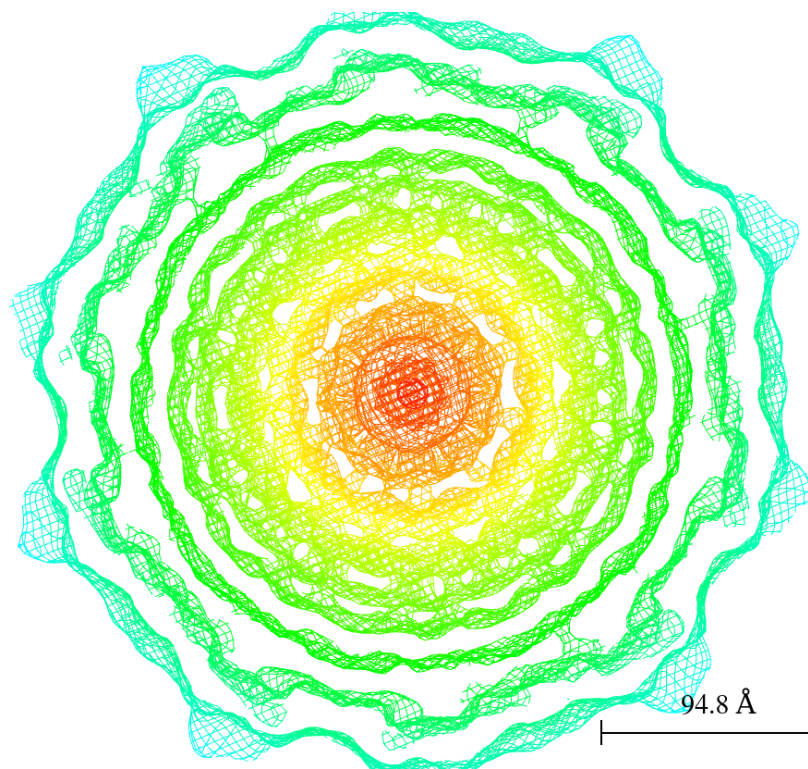
EMD 5580



124.8 Å



124.8 Å

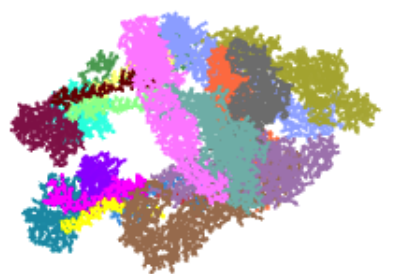


94.8 Å

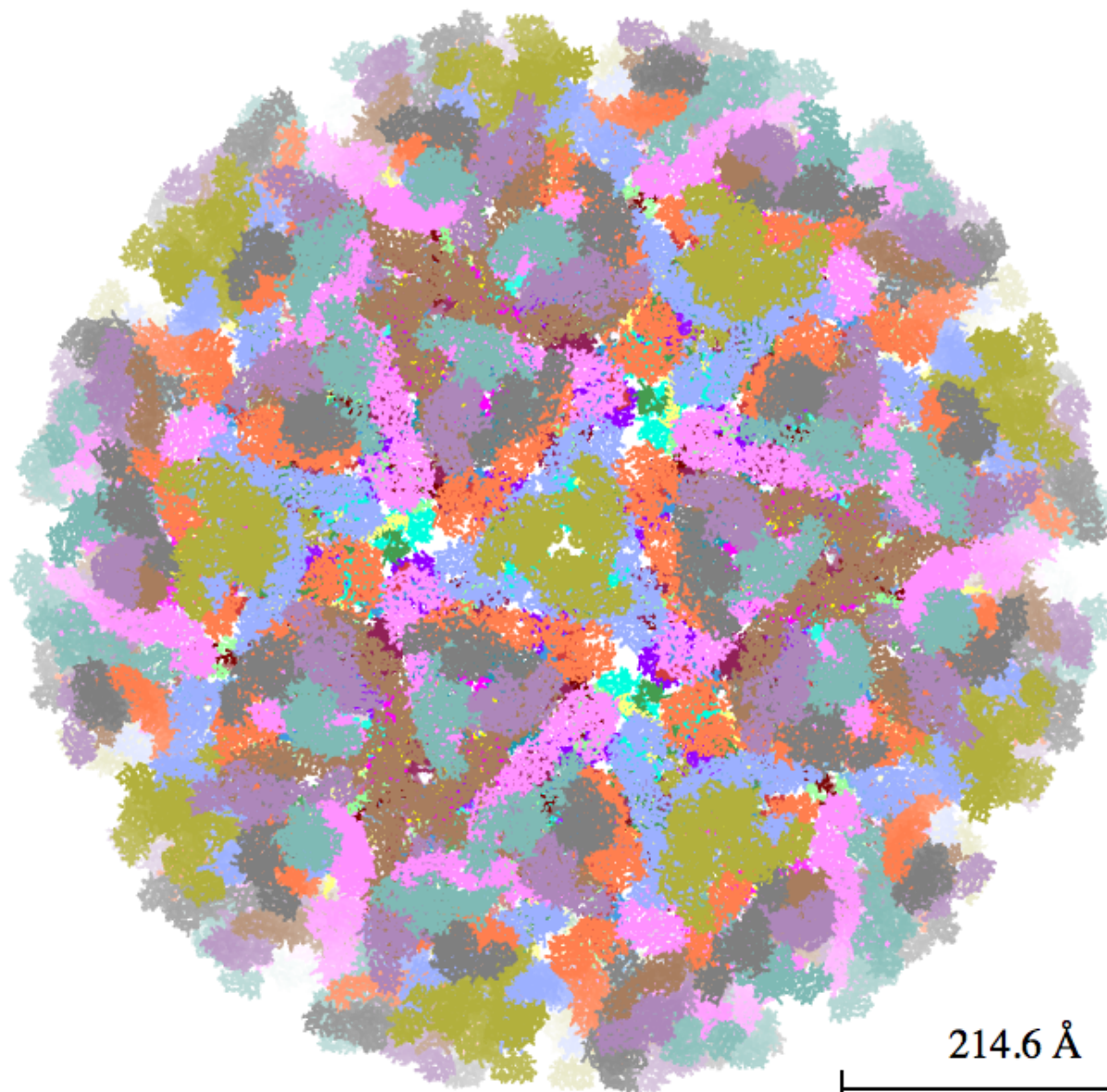
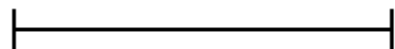
EMD 5580

# Biological Assemblies

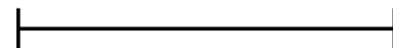
- Nightly builds can now parse the biological assembly information contained in PDB files.
  - Set of transformation matrices that create symmetry mates of model information to create a complete assembly.
  - Does not do PISA calculation – much simpler and faster – matrices used to redraw pictures without generating transformed atoms.



214.6 Å



214.6 Å



PDB 3j2w

# Acknowledgements

- Programming:
  - Liz Potterton
  - Eugene Krissinel
  - Kevin Cowtan
  - Paul Emsley
  - Martin Noble
  - Jan Gruber
  - Bernhard Lohkamp
  - Rob Nicholls
- General help:
  - Keith Wilson
  - Phil Evans
  - CCP4 staff: Eugene Krissinel, Charles Ballard, Ronan Keegan, Marcin Wojdyr, Andrey Lebedev, Ville Uski, David Waterman.
- Funding:
  - CCP4