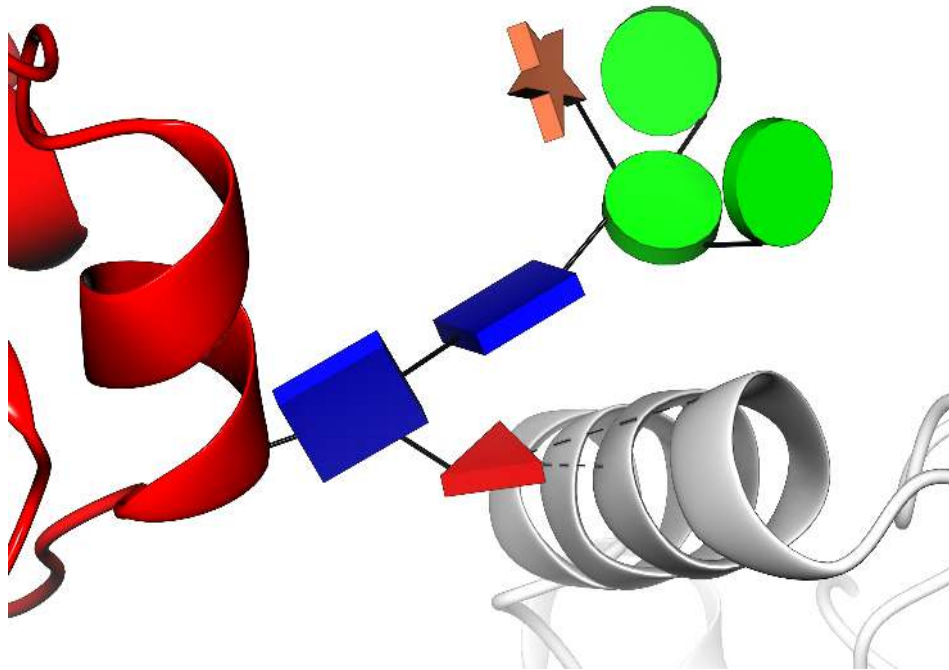


CCP4MG

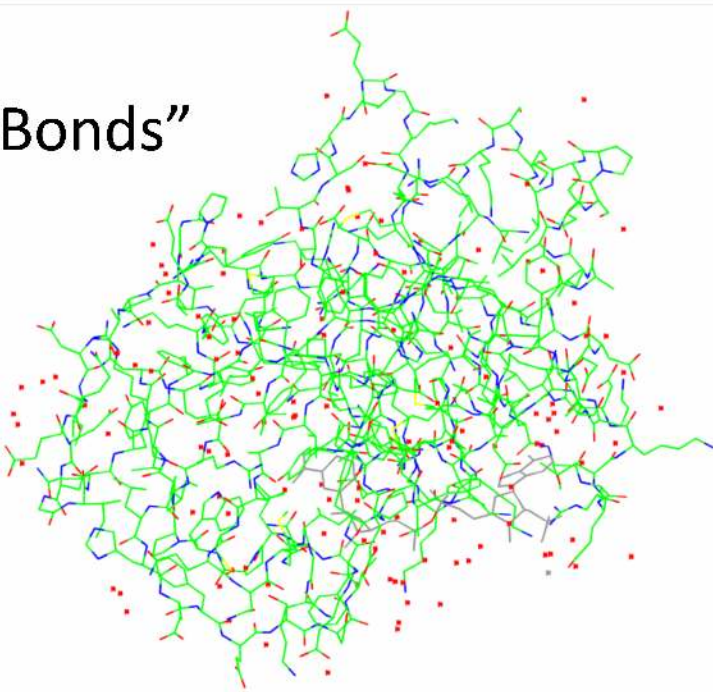


Stuart McNicholas, CCP4MG
Diamond/CCP4 Workshop 2015

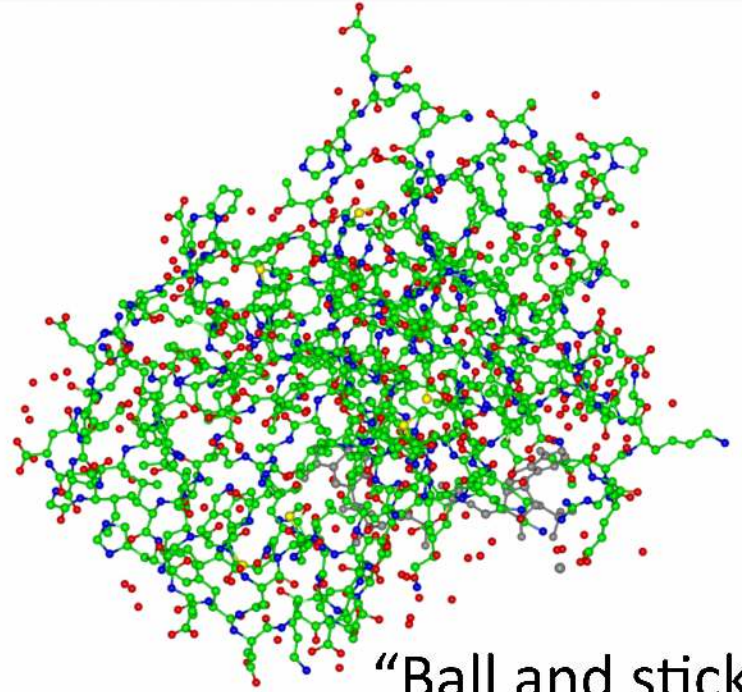
Introduction

- 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.
 - Source code freely available.

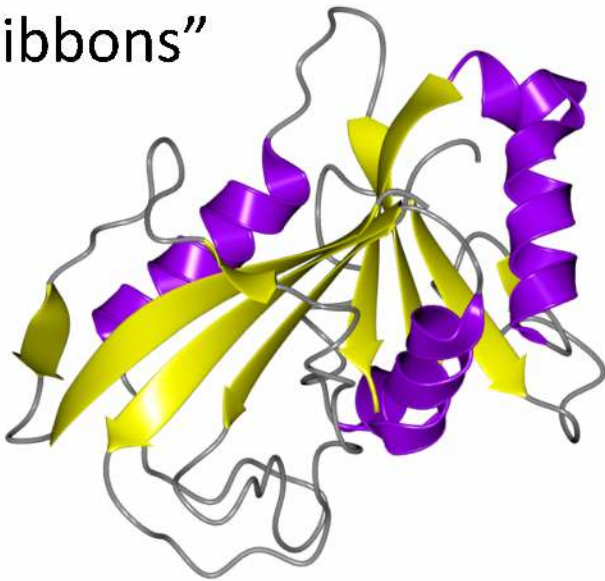
“Bonds”



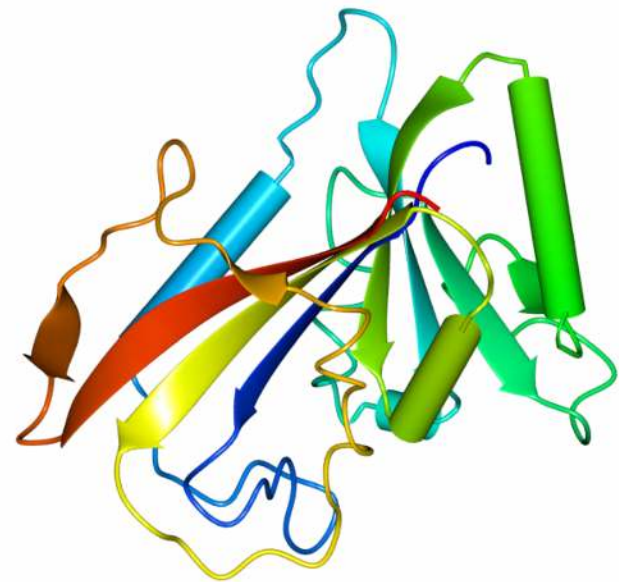
“Ball and stick”

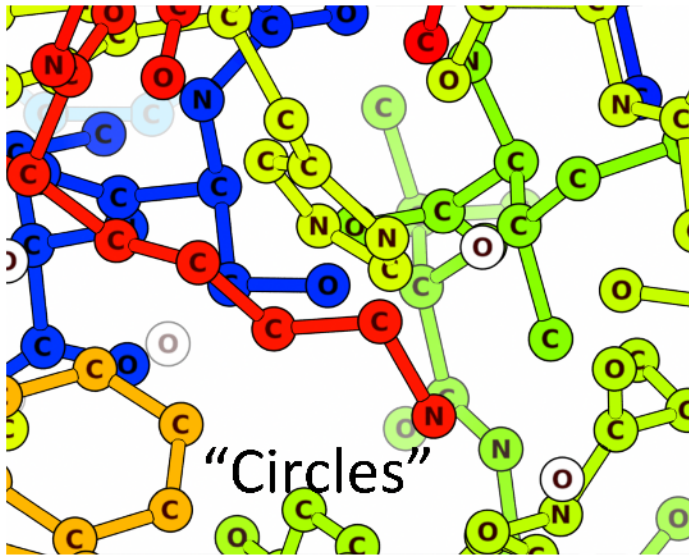


“Ribbons”

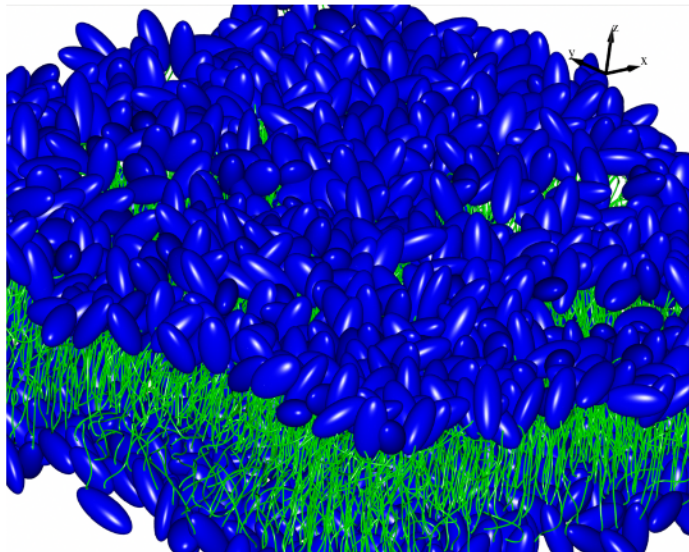
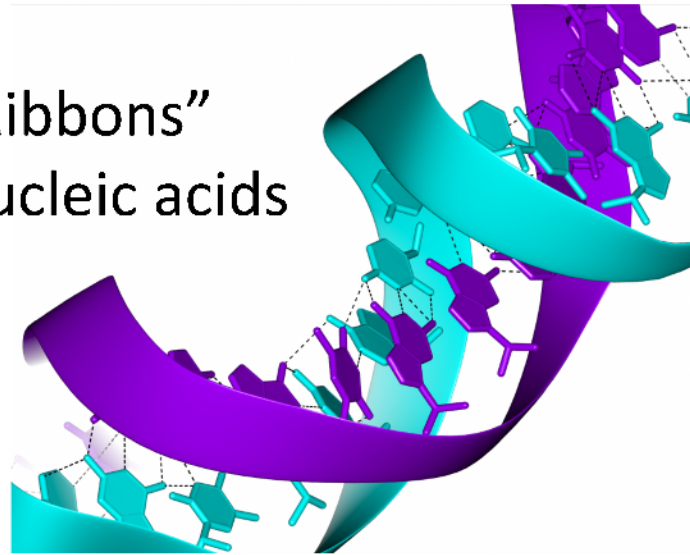


“Worms/tubes”

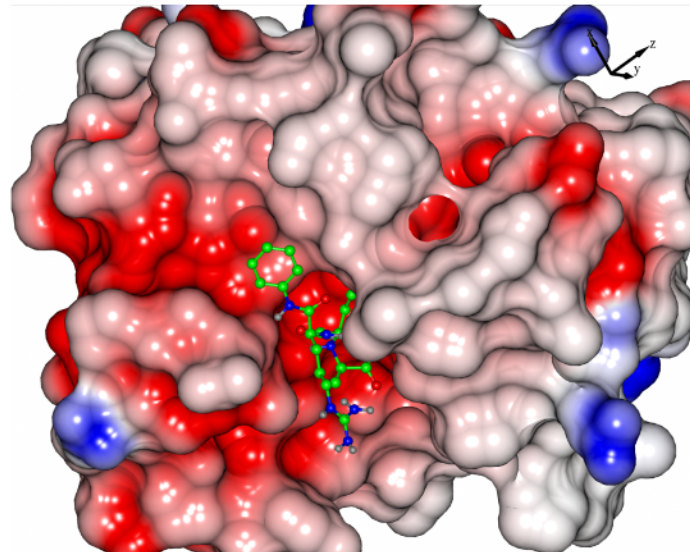




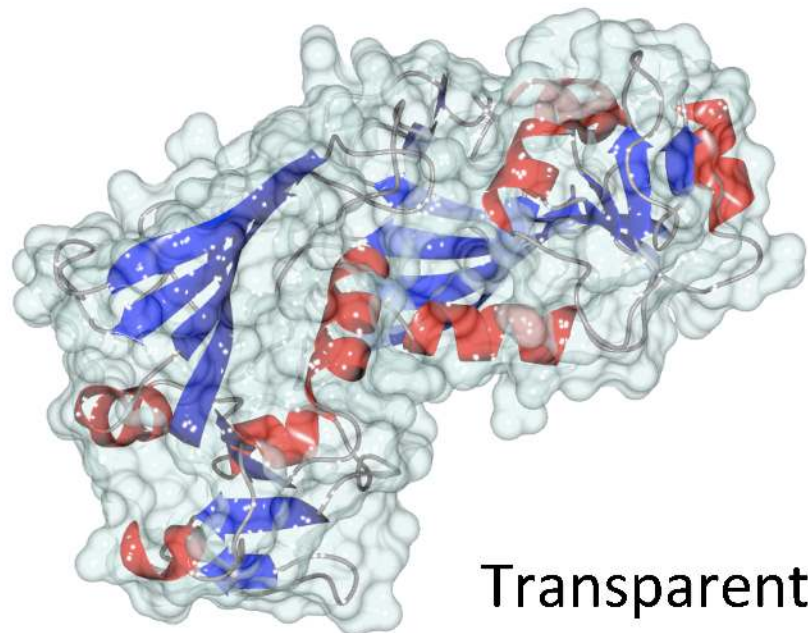
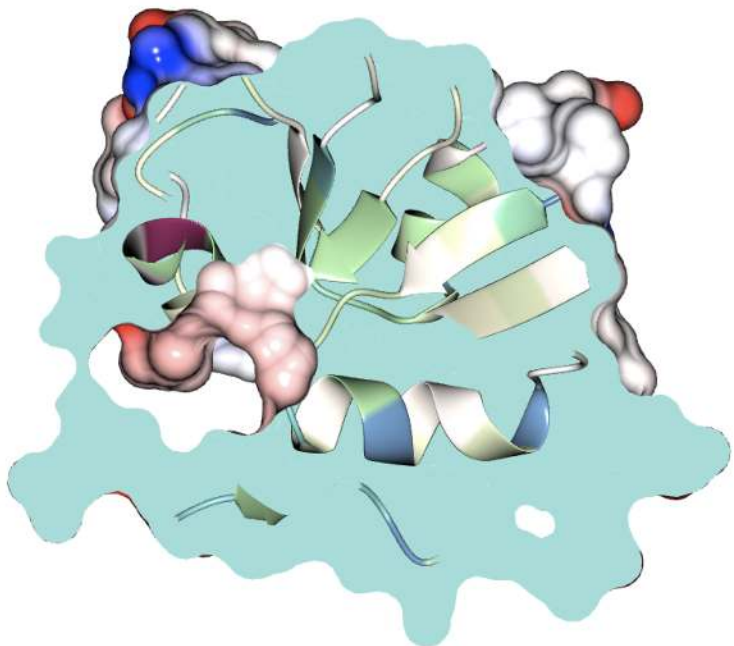
"Ribbons"
Nucleic acids



