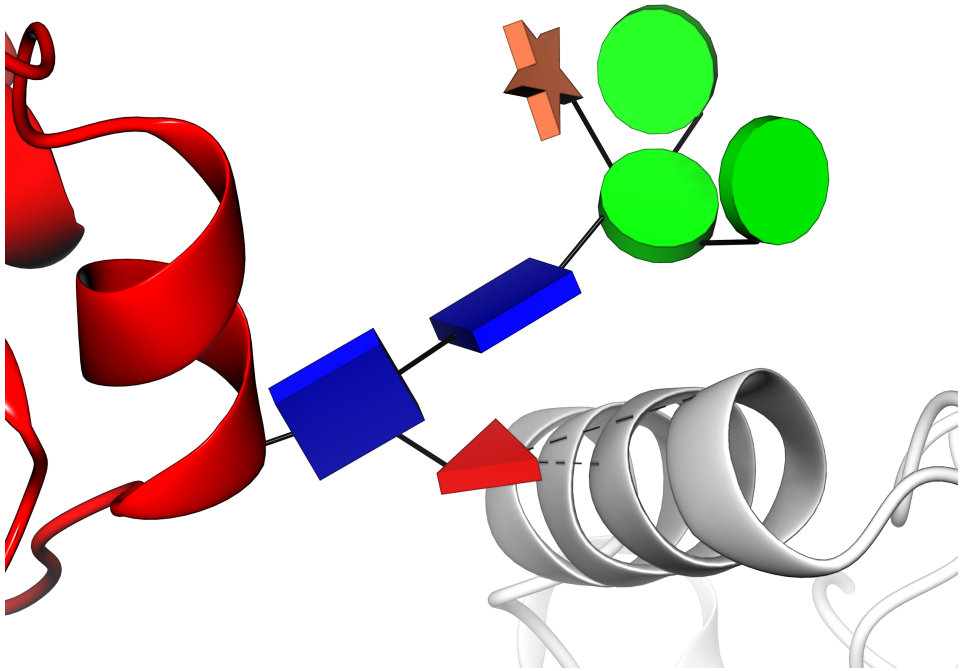
CCP4MG

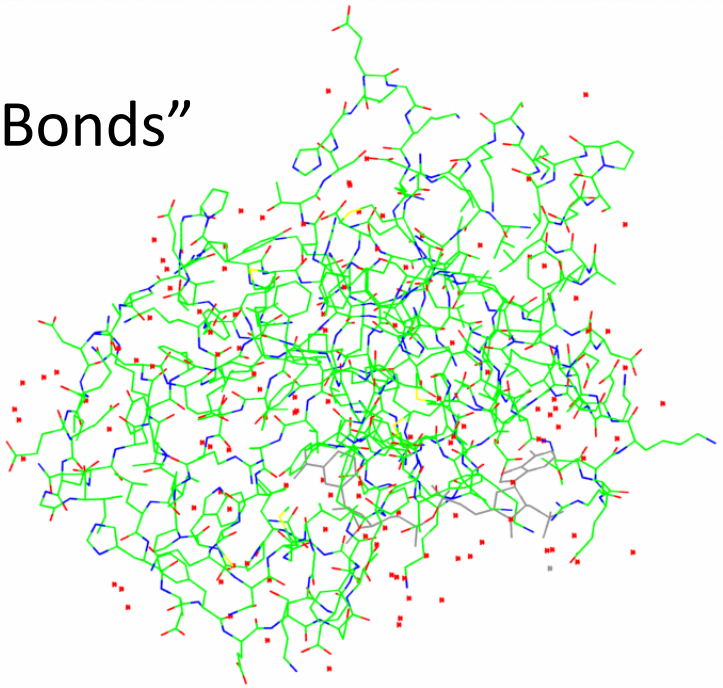


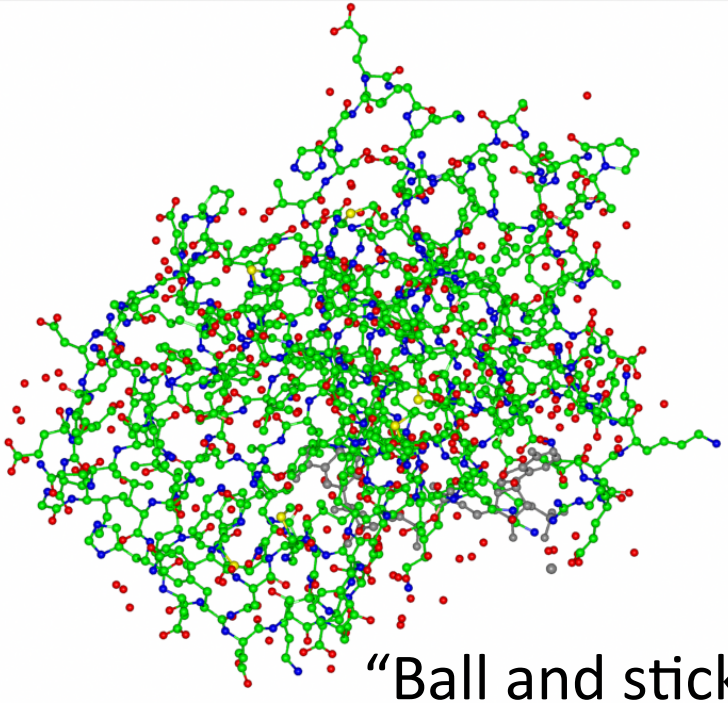
Diamond/CCP4 Workshop 2017

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.

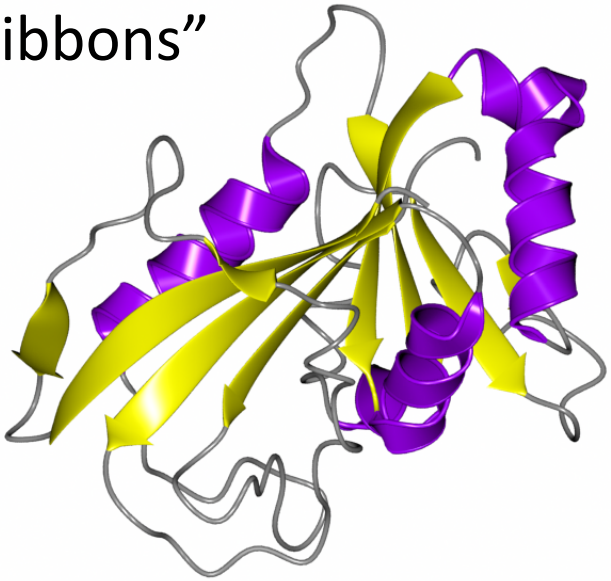
"Bonds"

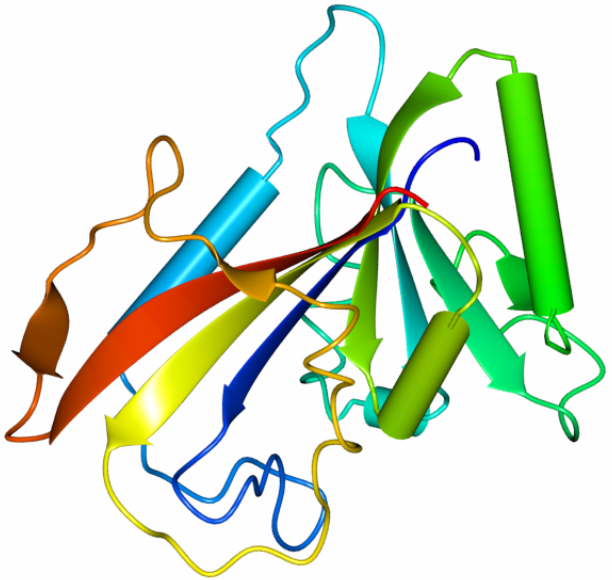




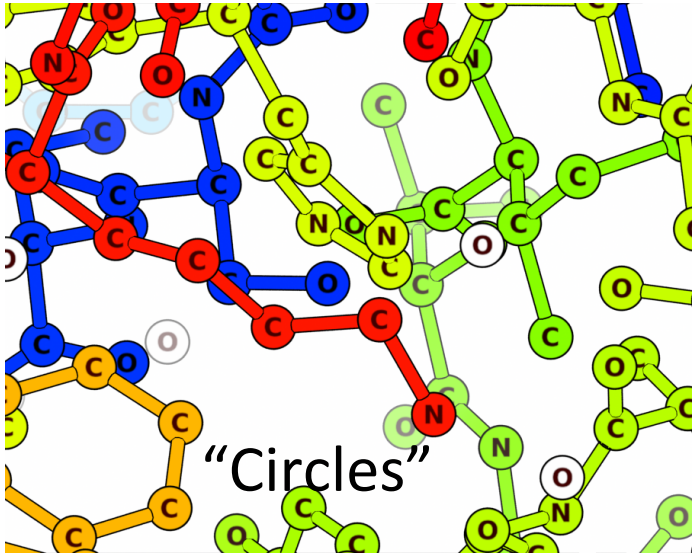
"Ball and stick"

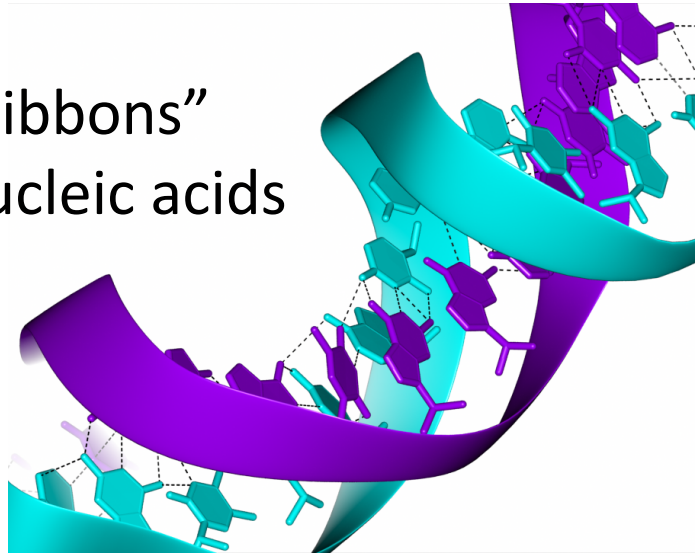
"Ribbons"

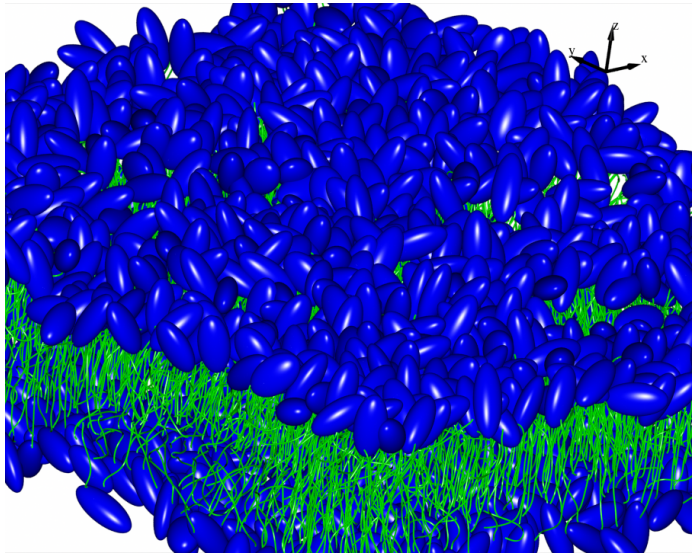




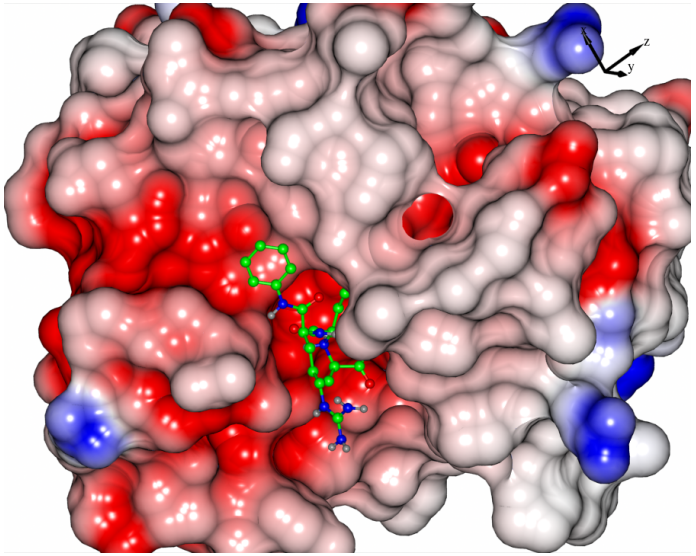
"Worms/tubes"



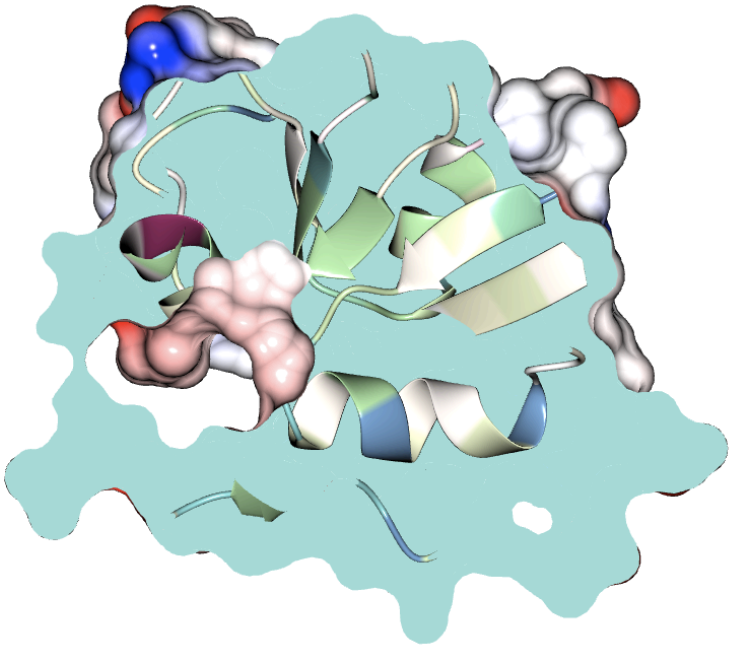


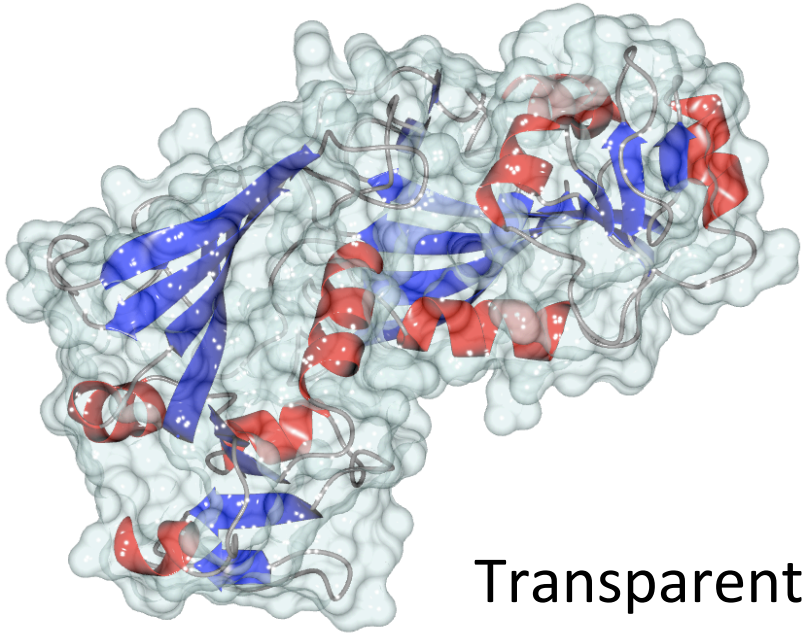


“Lipid Cartoon”



