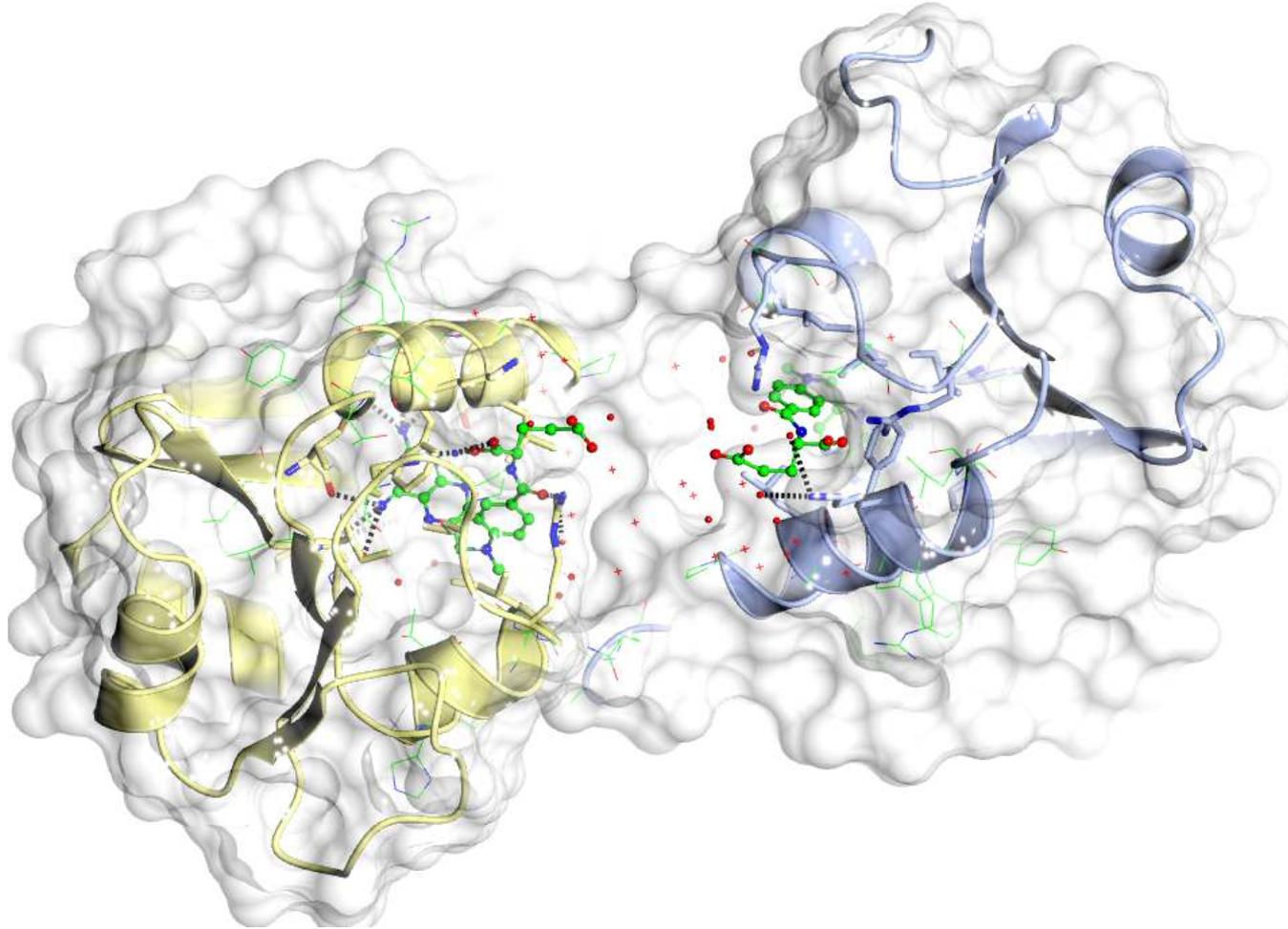


# CCP4MG



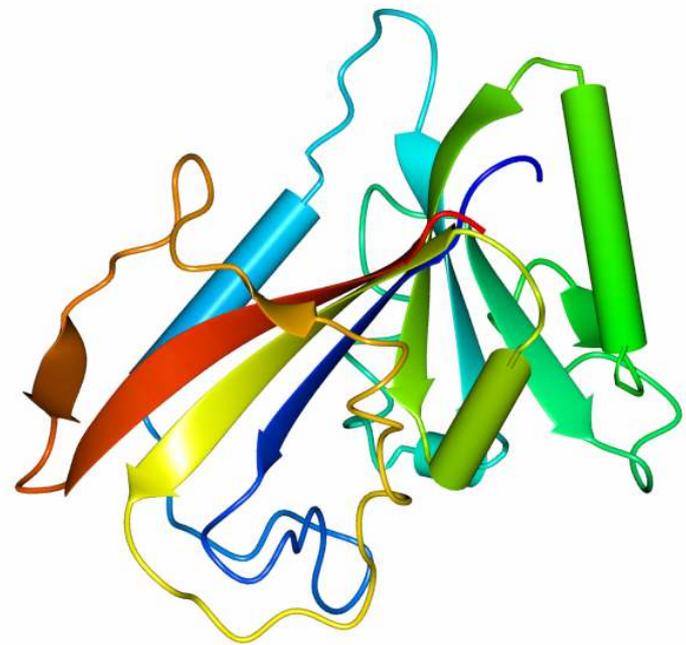
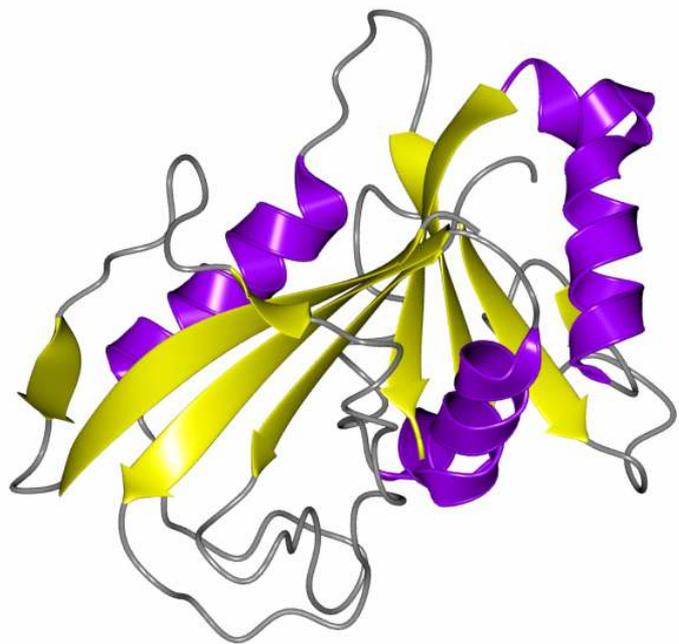
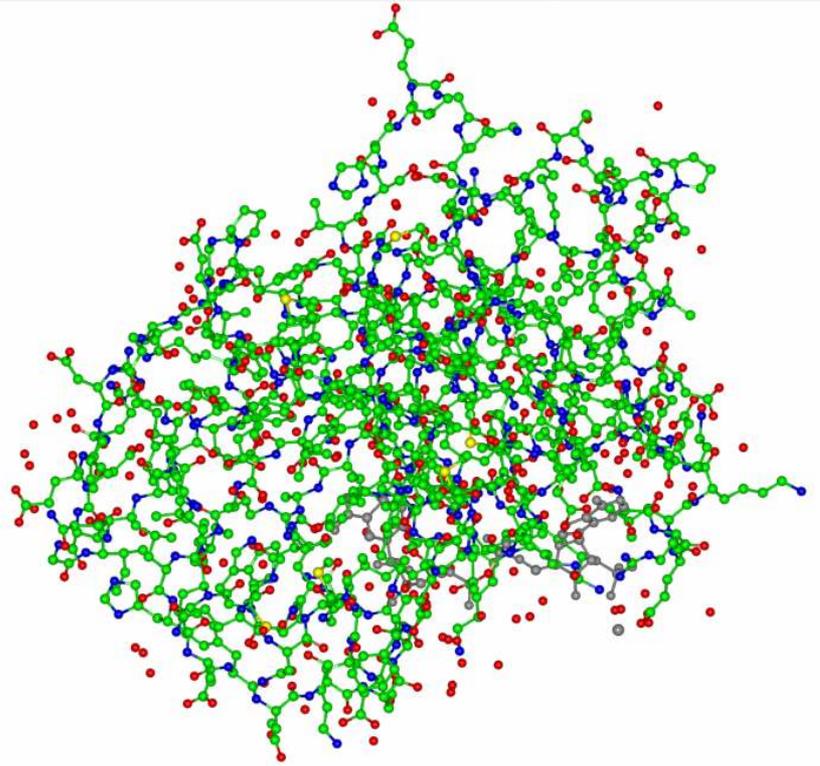
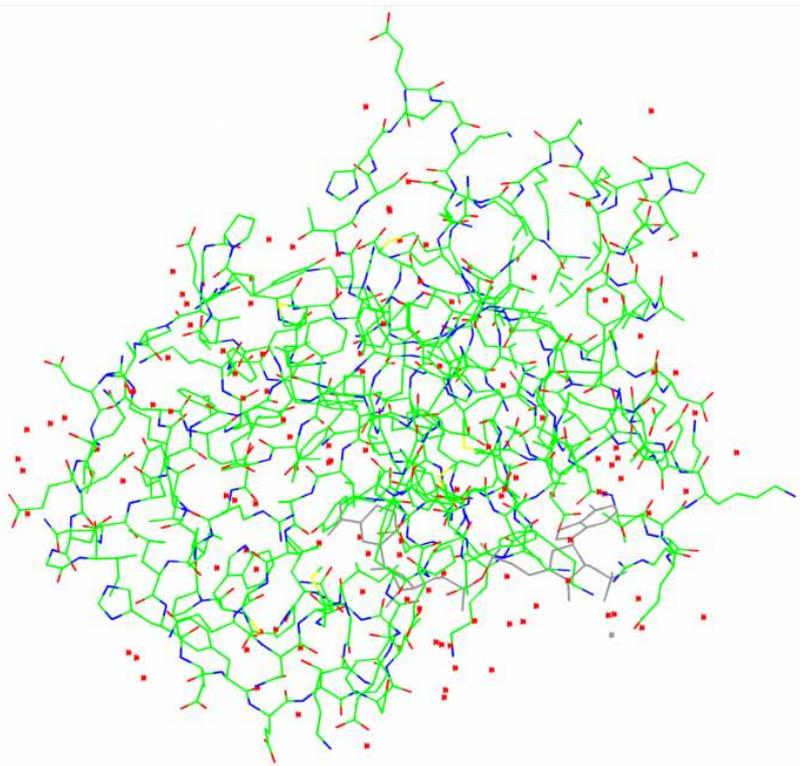
CCP4 Molecular Graphics Program

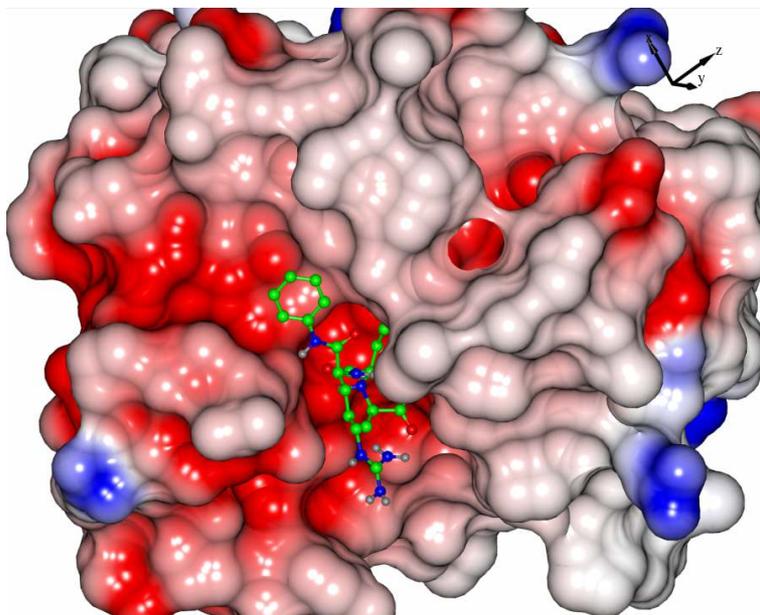
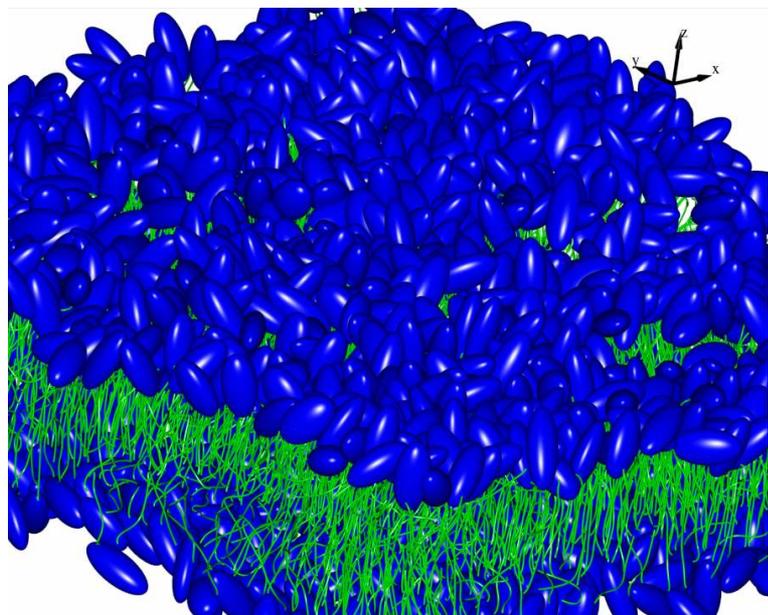
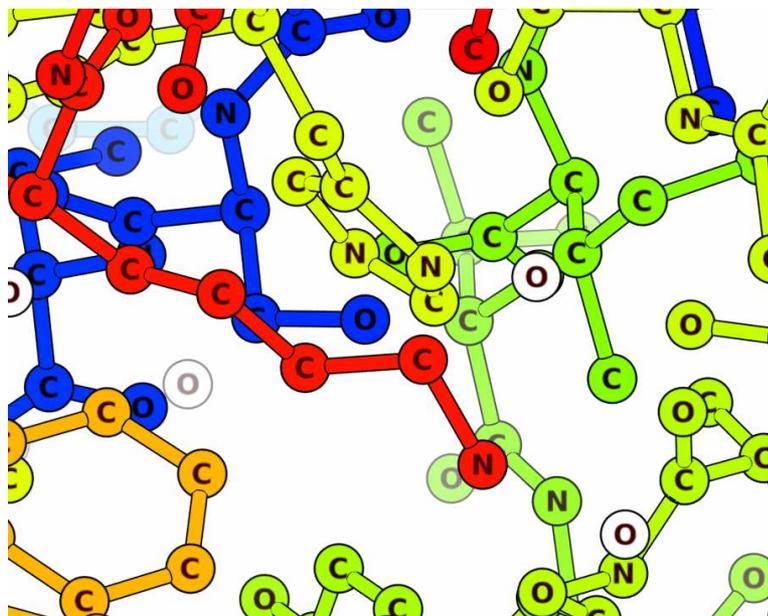
# Introduction

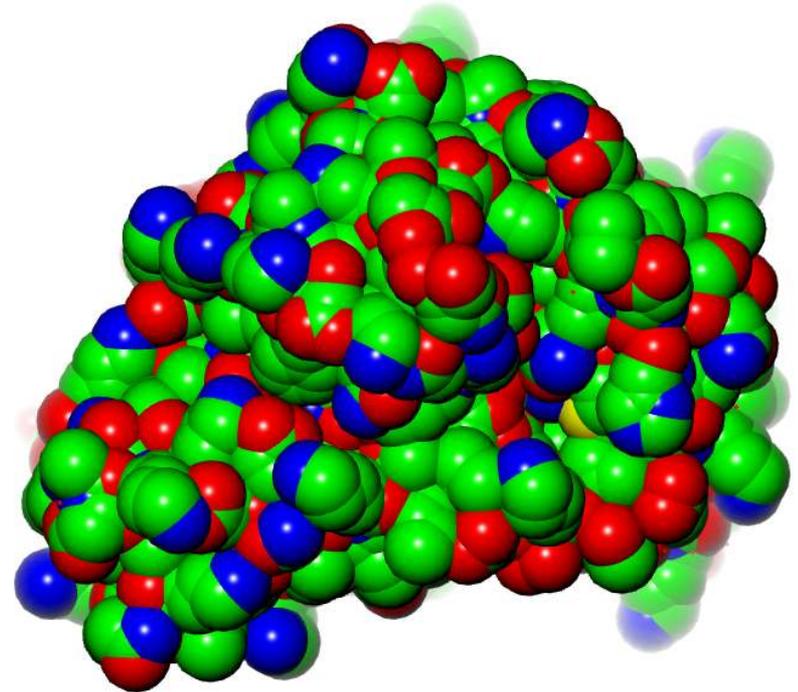
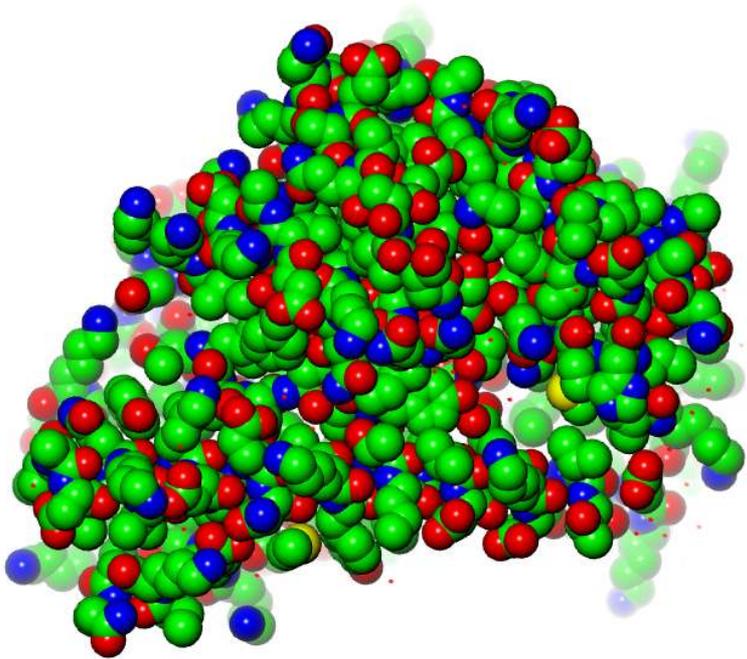
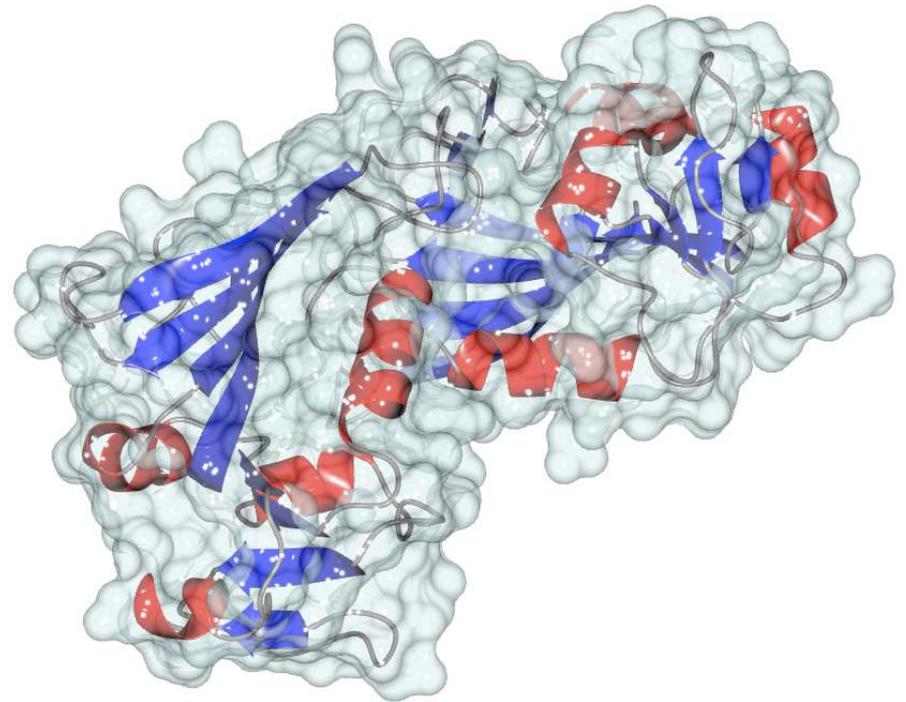
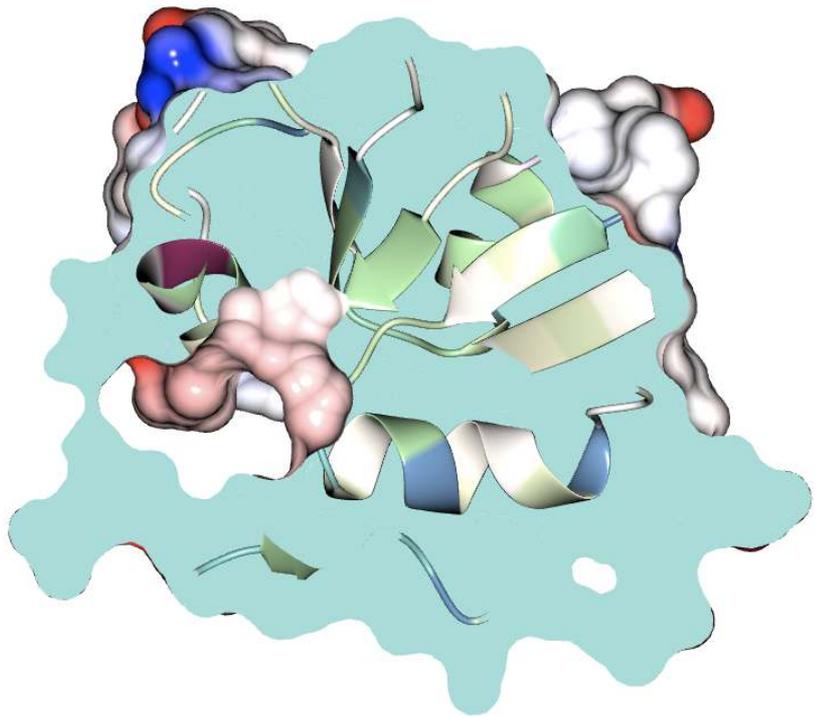
- CCP4MG is a molecular graphics program funded by CCP4.
- Its primary focus is the visualization and analysis of macromolecular structure.
- It produces high quality rendered images and movies.
- <http://www.ccp4.ac.uk/MG/>
  - Binaries for Windows, Mac and Linux.

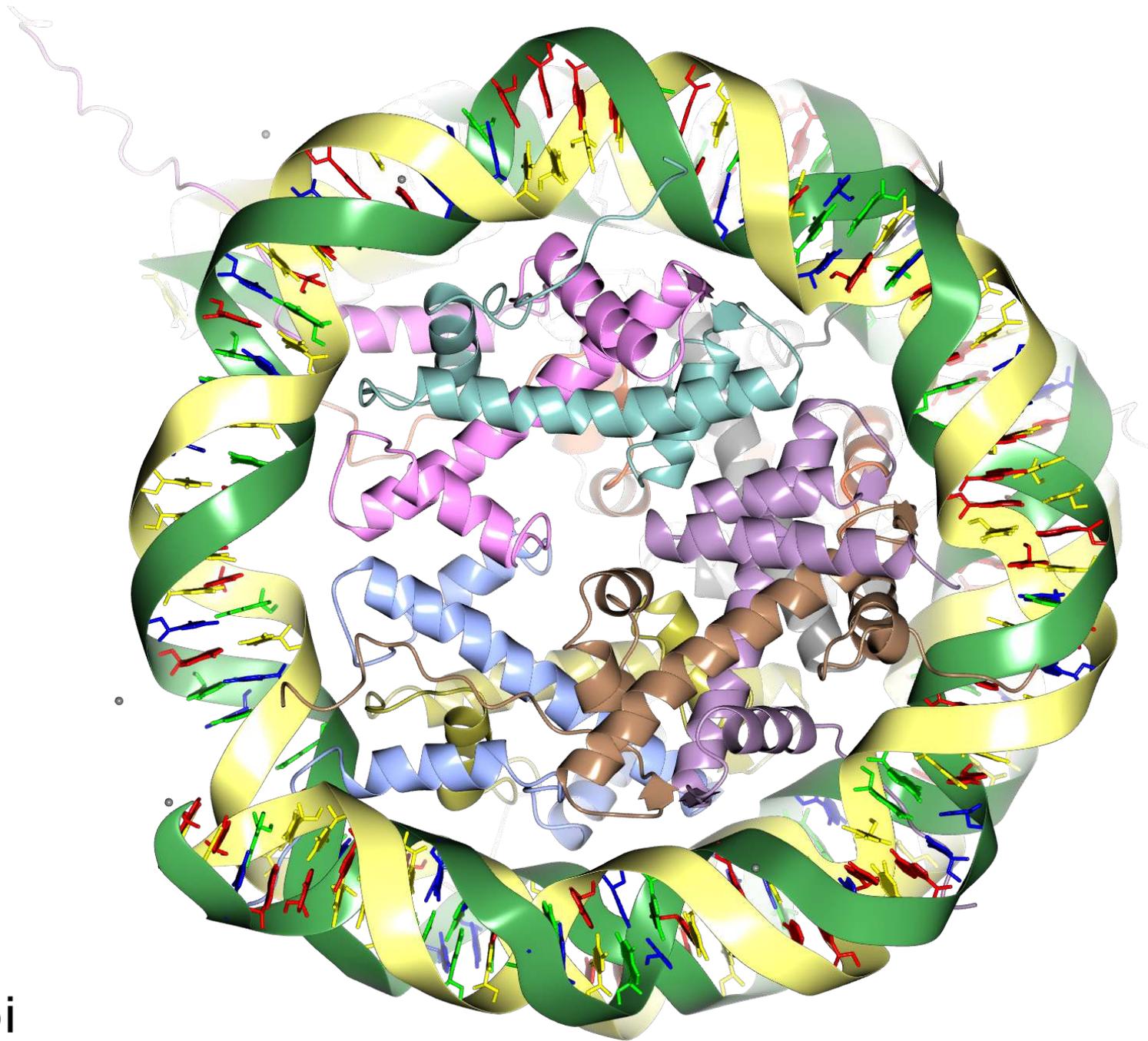
# Displaying Molecules (styles)