"Lipid Cartoon"

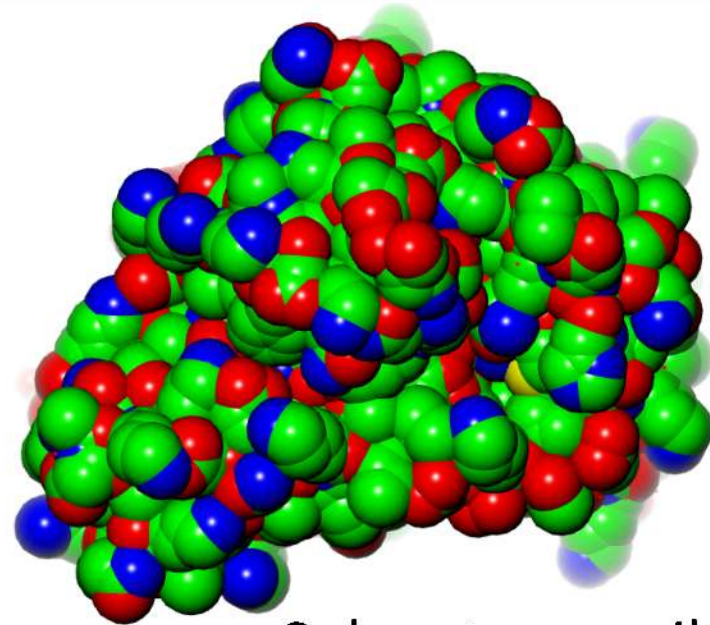
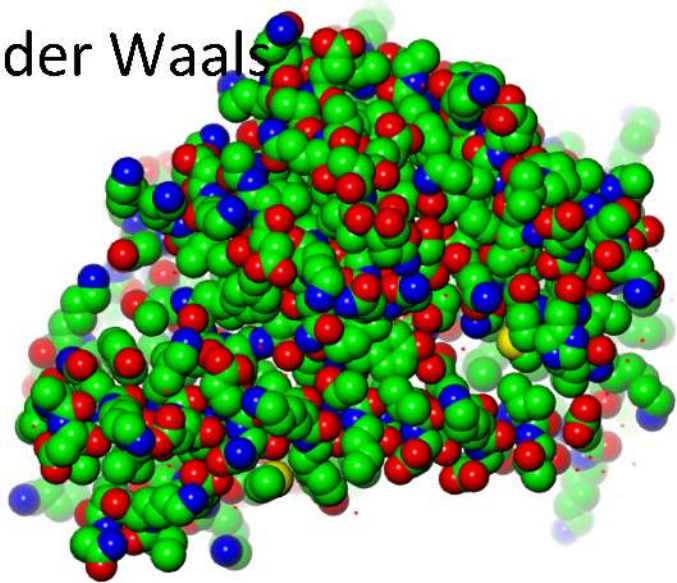


Electrostatic surface

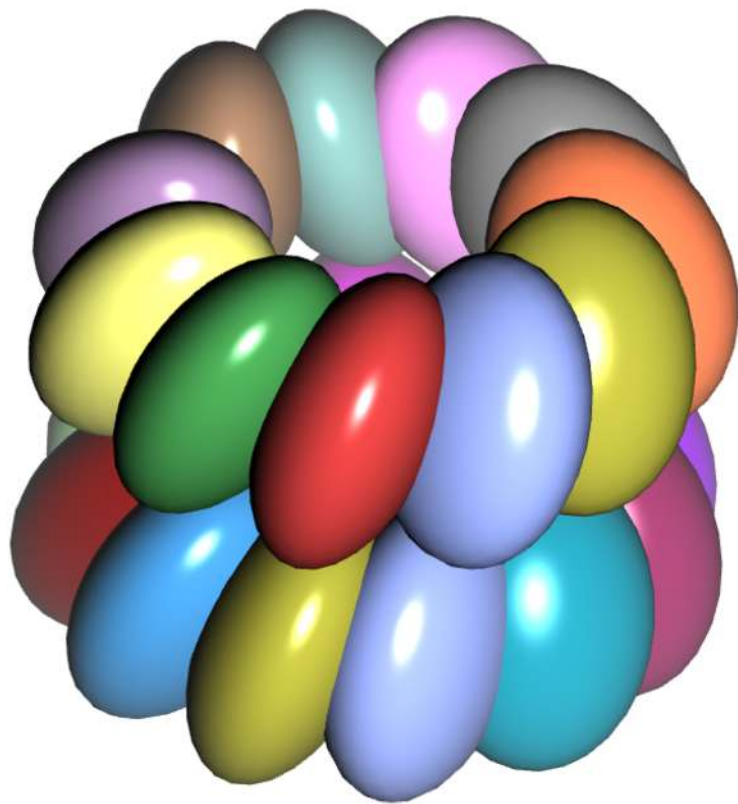


Transparent

Van der Waals

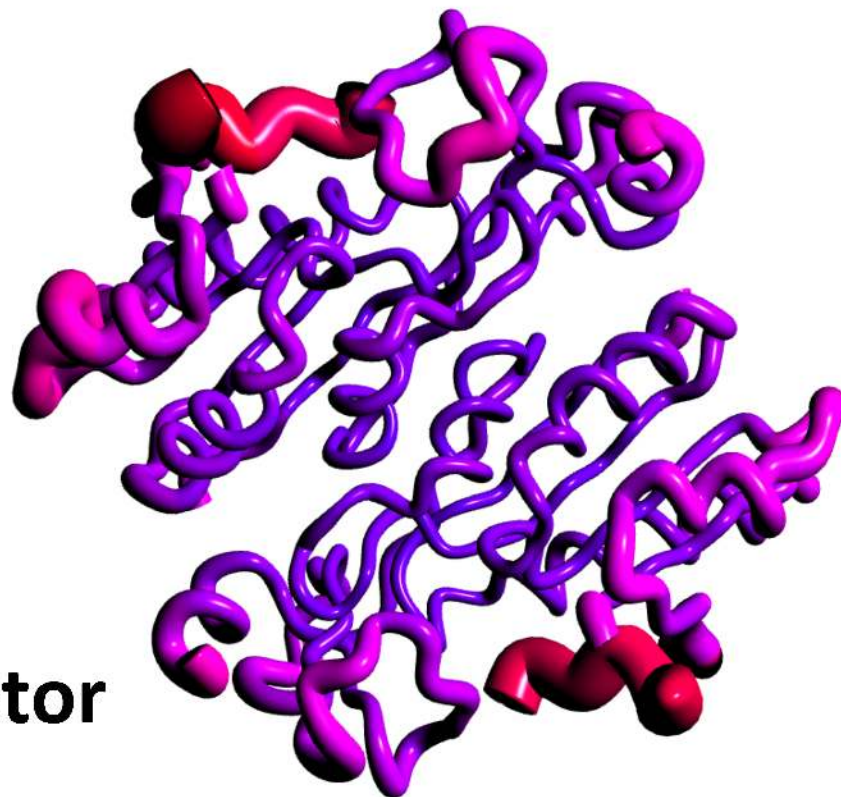


Solvent accessible



Bloboids

**Worm scaled by
Temperature factor**



Basic user Interface

CCP4MG version 2.7.1

Drawing style

Colour

Atom selection

Data object

Display object

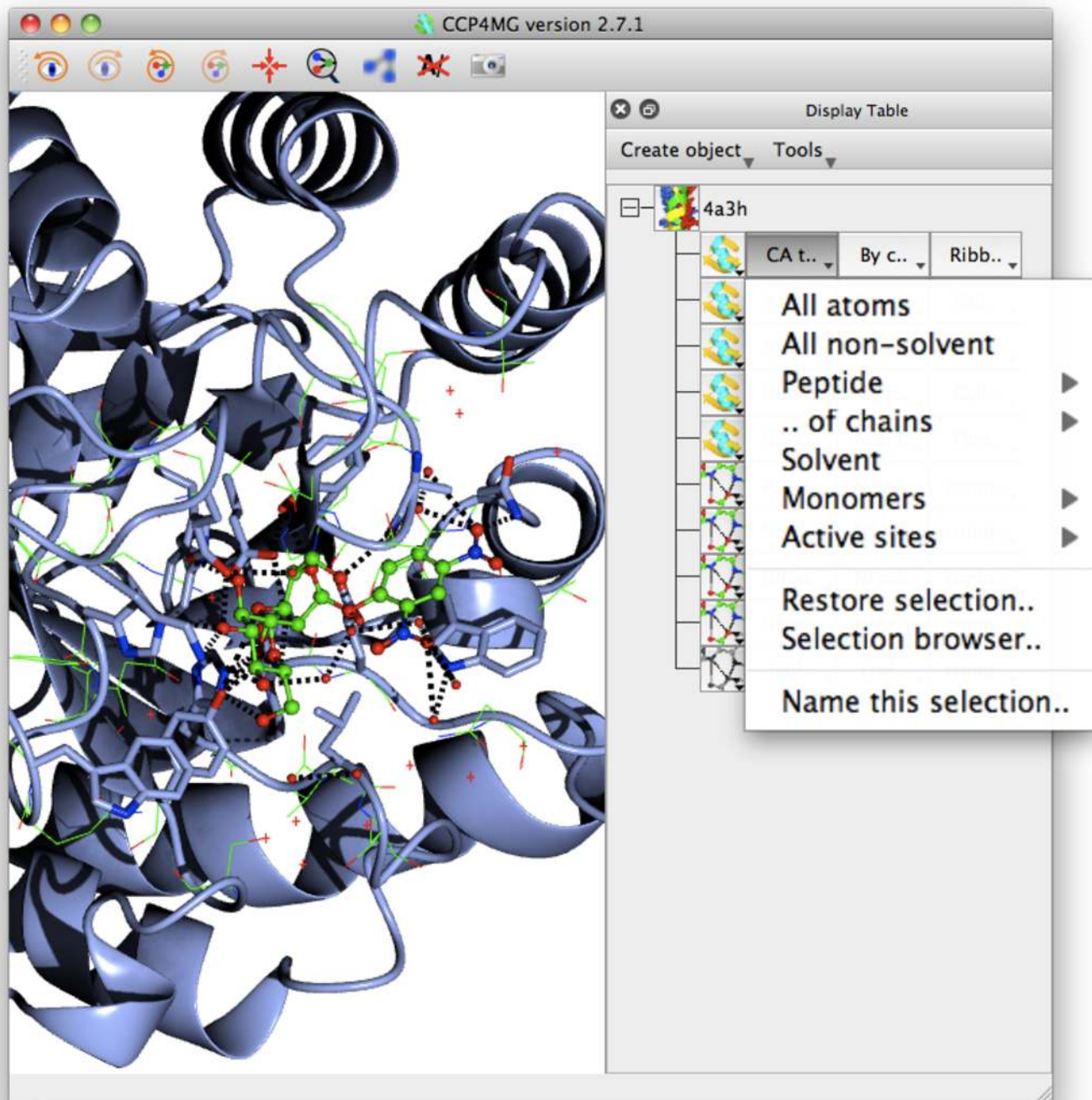
Display Table

Create object

Tools

4a3h

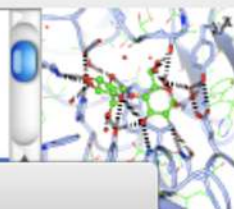
	CA t..	By c..	Ribb..
	A/30..	Atom..	Ball..
	Nhoo..	By c..	Cyli..
	HBon..	By c..	Cyli..
	Nhoo..	Atom..	Thin..
	A/30..	Nhoo..	comp..
	Nhoo..	Nhoo..	comp..
	HBon..	Nhoo..	comp..
	Nhoo..	Nhoo..	comp..
	{sol..	{sol..	comp..



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.

