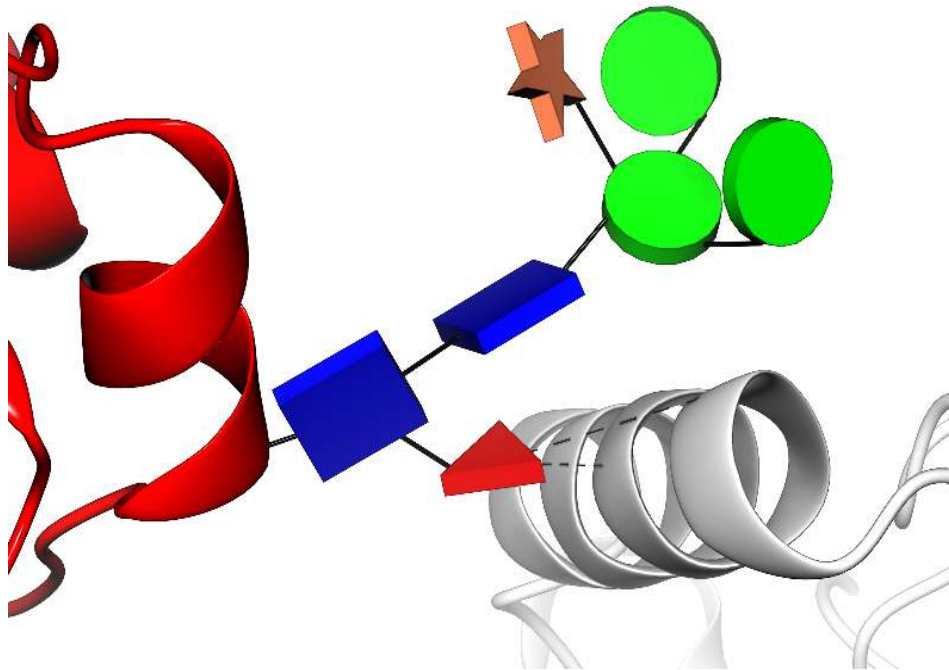


CCP4MG

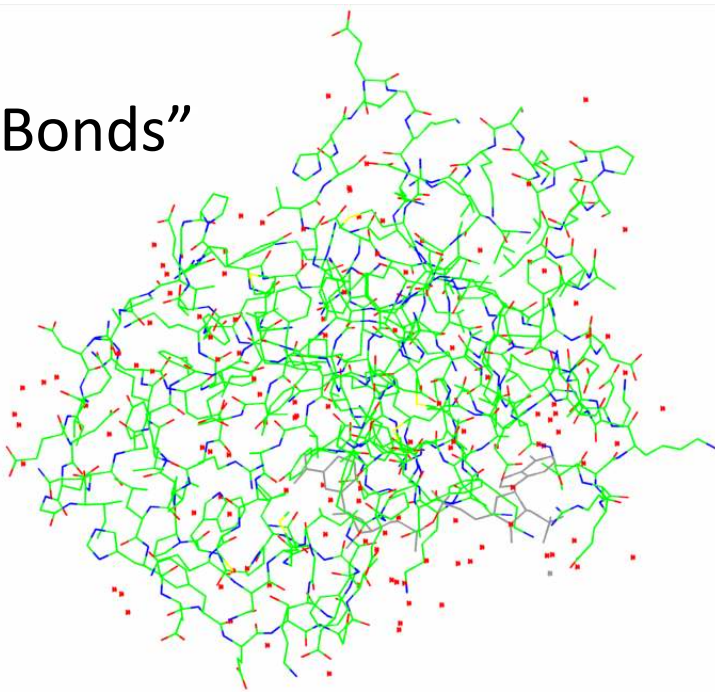


Diamond/CCP4 Workshop 2018

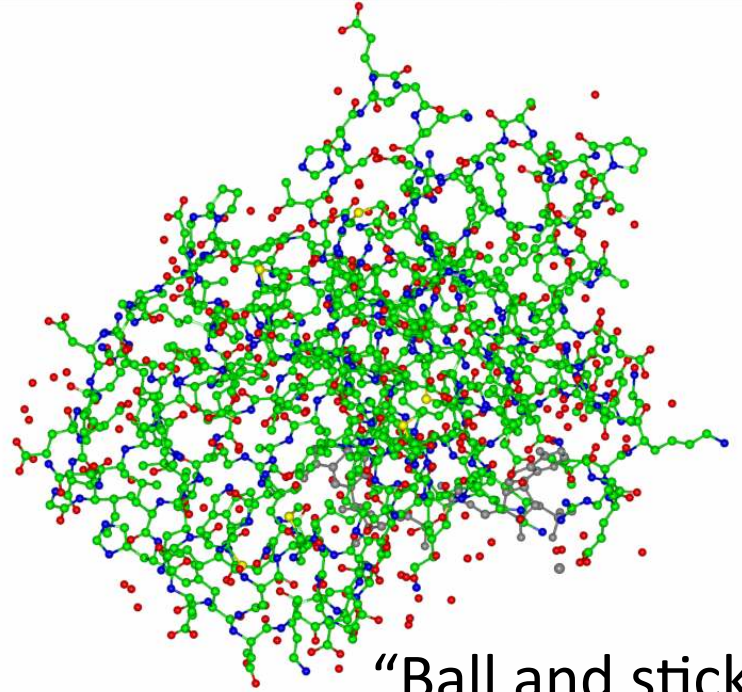
Introduction

- 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.
- Distributed as part of CCP4 and also:
 - <http://www.ccp4.ac.uk/MG/>
- Binaries for Windows, Mac and Linux.
- Source code freely available.

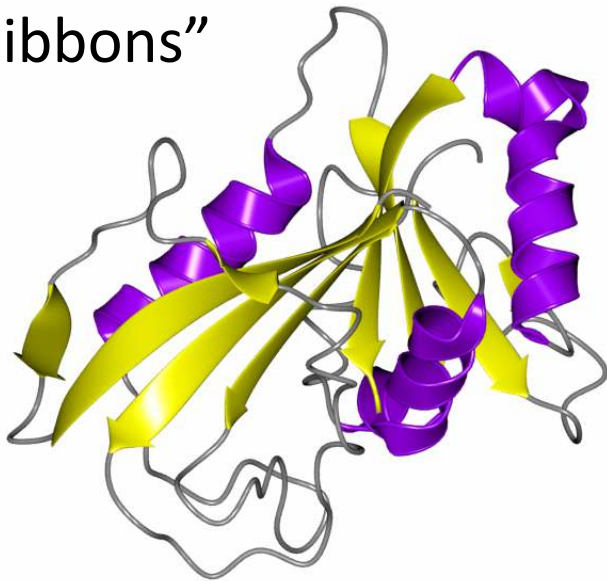
“Bonds”



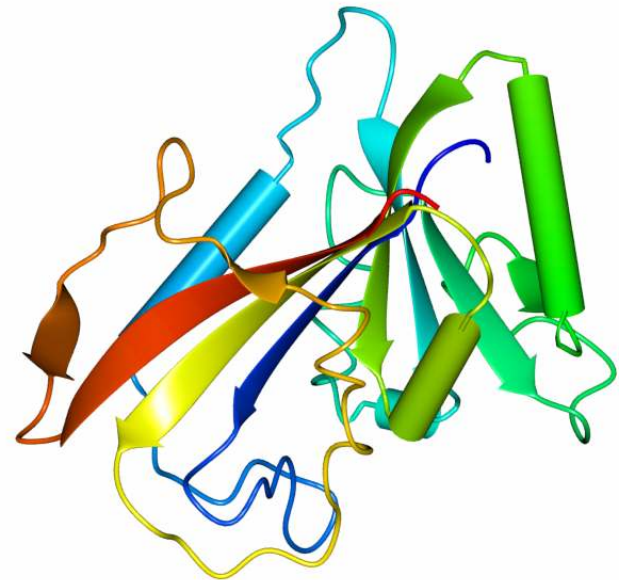
“Ball and stick”

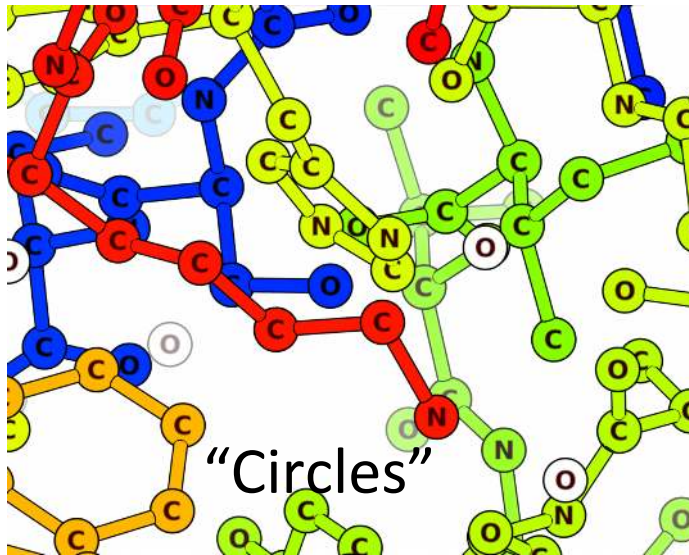


“Ribbons”

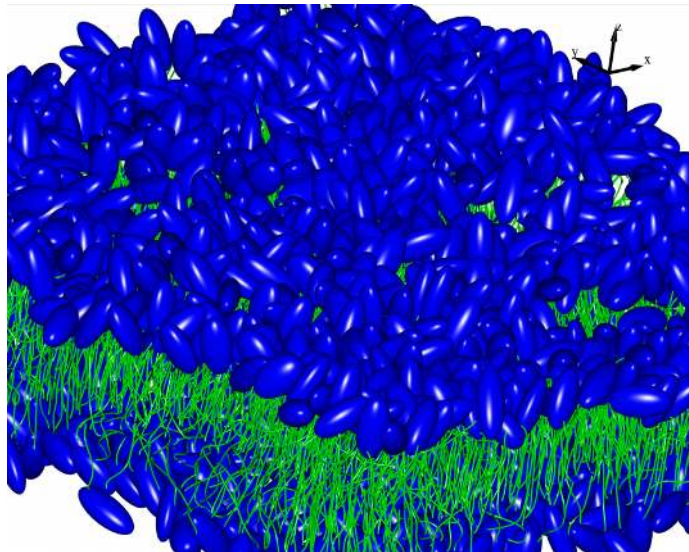
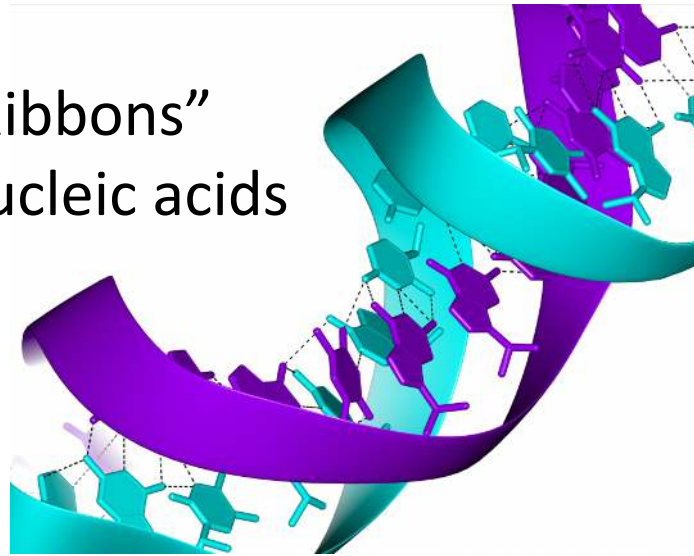


“Worms/tubes”

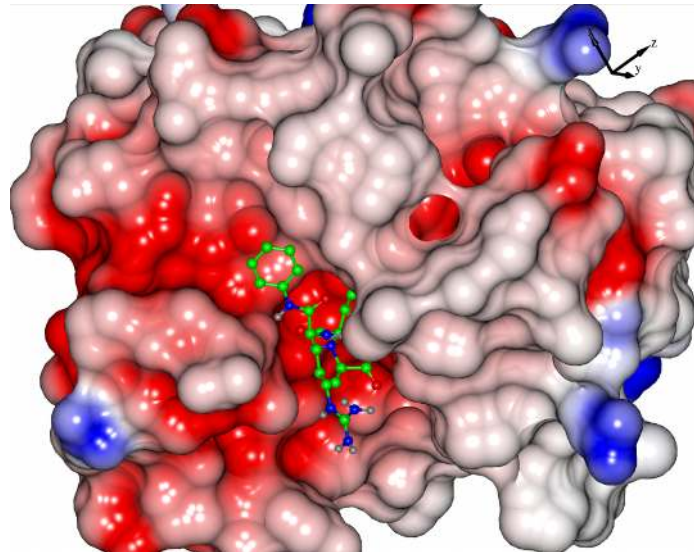




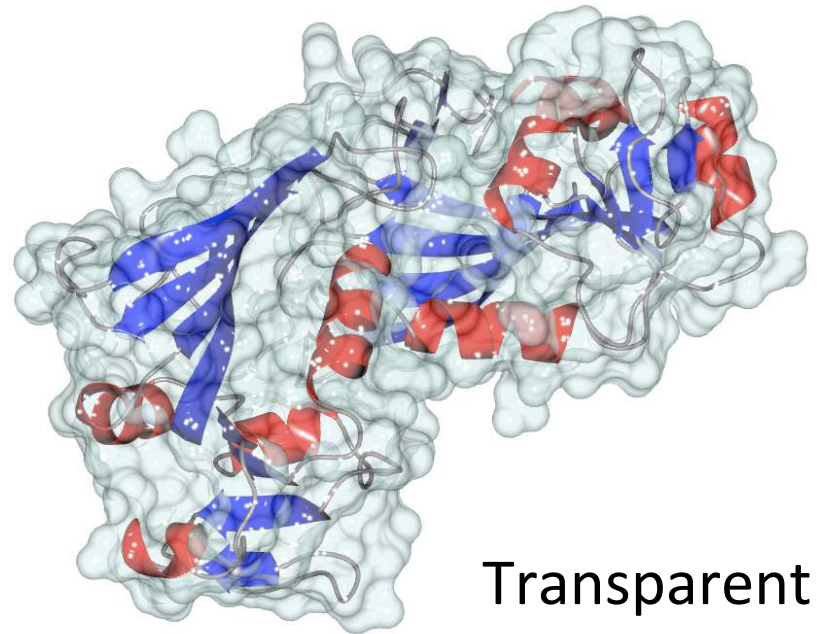
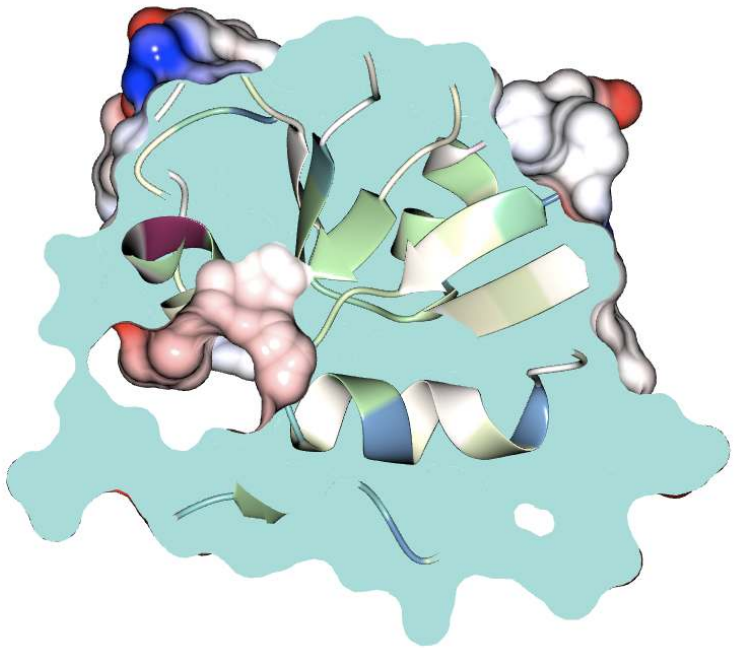
"Ribbons"
Nucleic acids



"Lipid Cartoon"

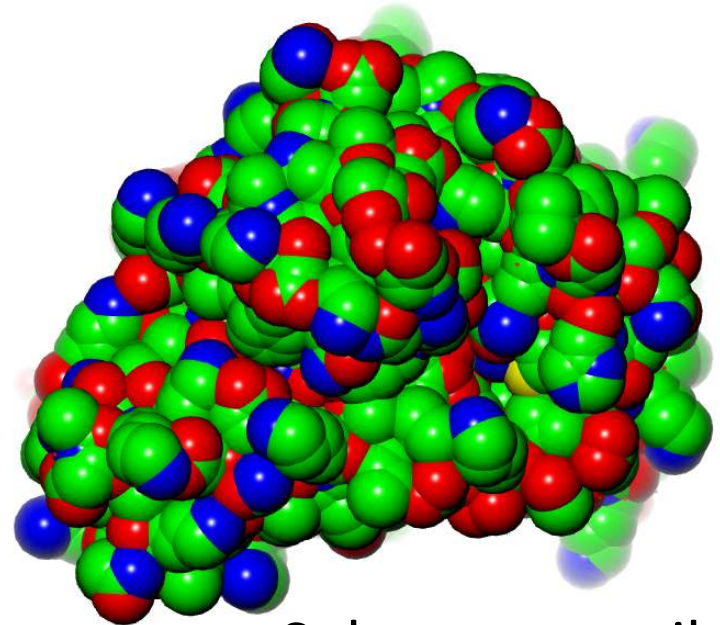
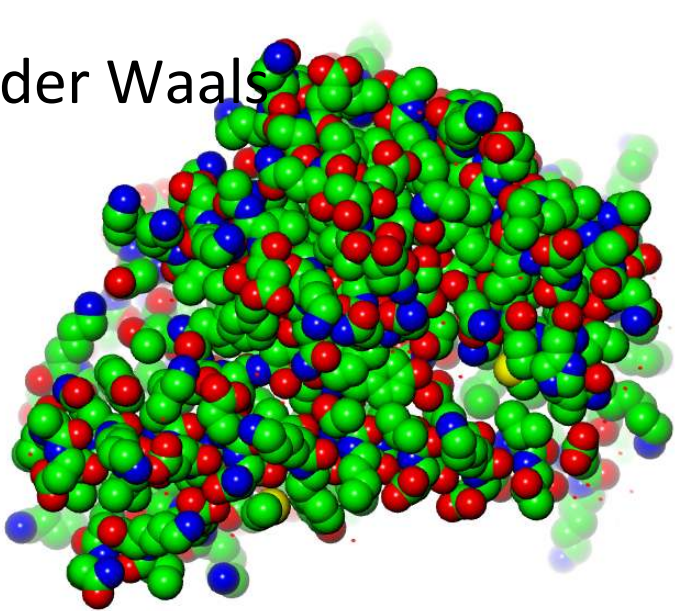