- 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

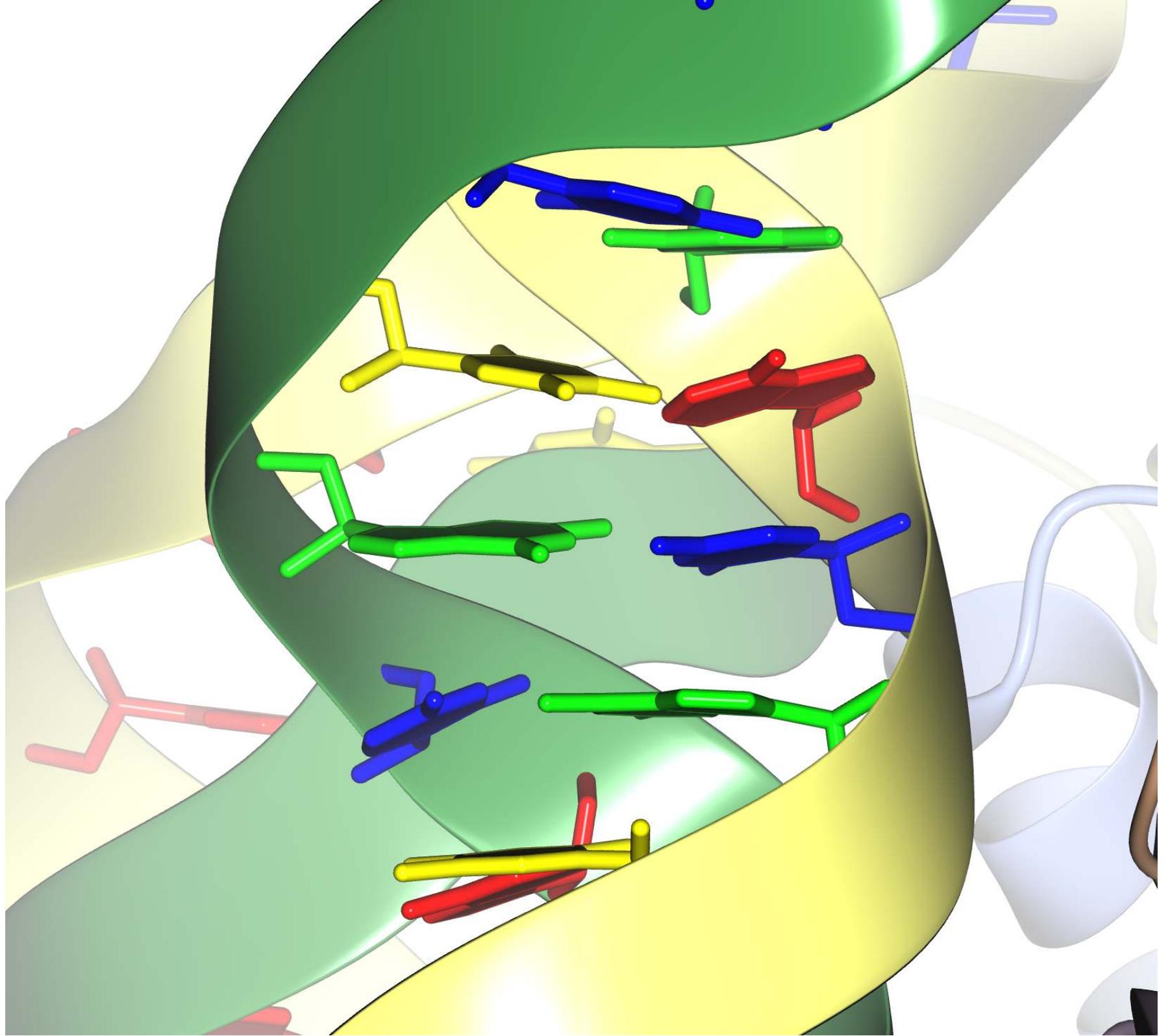


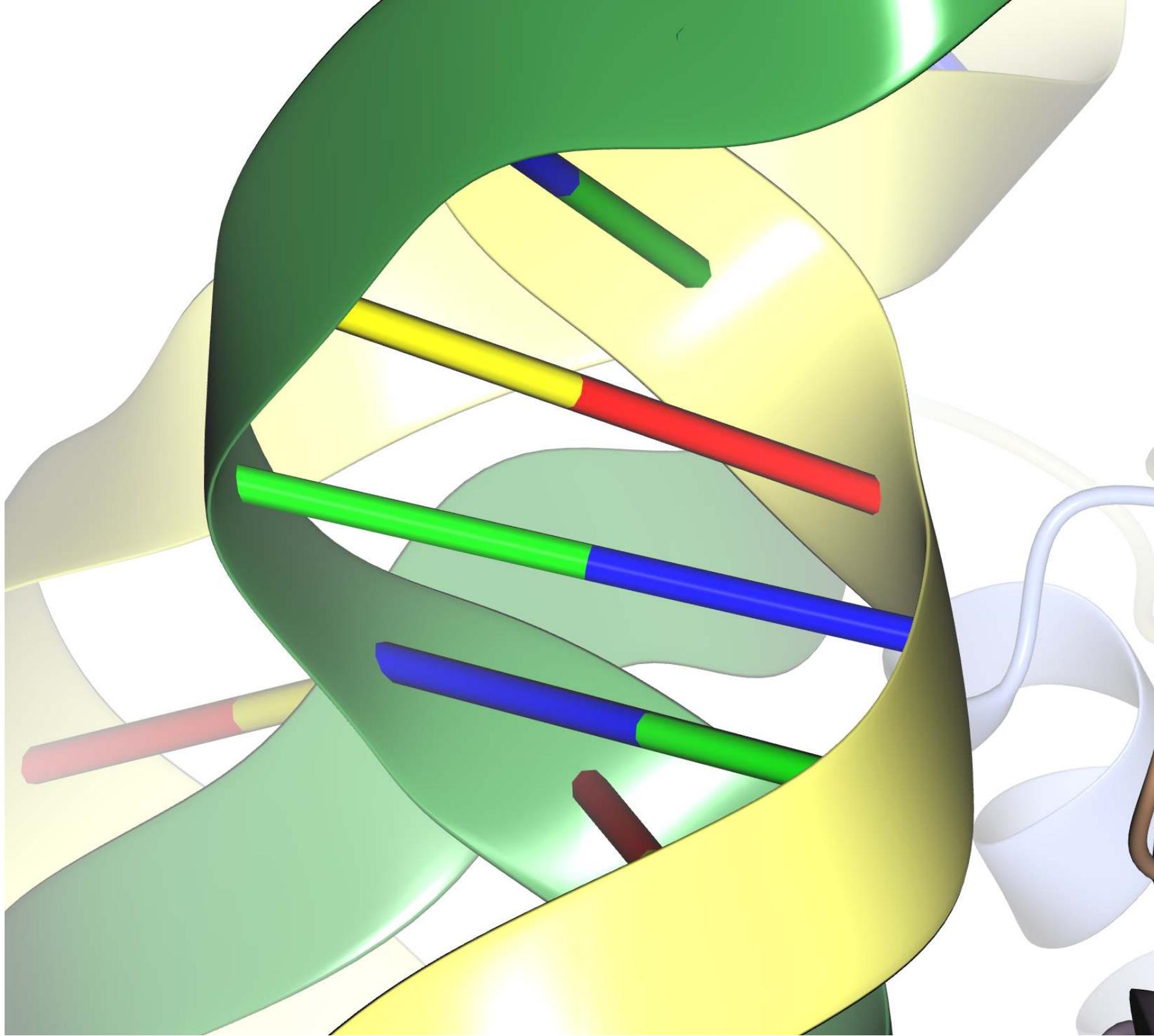




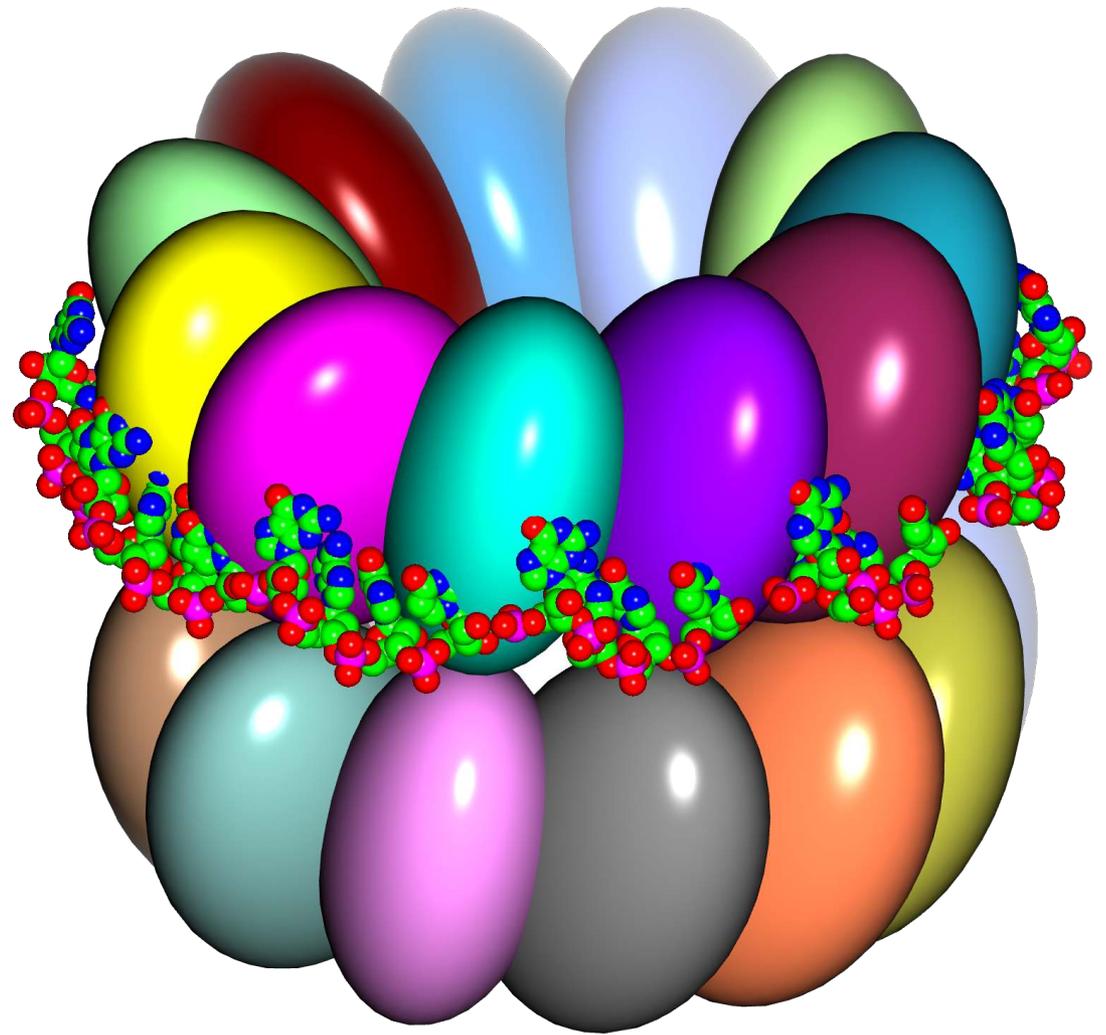
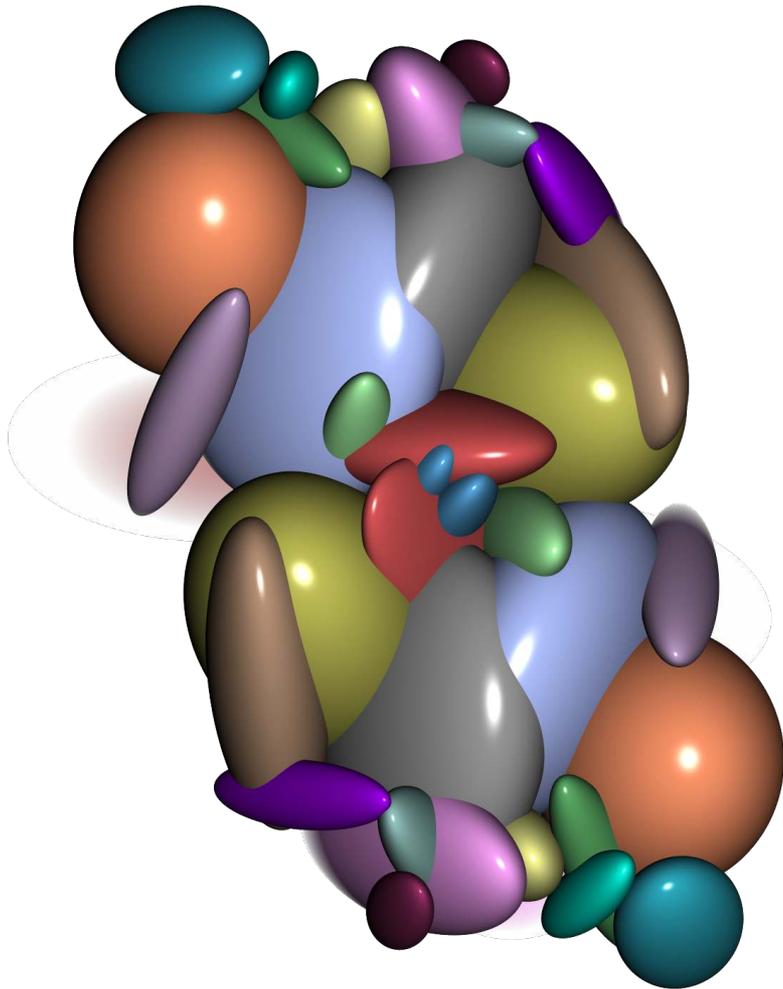


1aoi

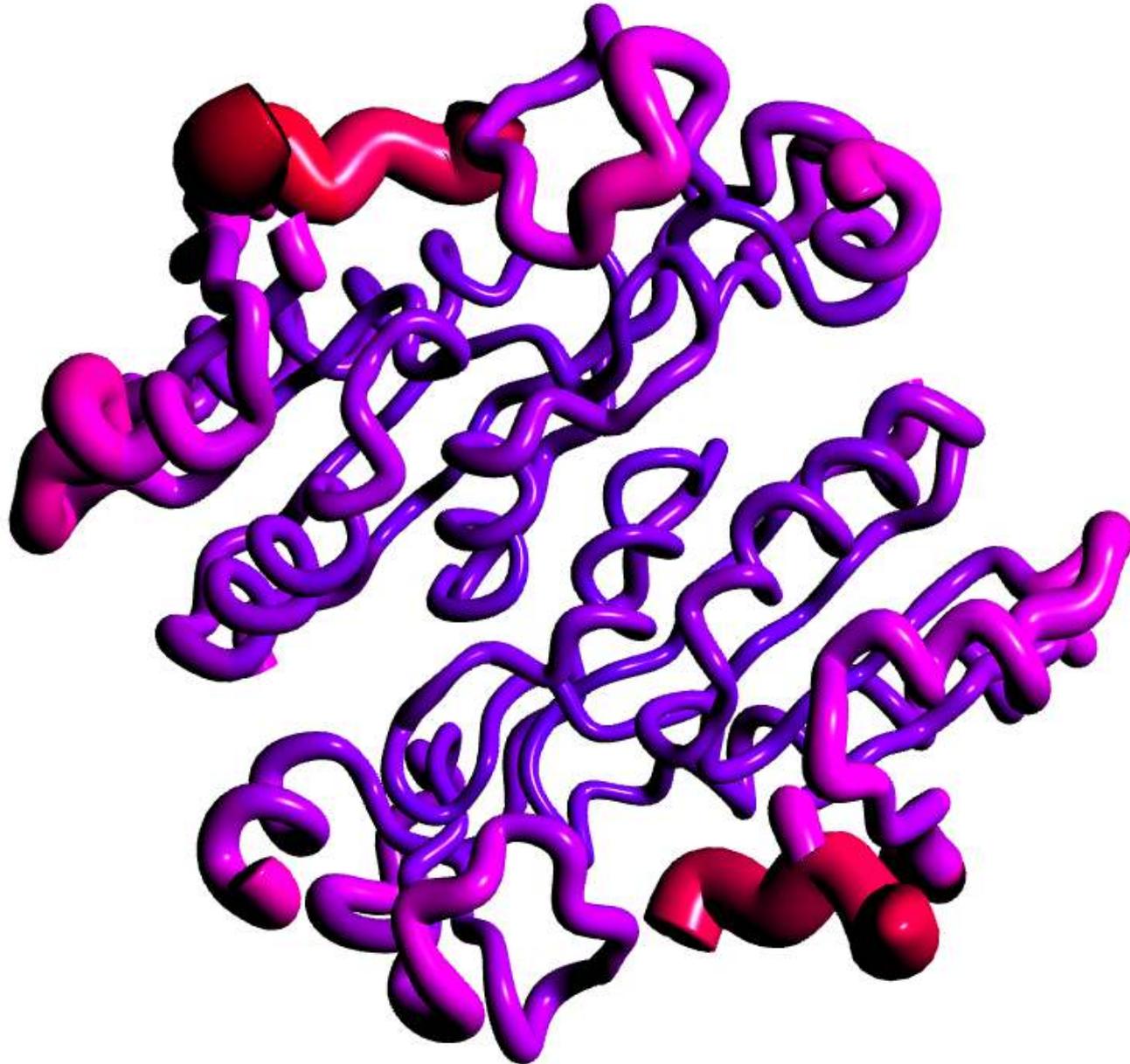




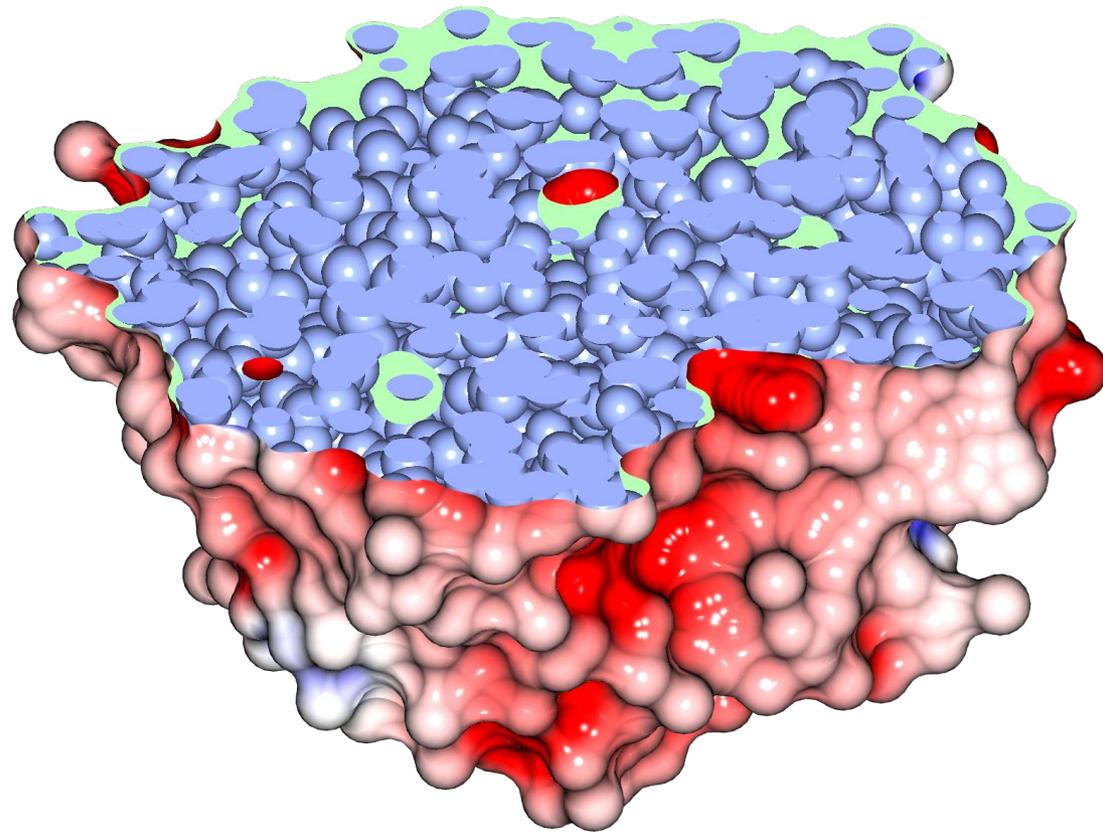
# Bloboids



# Worm scaled by B-factor

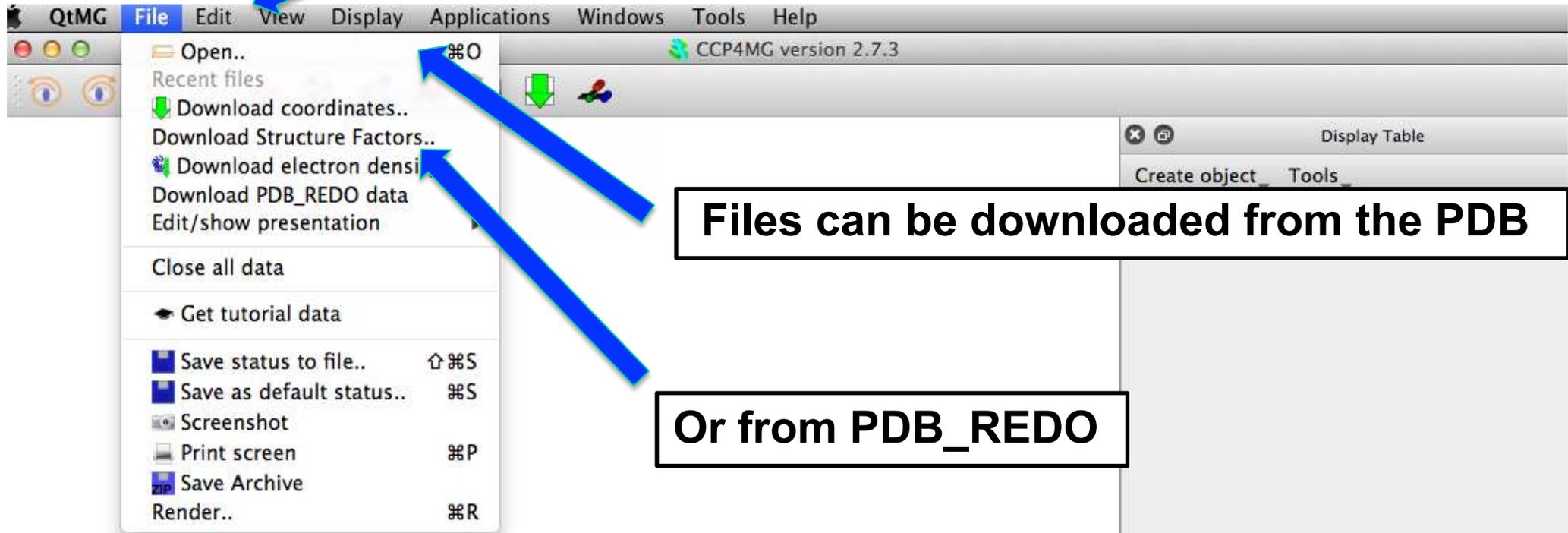


# “Custom clip planes”



**Getting started**

# Open a file

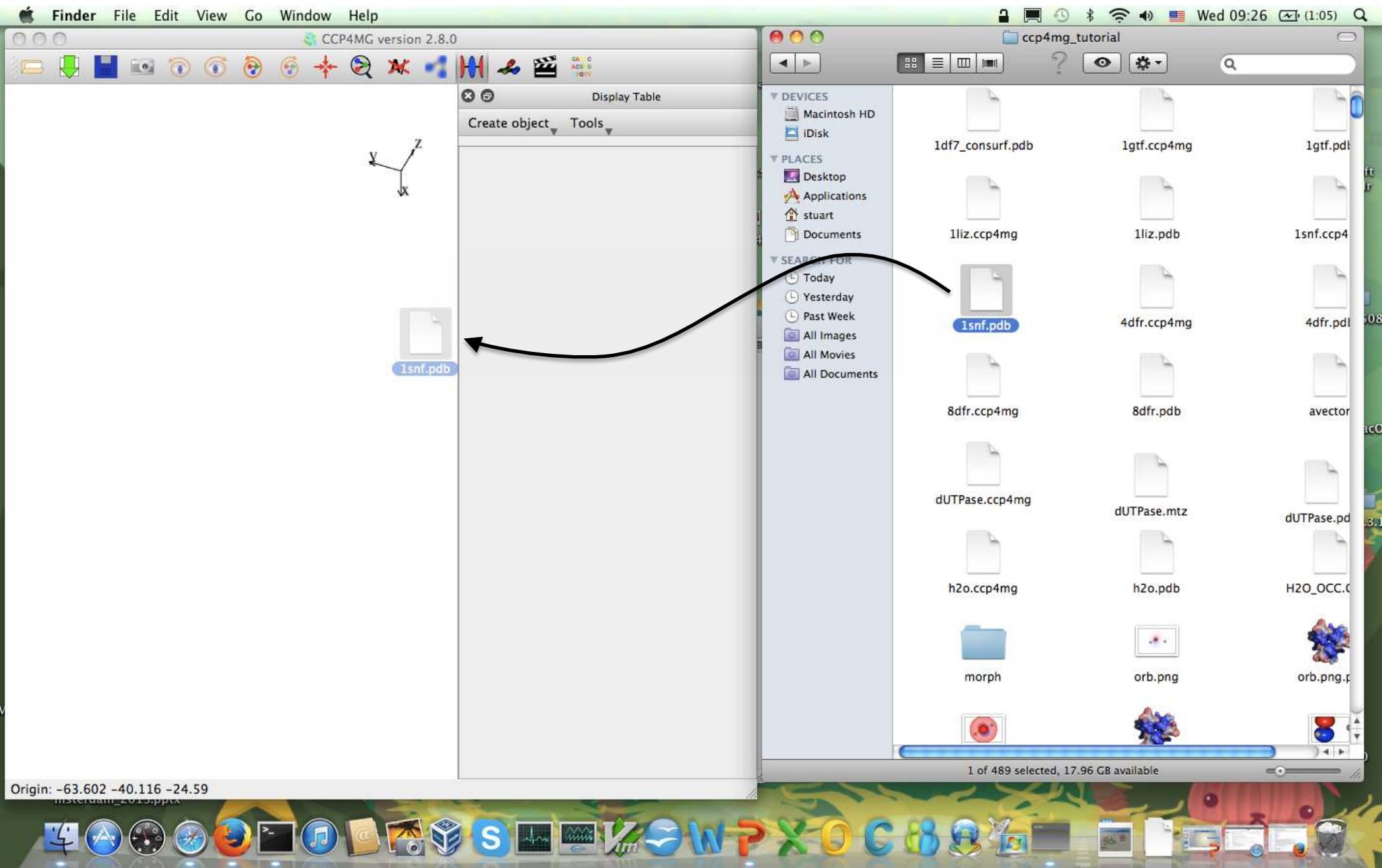


Files can be downloaded from the PDB

Or from PDB\_REDO

Easy access to the Protein Data Bank: PDB

# Open a file: Drag and Drop



Drawing style

Colour

Atom selection

Data object

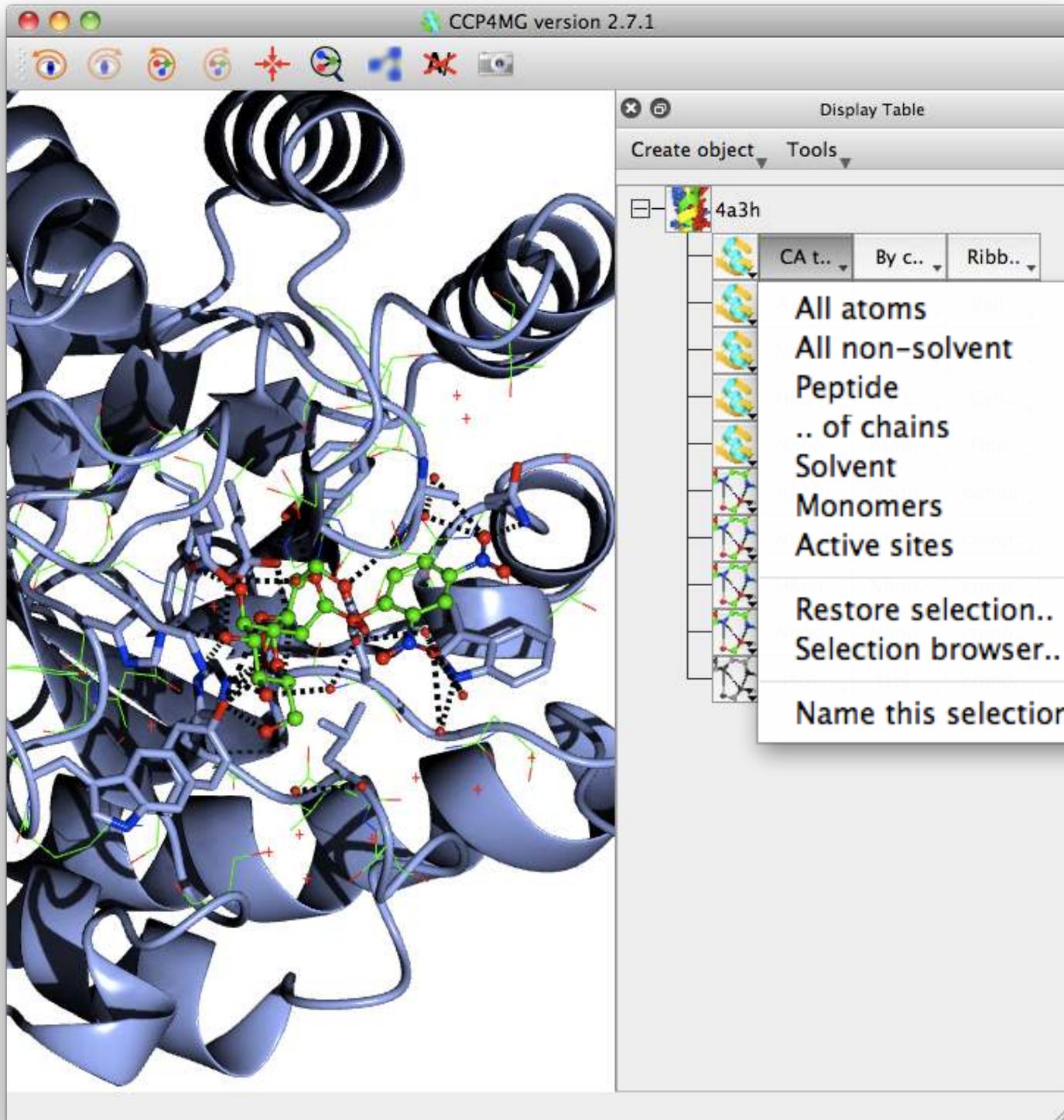
Display object

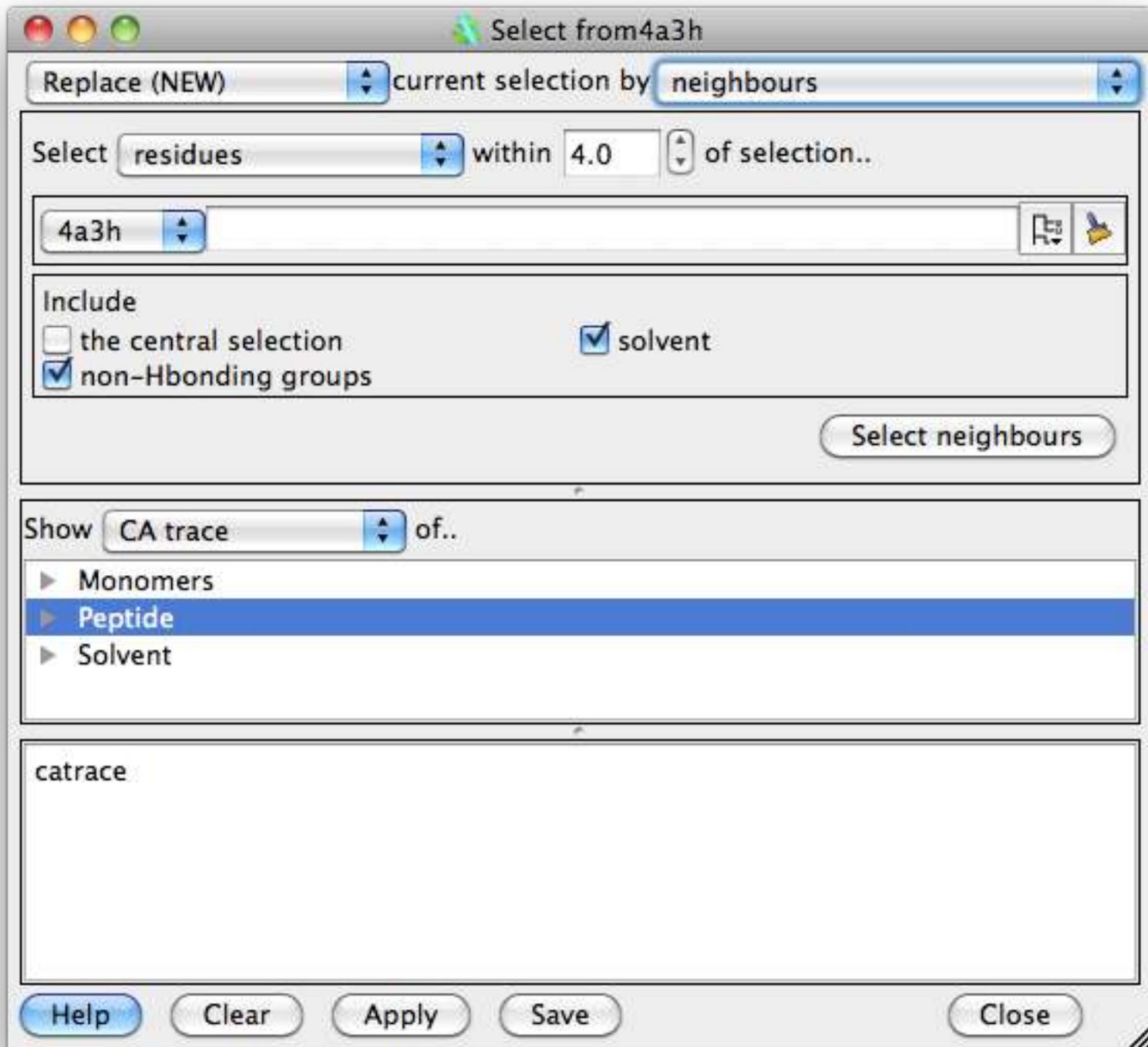
The image shows a screenshot of the CCP4MG software interface (version 2.7.1). The main window displays a 3D molecular model of a protein structure, rendered as a blue ribbon with a central ligand molecule shown in ball-and-stick representation. A 'Display Table' window is open on the right side of the interface. Red arrows point from text labels to specific elements in the software: 'Drawing style' points to the 'Tools' menu; 'Colour' points to the 'By c..' column in the table; 'Atom selection' points to the 'CA t..' column; 'Data object' points to the '4a3h' object in the table; and 'Display object' points to the 'Ribb..' column in the table.