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



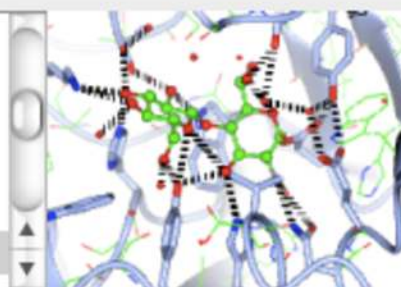
Picture wizard

- ☒ 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

Open file(s)

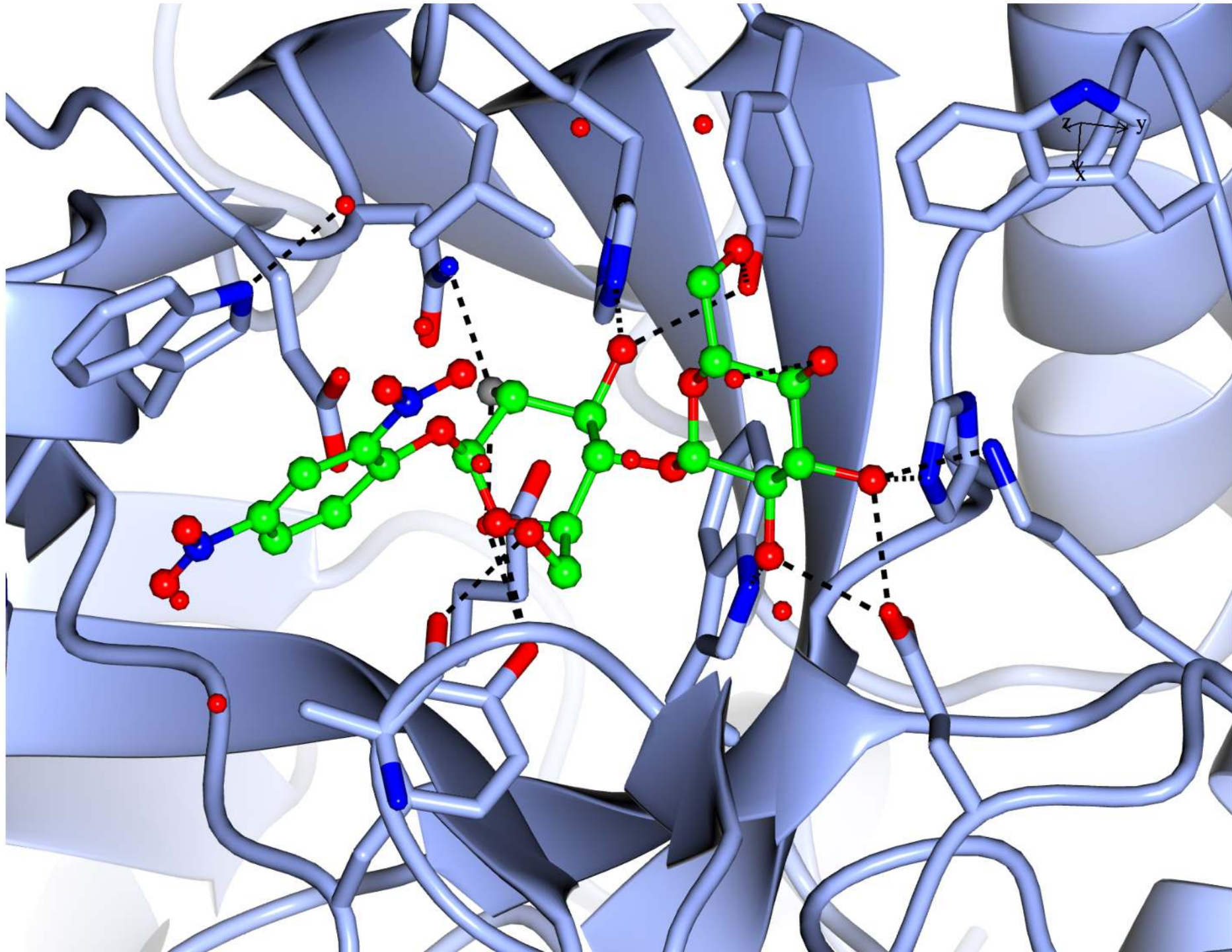
Projects- or ...

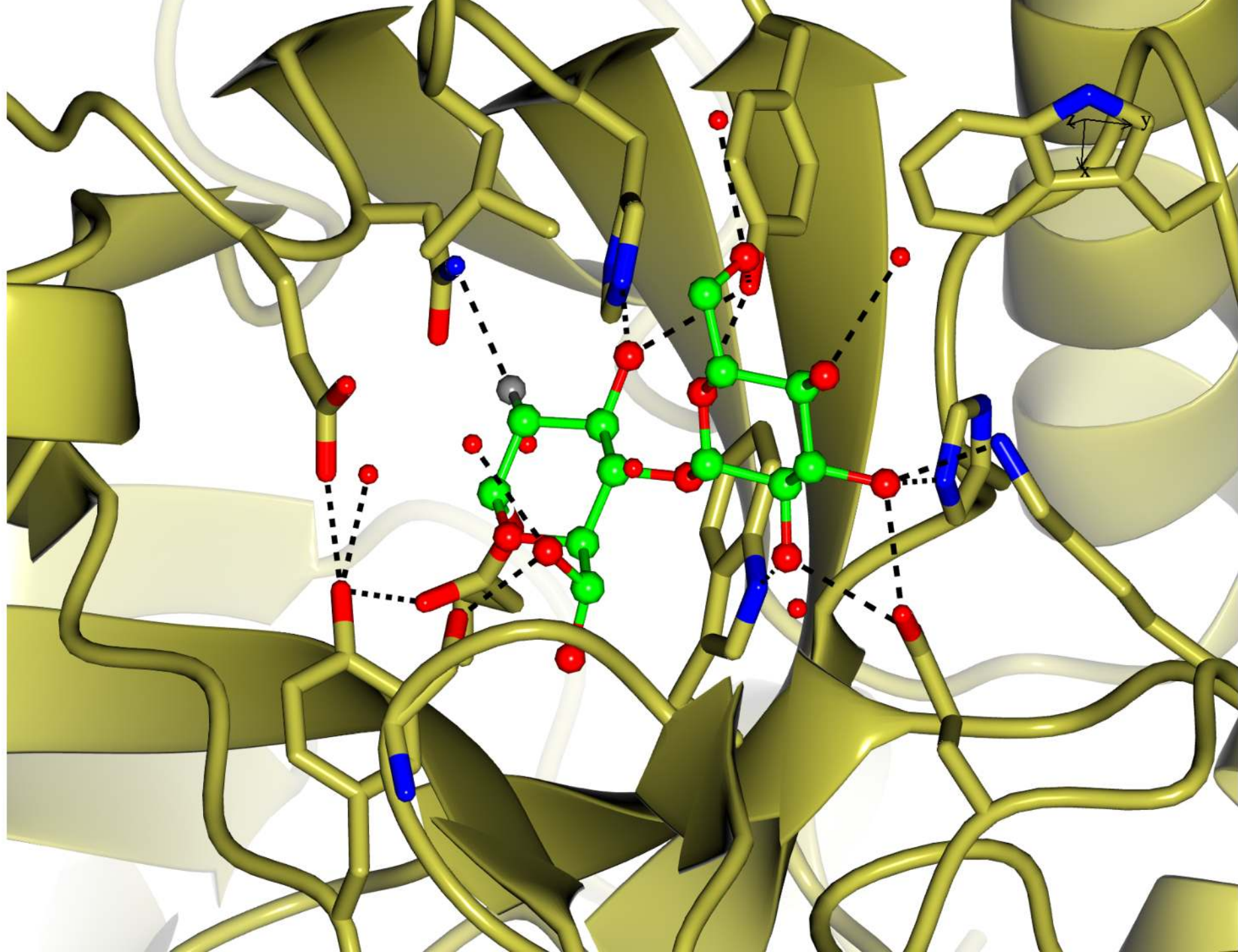


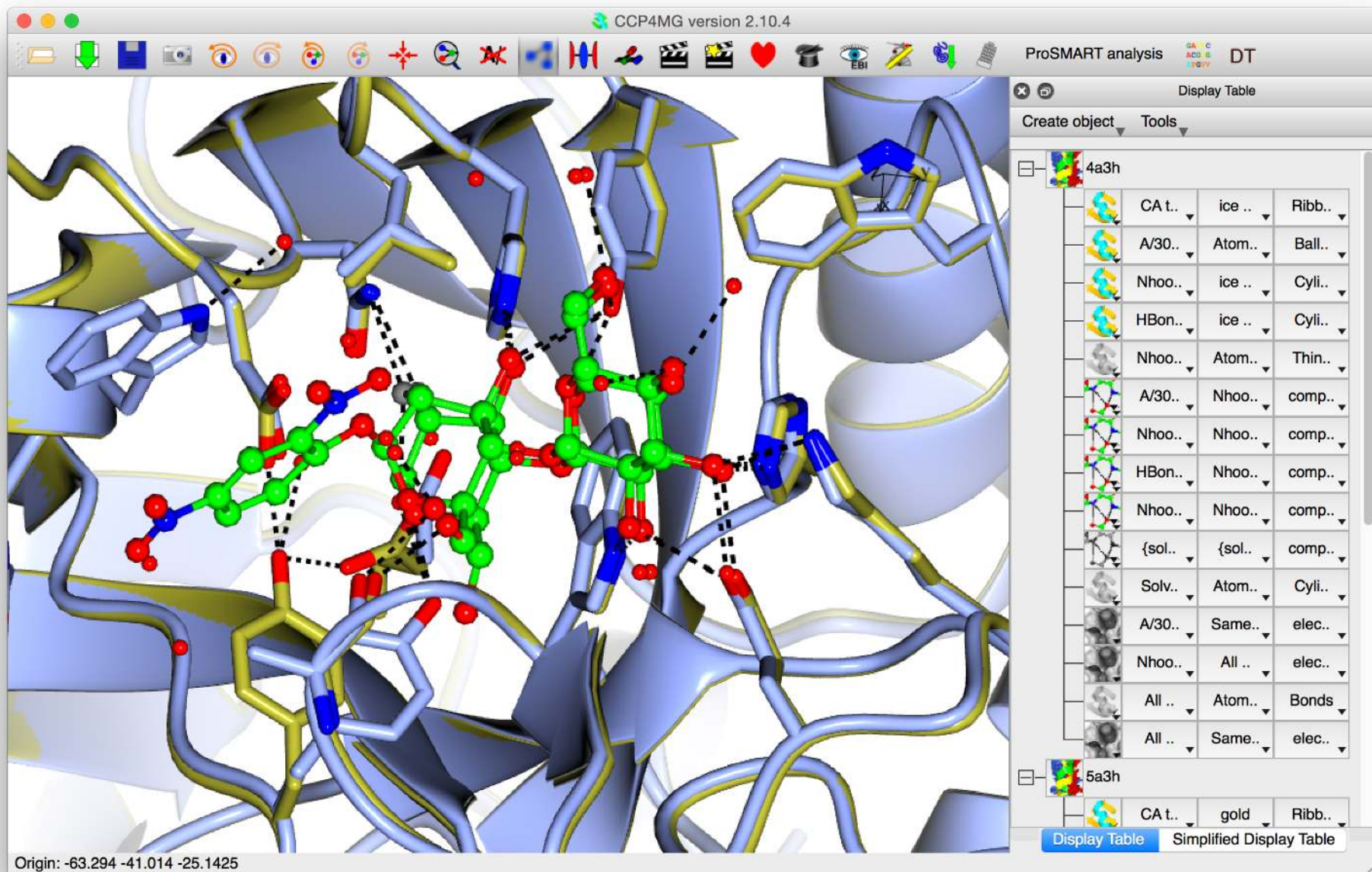
	Size	Kind
aw_BASEES.ppt	241 KB	ppt File
	--	Folder
156.jpg	1.7 MB	jpg File
resentation	--	Folder
er.docx	16 KB	docx File
	2.3 MB	png File
rogramme.pdf	101 KB	pdf File
	683 bytes	zip File
	38 KB	py File
at SMCPs.doc	15 KB	doc File
at SMCPs.odt	10 KB	odt File