Electrostatic surface

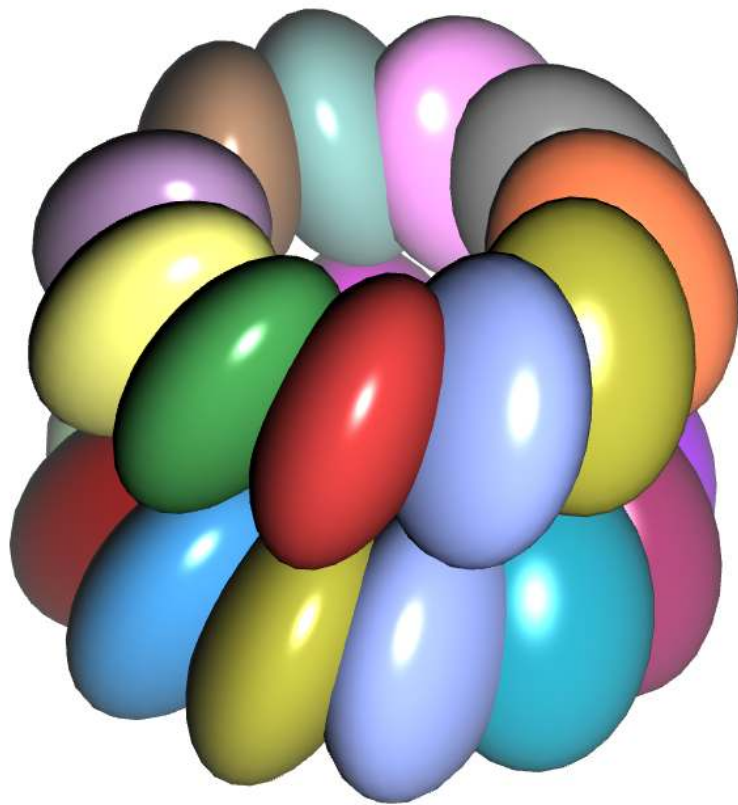


Transparent

Van der Waals

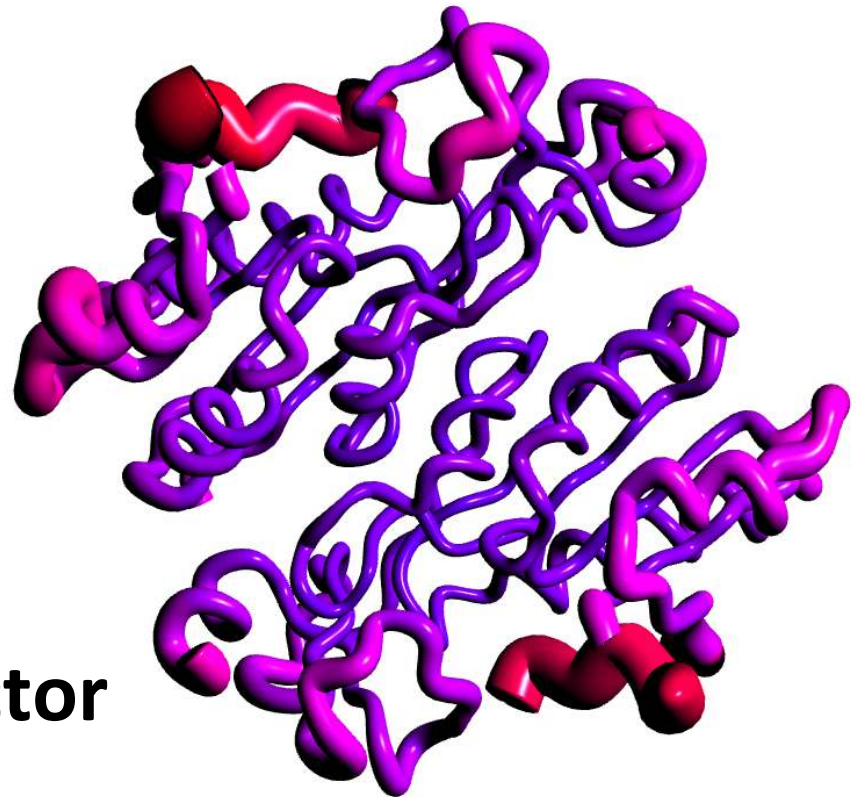


Solvent accessible



Bloboids

**Worm scaled by
Temperature factor**



Basic user Interface

CCP4MG version 2.7.1

Drawing style

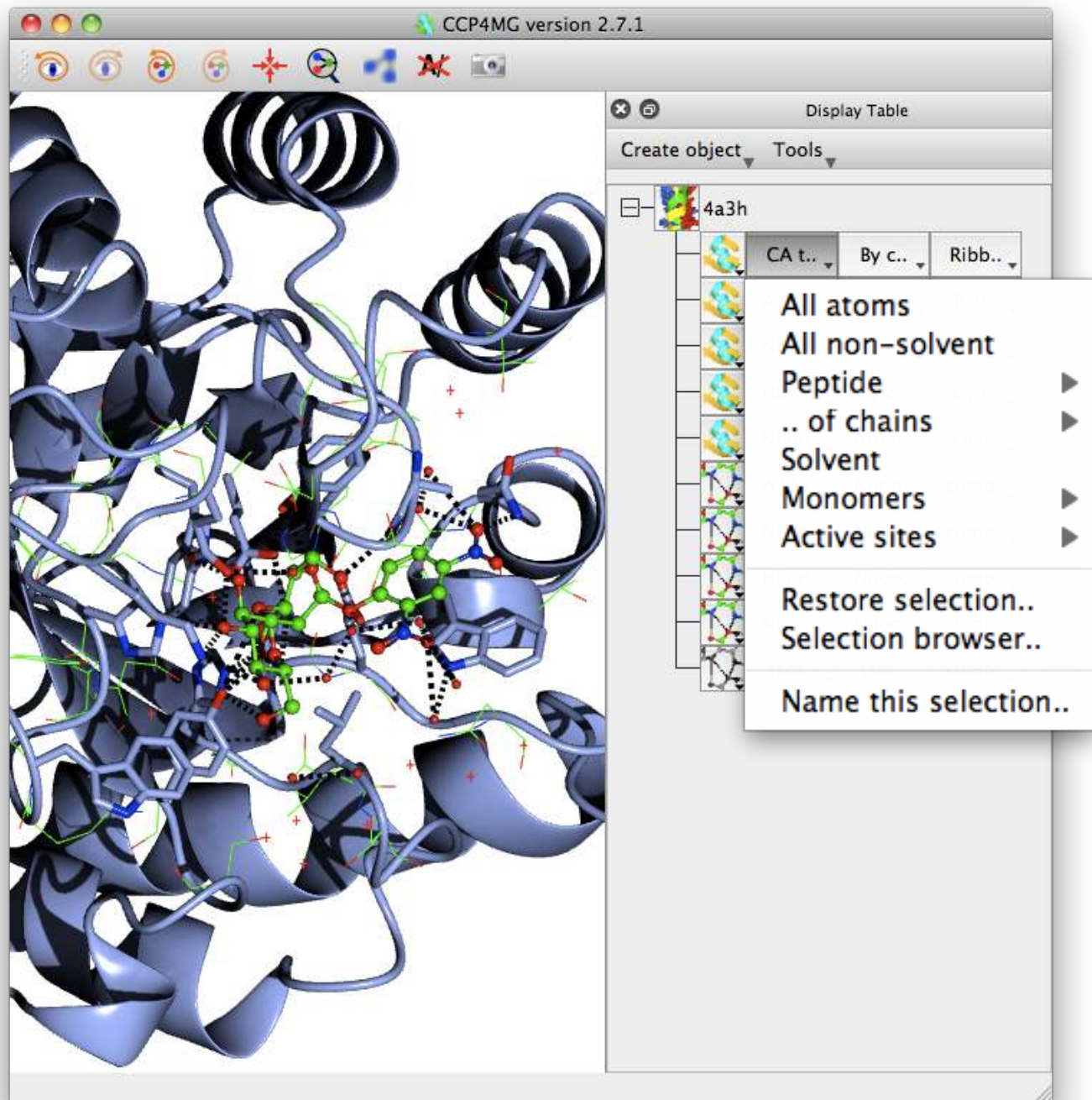
Colour

Atom selection

Data object

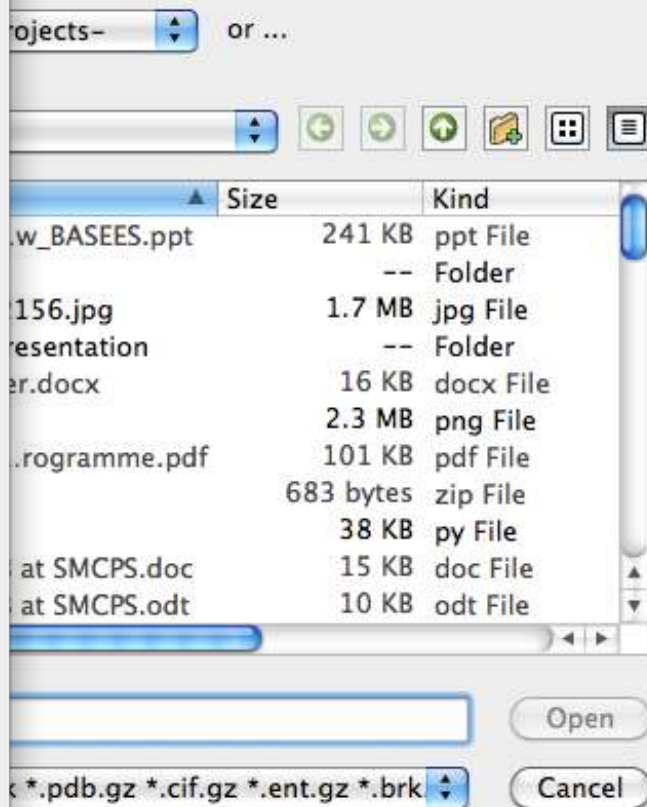
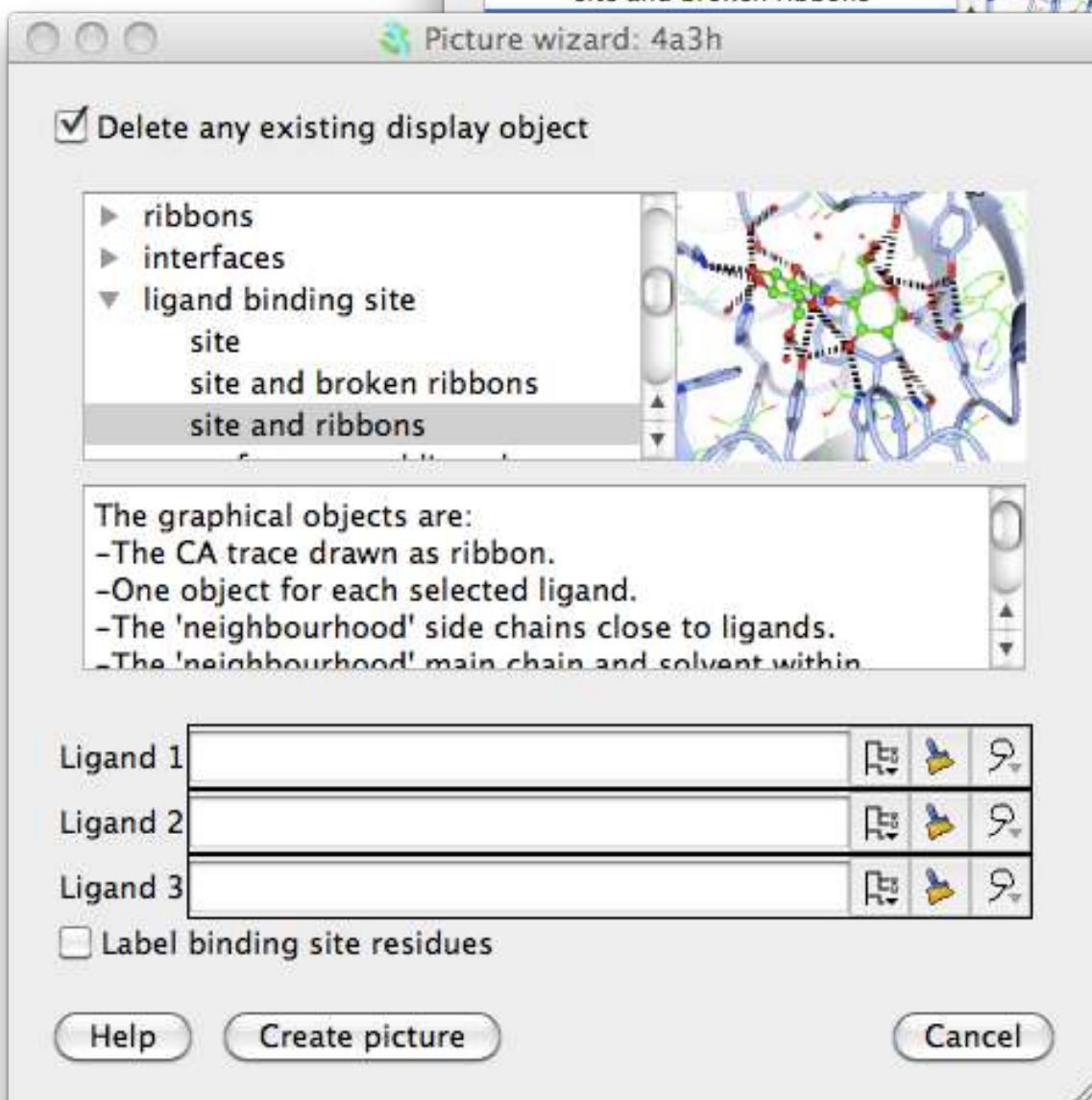
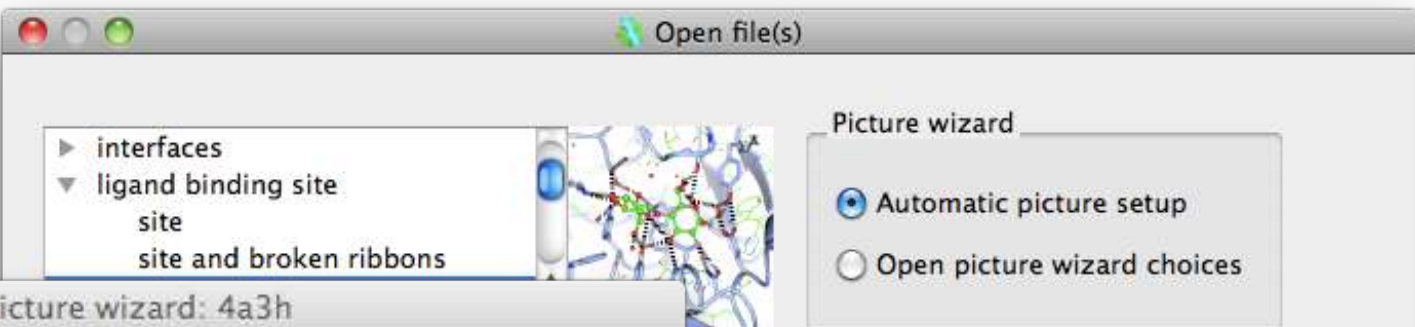
Display object

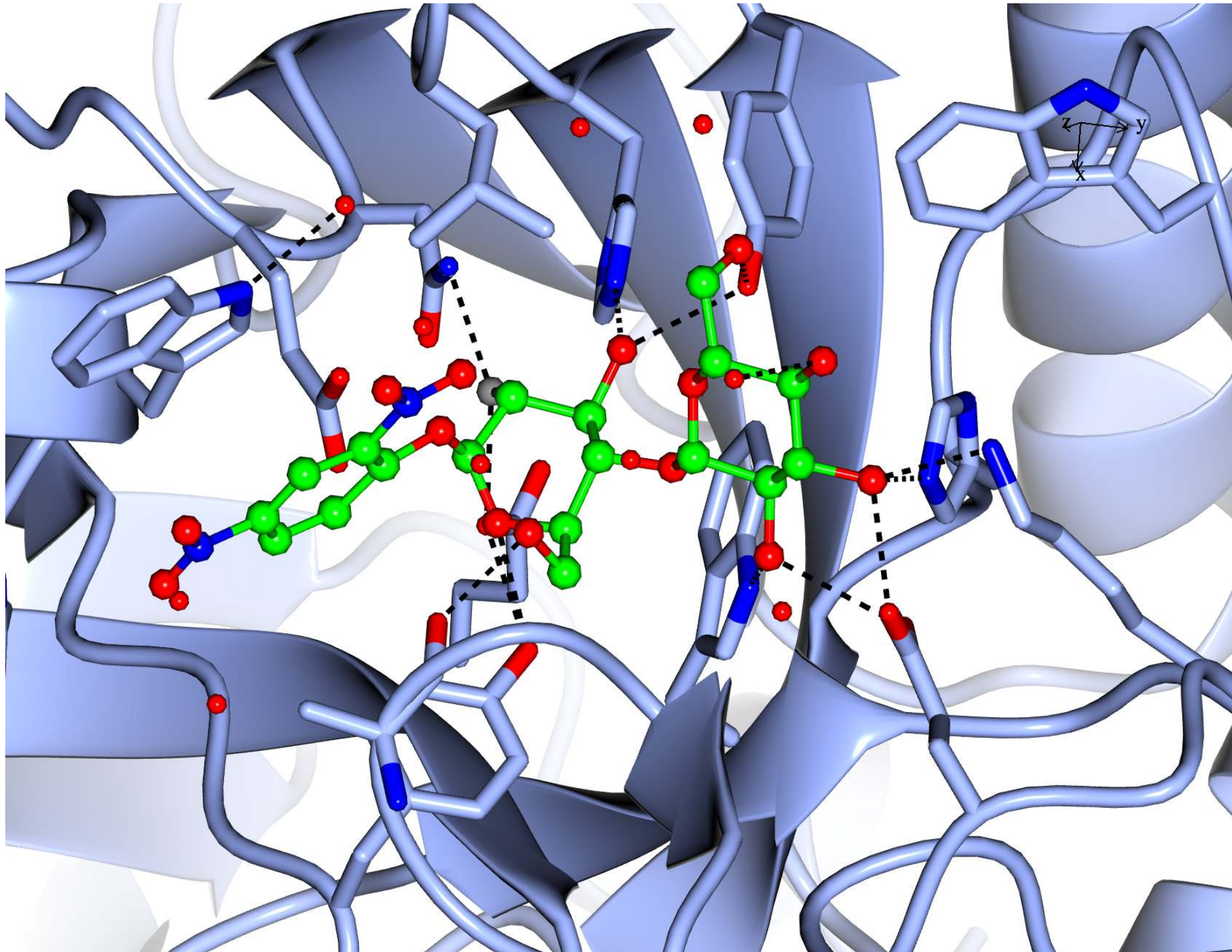
	CA t..	By c..	Ribb..
A/30..	Atom..	Ball..	
Nhoo..	By c..	Cyli..	
HBon..	By c..	Cyli..	
Nhoo..	Atom..	Thin..	
A/30..	Nhoo..	comp..	
Nhoo..	Nhoo..	comp..	
HBon..	Nhoo..	comp..	
Nhoo..	Nhoo..	comp..	
{sol..	{sol..	comp..	

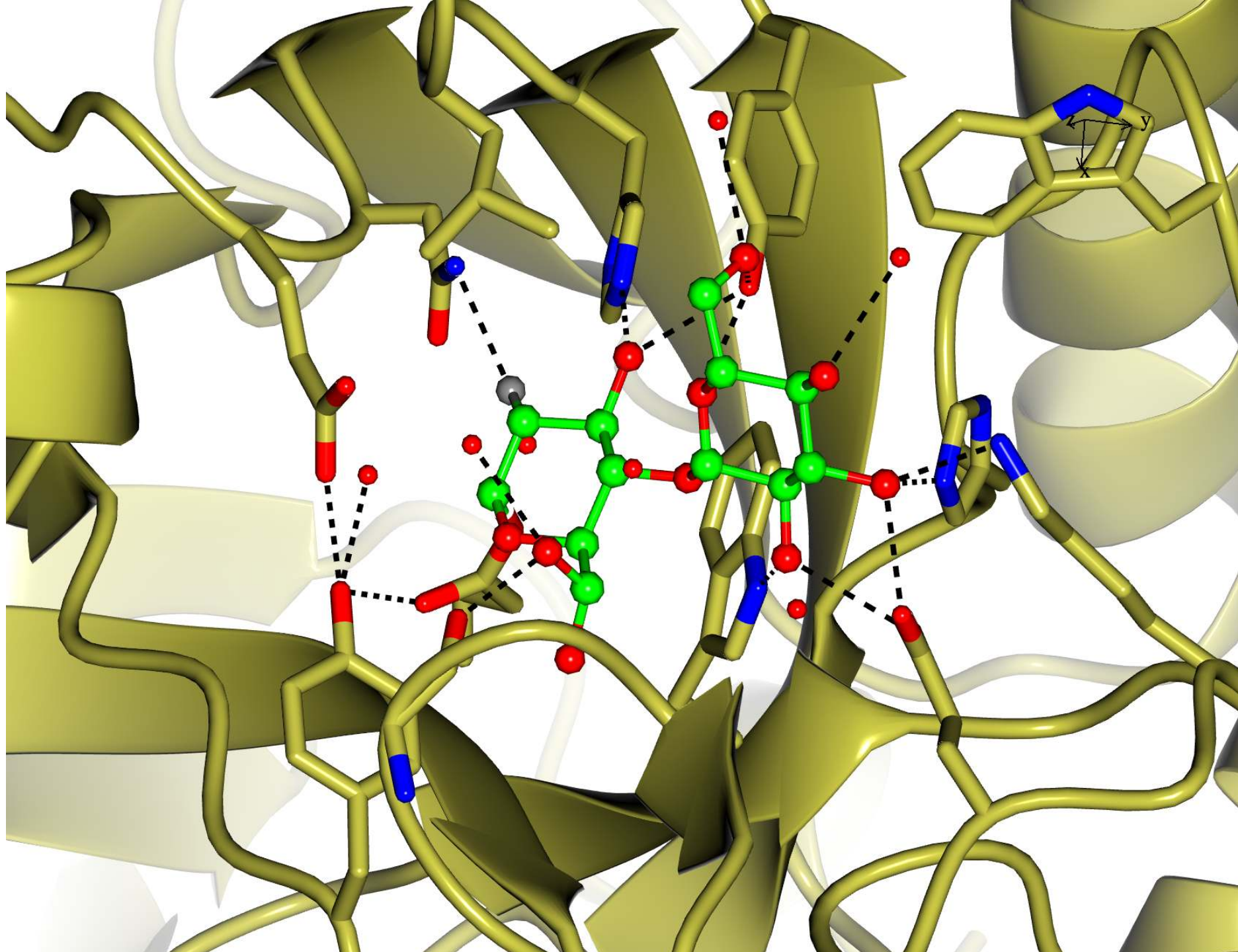


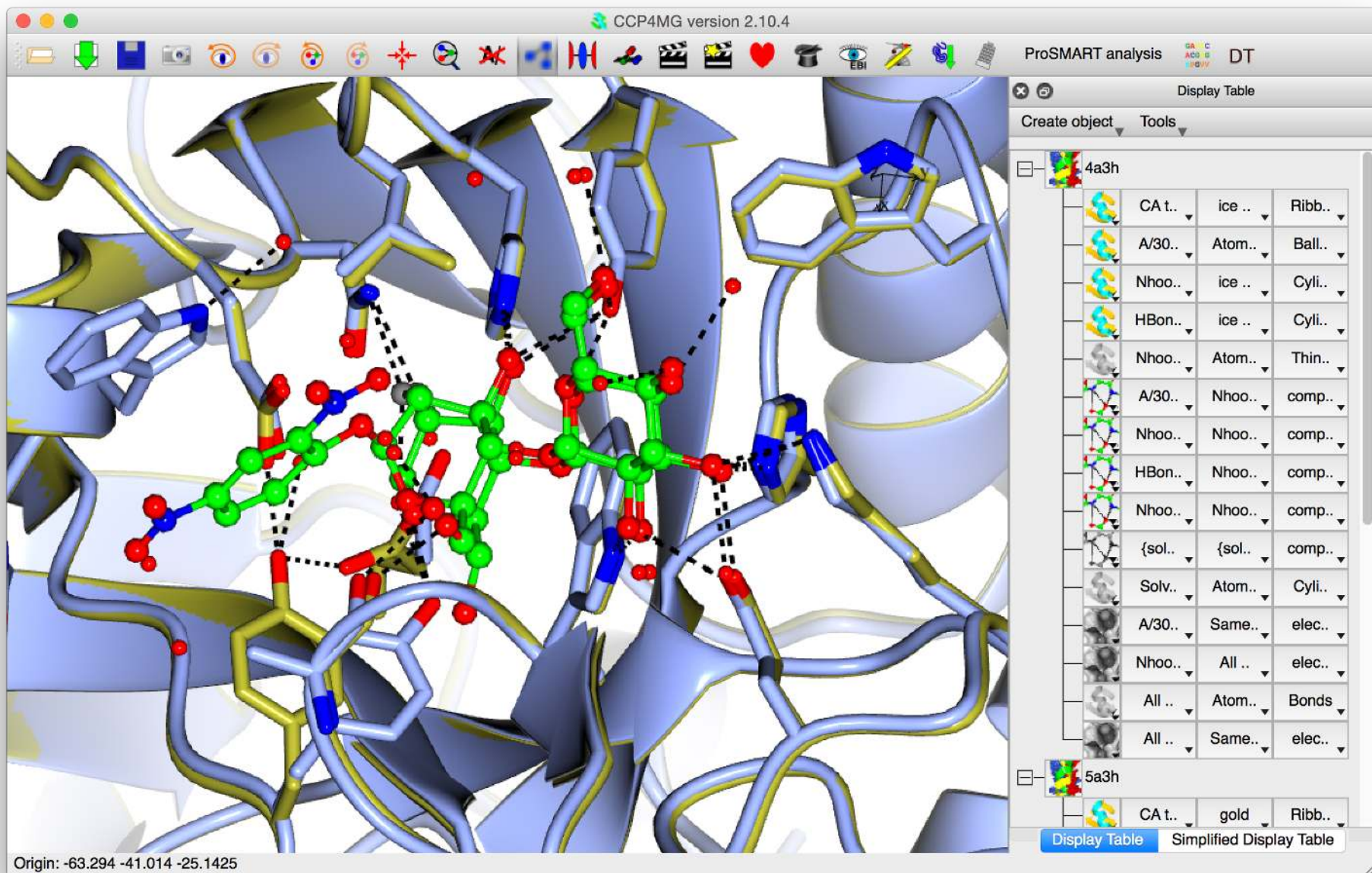
Picture Wizard

- 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.