Object	CA t..	By c..	Ribb..
A/30..	A/30..	Atom..	Ball..
Nhoo..	Nhoo..	By c..	Cyli..
HBon..	HBon..	By c..	Cyli..
Nhoo..	Nhoo..	Atom..	Thin..
A/30..	A/30..	Nhoo..	comp..
Nhoo..	Nhoo..	Nhoo..	comp..
HBon..	HBon..	Nhoo..	comp..
Nhoo..	Nhoo..	Nhoo..	comp..
{sol..	{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





# 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.

Open file(s)

▶ interfaces  
 ▼ ligand binding site  
   site  
   site and broken ribbons

Picture wizard

Automatic picture setup  
 Open picture wizard choices

Picture wizard: 4a3h

Delete any existing display object

▶ ribbons  
 ▶ interfaces  
 ▼ ligand binding site  
   site  
   site and broken ribbons  
   site and ribbons

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 solvent within

Ligand 1    

Ligand 2    

Ligand 3    

Label binding site residues

Help    Create picture    Cancel

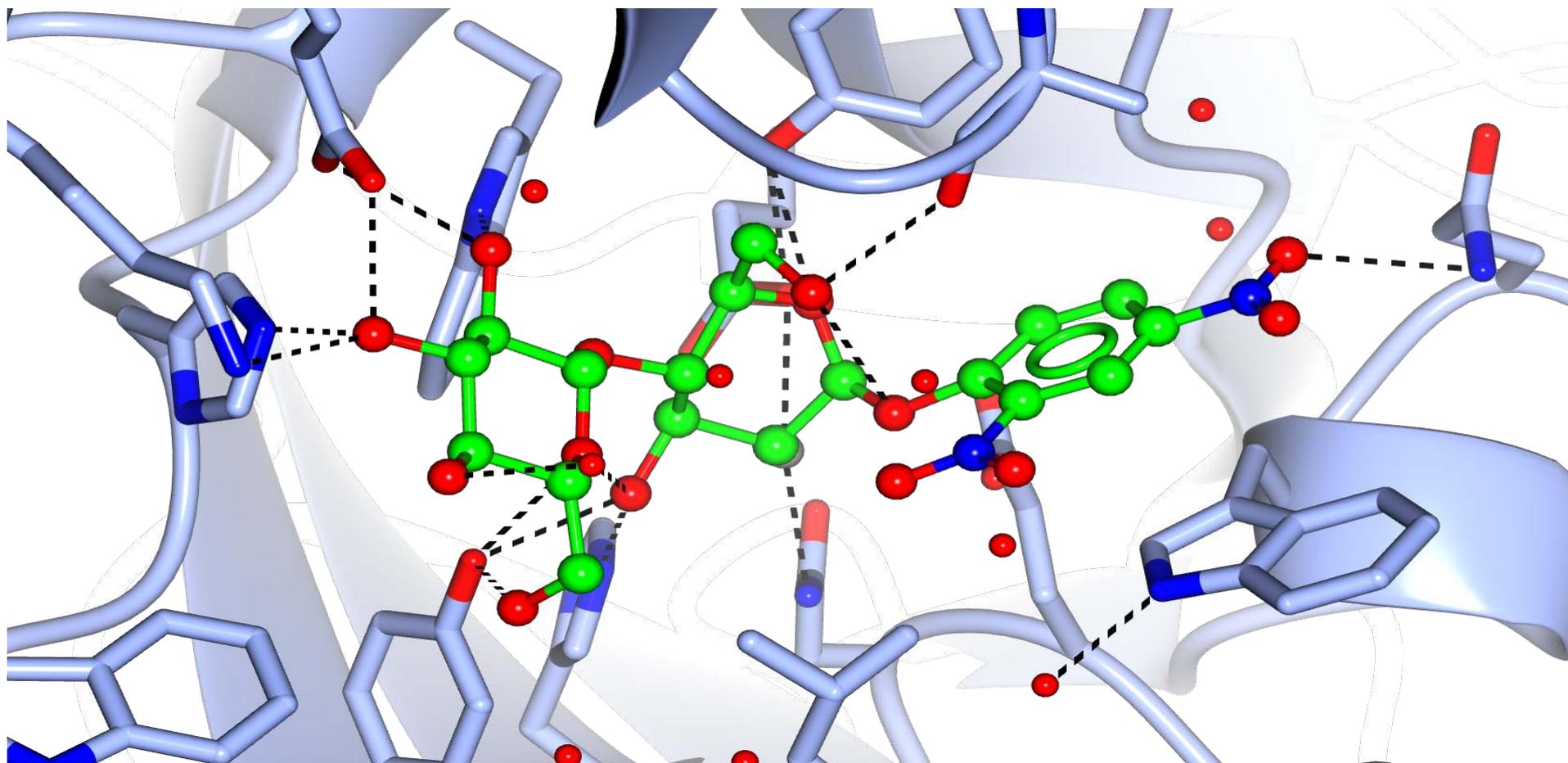
Projects- or ...

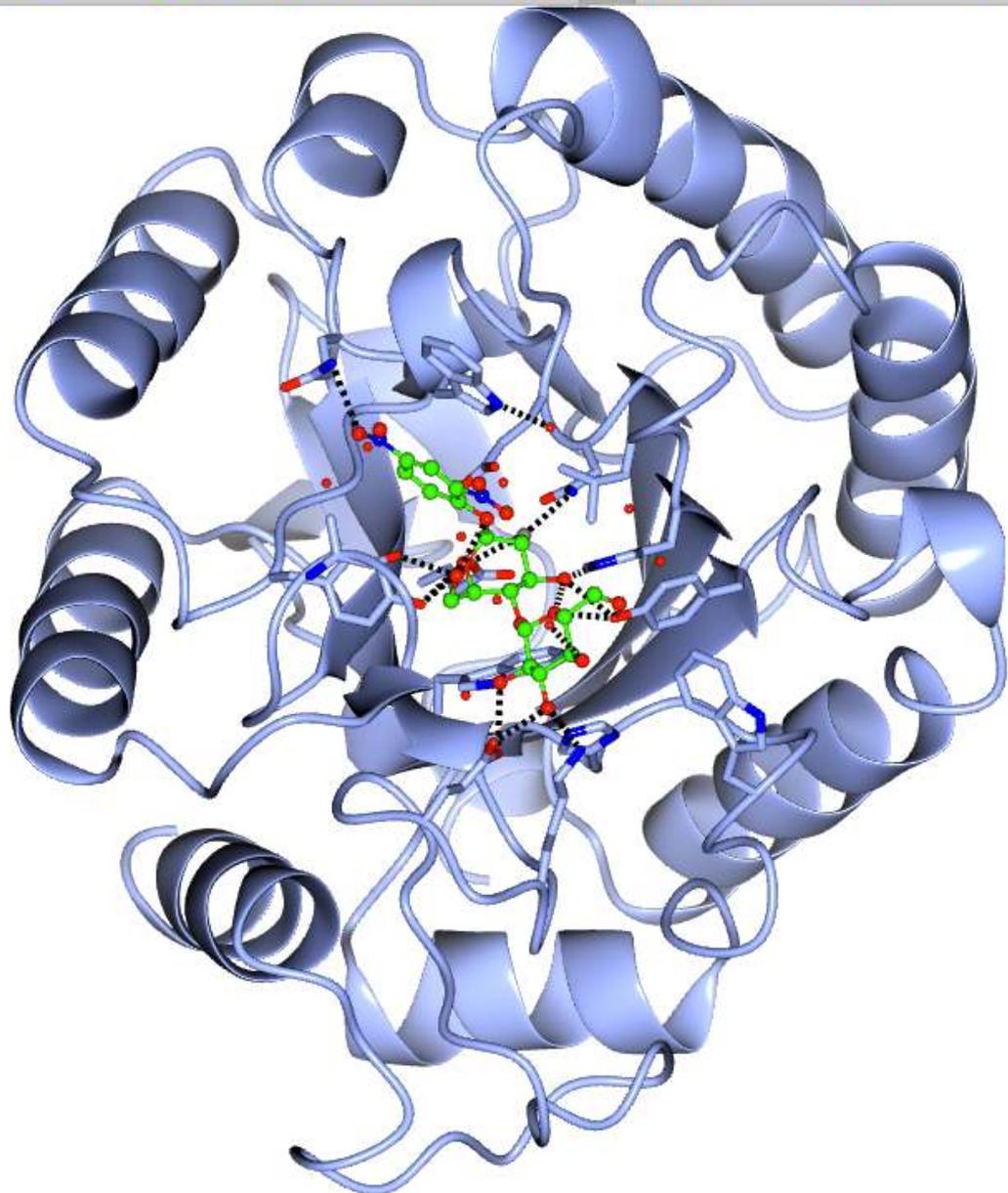
	Size	Kind
w_BASEES.ppt	241 KB	ppt File
	--	Folder
156.jpg	1.7 MB	jpg File
resentation	--	Folder
er.docx	16 KB	docx File
rogramme.pdf	2.3 MB	png File
	101 KB	pdf File
	683 bytes	zip File
	38 KB	py File
at SMCPS.doc	15 KB	doc File
at SMCPS.odt	10 KB	odt File

Open    Cancel

\*.pdb.gz \*.cif.gz \*.ent.gz \*.brk

# “Site and ribbons” wizard

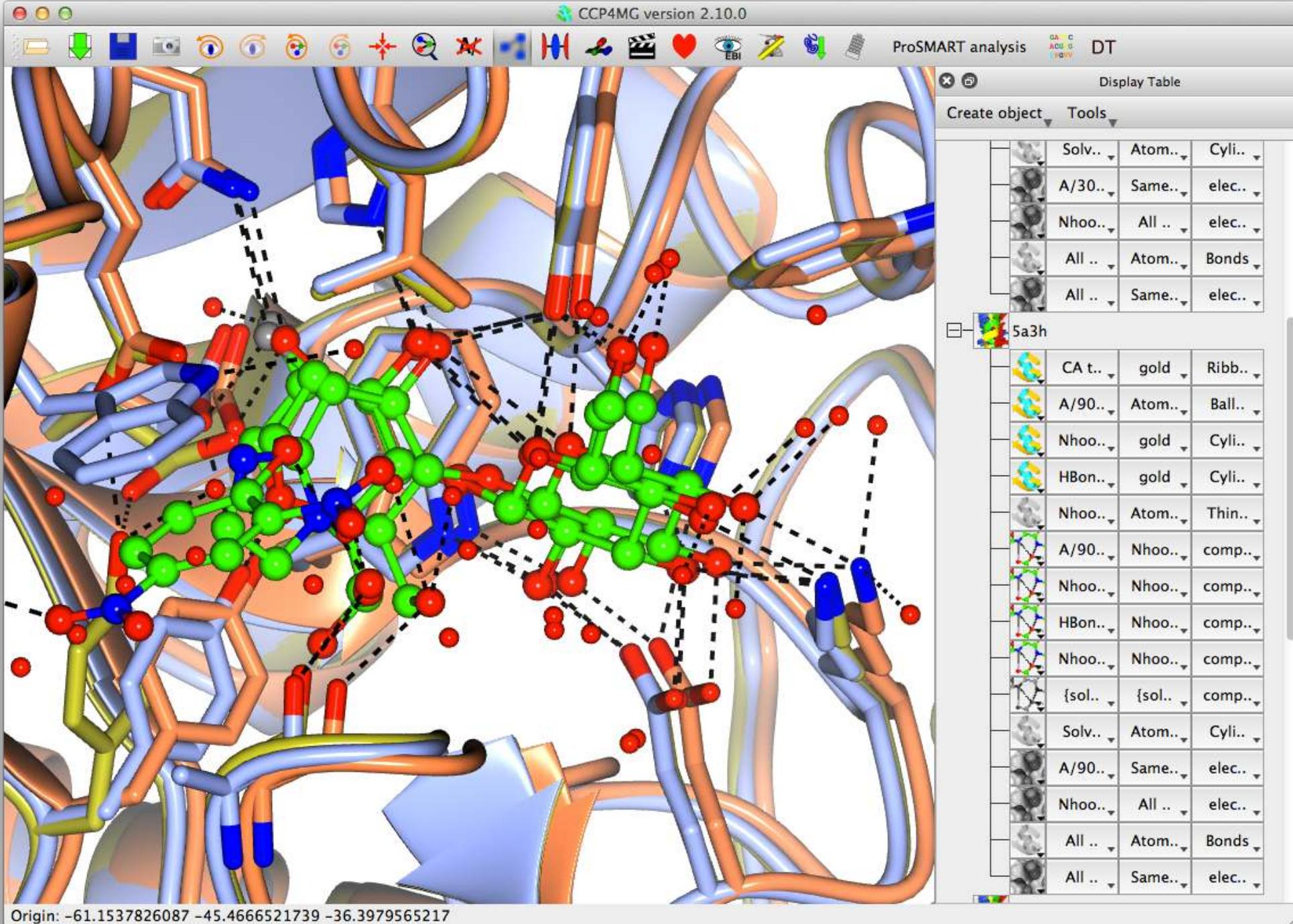




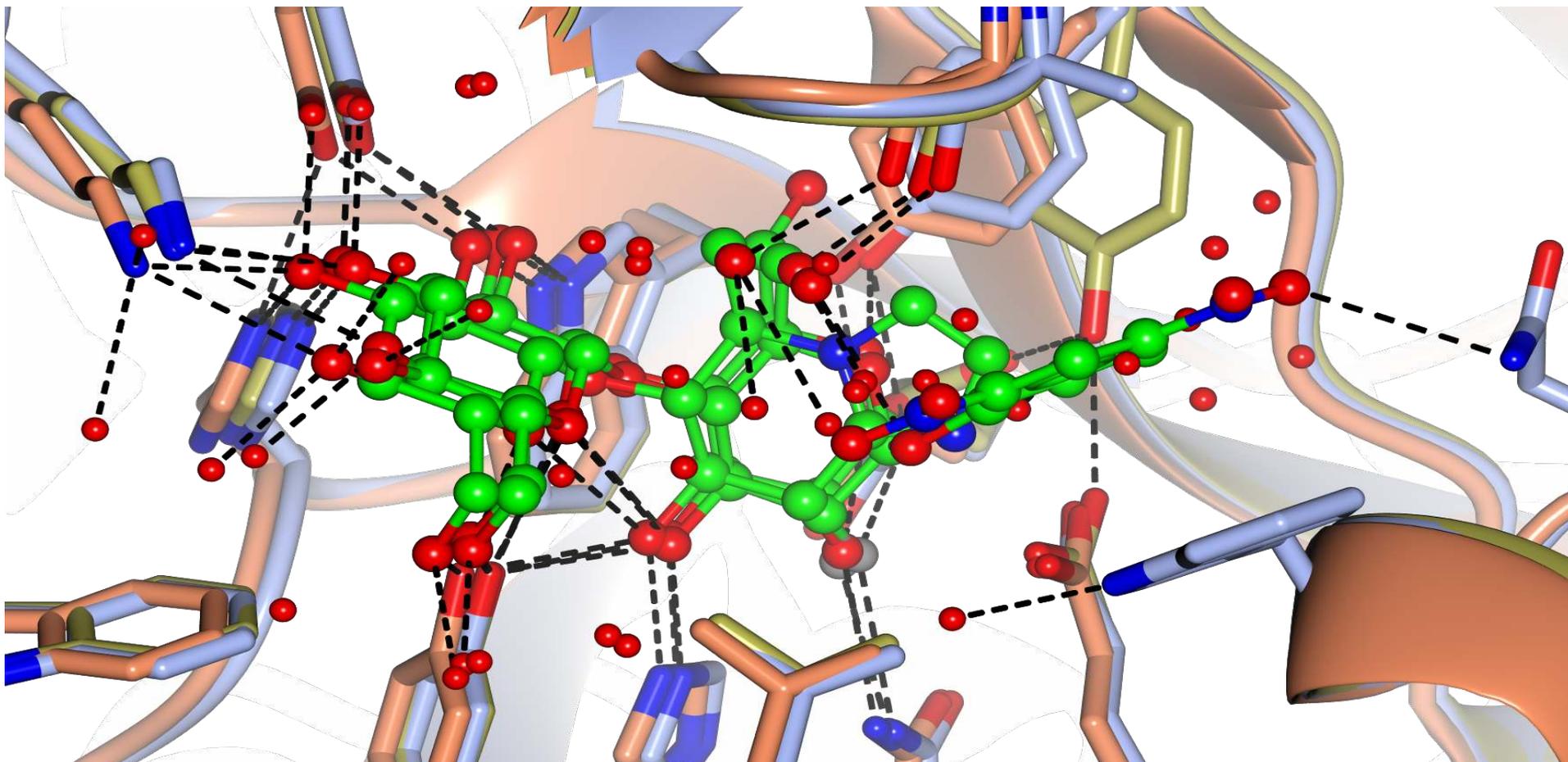
Display Table

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..

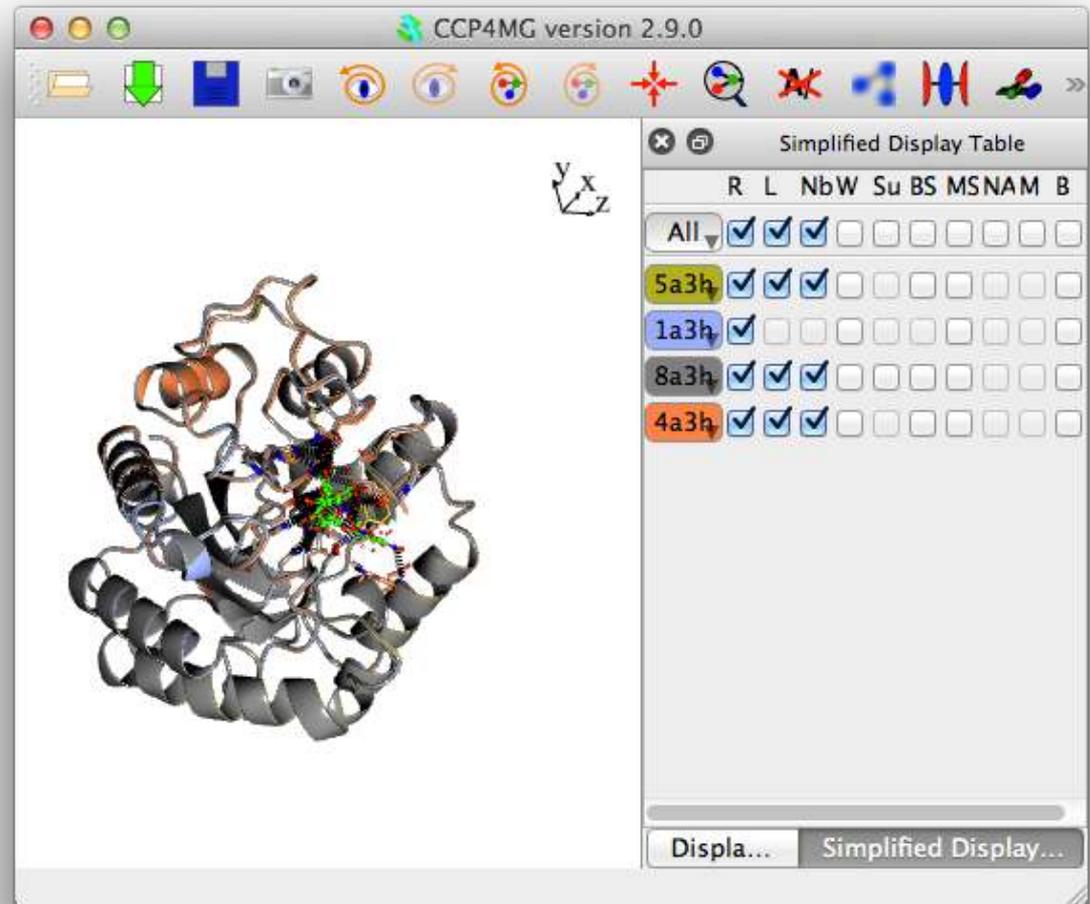


... with multiple files



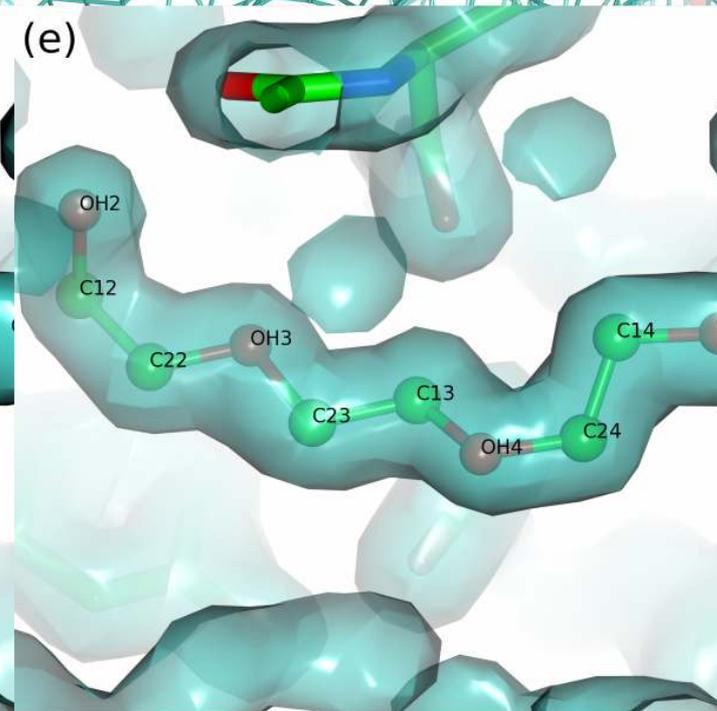
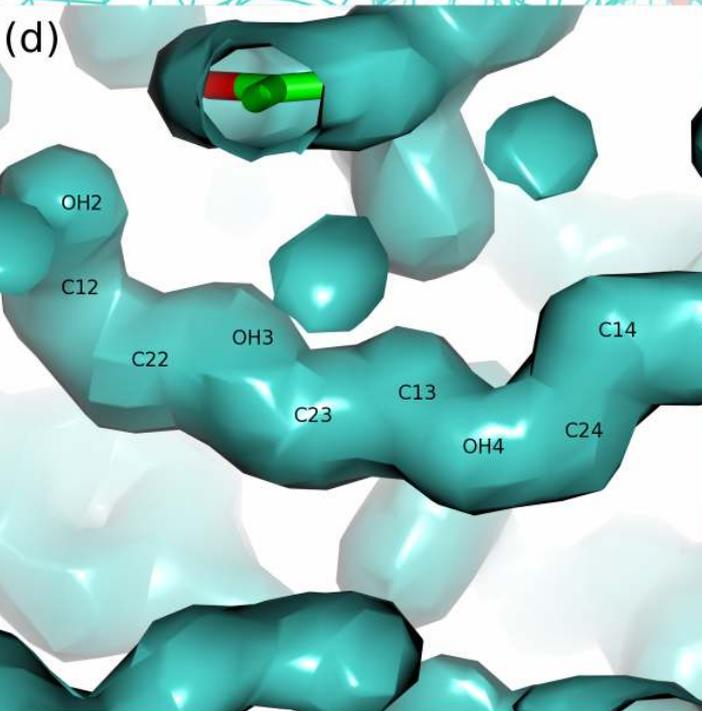
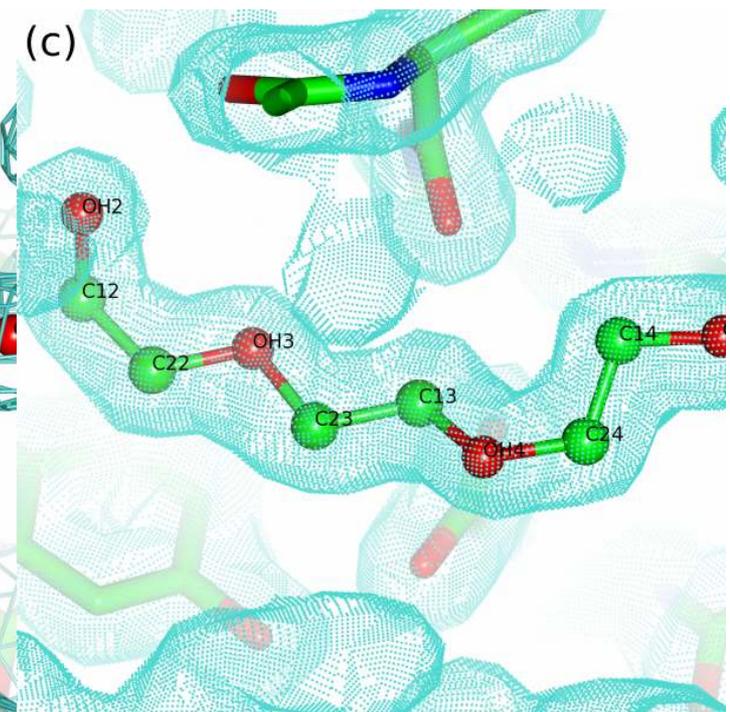
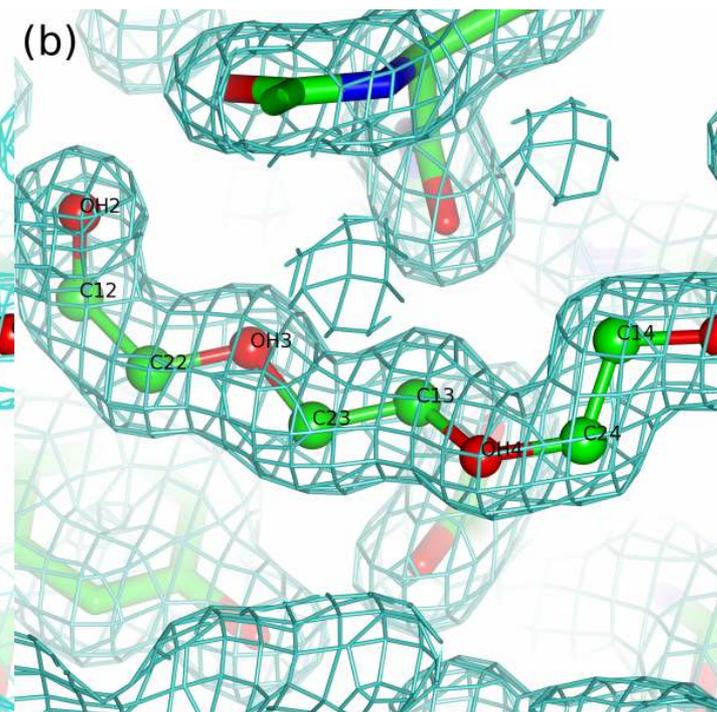
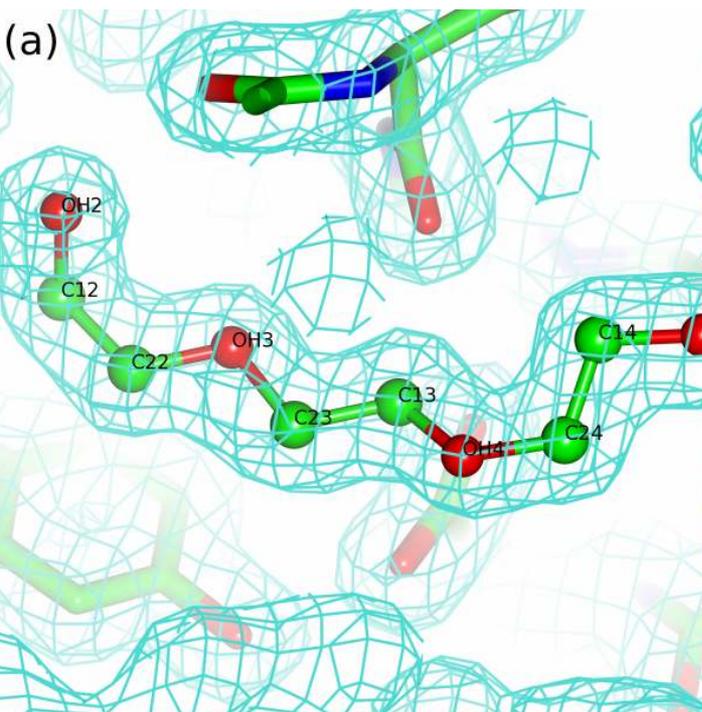
# Simple Display Table

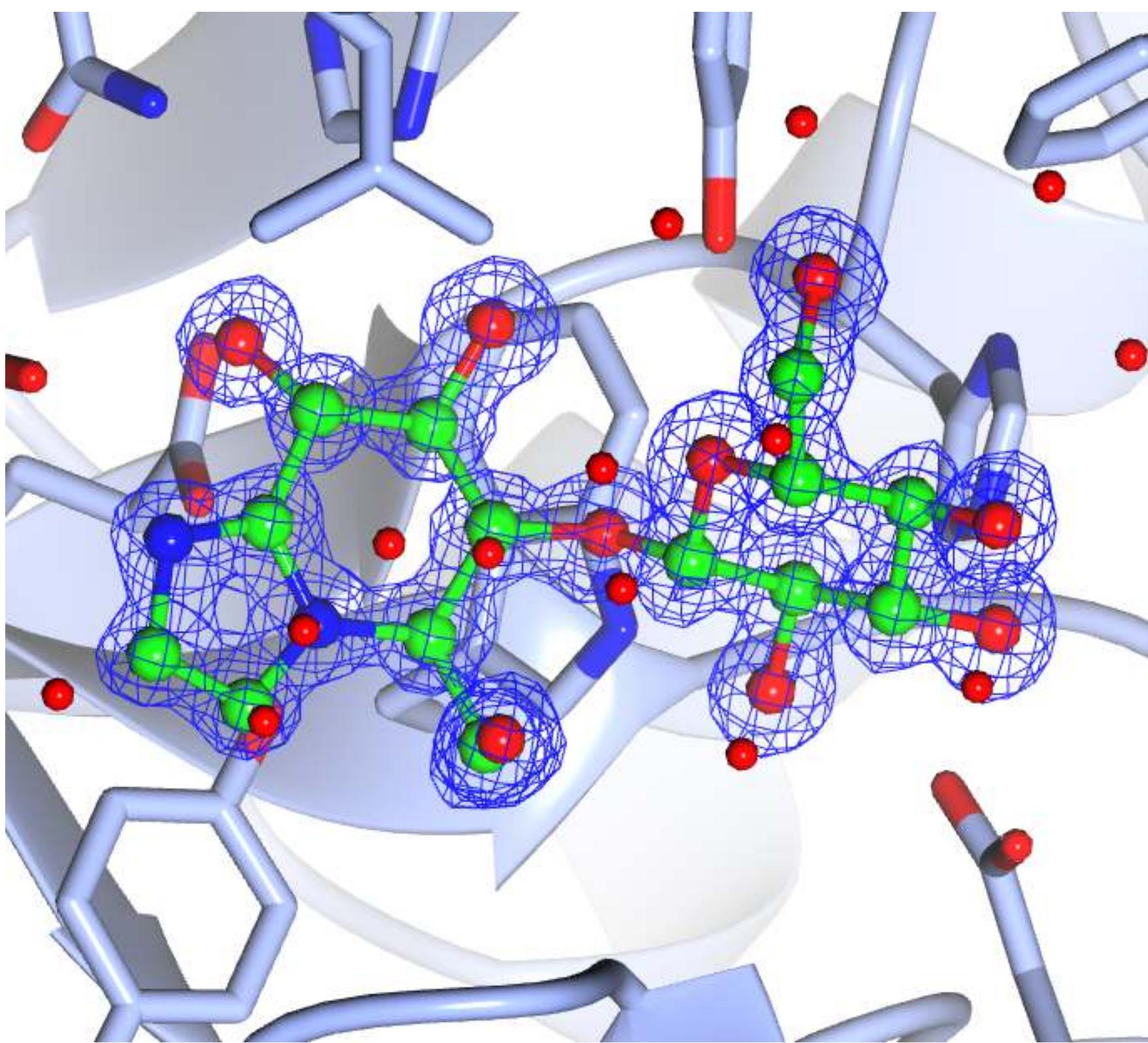
“Simple Display Table” added. New tool for quickly turning on/off lots of related display objects. Particularly useful for looking at large numbers of similar files. (Not a replacement for “full” Display Table, but a useful alternative for some use cases).