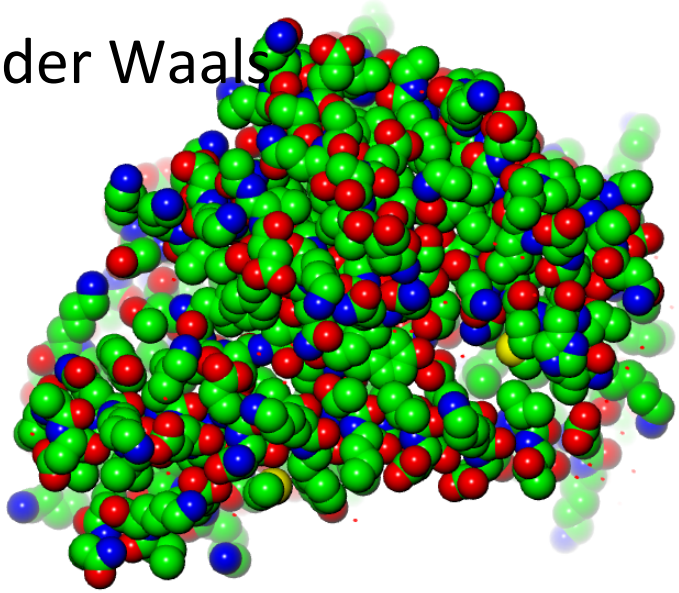
Electrostatic surface

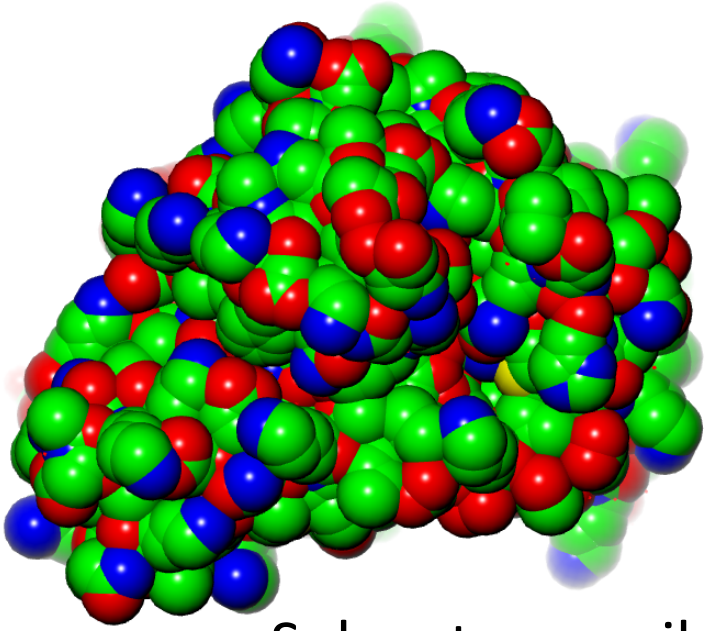




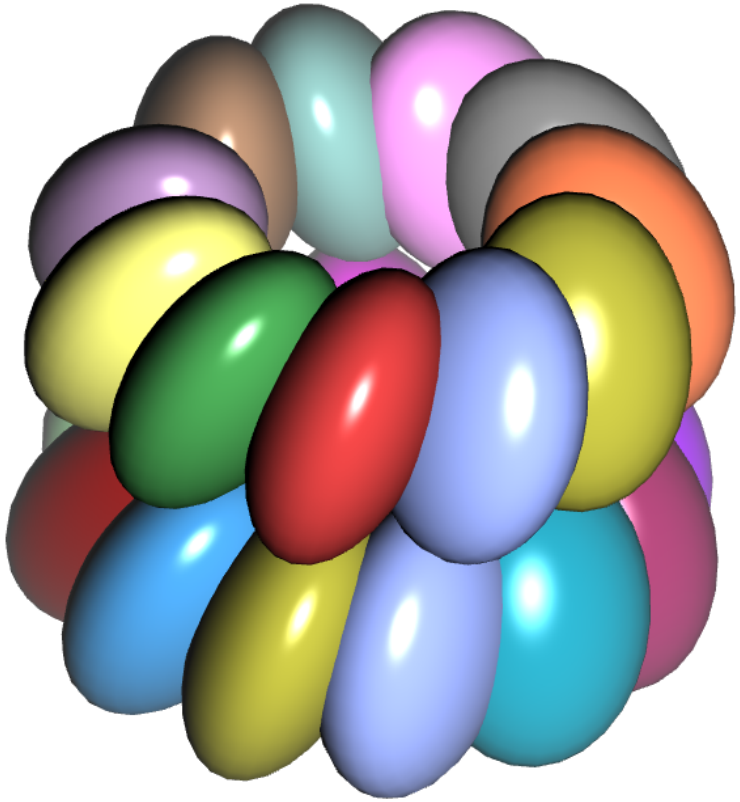
Transparent

Van der Waals

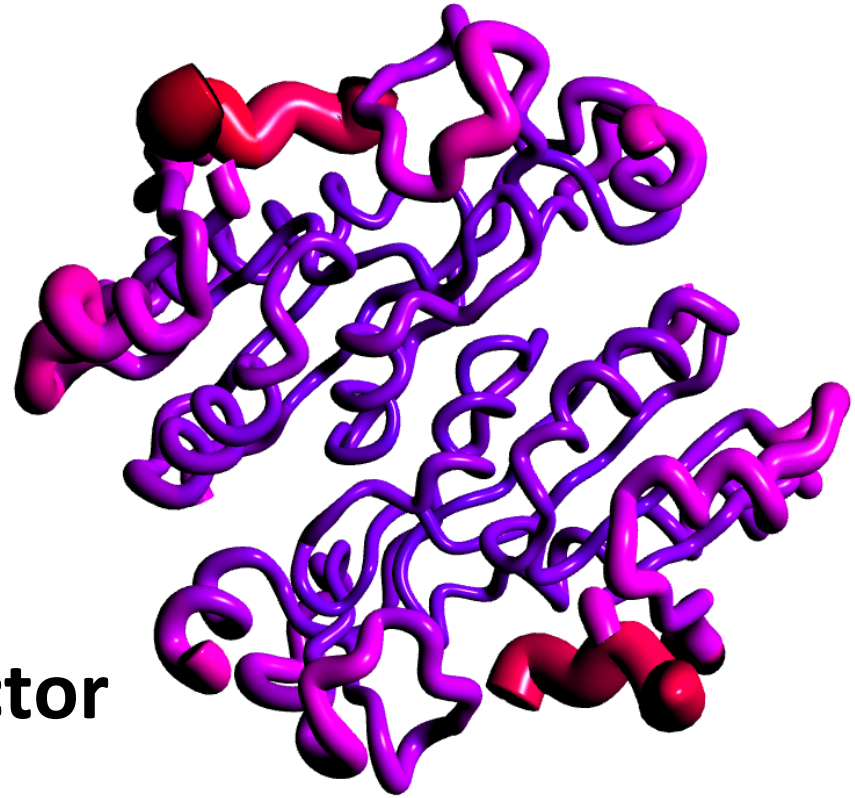




Solvent accessible

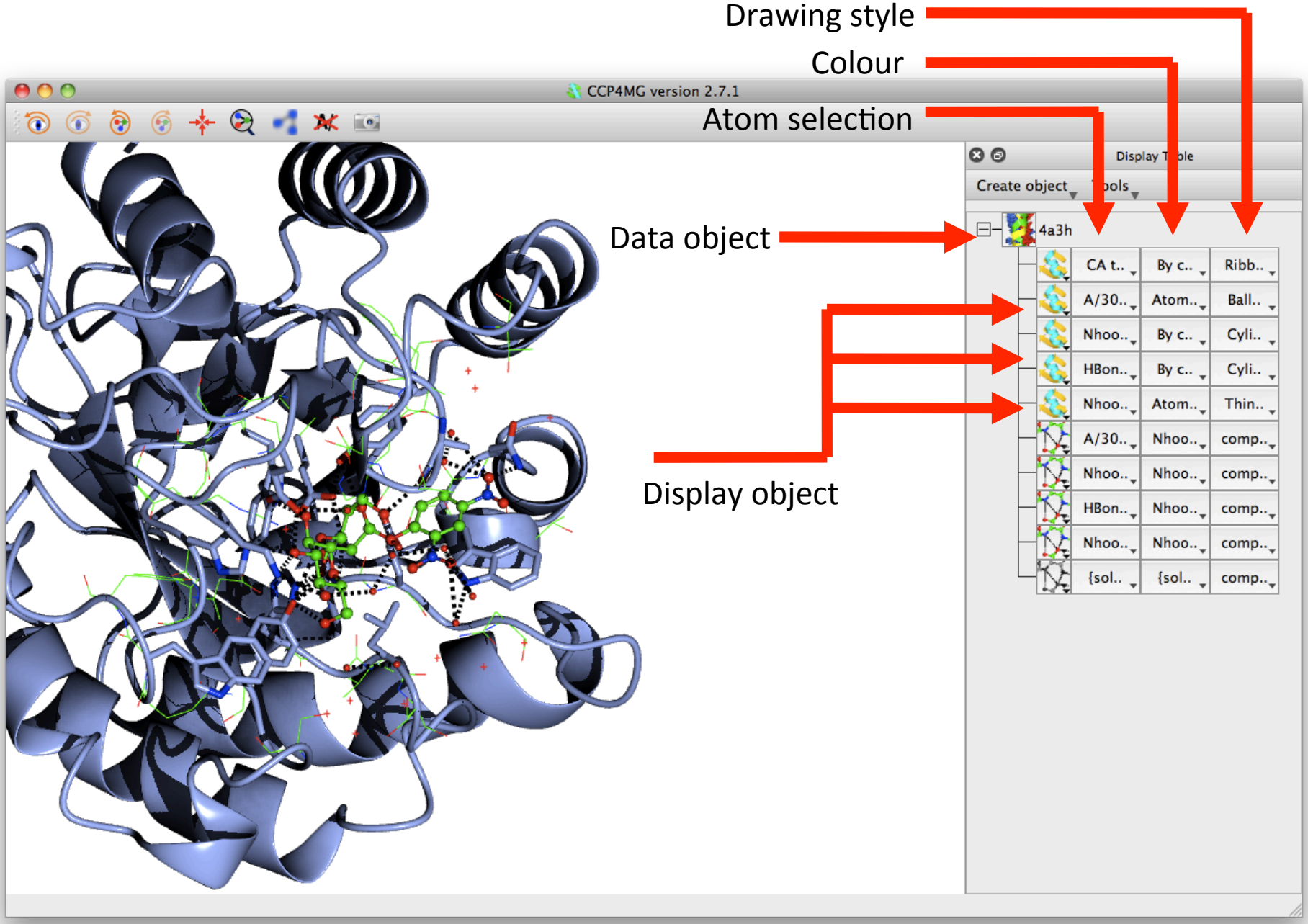


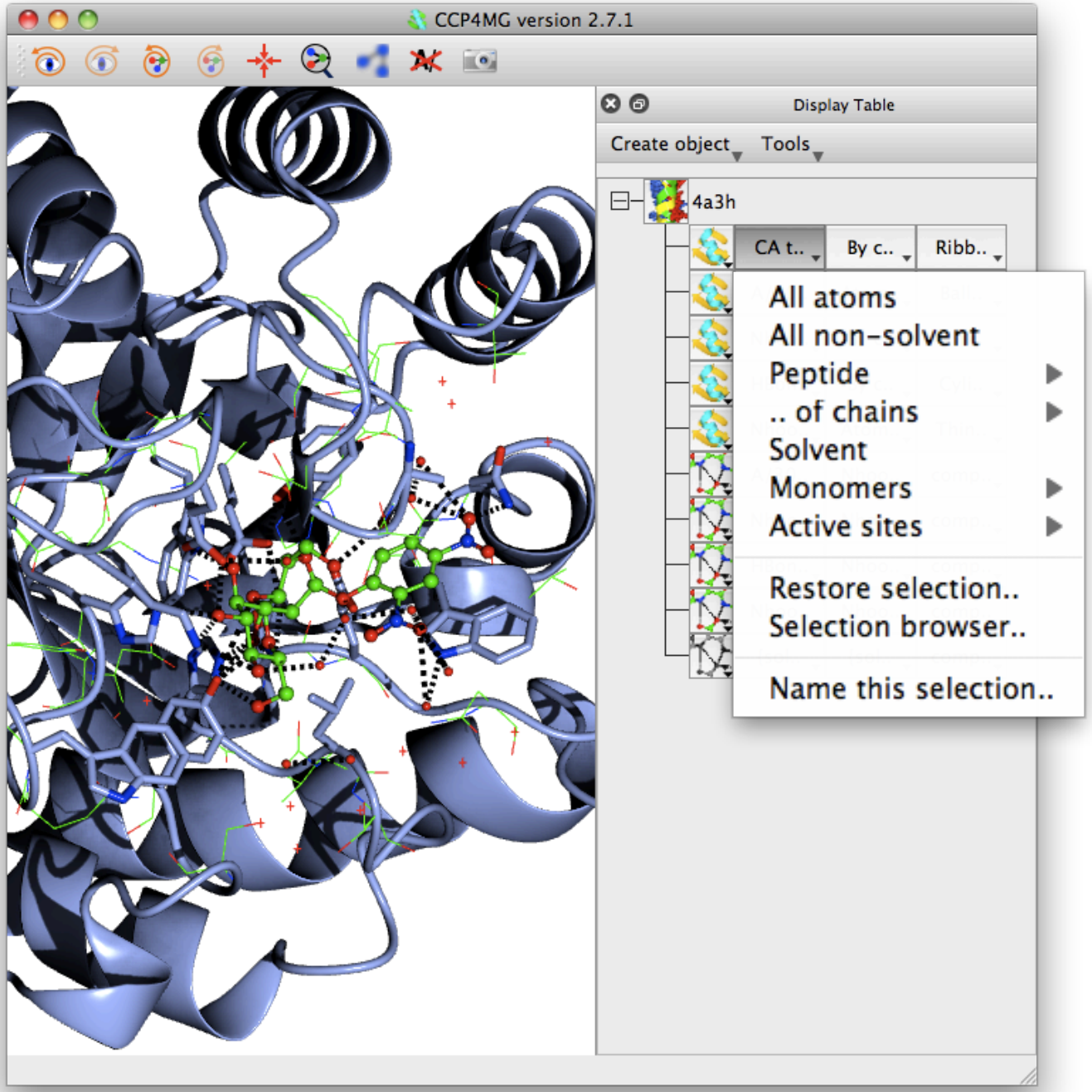
Bloboids



Worm scaled by Temperature factor

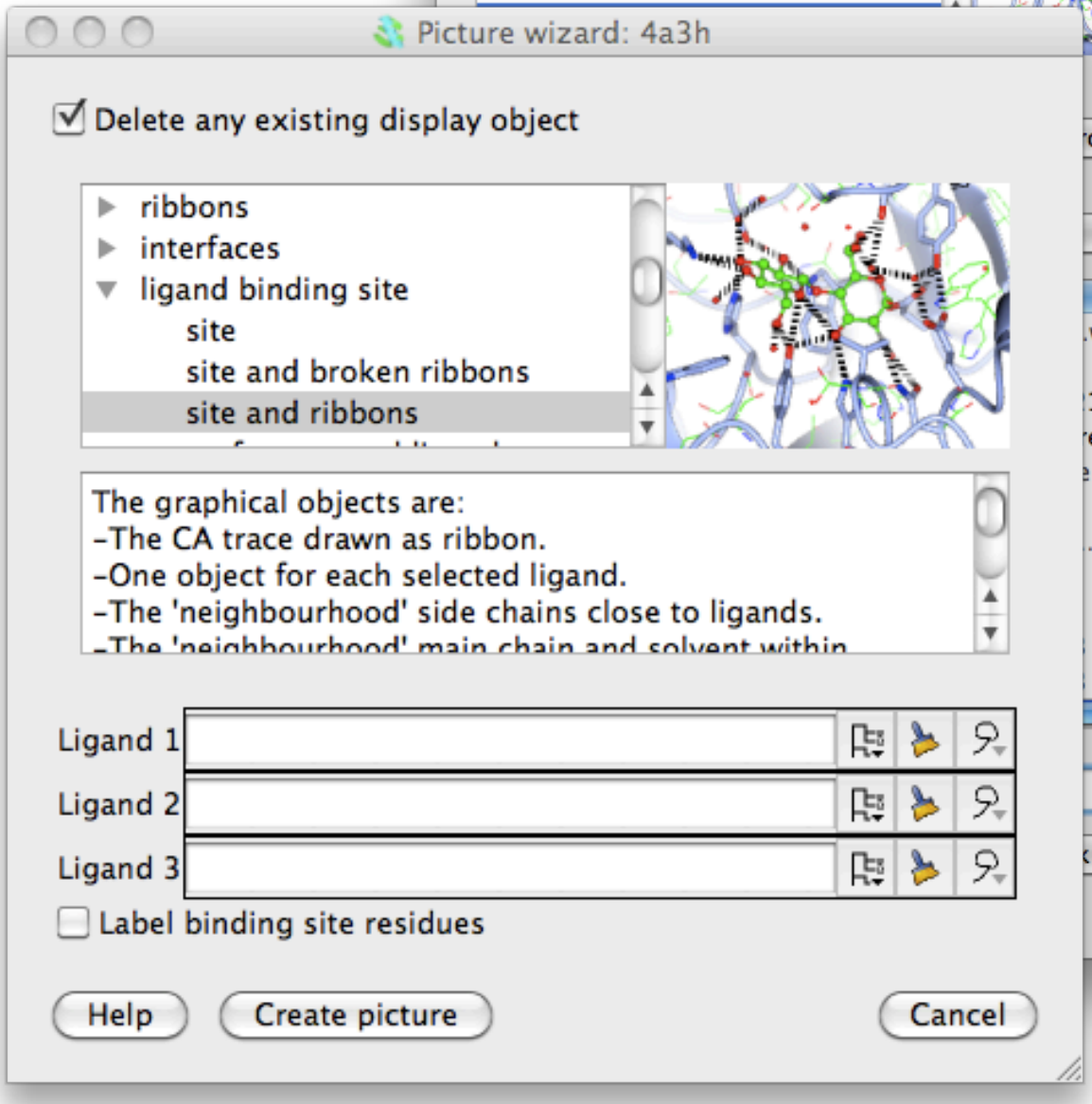
Basic user Interface


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

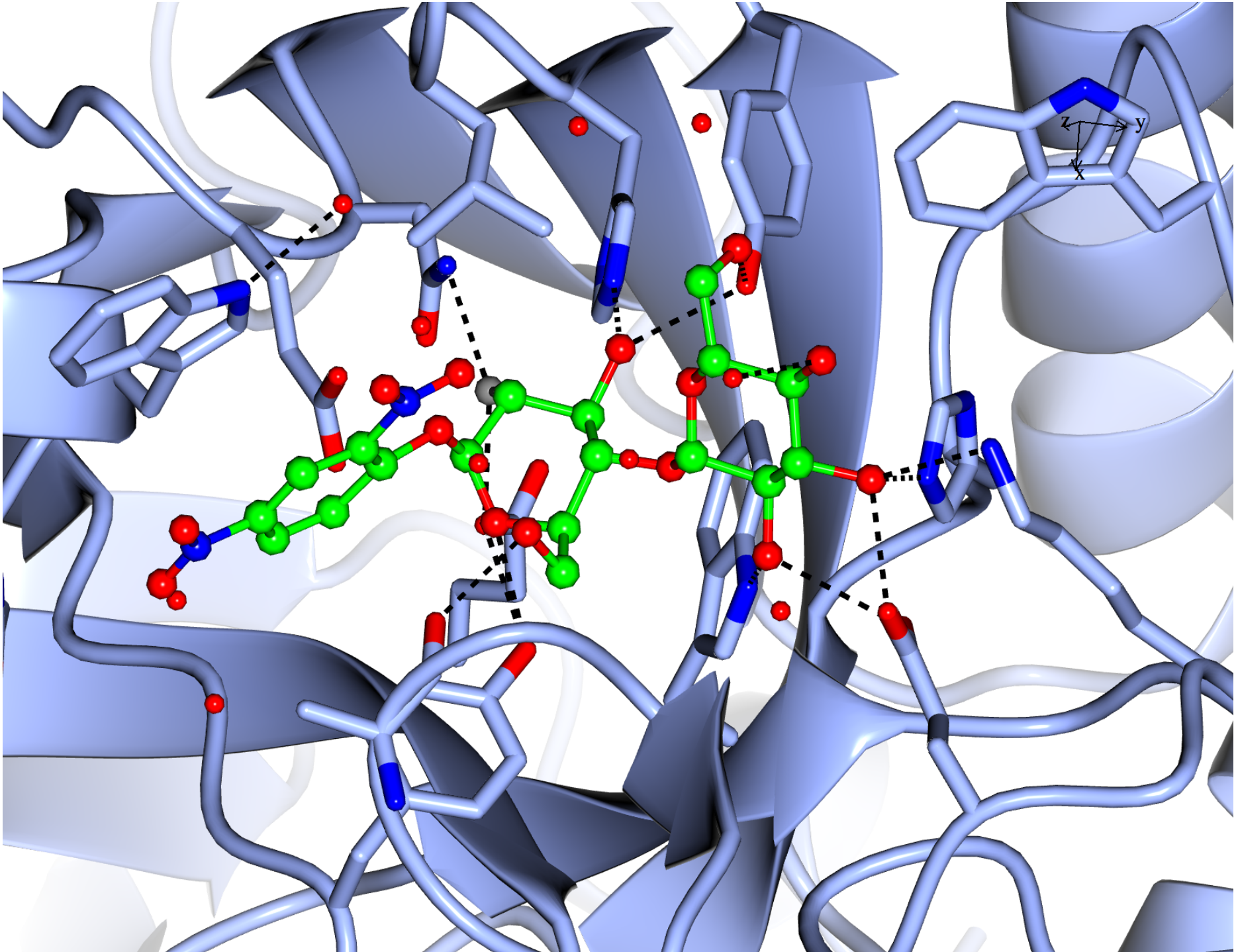

CCP4MG version 2.7.1
Display Table
Create object
Tools
4a3h
CA t..
By c..
Ribb..
All atoms
All non-solvent
Peptide
.. of chains
Solvent
Monomers
Active sites
Restore selection..
Selection browser..
Name this selection..

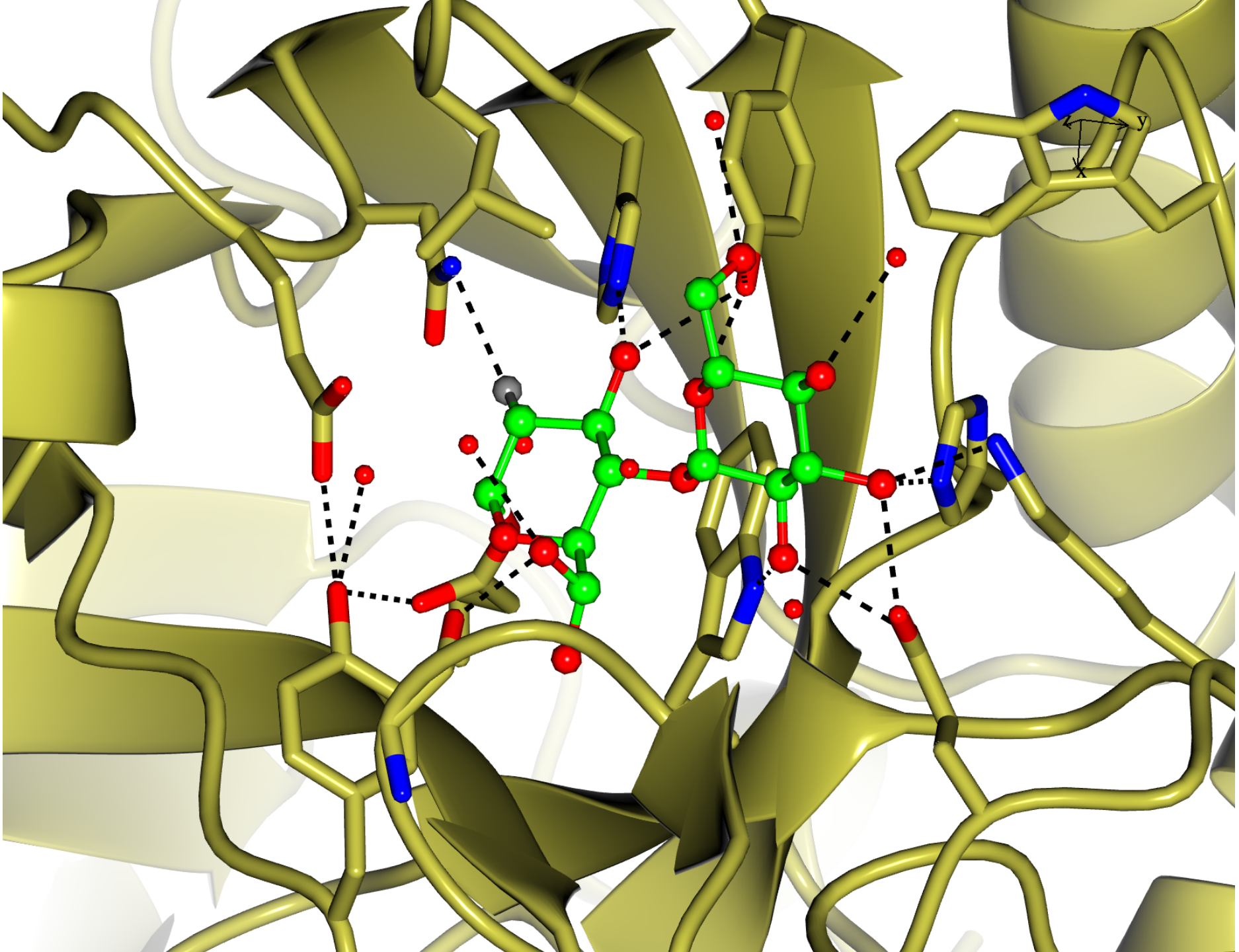
Picture Wizard

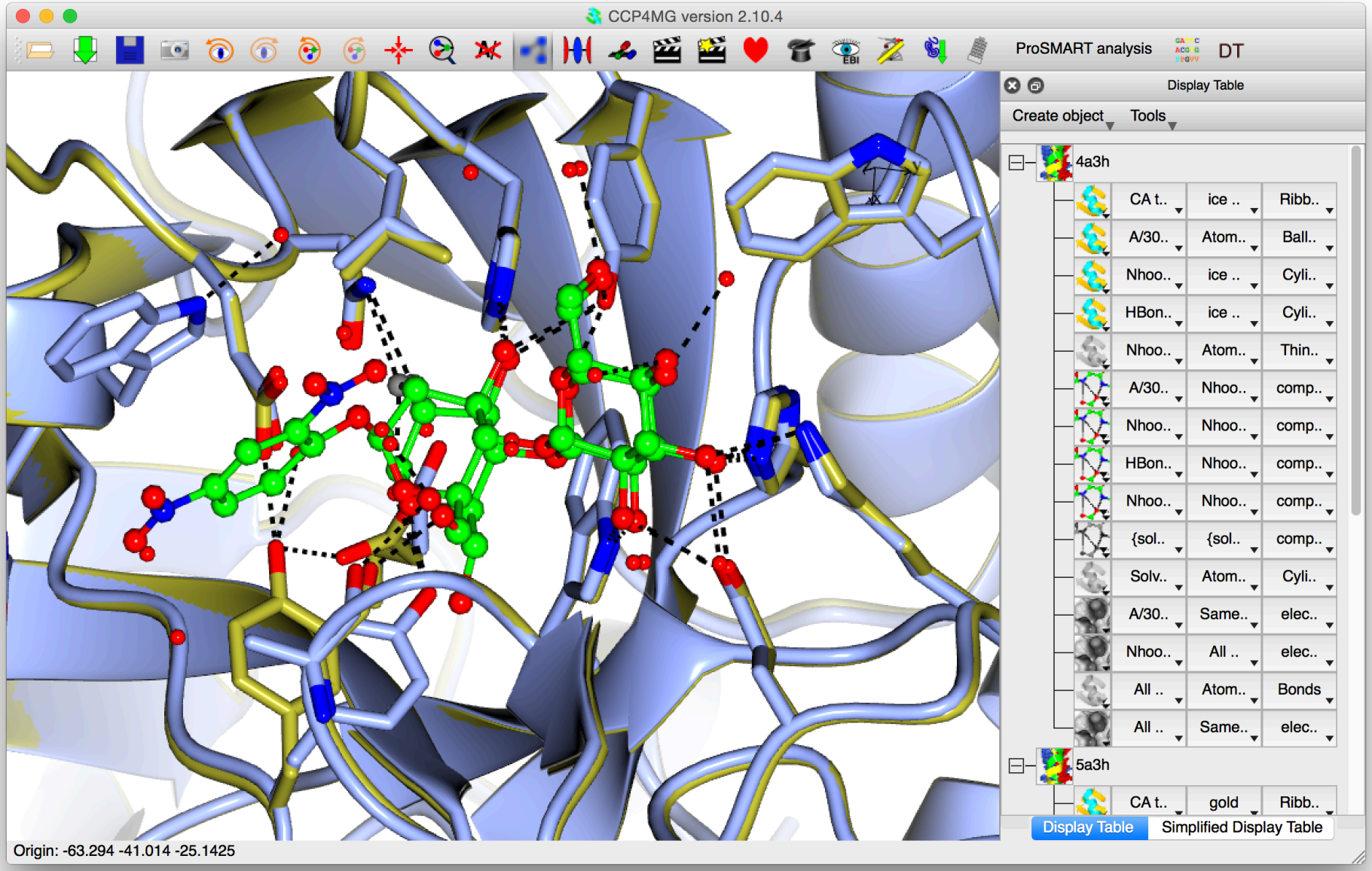
- The picture wizard is an automatic way of generating complex scenes with multiple selections, colouring, styles, etc.
- Representations are organised into various “styles”
- The picture wizard is shown at the top of the file browser window when a coordinate file is loaded, or can be accessed from the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


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.
Ligand 1
Ligand 2
Ligand 3
Label binding site residues
Help
Create picture
Cancel

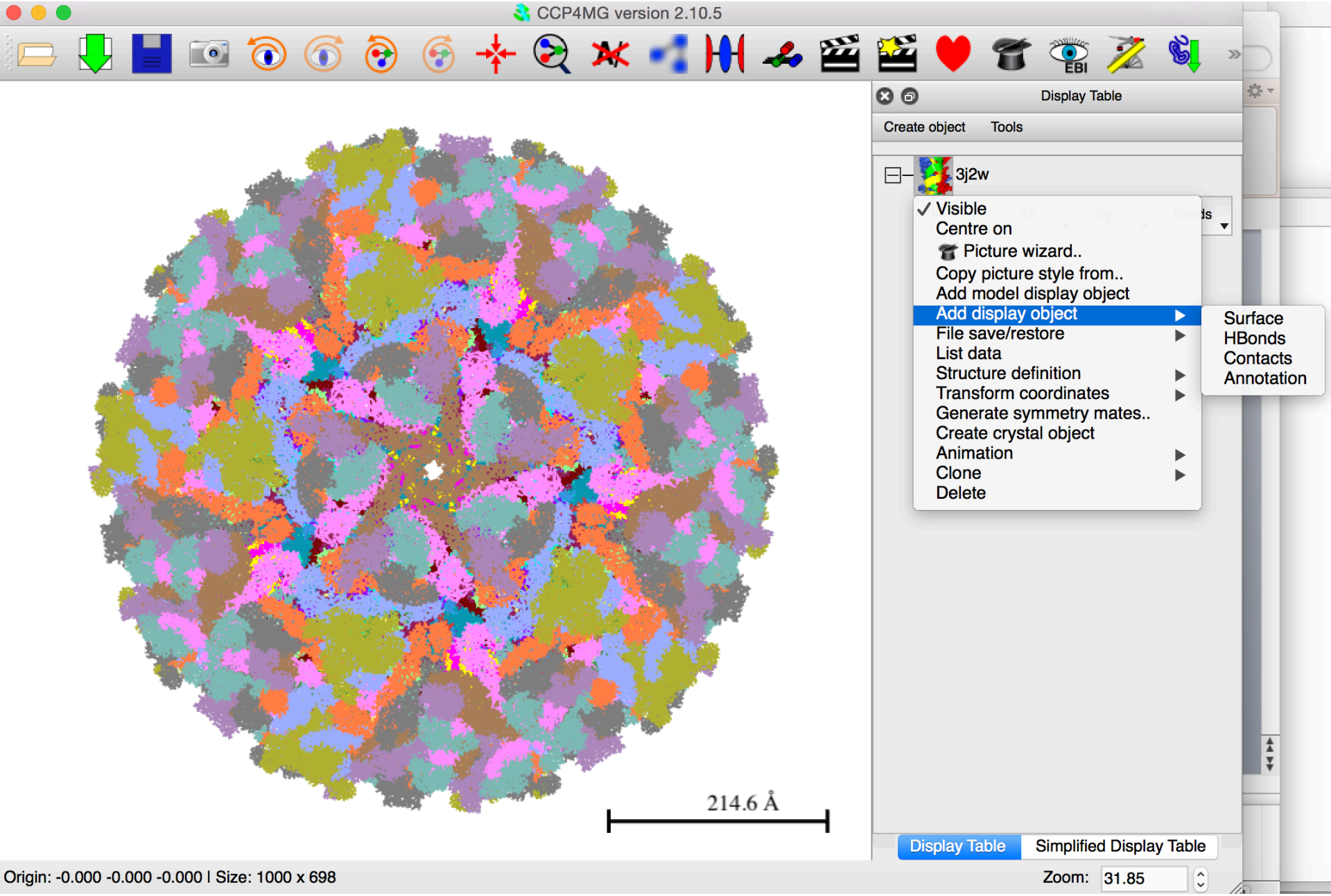
Open file(s)
interfaces
ligand binding site
site
site and broken ribbons
Picture wizard
Automatic picture setup
Open picture wizard choices
or ...
Size
Kind
241 KB
ppt File
Folder
1.7 MB
jpg File
Folder
16 KB
docx File
2.3 MB
png File
101 KB
pdf File
683 bytes
zip File
38 KB
py File
15 KB
doc File
10 KB
odt File
Open
Cancel

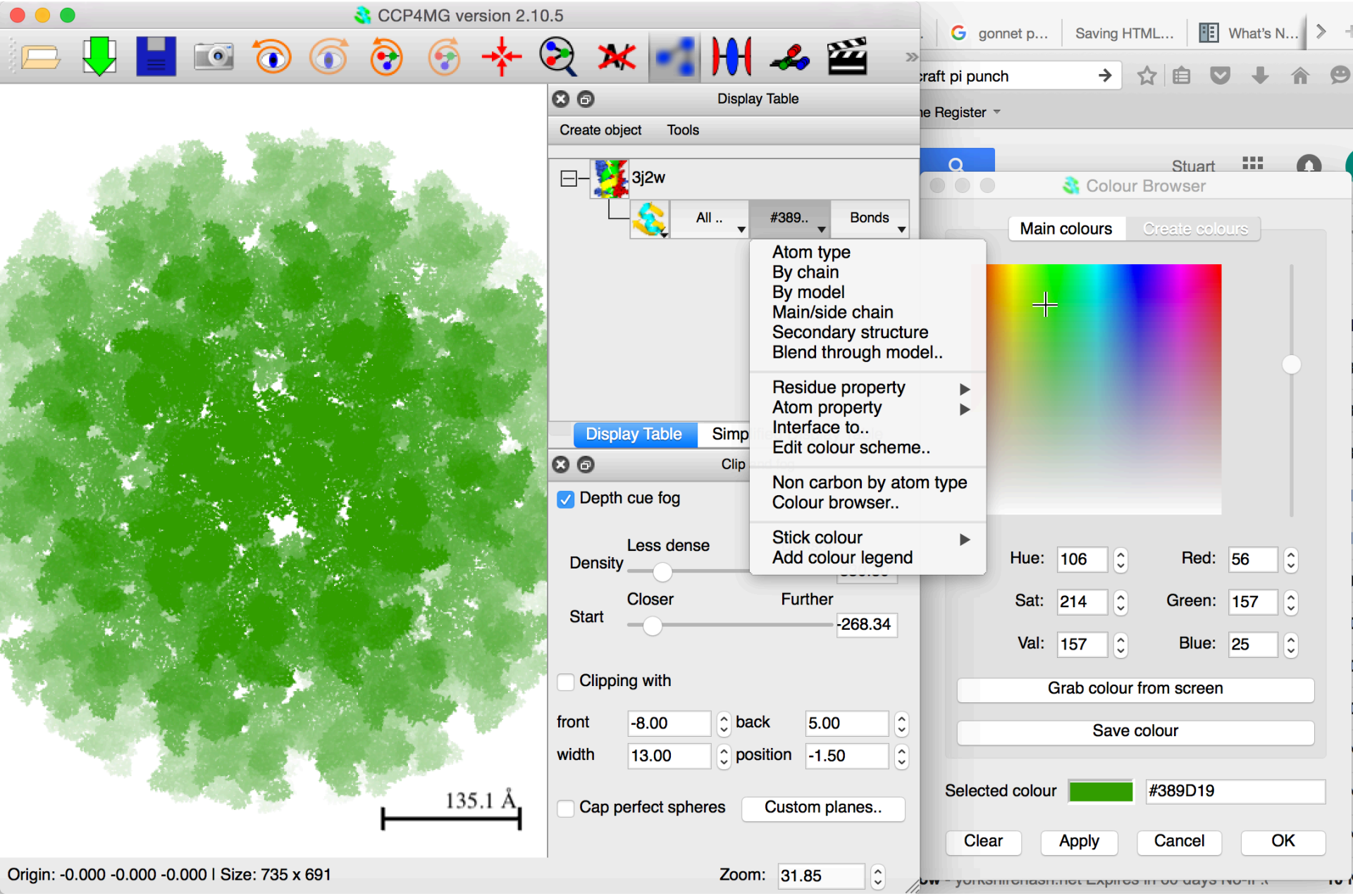

z
y
x

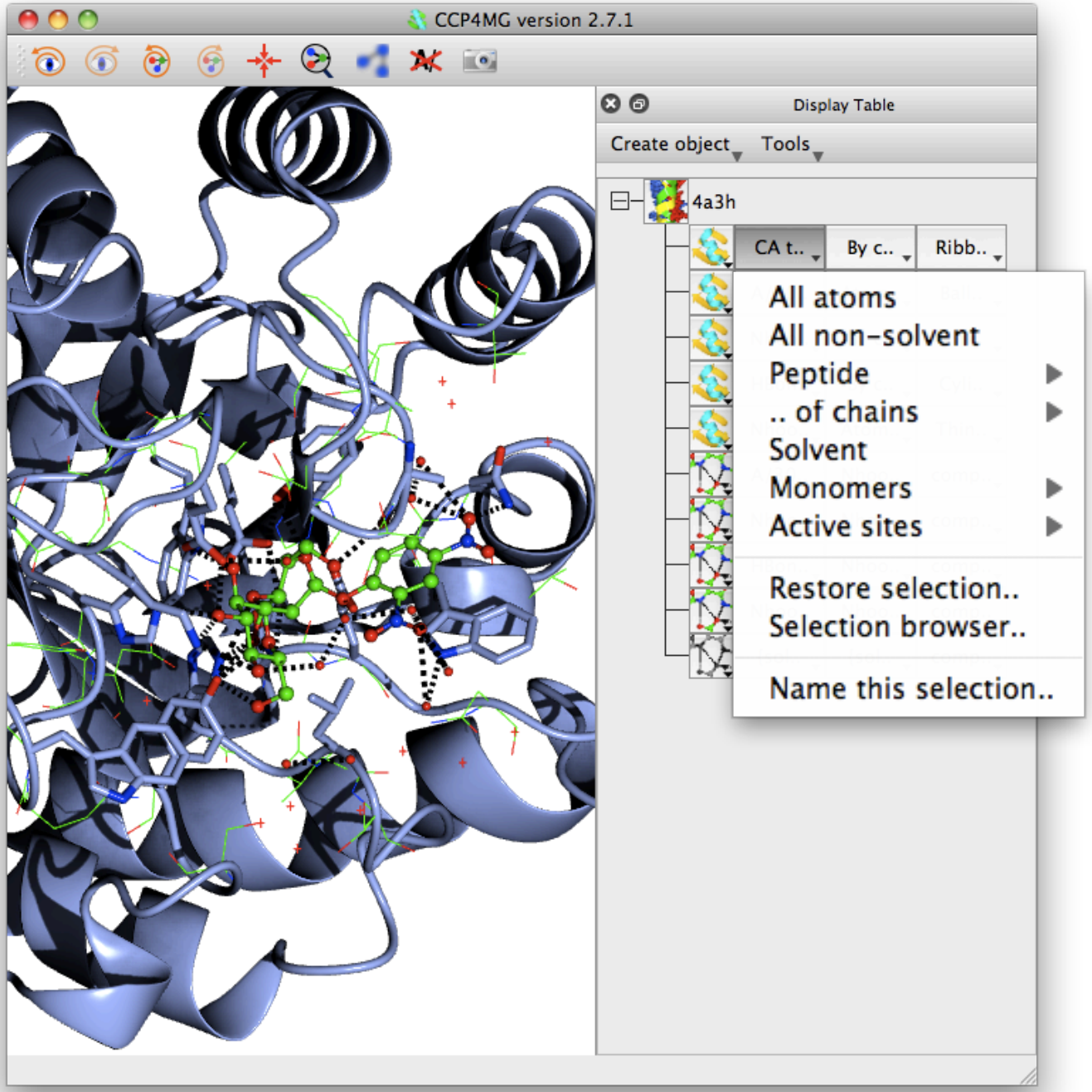

z
y
x

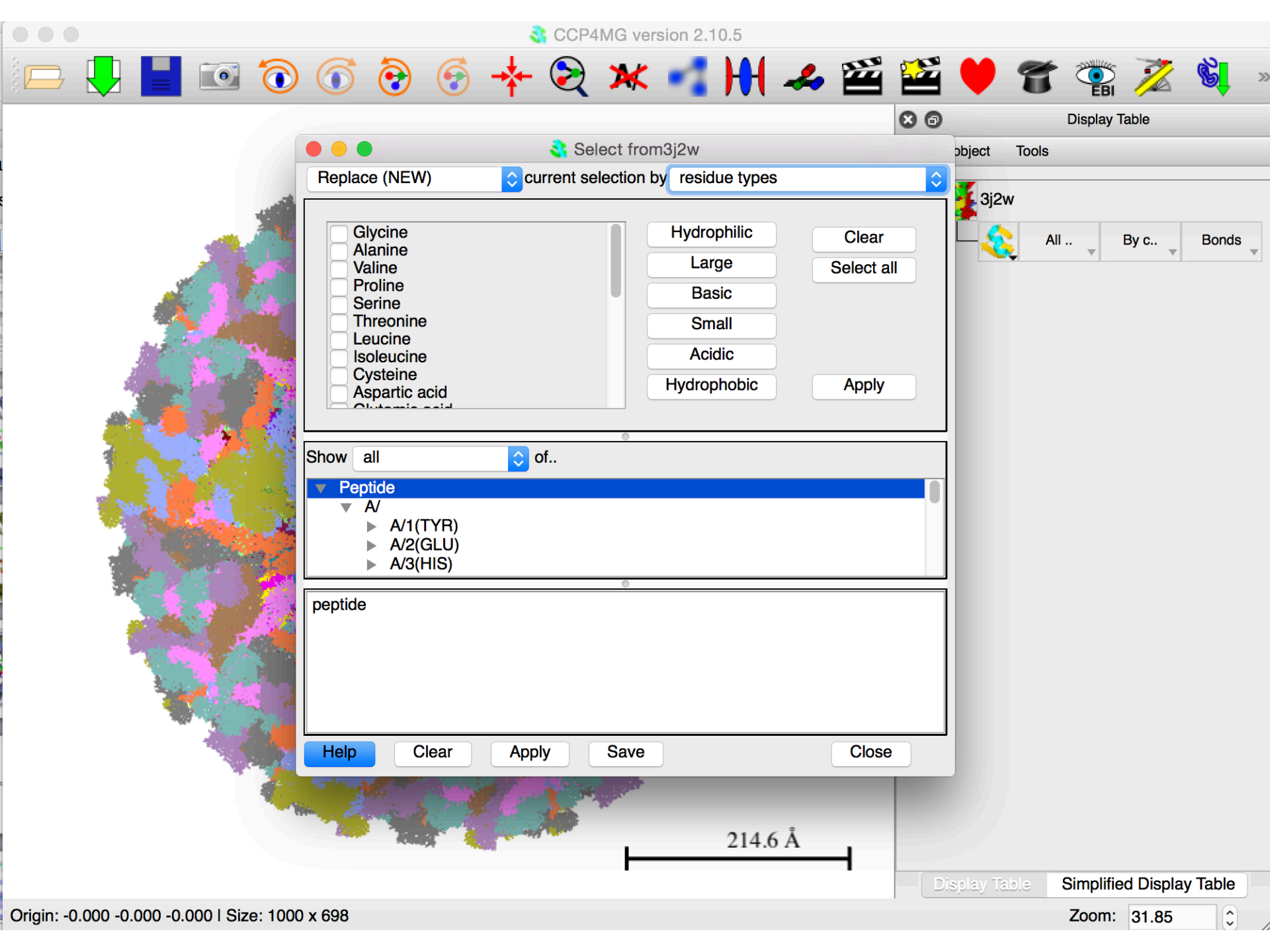

CCP4MG version 2.10.4
ProSMART analysis
DT
Display Table
Create object
Tools
4a3h
CA t.. ice .. Ribb..
A/30.. Atom.. Ball..
Nhoo.. ice .. Cyli..
HBon.. ice .. Cyli..
Nhoo.. Atom.. Thin..
A/30.. Nhoo.. comp..
Nhoo.. Nhoo.. comp..
HBon.. Nhoo.. comp..
Nhoo.. Nhoo.. comp..
{sol.. {sol.. comp..
Solv.. Atom..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