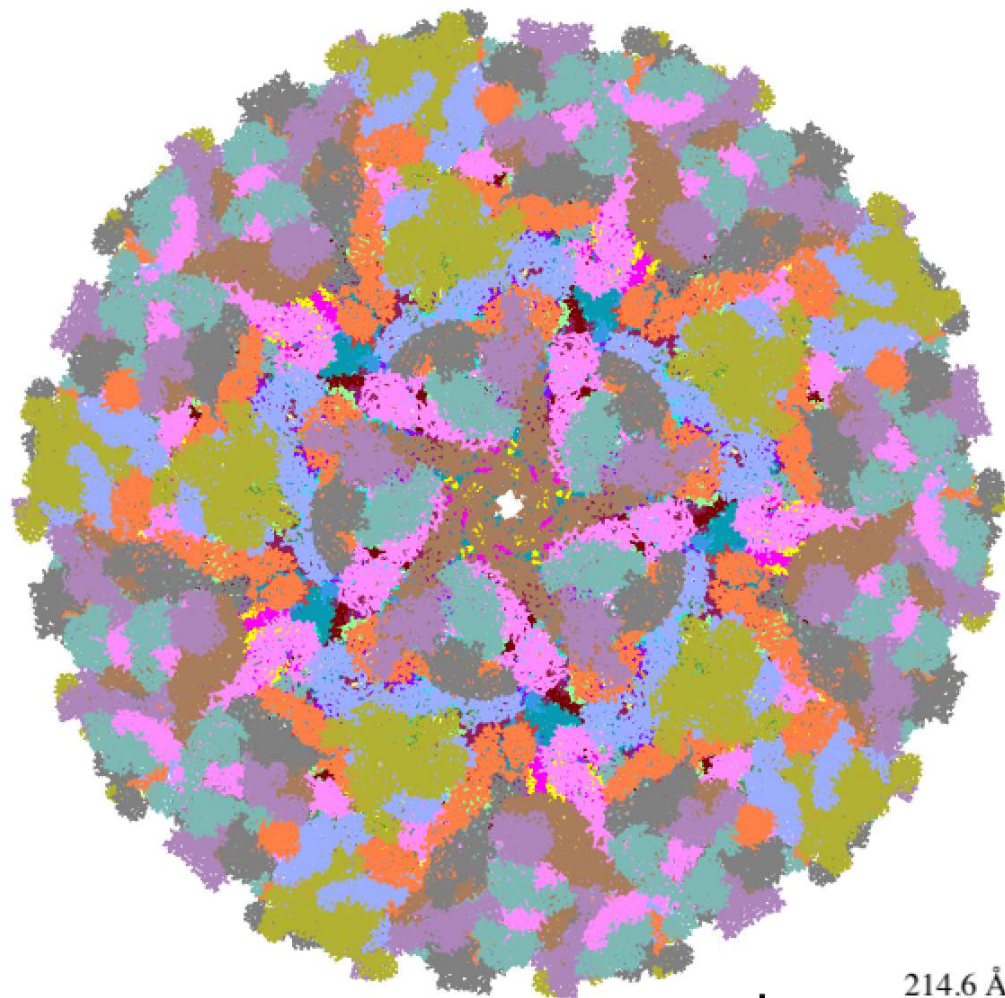








Doing it all Manually



214.6 Å

Display Table

Create object Tools

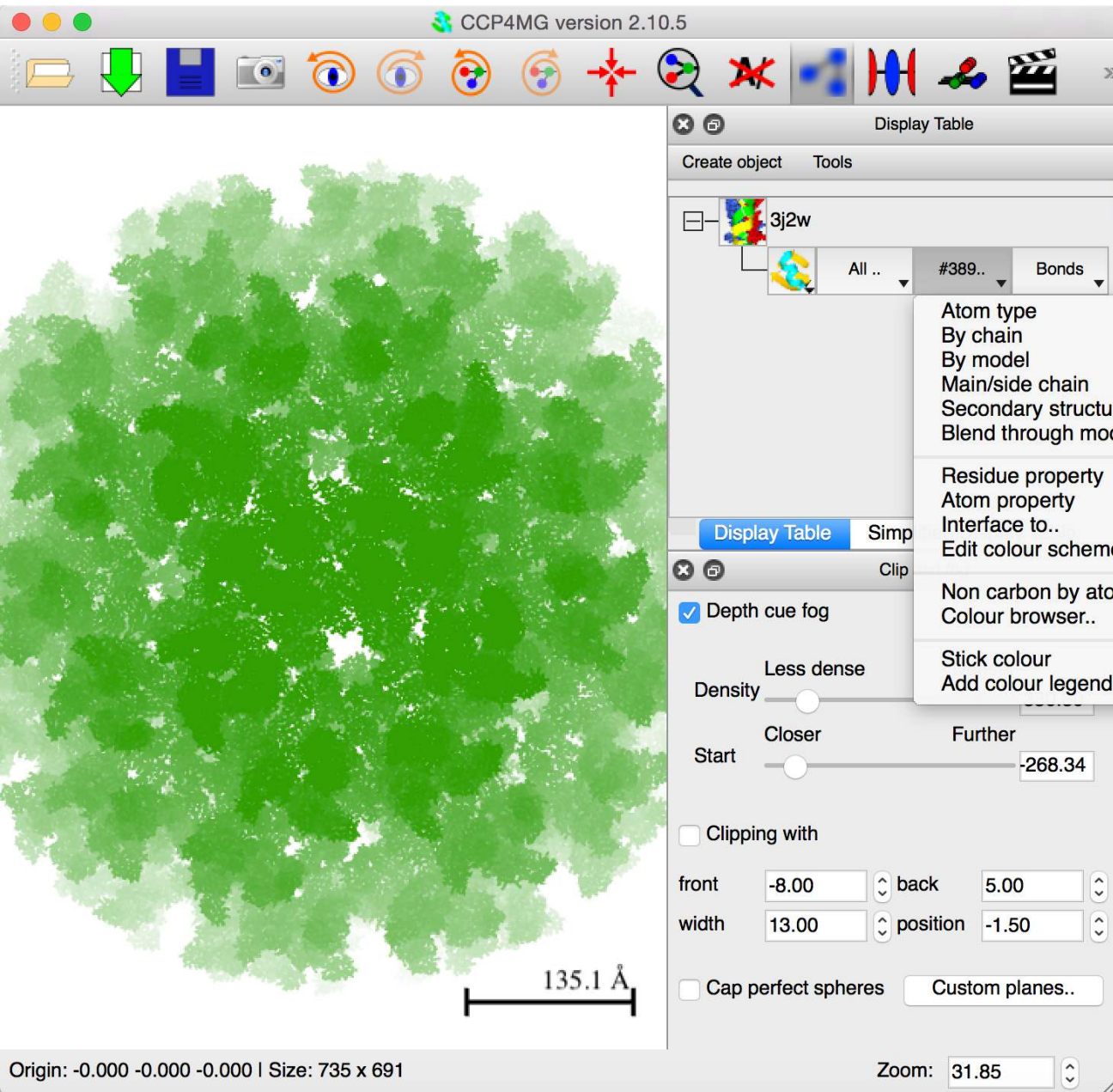
3j2w

☒ Visible
Centre on
 Picture wizard..
Copy picture style from..
Add model display object
Add display object
File save/restore
List data
Structure definition
Transform coordinates
Generate symmetry mates..
Create crystal object
Animation
Clone
Delete

Surface
HBonds
Contacts
Annotation

Display Table Simplified Display Table

Zoom: 31.85



gonnet p... Saving HTML... What's N...

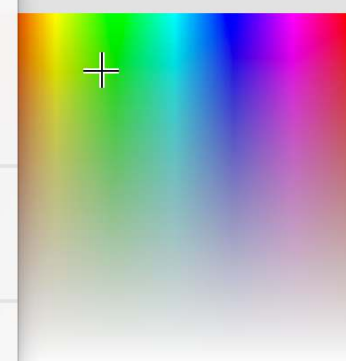
craft pi punch

Register

Stuart

Colour Browser

Main colours Create colours



Hue: 106 Red: 56

Sat: 214 Green: 157

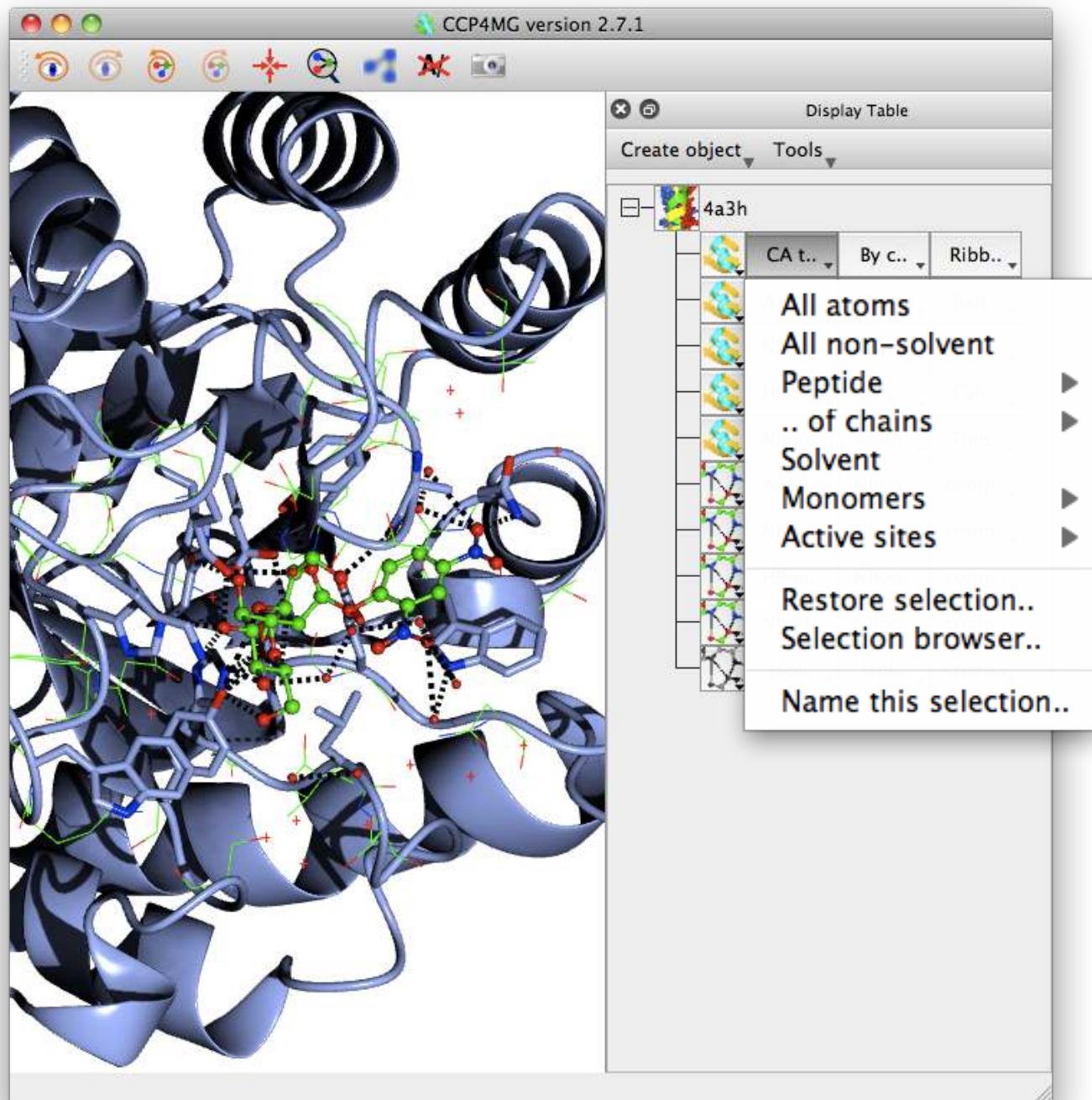
Val: 157 Blue: 25

Grab colour from screen

Save colour

Selected colour #389D19

Clear Apply Cancel OK





Display Table

Object Tools

3j2w

All ..

By c..

Bonds

Select from 3j2w

Replace (NEW) current selection by residue types

☐ Glycine	Hydrophilic	Clear
☐ Alanine	Large	Select all
☐ Valine	Basic	
☐ Proline	Small	
☐ Serine	Acidic	
☐ Threonine	Hydrophobic	Apply
☐ Leucine		
☐ Isoleucine		
☐ Cysteine		
☐ Aspartic acid		
☐ Glutamic acid		

Show all of..

▼ Peptide

- ▼ A/
 - ▶ A/1(TYR)
 - ▶ A/2(GLU)
 - ▶ A/3(HIS)

peptide

Help Clear Apply Save Close

214.6 Å

Display Table

Simplified Display Table

Zoom: 31.85

The screenshot displays the CCP4MG version 2.10.5 software interface. On the left, a large, multi-colored protein structure is visible. A scale bar at the bottom indicates a distance of 214.6 Å. The top toolbar contains various icons for file operations, viewing, and analysis. A 'Select from' dialog box is open, showing options for selecting residues and their neighbors. The 'neighbours' option is selected in the dropdown menu. The 'Include' section shows 'non-Hbonding groups' checked. The 'Show' section shows 'all' of the selected items. The 'Peptide' section lists 'A/1(TYR)', 'A/2(GLU)', and 'A/3(HIS)'. The 'peptide' section is empty. The 'Display Table' panel on the right shows the '3j2w' object and various display options. The status bar at the bottom shows the origin coordinates (-0.000 -0.000 -0.000) and the image size (1000 x 698).

saved selection
interactive selection
✓ neighbours
buried area
atomic elements
residue types
residue ranges
secondary structure elements
properties (eg temp factor)
NMR/symmetry models

Replace (NEW) current selection b
Select residues within 4.0
3j2w
Include
☐ the central selection
☒ non-Hbonding groups
☒ solvent
Select neighbours

Show all of..
▼ Peptide
▼ A/
▶ A/1(TYR)
▶ A/2(GLU)
▶ A/3(HIS)
peptide

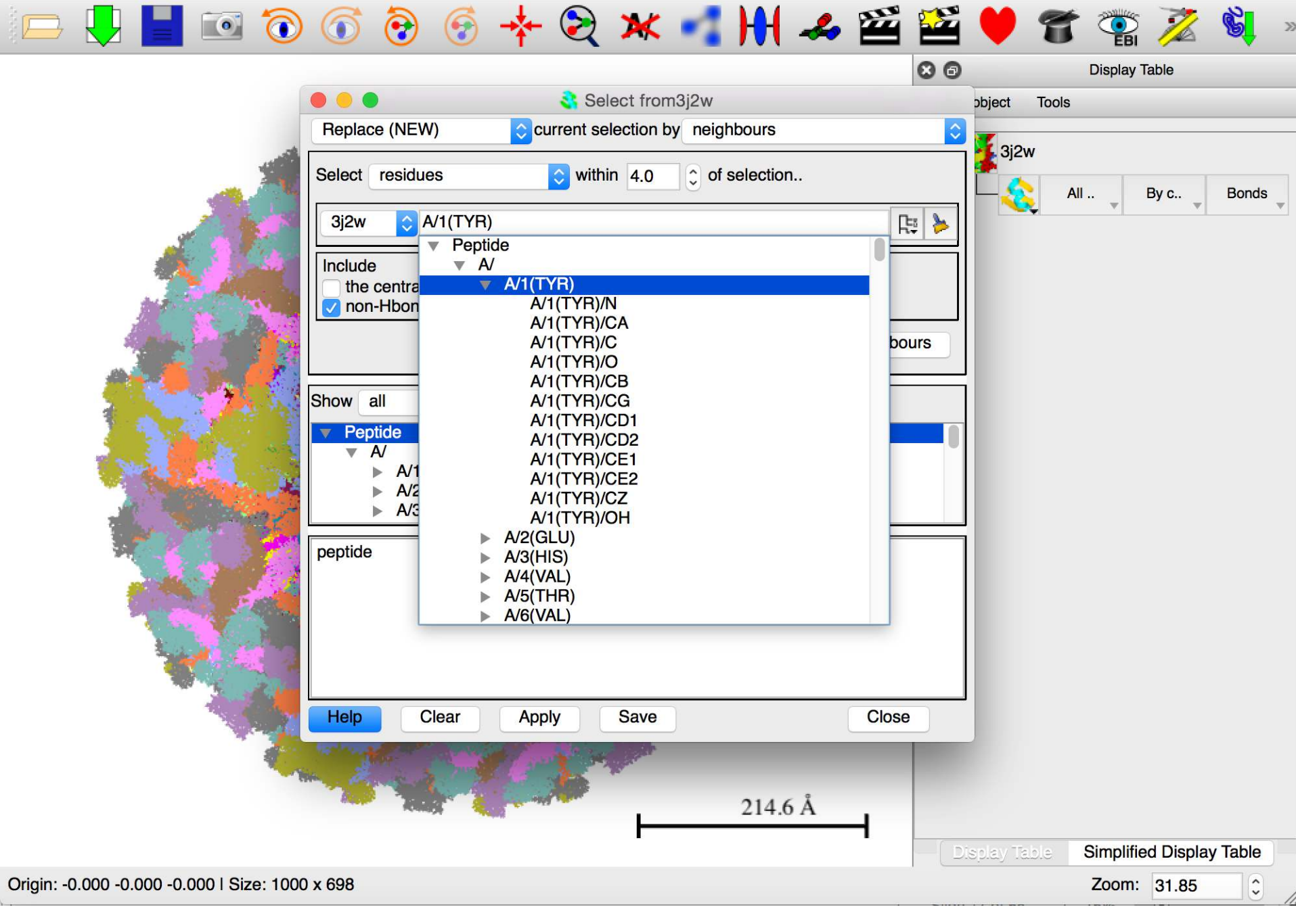
Help Clear Apply Save Close

214.6 Å

Display Table Simplified Display Table

Zoom: 31.85

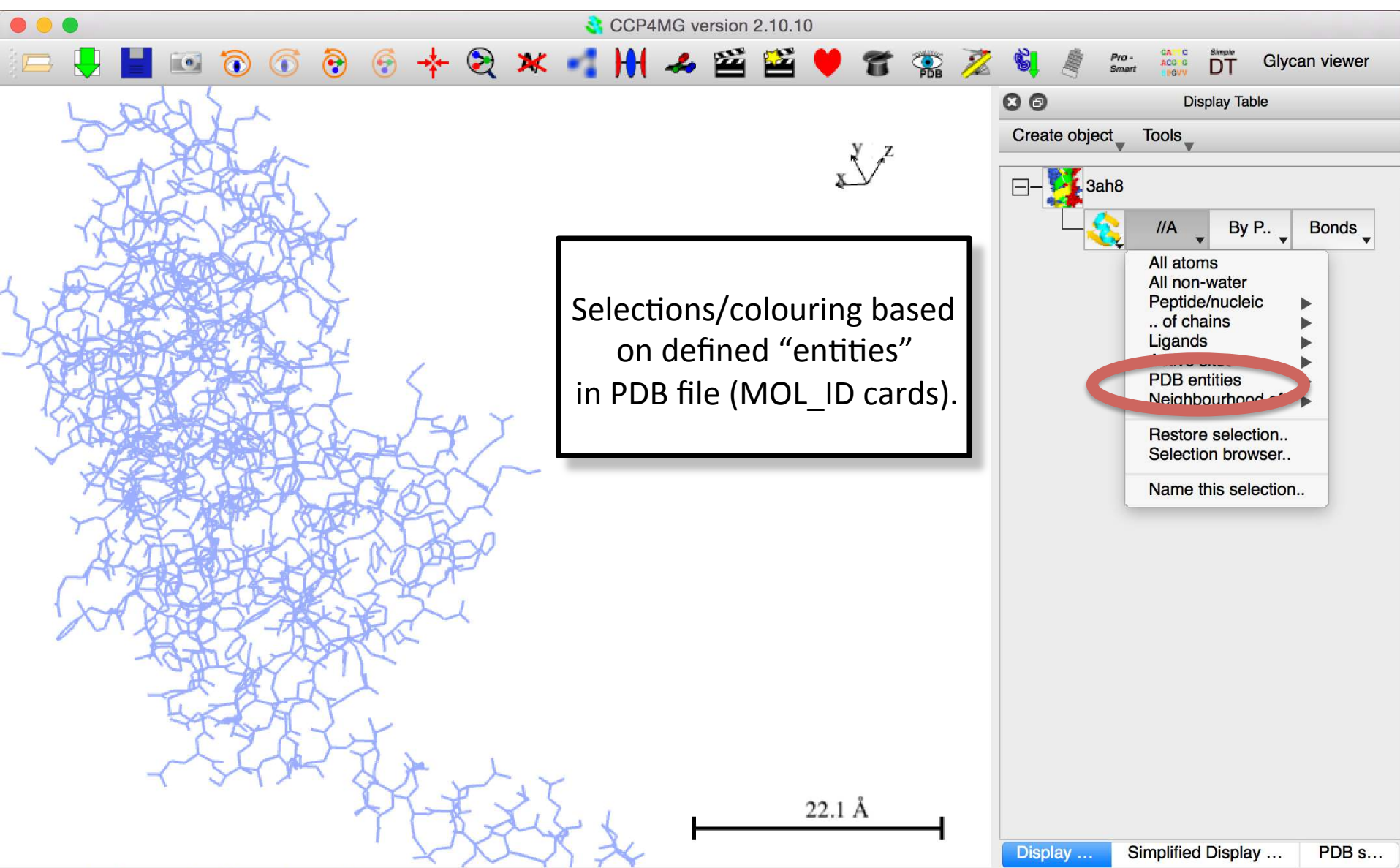
Origin: -0.000 -0.000 -0.000 | Size: 1000 x 698



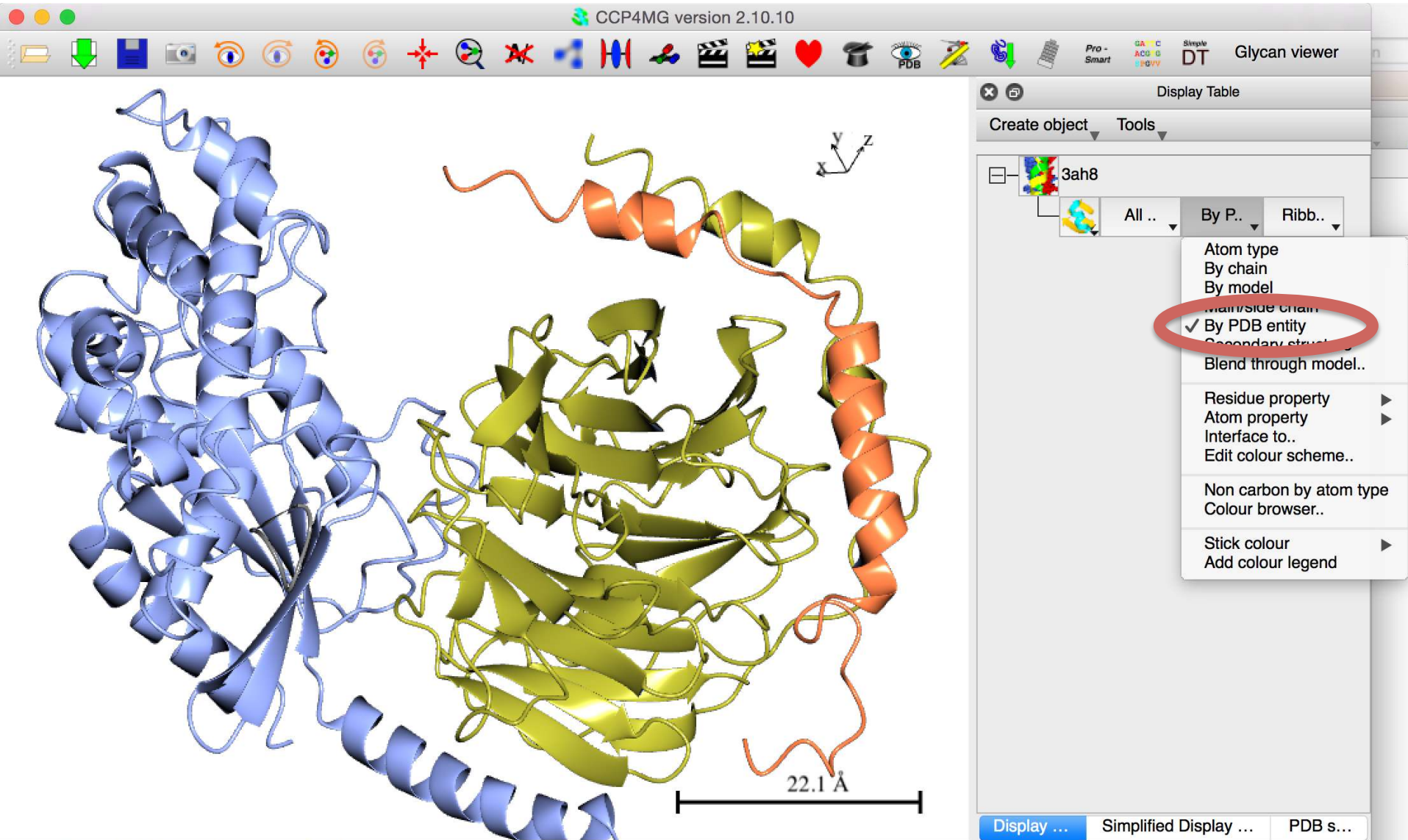
PDB Entities

```
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: RESPONSE REGULATOR RECEIVER DOMAIN PROTEIN;
COMPND      3 CHAIN: A, B;
COMPND      4 FRAGMENT: DNA BINDING DOMAIN;
COMPND      5 ENGINEERED: YES;
COMPND      6 MOL_ID: 2;
COMPND      7 MOLECULE: DNA (5'-
COMPND      8 D(P*GP*GP*AP*CP*TP*TP*AP*AP*GP*AP*AP*CP*GP*AP*TP*TP*T)-3');
COMPND      9 CHAIN: G;
COMPND     10 ENGINEERED: YES;
COMPND     11 MOL_ID: 3;
COMPND     12 MOLECULE: DNA (5'-D(P*TP*TP*CP*TP*TP*AP*AP*GP*TP*CP*C)-3');
COMPND     13 CHAIN: H;
COMPND     14 ENGINEERED: YES;
COMPND     15 MOL_ID: 4;
COMPND     16 MOLECULE: DNA (5'-D(P*AP*AP*AP*TP*CP*G)-3');
COMPND     17 CHAIN: C;
COMPND     18 ENGINEERED: YES
```