# Electron Density

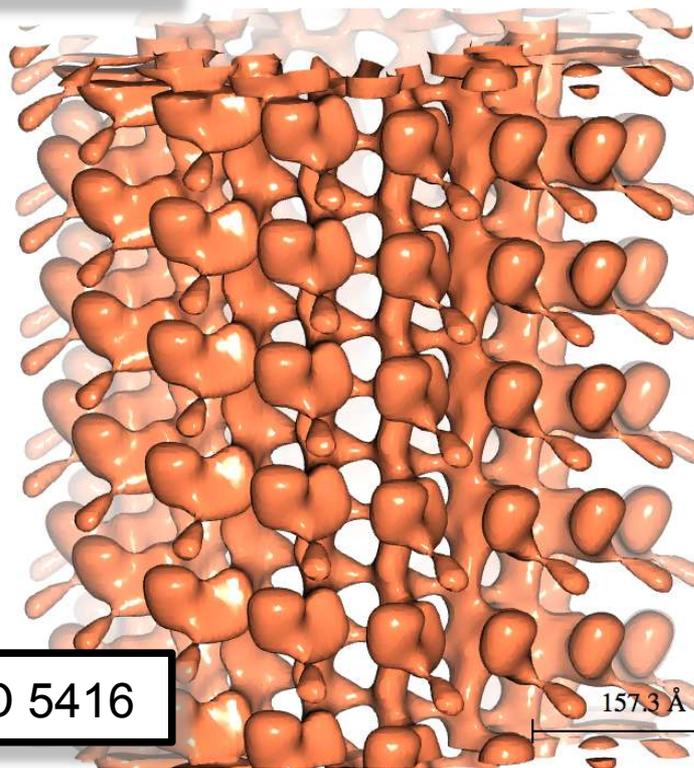
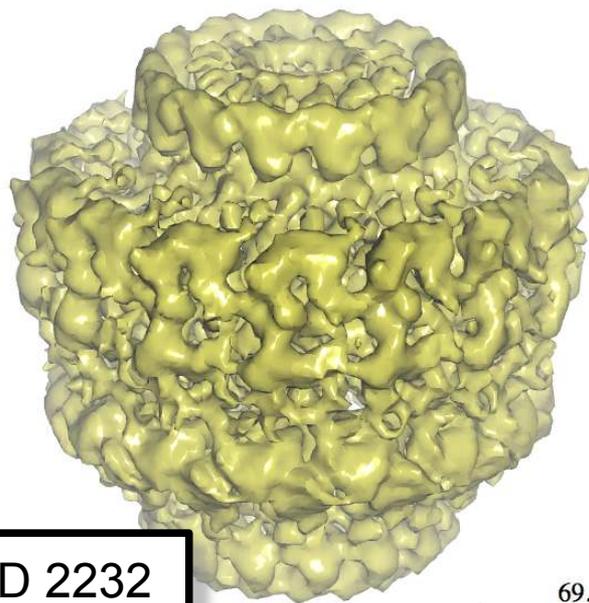
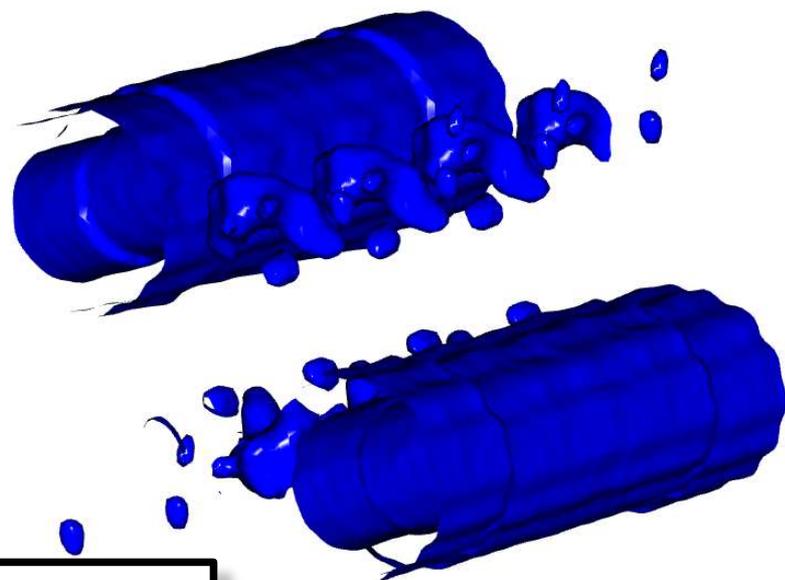
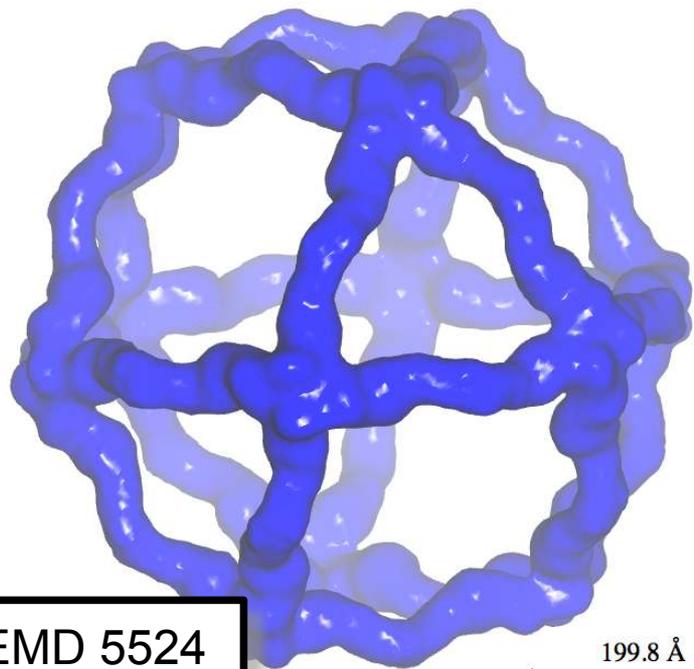
- Electron density maps can be read/created from any CCP4 supported file format, downloaded from EDS or generated from structure factors.
- Density can be represented as chickenwire lines, chickenwire cylinders, solid surface or dots.
- By default a 10Å cube of density at centre of screen is drawn, this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

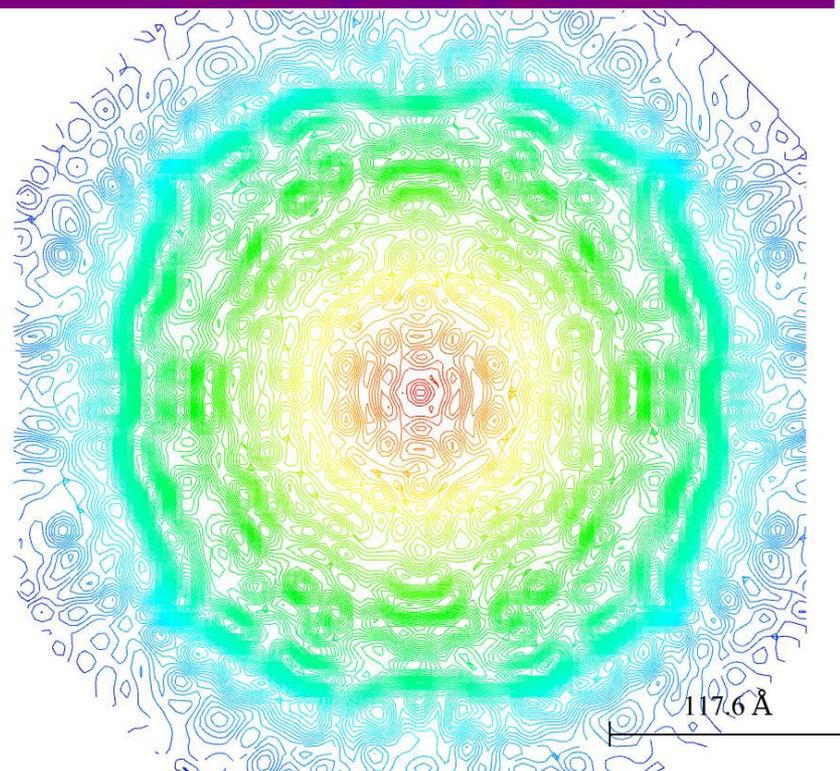
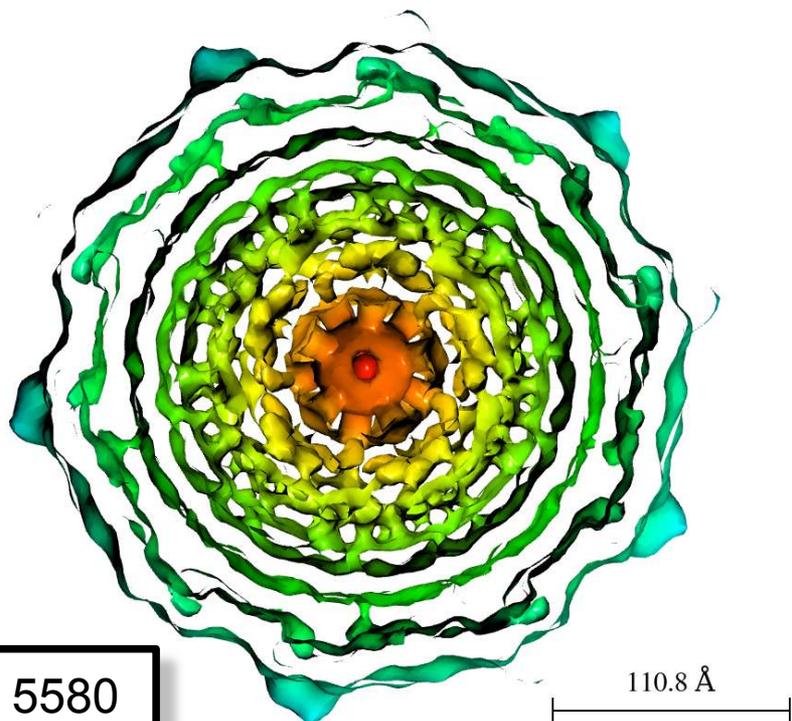
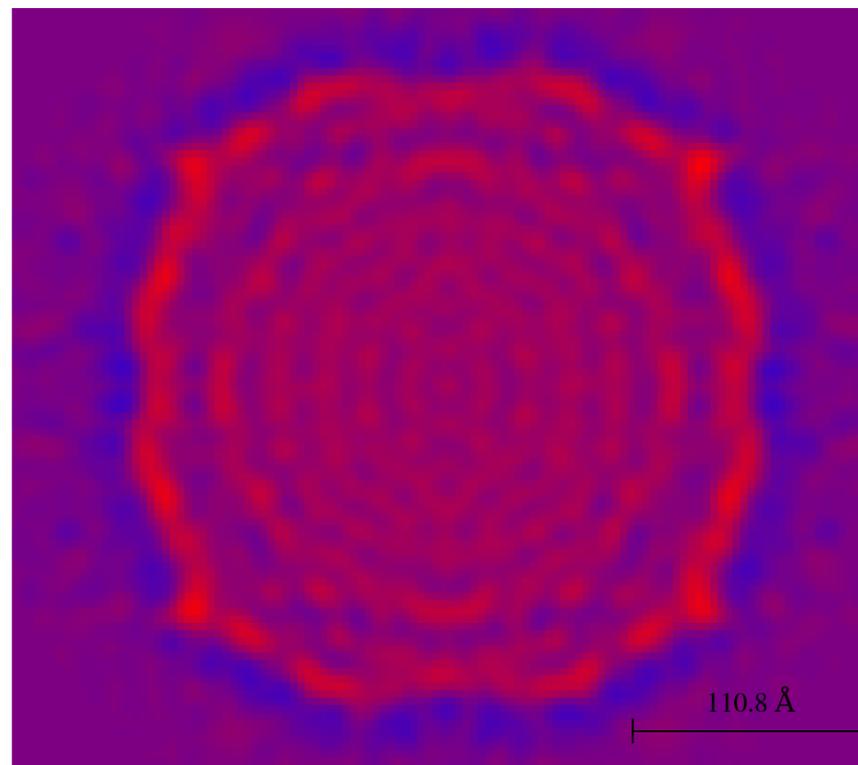
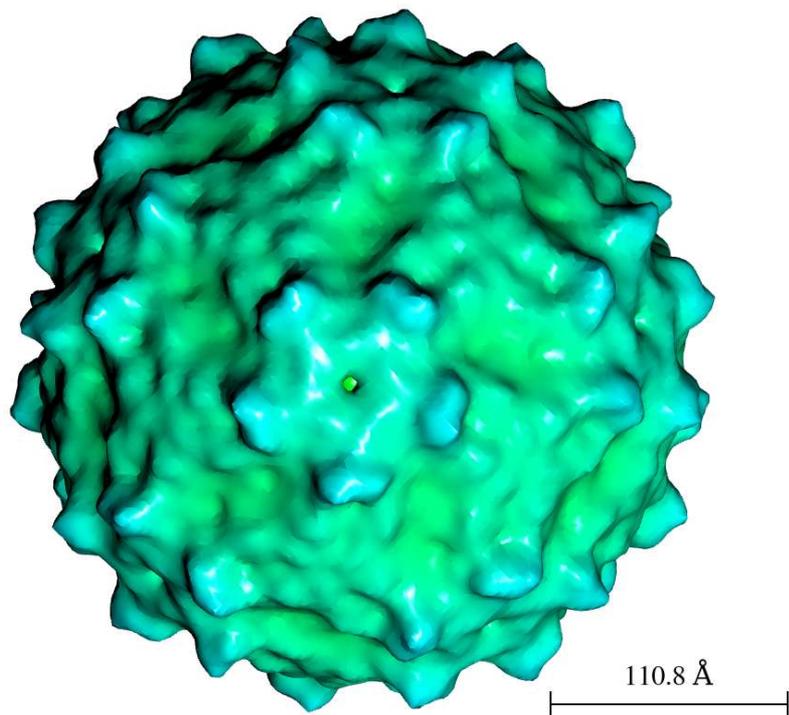




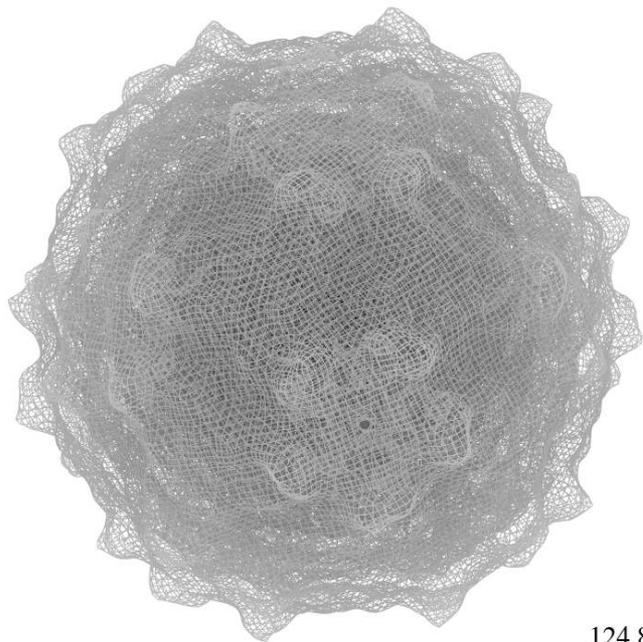
# Electron Microscopy Maps

- Changes made to CCP4MG to handle electron density maps larger than previous limit of about 200 angstroms. Can now cope with 1000 angstrom.
- 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.

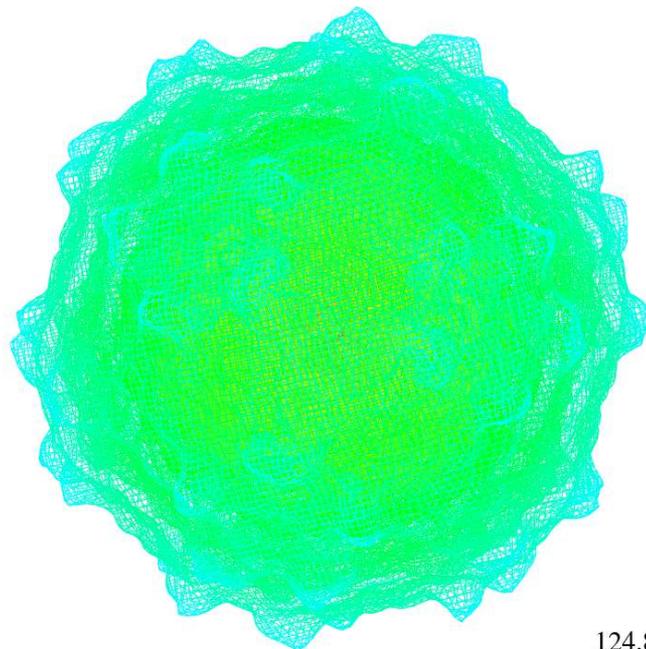




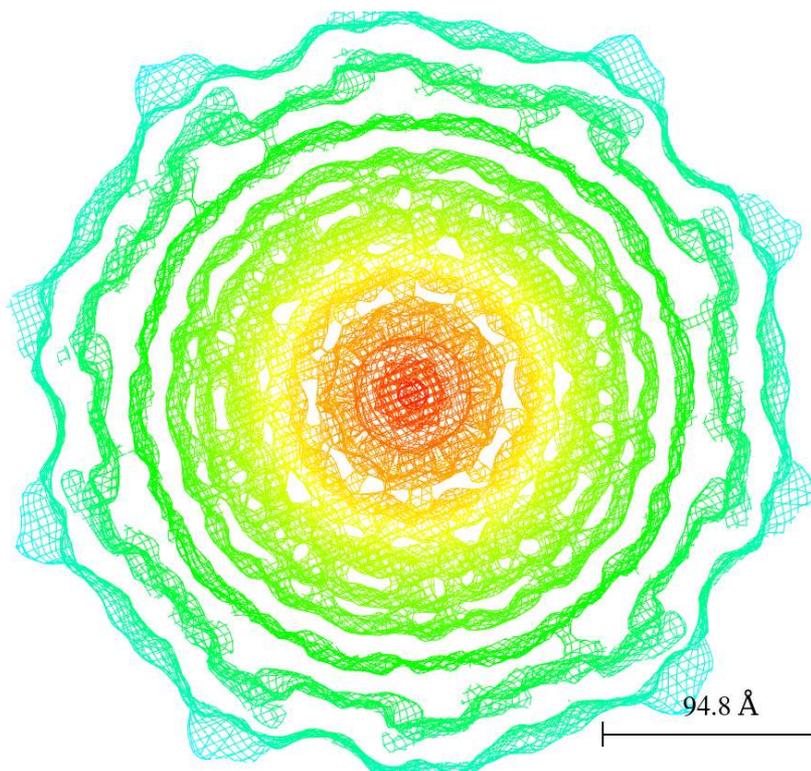
EMD 5580



124.8 Å

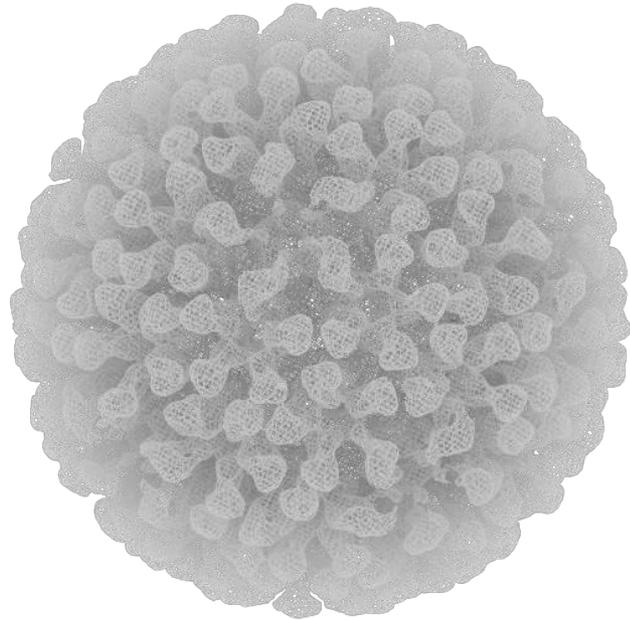
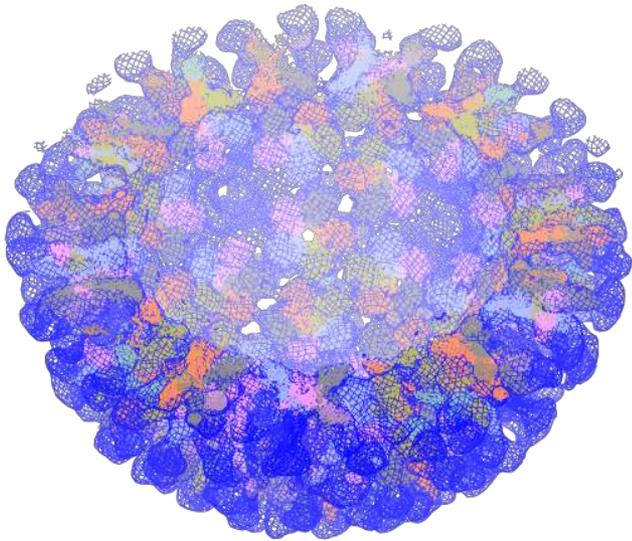
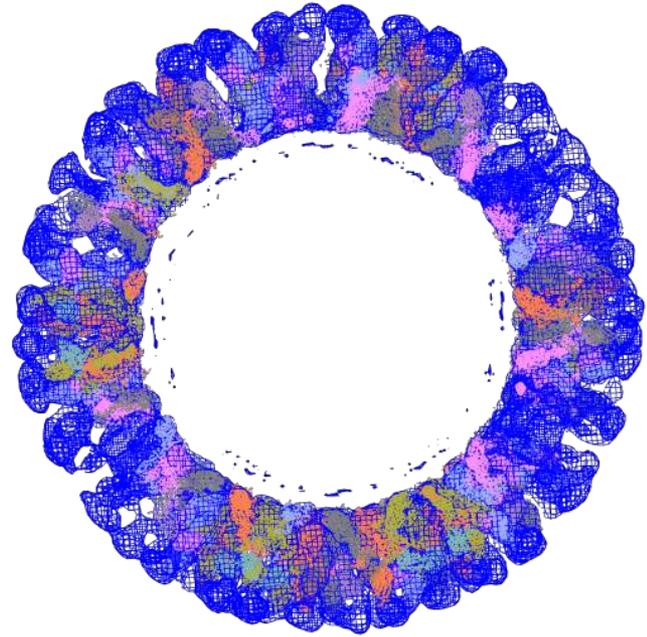
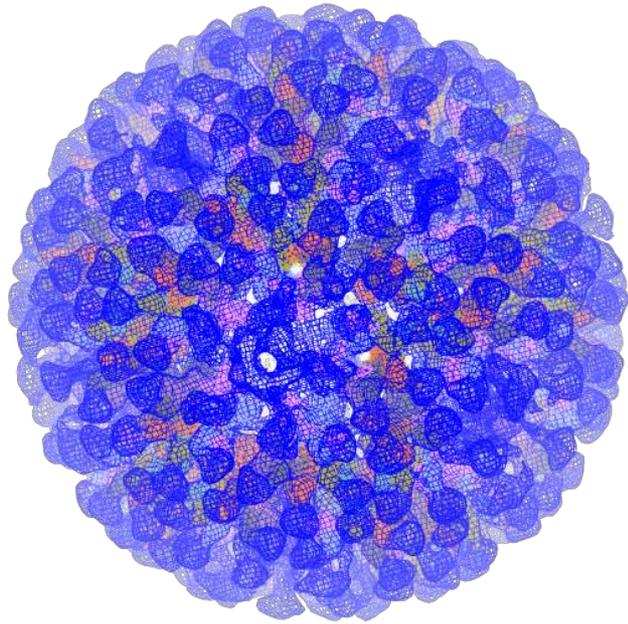


124.8 Å

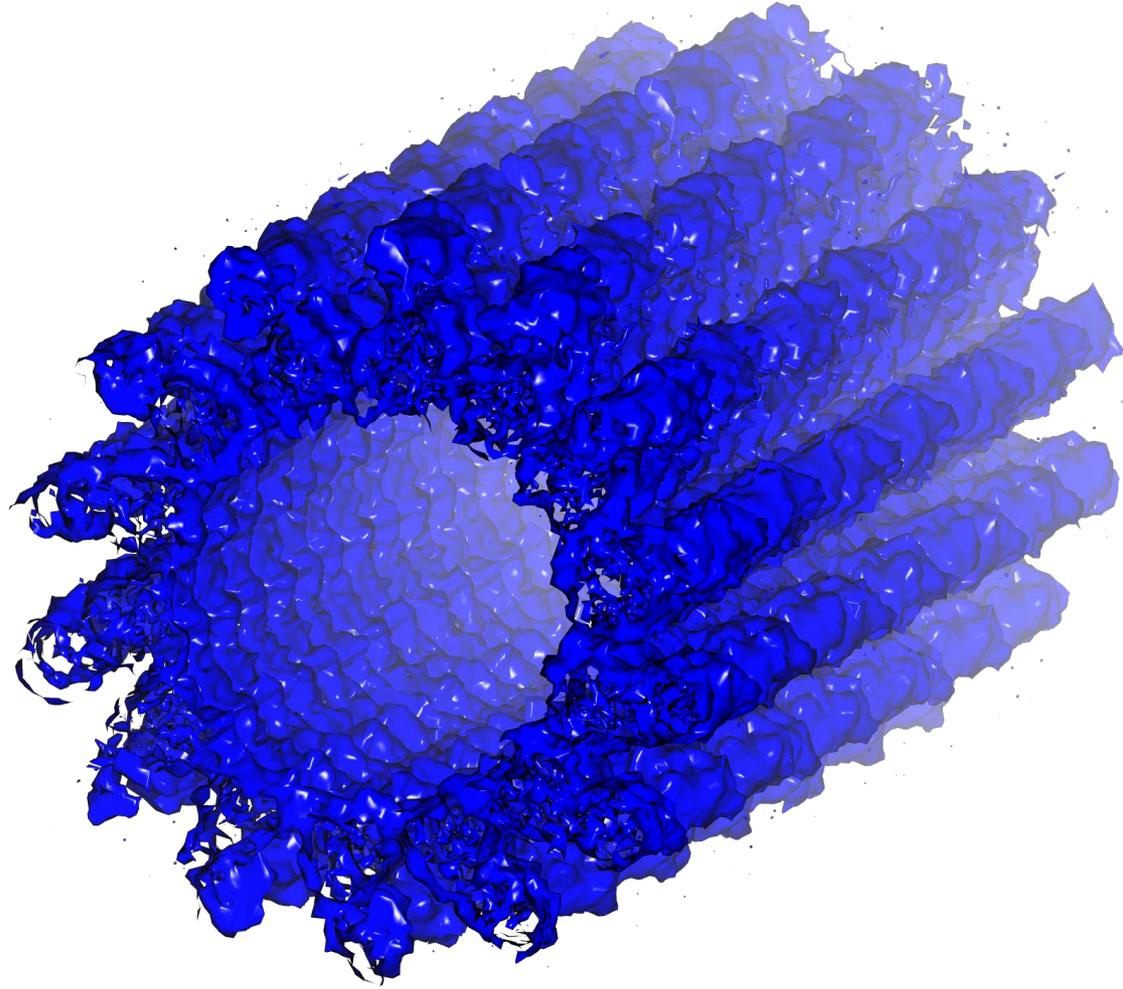


94.8 Å

EMD 5580



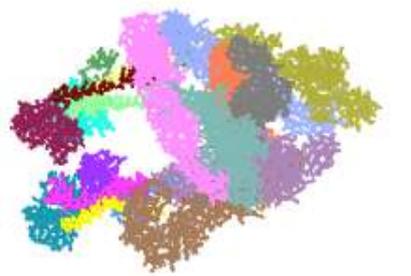
EMD 5994



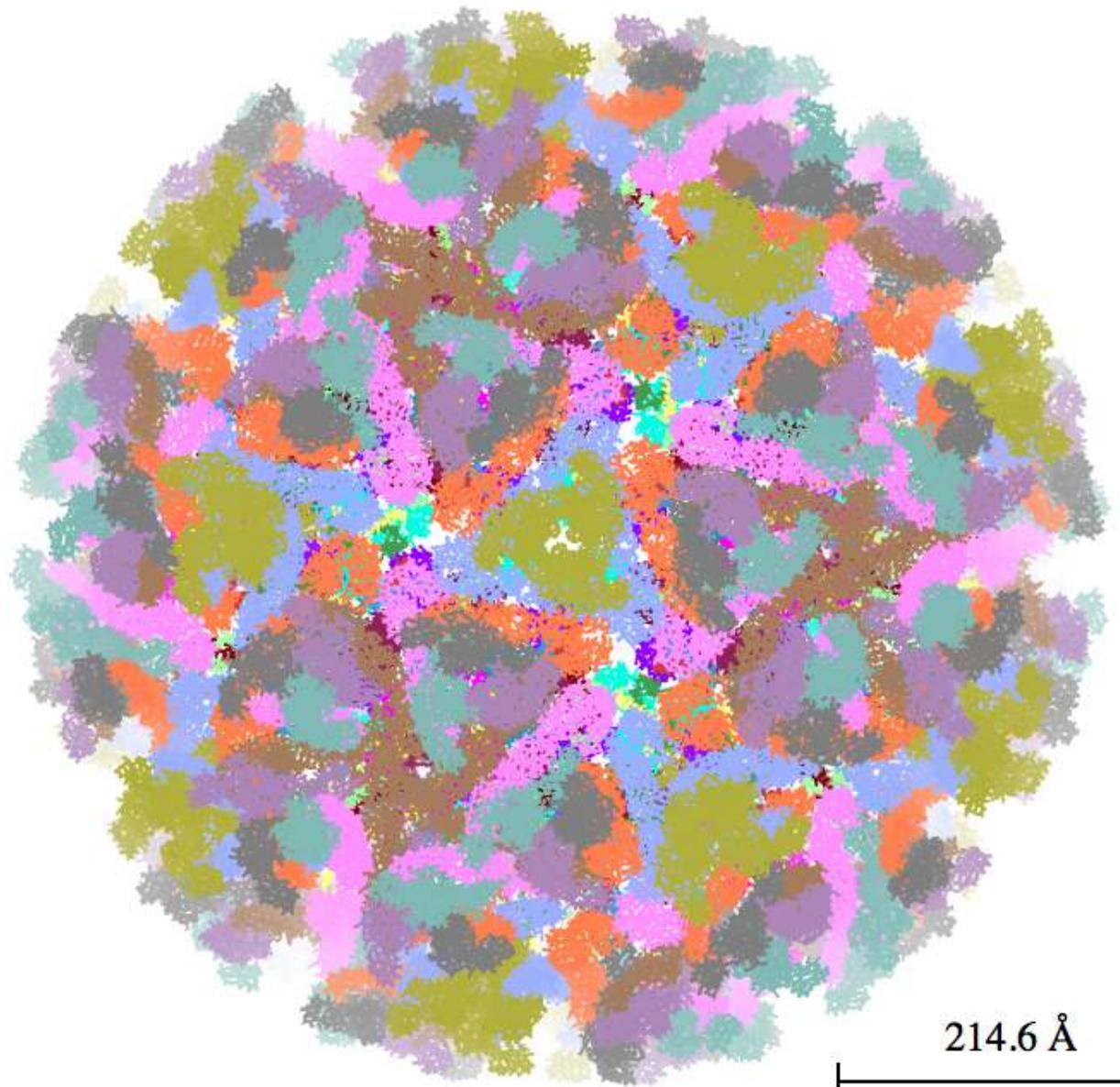
EMD 6188

# 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.
  - Does not do PISA calculation – much simpler and faster (instantaneous) – matrices used to redraw pictures without generating transformed atoms.