Open

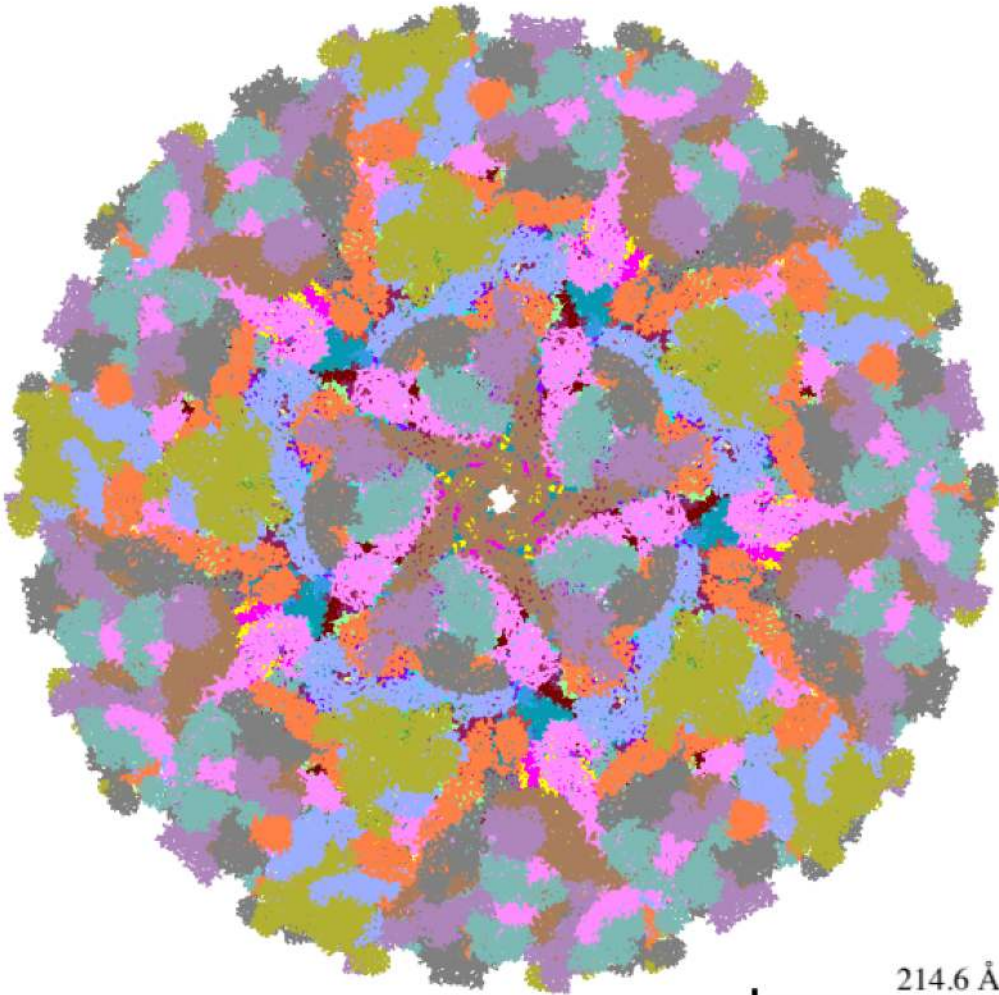
Cancel







Doing it all Manually



214.6 Å

Display Table

Create object Tools

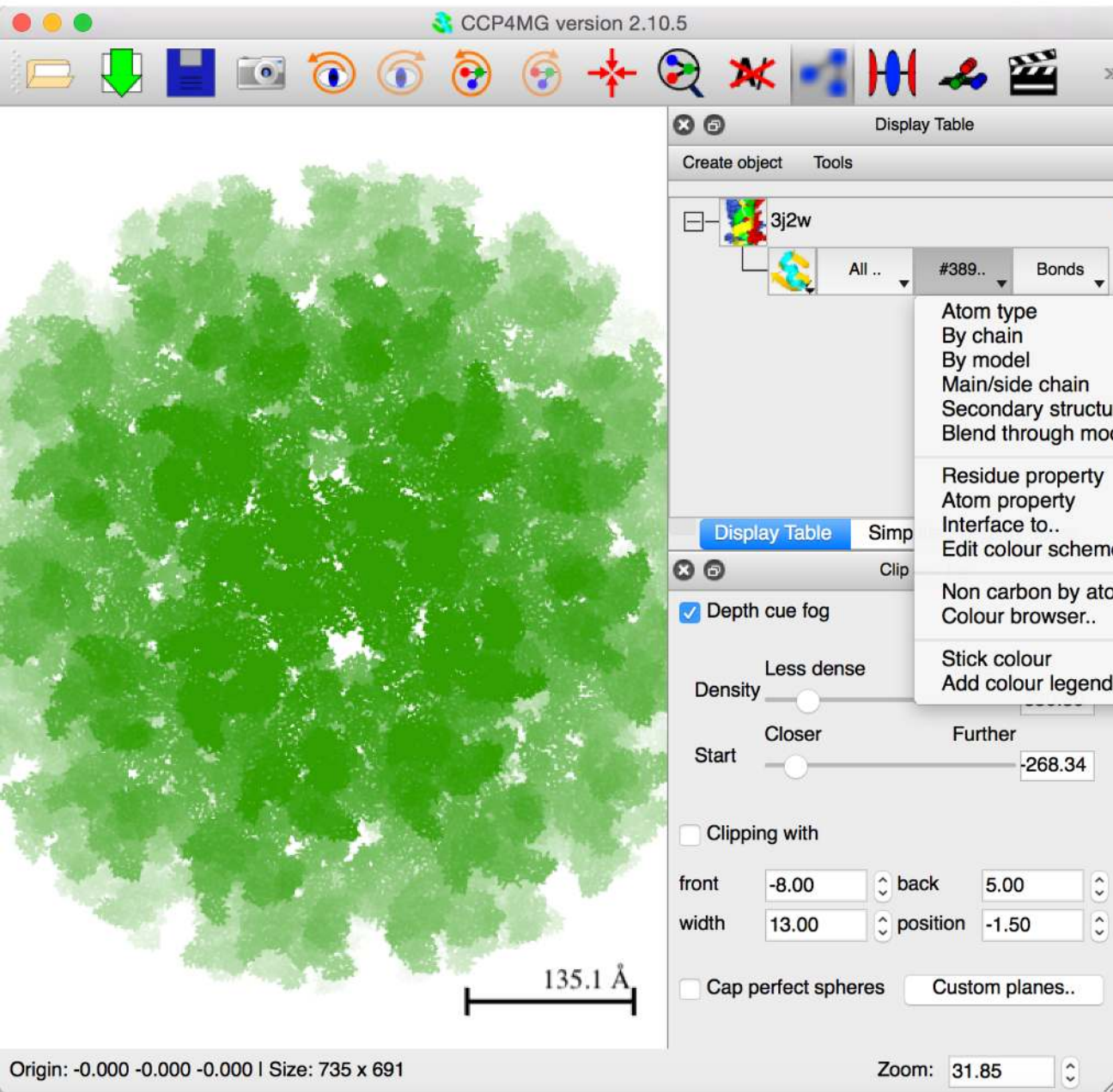
3j2w

- ✓ 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...