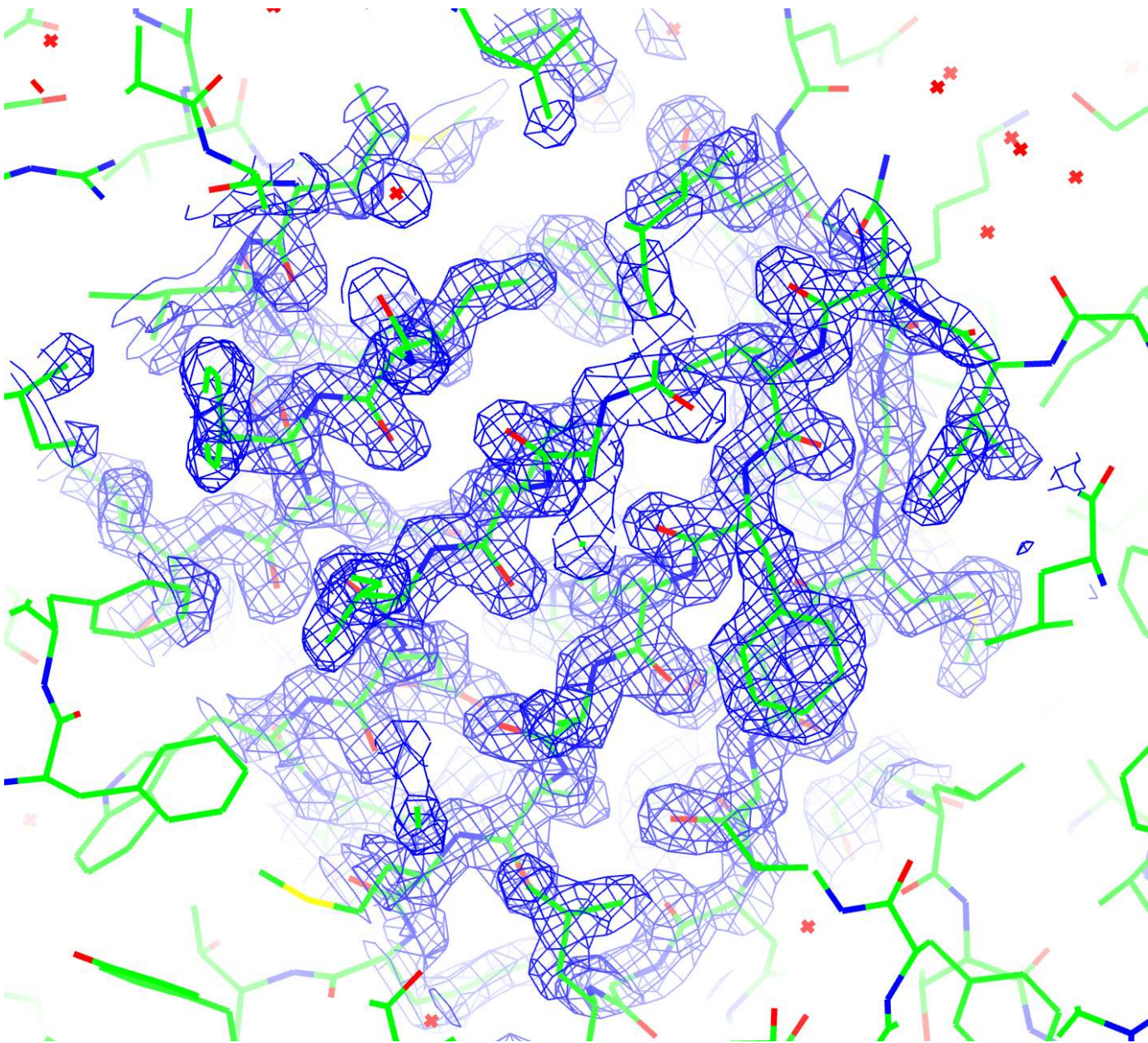
PDB Entities

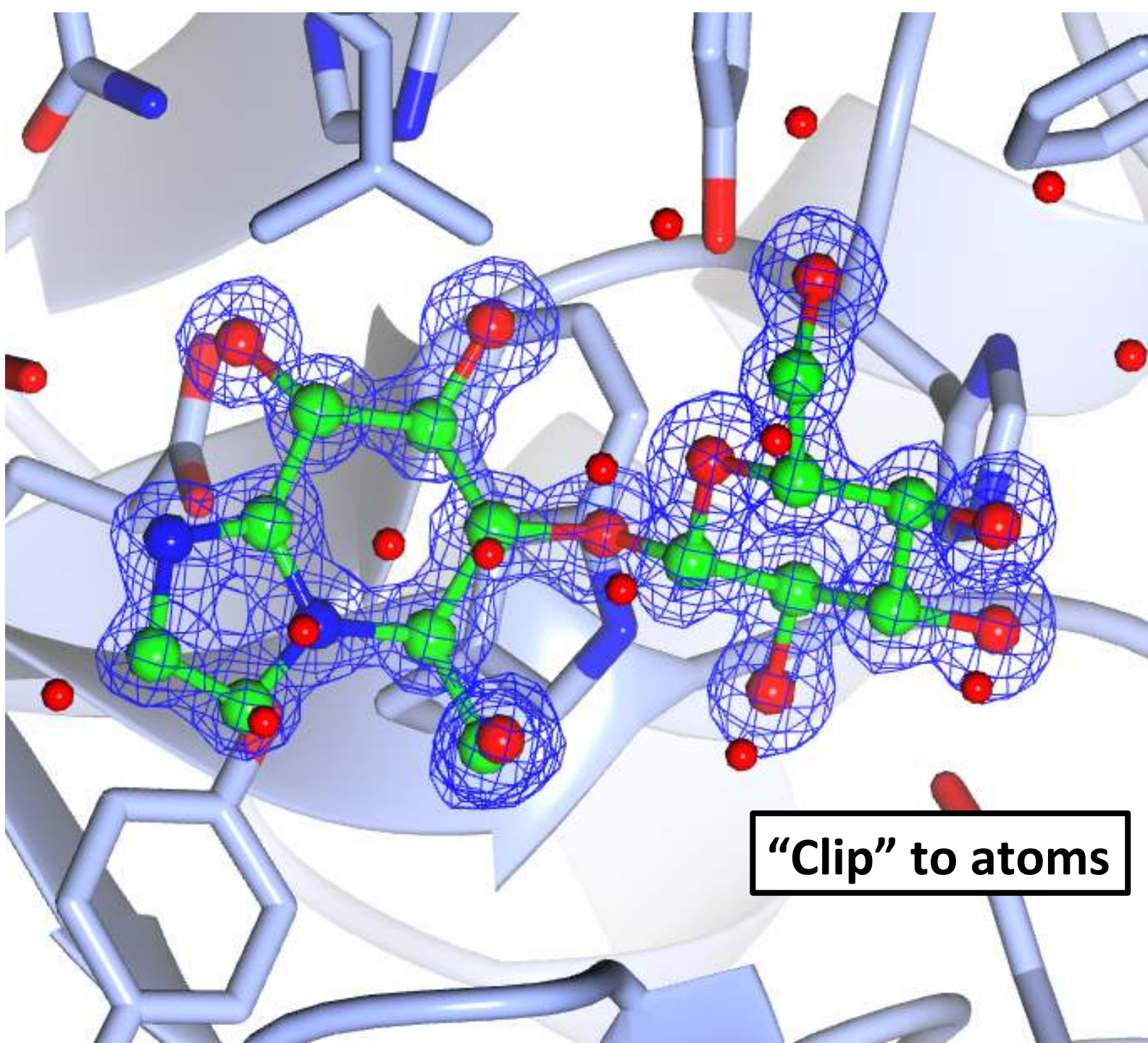


PDB Entities

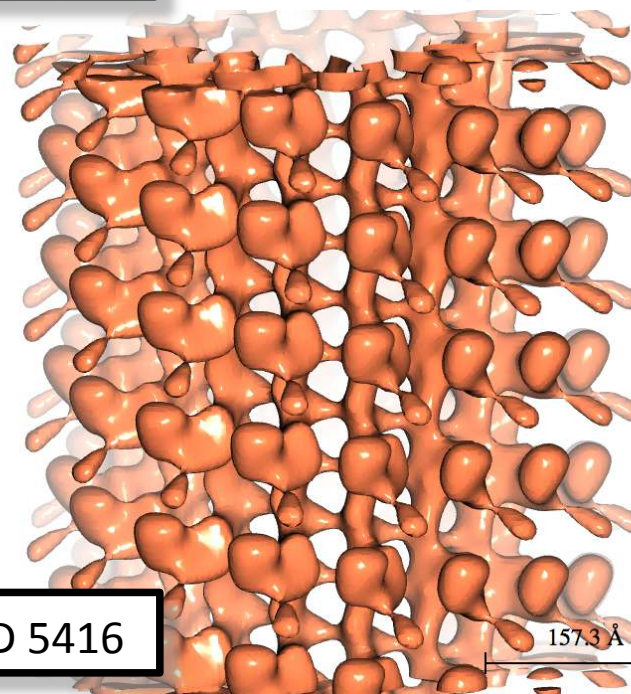
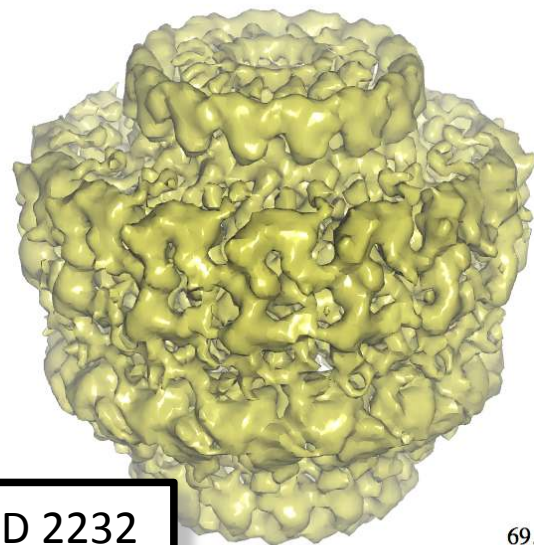
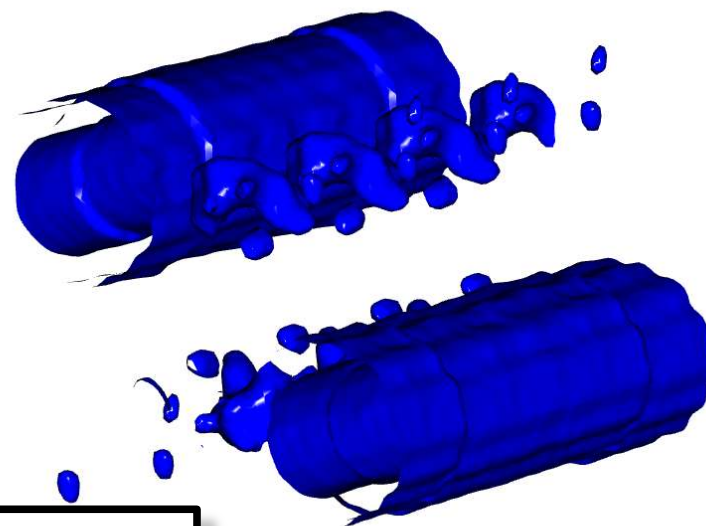
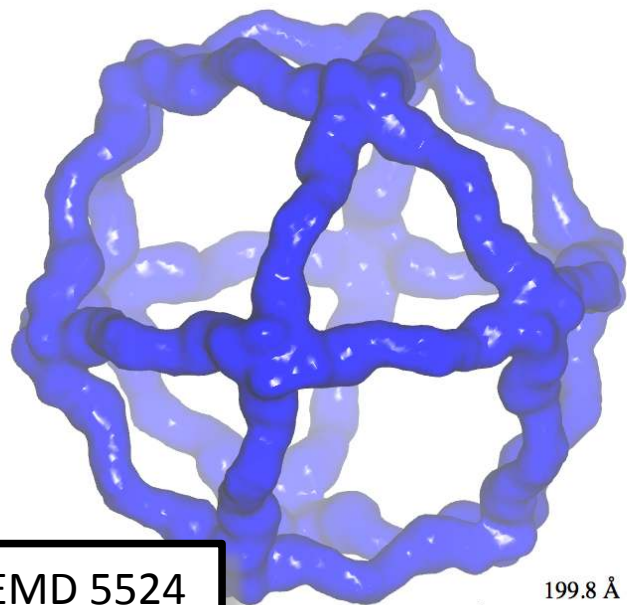


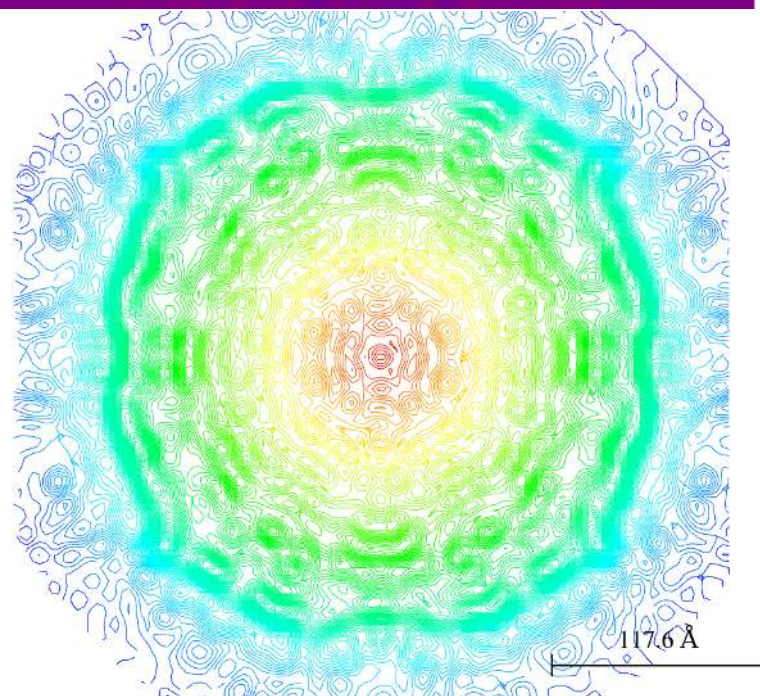
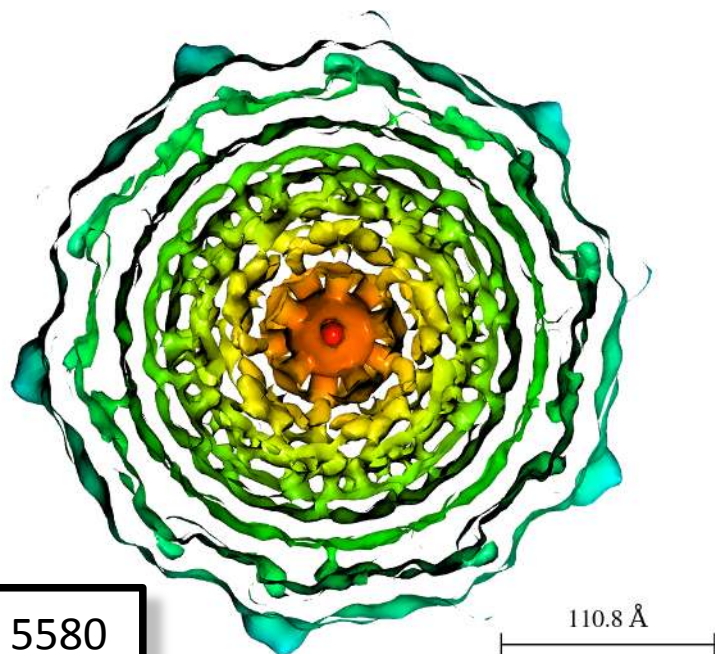
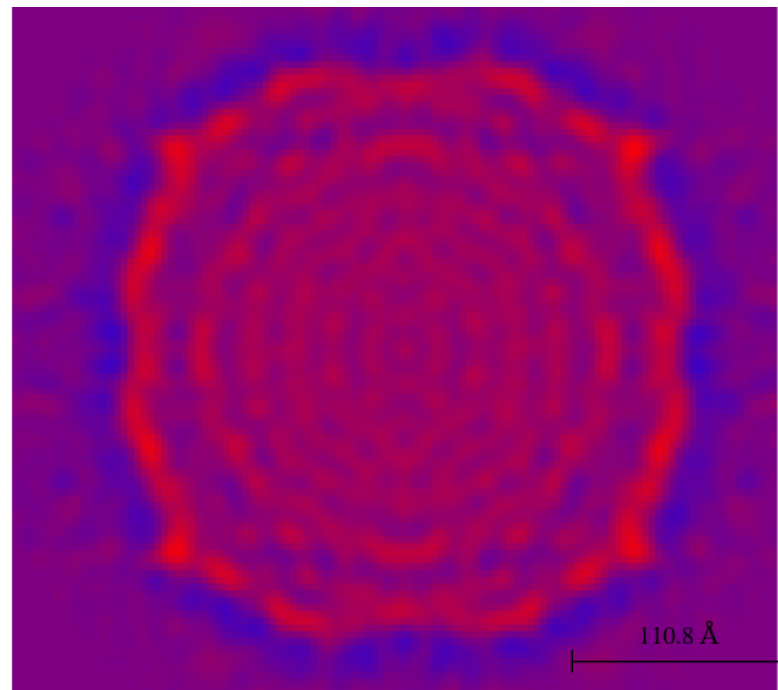
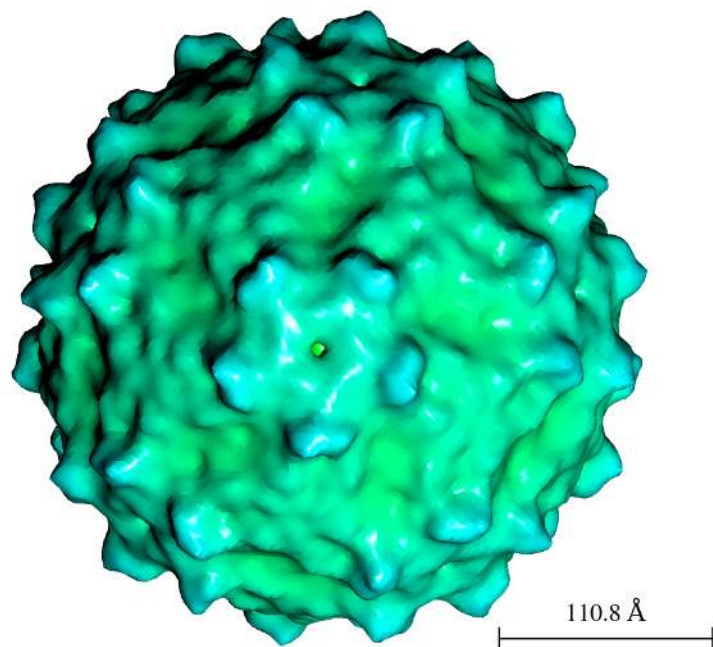
Electron Density



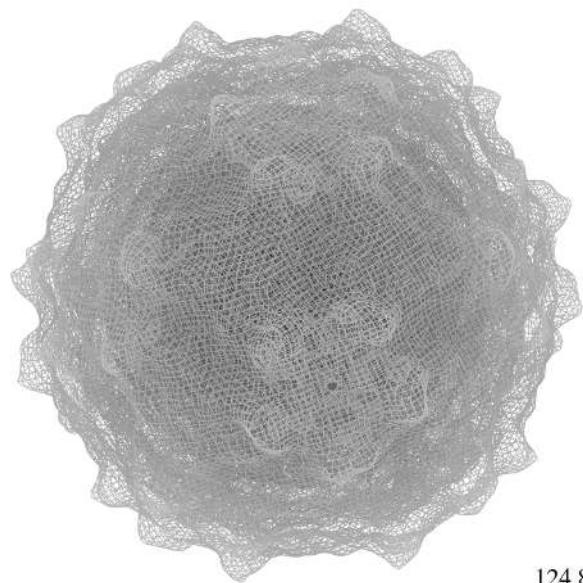


“Clip” to atoms

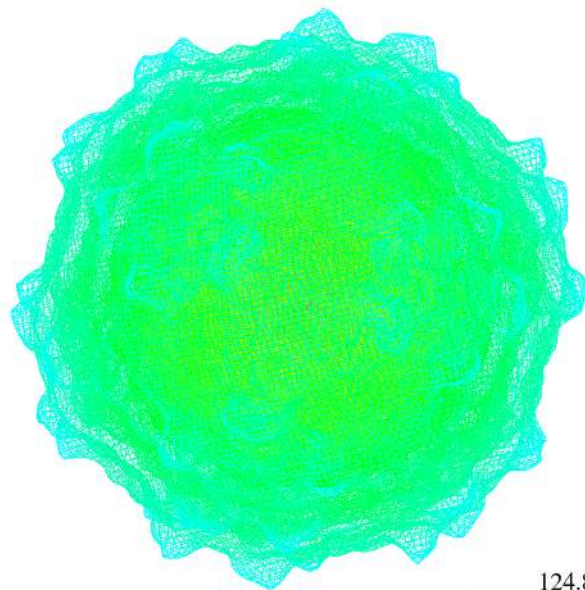




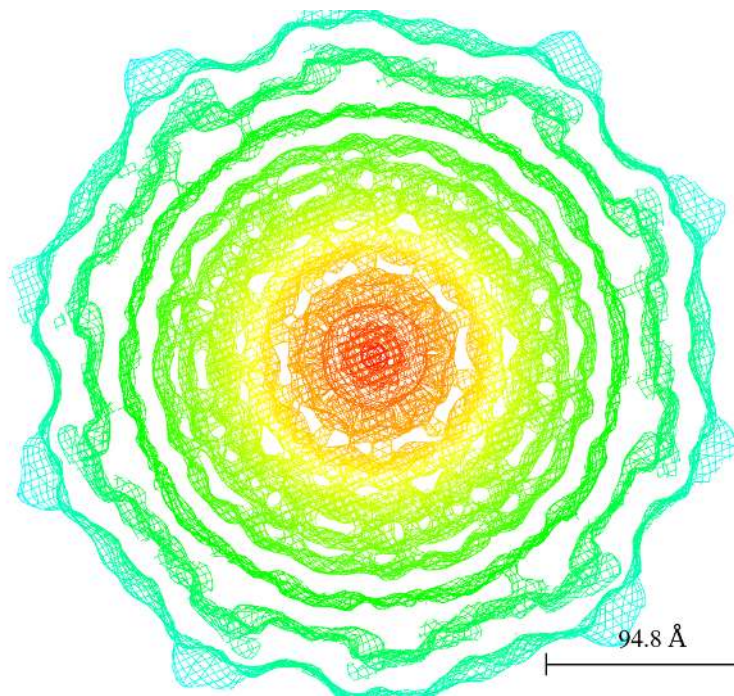
EMD 5580



124.8 Å



124.8 Å

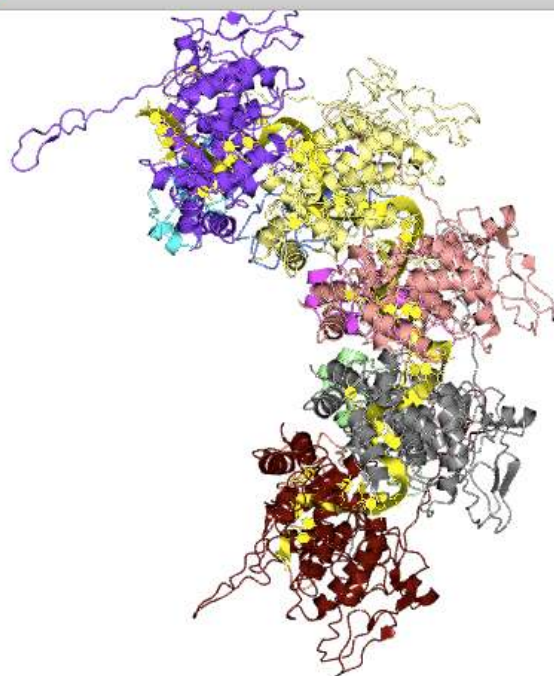


94.8 Å

EMD 5580

Other stuff

- PISA
- Structure superposition
- Sequence viewer/alignment/blast searches
- Biological assembly generation.
- Distance/angle measurement.
- Fancy lighting effects (shadows/occlusion).
- Normal modes calculation/visualization.
- Text/image overlays.