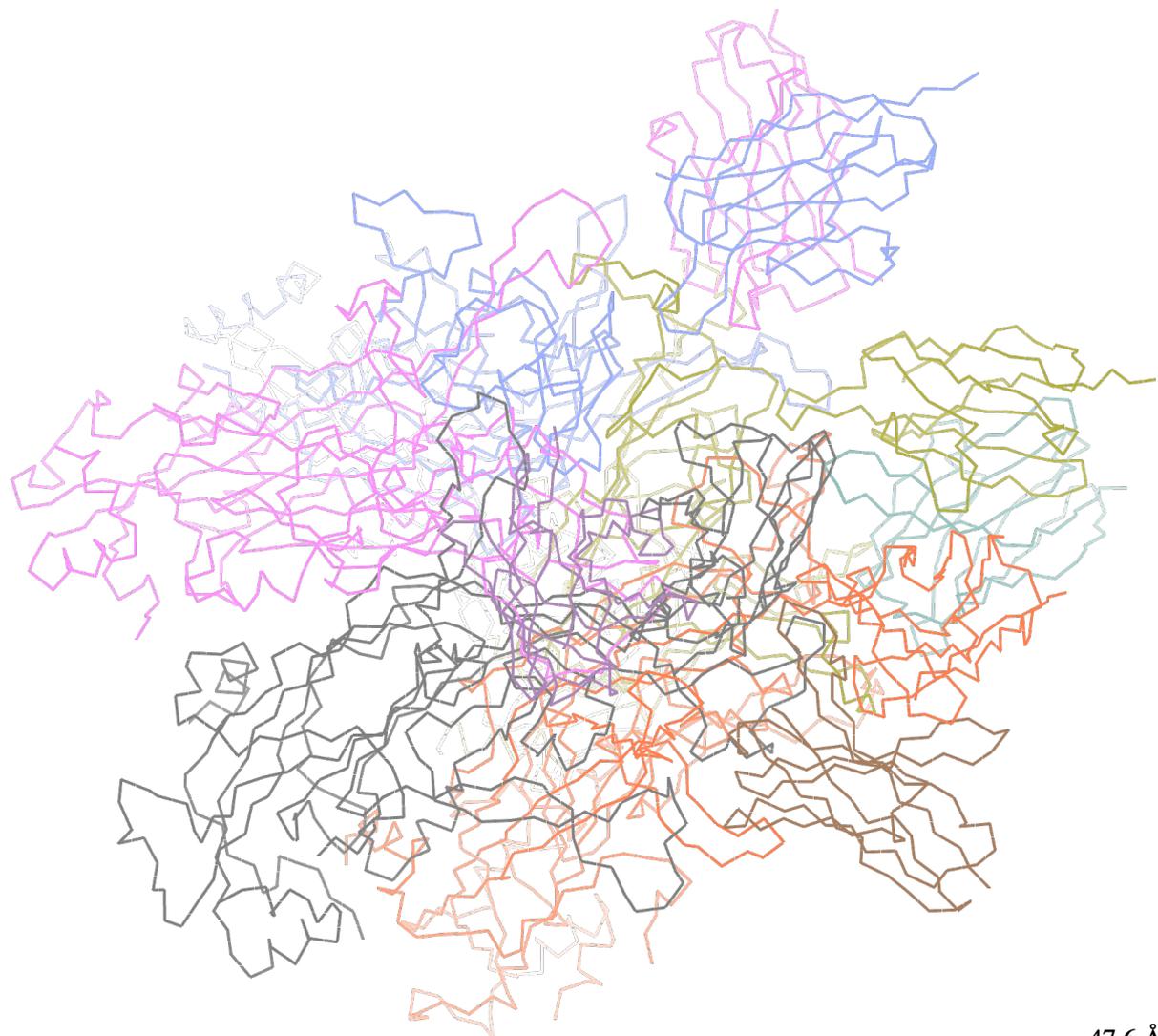
214.6 Å



214.6 Å

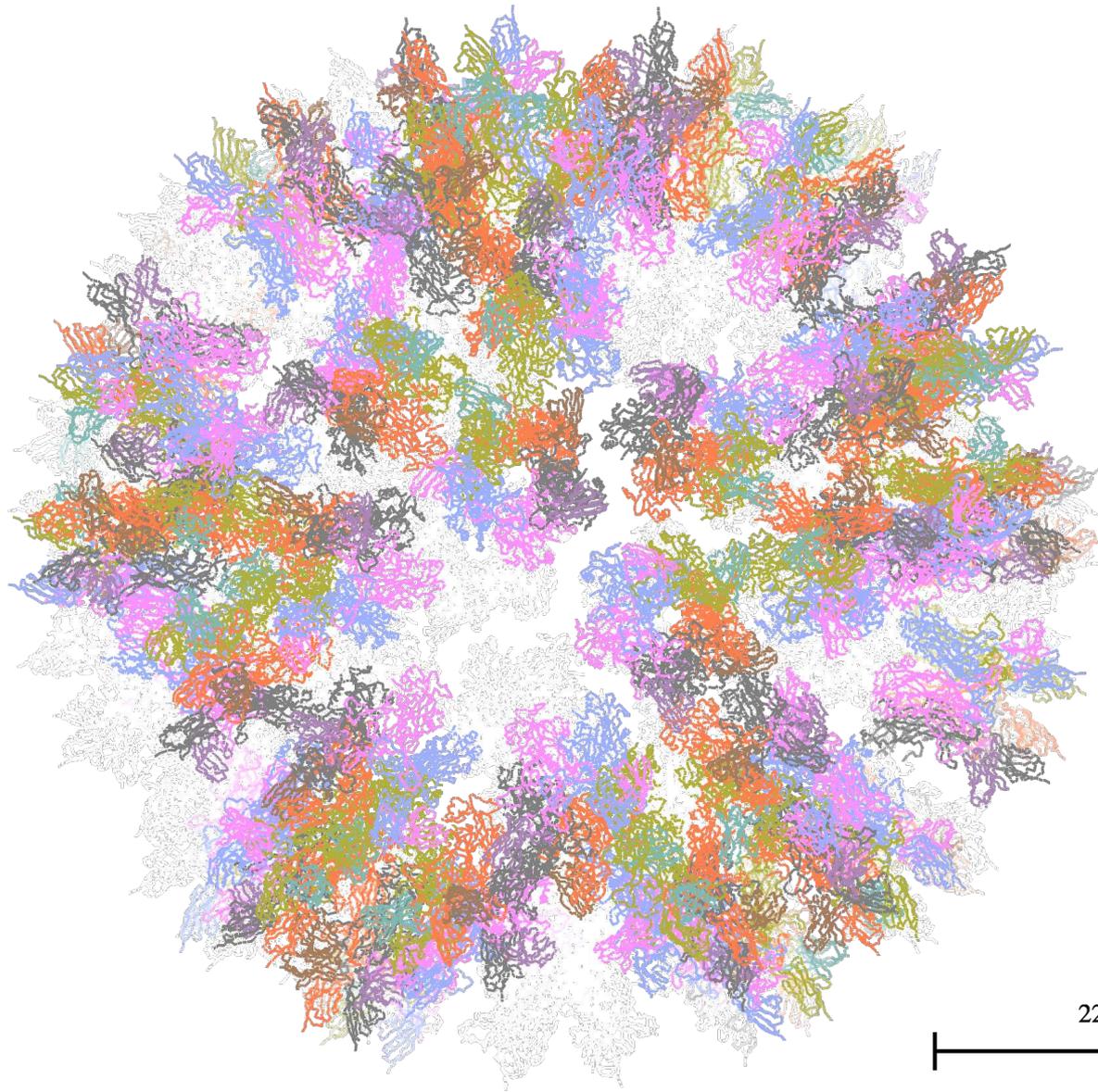


PDB 3j2w



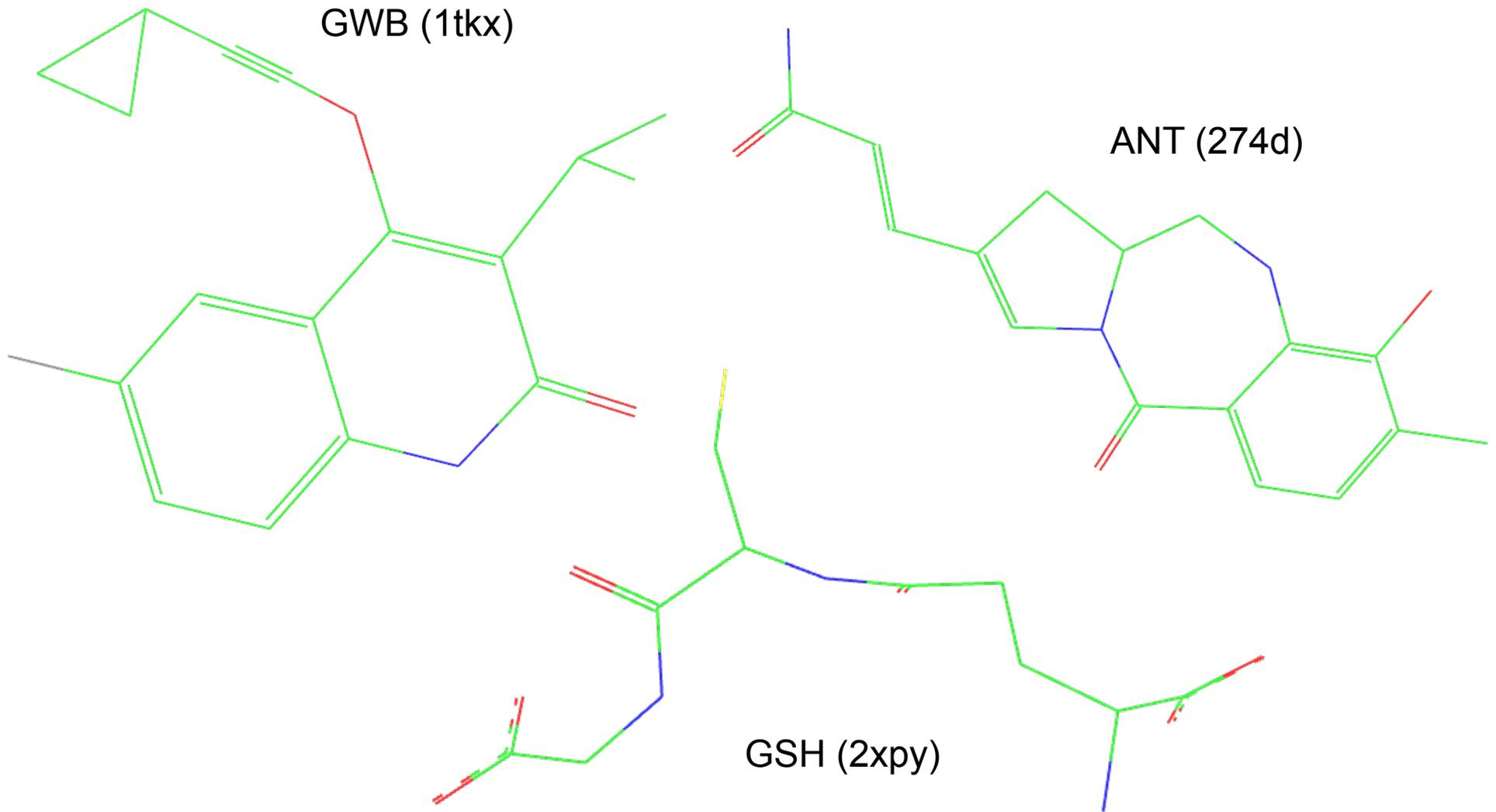
47.6 Å

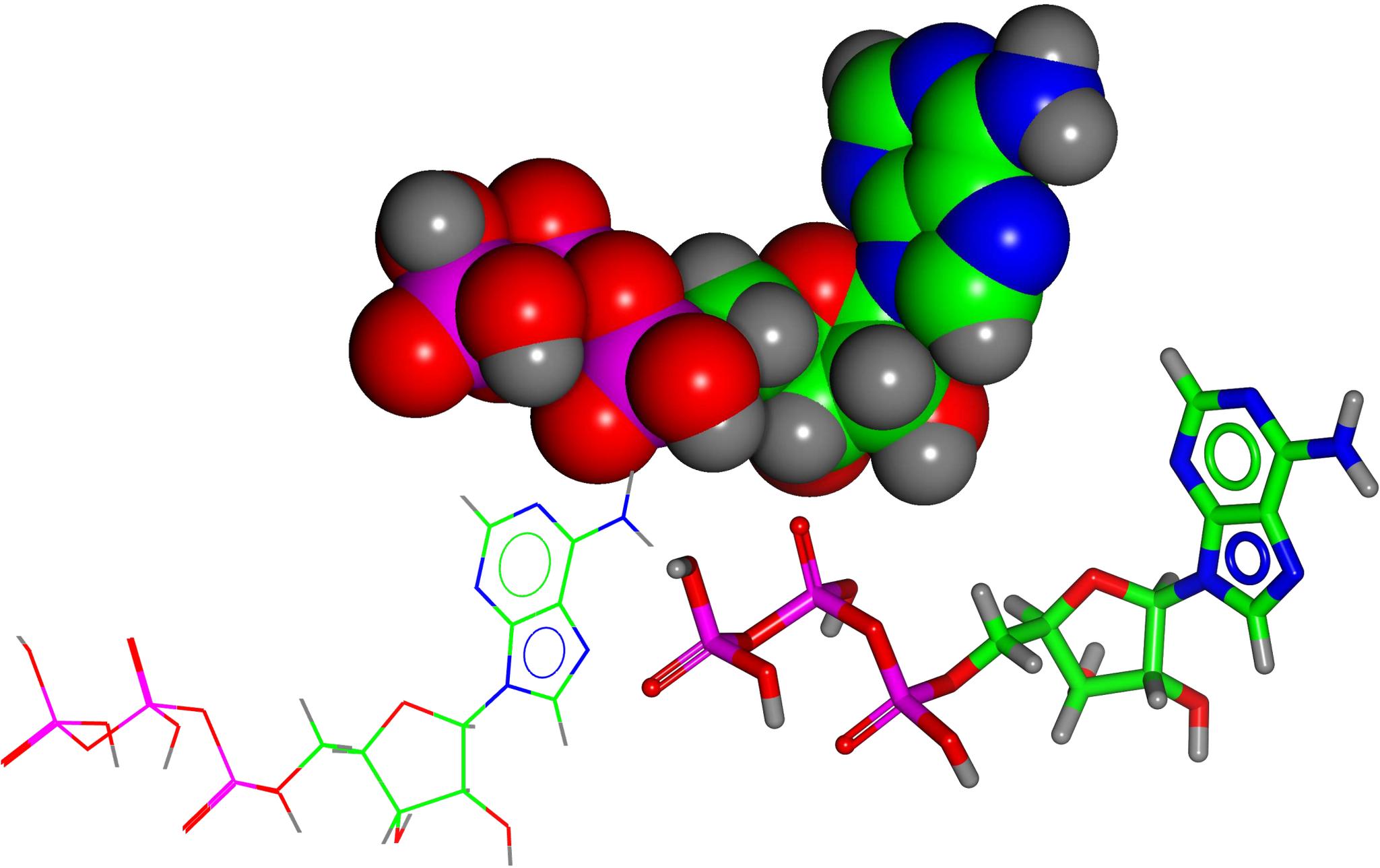
PDBs 3j7e, 3j7g



PDBs 3j7e, 3j7g

# Multiple bonds





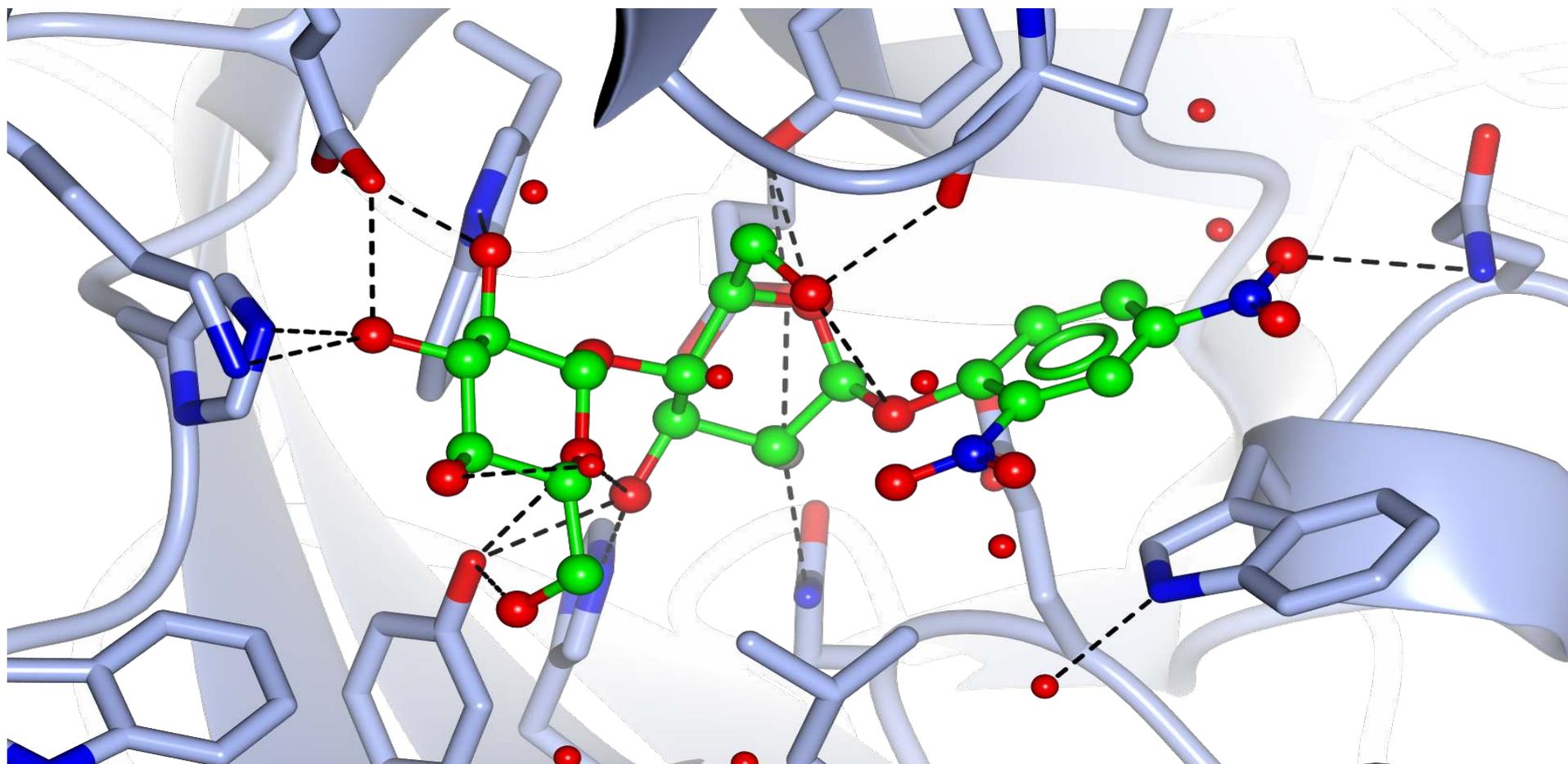
# Other Display Details

- 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))

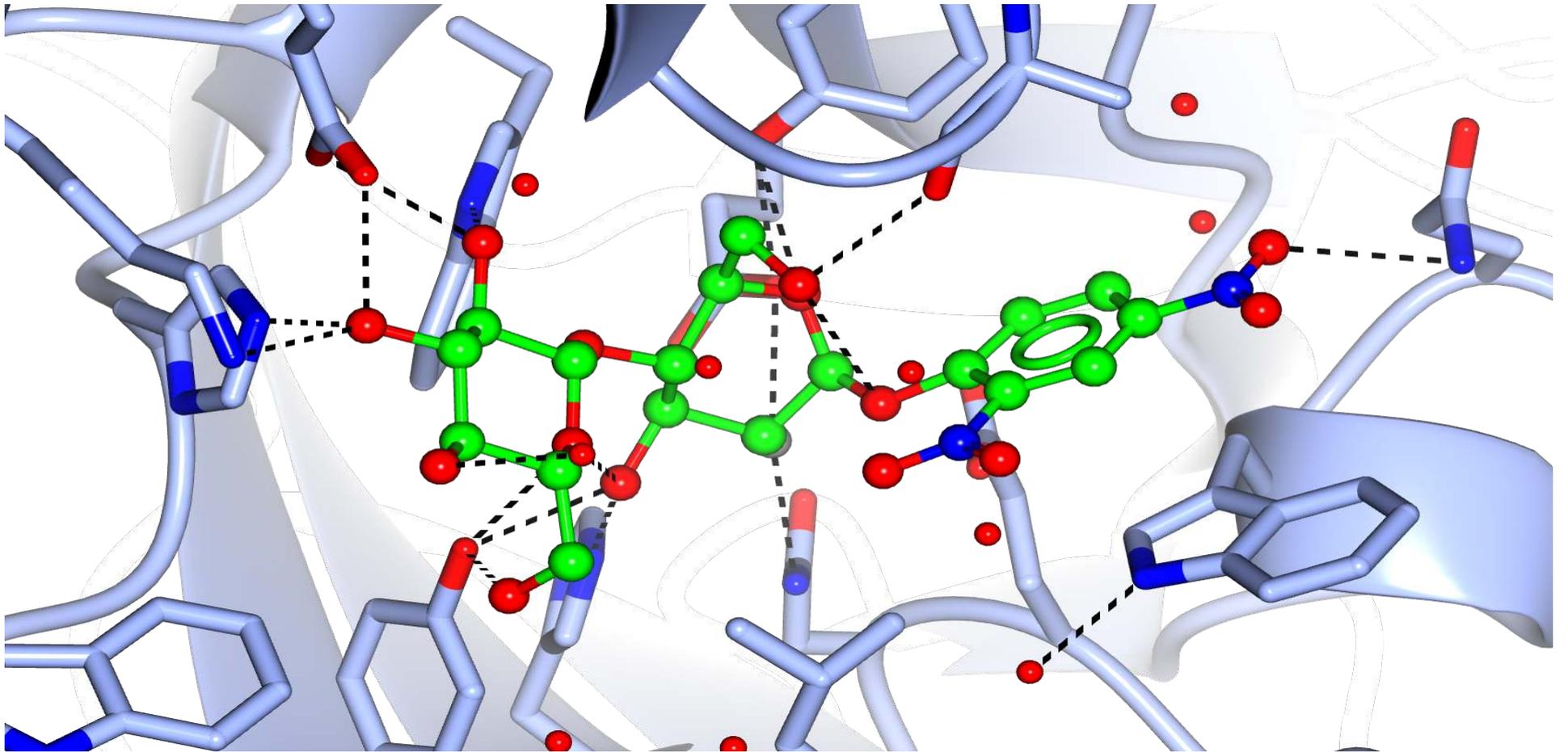
# Rendering

- 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 higher quality than the simple screen dump (spheres particularly). Better transparency with more than one transparent object is possible.