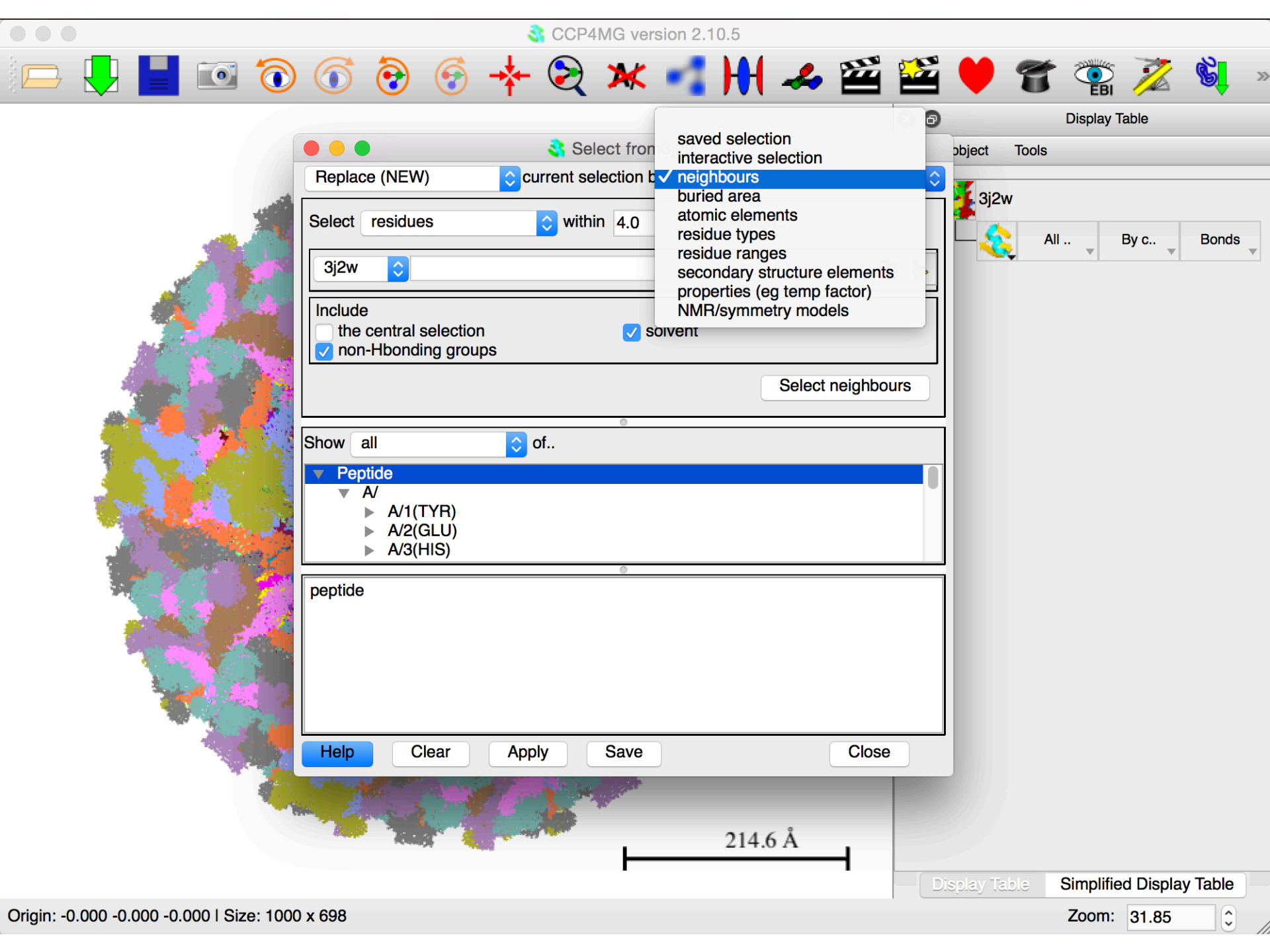
Doing it all Manually

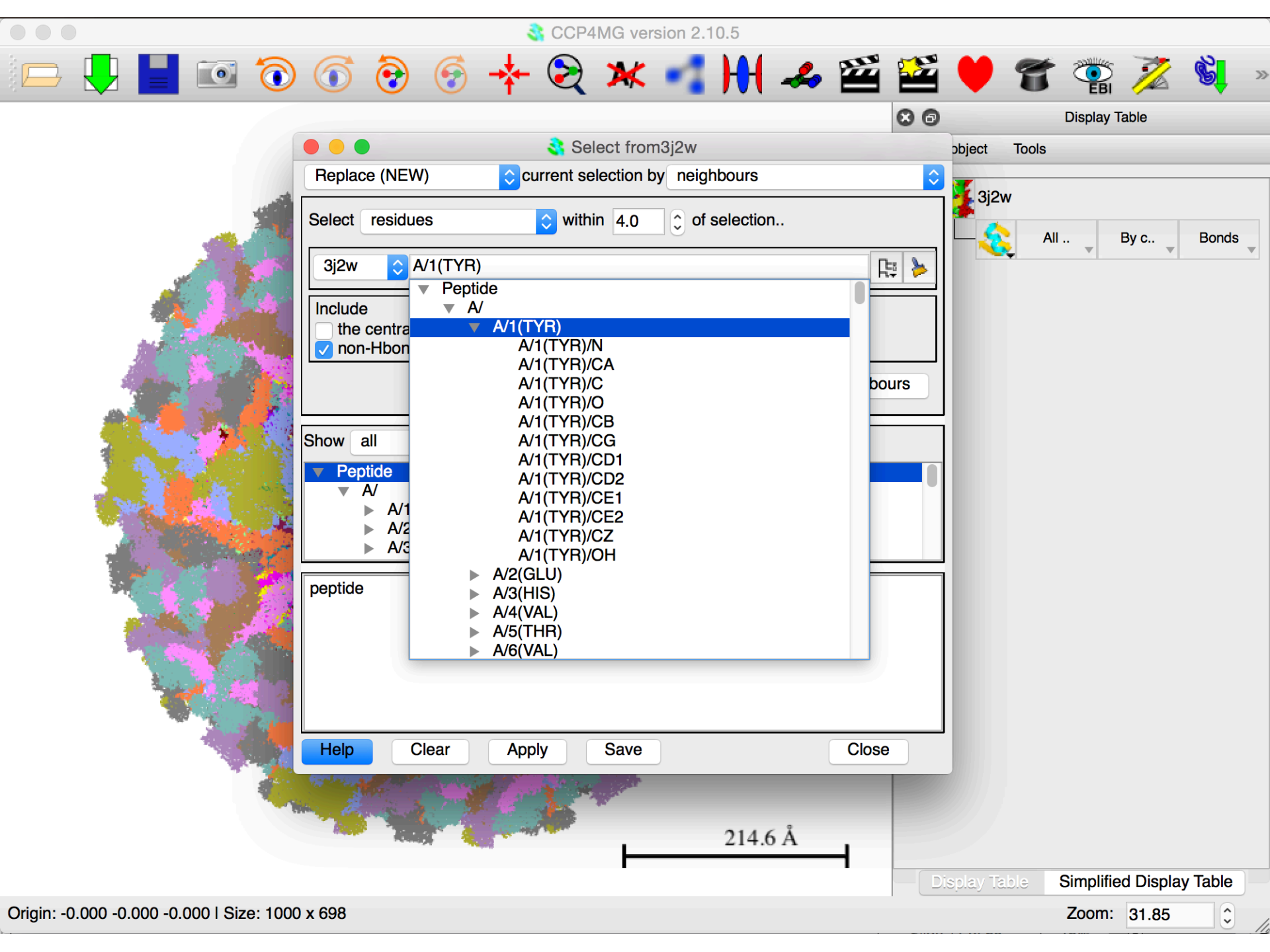

CCP4MG version 2.10.5
Display Table
Create object
Tools
3j2w
Visible
Centre on
Picture wizard..
Copy picture style from..
Add model display object
Add display object
File save/restore
List data
Structure definition
Transform coordinates
Generate symmetry mates..
Create crystal object
Animation
Clone
Delete
Surface
HBonds
Contacts
Annotation
214.6 Å
Display Table
Simplified Display Table
Origin: -0.000 -0.000 -0.000 | Size: 1000 x 698
Zoom:
31.85


CCP4MG version 2.10.5
Display Table
Create object
Tools
3j2w
All ..
#389..
Bonds
Atom type
By chain
By model
Main/side chain
Secondary structure
Blend through model..
Residue property
Atom property
Interface to..
Edit colour scheme..
Non carbon by atom type
Colour browser..
Stick colour
Add colour legend
Display Table
Simp
Clip
Depth cue fog
Density
Less dense
Start
Closer
Further
-268.34
Clipping with
front
-8.00
back
5.00
width
13.00
position
-1.50
Cap perfect spheres
Custom planes..
135.1 Å
Origin: -0.000 -0.000 -0.000 | Size: 735 x 691
Zoom:
31.85
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


CCP4MG version 2.7.1
Display Table
Create object
Tools
4a3h
CA t..
By c..
Ribb..
All atoms
All non-solvent
Peptide
.. of chains
Solvent
Monomers
Active sites
Restore selection..
Selection browser..
Name this selection..


CCP4MG version 2.10.5
Display Table
Select from3j2w
Replace (NEW)
current selection by
residue types
Glycine
Alanine
Valine
Proline
Serine
Threonine
Leucine
Isoleucine
Cysteine
Aspartic acid
Hydrophilic
Large
Basic
Small
Acidic
Hydrophobic
Clear
Select all
Apply
Show
all
of..
Peptide
A/
A/1(TYR)
A/2(GLU)
A/3(HIS)
peptide
Help
Clear
Apply
Save
Close
3j2w
All ..
By c..
Bonds
214.6 Å
Display Table
Simplified Display Table
Origin: -0.000 -0.000 -0.000 | Size: 1000 x 698
Zoom:
31.85

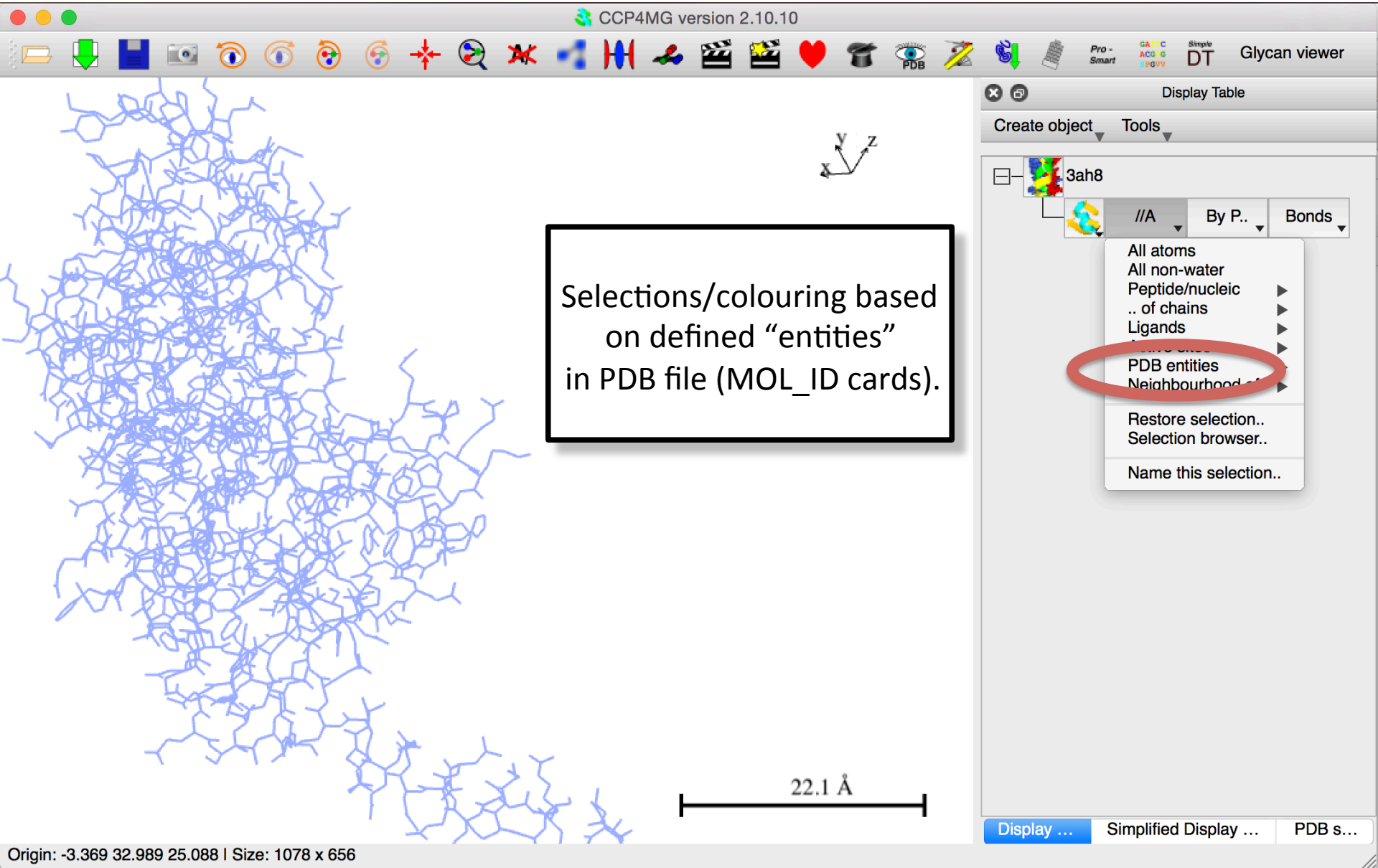

CCP4MG version 2.10.5
Display Table
Select from
saved selection
interactive selection
neighbours
buried area
atomic elements
residue types
residue ranges
secondary structure elements
properties (eg temp factor)
NMR/symmetry models
Replace (NEW)
current selection b
Select
residues
within
4.0
3j2w
Include
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
3j2w
All ..
By c..
Bonds
214.6 Å
Display Table
Simplified Display Table
Origin: -0.000 -0.000 -0.000 | Size: 1000 x 698
Zoom:
31.85


CCP4MG version 2.10.5
Display Table
Select from3j2w
Replace (NEW)
current selection by
neighbours
Select
residues
within
4.0
of selection..
3j2w
A/1(TYR)
Peptide
A/
A/1(TYR)
A/1(TYR)/N
A/1(TYR)/CA
A/1(TYR)/C
A/1(TYR)/O
A/1(TYR)/CB
A/1(TYR)/CG
A/1(TYR)/CD1
A/1(TYR)/CD2
A/1(TYR)/CE1
A/1(TYR)/CE2
A/1(TYR)/CZ
A/1(TYR)/OH
A/2(GLU)
A/3(HIS)
A/4(VAL)
A/5(THR)
A/6(VAL)
Include
Show
all
peptide
Help
Clear
Apply
Save
Close
Object
Tools
All ..
By c..
Bonds
214.6 Å
Display Table
Simplified Display Table
Origin: -0.000 -0.000 -0.000 | Size: 1000 x 698
Zoom:
31.85

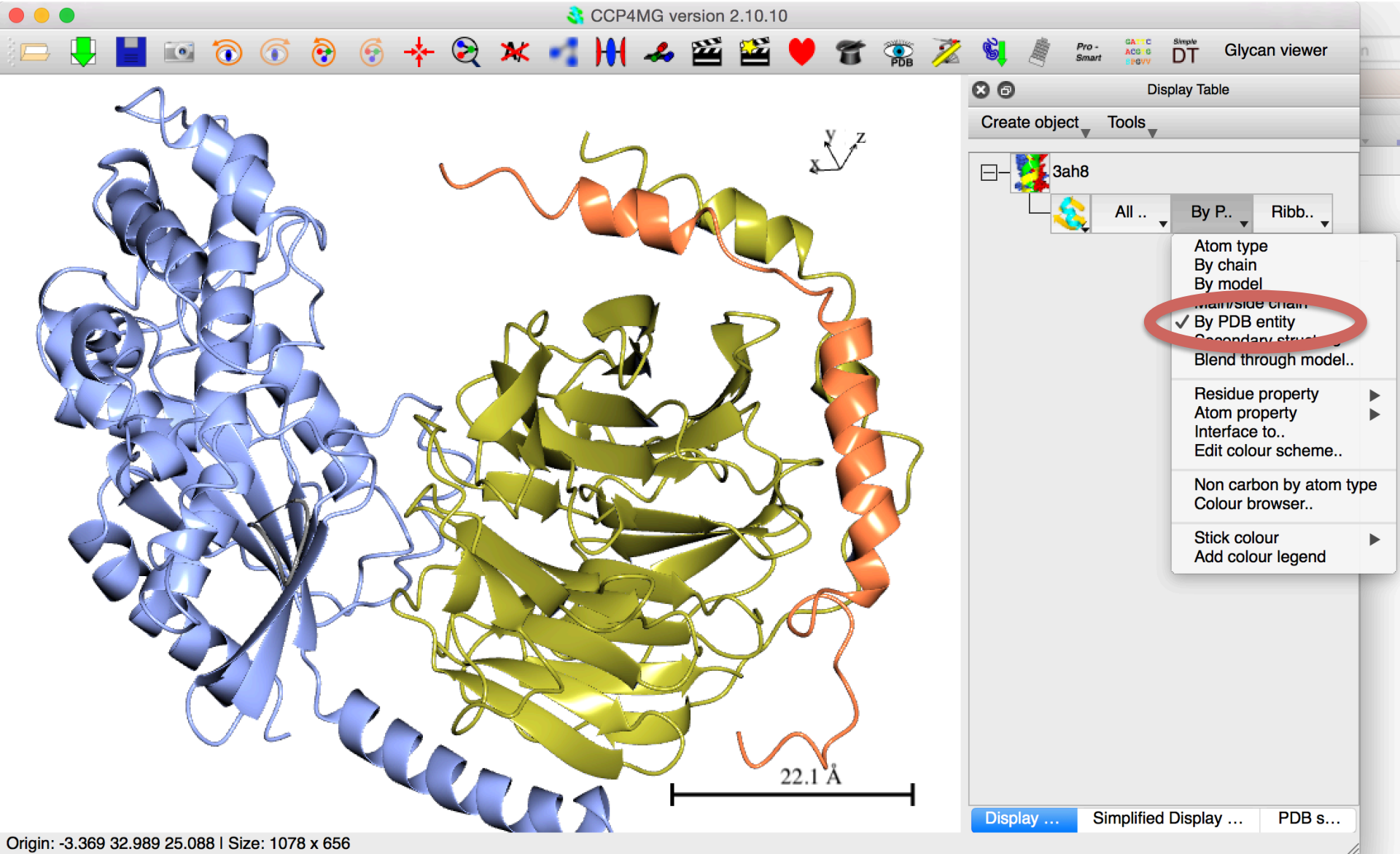
PDB Entities

```
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
```