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

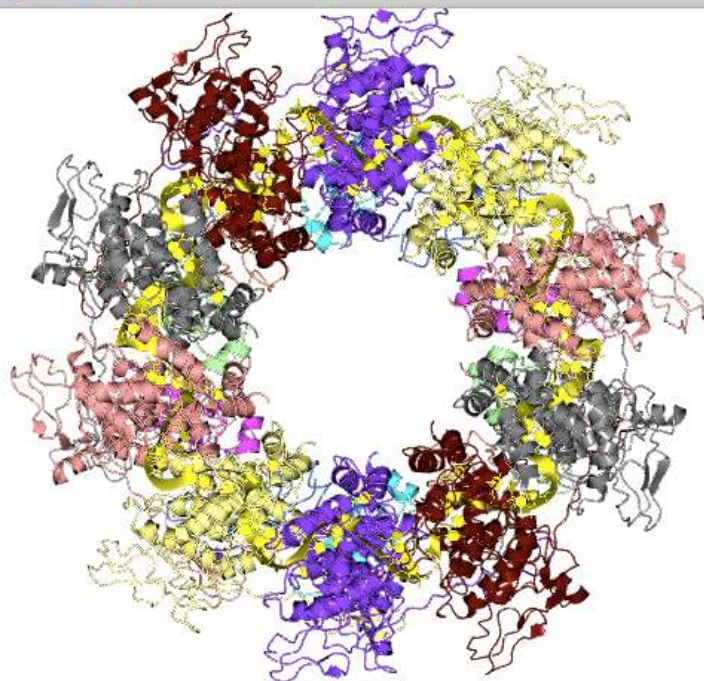
Close

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

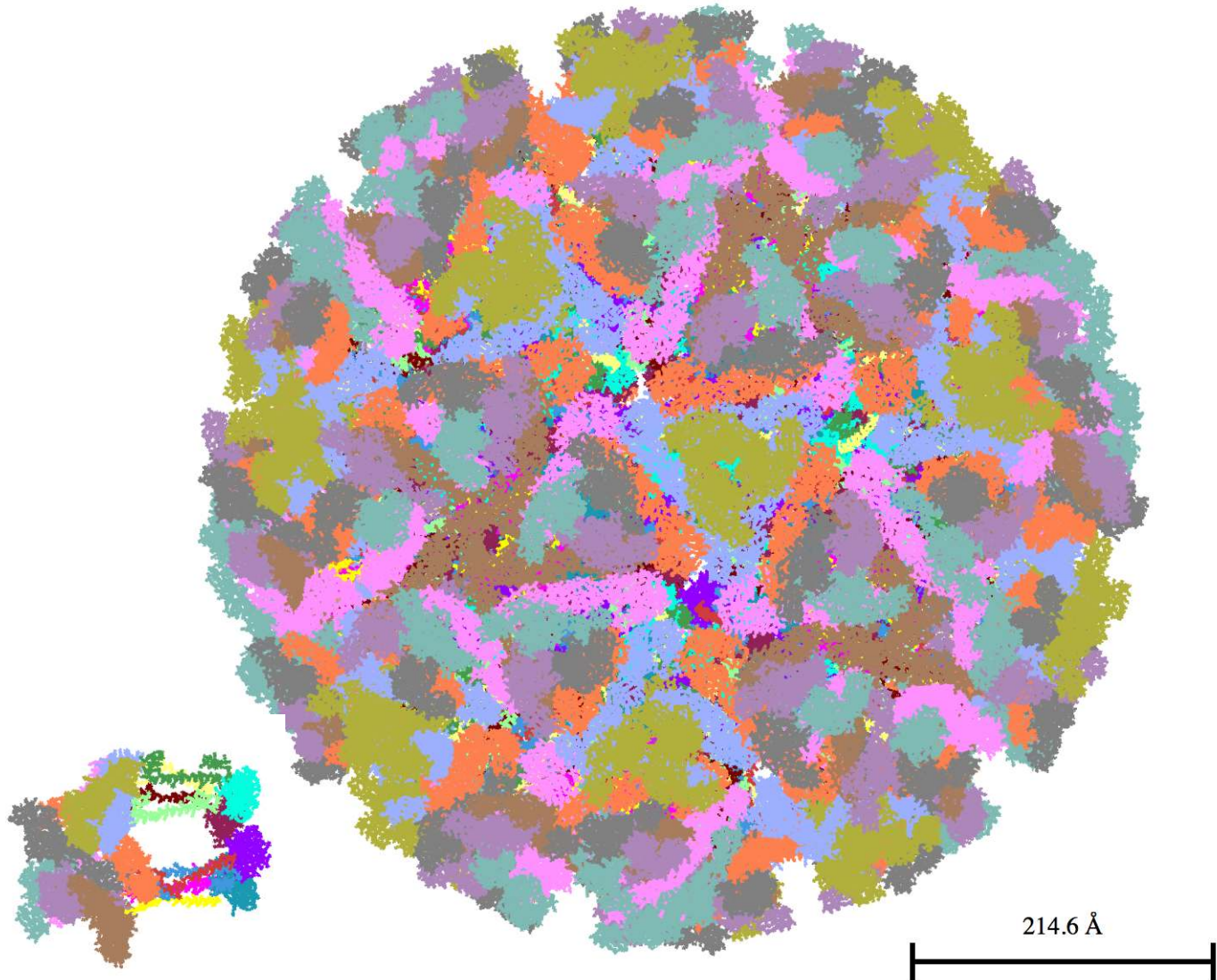
Structure Superposition

- CCP4MG has 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

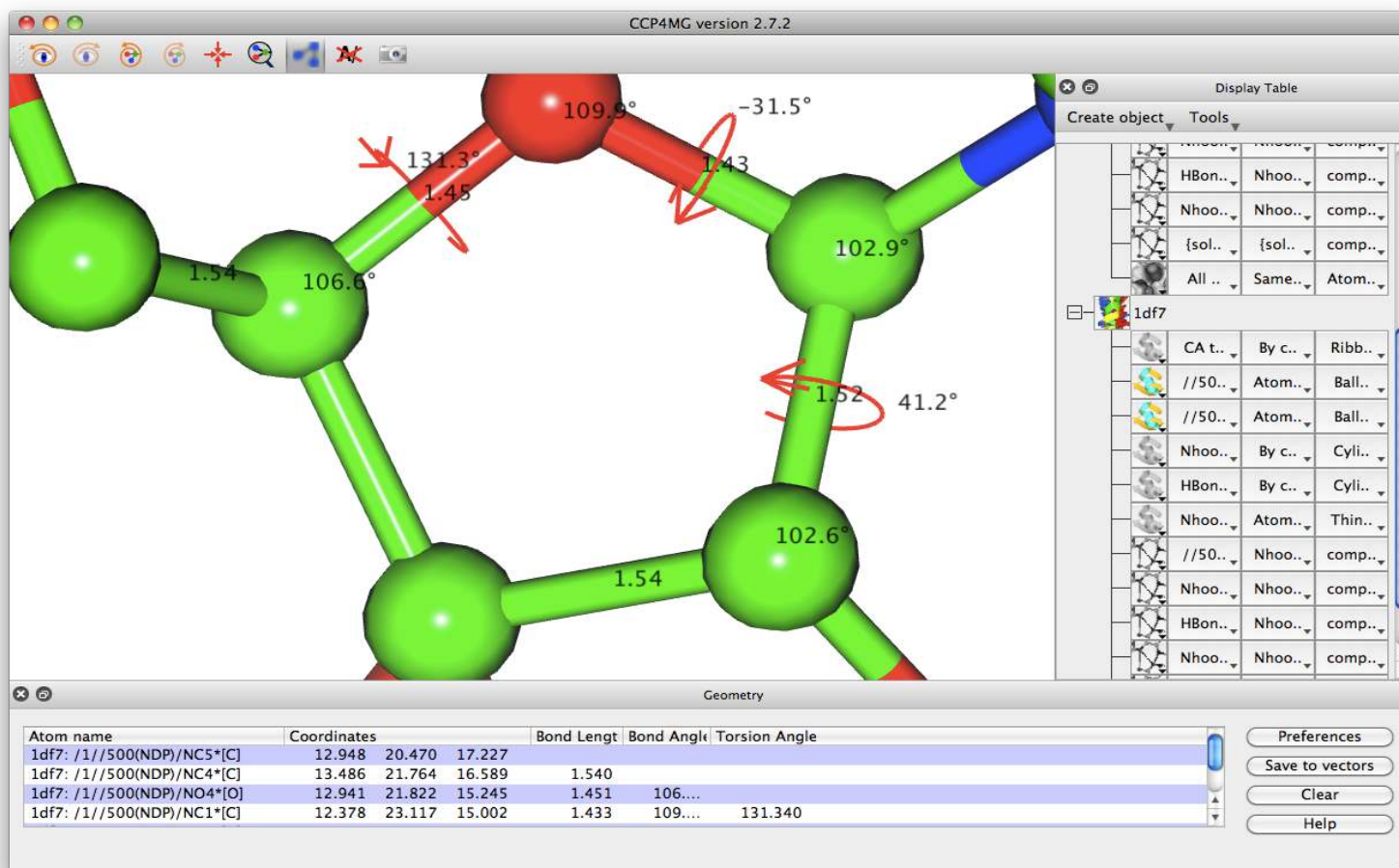
- Align sequences using muscle (a free multiple-alignment program) or ClustalW.
- Continuous (consurf style) or discrete traffic-light colour by conservation.
- Colour by secondary structure.
- Blastn/blastp interface. Blast results cached between sessions. Blast normally run remotely (EBI) with explicit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

Biological assemblies (3j2w)

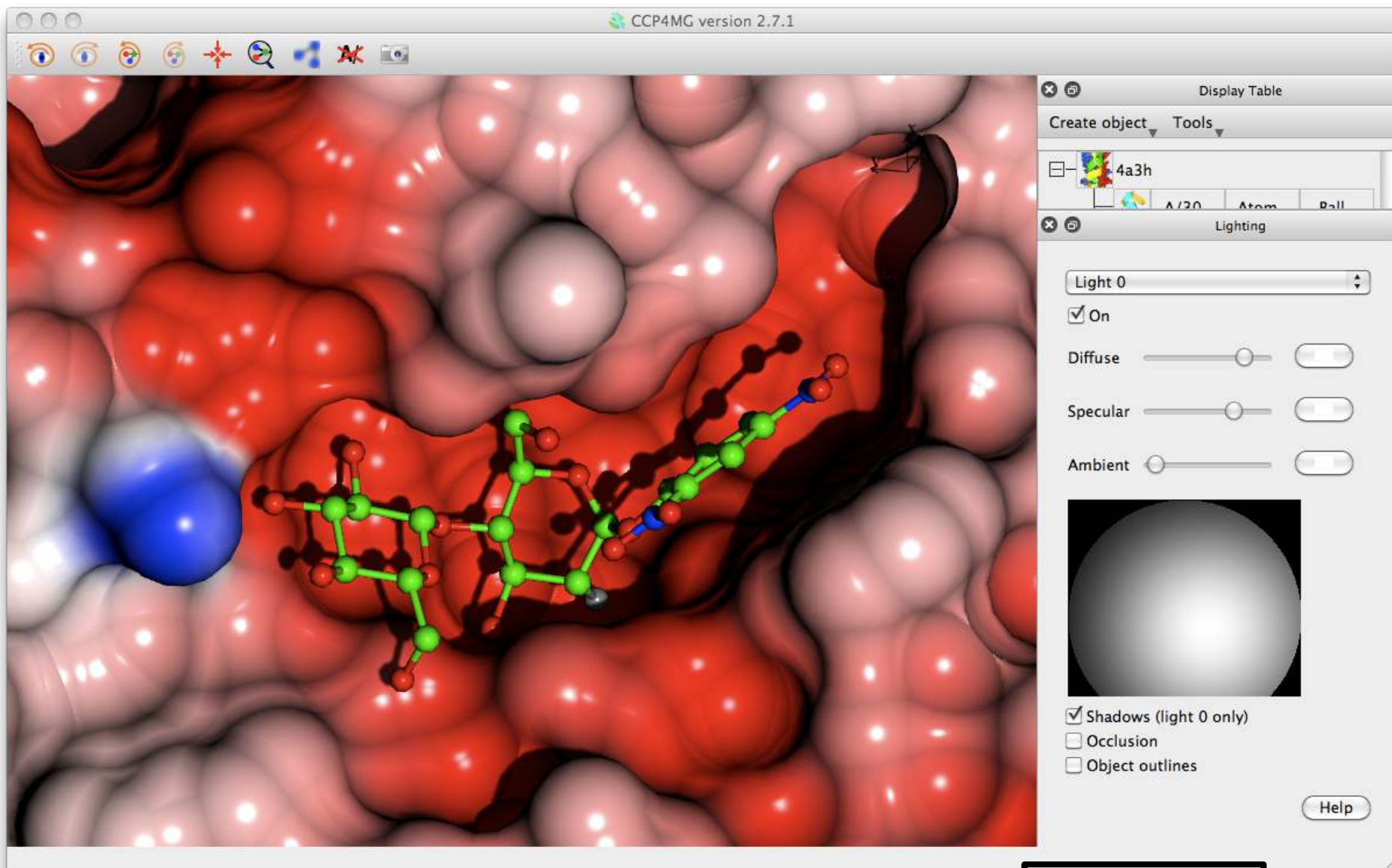


Distances and angles

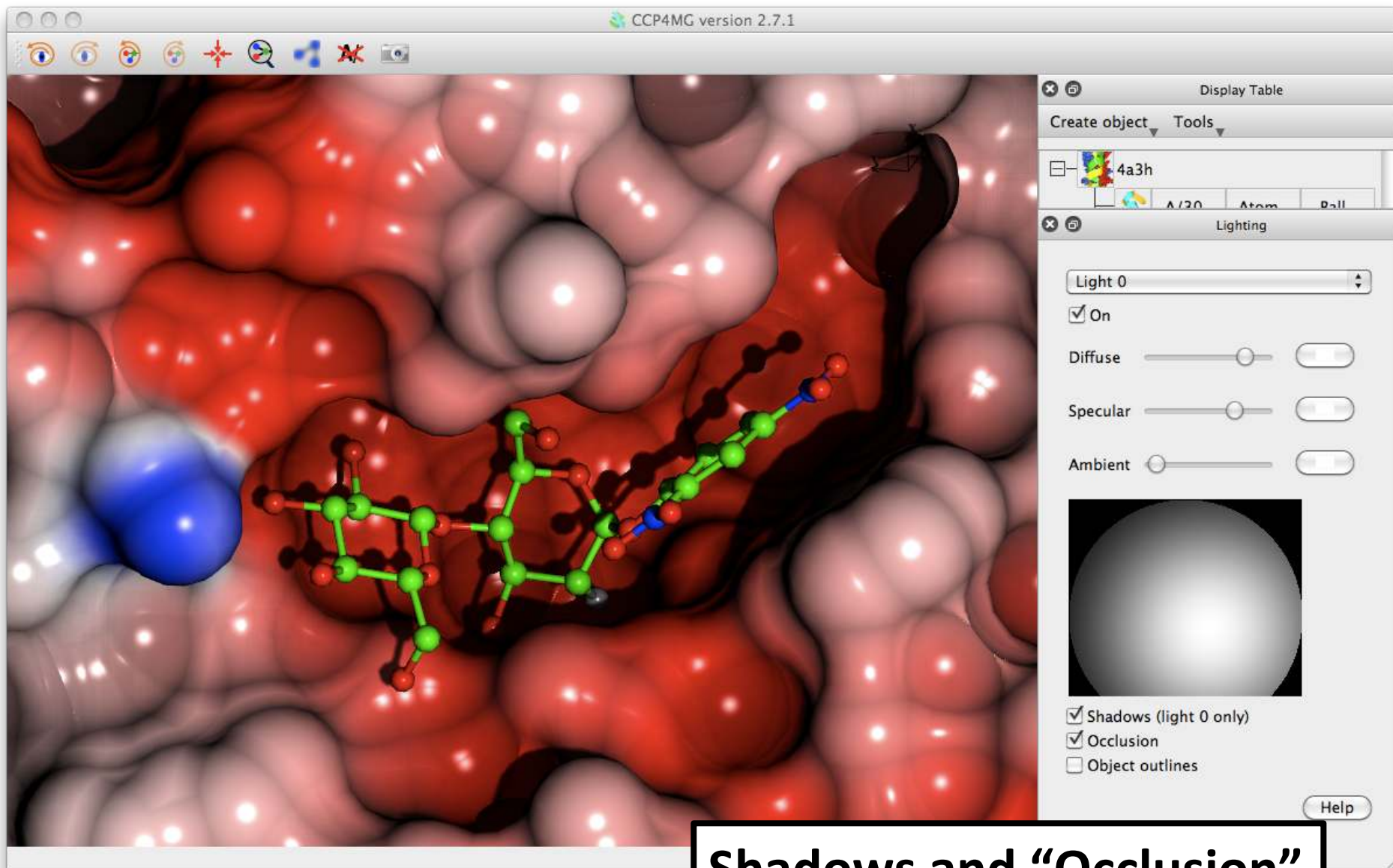
- Open “Geometry window” : Applications -> Geometry
- Double-click on one atom then another to measure bonds.
- Shift-double click on other atoms will measure angles.
- Results appear in table below and in graphics window.



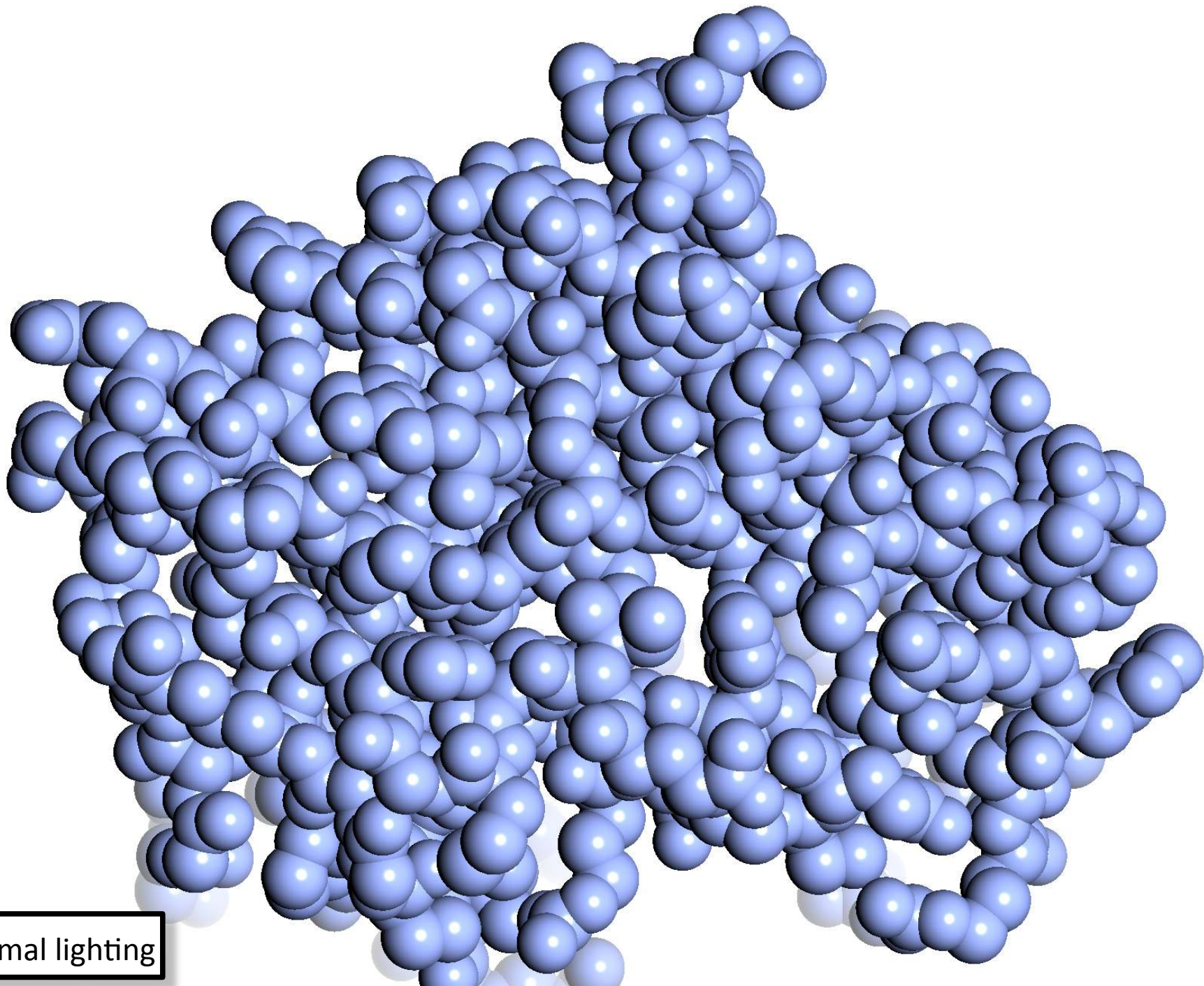
Lighting and Shadows



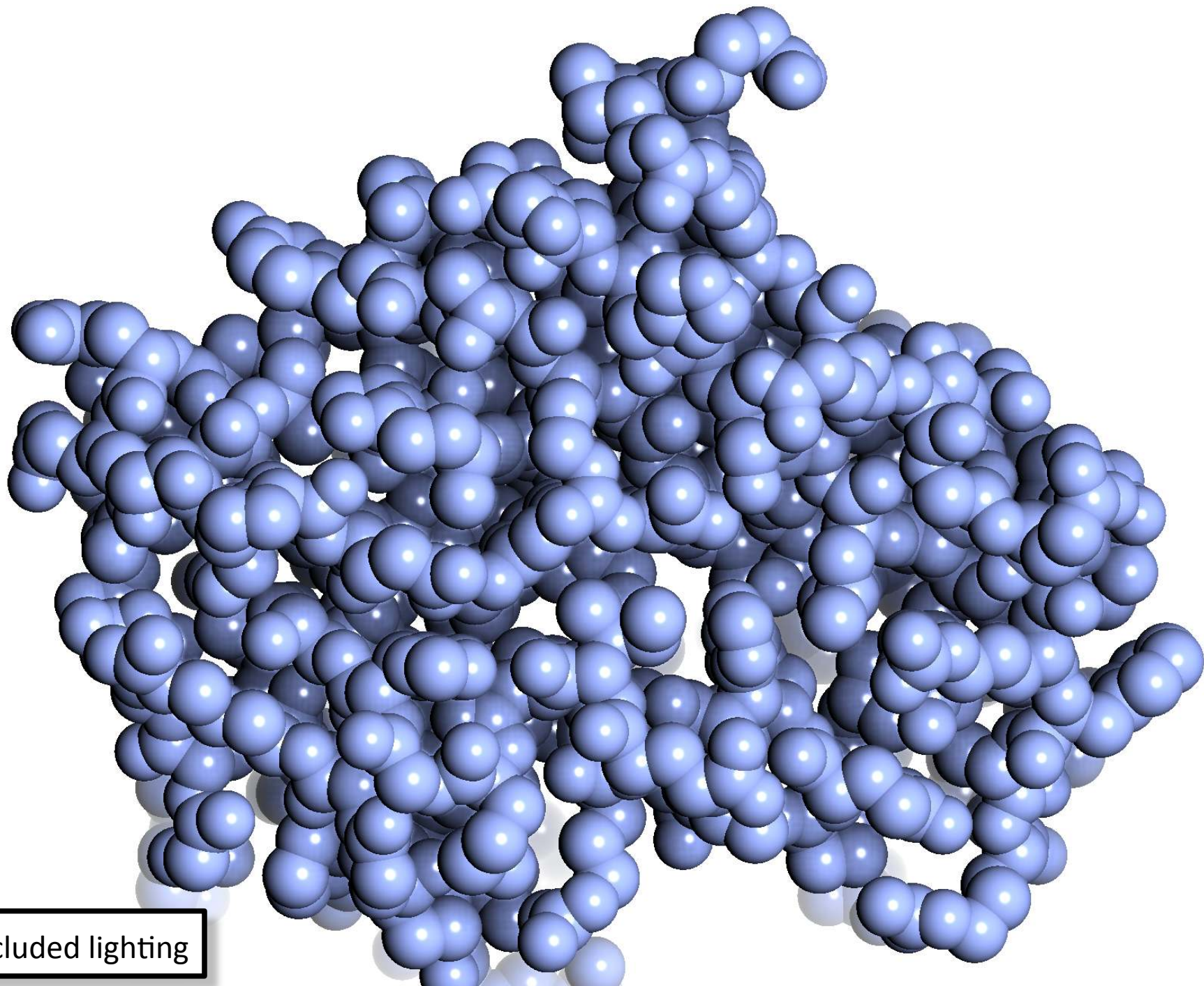
Shadows



Shadows and “Occlusion”