# Screenshot

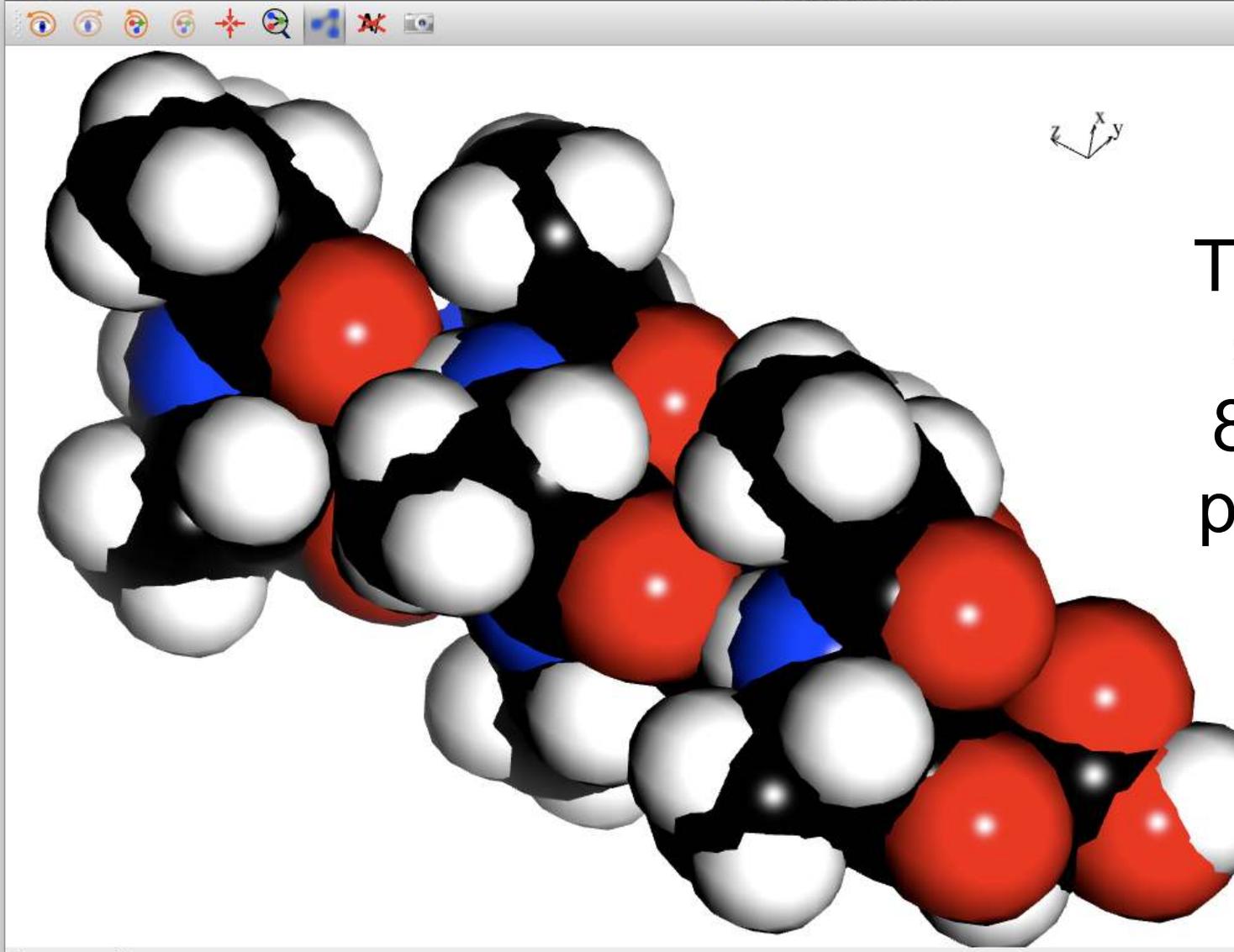


# Render



# “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 ....)



Display Table

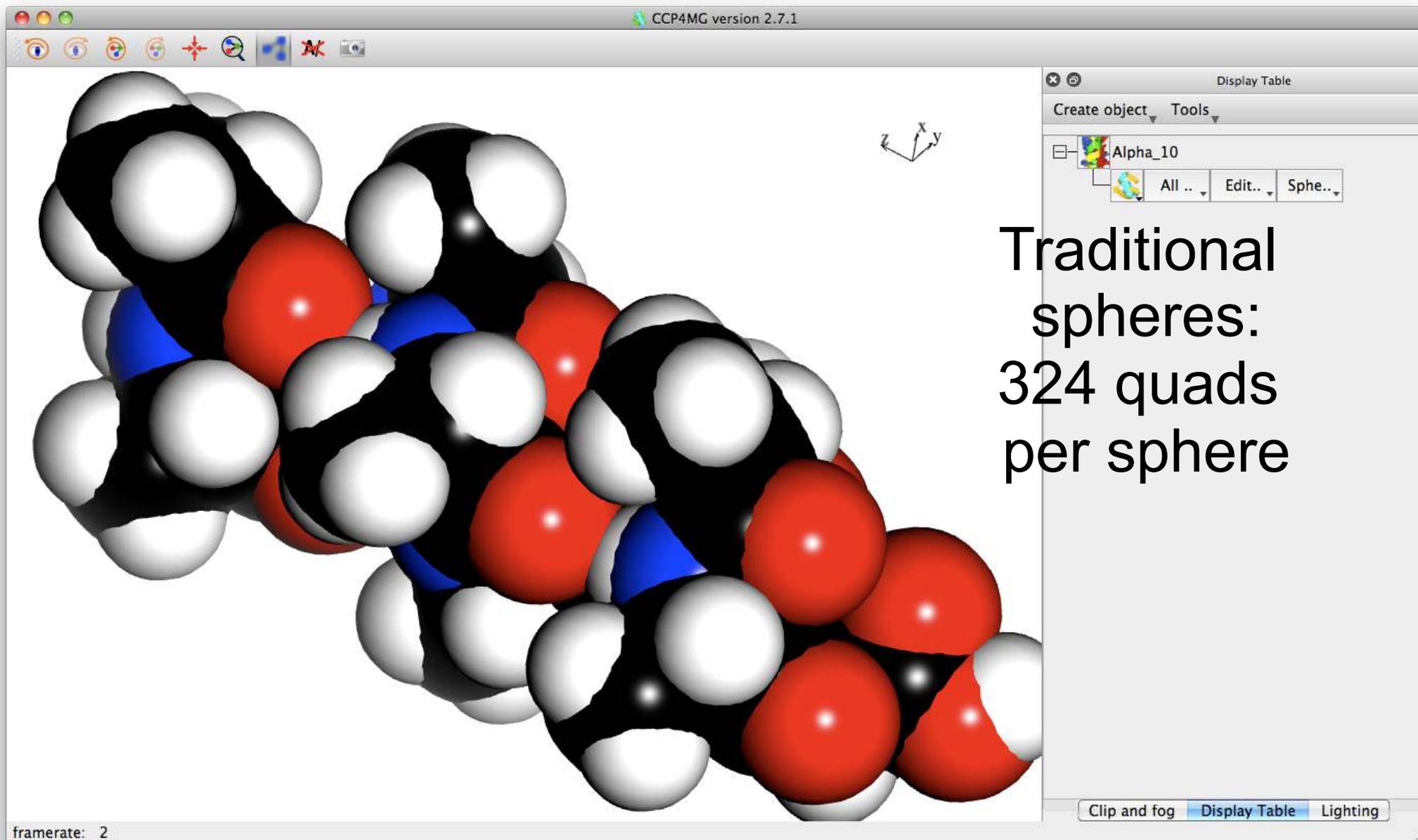
Create object Tools

Alpha\_10

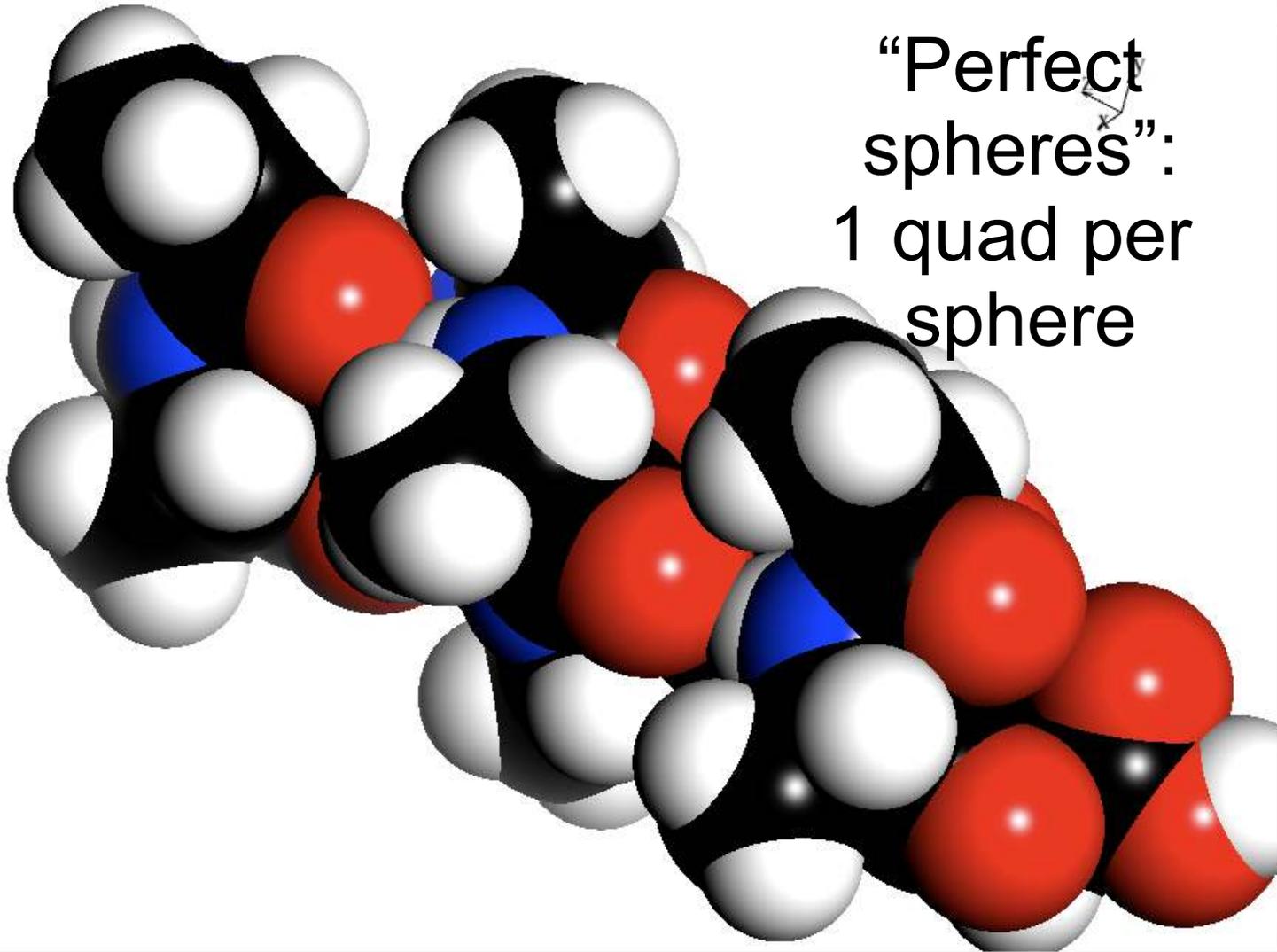
All .. Edit.. Sphe..

Clip and fog Display Table Lighting

Traditional  
spheres:  
81 quads  
per sphere



“Perfect spheres”:  
1 quad per sphere



Lighting

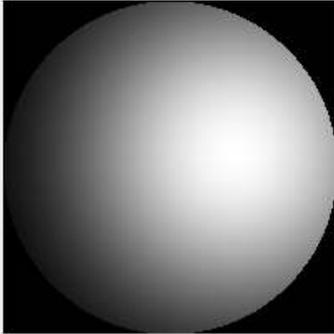
Light 0

On

Diffuse

Specular

Ambient



Shadows (light 0 only)

Occlusion

Object outlines

Help

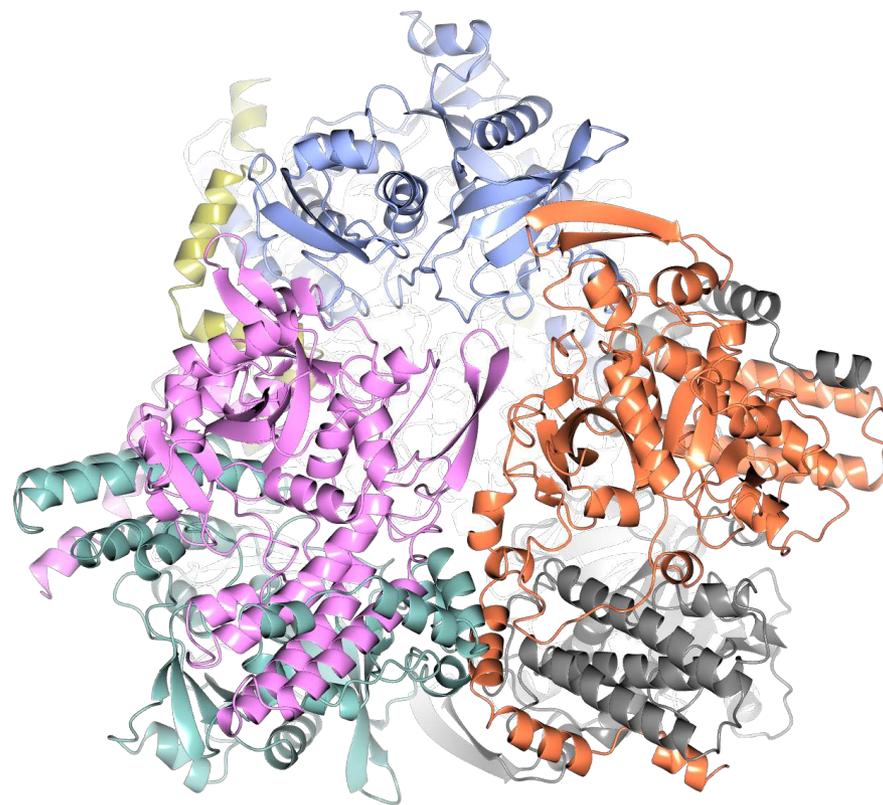
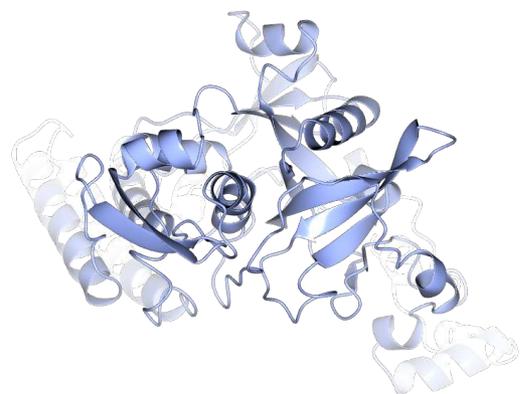
Display Table Clip and fog Lighting

# Render vs. Screenshot

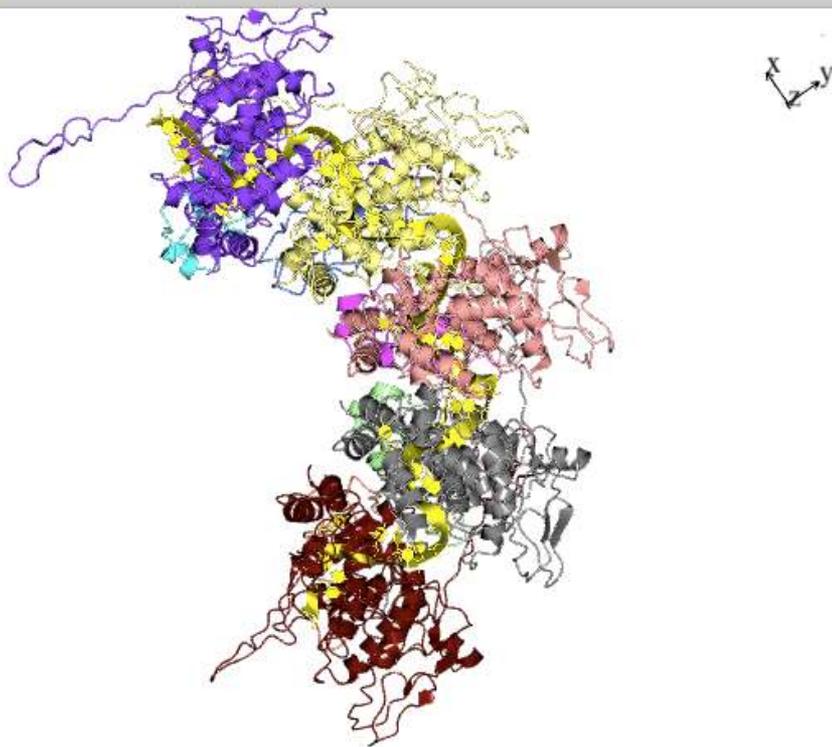
- Some new features mean that OpenGL is now *arguably* a better choice for rendering than “Render” module.
  - Screenshot pros:
    - Shadows make “Render” slow, but bearable.
    - Ambient occlusion makes “Render” really, really slow.
    - Darkness of OpenGL shadows could be changeable, “Render” ones 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.

# 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.



PDB 3gcb



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

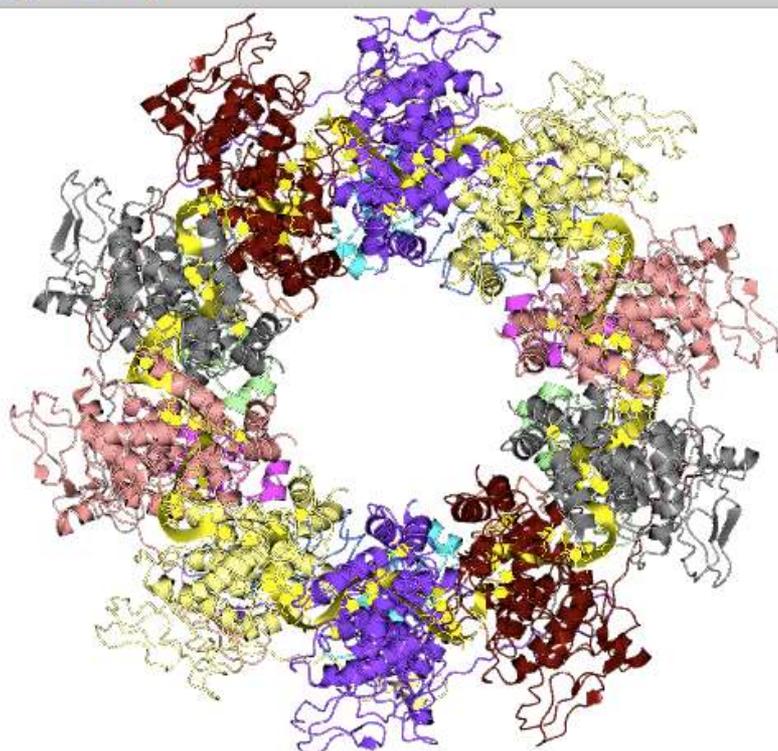
Analyse model

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

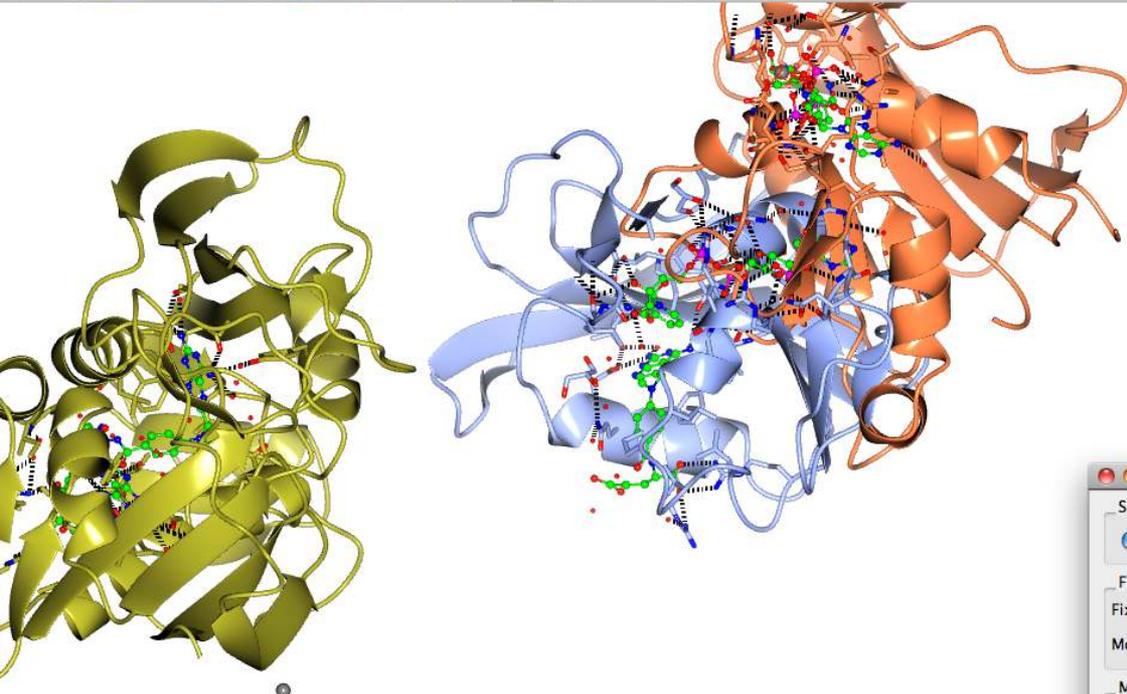
monomers interfaces **assemblies**

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.



Display Table

Create object Tools

1df7

CA t..	ice ..	Ribb..
A/50..	Atom..	Ball..
A/50..	Atom..	Ball..
Nhoo..	ice ..	Cyli..
HBon..	ice ..	Cyli..
Nhoo..	Atom..	Thin..
A/50..	Nhoo..	comp..
A/50..	Nhoo..	comp..
Nhoo..	Nhoo..	comp..

Superpose models

Superpose method

Gesamt/SSM  Match close residues  User defined matches

Fixed and moving models

Fixed model: 1df7

Moving model: 4dfr

Display of matches

Show matches with  distance labels (black)

Highlight selected atoms (yellow) (magenta)

Models to superpose

Active Selection

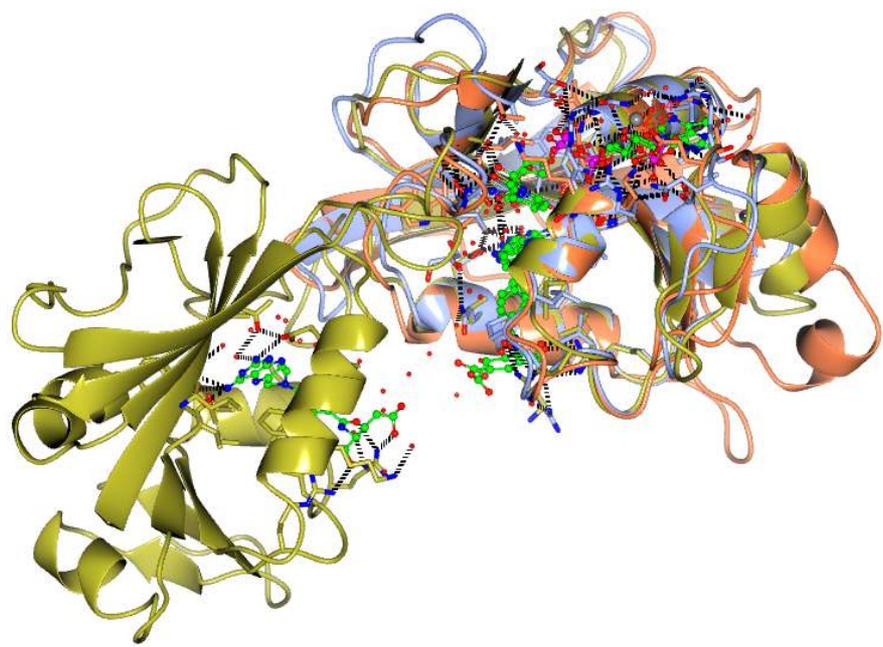
Model	Selection	Show match RMS
1df7	all	<input type="checkbox"/>
4dfr	all	<input type="checkbox"/>
8dfr	all	<input type="checkbox"/>

(or select chain [ ] in all objects)

Options

Method: SSM

Buttons: Help Superpose Undo Export matches List results Show axes Save all data files Close



Display Table

Create object Tools

1df7	CA t..	ice ..	Ribb..
	A/50..	Atom..	Ball..
	A/50..	Atom..	Ball..
	Nhoo..	ice ..	Cyli..
	HBon..	ice ..	Cyli..
	Nhoo..	Atom..	Thin..
	A/50..	Nhoo..	comp..
	A/50..	Nhoo..	comp..
	Nhoo..	Nhoo..	comp..

Superpose models

Superpose method

Gesamt/SSM  Match close residues  User defined matches

Fixed and moving models

Fixed model: 1df7

Moving model: 4dfr

Display of matches

Show matches with  distance labels (black)

Highlight selected atoms (yellow, magenta)

Models to superpose

	Active Selection	Show match	RMS
1df7	<input checked="" type="checkbox"/> all		
4dfr	<input checked="" type="checkbox"/> all	6	1.40/146
8dfr	<input checked="" type="checkbox"/> all	2	1.26/145

(or select chain [ ] in all objects)

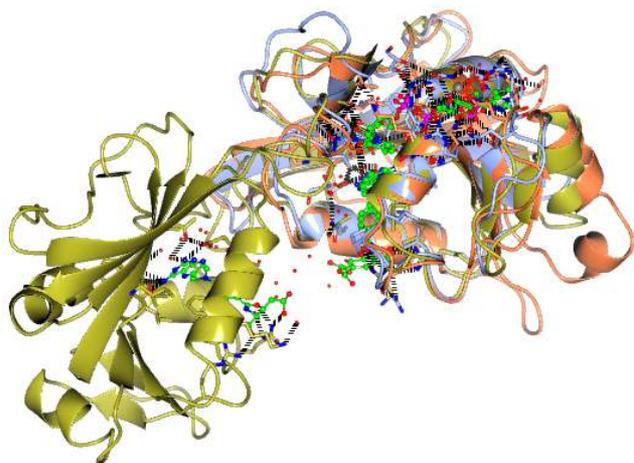
Options

Method: SSM

Buttons: Help, Superpose, Undo, Export matches, List results, Show axes, Save all data files, Close

# Sequence Viewer

- Align sequences using muscle (a free multiple-alignment program).
- 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 as PDF/bitmap. Will add text file very shortly.
- Click, shift-click, ctrl-click, etc. on residues in sequence to display atoms in the mail window.



Display Table

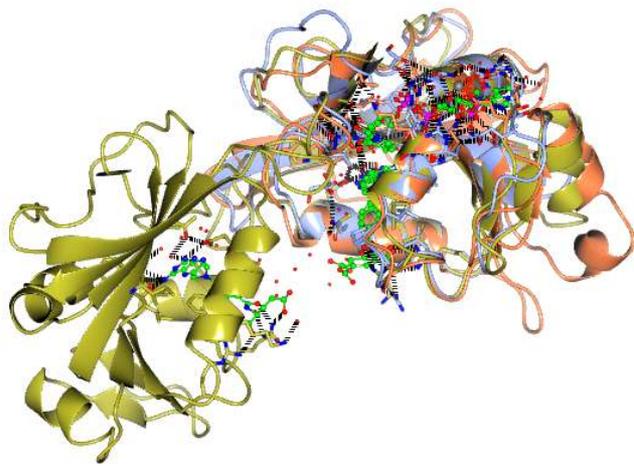
Create object Tools

1df7		
	CA t...	Ribb..
	A/50..	Ball..
	A/50..	Ball..
	Nhoo..	Cyli..
	HBon..	Cyli..
	Nhoo..	Thin..
	A/50..	comp..
	A/50..	comp..
	Nhoo..	comp..
	HBon..	comp..
	Nhoo..	comp..
	{sol..	comp..
	Solv..	Cyli..
	Solute	Cyli..
	A/50..	comp..

Display ... Simplified Display ... Lig...

Sequence Viewer

	10	20	30	40	50	60	70	80	90	100	110	120	130	140	150	506																						
1df7_A	GLIWAQATSGVIG	GGDIPWLPEDQARF	ETIMGETIVMG	ETWDSLPA	VPLPG	NVVLV	QANFMSGARVVG	SLREALTSP	ETWVIGGG	QVIALALPHAT	CHVT	EVDIGLP	REGALAPVLOETW	GTG	WVFS	SGLAYLLESH	S:XXXXXXXX																					
4dfr_A	SLIAALAVD	VIGM	NAMPNLPALANF	ENTLQ	PVING	ETWESIG	PLPG	NIISSQP	QTDV	VTWV	SVDEAIAACG	VPEIMVIGG	VTRQFLP	AQ	LYLTHIDAEV	GTRFPPD	YEPDWE	SVFS	SFHADAQNS	RSYCP	ILR	WXX																
4dfr_B	SLIAALAVD	VIGM	NAMPNLPALANF	ENTLQ	PVING	ETWESIG	PLPG	NIISSQP	QTDV	VTWV	SVDEAIAACG	VPEIMVIGG	VTRQFLP	AQ	LYLTHIDAEV	GTRFPPD	YEPDWE	SVFS	SFHADAQNS	RSYCP	ILR	WXX																
8dfr_A	SLNSIVAVC	QNMGLG	EGMLP	WPLP	NET	YFQ	MCSTSEV	EG	QNAVING	ETWPSIP	N	PLD	INIVLS	EL	RAP	GARYLS	SLDQALALL	SP	EL	S	VEMVIVGG	RAVY	AAM	PINR	LFVT	ILR	SFES	TFFP	PIQ	DP	LLR	STPGVP	ADIQ	SRD	GIQ	EFV	YQ	SVXX



Display Table

Create object Tools

1df7		
CA t..	ice ..	Ribb..
A/50..	Atom..	Ball..
A/50..	Atom..	Ball..
Nhoo..	ice ..	Cyli..
HBon..	ice ..	Cyli..
Nhoo..	Atom..	Thin..
A/50..	Nhoo..	comp..
A/50..	Nhoo..	comp..
Nhoo..	Nhoo..	comp..
HBon..	Nhoo..	comp..
Nhoo..	Nhoo..	comp..
{sol..	{sol..	comp..
Solv..	Atom..	Cyli..
Solute	Atom..	Cyli..
A/50..	Same	oloc

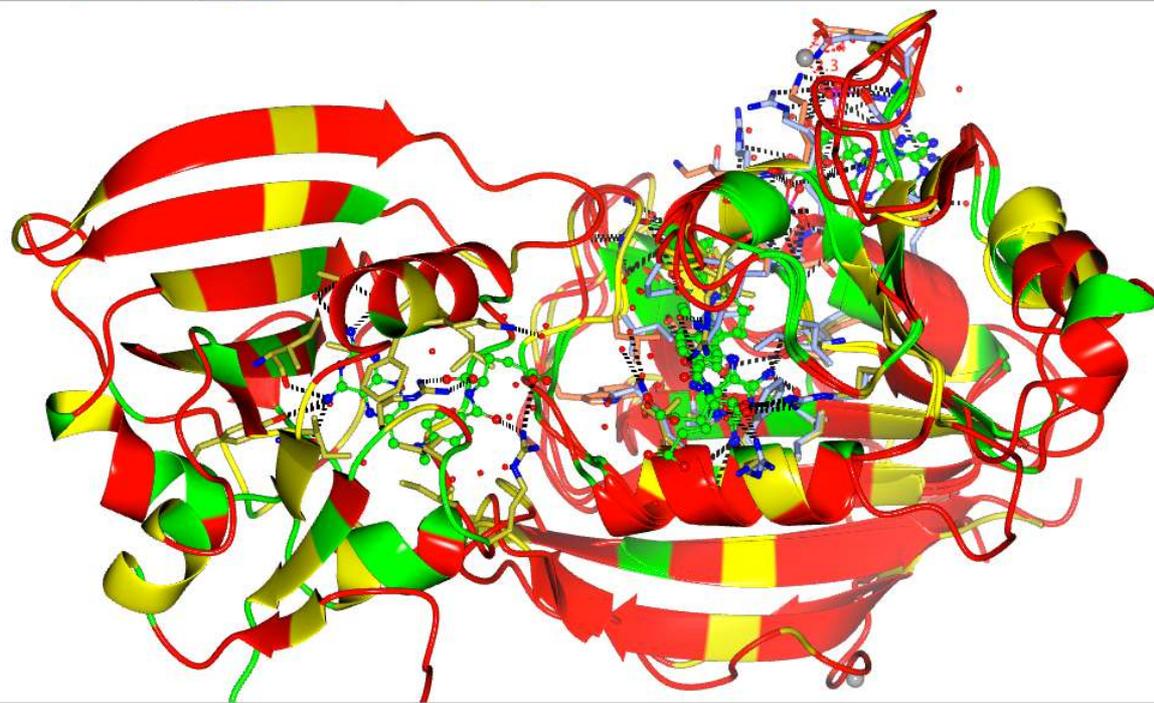
Display ... Simplified Display ... Lig...

Sequence Viewer

	8	18	27	40	50	60	70	98	106	116	126	135	142	150	506
1df7_A	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
4dfr_A	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
4dfr_B	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
8dfr_A	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

```

  MVGLIWAQATSGVIGRGGIPIW-ELPEDQAFRBIT-----MERTIVMGRRTWDSLPAKVRPLGRGIVVLSKQDFPAGCANVY-GLLEAL-----TSPE-----IVVIGGQVYALAL--PFAFRCEVTEVDICLPHRGGALAPVLD-ETWQST---GMR--PSPGSLRYLISTERSIXXXXX
  MISLIAALAVDRVIGHENMPW-ELPADLAWFKRPT-----LKPVINGRHTWESI---GRPLPGRNIIILSQQOTDDRTWV--FSVDEAIACGDVPE-----DAVIGGGRVYRQL--PKAQLILFIDAEV---EGDTFFPDEFDWSSVY--SPFDADAQNSRSTCPKILRRX
  MISLIAALAVDRVIGHENMPW-ELPADLAWFKRPT-----LKPVINGRHTWESI---GRPLPGRNIIILSQQOTDDRTWV--FSVDEAIACGDVPE-----DAVIGGGRVYRQL--PKAQLILFIDAEV---EGDTFFPDEFDWSSVY--SPFDADAQNSRSTCPKILRRX
  ELNSIVAVCONAGIGRGGLPWPLRNEIKYFQRWSTSHVGGKNAVINGKKTWPSIPEKRRPLDRINIVLSRELRKAPKCAIYLSLDDALALL-DSPELRKVDVIVGGIAYVKAMSPINERLVPVILRFP---SDTFFPDEIDKPKALLTEYFVPPADIQEDG!QYSPVYKSVY
  
```



Display Table

Create object Tools

	HBon...	Nhoo...	comp...
	Nhoo...	Nhoo...	comp...
	{sol..	{sol..	comp...
	Metal	Atom..	Sphe..
	Solv..	Atom..	Cyli..
	Solute	Atom..	Cyli..
	A/16..	Same..	elec..
	Nhoo...	All ..	elec..
	All ..	Atom..	Bonds
	All ..	Same..	elec..