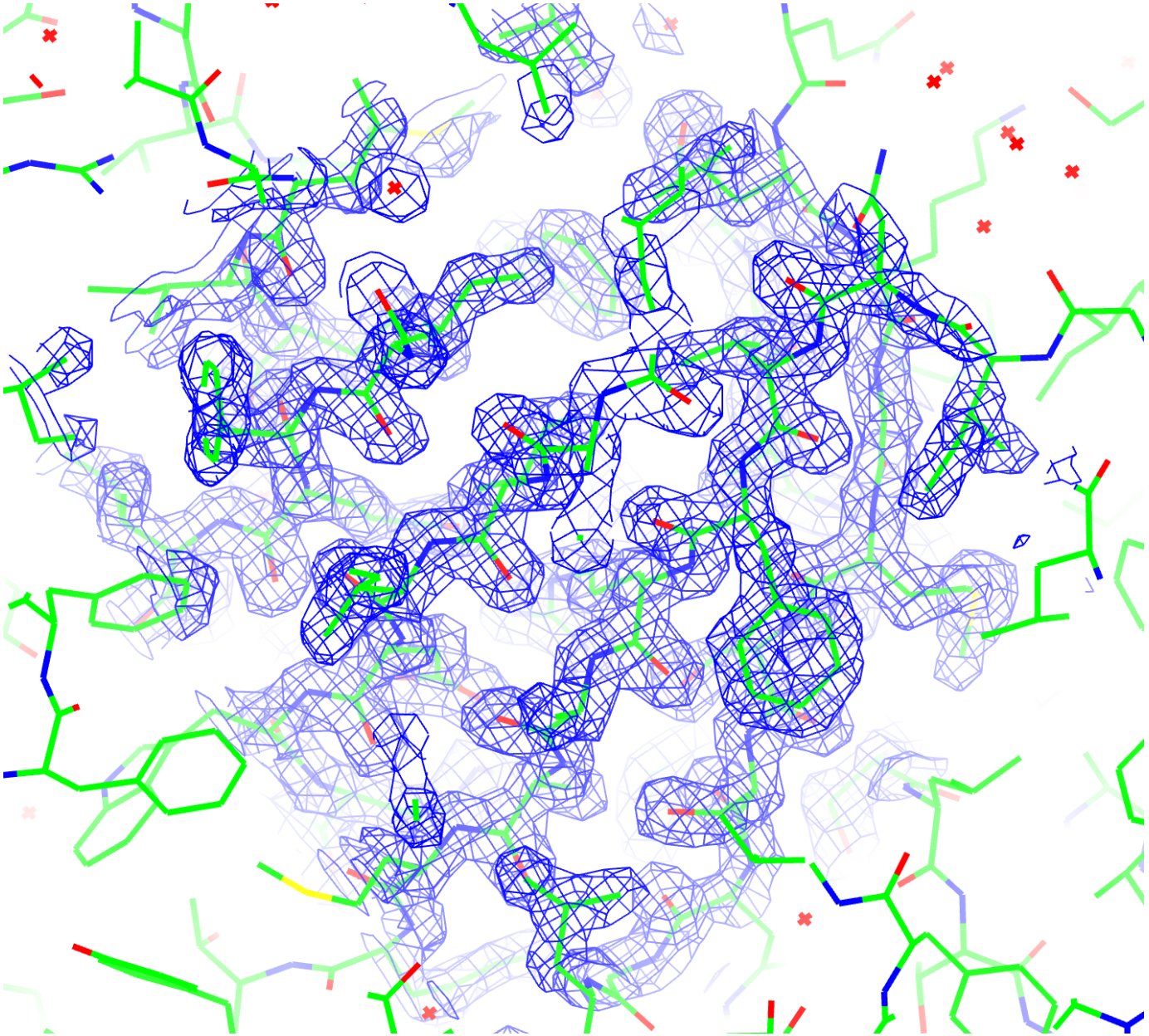
PDB Entities

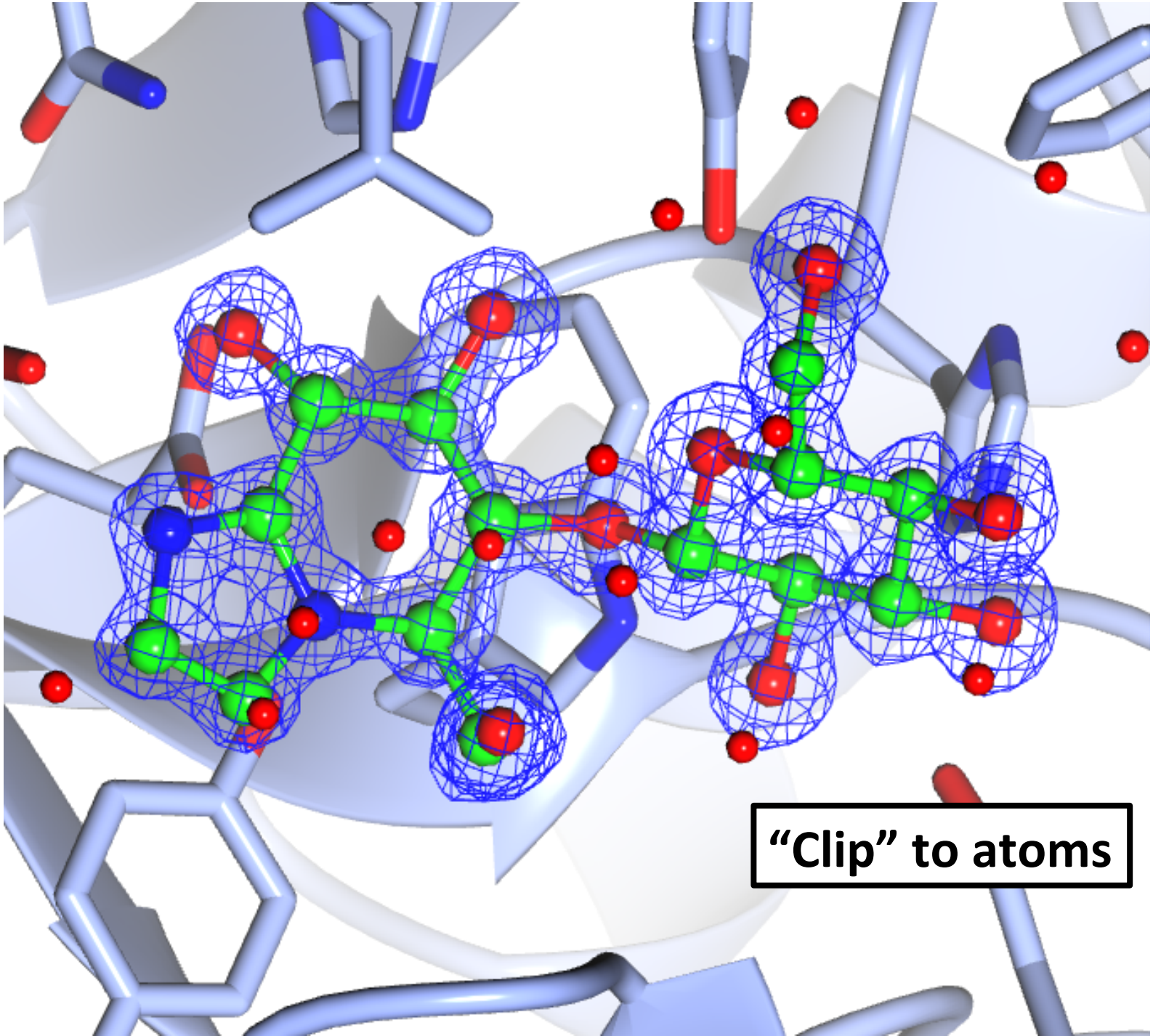


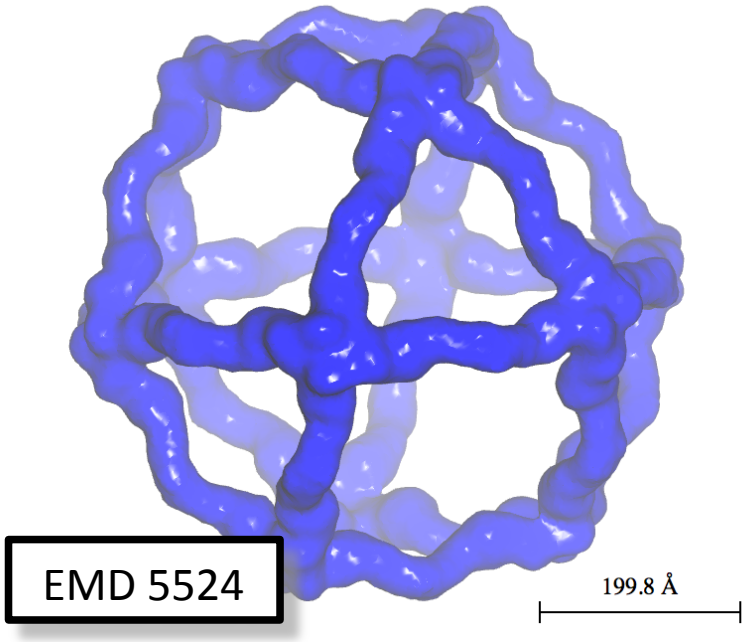
PDB Entities

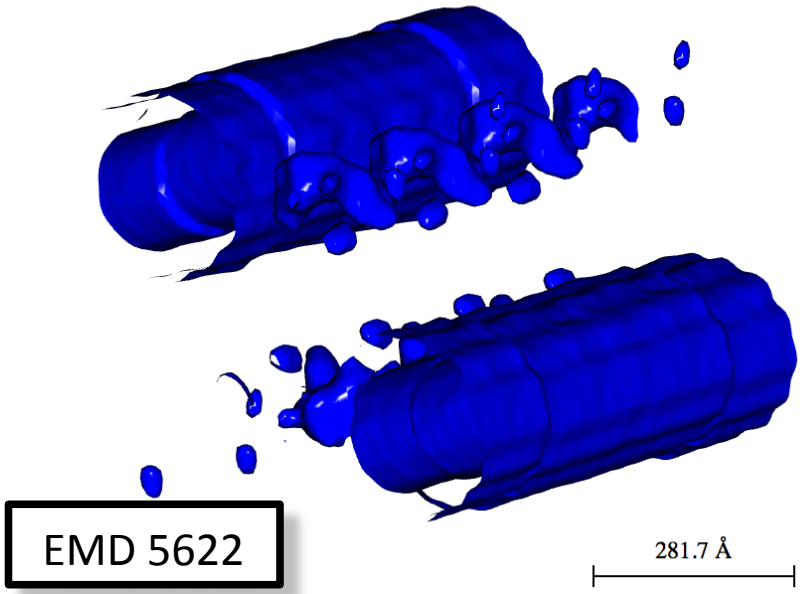


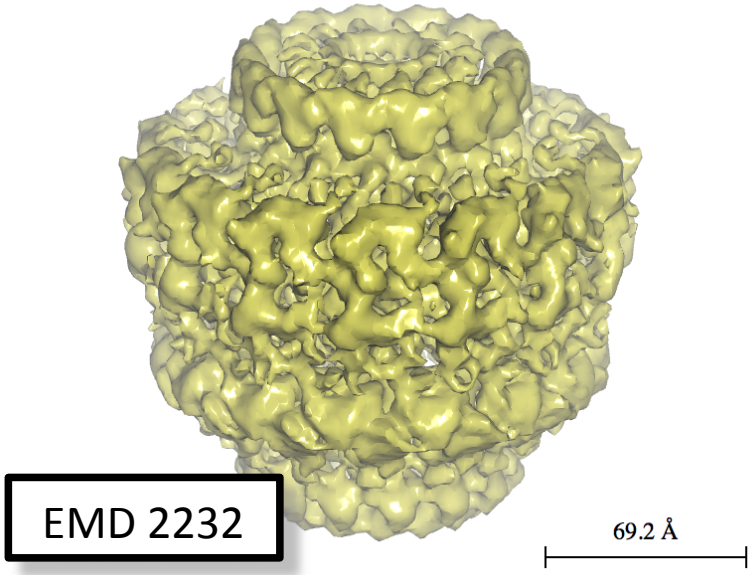
Electron Density

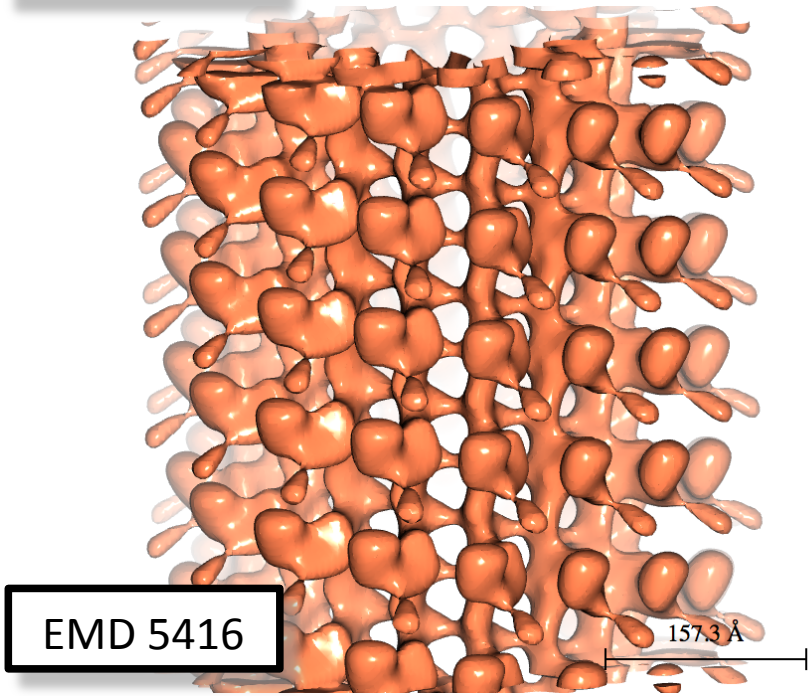


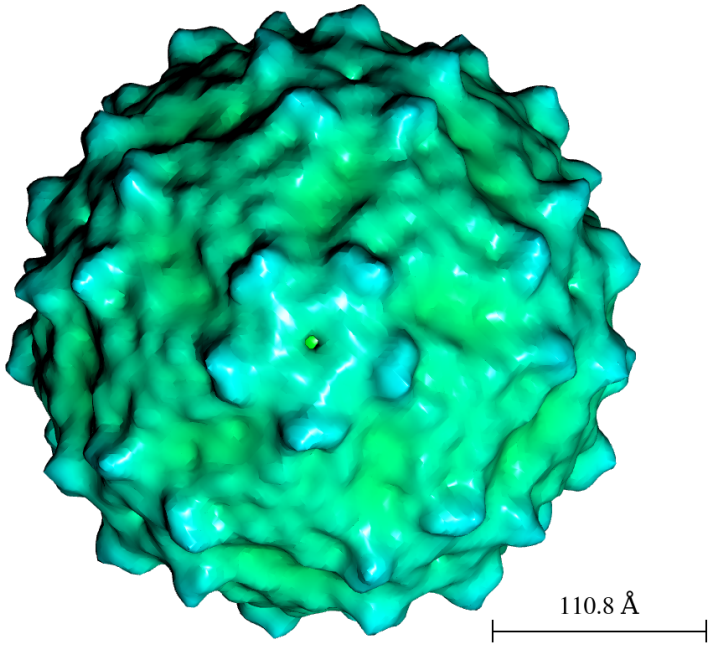

“Clip” to atoms

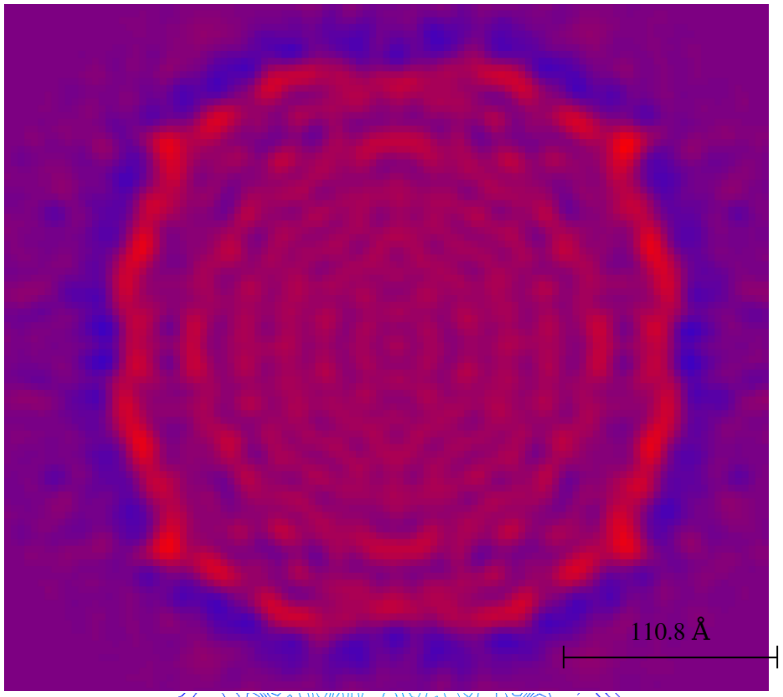

EMD 5524
199.8 Å

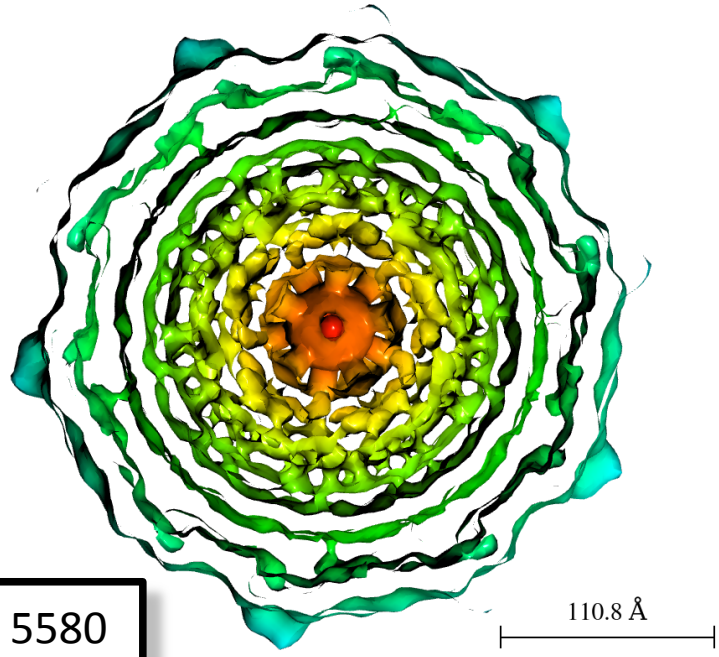

EMD 5622
281.7 Å

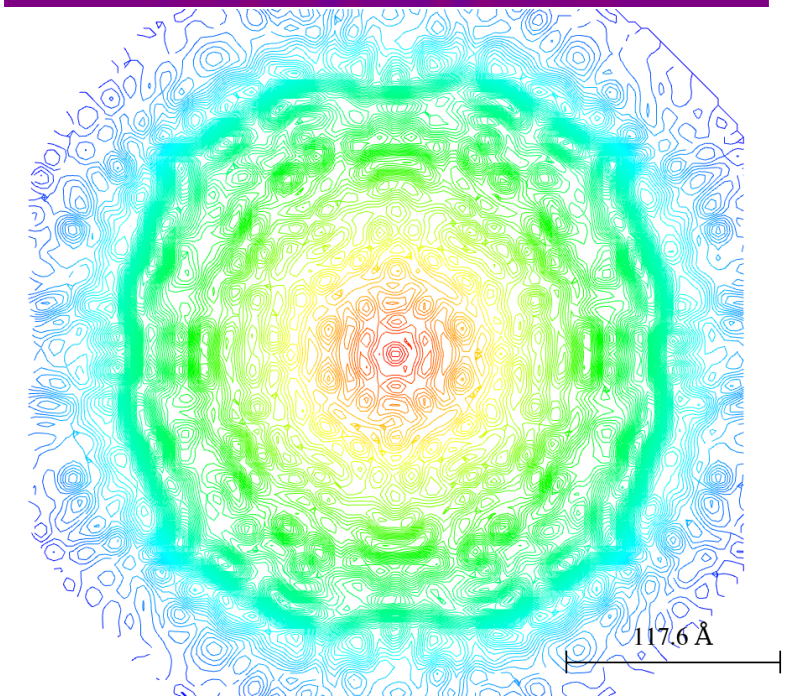

EMD 2232
69.2 Å


EMD 5416
157.3 Å

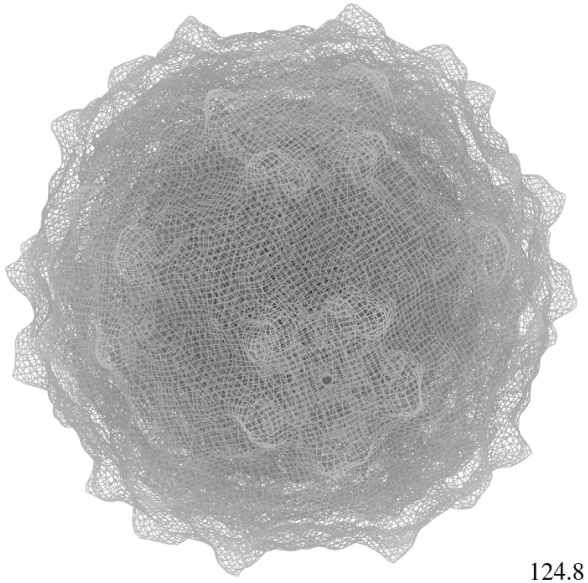




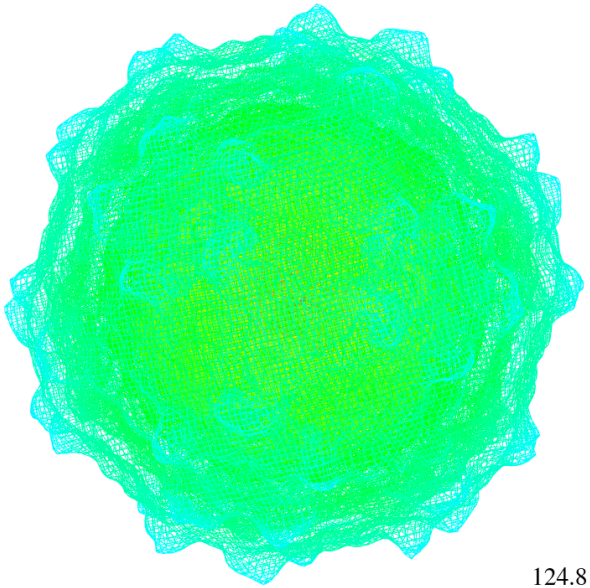




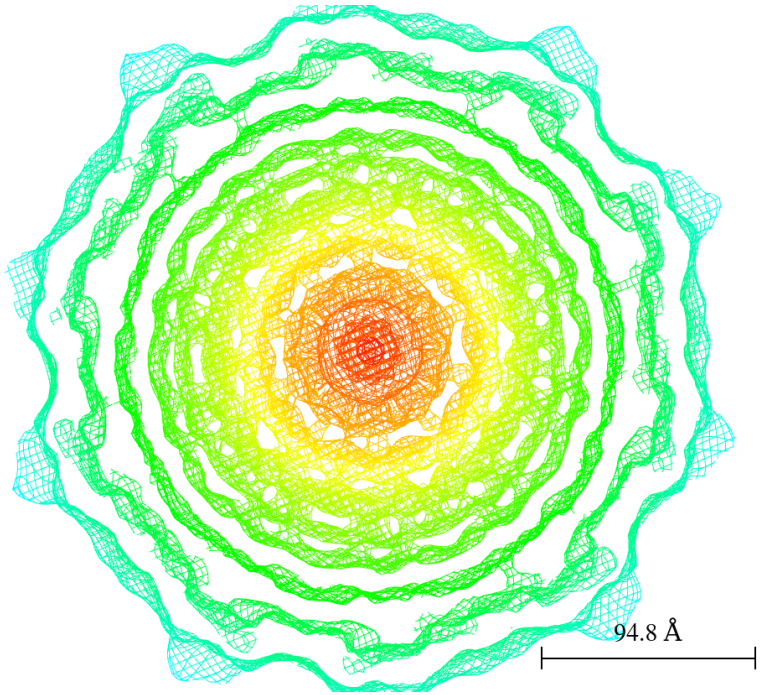
EMD 5580



124.8 Å



124.8 Å

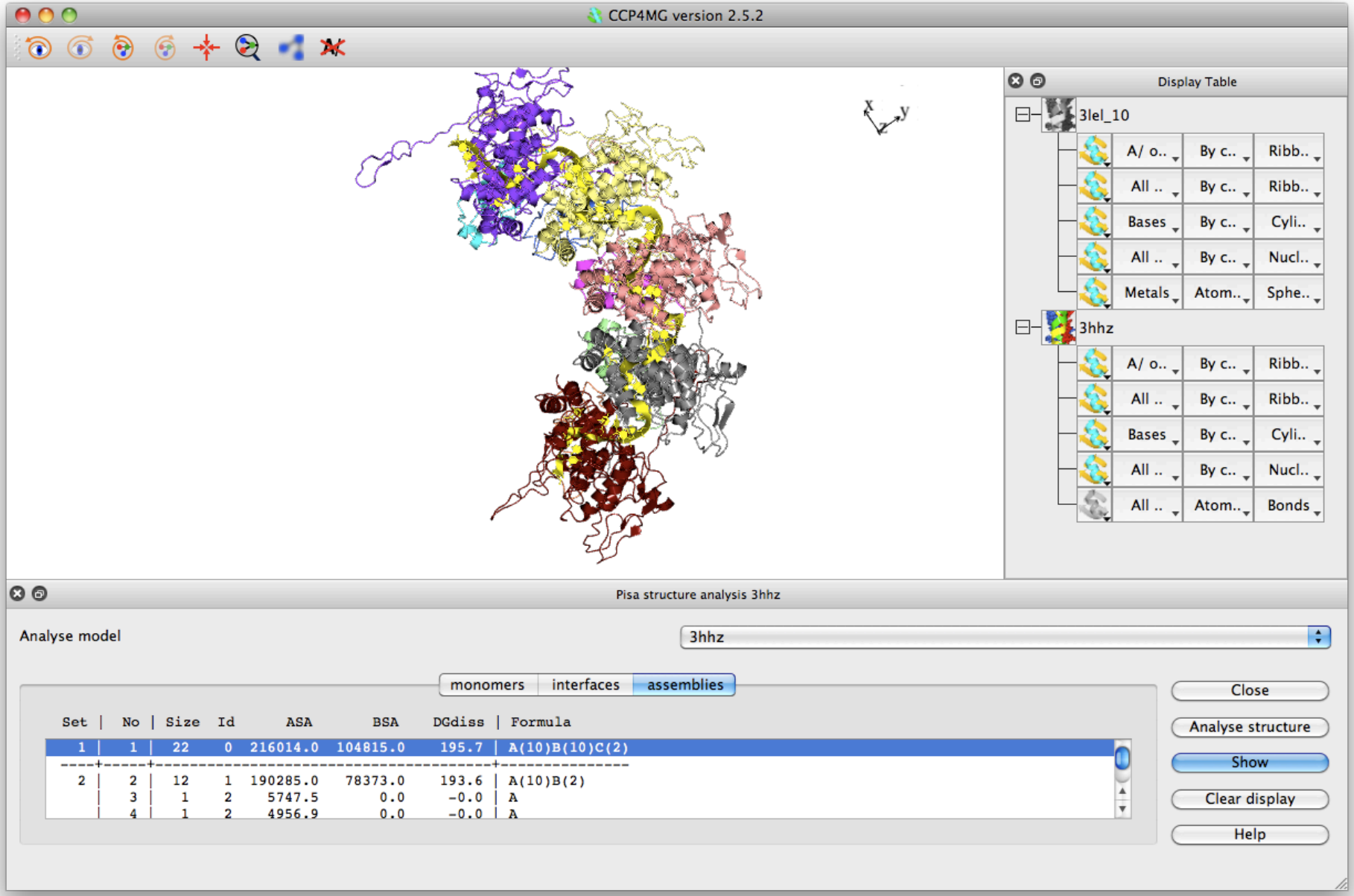


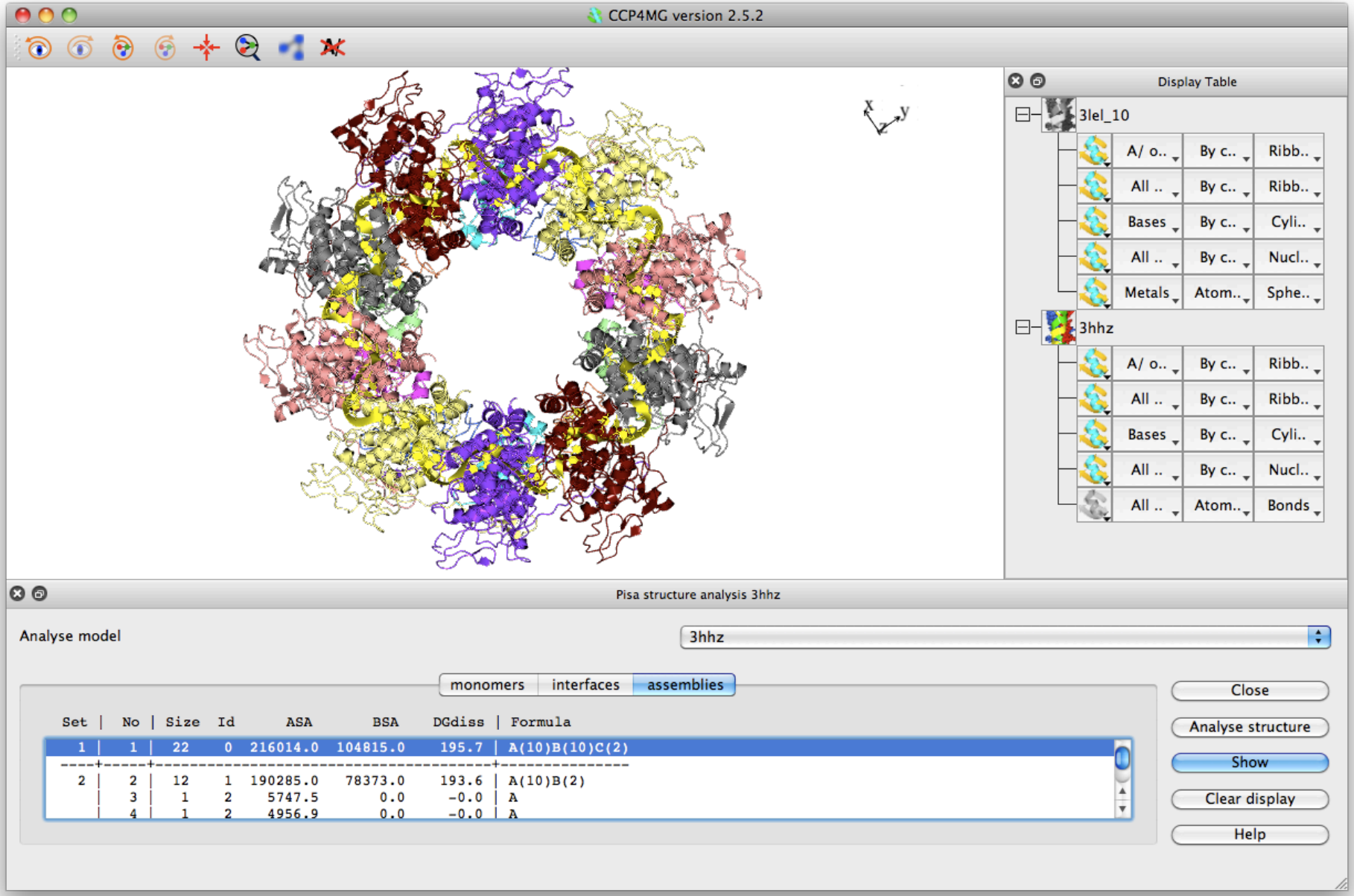
94.8 Å

EMD 5580

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.


CCP4MG version 2.5.2
Display Table
3lel_10
A/ o..
By c..
Ribb..
All ..
By c..
Ribb..
Bases
By c..
Cyli..
All ..
By c..
Nucl..
Metals
Atom..
Sphe..
3hhz
A/ o..
By c..
Ribb..
All ..
By c..
Ribb..
Bases
By c..
Cyli..
All ..
By c..
Nucl..
All ..
Atom..
Bonds
Pisa structure analysis 3hhz
Analyse model
3hhz
monomers
interfaces
assemblies
Set | No | Size Id ASA BSA DGdiss | Formula
1 | 1 | 22 0 216014.0 104815.0 195.7 | A(10)B(10)C(2)
2 | 2 | 12 1 190285.0 78373.0 193.6 | A(10)B(2)
3 | 1 2 5747.5 0.0 -0.0 | A
4 | 1 2 4956.9 0.0 -0.0 | A
Close
Analyse structure
Show
Clear display
Help


CCP4MG version 2.5.2
Display Table
3lel_10
A/ o..
By c..
Ribb..
All ..
By c..
Ribb..
Bases
By c..
Cyli..
All ..
By c..
Nucl..
Metals
Atom..
Sphe..
3hhz
A/ o..
By c..
Ribb..
All ..
By c..
Ribb..
Bases
By c..
Cyli..
All ..
By c..
Nucl..
All ..
Atom..
Bonds
Pisa structure analysis 3hhz
Analyse model
3hhz
monomers
interfaces
assemblies
Set | No | Size Id ASA BSA DGdiss | Formula
1 | 1 | 22 0 216014.0 104815.0 195.7 | A(10)B(10)C(2)
2 | 2 | 12 1 190285.0 78373.0 193.6 | A(10)B(2)
3 | 1 2 5747.5 0.0 -0.0 | A
4 | 1 2 4956.9 0.0 -0.0 | A
Close
Analyse structure
Show
Clear display
Help

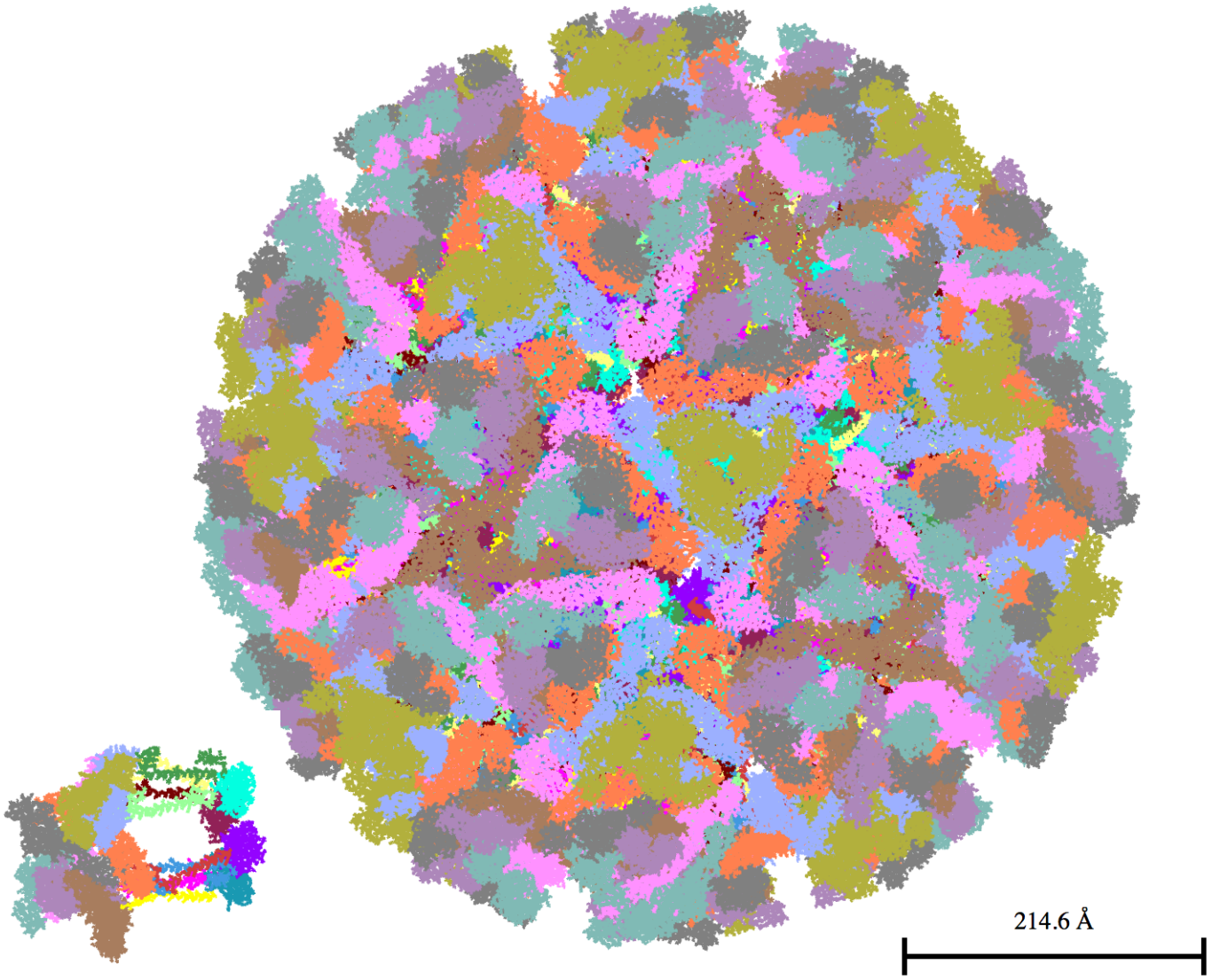
Structure Superposition

- 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

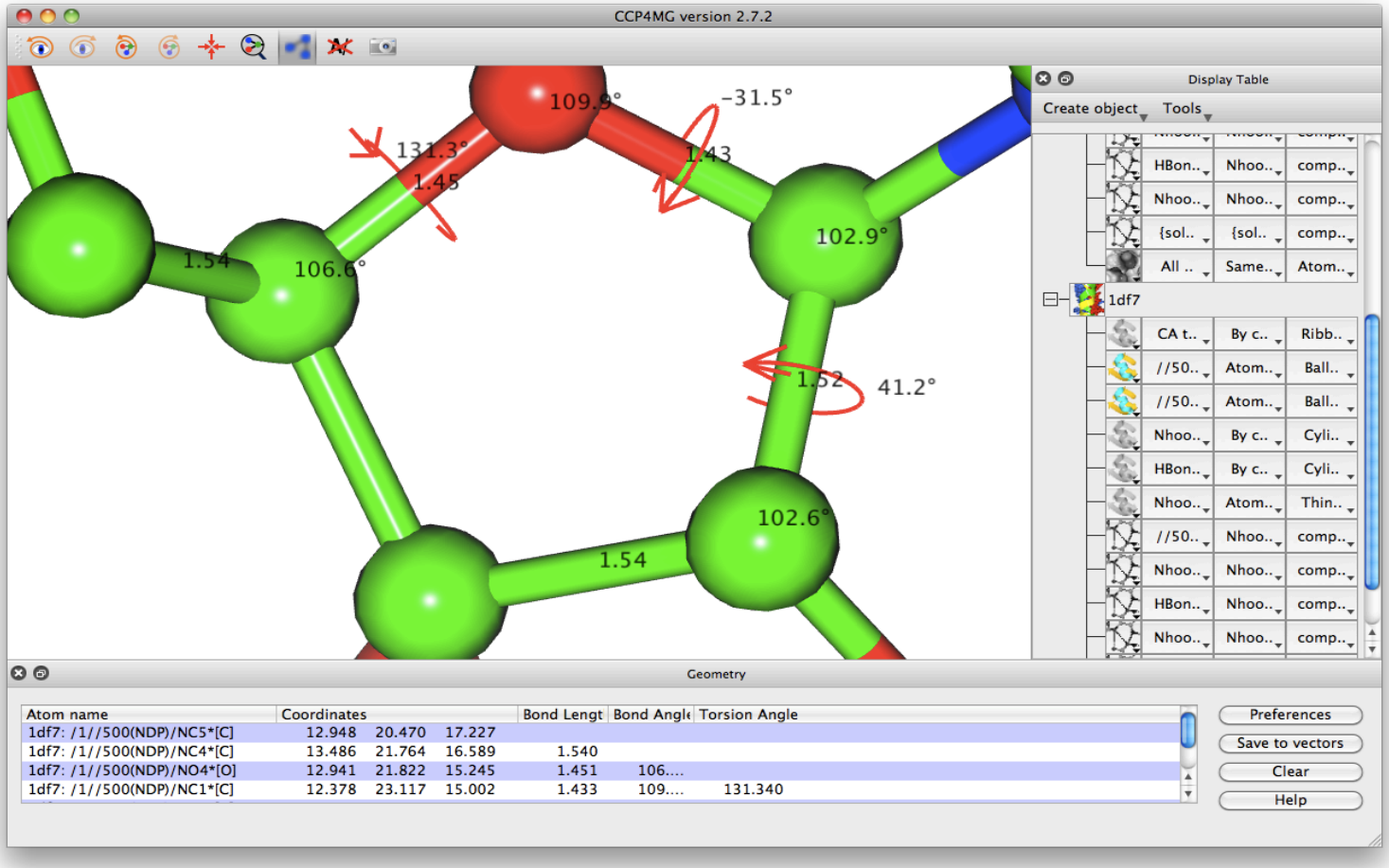
- Align sequences using muscle (a free multiple-alignment program) or ClustalW.
- Continuous (consurf style) or discrete traffic-light colour by conservation.
- Colour by secondary structure.
- Blastn/blastp interface. Blast results cached between sessions. Blast normally run remotely (EBI) with explicit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