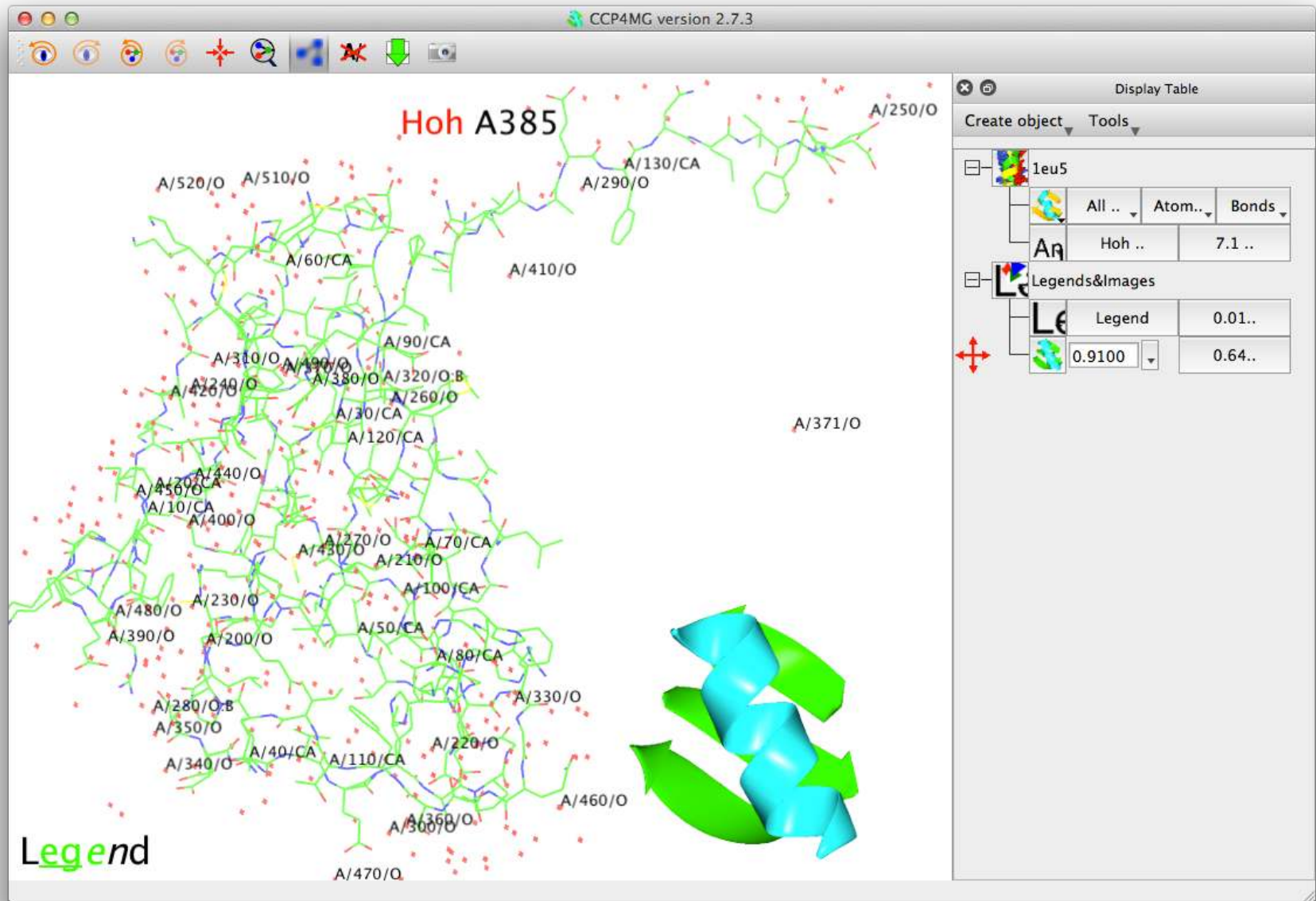


Normal lighting

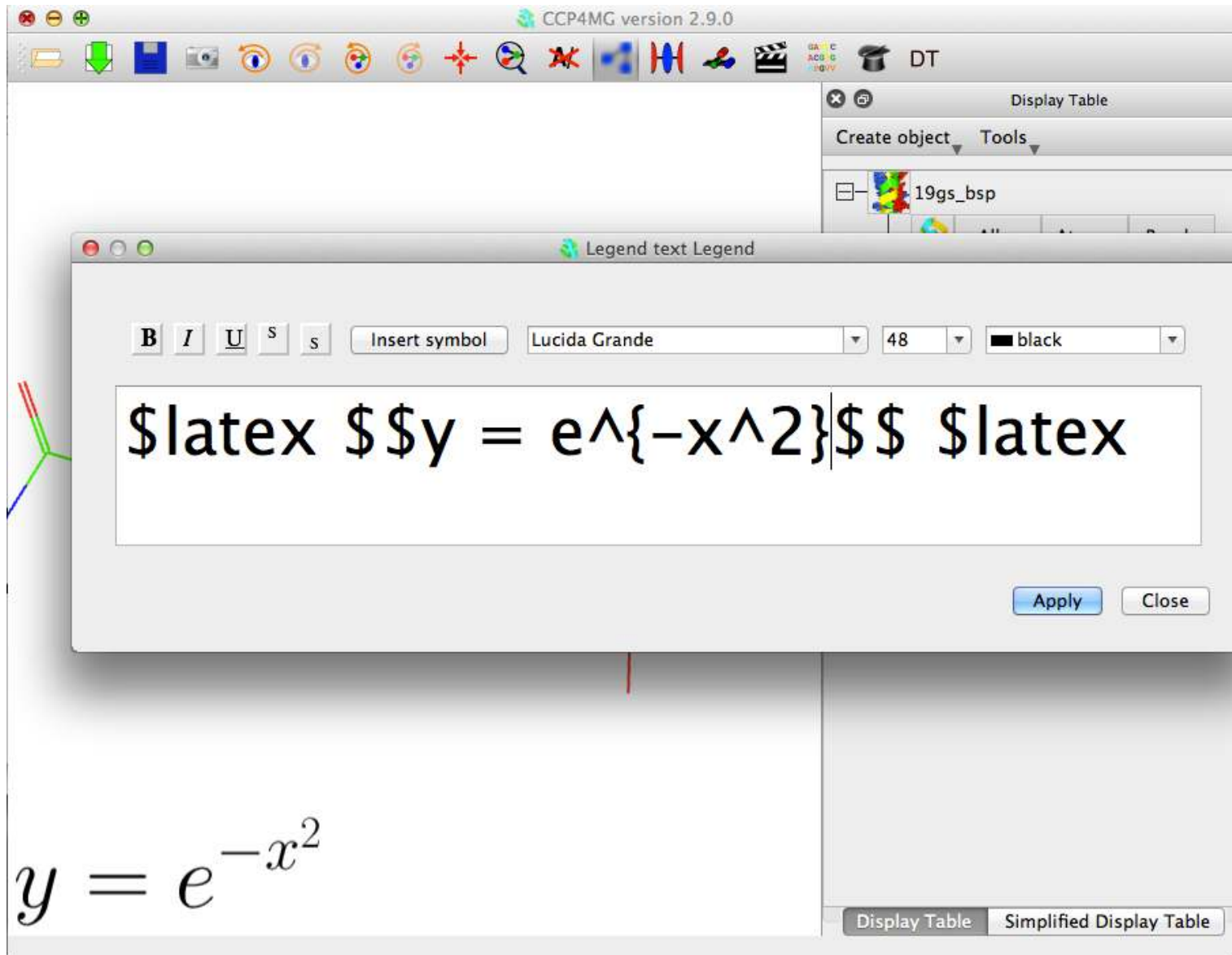


Occluded lighting

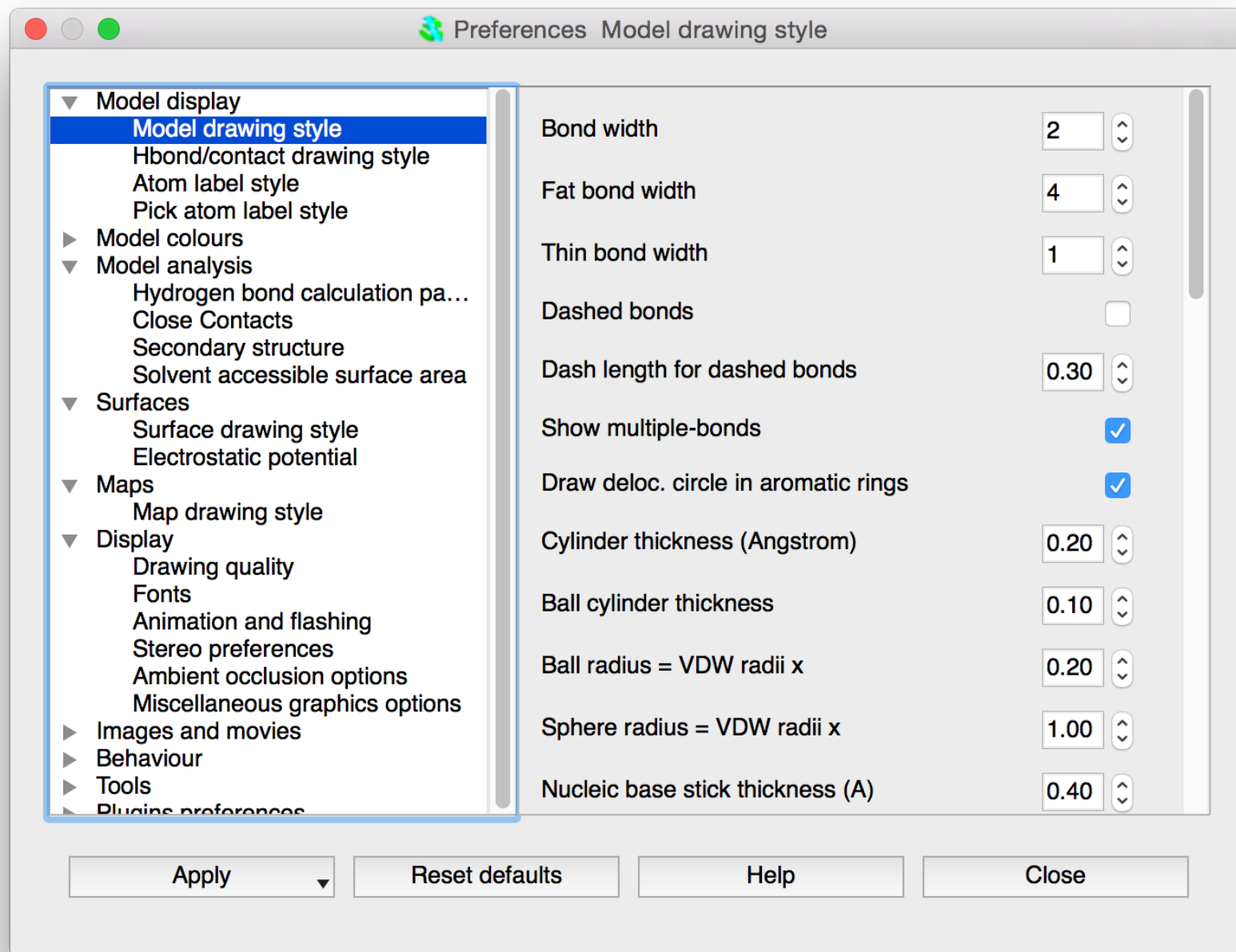
On screen text and images



On screen text and images



Preferences



“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.* Very fast, even with shadows and occlusion.
 - “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. Slower with shadows; impossibly slow with occluded lighting.

Save screenshot to image file

Note that the Render tool (on the File menu) will produce better quality pictures than this screenshot

Output image size

☒ Display window size x 1.00

☐ Width (in pixels) 600 height 600

☐ Use dpi 300 width (in) 6.00 height 4.00

☐ Keep graphics window aspect

☒ Scale font sizes

☒ Scale line widths

☒ Scale image sizes

☐ Transparent background

☐ Stereo image

☐ Shear stereo with separation 0.10

☐ Rotation stereo with angle 6.00

☒ Output text on scale bar

☒ Save status file

☒ View output

Look in ccp4 project or aliased directory: -Projects- or ...

Look in:

/Users/stuart

	Name	Size	Kind	Date Modified
Computer	Desktop	--	Folder	07/12/2017 08:19
stuart	Documents	--	Folder	06/12/2017 17:52
Desktop	1yp8.ccp4mg	221...tes	ccp4mg File	06/12/2017 15:52
Document	1yp8.pdb	729 KB	pdb File	06/12/2017 14:31
Macintos..	1WN4.ccp4mg	202...tes	ccp4mg File	06/12/2017 13:20
	3H8T.ccp4mg	267...tes	ccp4mg File	06/12/2017 13:20
	4T8D.ccp4mg	267...tes	ccp4mg File	06/12/2017 13:20

File name:

Save

Files of type: PNG files (*.png)



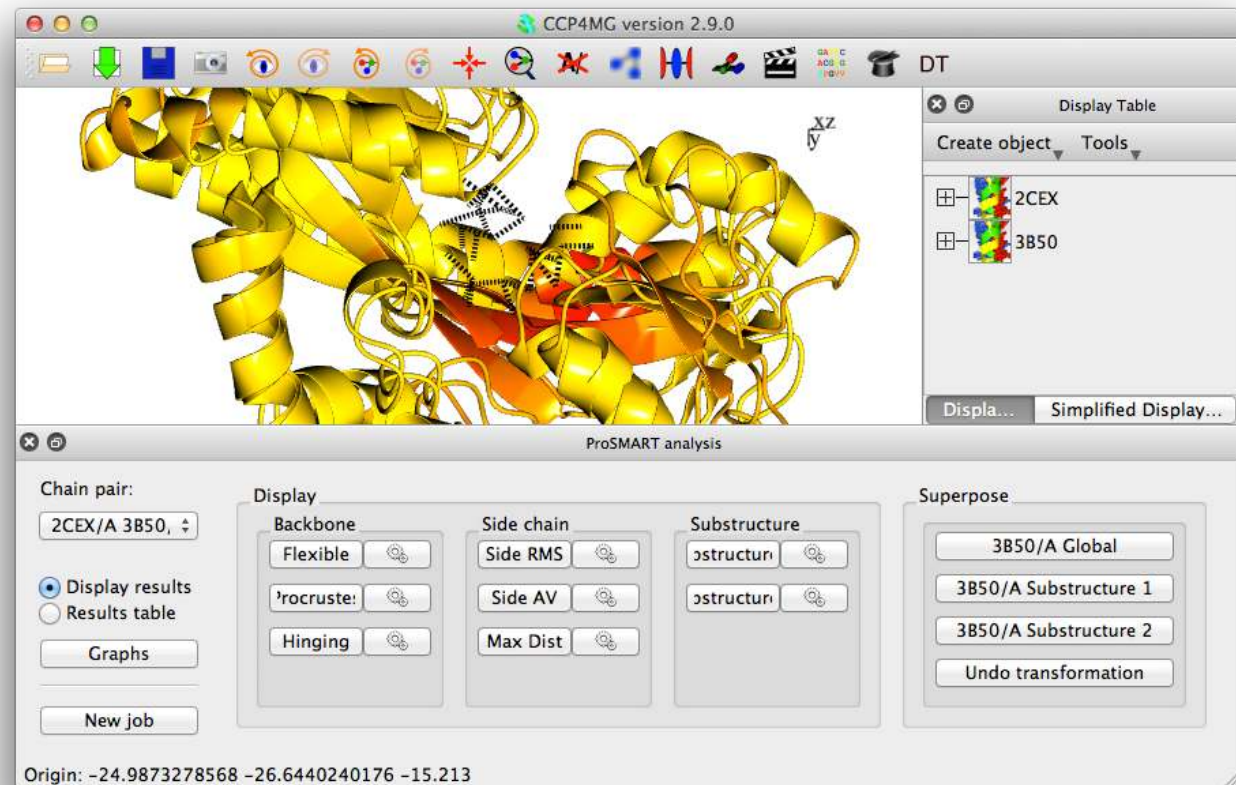
Cancel

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
- 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.

ProSMART interface

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



Ebeye – search (obsolete)

- Interface to simple search facility of PDB-E.

The screenshot shows the CCP4MG version 2.7.3 interface. On the left, a 3D ribbon diagram of a protein structure is displayed. On the right, the 'Ebeye search' window is open, showing a search for 'cyclotide'. The search results list several PDB IDs with checkboxes and descriptions. Annotations with arrows point to specific parts of the interface:

- Type search string here**: Points to the search input field containing 'cyclotide'.
- Check boxes and click download to get files**: Points to the checkboxes next to the search results.
- Click on links to view details in web browser**: Points to the PDB IDs in the search results.

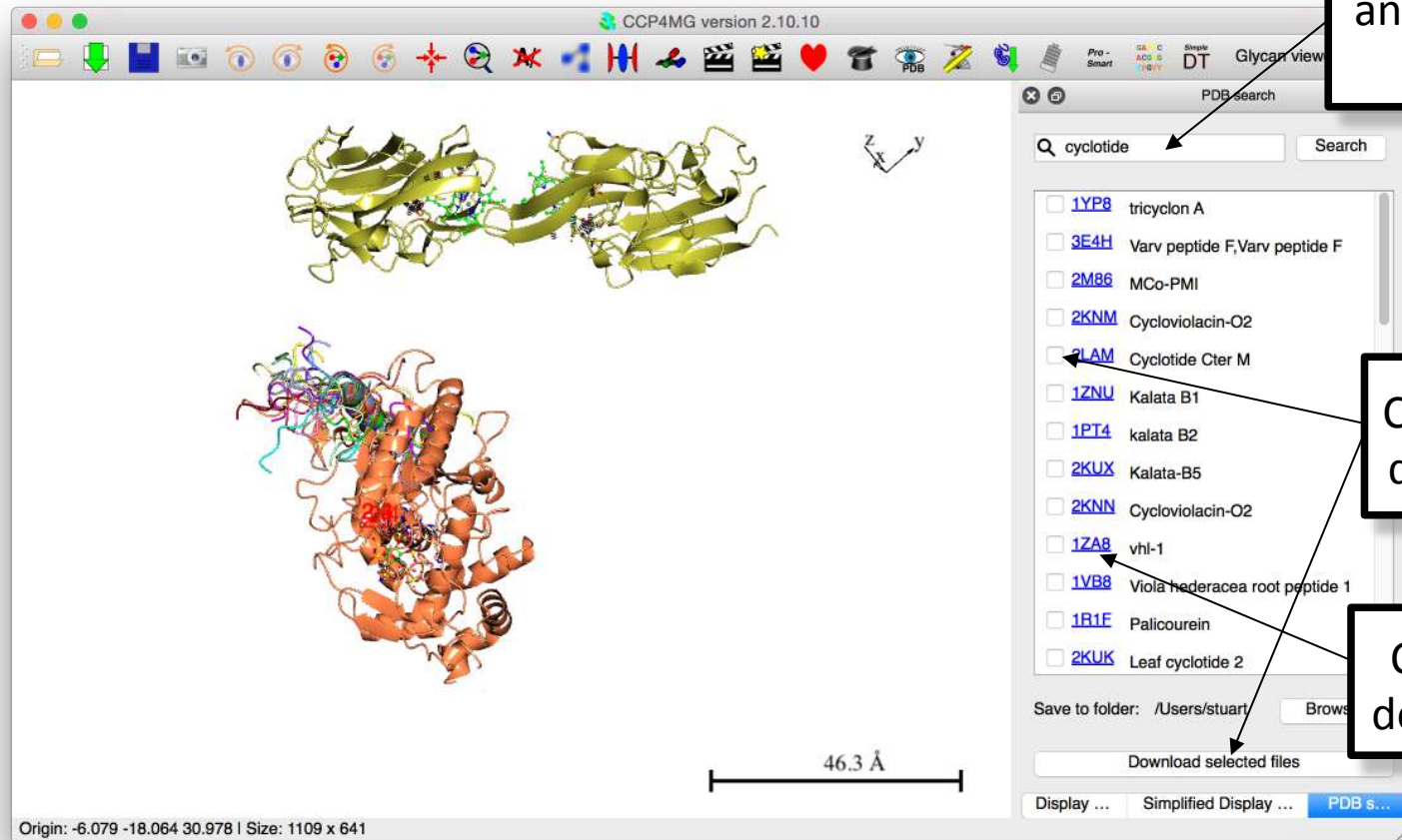
The search results table is as follows:

PDB ID	Description
☒ 2lam	Three-dimensional str
☒ 1r1f	Solution Structure of t
☒ 3e4h	Crystal structure of th
☒ 1yp8	Solution structure of t
☒ 1pt4	Solution structure
☐ 1vb8	solution structure
☐ 2knm	Solution structure
☐ 1znu	Structure of cycloti
☐ 2knn	Solution structure
☐ 2kux	Solution structure of t
☐ 1za8	NMR solution structure
☐ 2qi0	Cycloviolacin O14
☐ 2kuk	Solution structure of
☐ 2k7g	Solution Structure
☐ 1nb1	High resolution sol
☐ 1nbi	High-resolution so

At the bottom of the window, there is a 'Save to folder: /Users/stuart' field with a 'Browse' button, a 'Download selected files' button, and 'Display Table' and 'Ebeye search' buttons.

PDB/EBI – search (coming soon)

- Interface to simple search facility of PDB.



Type search string here
and press Enter or click
search button

Check boxes and click
download to get files

Click on links to view
details in web browser

“Batch” rendering

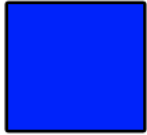
- Images may be rendered from command line or from scripts without starting up the main program.
- `ccp4mg -norestore -picture
mypic.mgpic.py -R test.png -RO
'{"size":"1600x1600","smoothribbons":
"1", "raytrace":"1"}' -quit`
- The file `mypic.mpic.py` is a file containing a scene description: lists of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

Glycoblocks

Glycosylation depiction in 3D

- Electrostatic interactions provided by N- and O-linked glycans are essential for correct folding of glycoproteins.
- Depicting these protein-glycan contacts can be challenging; glycans can have many branched sugars.
- CCP4MG brings the familiar two-dimensional identification convention used by the glycobiology community into three dimensions.