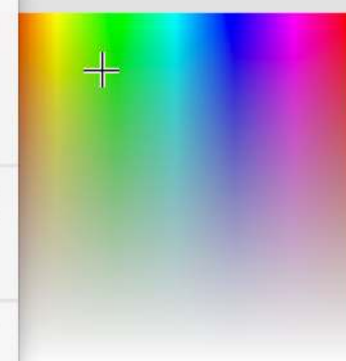
craft pi punch

Register

Stuart

Colour Browser

Main colours Create colours



Hue: 106 Red: 56

Sat: 214 Green: 157

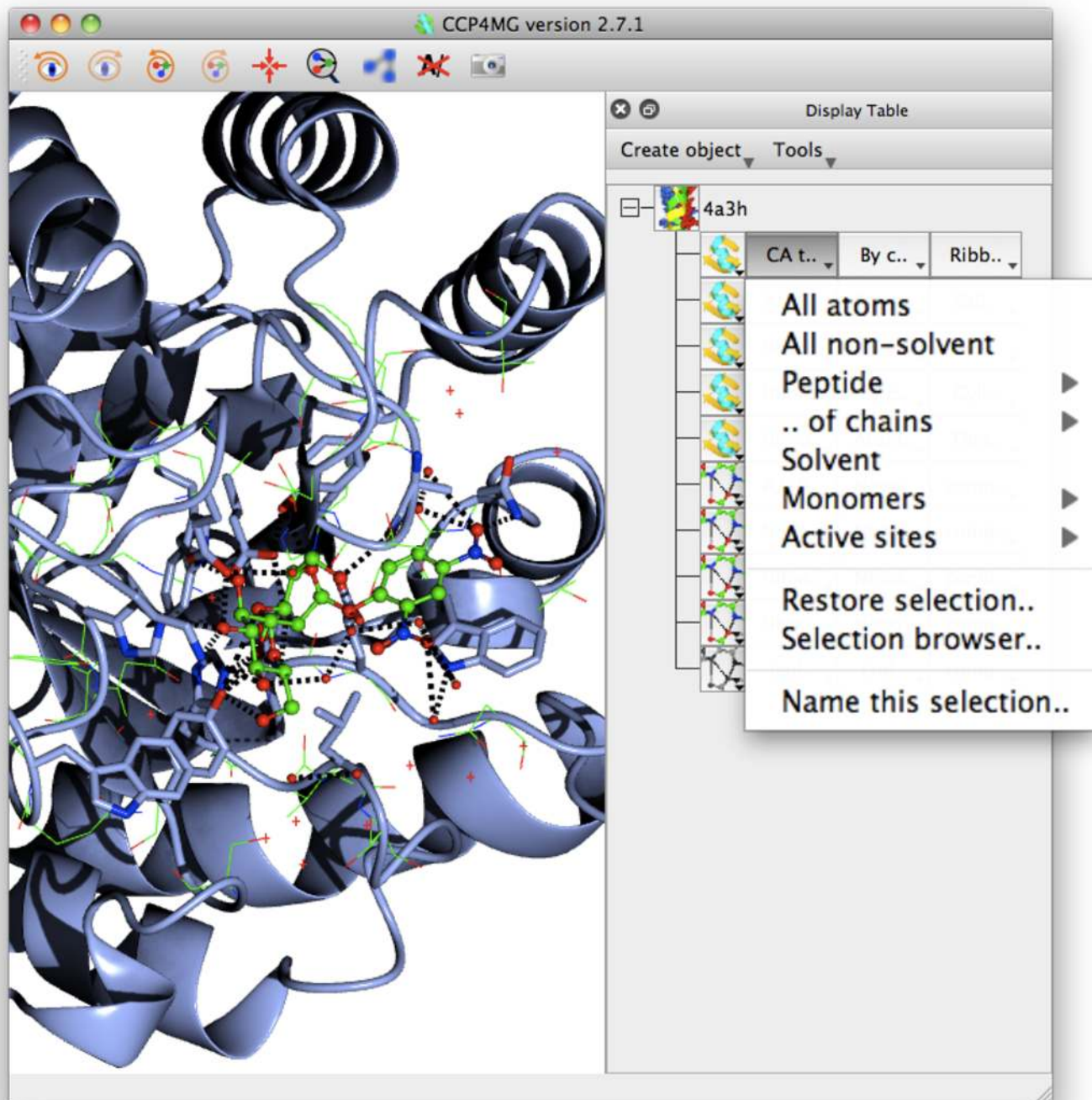
Val: 157 Blue: 25

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

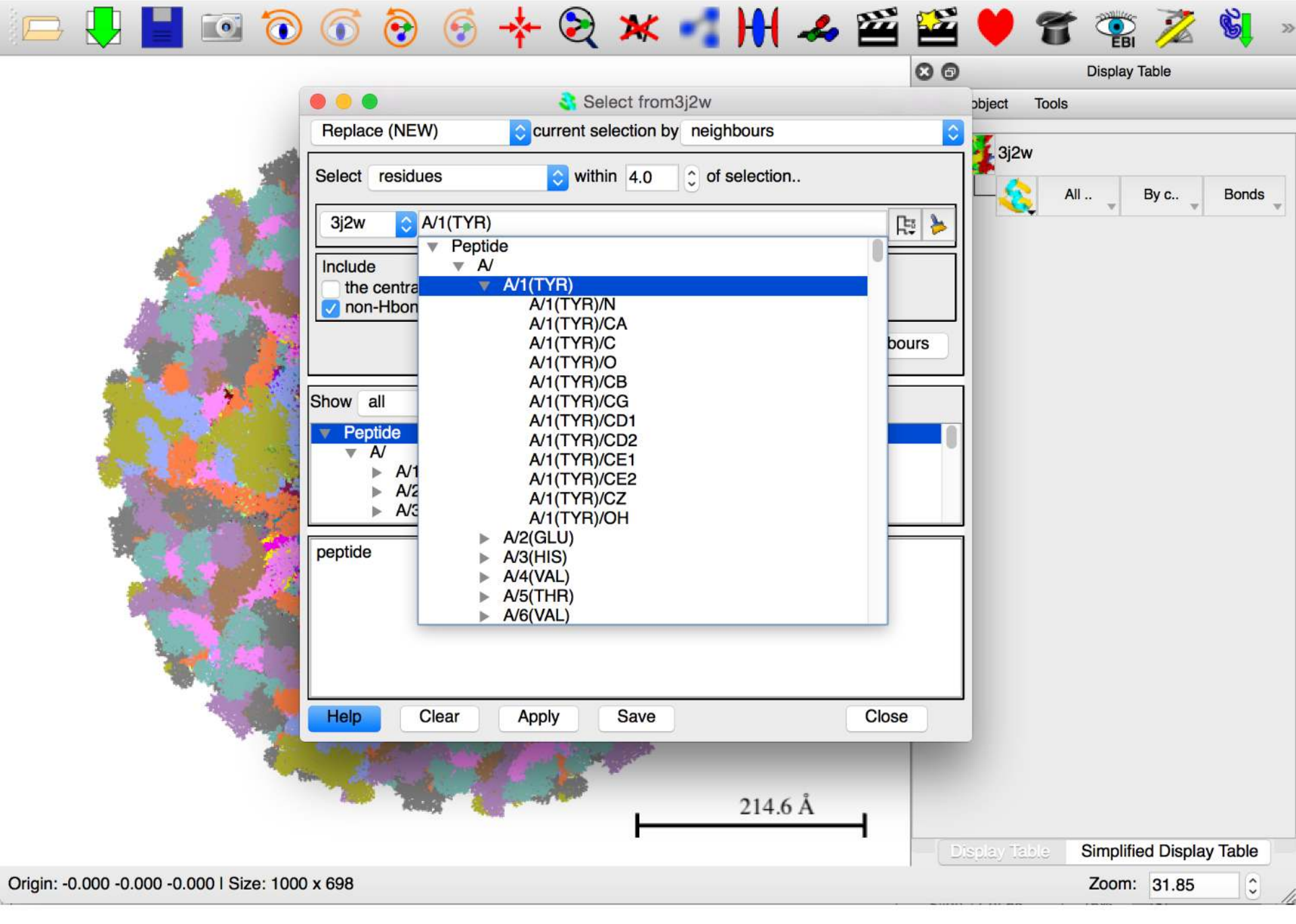
Simplified Display Table

Zoom: 31.85

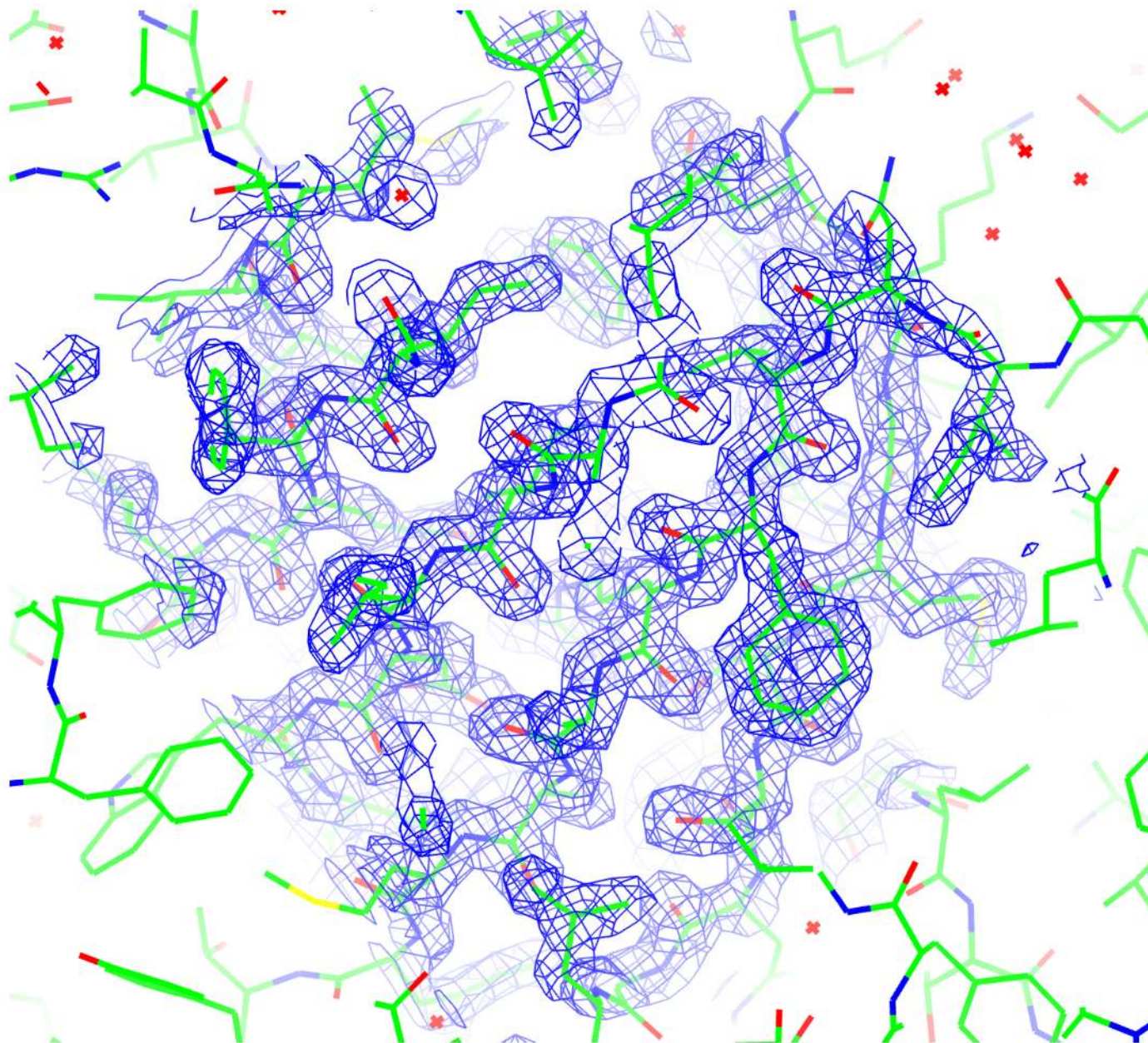
The screenshot displays the CCP4MG version 2.10.5 software interface. On the left, a large, multi-colored protein structure is visible. A scale bar at the bottom indicates a distance of 214.6 Å. The top toolbar contains various icons for file operations, viewing, and analysis. The 'Select from' dialog box is open, showing options for selecting residues within a 4.0 Å radius of the selected peptide (3j2w). The 'neighbours' option is selected in the dropdown menu. The 'Include' section shows 'non-Hbonding groups' checked. The 'Show' section lists 'Peptide' and 'A1' (TYR, GLU, HIS). The 'peptide' text box is empty. The 'Display Table' panel on the right shows the '3j2w' object and 'Tools' for 'All ..', 'By c..', and 'Bonds'.

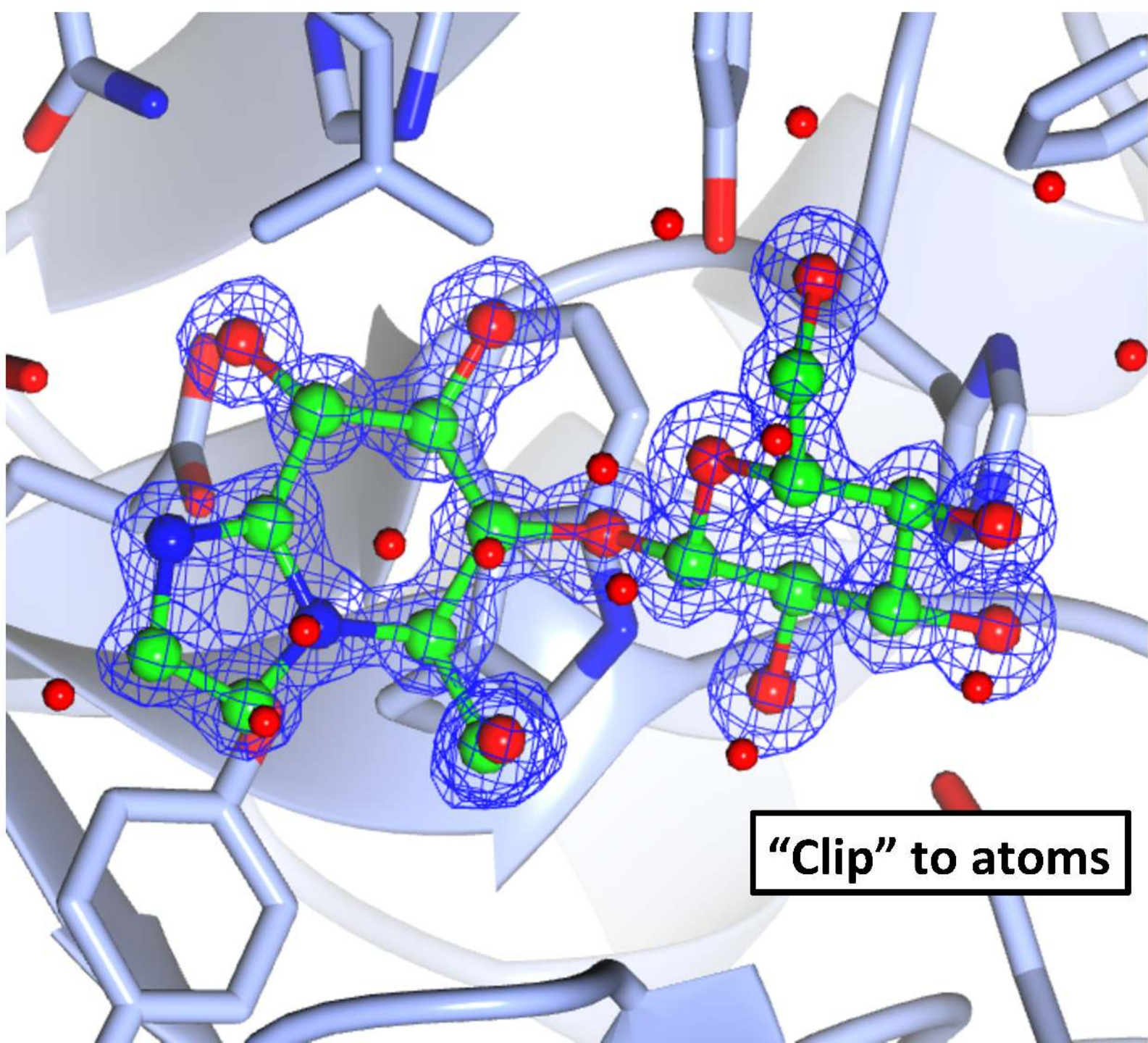
saved selection
interactive selection
✓ neighbours
buried area
atomic elements
residue types
residue ranges
secondary structure elements
properties (eg temp factor)
NMR/symmetry models

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
▼ A1
▶ 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

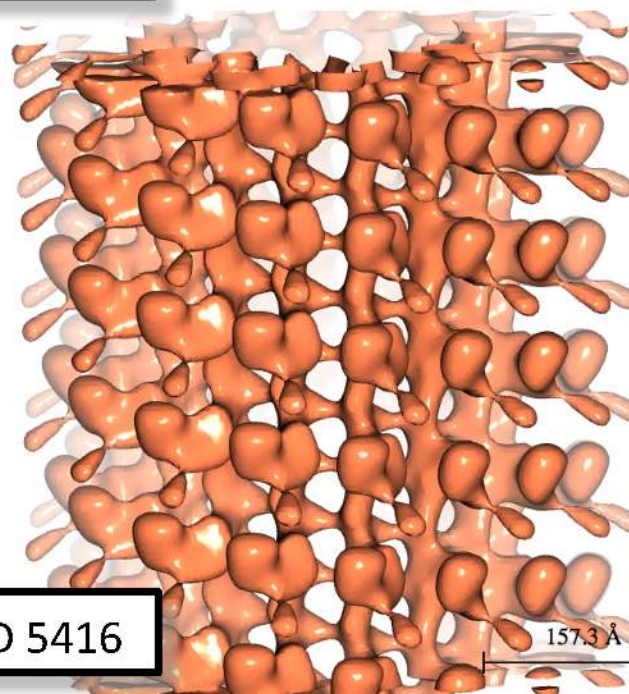
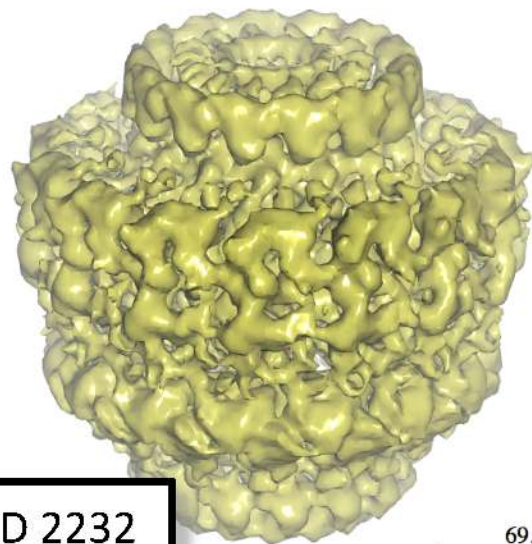
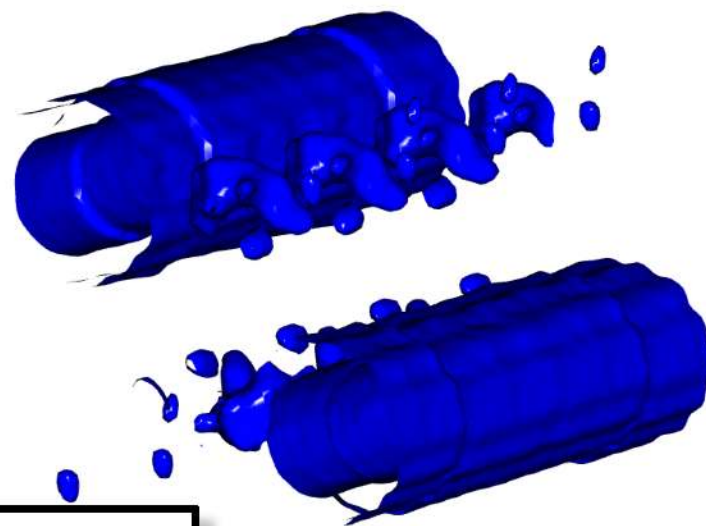
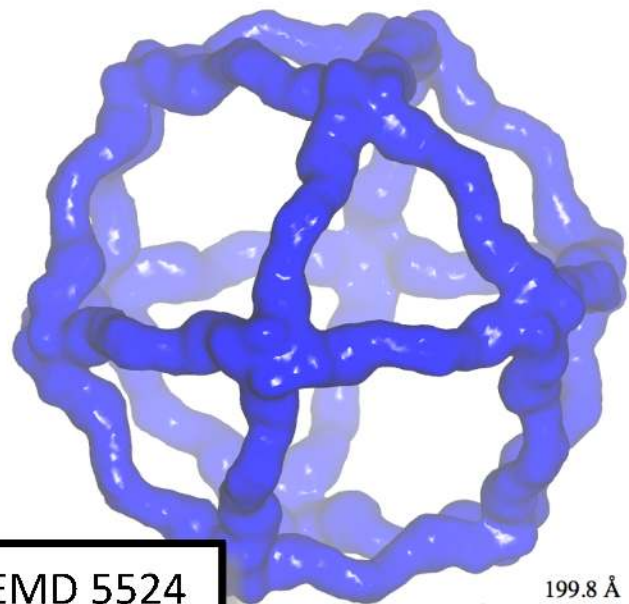