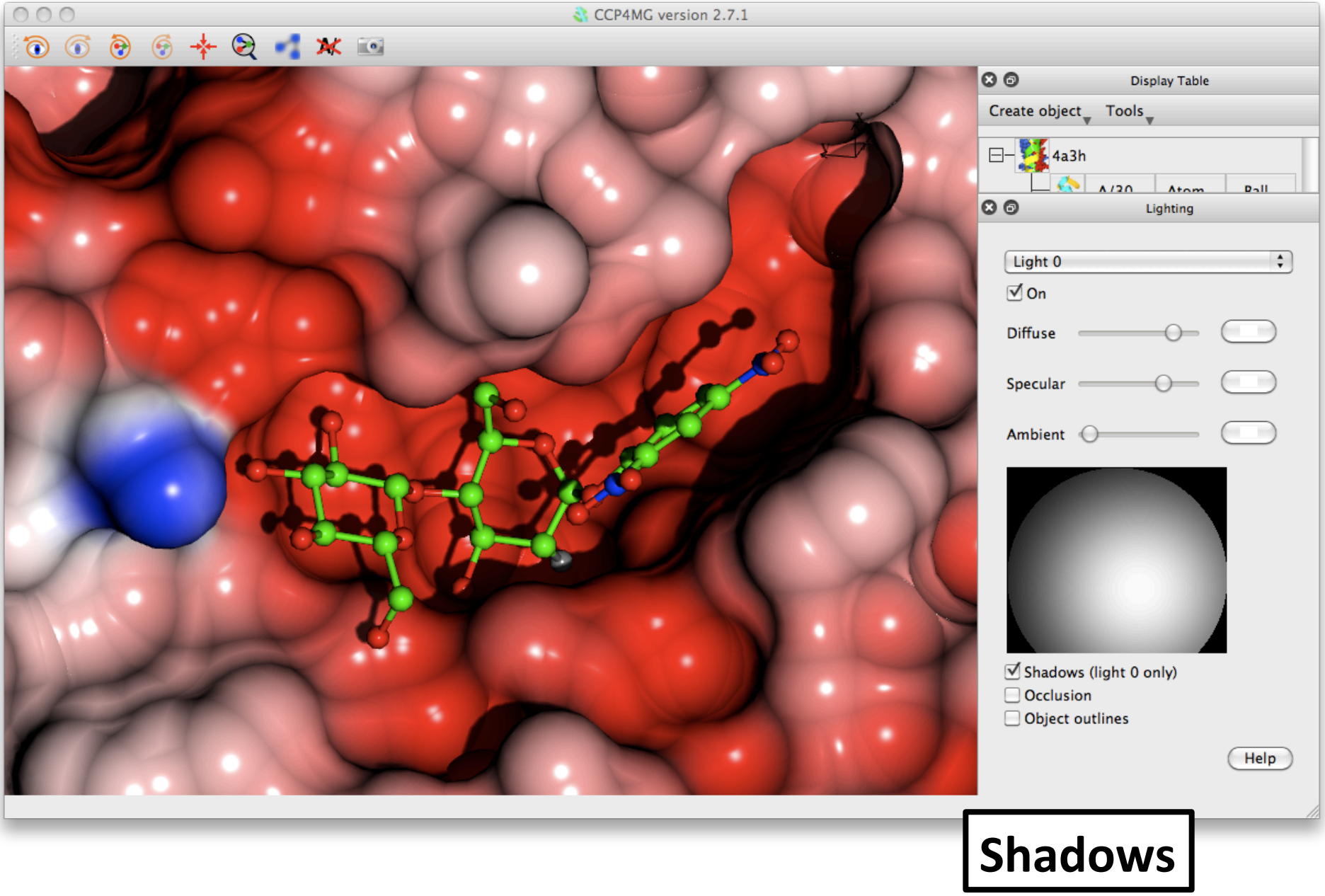


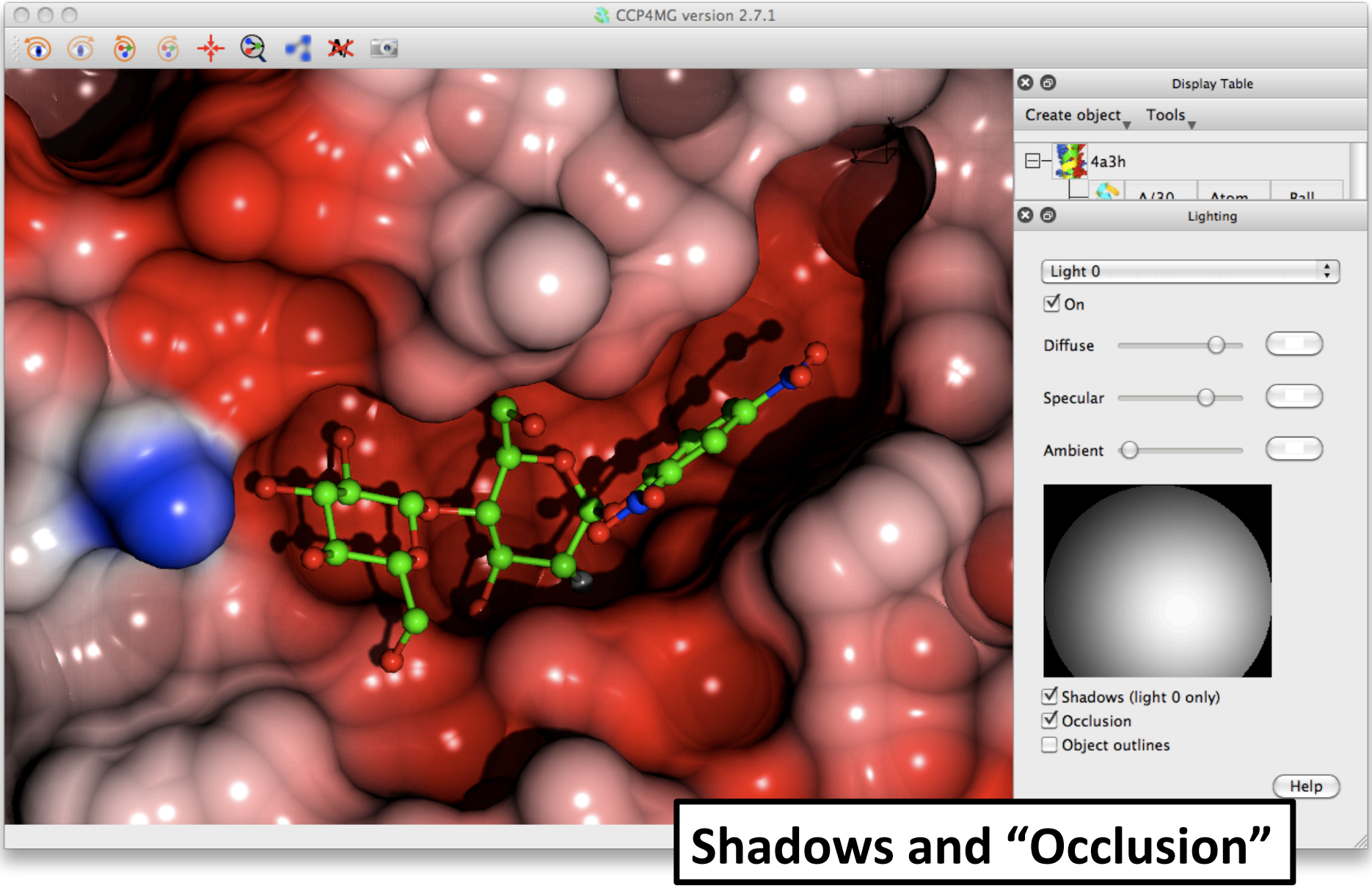
Distances and angles

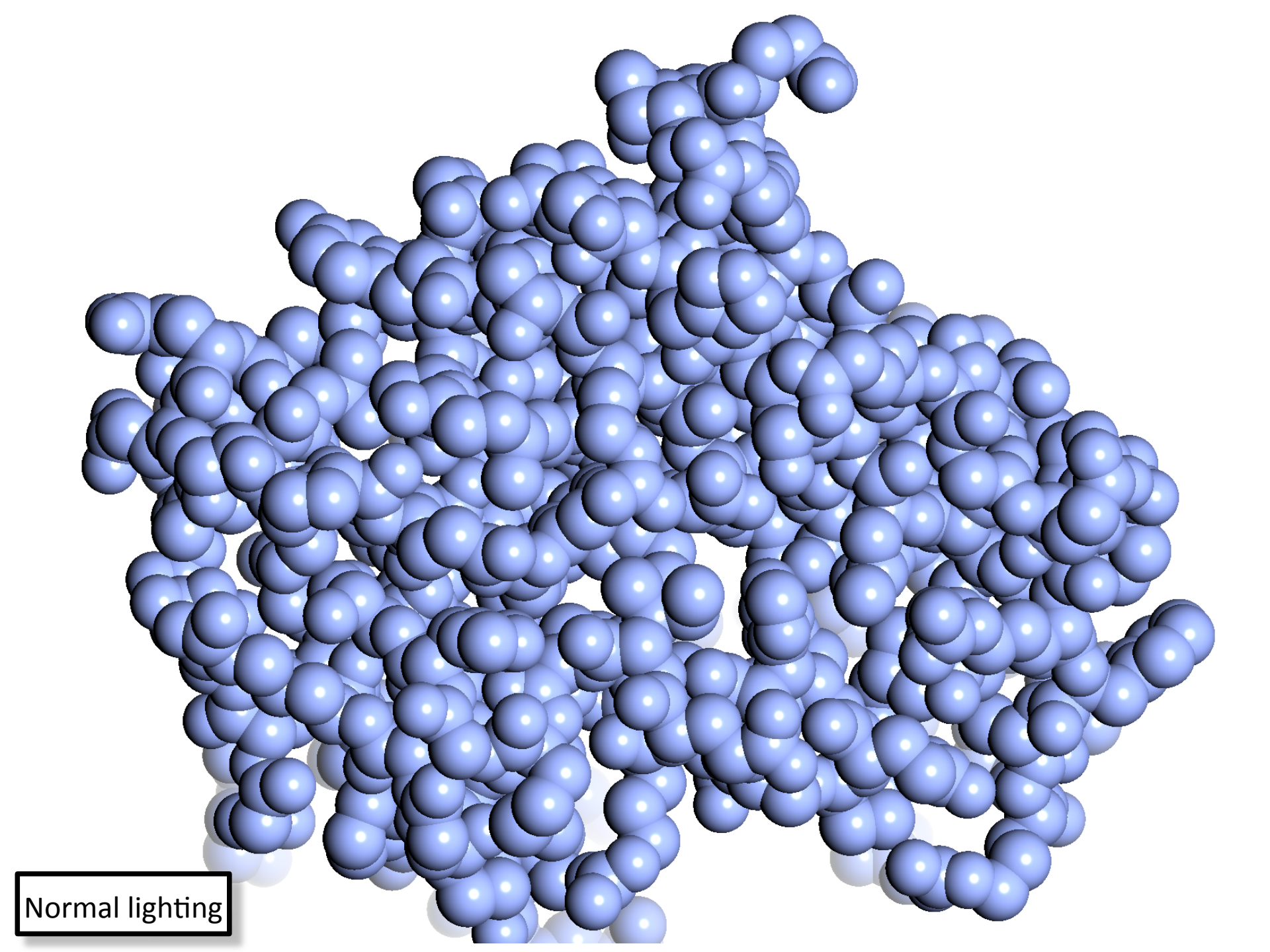
- Open “Geometry window” : Applications -> Geometry
- Double-click on one atom then another to measure bonds.
- Shift-double click on other atoms will measure angles.
- Results appear in table below and in graphics window.

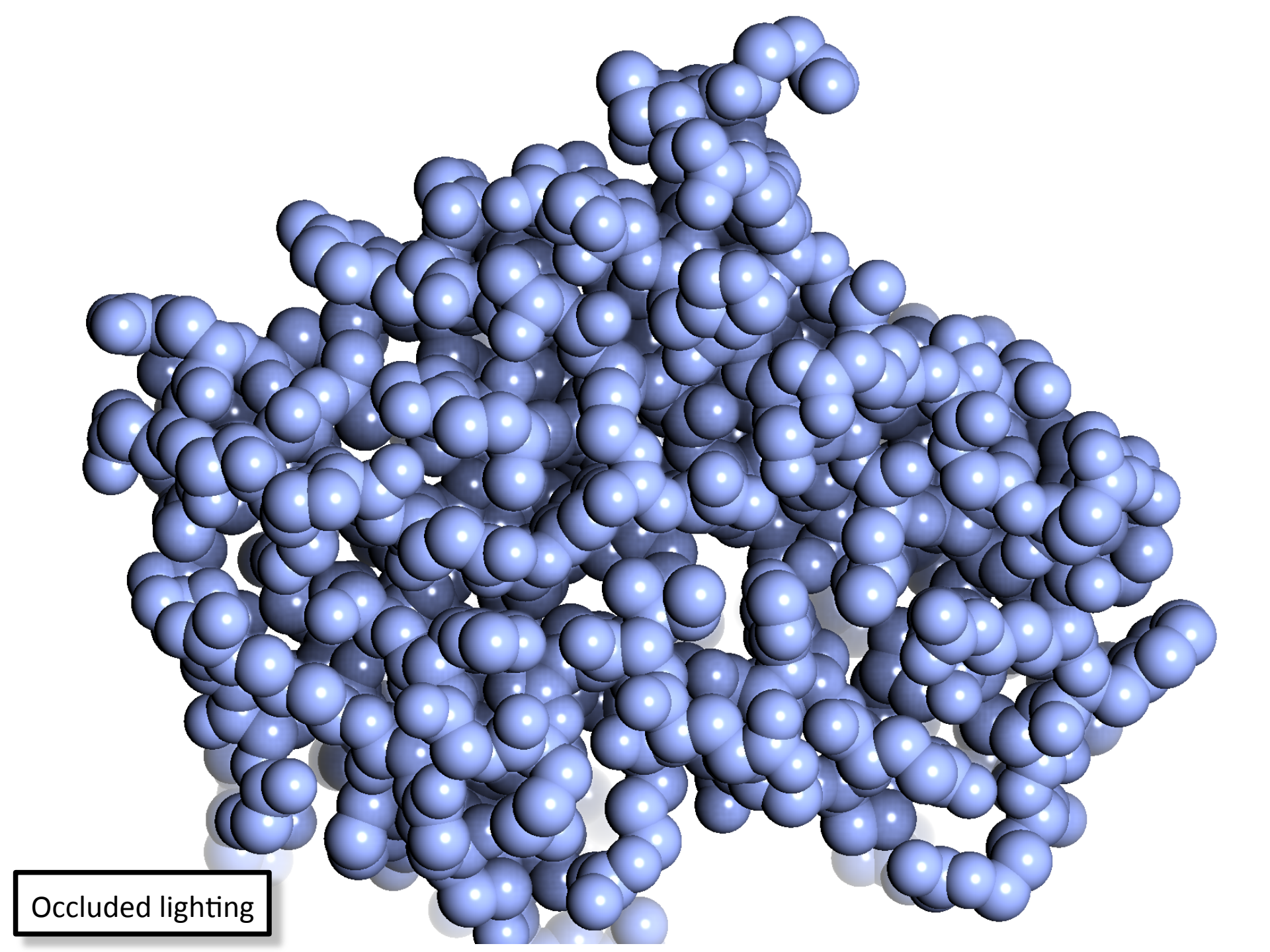


Lighting and Shadows

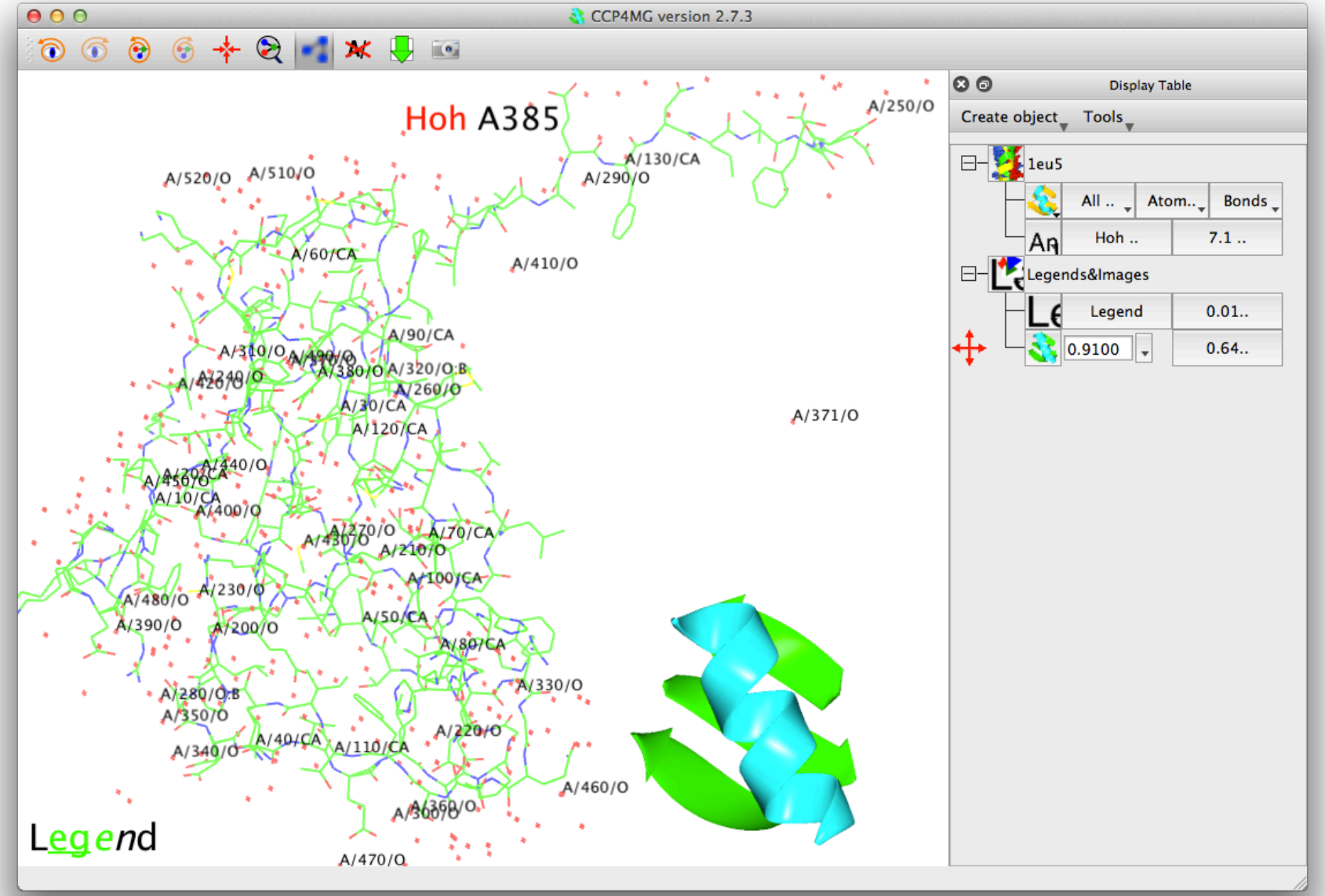

CCP4MG version 2.7.1
Display Table
Create object
Tools
4a3h
Lighting
Light 0
On
Diffuse
Specular
Ambient
Shadows (light 0 only)
Occlusion
Object outlines
Help
Shadows


CCP4MG version 2.7.1
Display Table
Create object
Tools
4a3h
Lighting
Light 0
On
Diffuse
Specular
Ambient
Shadows (light 0 only)
Occlusion
Object outlines
Help
Shadows and “Occlusion”

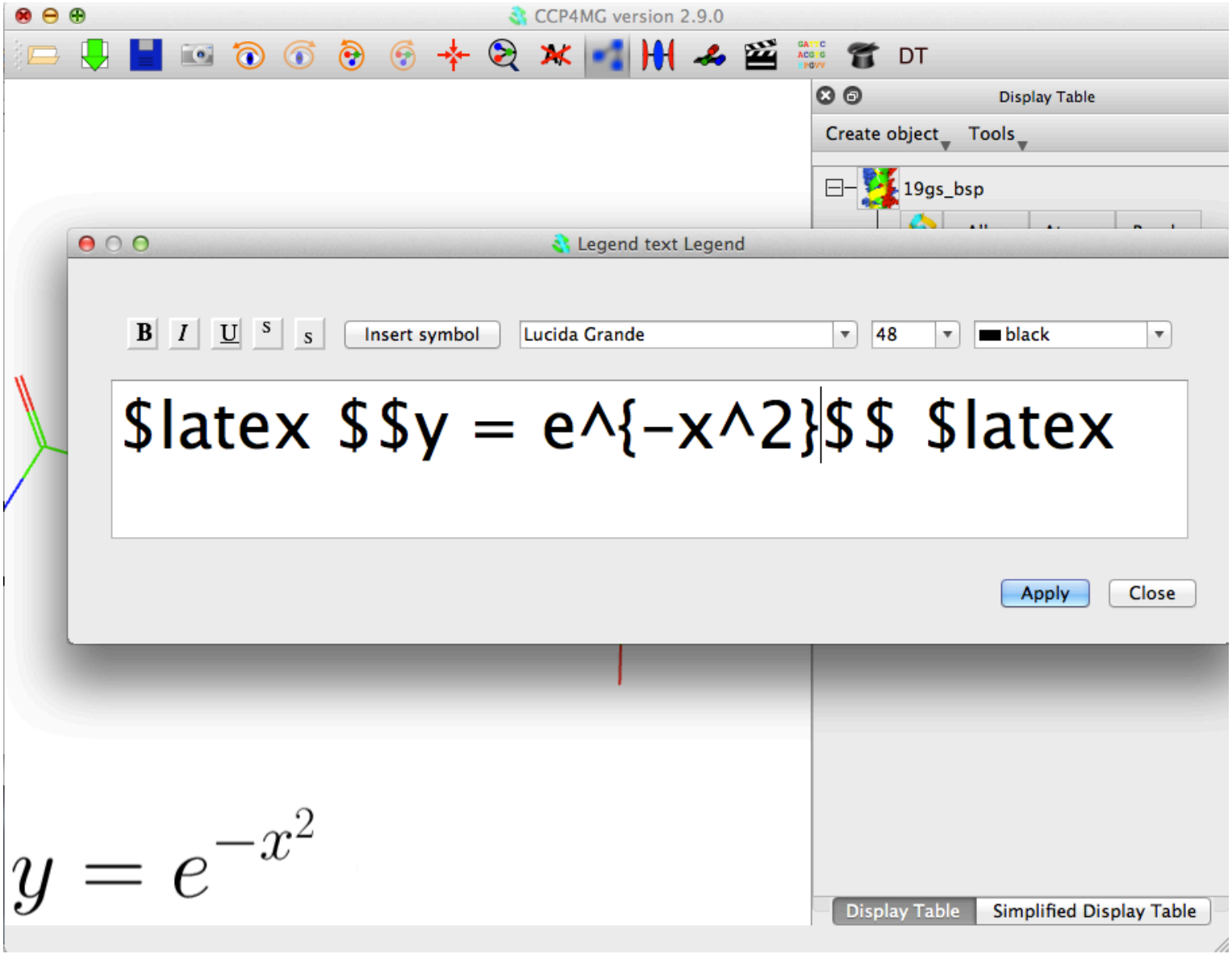

Normal lighting


Occluded lighting

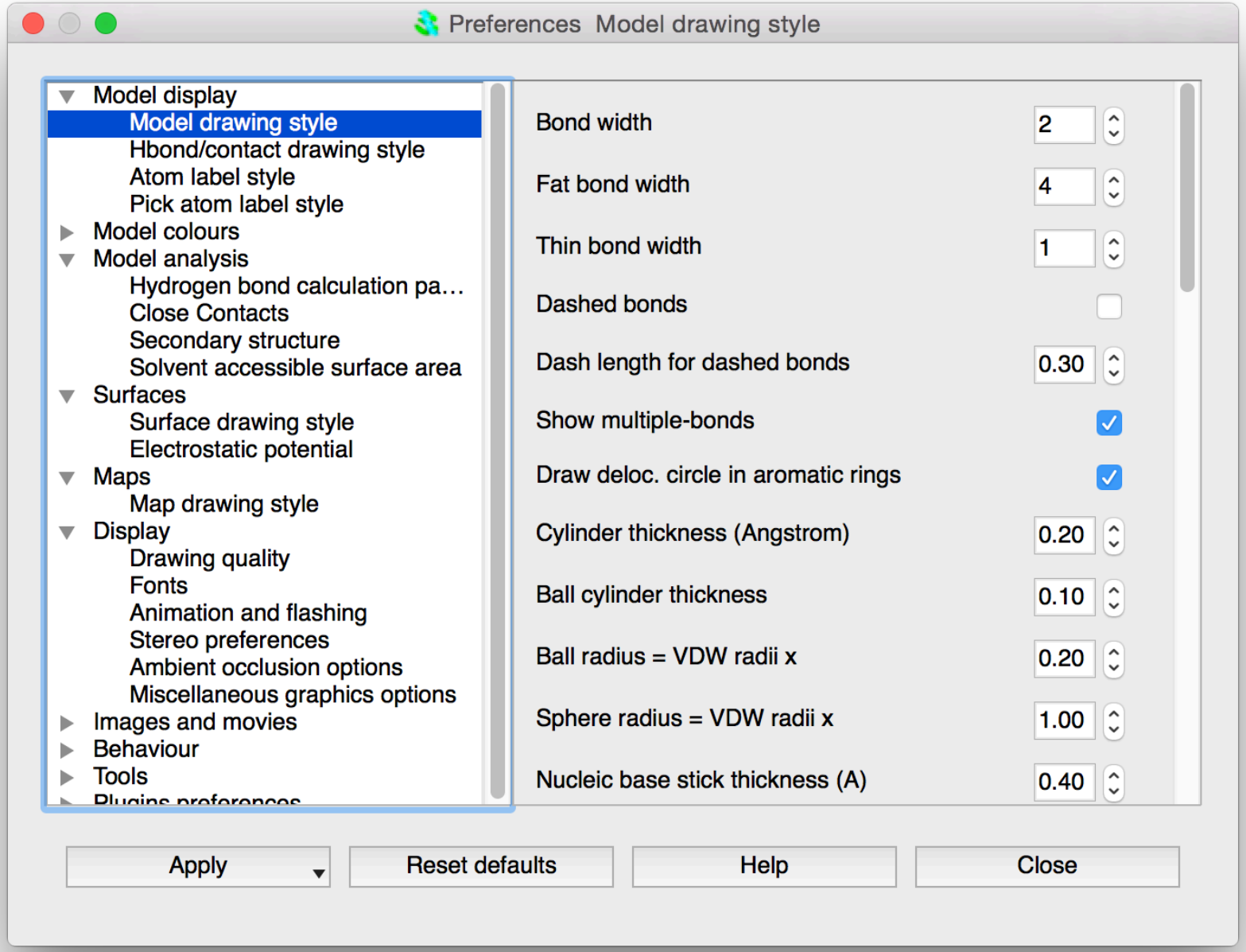
On screen text and images



On screen text and images

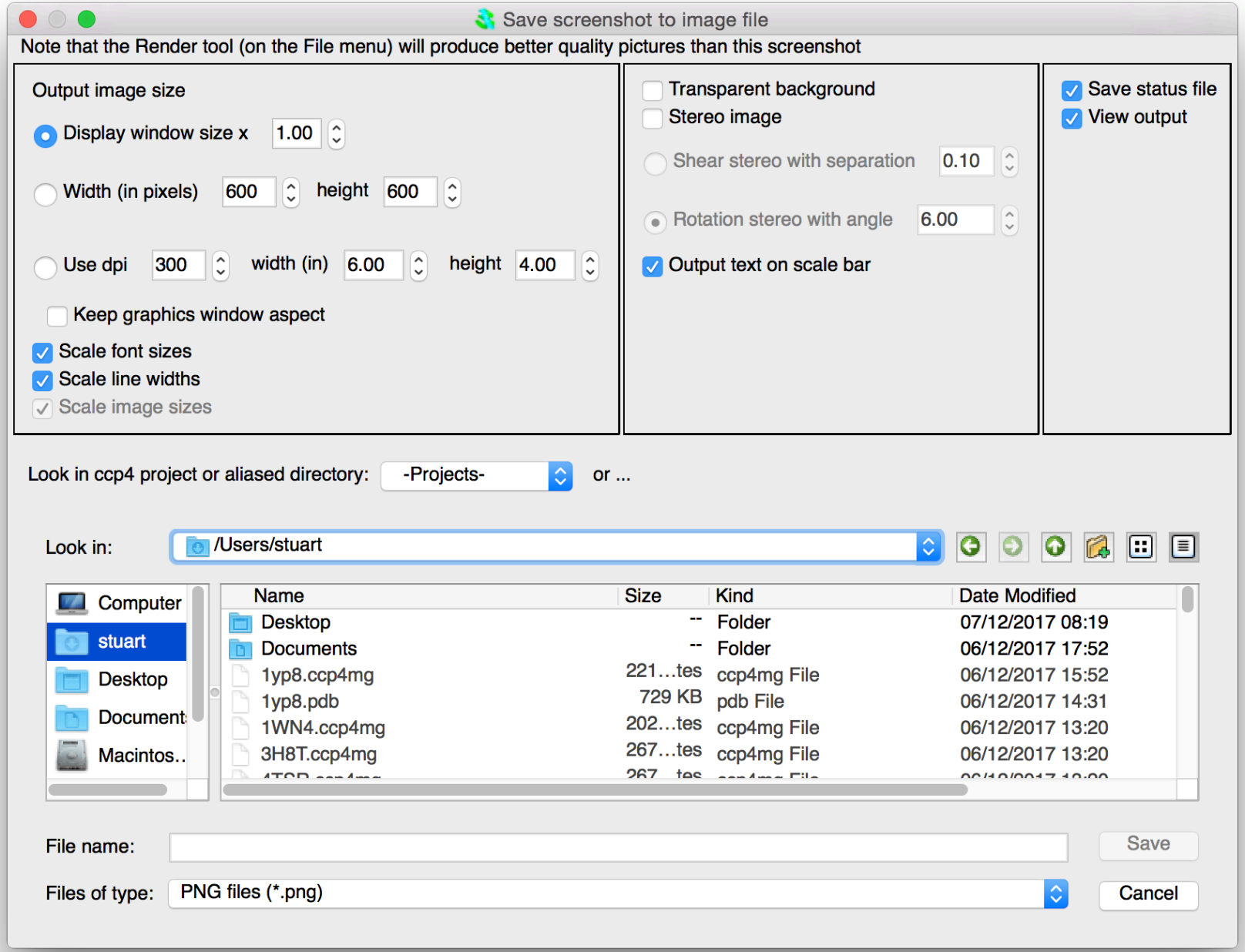


Preferences



“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.