8dfr

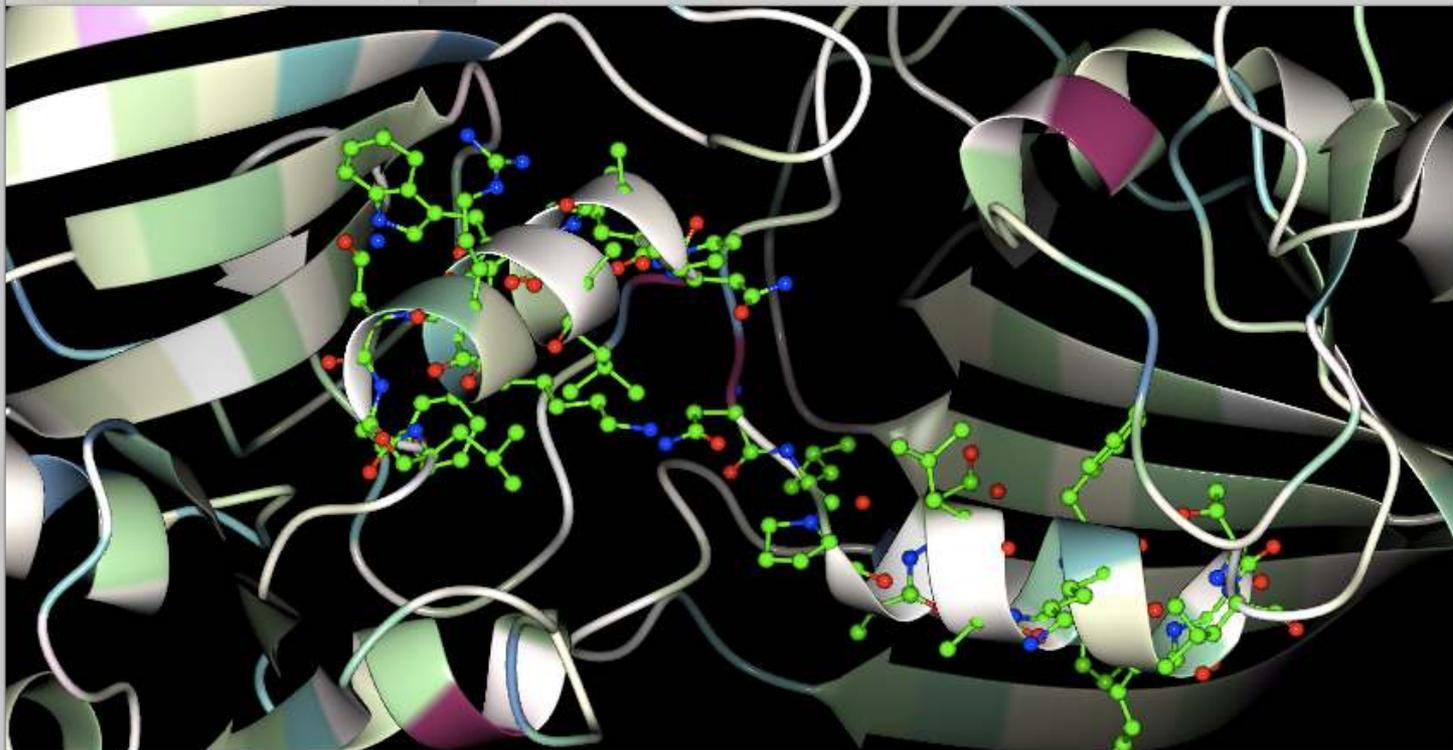
	CA t..	Cons..	Ribb..
	A/19..	Atom..	Ball..
	Nhoo...	coral	Cyli..
	HBon...	coral	Cyli..

Display ... Simplified Display ... Lig...

Sequence Viewer

	8	18	27	40	50	60	70	98	106	116	126	135	142	150	506																					
1df7_A	MVGLIWAQATS	SVVIGRGGIPW	ELPEDQARFRIT	-----	MEETIVMGRRTW	DELPAKVRPL	GRGNVVL	EQADFMASQAVV	CSLEEAR	-----	TSPE	-----	IVVIGGQVYALAL	PKATRCVET	VDIQLPREGDALAP	WLD	SWAGST	-----	GMML	FSRSGLYL	LYSTER	SIK	IKIKI													
4dfr_A	MISLIAALAV	DRVIGHENMPW	ELPADANFKRST	-----	LKPVIMGRHTW	ESI	-----	GRPLGRGNILLS	QVQEDDRVTW	-----	ISVDEAIAACGDVPE	-----	IVVIGGGRVYRQPL	PKAKLILTSIDAV	-----	EGDTRFPPE	PDWSSVF	-----	SPHDADA	NS	SY	CP	KILERR	IK												
4dfr_B	MISLIAALAV	DRVIGHENMPW	ELPADANFKRST	-----	LKPVIMGRHTW	ESI	-----	GRPLGRGNILLS	QVQEDDRVTW	-----	ISVDEAIAACGDVPE	-----	IVVIGGGRVYRQPL	PKAKLILTSIDAV	-----	EGDTRFPPE	PDWSSVF	-----	SPHDADA	NS	SY	CP	KILERR	IK												
8dfr_A	SLNSIVAVC	QNNIGIGG	LWPFLLRSE	IKYFQKST	STSRVGRGQ	NAVIMGKKTW	PSIPEKRRPL	DRINIVLS	SEIKRAPRC	ANTLSE	SLDDALALL	-----	DGPELRSKVDHVV	IGGTA	VYKAMSE	PIMRSLV	TSILRFP	-----	ESDTFFP	PD	EKQ	P	LLCET	FG	PADIQ	SE	DG	IQ	Y	SP	VY	Q	K	S	V	I

Origin: -9.41521547397 -34.0333911405 -15.1800613056



Display Table

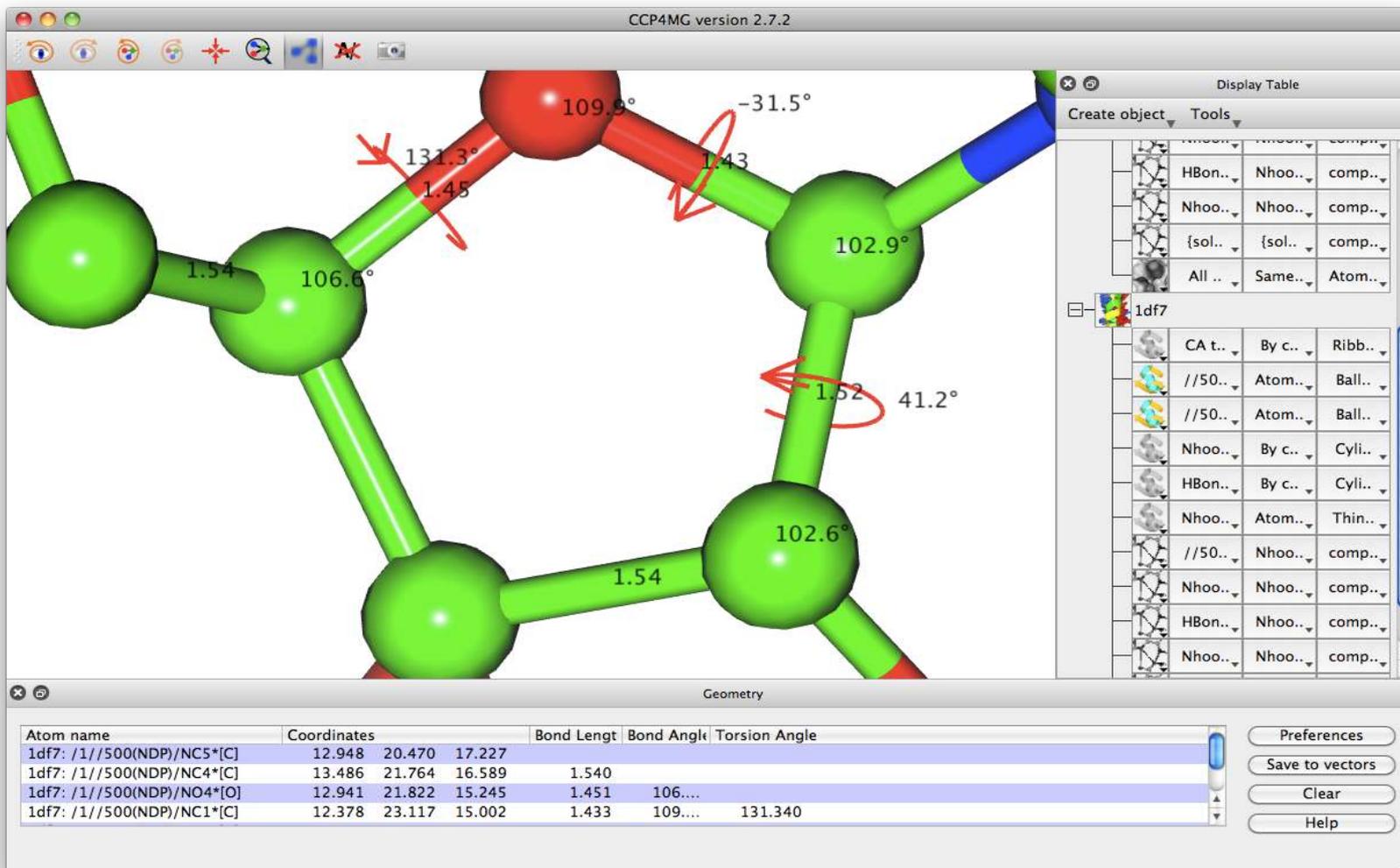
4dfr	All ..	Cons..	Ribb..
//A/..	Atom..	Ball..	
//B/..	Atom..	Ball..	
8dfr	All ..	Atom..	Bonds
// /..	Atom..	Fat ..	
1sar	A/	Blen..	Ribb..
B/	Blen..	Ribb..	
Solv..	Atom..	Ball..	
Solute	Atom..	Ball..	
	Atom..	Fat ..	

Sequence Viewer

4dfr_A	<input type="checkbox"/>			--MISLIAALAVDRVIGMENAMPW-NLPADLAWFKRNTL-----DKPVIMGRHTWESI---GRPLPGRKNIILSSQPGTDDRVT--WVK
4dfr_B	<input type="checkbox"/>			--MISLIAALAVDRVIGMENAMPW-NLPADLAWFKRNTL-----DKPVIMGRHTWESI---GRPLPGRKNIILSSQPGTDDRVT--WVK
8dfr_	<input type="checkbox"/>			VRSLSNIVAVCQNMIGKDGNLWPPLRNEYKYFQRMSTSHVEGKQNAVIMGKKTWFSIPEKNRPLKDRINIVLSRELKEAPKGAHYLSK
1sar_A	<input type="checkbox"/>			DVSGTVCLLSALPPEATDTLNLIASDGPPFPYSQDGVVFQNRRESVLPTQSYGYTHEYTVITPGARTRGTRRIICGEATQEDYTTGDHYATFSL
1sar_B	<input type="checkbox"/>			DVSGTVCLLSALPPEATDTLNLIASDGPPFPYSQDGVVFQNRRESVLPTQSYGYTHEYTVITPGARTRGTRRIICGEATQEDYTTGDHYATFSL
1aim_A	<input type="checkbox"/>			APAAVDWRARGAVTAVKDQGQCGSCWAFSAIGNVECQWFLAGHPLTNLSEQMLVSCDKTDSGCBSGLMNAFEWIVQENNGAVYTEDSYPY
3ljb_A	<input type="checkbox"/>			EDENEKMFLLIDKVNAPNQDITALMQGEETVGEEDIRLFTRLRHEFHKWTIENNFOEGHKILSRKIQKFNFNVRTFETIVKQIQIKALI
3ljb_B	<input type="checkbox"/>			DENEKMFLLIDKVNAPNQDITALMQGEETVGEEDIRLFTRLRHEFHKWTIENNFOEGHKILSRKIQKYRTFETIVKQIQIKALEEPAVDM

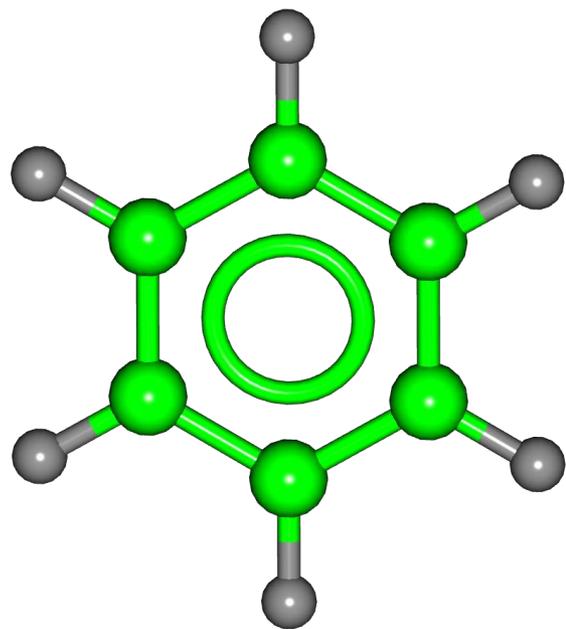
# Distances and angles

- 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.

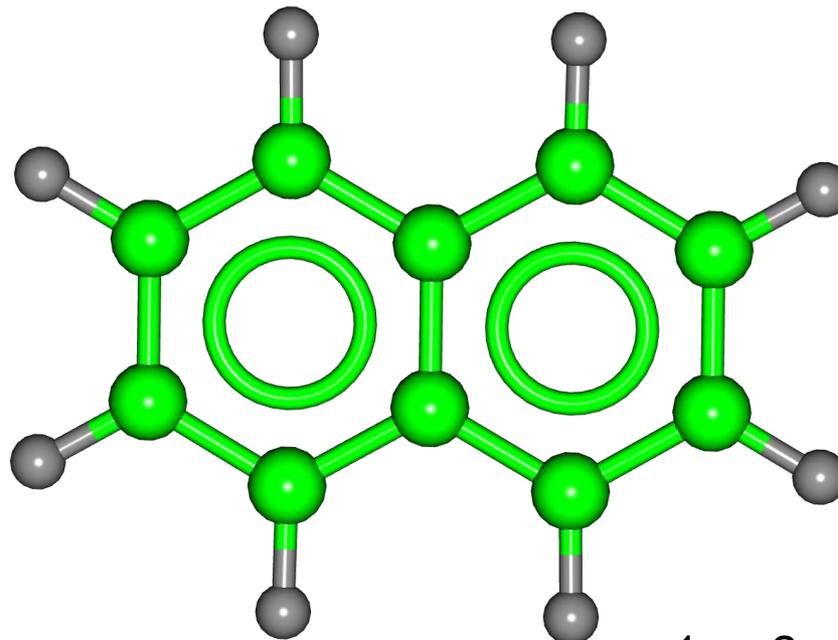


# “Get SMILES”

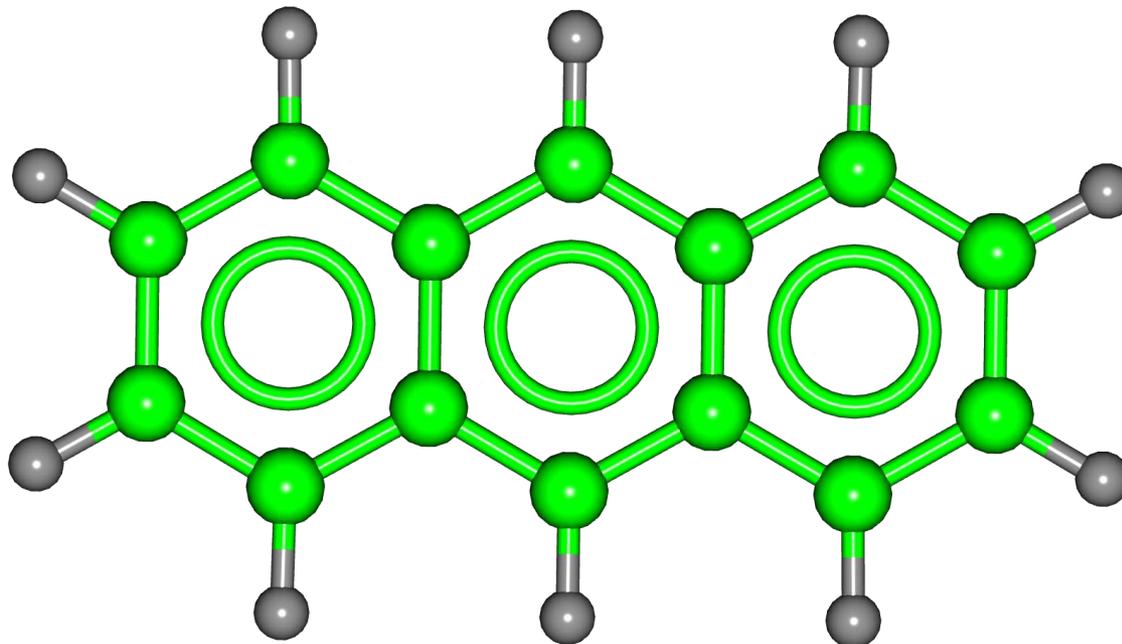
- SMILES string interpretation
- Type in string and molecule is loaded hopefully with correct chemistry.
- (Applications -> Get SMILES)



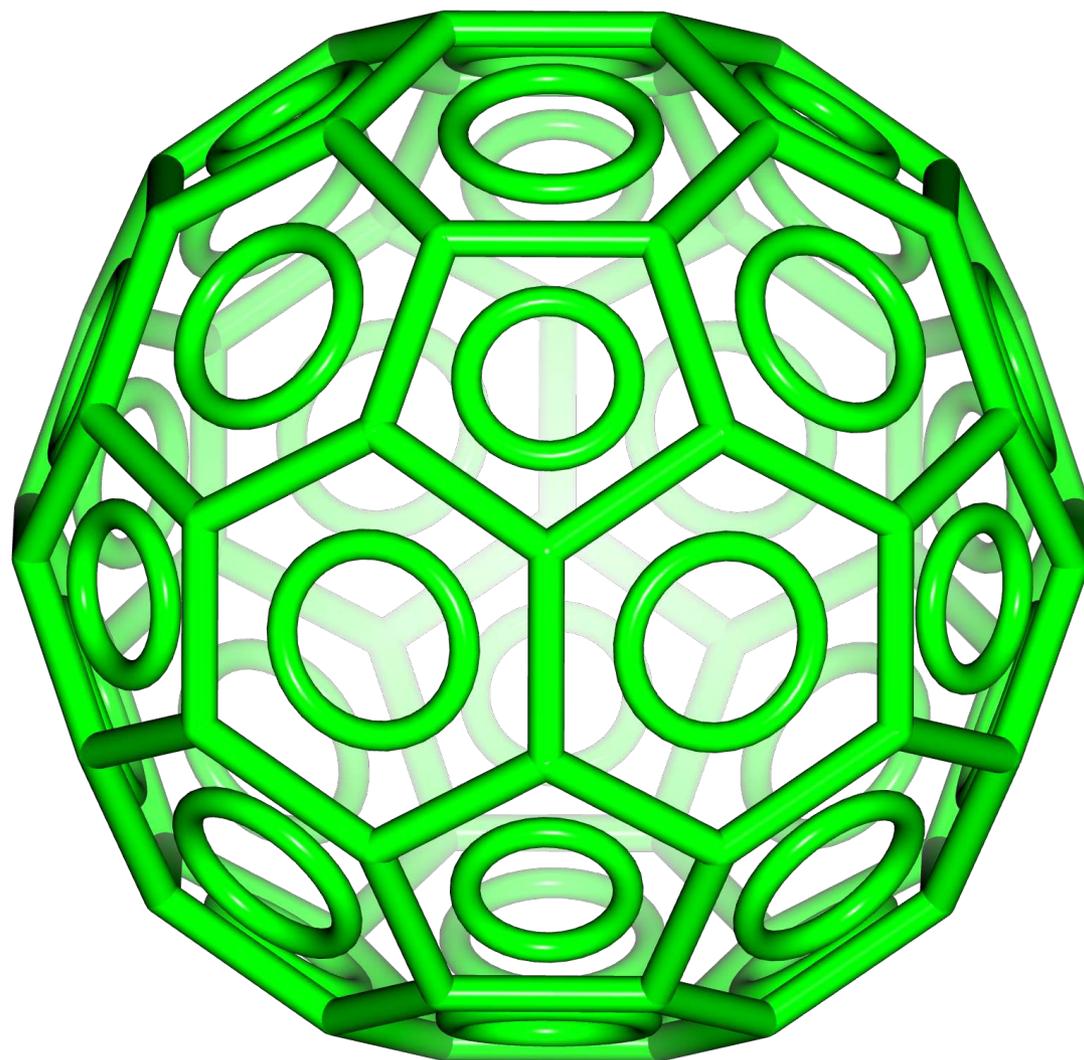
c1ccccc1



c1ccc2ccccc2c1



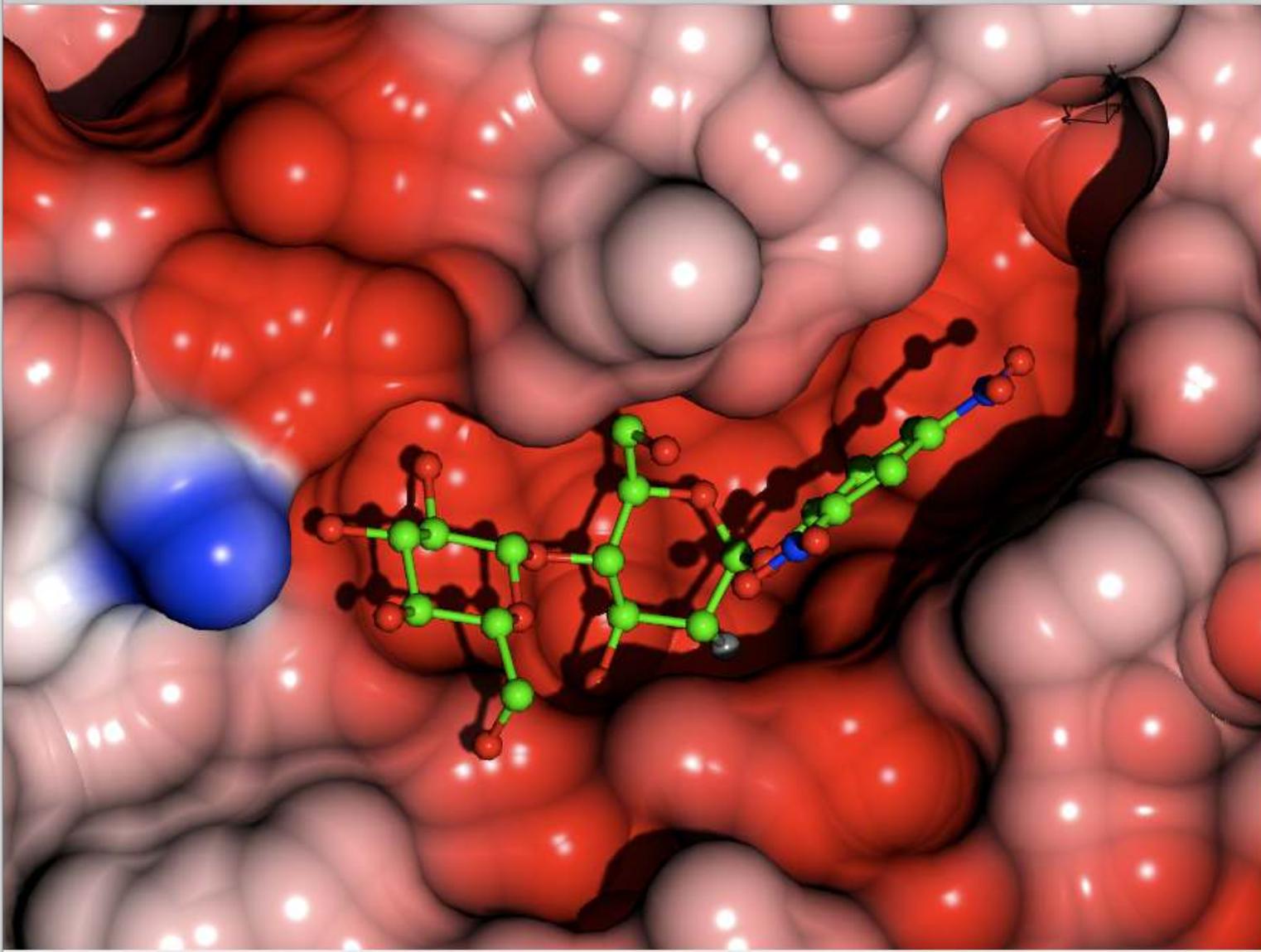
c3ccc2cc1ccccc1cc2c3



c12c3c4c5c1c6c7c8c2c9c1c3c2c3c4c4c%10c5c5c6c6c7c7c%11c8c9c8c9c1c2c1c2c3c4c3c4c  
%10c5c5c6c6c7c7c%11c8c8c9c1c1c2c3c2c4c5c6c3c7c8c1c23

# 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

A/20 Atom Ball

Lighting

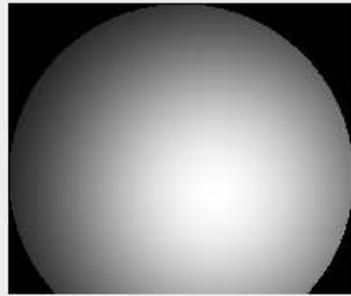
Light 0

On

Diffuse

Specular

Ambient

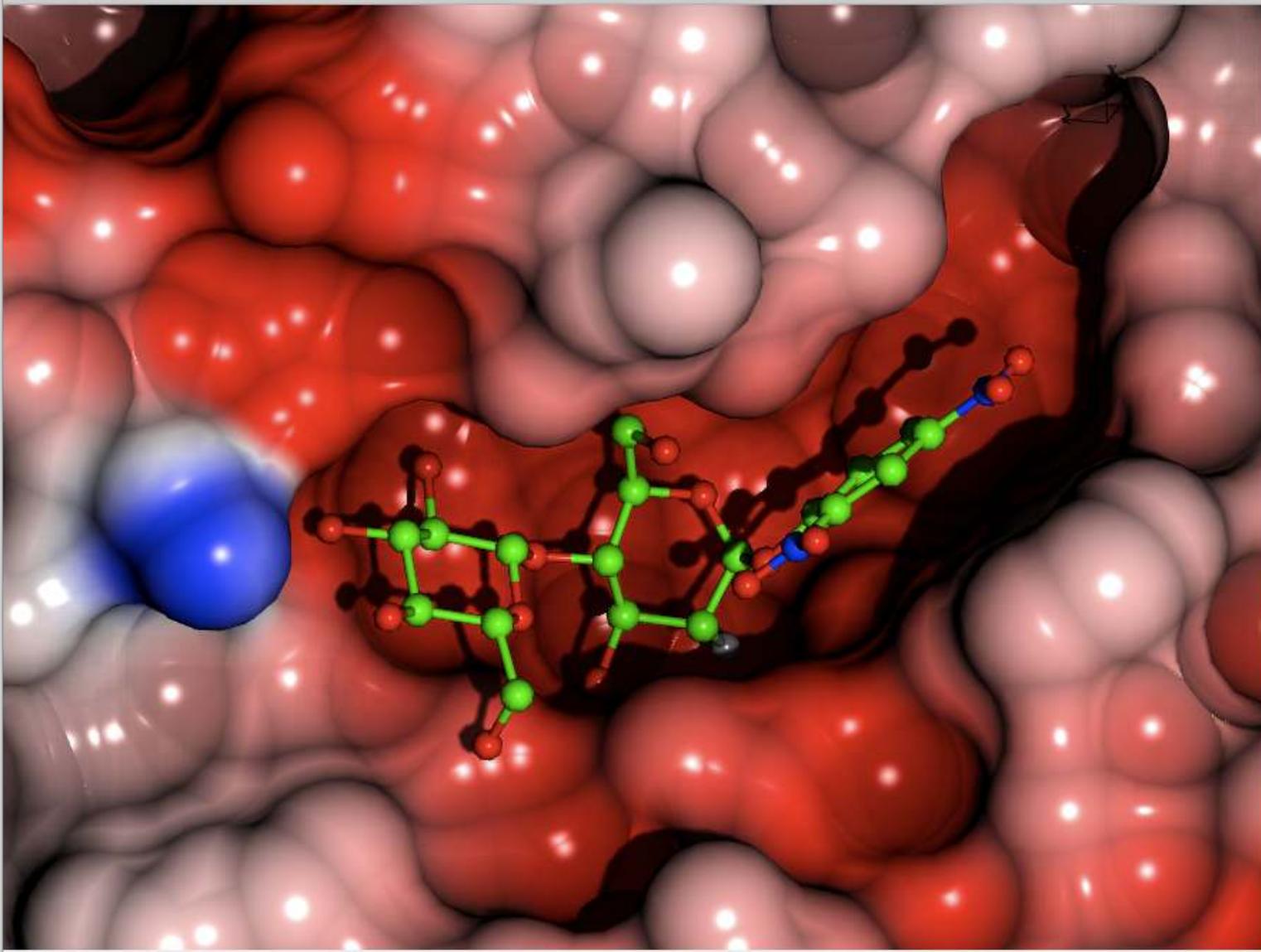


Shadows (light 0 only)

Occlusion

Object outlines

Help



Display Table

Create object Tools

4a3h

A/20 Atom Ball

Lighting

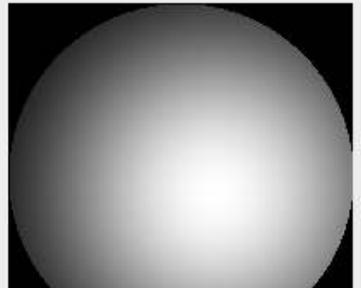
Light 0

On

Diffuse

Specular

Ambient

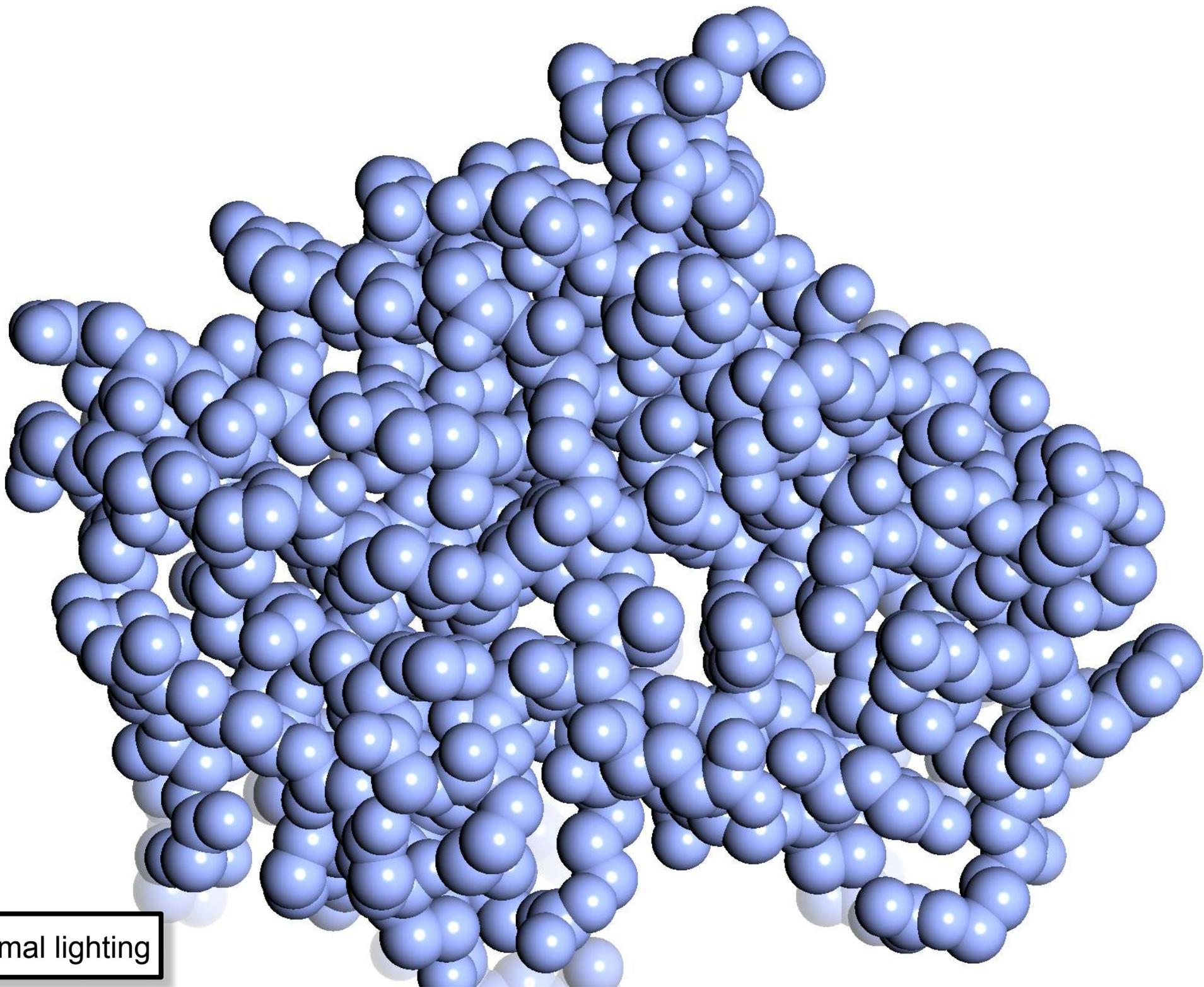


Shadows (light 0 only)