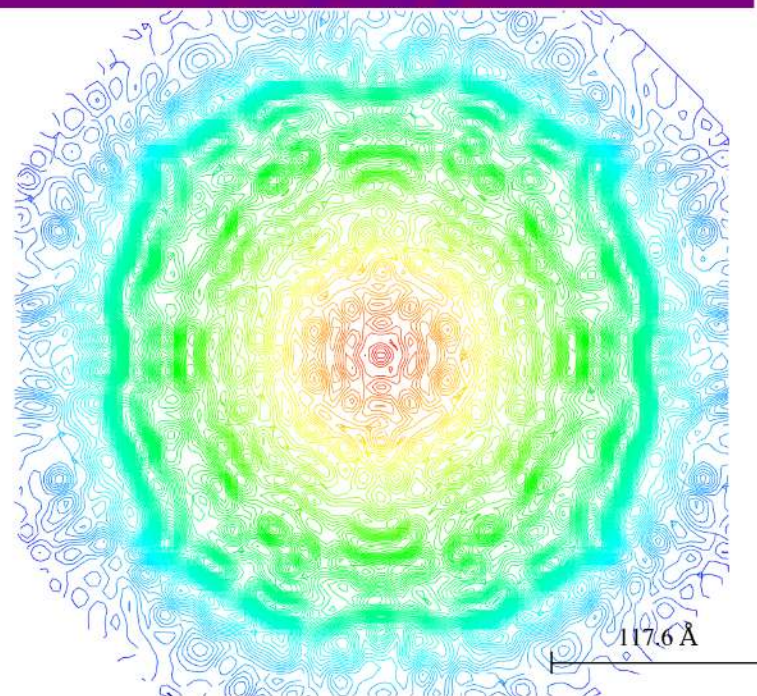
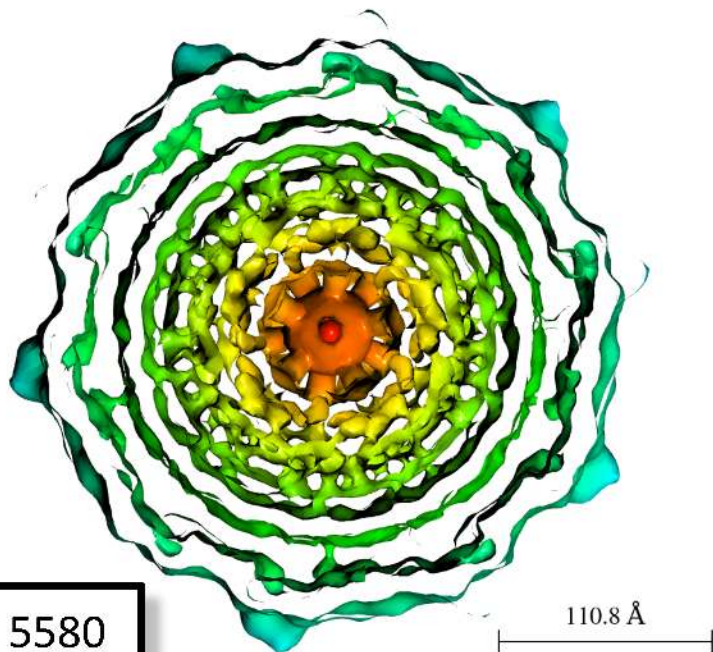
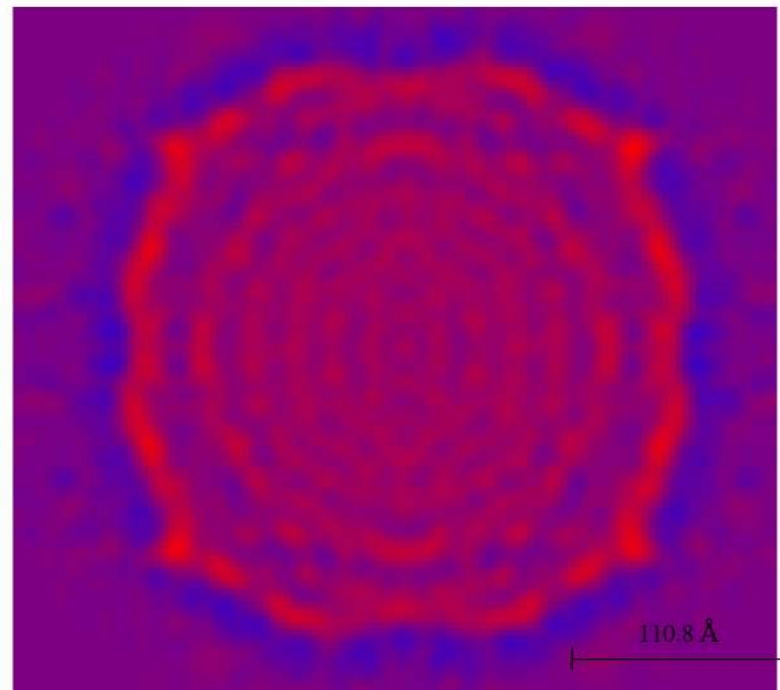
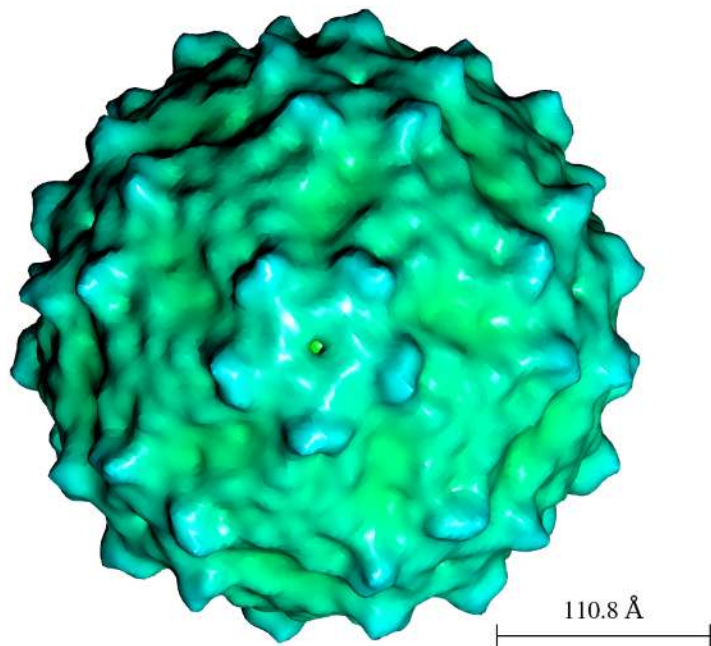
Electron Density



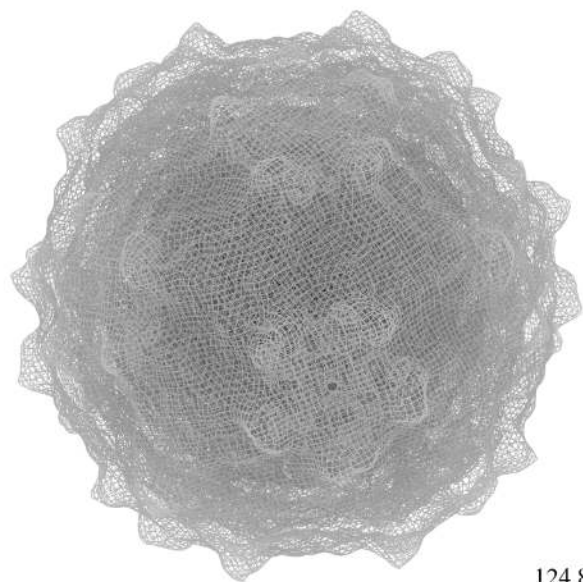


“Clip” to atoms

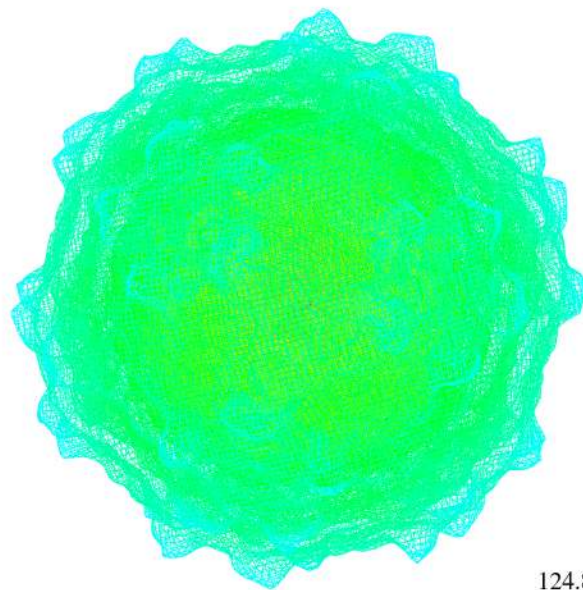




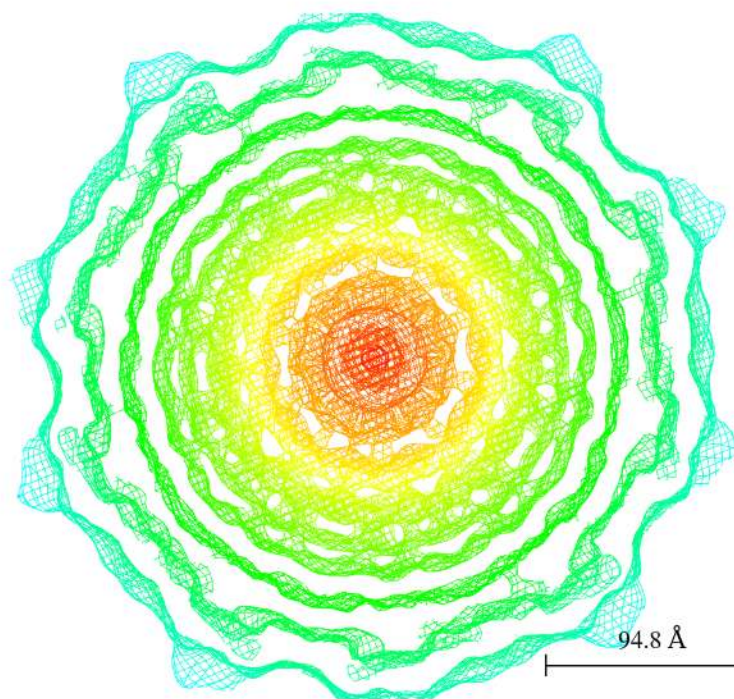
EMD 5580



124.8 Å



124.8 Å

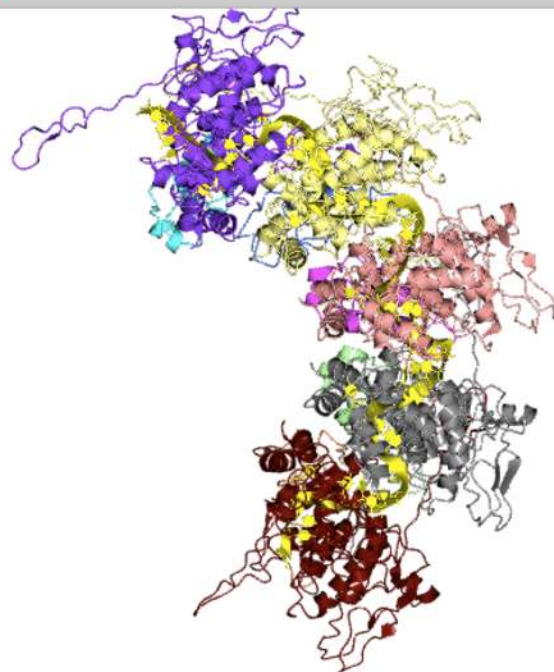


94.8 Å

EMD 5580

Other stuff

- PISA
- Structure superposition
- Sequence viewer/alignment/blast searches + more (see later).
- 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