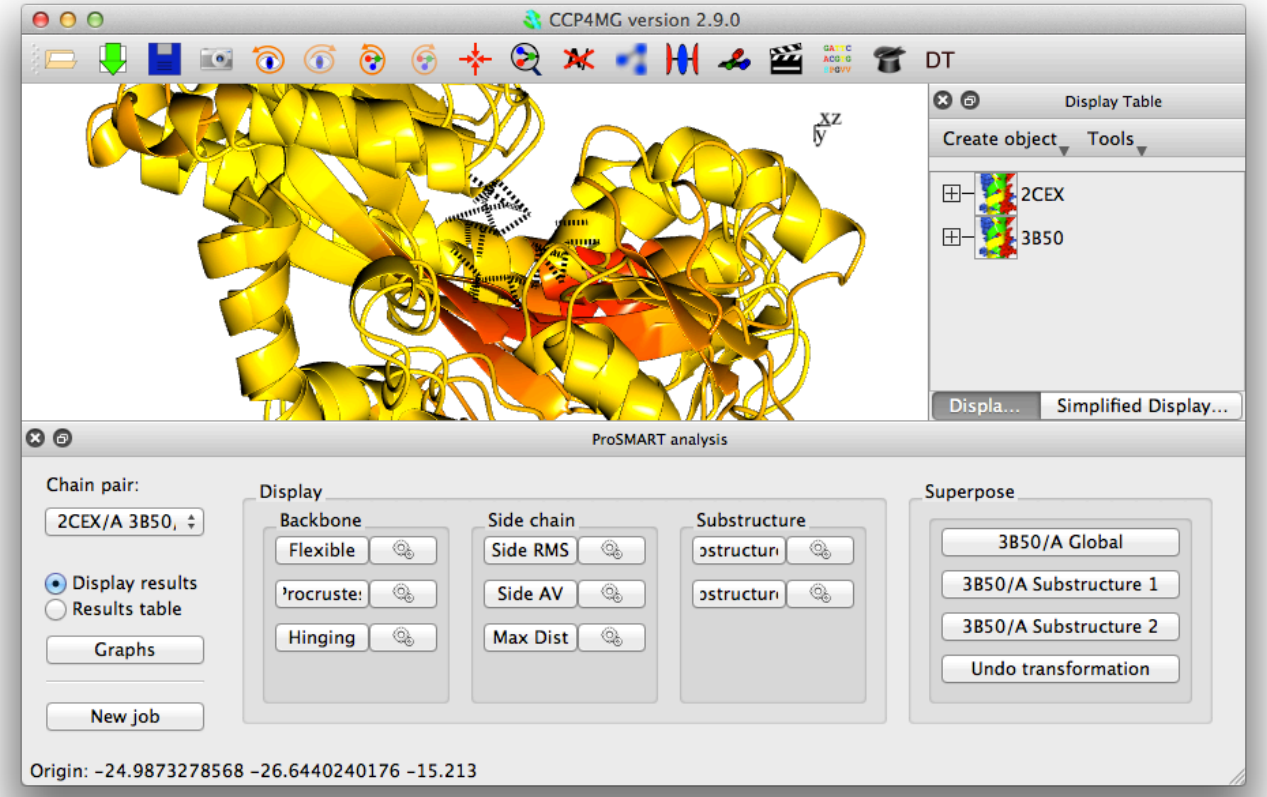

Save screenshot to image file
Note that the Render tool (on the File menu) will produce better quality pictures than this screenshot
Output image size
Display window size x 1.00
Width (in pixels) 600 height 600
Use dpi 300 width (in) 6.00 height 4.00
Keep graphics window aspect
Scale font sizes
Scale 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
Computer
stuart
Desktop
Document
Macintos..
Name Size Kind Date Modified
Desktop -- Folder 07/12/2017 08:19
Documents -- Folder 06/12/2017 17:52
1yp8.ccp4mg 221...tes ccp4mg File 06/12/2017 15:52
1yp8.pdb 729 KB pdb File 06/12/2017 14:31
1WN4.ccp4mg 202...tes ccp4mg File 06/12/2017 13:20
3H8T.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.

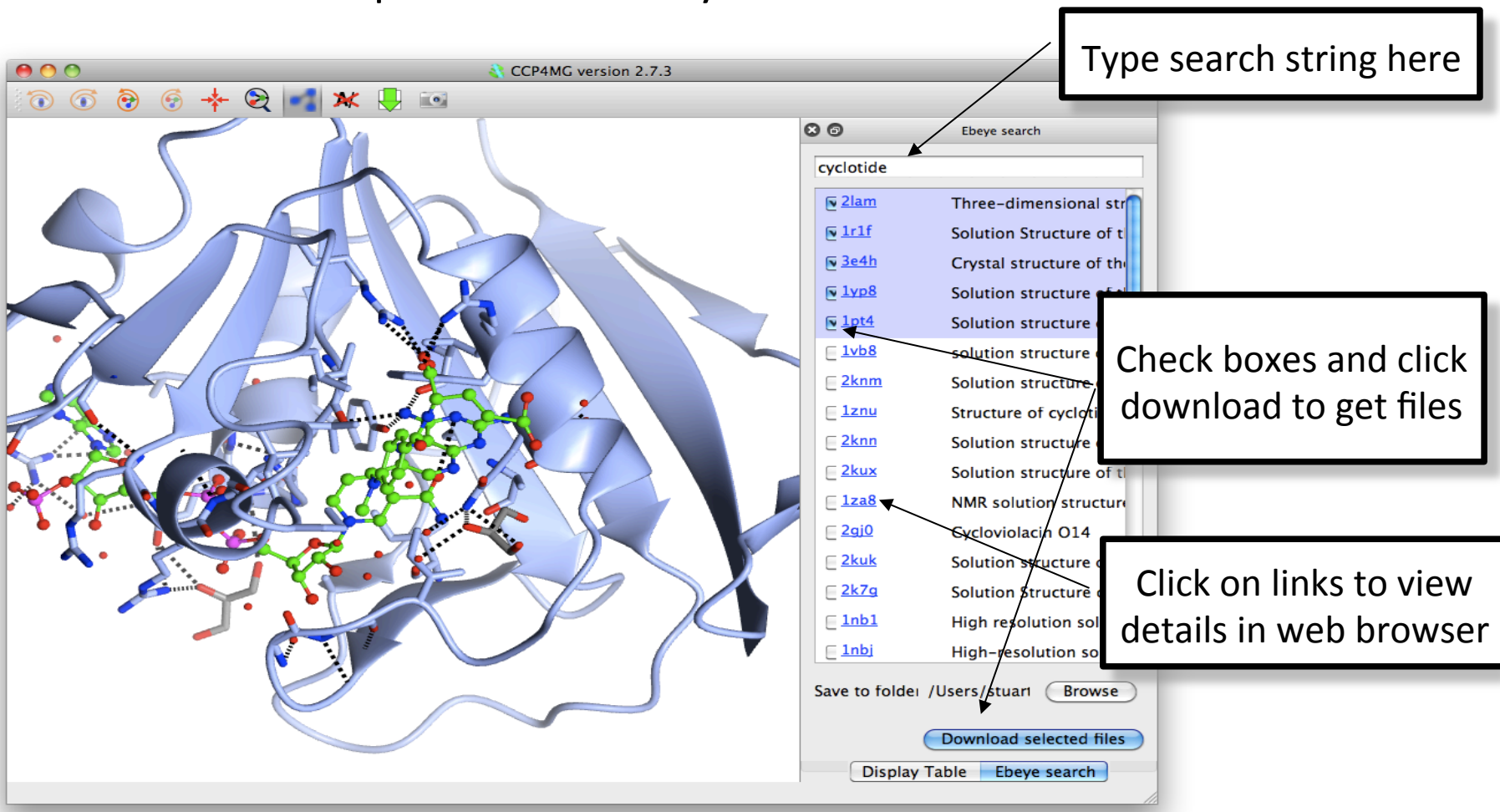
ProSMART interface

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



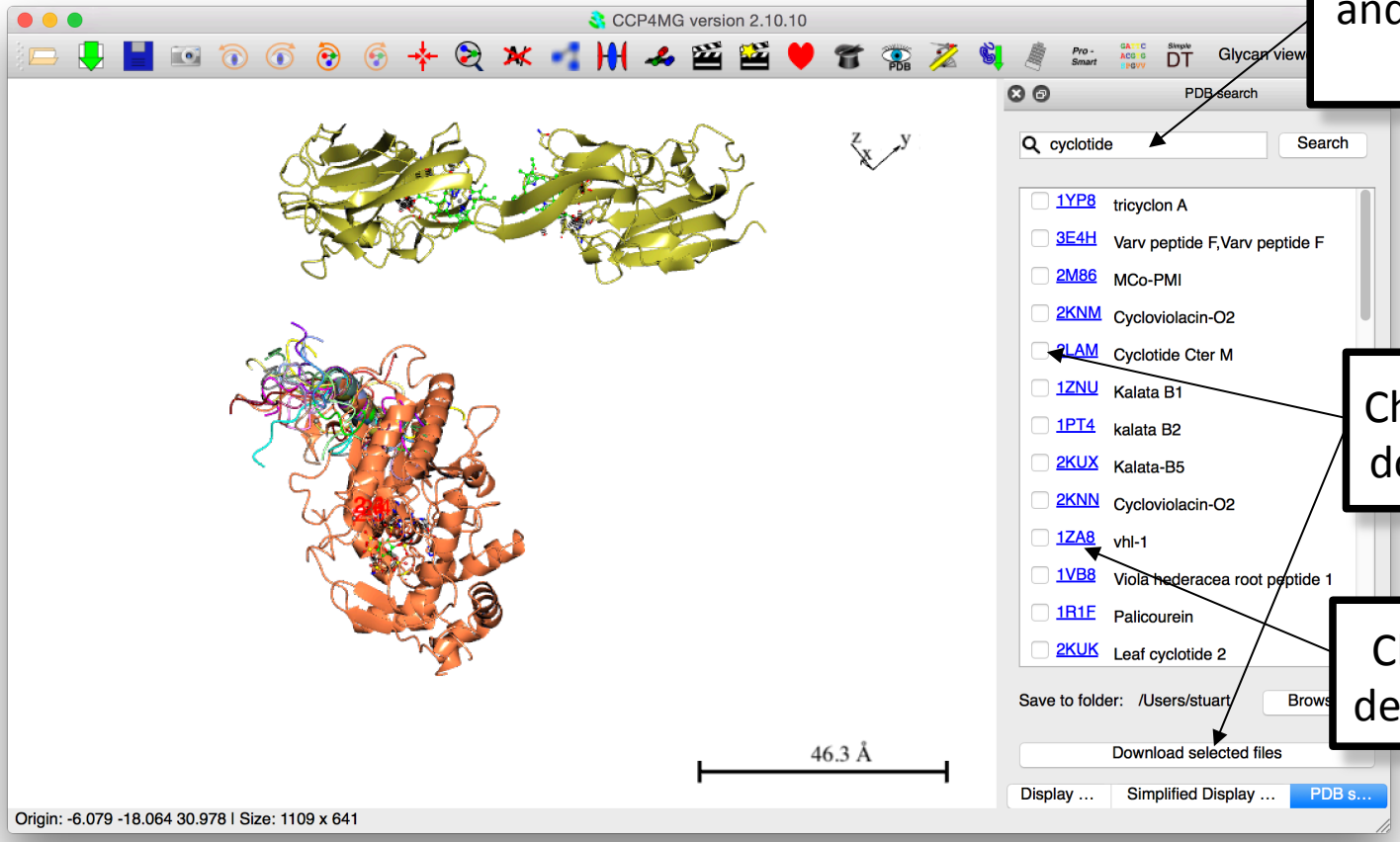
Ebeye – search (obsolete)

- Interface to simple search facility of PDB-E.



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

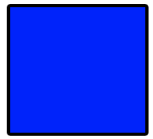
- Images may be rendered from command line or from scripts without starting up the main program.
- `ccp4mg -norestore -picture mypic.mgpic.py -R test.png -RO '{"size":"1600x1600","smoothribbons":"1", "raytrace":"1"}' -quit`
- The file mypic.mpic.py is a file containing a scene description: lists of data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

Glycoblocks

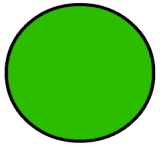
Glycosylation depiction in 3D

- 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.

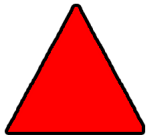
Saccharide display in 2D



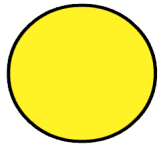
N-Acetyl-glucosamine
(NAG)



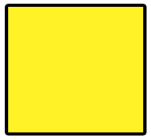
Mannose
(BMA, MAN)



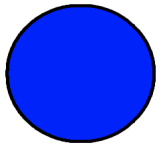
Fucose
(FCA, FCB, FUC)



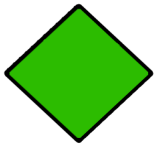
Galactose
(GAL)



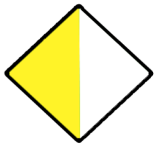
N-Acetyl-galactosamine
(NGA)



Glucose
(GLC, BGC)



2-keto-3-deoxynononic acid
(KDN)



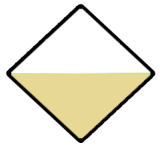
Galacturonic acid
(ADA, GTR)



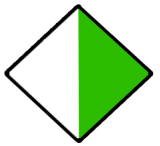
Glucosamine
(GCS)



Xylose
(XYS, XYP)

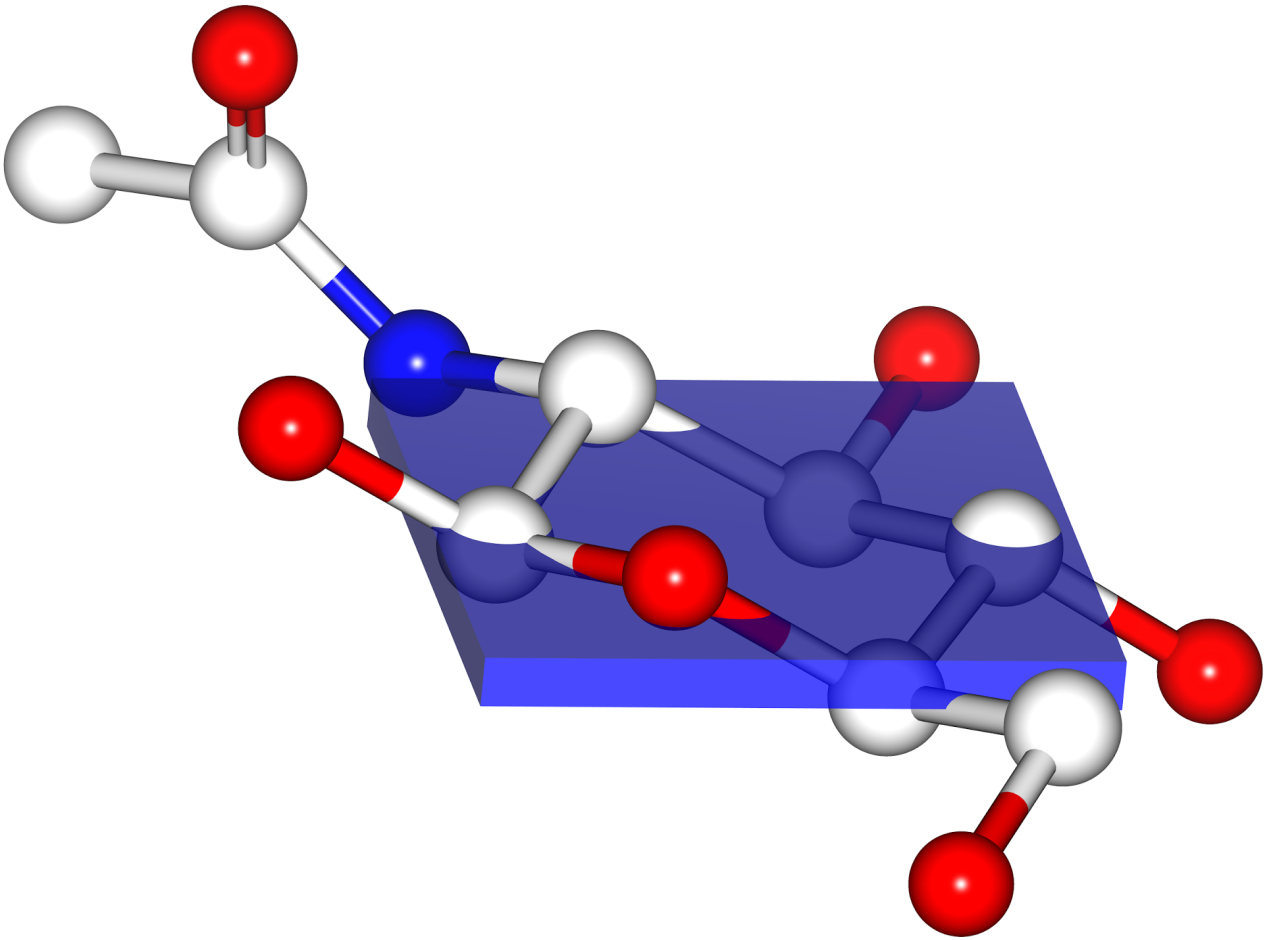


Iduronic acid
(IDR)

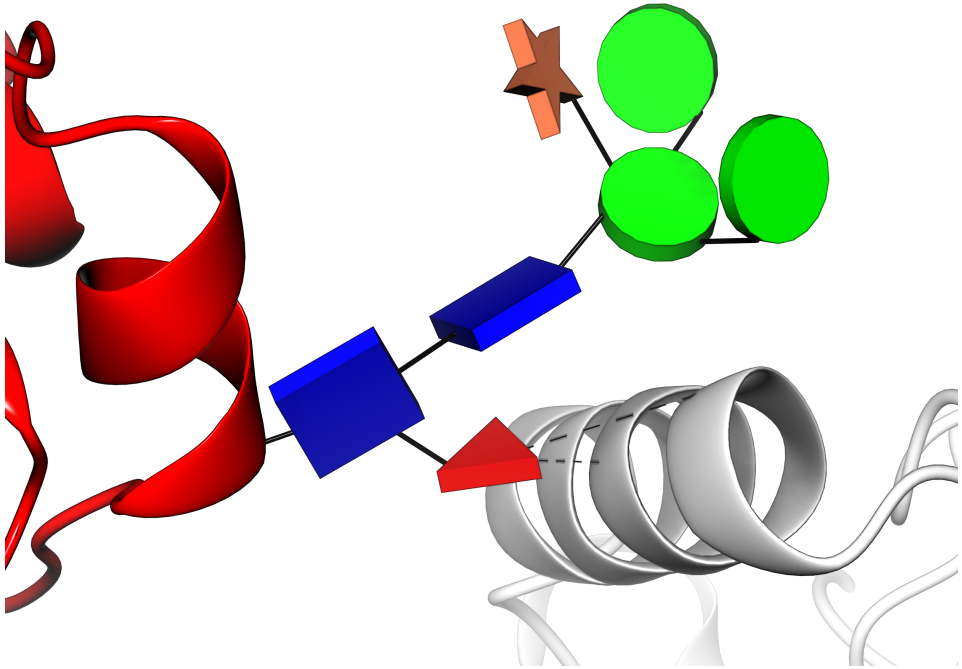


Mannuronic acid
(BEM)

Saccharide display in 3D

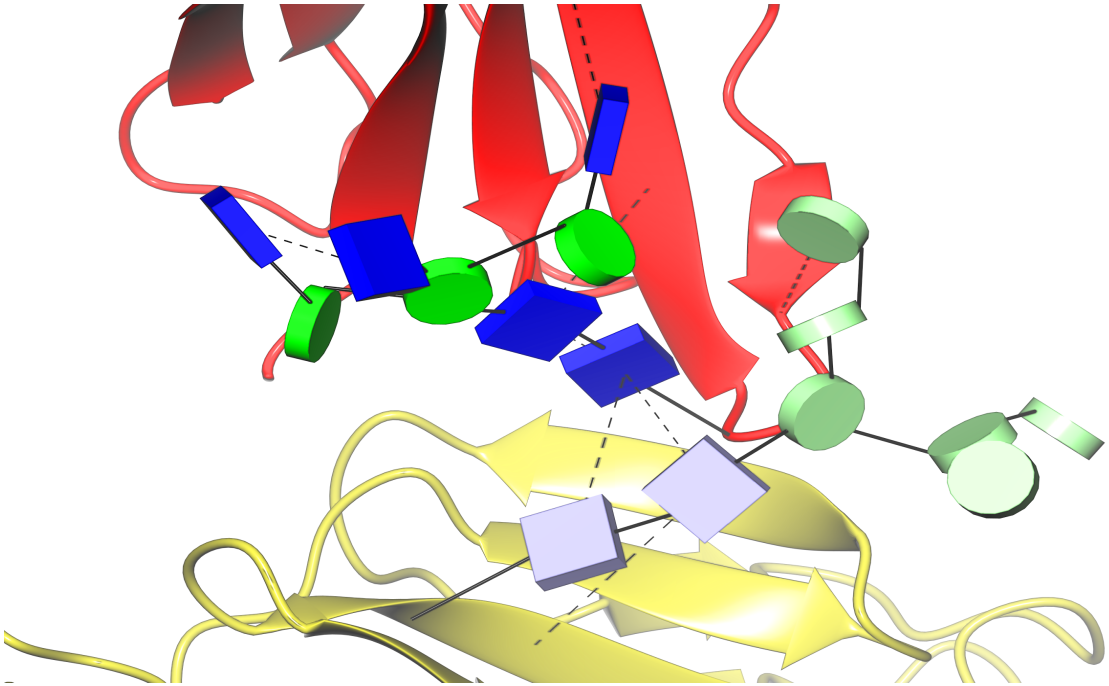


Saccharide display in 3D



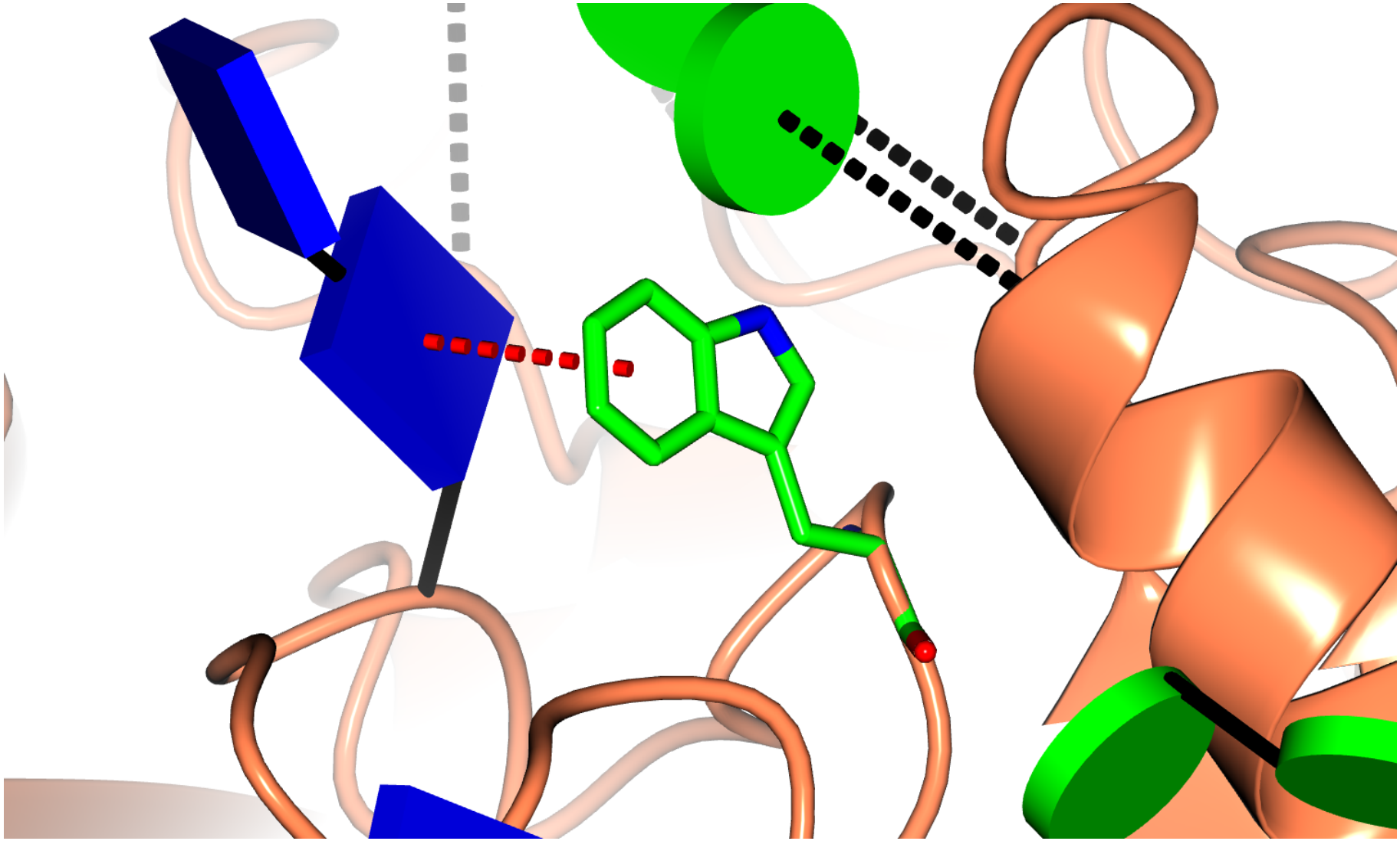
Glycoblocks representation of a plant N-glycan and its interactions (PDB 4CUO). In this structure, the Fucose sugar attached to the first N-acetyl-β-D-glucosamine residue establishes two hydrogen bonds to a neighbouring chain (depicted in white) that is related by crystallographic symmetry to the one 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.