Saccharide display in 2D



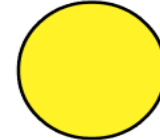
N-Acetyl-glucosamine
(NAG)



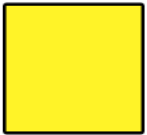
Mannose
(BMA, MAN)



Fucose
(FCA, FCB, FUC)



Galactose
(GAL)



N-Acetyl-galactosamine
(NGA)



Glucose
(GLC, BGC)



2-keto-3-deoxynononic acid
(KDN)



Galacturonic acid
(ADA, GTR)



Glucosamine
(GCS)



Xylose
(XYS, XYP)

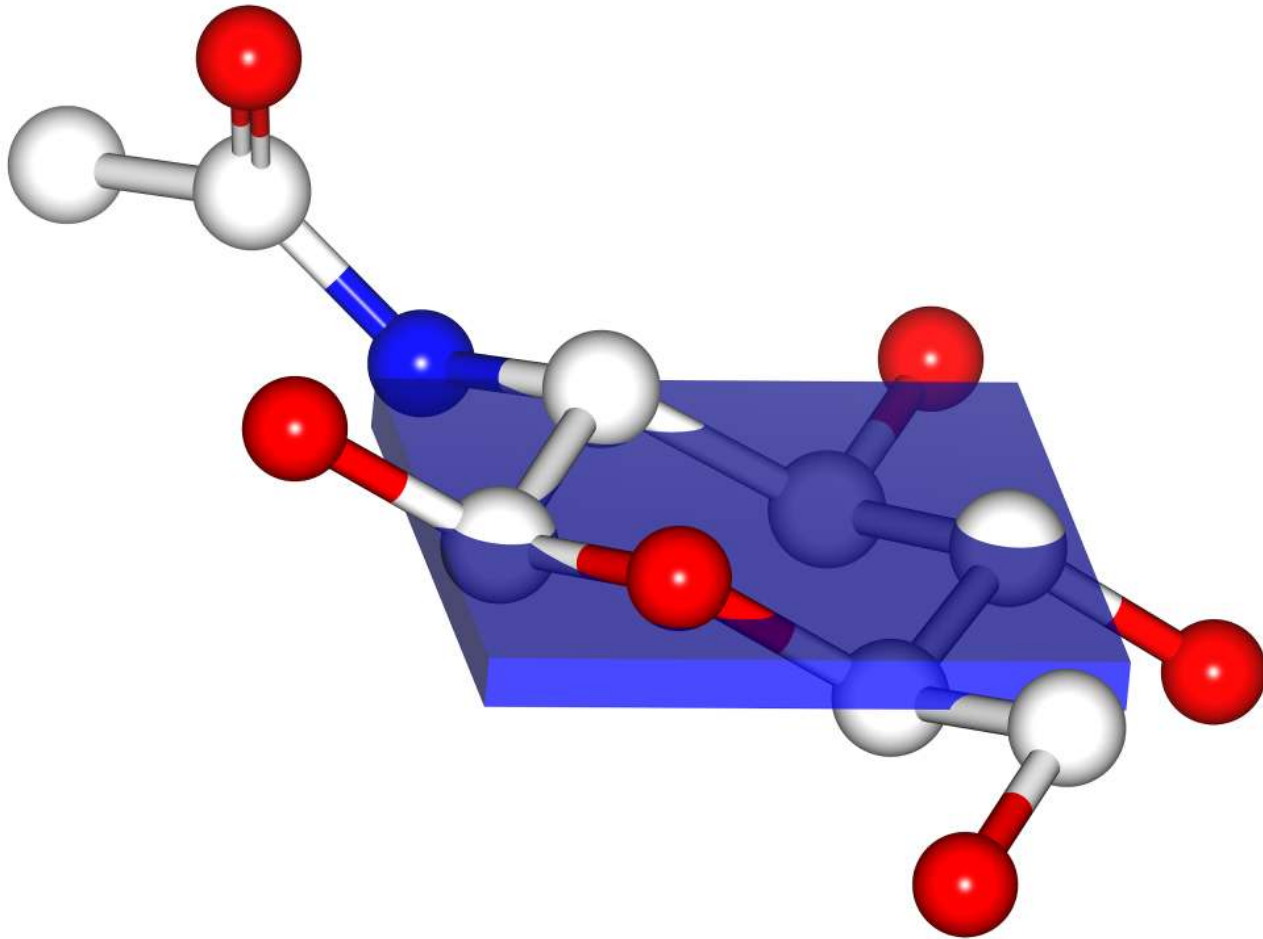


Iduronic acid
(IDR)

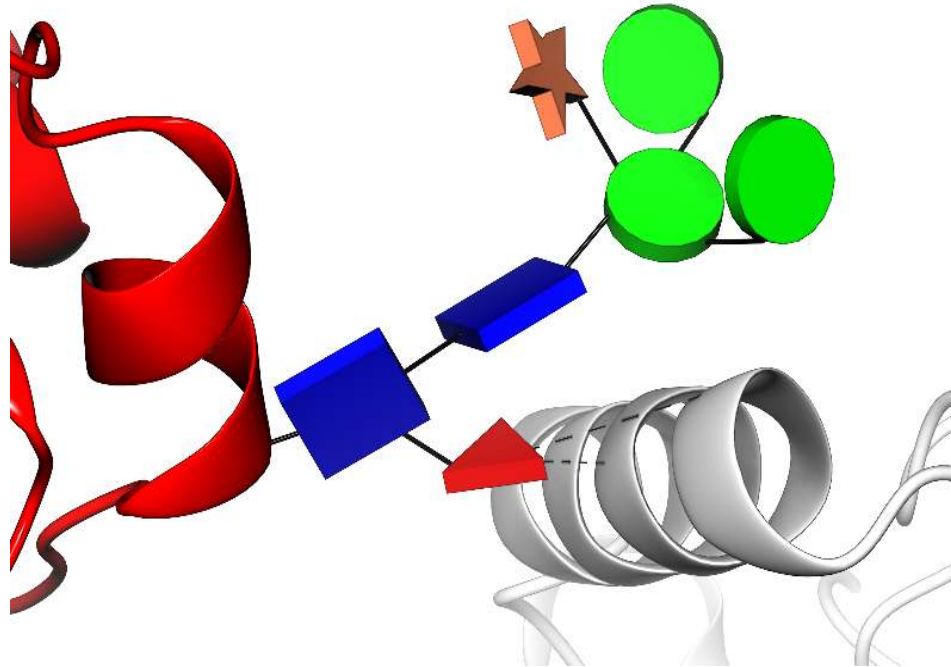


Mannuronic acid
(BEM)

Saccharide display in 3D

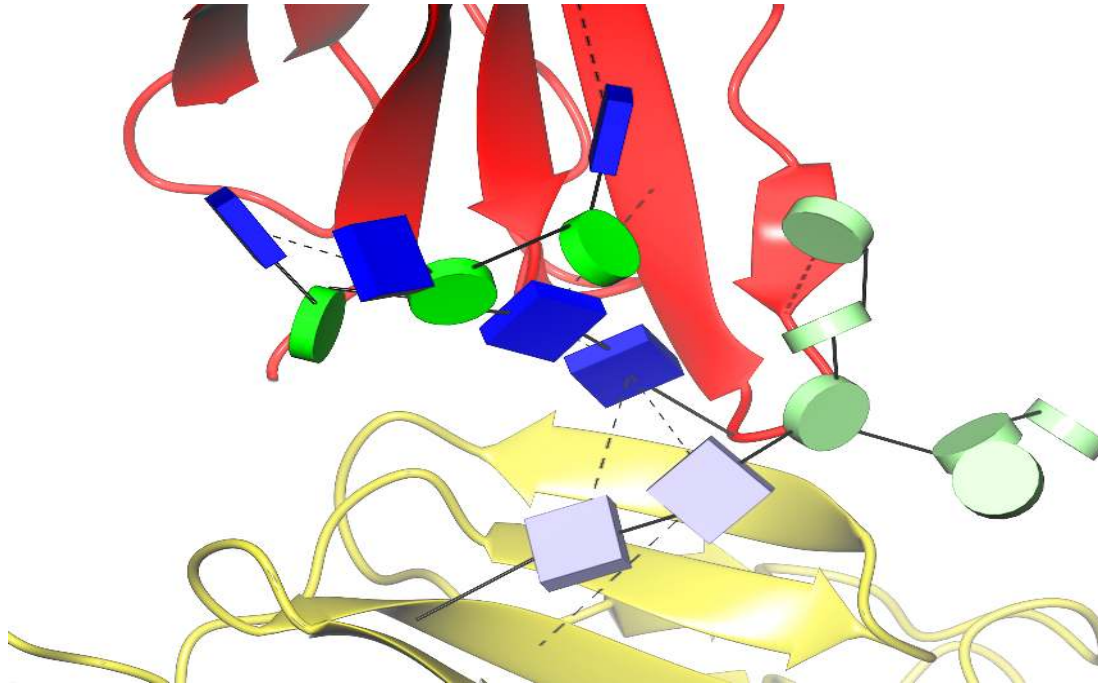


Saccharide display in 3D



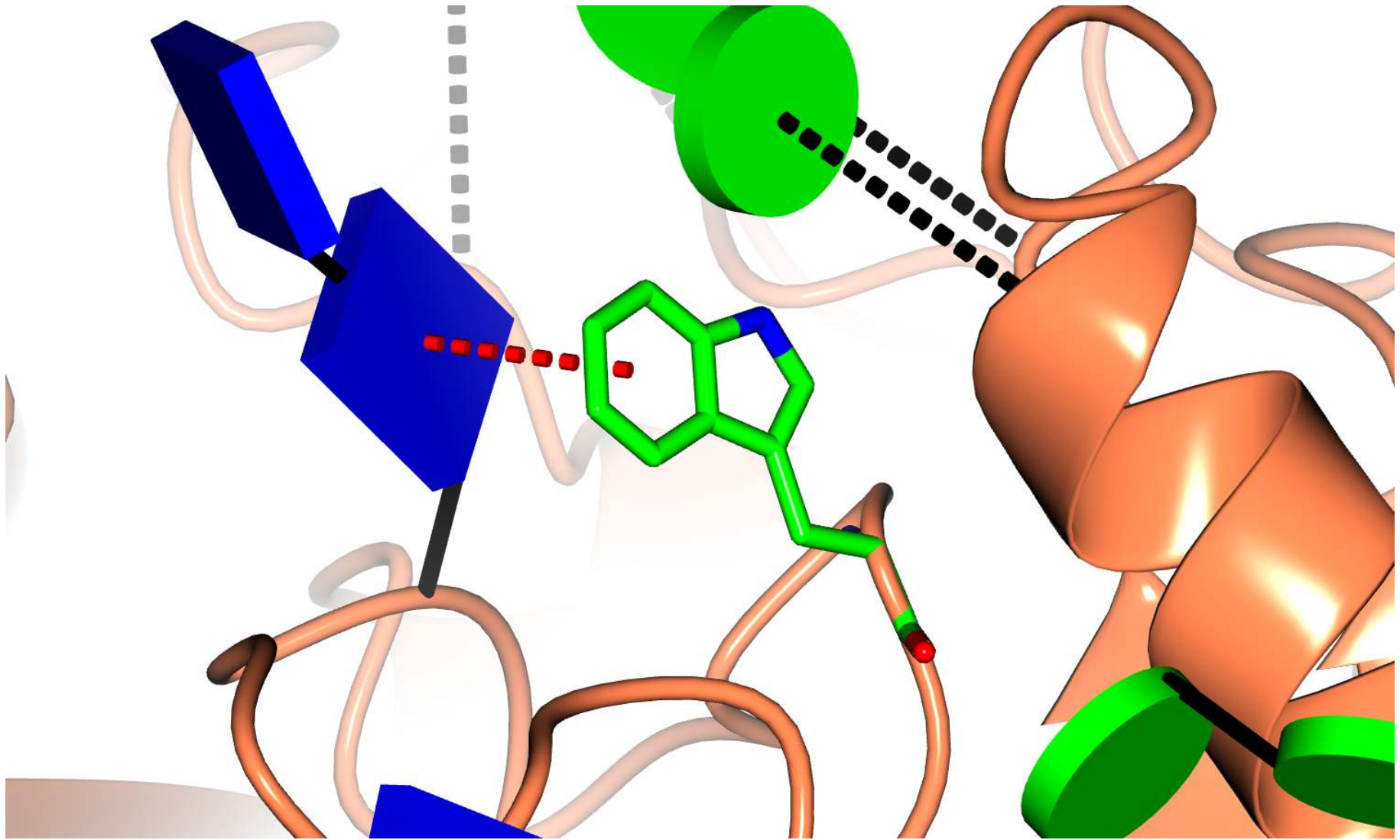
Glycoblocks representation of a plant N-glycan and its interactions (PDB 4CUO). In this structure, the Fucose sugar attached to the first N-acetyl- β -D-glucosamine residue establishes two hydrogen bonds to a neighbouring chain (depicted in white) that is related by crystallographic symmetry to the one the tree is covalently bound to (in red). L-sugars (Fucose, red triangle, and Xylose, orange star) are only present in plant glycans and make for less than 1% of all the N-glycan forming pyranosides deposited in the wwPDB.

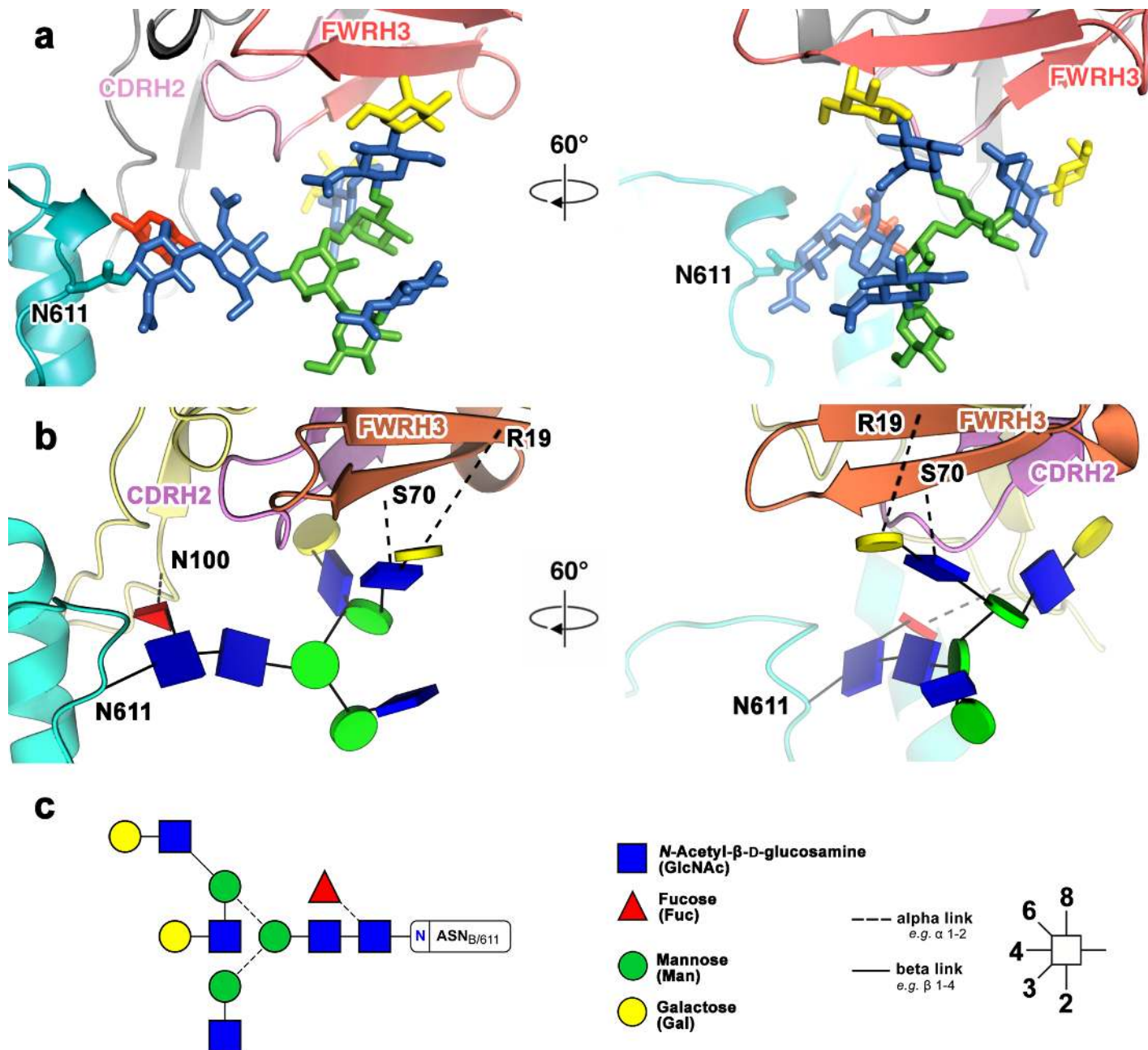
Saccharide display in 3D



Glycoblocks view of carbohydrate-carbohydrate interactions (PDB 3SGK). Two N-glycans attached to two separate Fc fragments (depicted in red and gold) establish hydrogen bonds with each other and the protein part. These interactions, along with others that are described in Ferrara et al. (2011), make a key contribution to the increased binding between these two antibody fragments. The representation shows a clean view of an otherwise very complex network of H-bonds.

Interactions





Privateer Mk III

- Validation of glycosylation structures based on the expression system (fungal, mammalian, plant, etc.)
- Generates pretty SVG diagrams which also happen to be interactive - i2 and MG can use these
- Python interface for easy connection with other programs/pipelines. Example: Glycoblocks in MG

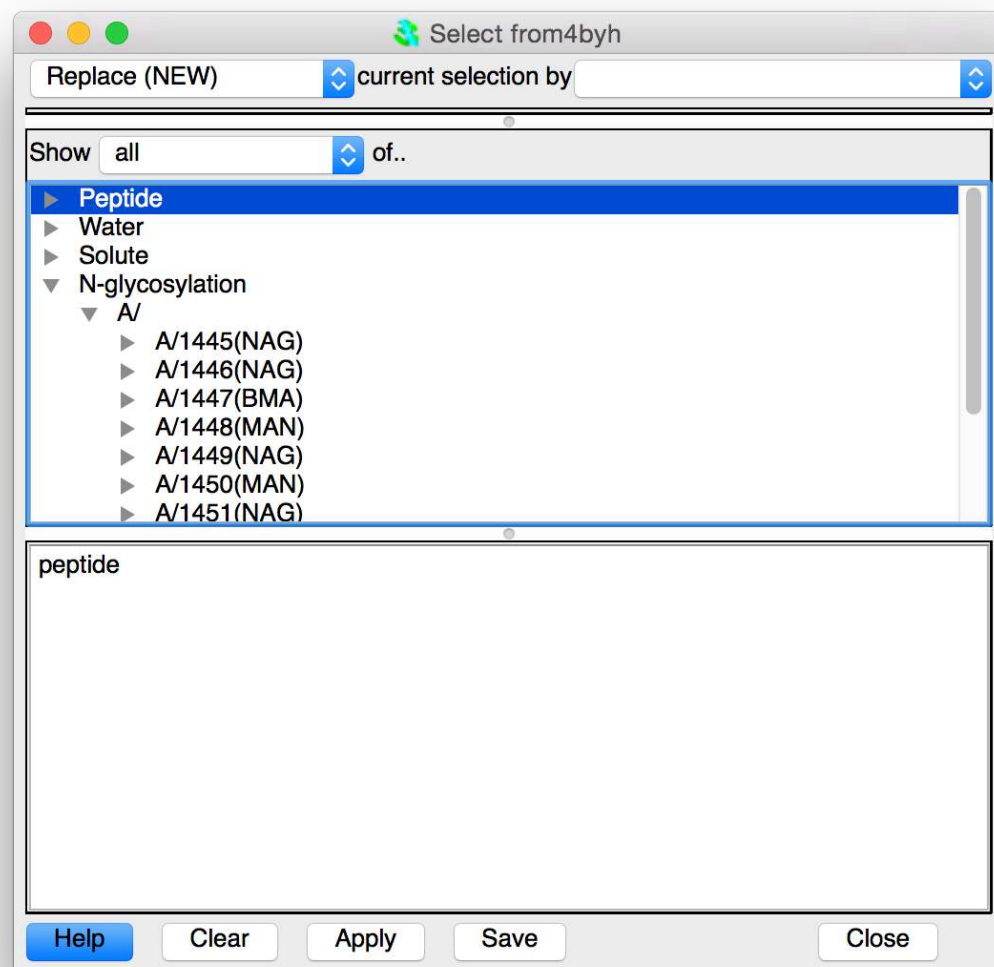
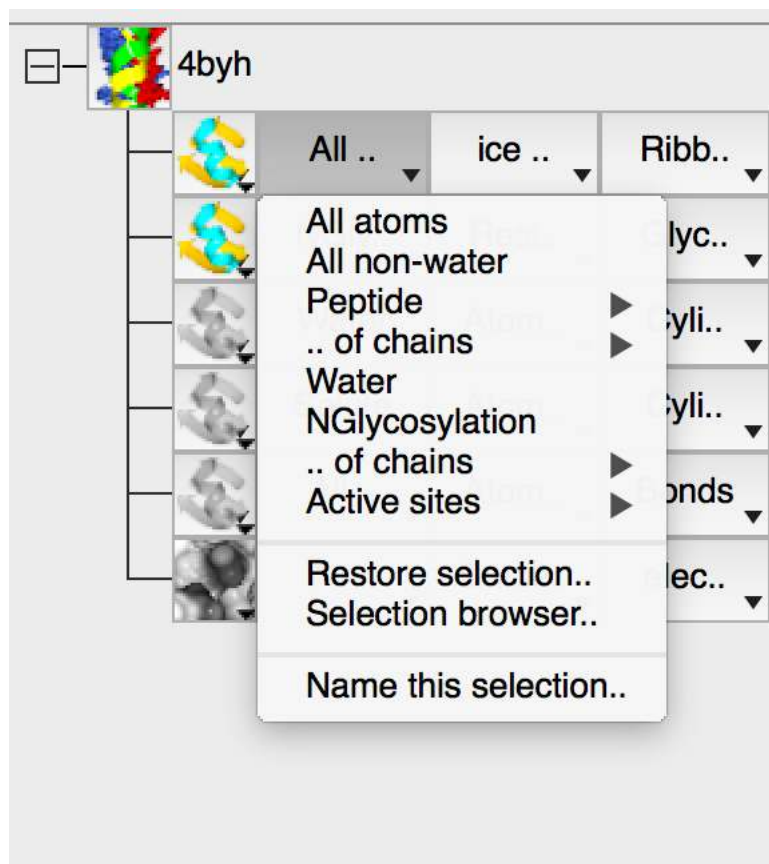
Privateer: software for the conformational validation of carbohydrate structures.

Jon Agirre, Javier Iglesias-Fernández, Carme Rovira, Gideon Davies, Keith Wilson and Kevin Cowtan. *Nature Structural & Molecular Biology*, 2015, **22**(11), 833-834.

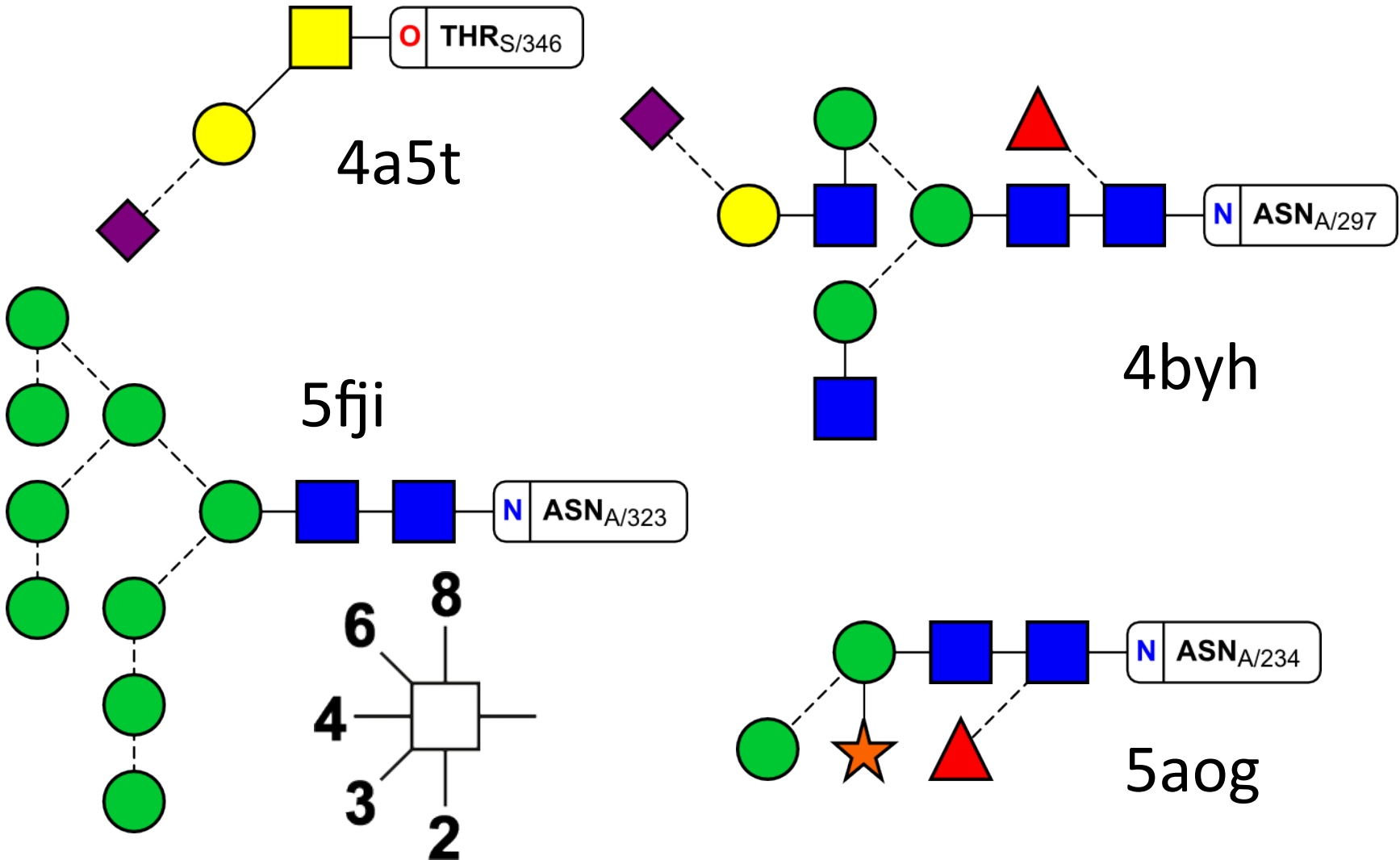
Glycosylation in selections

- N- and O- glycosylation sites are now identified when file is loaded into CCP4MG using *Privateer* and appear in selection menus.
- Picture wizards automatically generate Glycoblocks.