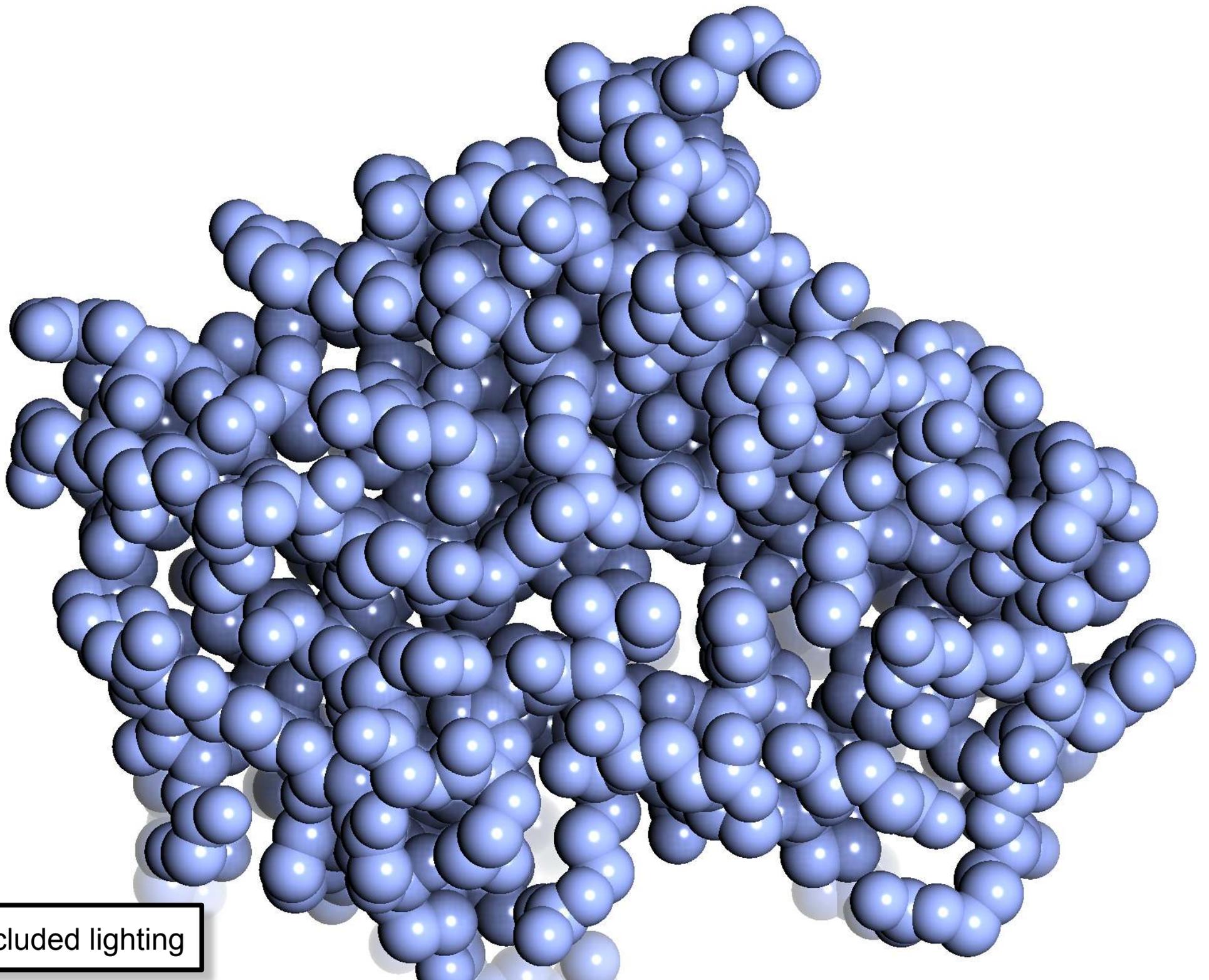
Occlusion

Object outlines

Help

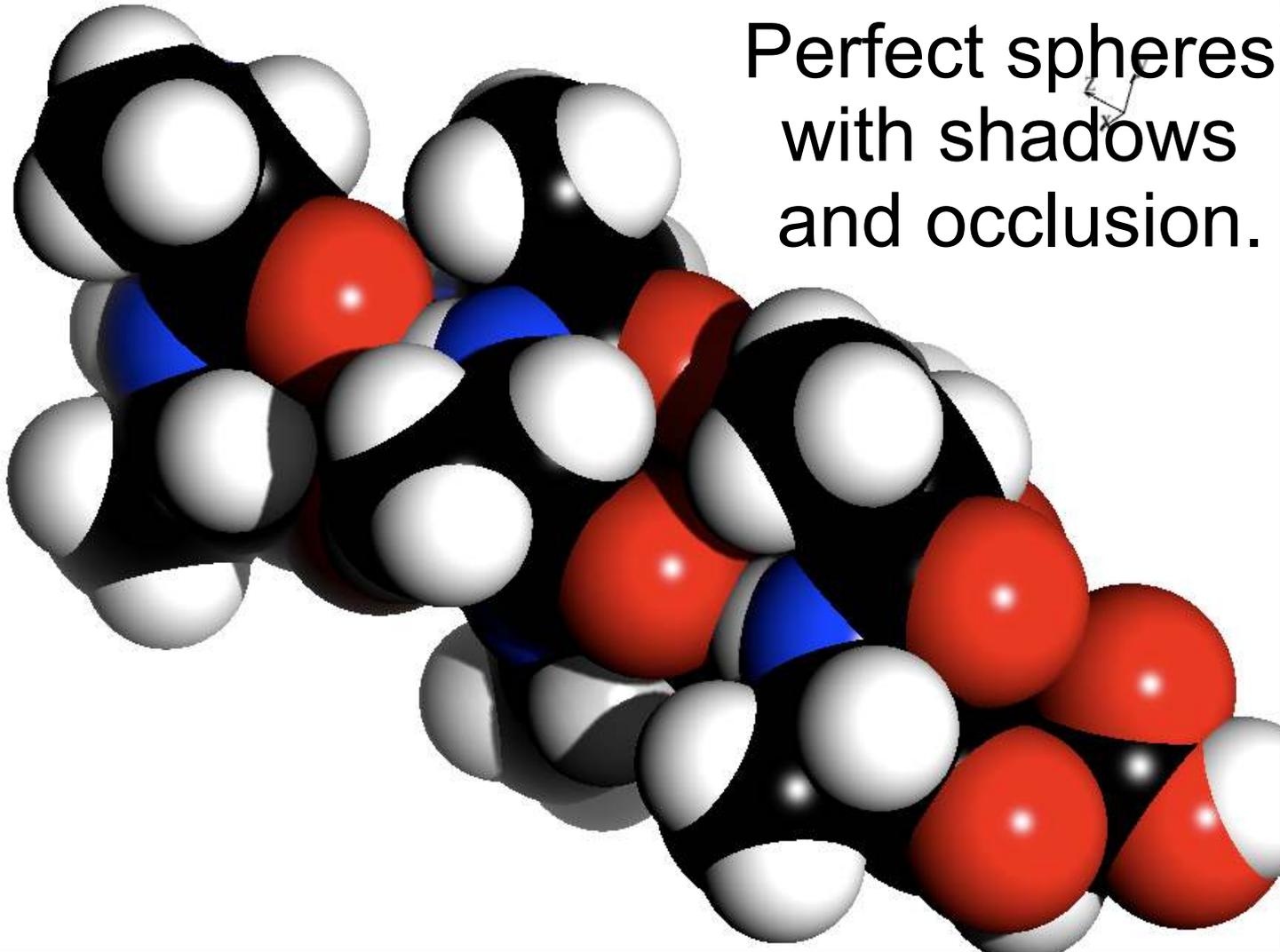


Normal lighting



Occluded lighting

Perfect spheres  
with shadows  
and occlusion.



Lighting

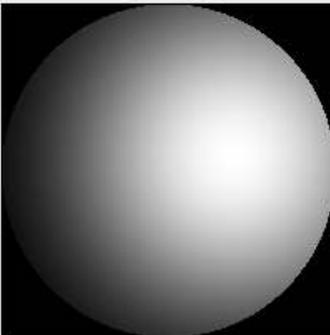
Light 0

On

Diffuse

Specular

Ambient



Shadows (light 0 only)

Occlusion

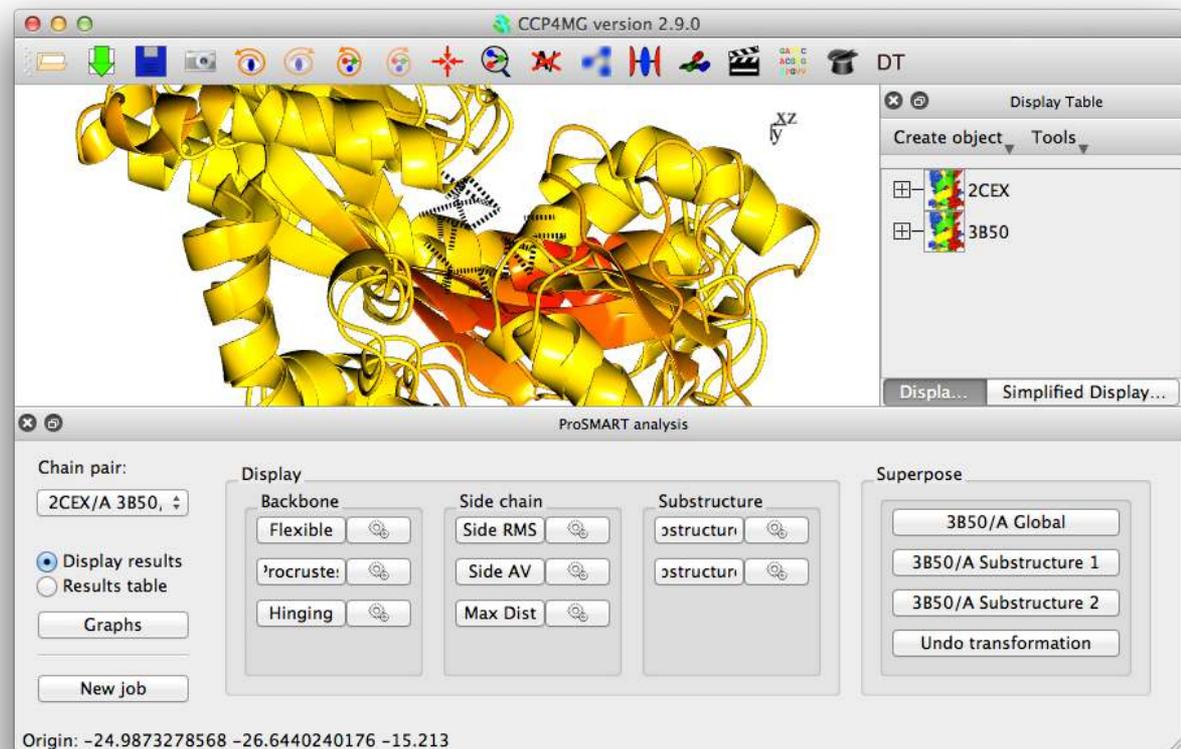
Object outlines

Help

Display Table | Clip and fog | **Lighting**

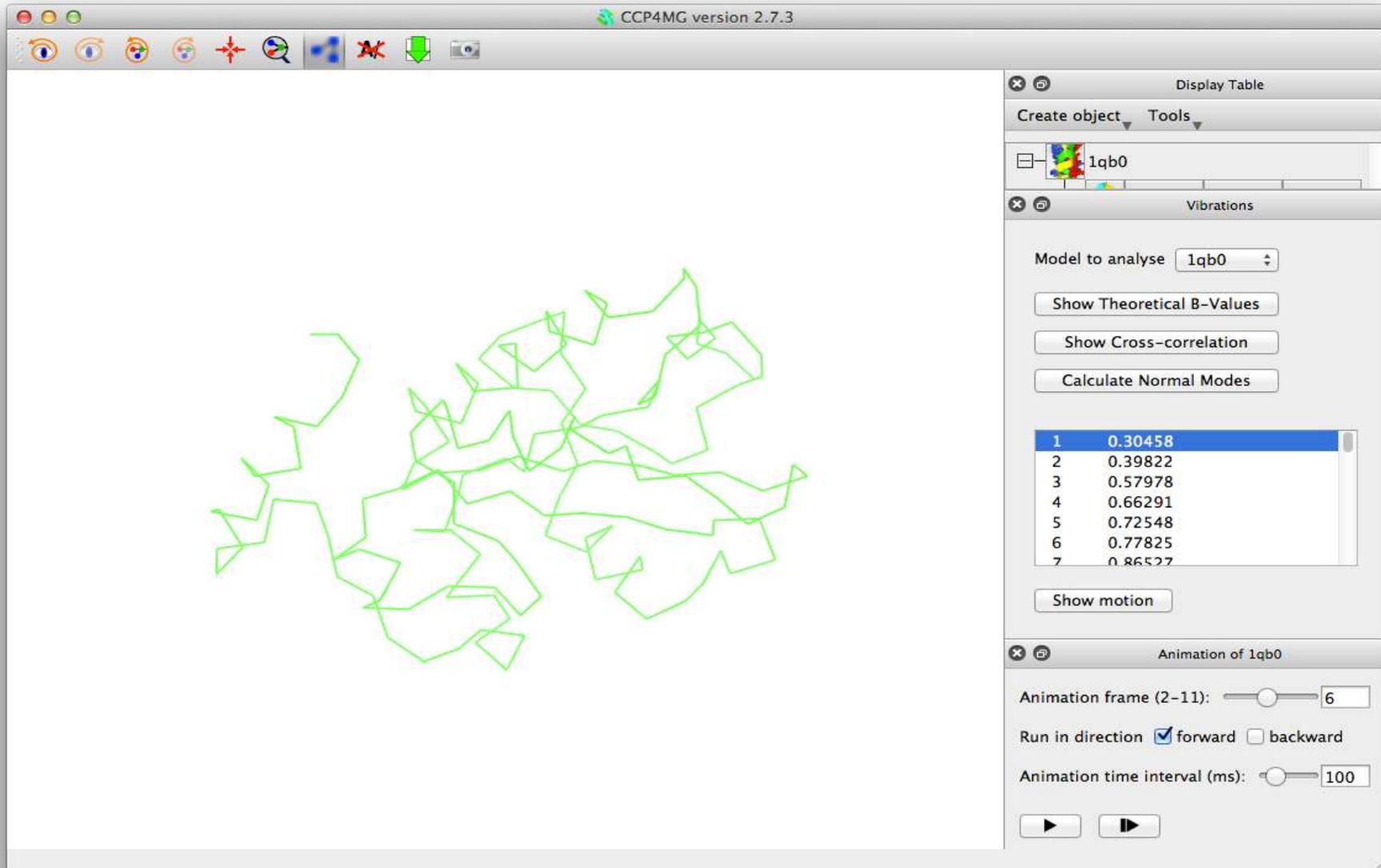
# ProSMART interface

ProSMART interface completely overhauled. Now has tool buttons as major feature and graphs to visualize results.



# Normal Modes

- Simple approximate elastic network model.



The screenshot displays the CCP4MG version 2.7.3 software interface. The main window shows a protein structure rendered in green lines. 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 small icon.
- Vibrations:** Shows 'Model to analyse' set to '1qb0'. It includes buttons for 'Show Theoretical B-Values', 'Show Cross-correlation', and 'Calculate Normal Modes'. Below these is a table of results:

1	0.30458
2	0.39822
3	0.57978
4	0.66291
5	0.72548
6	0.77825
7	0.86527

- Animation of 1qb0:** Features an 'Animation frame (2-11)' slider set to 6, a 'Run in direction' checkbox with 'forward' selected and 'backward' unselected, and an 'Animation time interval (ms)' slider set to 100. Playback buttons are located at the bottom.

# On screen text and images

CCP4MG version 2.7.3

**Hoh A385**

A/520/O A/510/O A/60/CA A/410/O A/310/O A/490/O A/380/O A/320/O A/260/O A/30/CA A/120/CA A/90/CA A/440/O A/450/O A/10/CA A/400/O A/270/O A/430/O A/70/CA A/210/O A/100/CA A/480/O A/230/O A/390/O A/200/O A/50/CA A/80/CA A/280/O A/350/O A/340/O A/40/CA A/110/CA A/220/O A/360/O A/300/O A/460/O A/470/O

**Legend**

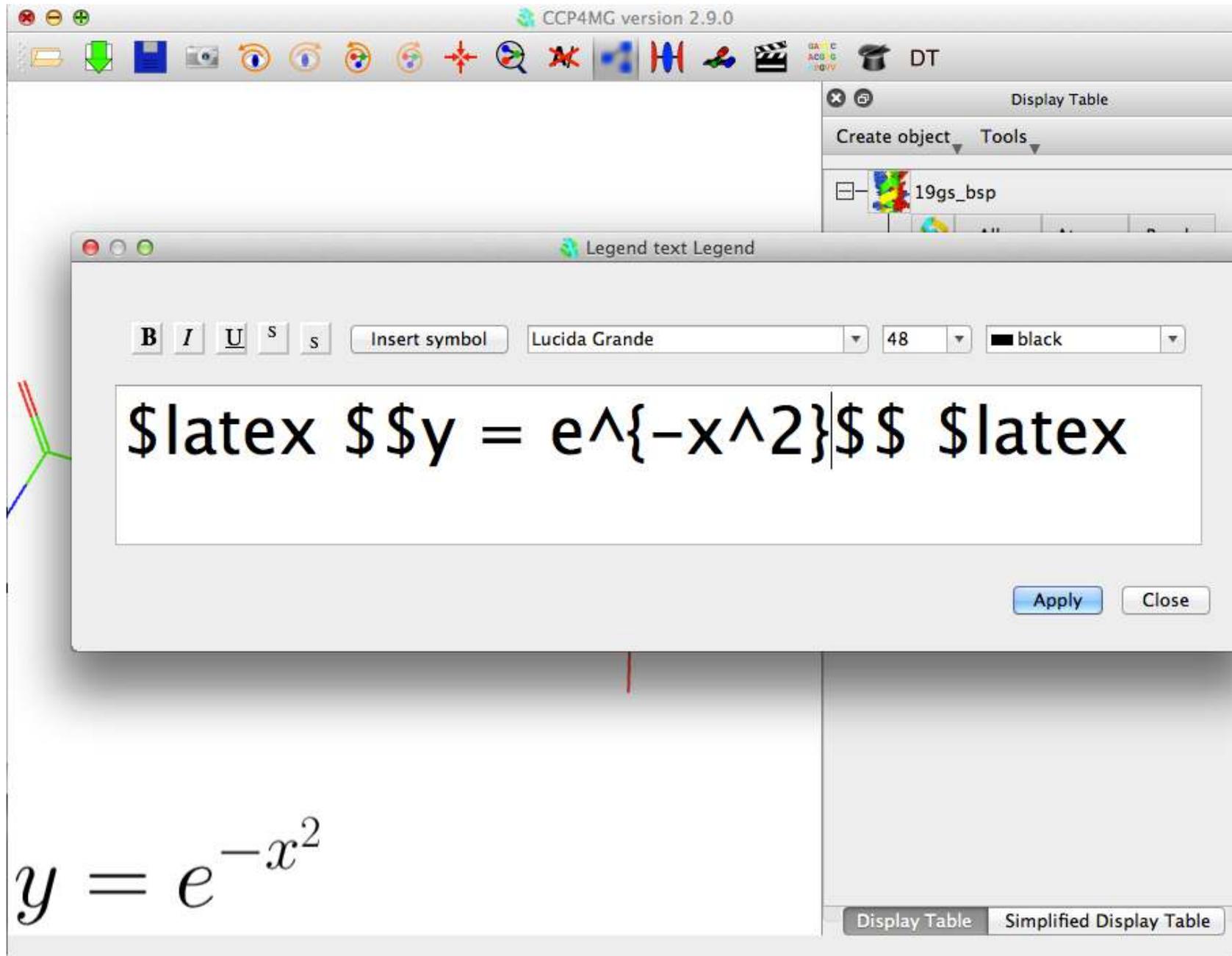
**Display Table**

Create object Tools

1eu5	All ..	Atom..	Bonds
A	Hoh ..	7.1 ..	

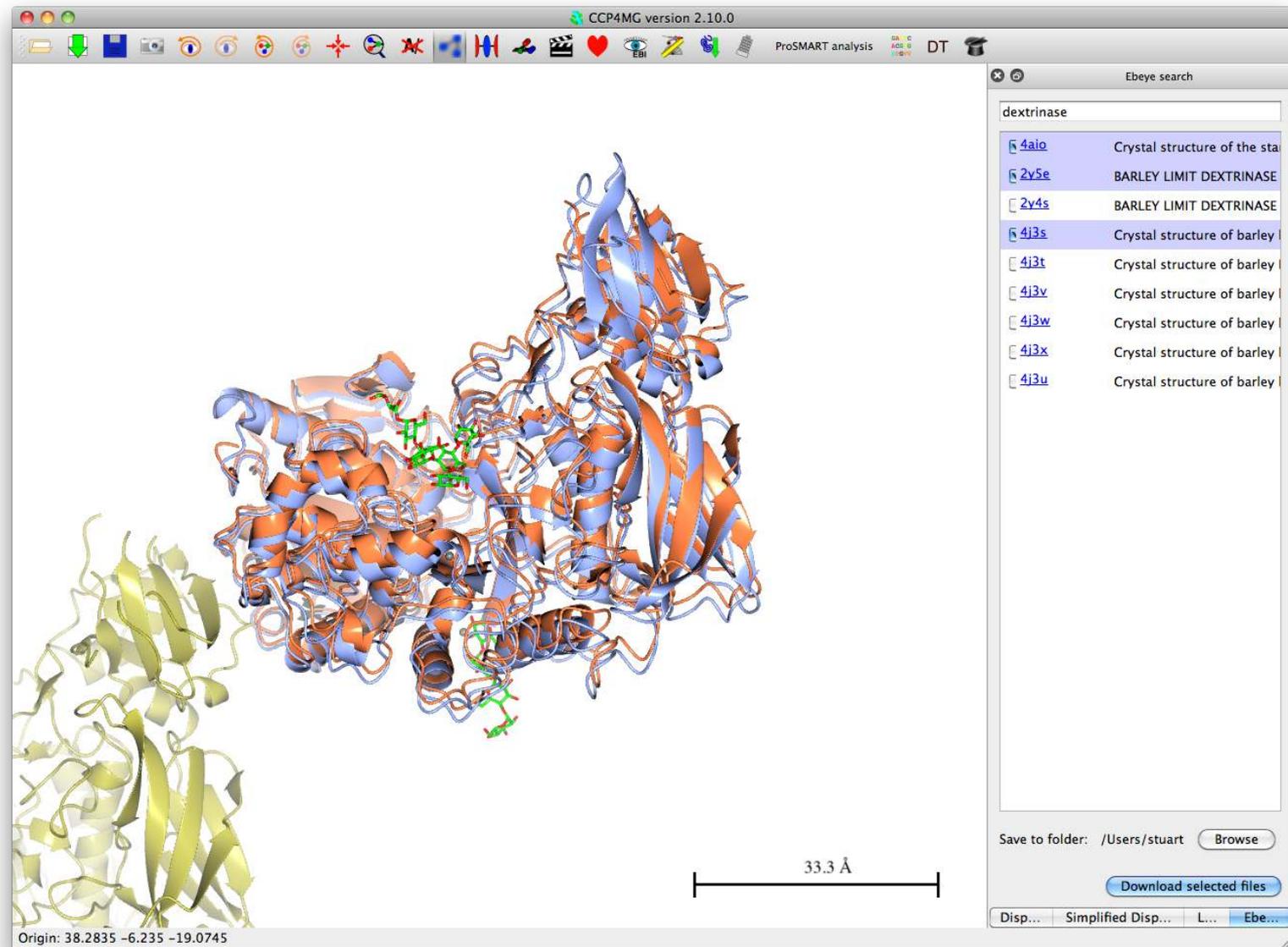
Legend	Legend	0.01..	
0.9100		0.64..	

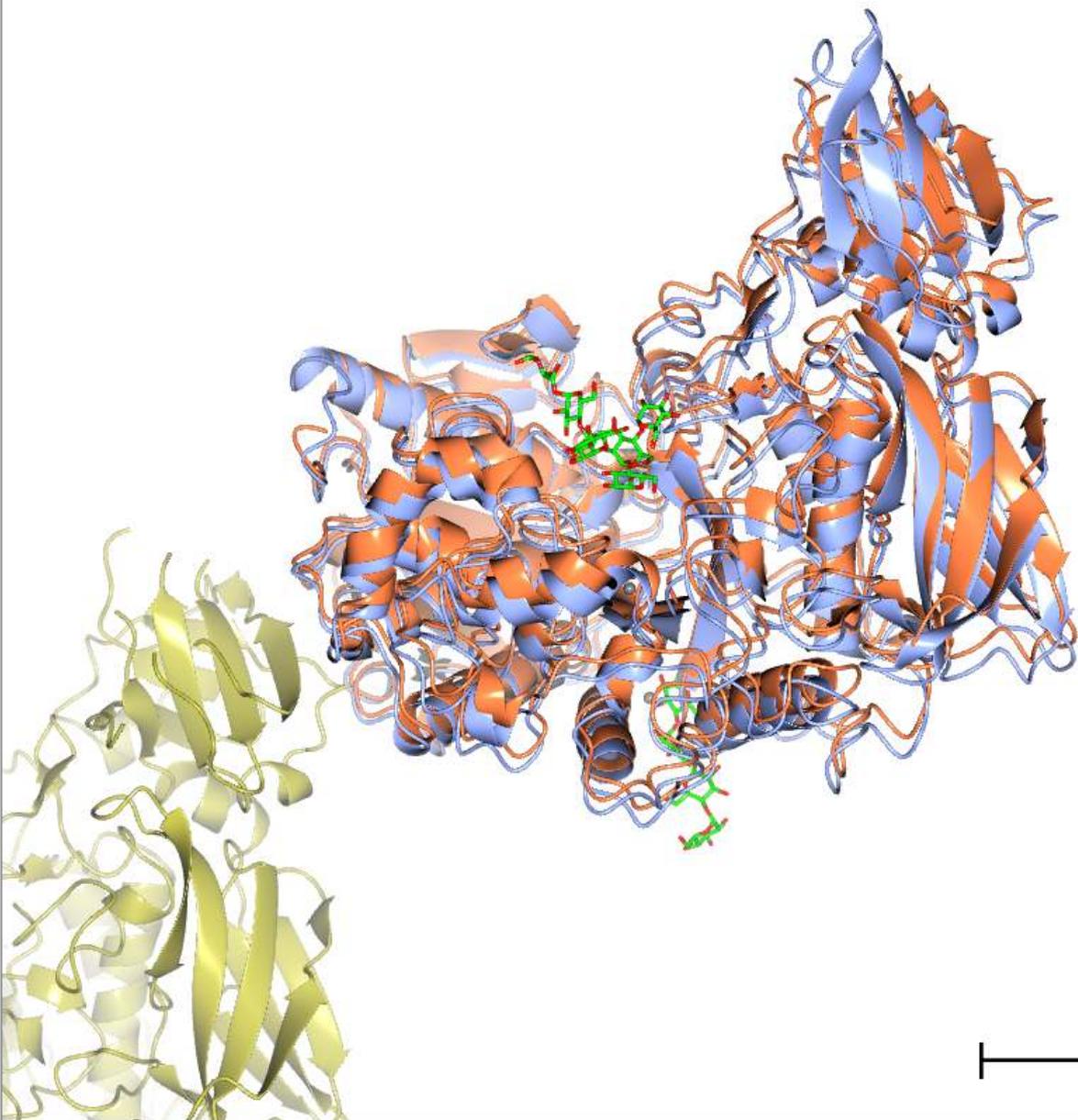
# On screen text and images



# Ebeye search

- Simple box to search ebeye.





Origin: 38.2835 -6.235 -19.0745

Ebeye search

dextrinase

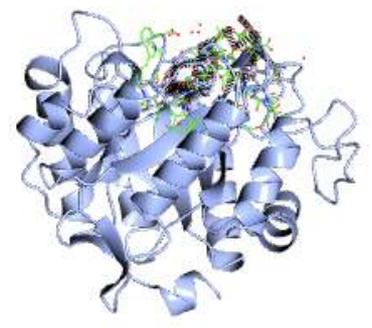
- [4aio](#) Crystal structure of the sta
- [2v5e](#) BARLEY LIMIT DEXTRINASE
- [2v4s](#) BARLEY LIMIT DEXTRINASE
- [4j3s](#) Crystal structure of barley l
- [4j3t](#) Crystal structure of barley l
- [4j3v](#) Crystal structure of barley l
- [4j3w](#) Crystal structure of barley l
- [4j3x](#) Crystal structure of barley l
- [4j3u](#) Crystal structure of barley l

Save to folder: /Users/stuart

Disp... Simplified Disp... L...

# 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.



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

<p>00003</p> <p>Record 4.00 secs</p> <p>View rotate abou</p> <p>Details</p>	<p>00004</p> <p>Record 4.00 secs</p> <p>View glid 000</p> <p>Details</p>	<p>00005</p> <p>..glide through.. for time proportio</p> <p>1.00</p>	<p>00006</p> <p>Record 4.00 secs</p> <p>View rock</p> <p>Details</p>
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Save snapshot here

- Action
- Edit
- Help

framerate: 15

# Getting CCP4MG

- Available from CCP4 download pages (next version 2.10.0 to be released with CCP4 6.5) or ...
- <http://www.ccp4.ac.uk/MG/download/>
- Available for Mac, Windows and Linux.
- Source code available for those who wish to try other operating systems.

# Acknowledgements

- Programming:

- Liz Potterton
- Eugene Krissinel
- Kevin Cowtan
- Paul Emsley
- Martin Noble
- Jan Gruber
- Bernhard Lohkamp
- Rob Nicholls
- Robbie Joosten

- General help:

Keith Wilson

Phil Evans

CCP4 staff: Eugene Krissinel, Charles Ballard, Ronan Keegan, Marcin Wojdyr, Andrey Lebedev, Ville Uski, David Waterman.

- Funding:

CCP4

Gwyndaf Evans and David Waterman for inviting me to speak