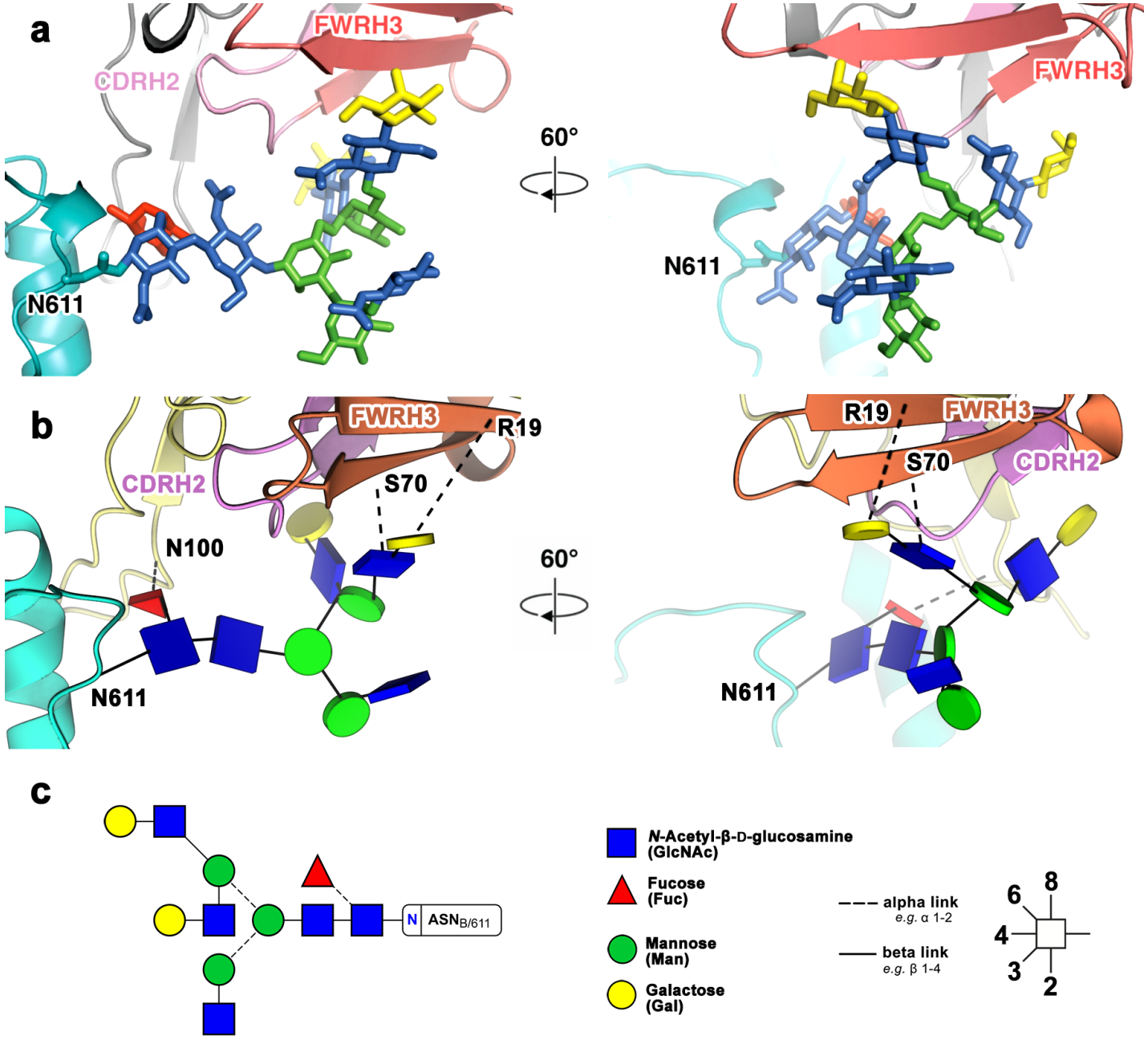
Saccharide display in 3D



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




a
FWRH3
CDRH2
N611
60°
FWRH3
N611
b
FWRH3
R19
CDRH2
S70
N100
N611
60°
R19
FWRH3
S70
CDRH2
N611
c
N
ASN B/611
N-Acetyl-β-D-glucosamine (GlcNAc)
Fucose (Fuc)
Mannose (Man)
Galactose (Gal)
alpha link
e.g. α 1-2
beta link
e.g. β 1-4
6
8
4
3
2

Privateer Mk III

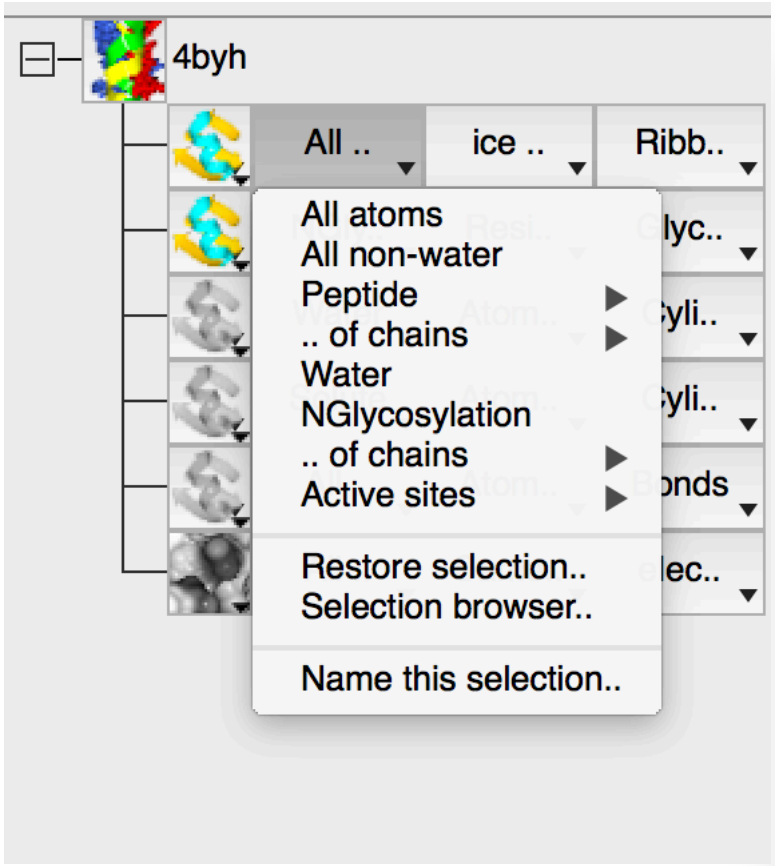
- Validation of glycosylation structures based on the expression system (fungal, mammalian, plant, etc.)
- Generates pretty SVG diagrams which also happen to be interactive - i2 and MG can use these
- Python interface for easy connection with other programs/pipelines. Example: Glycoblocks in MG

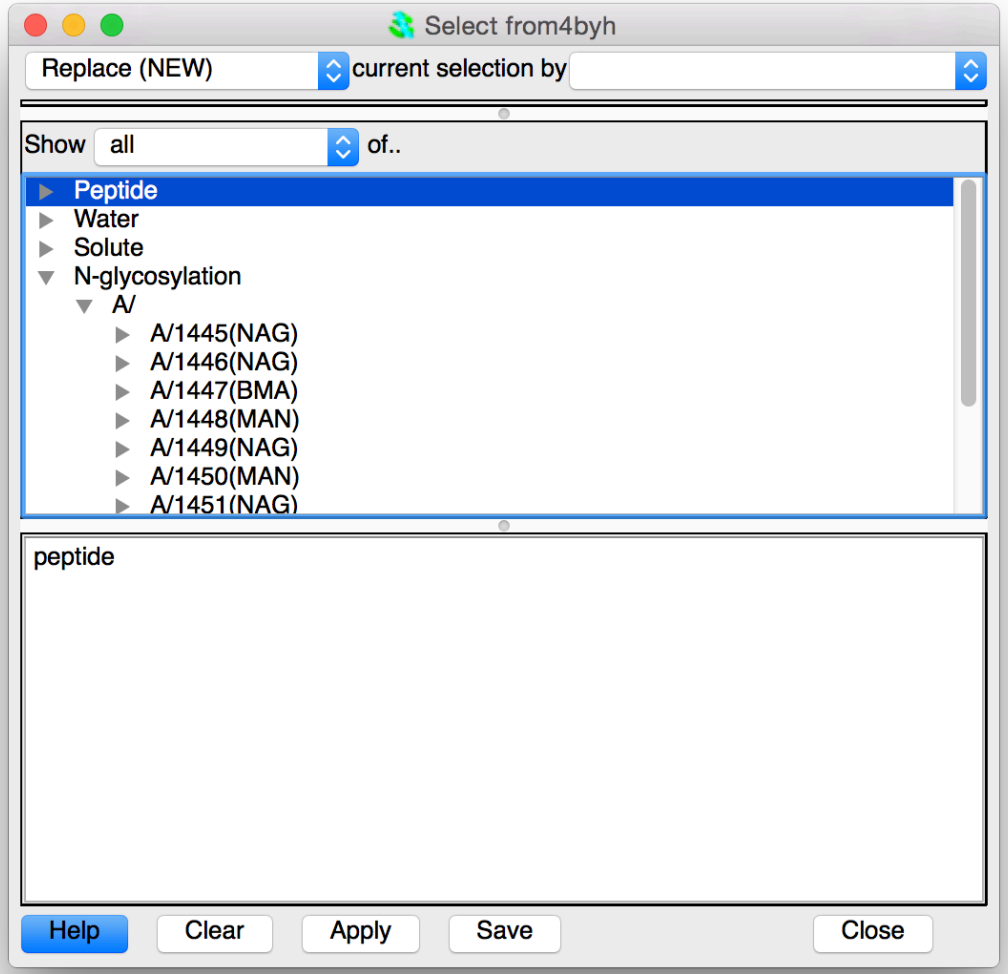
Privateer: software for the conformational validation of carbohydrate structures.
Jon Agirre, Javier Iglesias-Fernández, Carme Rovira, Gideon Davies, Keith Wilson and Kevin Cowtan. *Nature Structural & Molecular Biology,* 2015, **22**(11), 833-834.

Glycosylation in selections

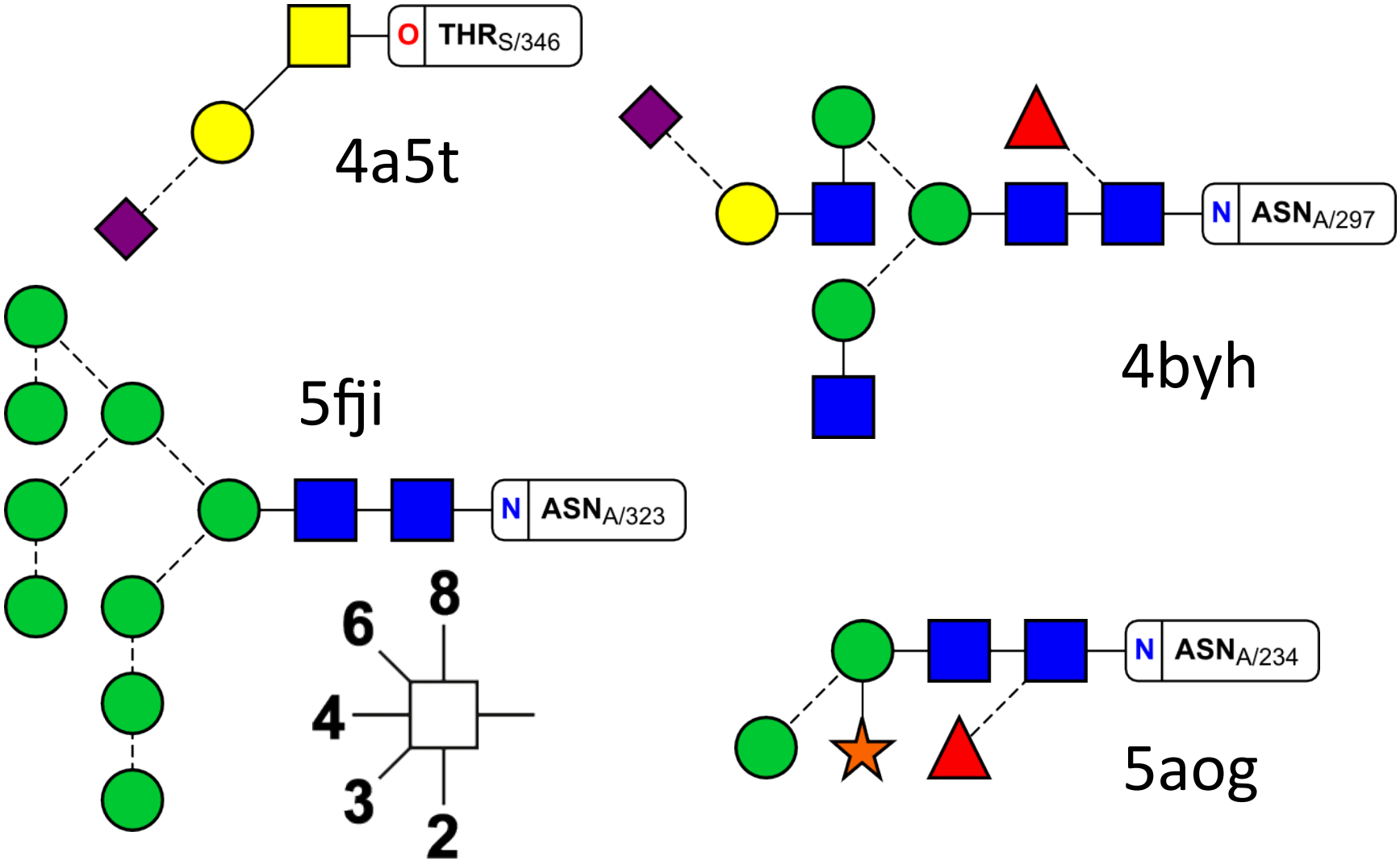
- N- and O- glycosylation sites are now identified when file is loaded into CCP4MG using *Privateer* and appear in selection menus.
- Picture wizards automatically generate Glycoblocks.

Glycosylation selections



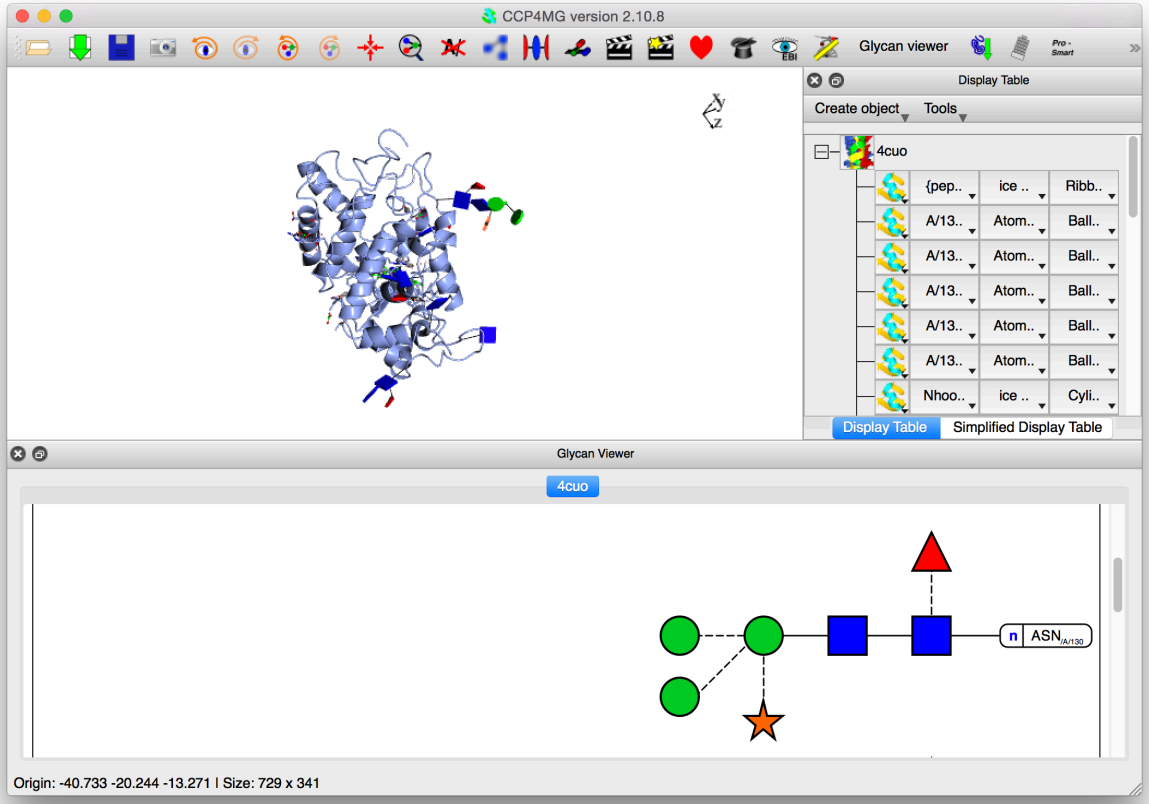


SVG Diagrams – “Essentials” notation



Glycan Viewer

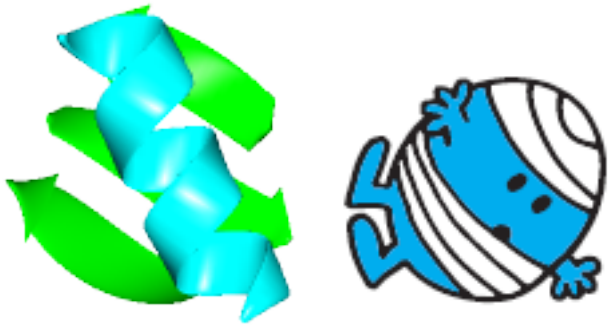
- Traditional 2D – representation with:
  - Hover over glycans/links for extra information
  - Click on glycan to centre 3D view on that glycan.



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

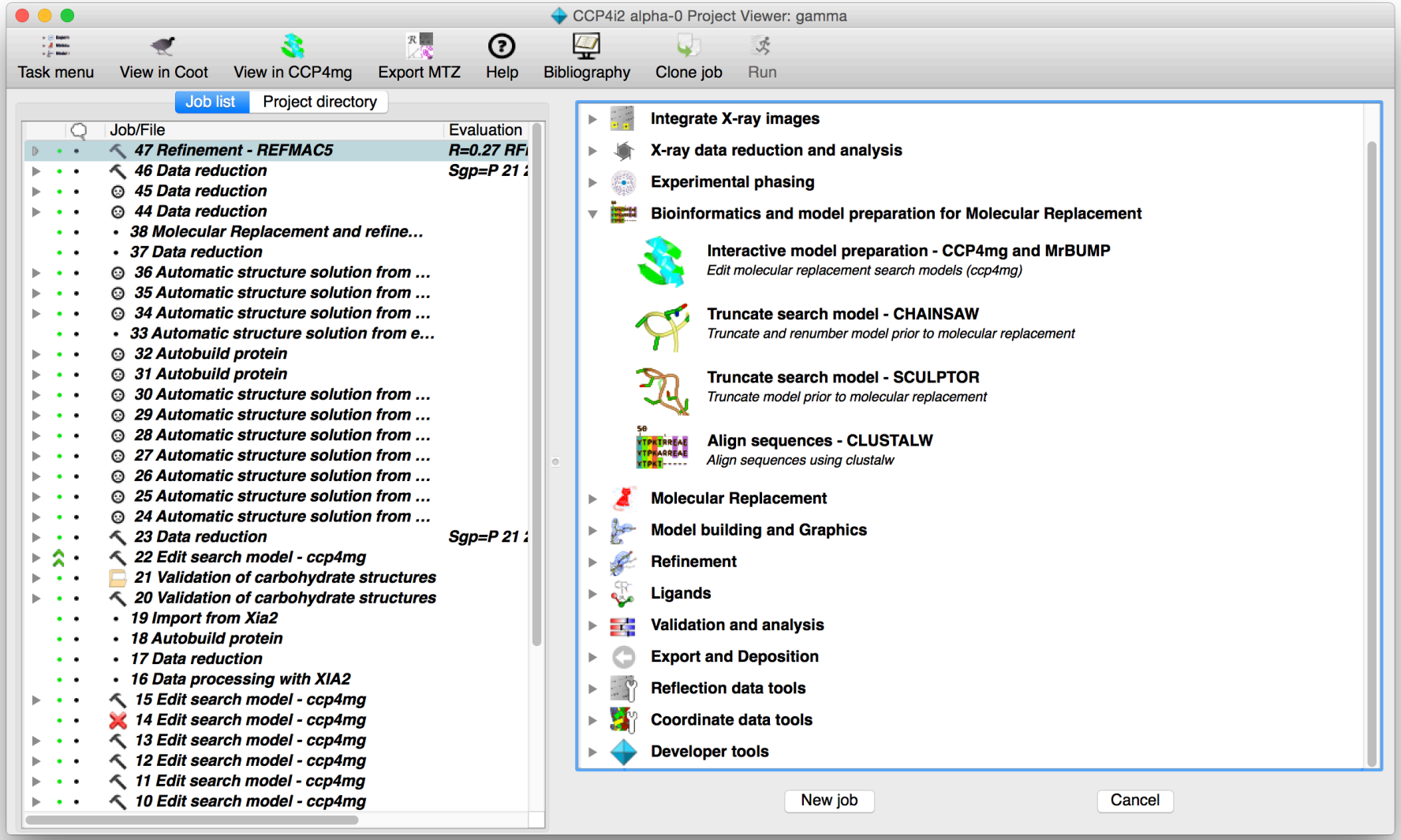
- Goal is to provide i2 users with a graphical driven interface to the model search and preparation steps for molecular replacement in MrBUMP. The intention is to derive a graphically-informed single “best” search model for passing back to i2 and the Phaser/ Molrep interfaces

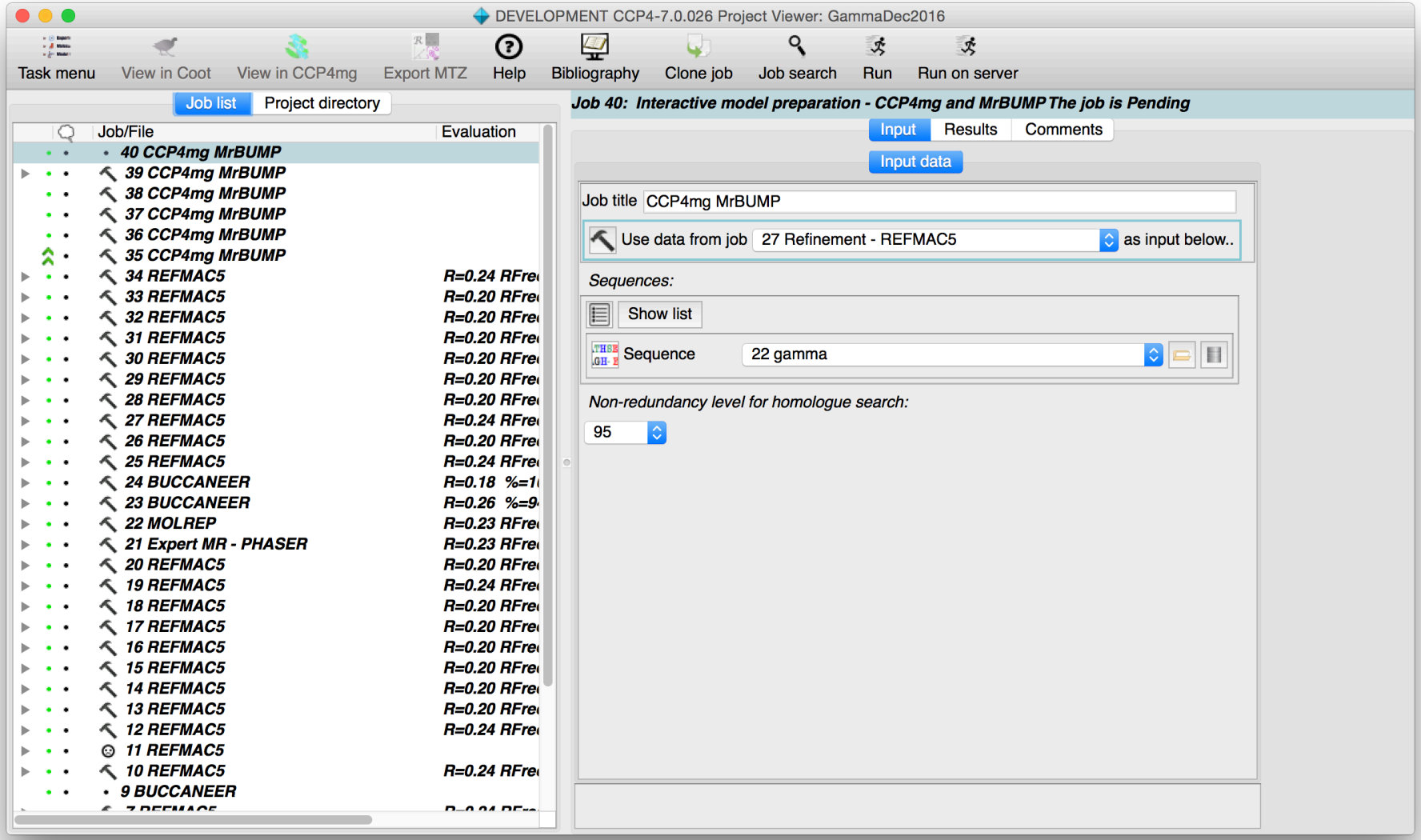
CCP4MG and MrBUMP

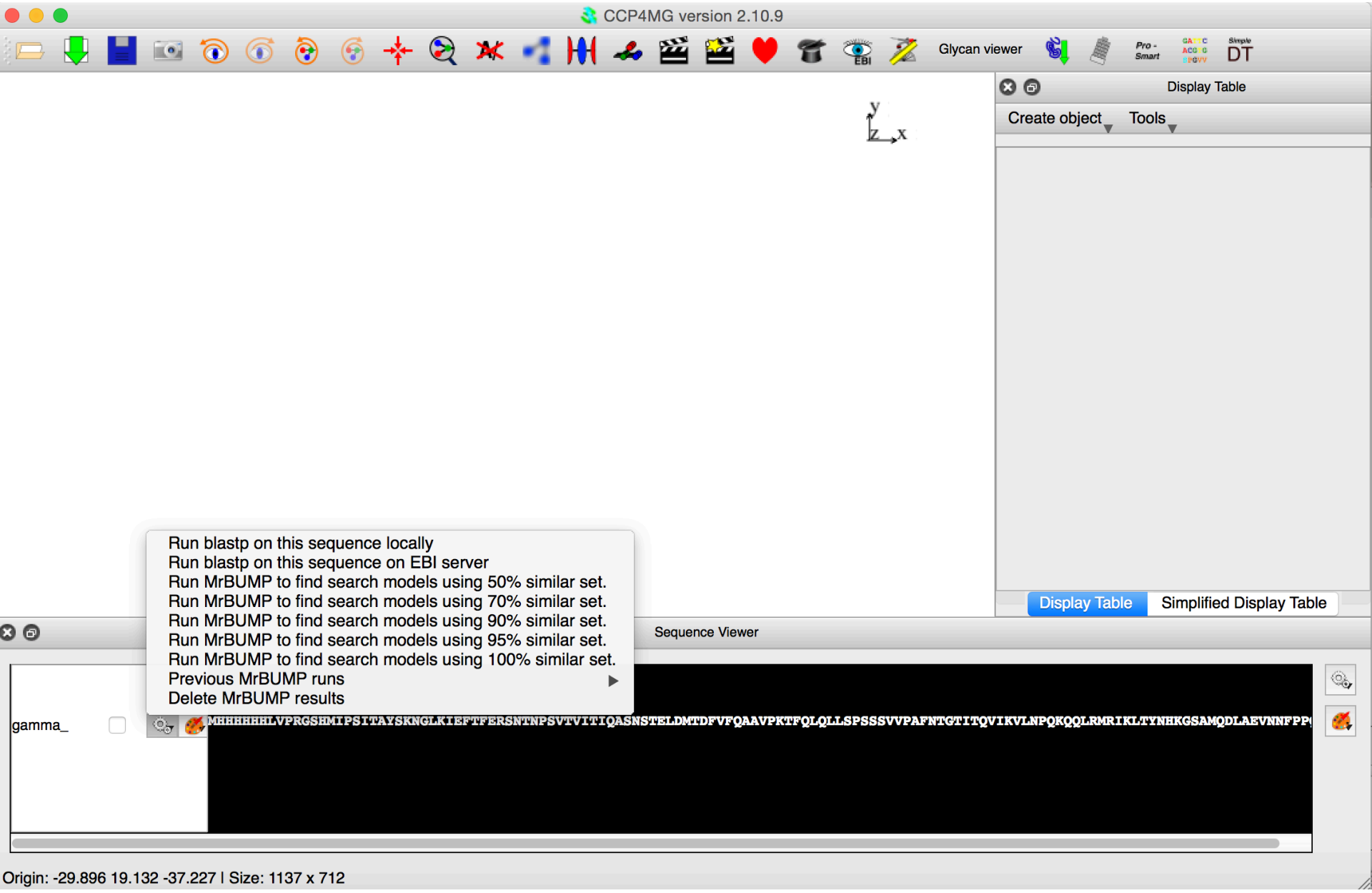
- CCP4MG uses initial steps of the MrBUMP to interactively edit molecular replacement models.
- Scheme:
  - MrBUMP is sent a sequence from CCP4MG
  - uses the phmmer tool to search for homologous structures with a maximum similarity between them of 100%, 95%, 90%, 70% or 50%.
  - select just the relevant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