Glycosylation selections

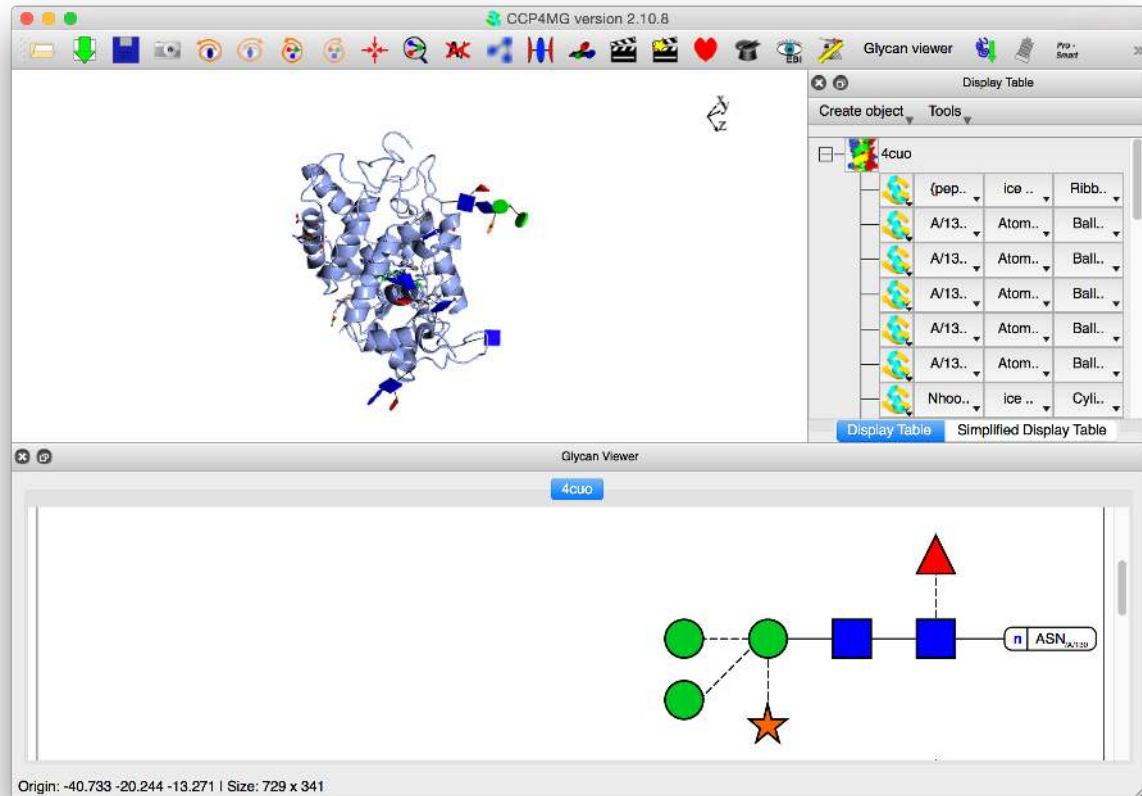


SVG Diagrams – “Essentials” notation



Glycan Viewer

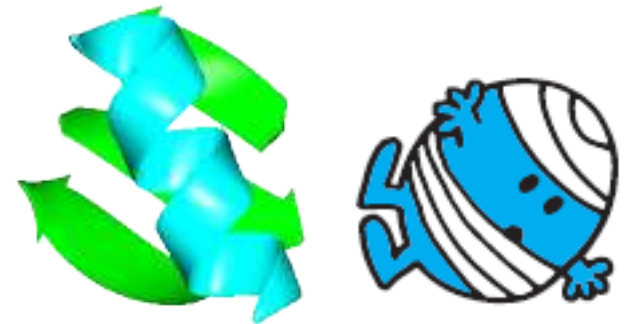
- Traditional 2D – representation with:
 - Hover over glycans/links for extra information
 - Click on glycan to centre 3D view on that glycan.



Glycoblocks/Glycan Viewer Video

- Video available at
<https://doi.org/10.1107/S2059798316013553>
(Or google 'Glycoblocks').

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.

CCP4i2 alpha-0 Project Viewer: gamma

Task menu View in Coot View in CCP4mg Export MTZ Help Bibliography Clone job Run

Job list Project directory

Job/File	Evaluation
47 Refinement - REFMAC5	R=0.27 RFI
46 Data reduction	Sgp=P 21
45 Data reduction	
44 Data reduction	
38 Molecular Replacement and refine...	
37 Data reduction	
36 Automatic structure solution from ...	
35 Automatic structure solution from ...	
34 Automatic structure solution from ...	
33 Automatic structure solution from e...	
32 Autobuild protein	
31 Autobuild protein	
30 Automatic structure solution from ...	
29 Automatic structure solution from ...	
28 Automatic structure solution from ...	
27 Automatic structure solution from ...	
26 Automatic structure solution from ...	
25 Automatic structure solution from ...	
24 Automatic structure solution from ...	
23 Data reduction	Sgp=P 21
22 Edit search model - ccp4mg	
21 Validation of carbohydrate structures	
20 Validation of carbohydrate structures	
19 Import from Xia2	
18 Autobuild protein	
17 Data reduction	
16 Data processing with XIA2	
15 Edit search model - ccp4mg	
14 Edit search model - ccp4mg	
13 Edit search model - ccp4mg	
12 Edit search model - ccp4mg	
11 Edit search model - ccp4mg	
10 Edit search model - ccp4mg	

Integrate X-ray images

X-ray data reduction and analysis

Experimental phasing

Bioinformatics and model preparation for Molecular Replacement

Interactive model preparation - CCP4mg and MrBUMP
Edit molecular replacement search models (ccp4mg)

Truncate search model - CHAINSAW
Truncate and renumber model prior to molecular replacement

Truncate search model - SCULPTOR
Truncate model prior to molecular replacement

Align sequences - CLUSTALW
Align sequences using clustalw

Molecular Replacement

Model building and Graphics

Refinement

Ligands

Validation and analysis

Export and Deposition

Reflection data tools

Coordinate data tools

Developer tools

New job Cancel

DEVELOPMENT CCP4-7.0.026 Project Viewer: GammaDec2016

Task menu

View in Coot

View in CCP4mg

Export MTZ

Help

Bibliography

Clone job

Job search

Run

Run on server

Job list

Project directory

Job/File	Evaluation
40 CCP4mg MrBUMP	
39 CCP4mg MrBUMP	
38 CCP4mg MrBUMP	
37 CCP4mg MrBUMP	
36 CCP4mg MrBUMP	
35 CCP4mg MrBUMP	
34 REFMAC5	R=0.24 RFre
33 REFMAC5	R=0.20 RFre
32 REFMAC5	R=0.20 RFre
31 REFMAC5	R=0.20 RFre
30 REFMAC5	R=0.20 RFre
29 REFMAC5	R=0.20 RFre
28 REFMAC5	R=0.20 RFre
27 REFMAC5	R=0.24 RFre
26 REFMAC5	R=0.20 RFre
25 REFMAC5	R=0.24 RFre
24 BUCCANEER	R=0.18 %=1
23 BUCCANEER	R=0.26 %=9
22 MOLREP	R=0.23 RFre
21 Expert MR - PHASER	R=0.23 RFre
20 REFMAC5	R=0.20 RFre
19 REFMAC5	R=0.24 RFre
18 REFMAC5	R=0.20 RFre
17 REFMAC5	R=0.20 RFre
16 REFMAC5	R=0.20 RFre
15 REFMAC5	R=0.20 RFre
14 REFMAC5	R=0.20 RFre
13 REFMAC5	R=0.20 RFre
12 REFMAC5	R=0.24 RFre
11 REFMAC5	
10 REFMAC5	R=0.24 RFre
9 BUCCANEER	
8 REFMAC5	

Job 40: Interactive model preparation - CCP4mg and MrBUMP The job is Pending

Input

Results

Comments

Input data

Job title

CCP4mg MrBUMP

Use data from job

27 Refinement - REFMAC5

as input below..

Sequences:

Show list

Sequence

22 gamma

Non-redundancy level for homologue search:

95



Display Table

Create object Tools

Display Table Simplified Display Table

Run blastp on this sequence locally
 Run blastp on this sequence on EBI server
 Run MrBUMP to find search models using 50% similar set.
 Run MrBUMP to find search models using 70% similar set.
 Run MrBUMP to find search models using 90% similar set.
 Run MrBUMP to find search models using 95% similar set.
 Run MrBUMP to find search models using 100% similar set.
 Previous MrBUMP runs
 Delete MrBUMP results

Sequence Viewer

gamma_ ☐

MHHHHHHLLVPRGSEMIPISTAYSKNGLKIEFTTFERSNTNPSTVTVITIQASNSTELDMTDFVFPQAAVPKTFQLQLLSPSSSVVPFNTCTITQVIKVLNPQKQQLRMRIKLTYNHKGSAQDLAEVNNFPPI

 Running MrBUMP search for gamma . Please wait...

Running MrBUMP search for gamma . Please wait...

☒ Show other log files

☐ Show MrBUMP output

☐ Show domains view

```
http_proxy not specified in environemnt
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
```

```
#####
#####
#####
### CCP4 7.0: MRBUMP                      version 00.9.00 : 26/01/15##
#####
User: stuart  Run date: 09/06/2017 Run time: 09:42:29
```

Display models for

Domain 1

Show residues with gesamt variance $\leq$: 0



☐ Show MrBUMP models

☐ Show unsculpted PDB models

Close MrBUMP models

Close

Cancel

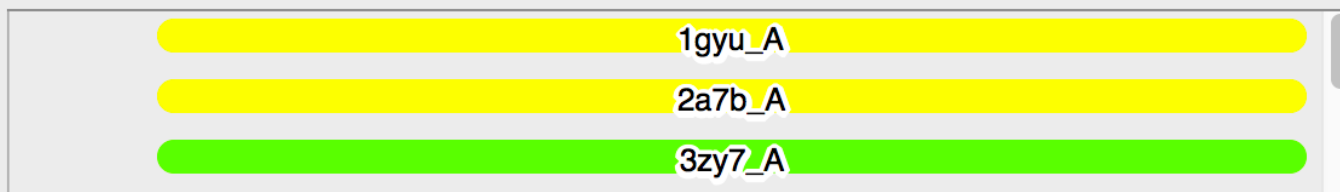
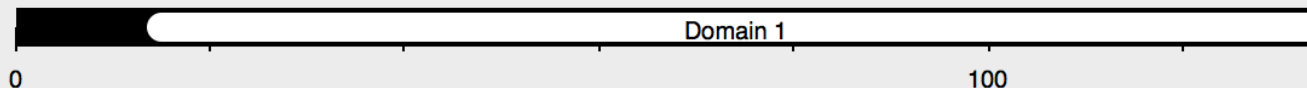
Finished MrBUMP search

Finished MrBUMP search

☐ Show other log files

☐ Show MrBUMP output

☒ Show domains view



Display models for

Domain 1

Show residues with gesamt variance $\leq$: 0



☒ Show MrBUMP models

☐ Show unsculpted PDB models

Close MrBUMP models

Close

Cancel

CCP4MG version 2.10.9

Glycan viewer

Display Table

Create object Tools

sculpt_2a7b_A1

All .. ice .. Ribb..

Finished MrBUMP search

Finished MrBUMP search

☐ Show other log files ☐ Show MrBUMP output ☒ Show domains view

Domain 1

0 100

1gyu_A

2a7b_A

3zy7_A

Display models for Domain 1

Show residues with gesamt variance <= : 0 110

☒ Show MrBUMP models ☐ Show unsculpted PDB models

Close MrBUMP models Close Cancel

gamma_ ☐ MHHHHHHLVPRGSEMIPSITAYSK

sculpt_2a7b_A1_A ☐ MIPSITAYS NGL I EFT F E S N T

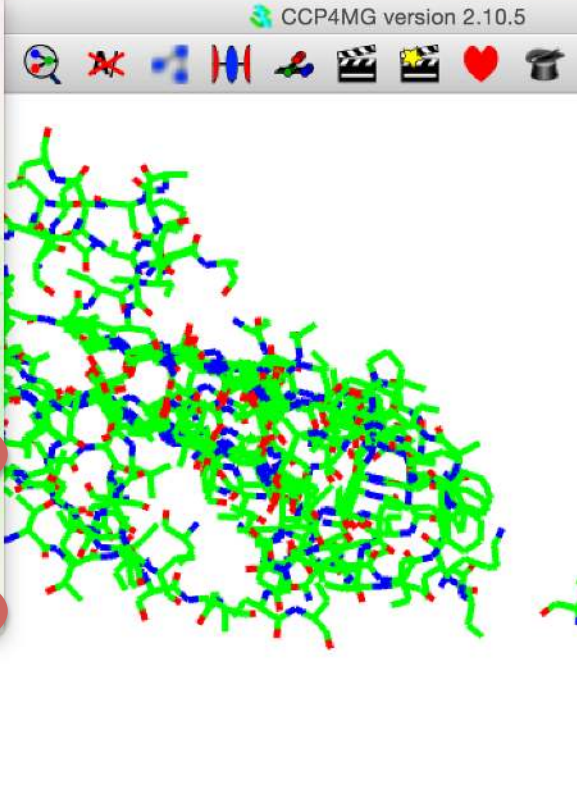
sculpt_1gyu_A1_A ☐ MIPSITAYS NGL I EFT F E S N T

sculpt_3zy7_A1_A ☐ MIPSITAYS NGL I EFT F E S S V

sculpt_2e9g_A1_A ☐ IPSITAYS NGL I EFT F E S N T

Origin: 1.319 -46.302 -27.456 | Size: 1028 x 615

Then use the variance slider to choose atoms.



Help

Display Table Simplified Display Table

Sequence Viewer

Model	Alignment	Score	Sequence
unkgamma_			HHHHHHLVPRGSHMIPSITAYSKNGLKIEFTFERSNTNPSTVITIQASNSTELDMTDFVPQAAVPKTFQLQLLSPSSSVVPAFNTTITQVVKVLNPKQQLRMRIKLTYNHRGSAMQDLAEV
sculpt_1gyu_A_A			-----MIPSITAYSKNGLKIEFTFERSNTNPSTVITIQASNSTELDMTDFVPQAAVPKTFQLQLLSPSSSVVPAFNTTITQVVKVLNPKQQLRMRIKLTYNHRGSAMQDLAEV
sculpt_1iu1_A_A			-----MIPSITAYSKNGLKIEFTFERSNTNPSTVITIQASNSTELDMTDFVPQAAVPKTFQLQLLSPSSSVVPAFNTTITQVVKVLNPKQQLRMRIKLTYNHRGSAMQDLAEV
sculpt_1iur_A_A			HHHHHHLVPRGS-----TVITIQASNS-----KTFQLQLLSPSSSVVPAFNTTITQVVKVLNPKQQLRMRIKLTYNHRGSAMQDLAEV-----RGS-----
sculpt_1p4u_A_A			---HHHVPRGSHMIPSITAYSKNGLKIEFTFERSNTNPSTVITIQASNSTELDMTDFVPQAAVPKTFQLQLLSPSSSVVPAFNTTITQVVKVLNPKQQLRMRIKLTYNHRGSAMQDLAEV
sculpt_2lxe_A_A			HHHHHHLVPRGSHM-----VTITIQASNSTELDMTDFVPQAAVPKTFQLQLLSPSSSVVPAFNTTITQVVKVLNPKQQLRMRIKLTYNHRGSAMQDLAEV-----KLTYNHRGS
sculpt_2m7a_A_A			HHHHHHLVPRGSHMIPSITAYSKN-----GLKIENPSTVITIQASNSTELDMTDFVPQAAVPKTFQLQLLSPSSSVVPAFNTTITQVVKVLNPKQQLRMRIKLTYNHRGSAMQDLAEV

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.



× 📄
Display Table

Create object
Tools

+

5a3h

Display Table
Simplified Display Table

Sequence Viewer

5a3h_A
☐

13
23
33
43
53
63
73
83
93
103
113
123

SVVEERGLSISNGELVNEGEQVQLGMSSEGLQWYGGFVNYESMMLDDWGINVFAAMYTSSGGYIDDPVKEVKEAVEAAIDLDIYVIIDWHILSDNDPNIXEEADFFDEMSELYG DY

Run blastp on this sequence locally
Run blastp on this sequence on EBI server
Run mrbump to find search models
Previous mrbump runs
Delete MrBump results

Thu Mar 10 12:01:47 2016
Fri Mar 11 13:29:52 2016
Fri Mar 11 13:35:35 2016
Fri Mar 11 13:37:48 2016

CCP4MG version 2.10.10

Display Table

Create object Tools

sculpt_2a7b_A1

Mr Bump results from Tue Nov 21 13:43:45 2017

Mr Bump results from Tue Nov 21 13:43:45 2017

Show other log files

Show MrBUMP output

Show domains view

Domain 1

0100

1gyu_A

2a7b_A

3zy7_A

2e9g_A

2dwy_A

1p4u_A

3im9_A

Display models for

Domain 1

Show residues with gesamt variance <= : 0110

Show MrBUMP models

Show unsculpted PDB models

Close MrBUMP models

gamma_

sculpt_2a7b_A1_A

sculpt_1gyu_A1_A

sculpt_3zy7_A1_A

MHHHHHHLVPRGSHMIPSITAYSK

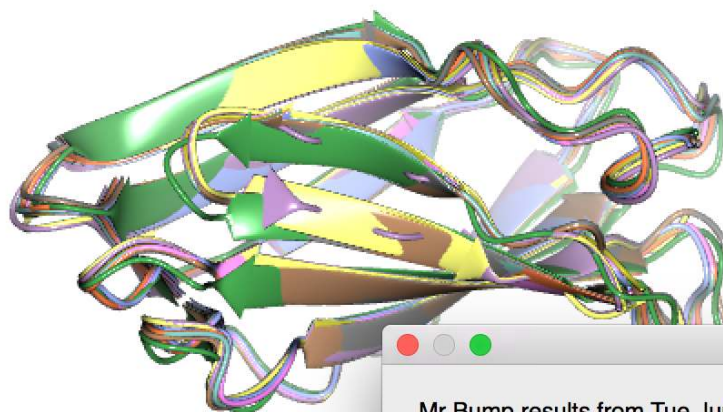
NIPSITAYSKNGLKIEFTFERSNT

NIPSITAYSKNGLKIEFTFERSNT

NIPSITAYSKNGLKIEFTFERSNV

TECTMAVGVVYVTEPDDC

Origin: 1.319 -46.302 -27.456 | Size: 753 x 411



Display Table

Create object Tools

	sculpt_2a7b_A
	sculpt_1gyu_A
	sculpt_1iu1_B
	sculpt_1iu1_A
	sculpt_1gyv_A
	sculpt_1gyw_B
	sculpt_1gyw_A

Mr Bump results from Tue Jun 7 13:27:46 2016

http_proxy not specified in environemnt
!--SUMMARY_BEGIN-->

```
#####  
#####  
#####  
### CCP4 7.0: MRBUMP          version 00.9.00 : 26/01/15##  
#####  
User: stuart  Run date: 07/06/2016 Run time: 13:27:27
```

Operating System: darwin
Python Version:
2.7.10 (default, Oct 2 2015, 00:28:39)
[GCC Intel(R) C++ gcc 4.2 mode]
Python location:

Show residues with gesamt variance <= : 0 110

☐ Show all log files ☒ Show simple log file

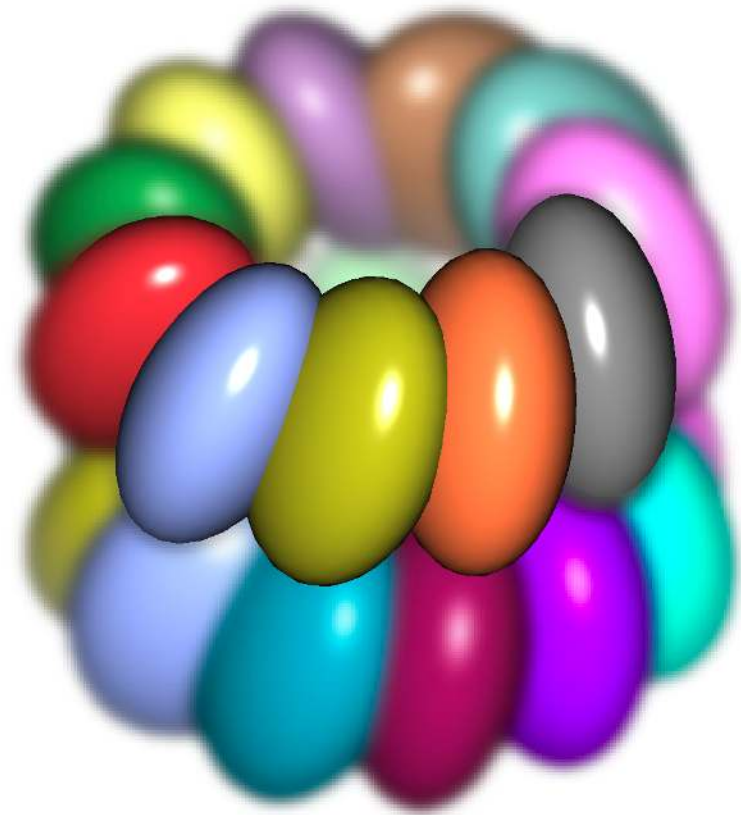
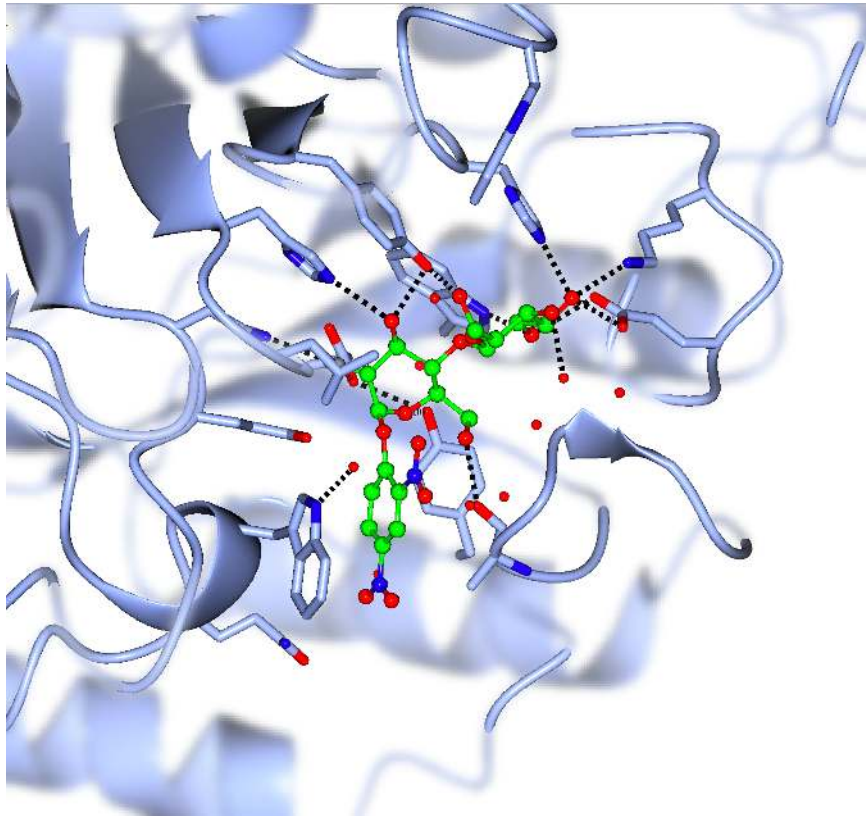
Load MrBump models

Close MrBump models

gamma_	☐			MHHHHHLLVPRGSEMI
sculpt_2a7b_A_A	☐			MIPSI
sculpt_1gyu_A_A	☐			MIPSI
sculpt_1iu1_B_B	☐			IPSI
sculpt_1iu1_A_A	☐			IPSI

Coming soon

Depth blur



Coming soon

- Better transparency
- (Python 3, purely technical)

Acknowledgements

- Programming:

- Liz Potterton
- Eugene Krissinel
- Kevin Cowtan
- Paul Emsley
- Martin Noble
- Jan Gruber

- Bernhard Lohkamp
- Rob Nicholls
- Ronan Keegan
- Jon Agirre

- General help:

Keith Wilson

Phil Evans

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

- Funding:

CCP4