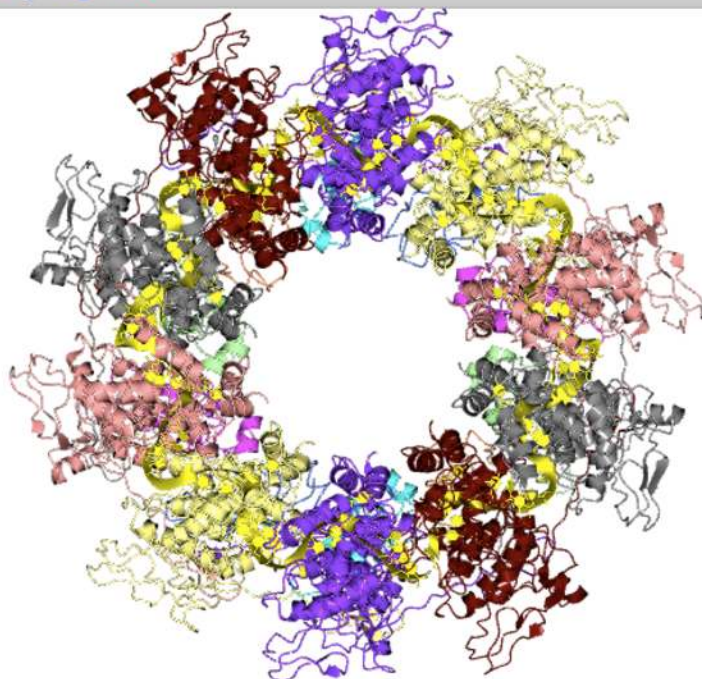
Close

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

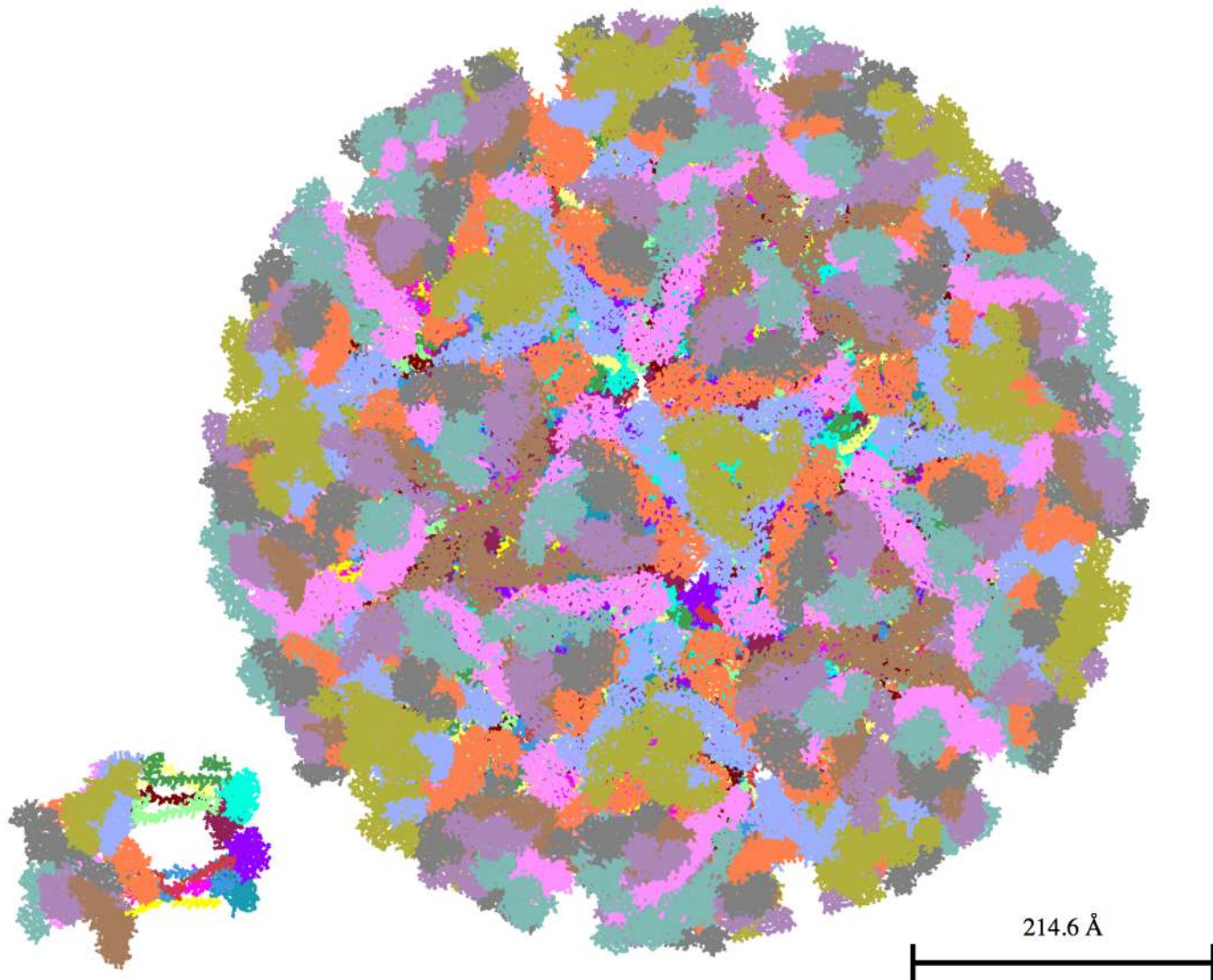
Analyse structure

Show

Clear display

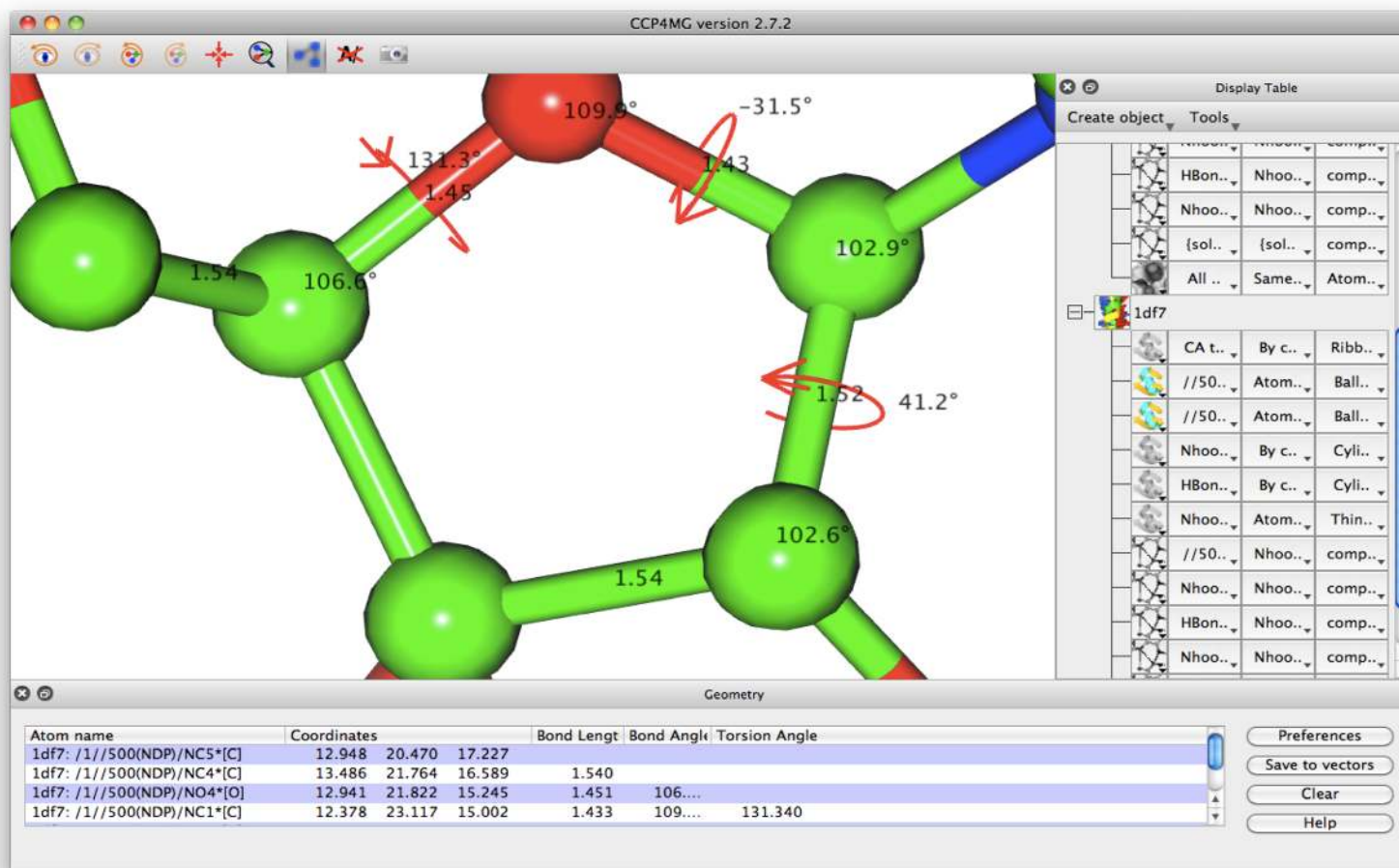
Help

Biological assemblies (3j2w)

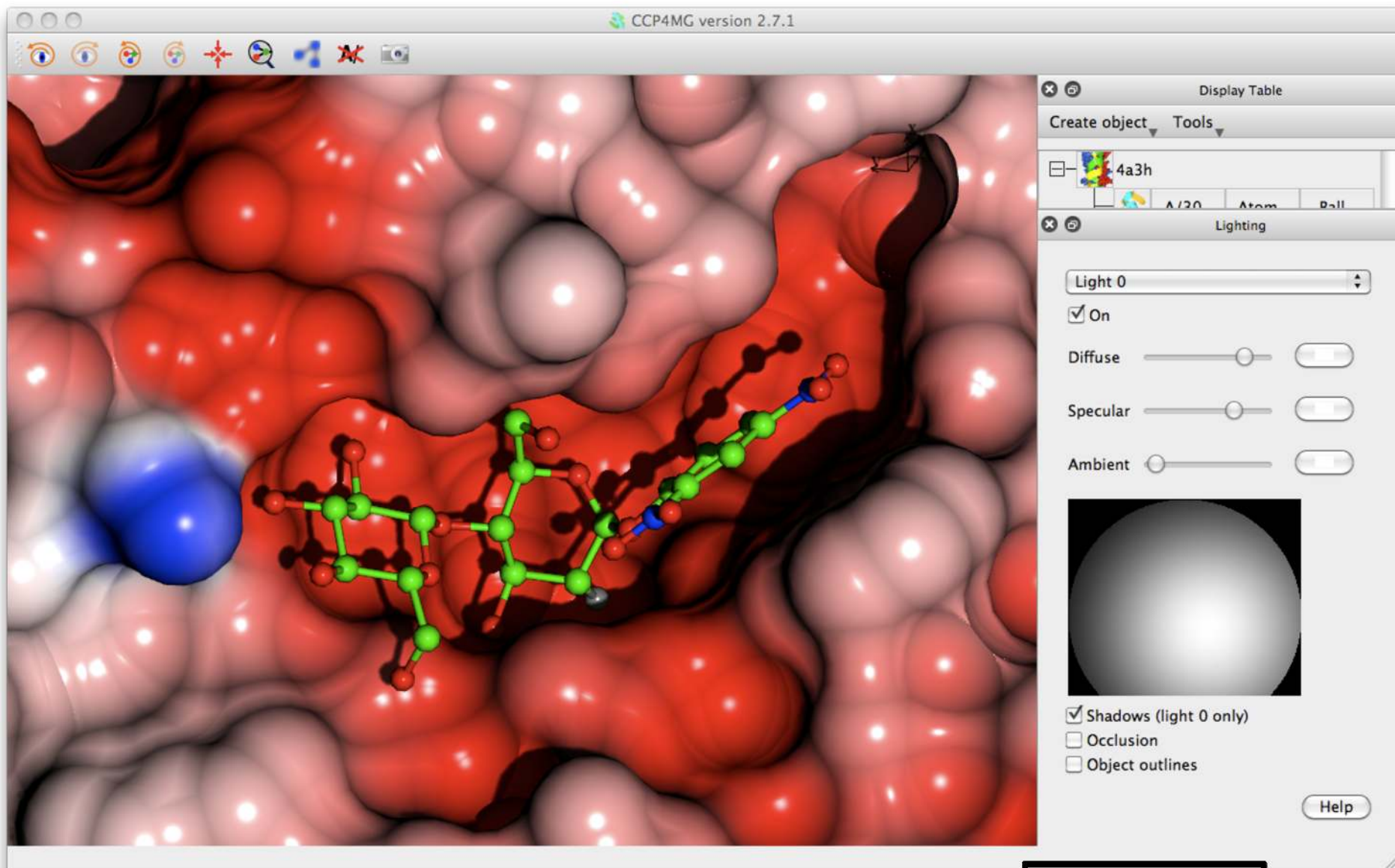


Distances and angles

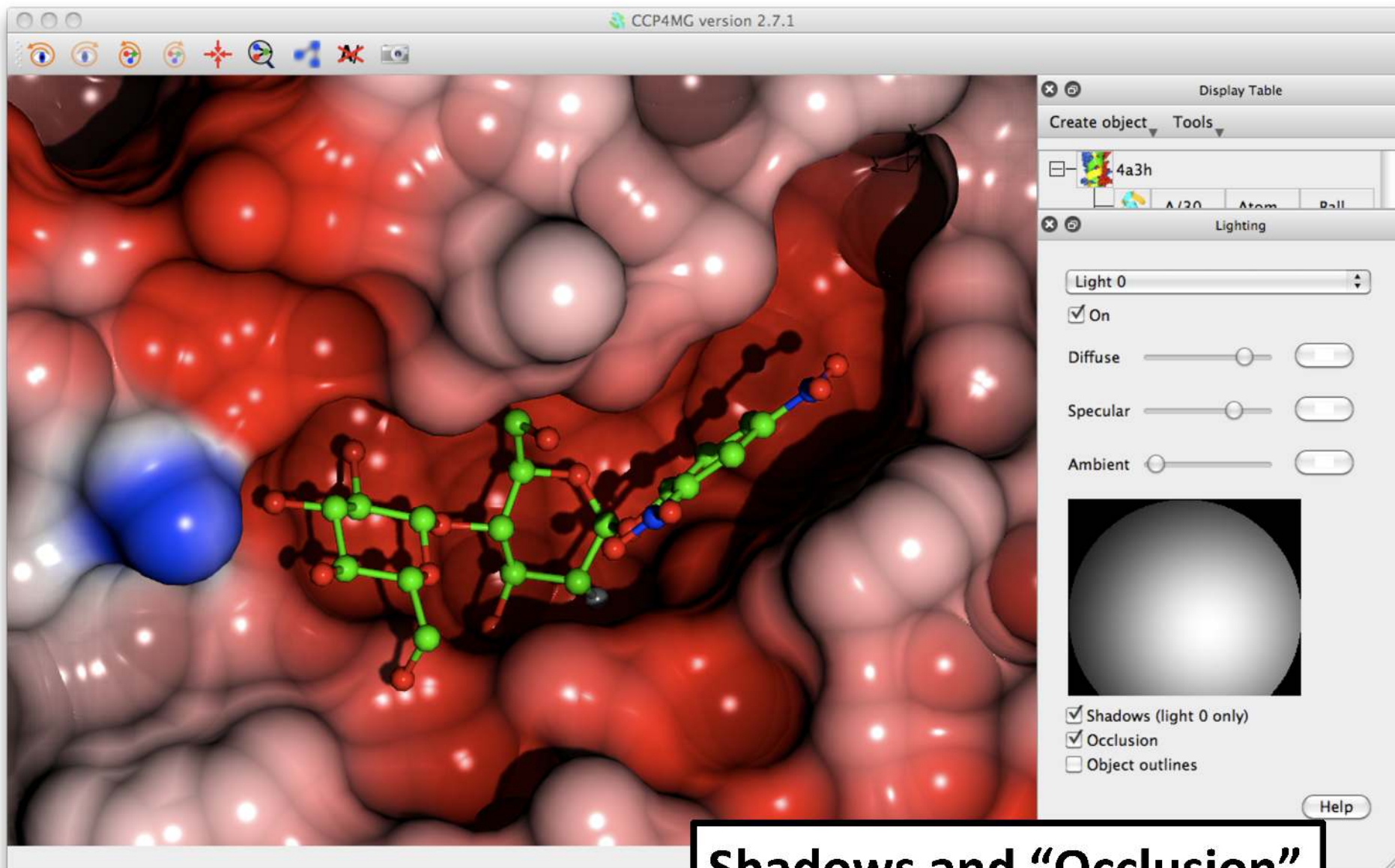
- Open “Geometry window” : Applications -> Geometry
- Double-click on one atom then another to measure bonds.
- Shift-double click on other atoms will measure angles.
- Results appear in table below and in graphics window.