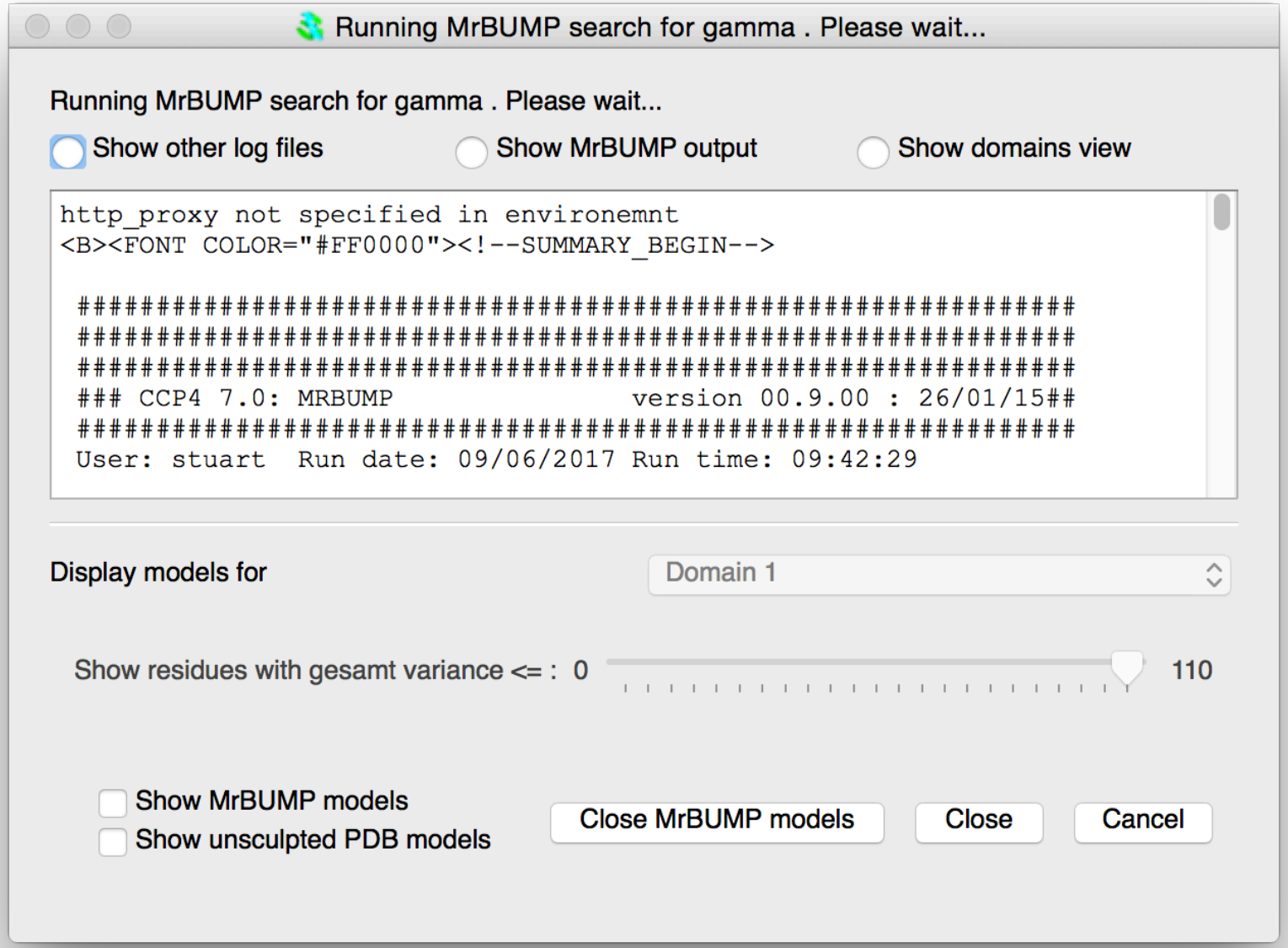
CCP4MG and MrBUMP

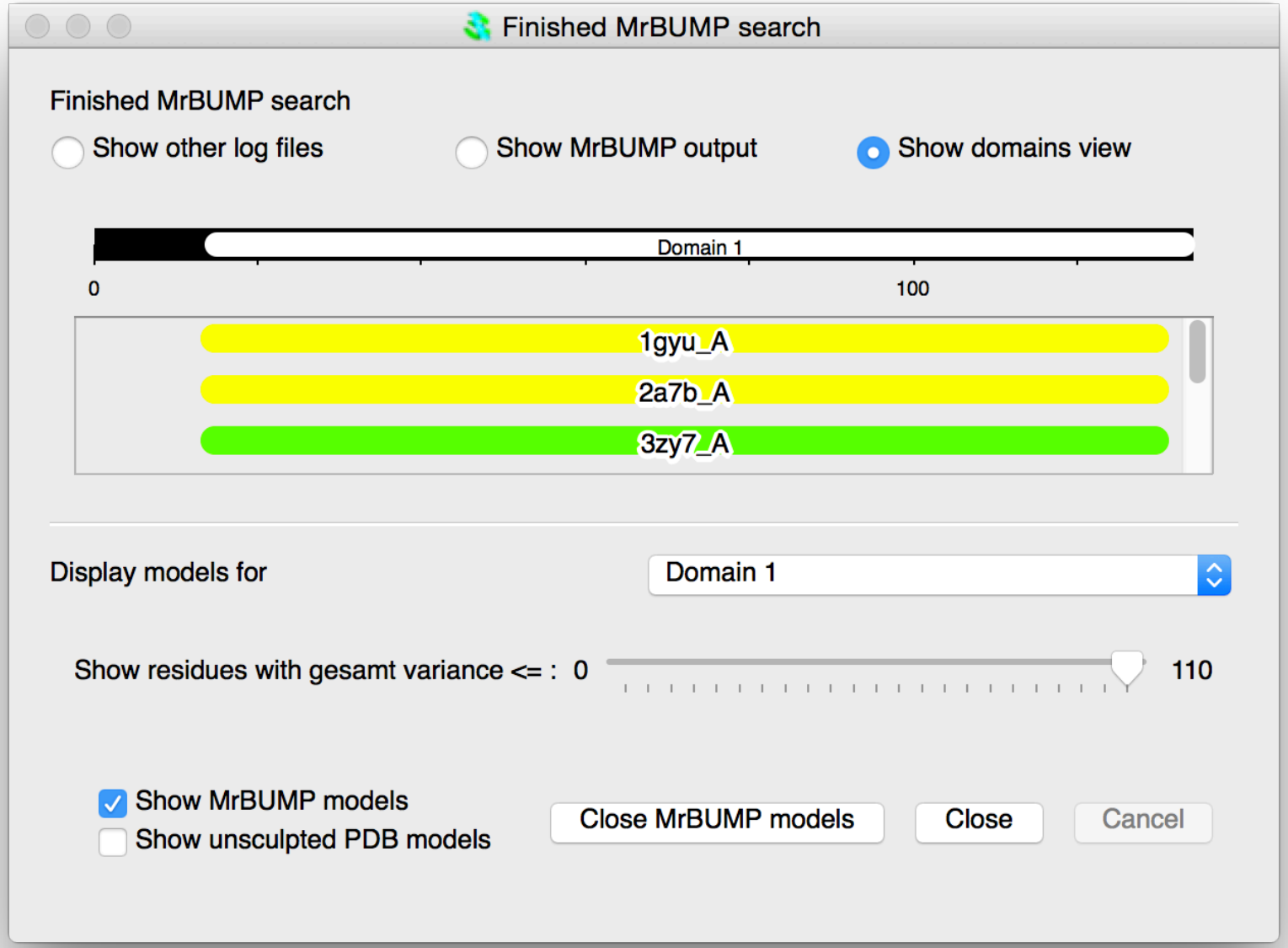
- Then CCP4MG can be used to select subsets of atoms from the newly loaded structures:
  - Completely hide some structures.
  - Select e.g. just alpha-helices
  - Prune terminating loops.
  - Whatever … (including “gesamt variance slider”).
- And then everything visible can be saved into one ensemble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

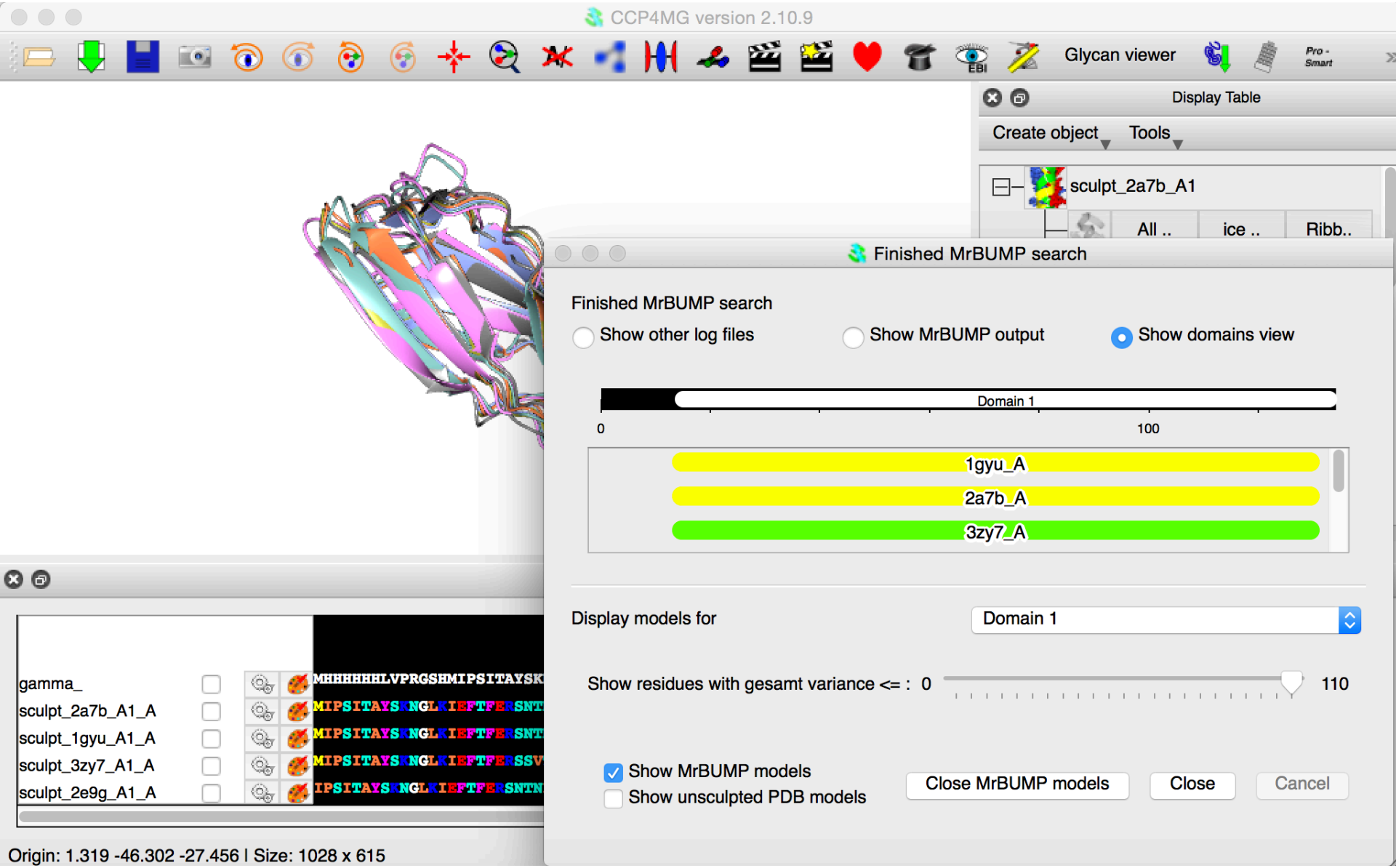

CCP4i2 alpha-0 Project Viewer: gamma
Task menu
View in Coot
View in CCP4mg
Export MTZ
Help
Bibliography
Clone job
Run
Job list
Project directory
Job/File
Evaluation
47 Refinement - REFMAC5
R=0.27 RF
46 Data reduction
Sgp=P 21 2
45 Data reduction
44 Data reduction
38 Molecular Replacement and refine...
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 2
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
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

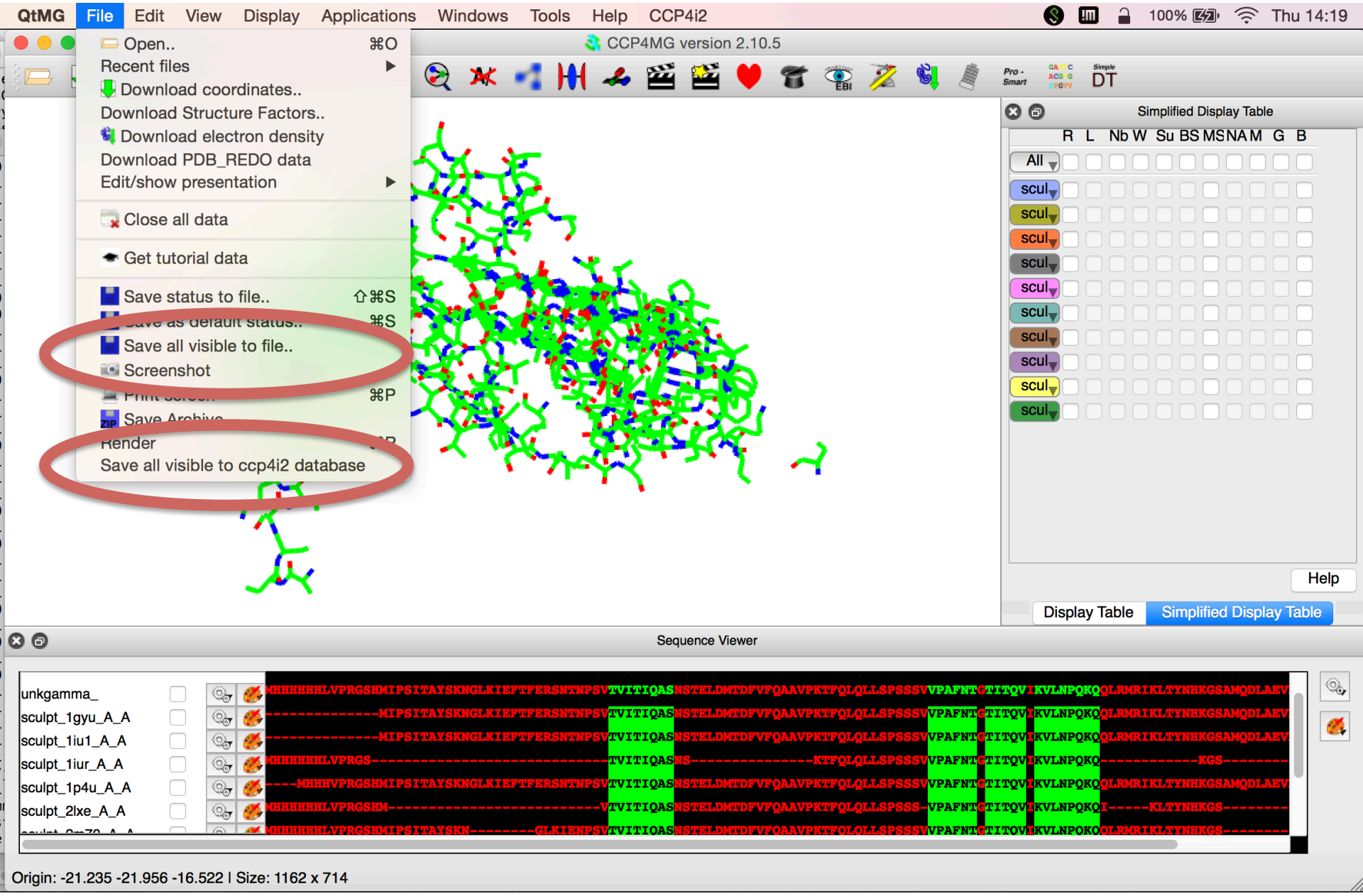

CCP4MG version 2.10.9
Glycan viewer
Display Table
Create object
Tools
Run blastp on this sequence locally
Run blastp on this sequence on EBI server
Run MrBUMP to find search models using 50% similar set.
Run MrBUMP to find search models using 70% similar set.
Run MrBUMP to find search models using 90% 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
Display Table
Simplified Display Table
Sequence Viewer
gamma_
MHHHHHHLVPRGSHMIPSITAYSKNGLKIEFTFERSNTNPSVTVITIQASNSTELDMTDFVFQAAVPKTFQLQLLSPSSSVVPAFNTGTITQVIKVLNPQKQQLRMRIKLTYNHKGSAMQDLAEVNNFPP
Origin: -29.896 19.132 -37.227 | Size: 1137 x 712


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 <= : 0
110
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
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

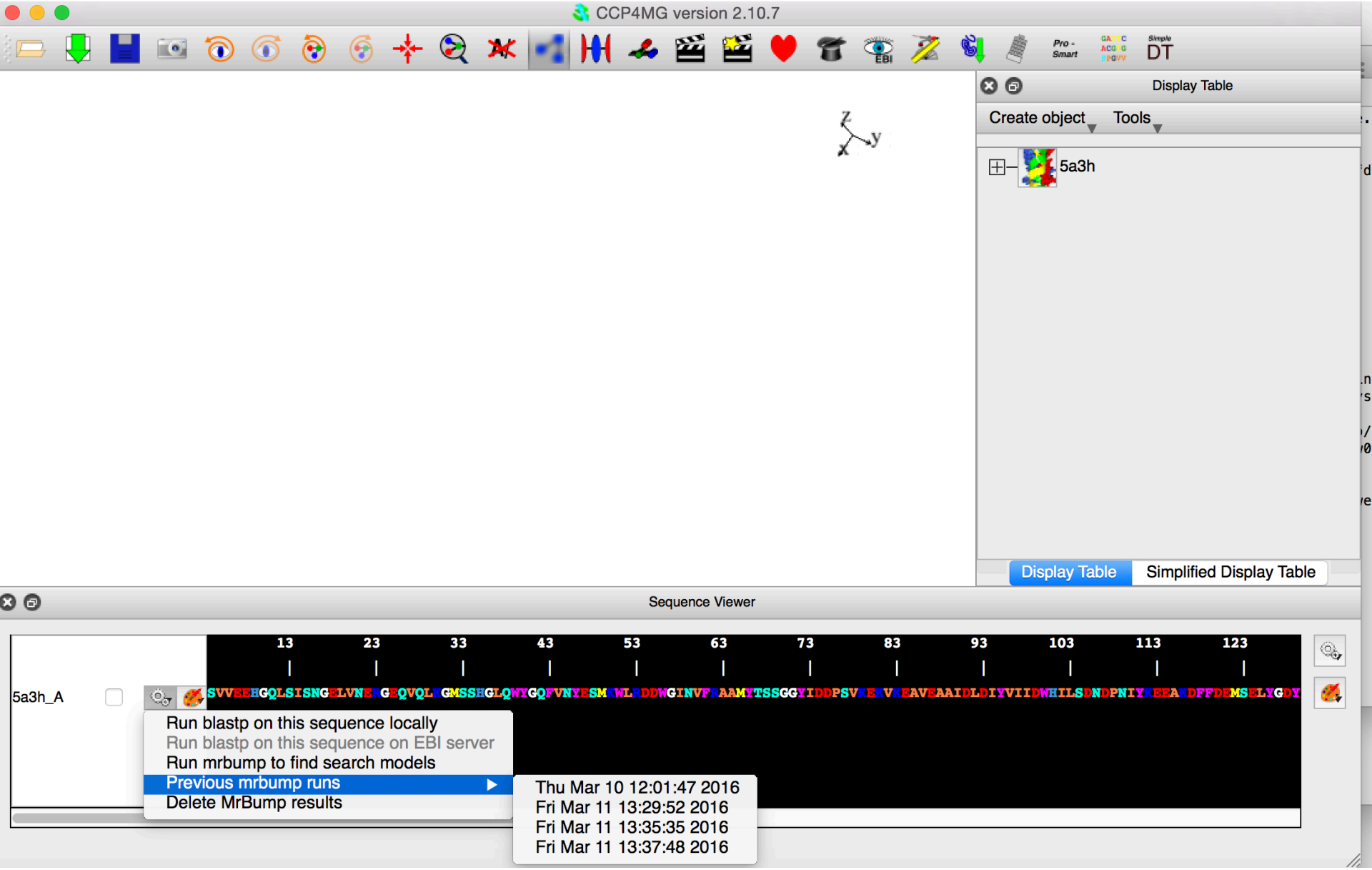


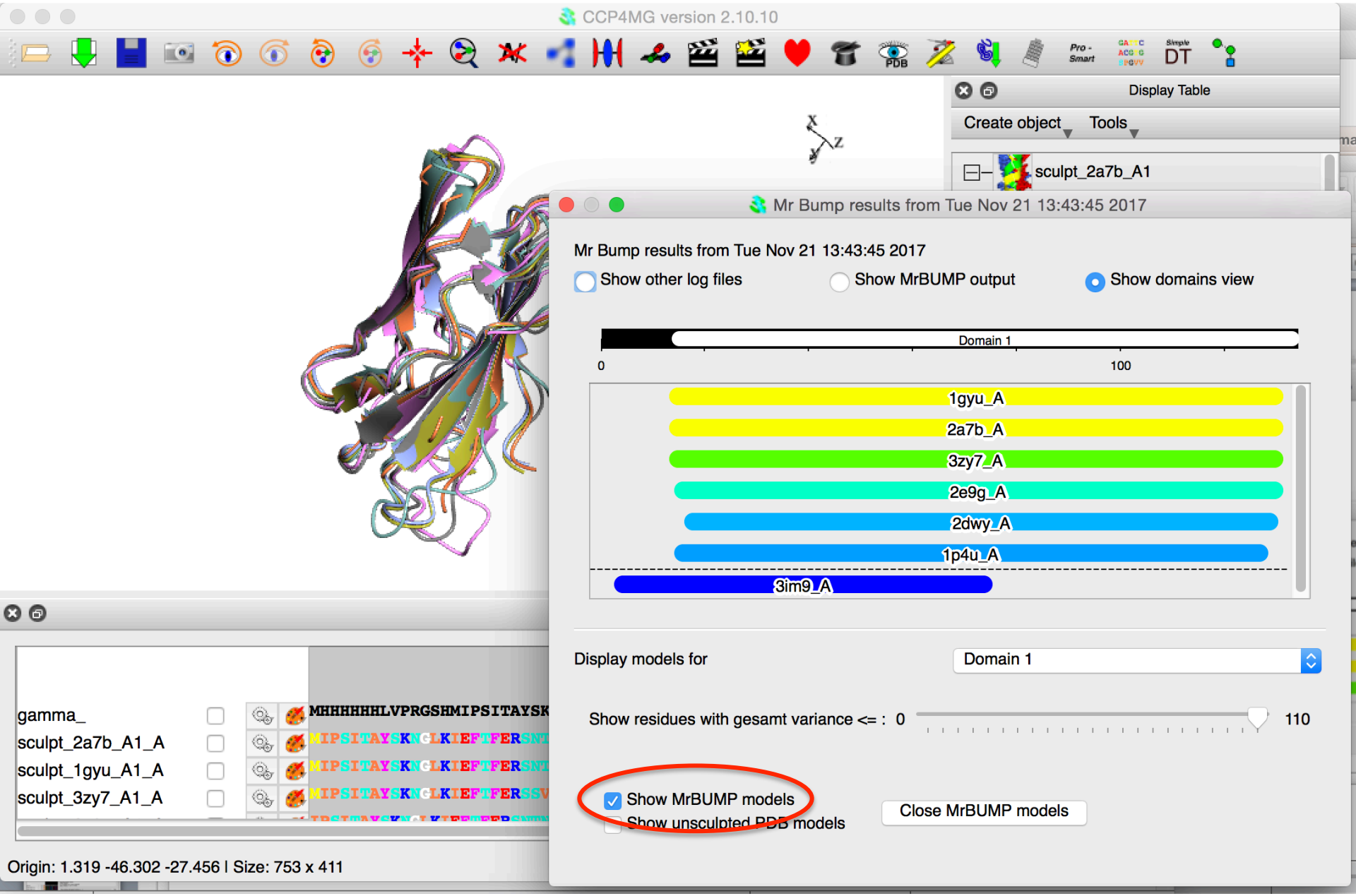
Then use the variance slider to choose atoms.

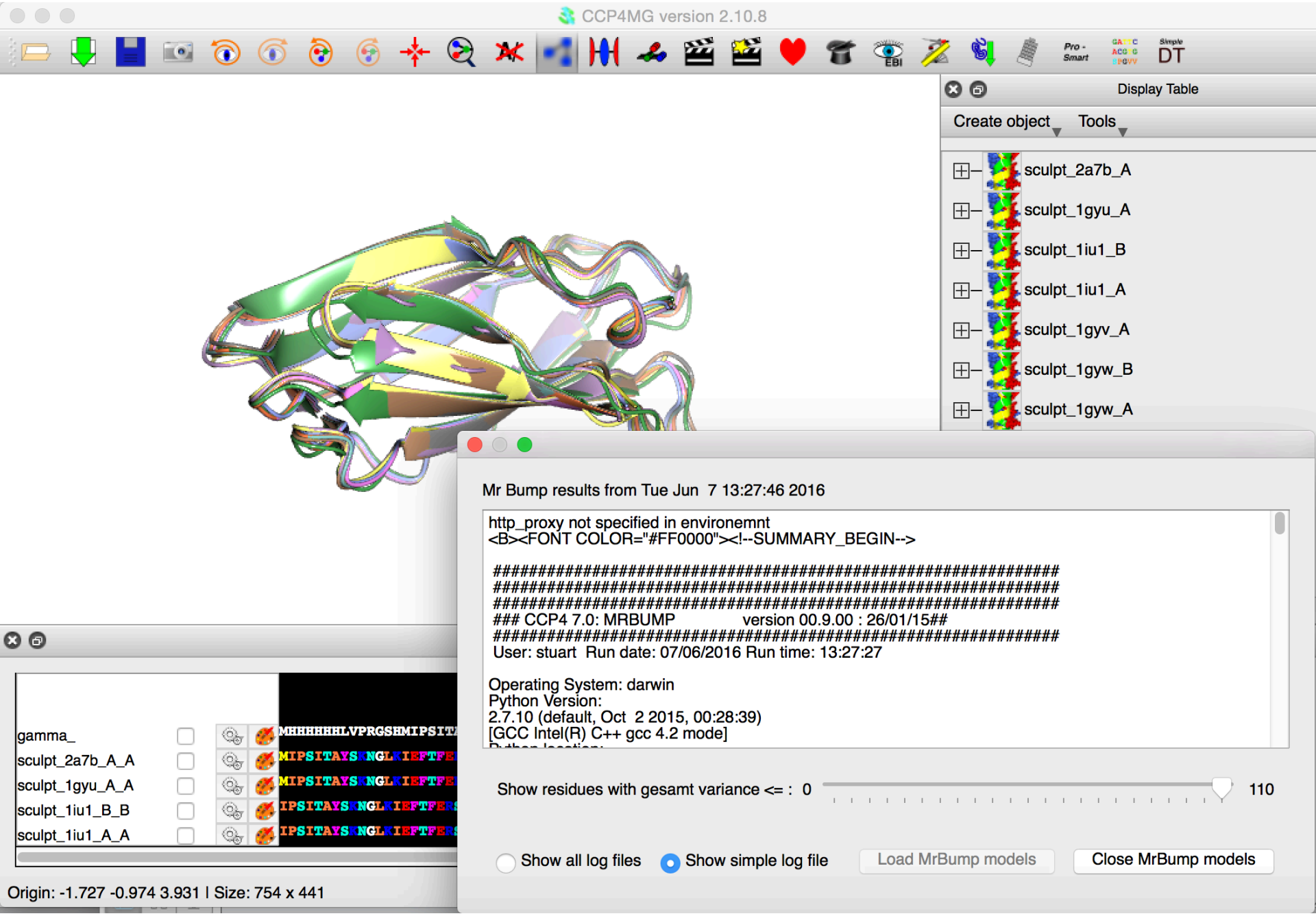

QtMG
File
Edit
View
Display
Applications
Windows
Tools
Help
CCP4i2
100%
Thu 14:19
CCP4MG version 2.10.5
Open..
⌘O
Recent files
Download coordinates..
Download Structure Factors..
Download electron density
Download PDB_REDO data
Edit/show presentation
Close all data
Get tutorial data
Save status to file..
⇧⌘S
⌘S
Save all visible to file..
Screenshot
⌘P
Save Archive
Render
Save all visible to ccp4i2 database
Simplified Display Table
R L Nb W Su BS MS NA M G B
All
Help
Display Table
Simplified Display Table
Sequence Viewer
unkgamma_
sculpt_1gyu_A_A
sculpt_1iu1_A_A
sculpt_1iur_A_A
sculpt_1p4u_A_A
sculpt_2lxe_A_A
Origin: -21.235 -21.956 -16.522 | Size: 1162 x 714

Other details

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


CCP4MG version 2.10.7
Display Table
Create object
Tools
5a3h
Display Table
Simplified Display Table
Sequence Viewer
13
23
33
43
53
63
73
83
93
103
113
123
5a3h_A
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
0
100
1gyu_A
2a7b_A
3zy7_A
2e9g_A
2dwy_A
1p4u_A
3im9_A
Display models for
Domain 1
Show residues with gesamt variance <= : 0
110
Show MrBUMP models
Show unsculpted PDB models
Close MrBUMP models
gamma_
sculpt_2a7b_A1_A
sculpt_1gyu_A1_A
sculpt_3zy7_A1_A
Origin: 1.319 -46.302 -27.456 | Size: 753 x 411


CCP4MG version 2.10.8
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
<B><FONT COLOR="#FF0000"><!--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]
Show residues with gesamt variance <= : 0
110
Show all log files
Show simple log file
Load MrBump models
Close MrBump models
gamma_
sculpt_2a7b_A_A
sculpt_1gyu_A_A
sculpt_1iu1_B_B
sculpt_1iu1_A_A
Origin: -1.727 -0.974 3.931 | Size: 754 x 441

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CCP4