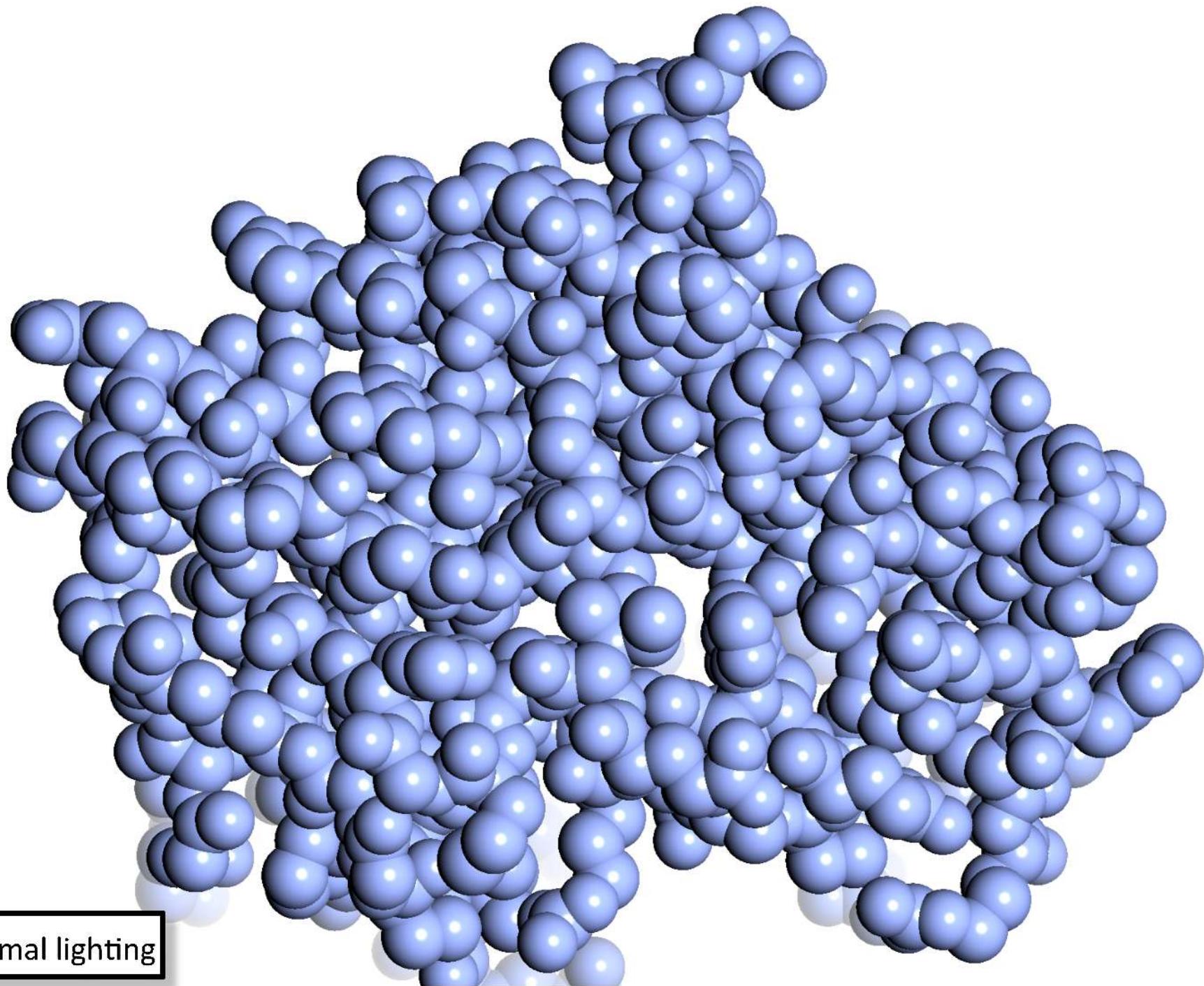
Lighting and Shadows



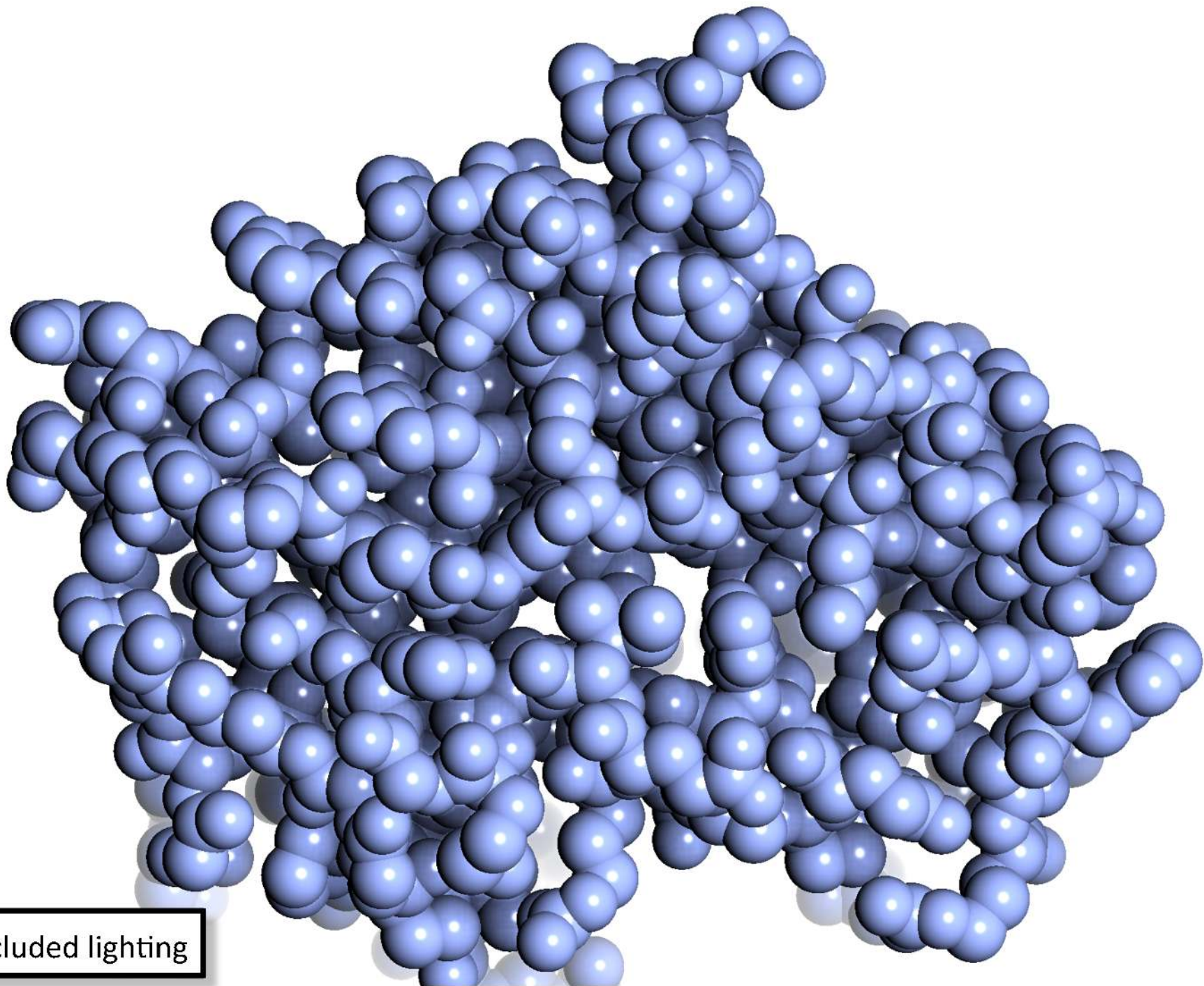
Shadows



Shadows and “Occlusion”

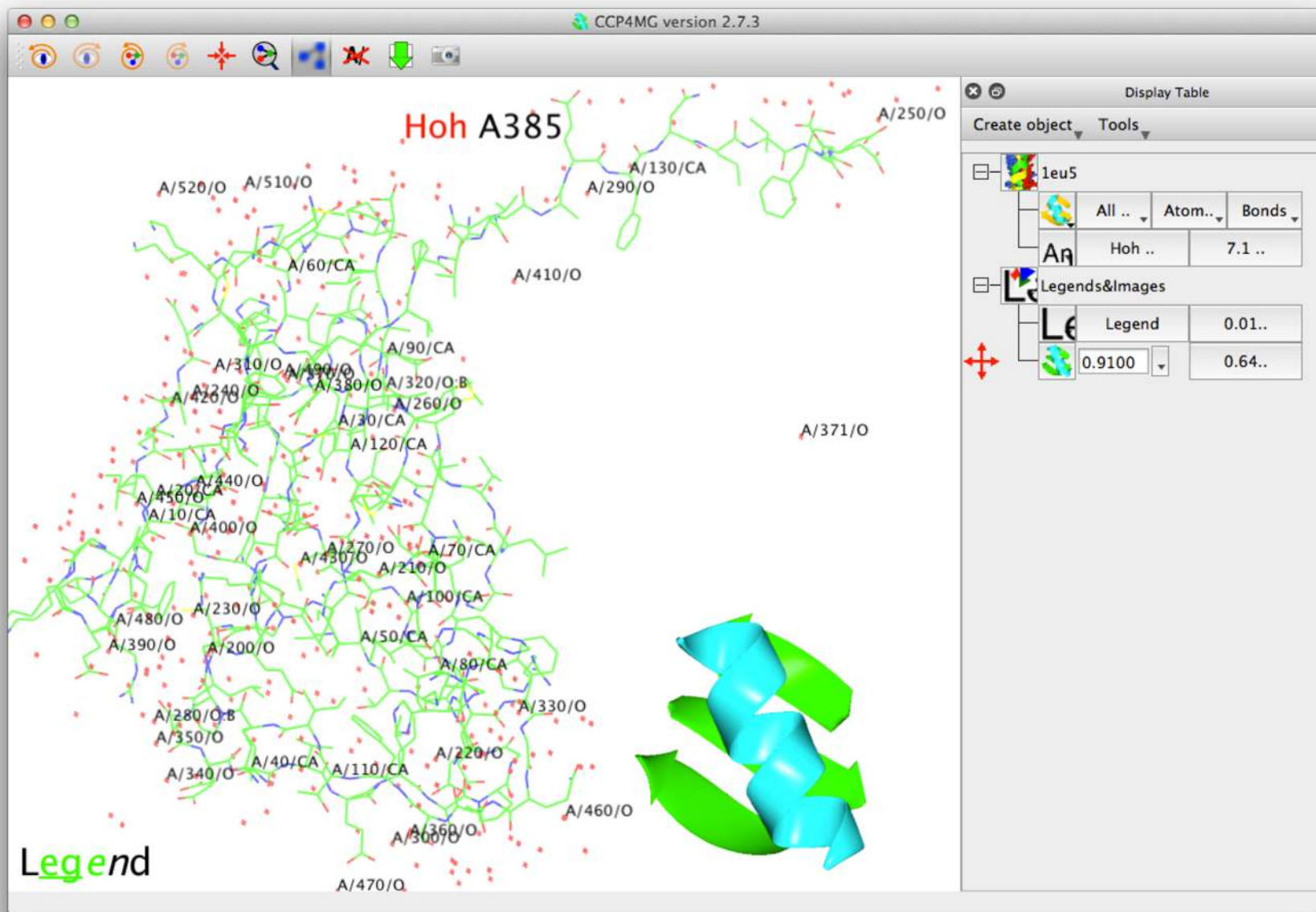


Normal lighting

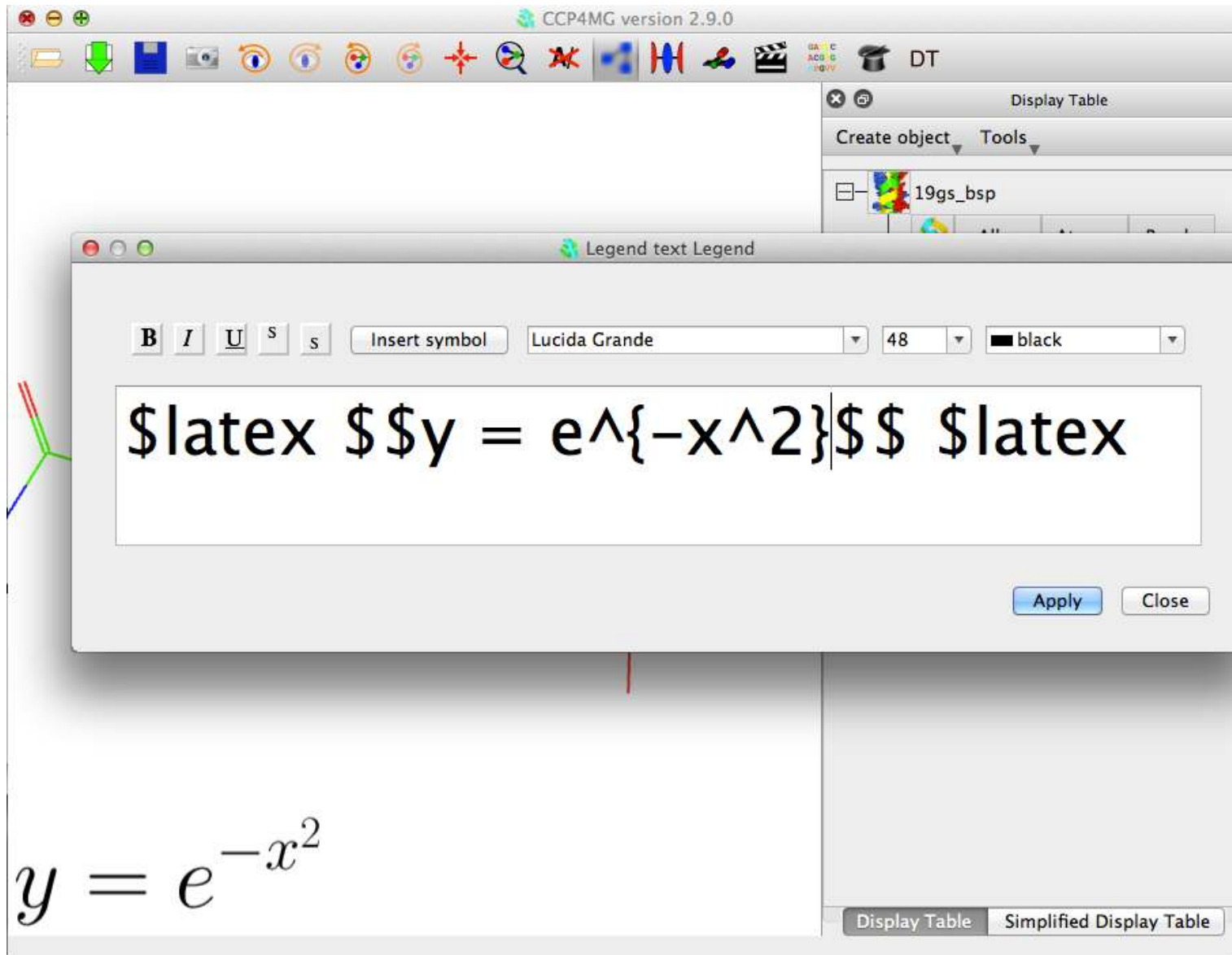


Occluded lighting

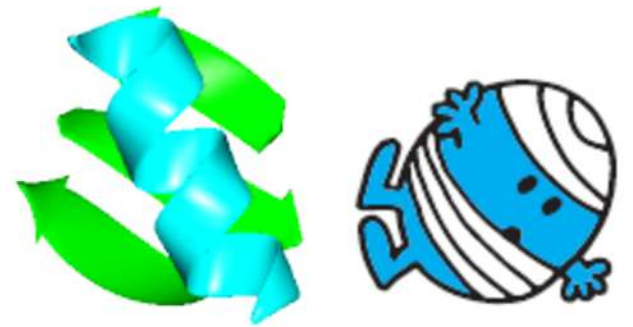
On screen text and images



On screen text and images



MrBump



Mr Bump

- Mr Bump 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.

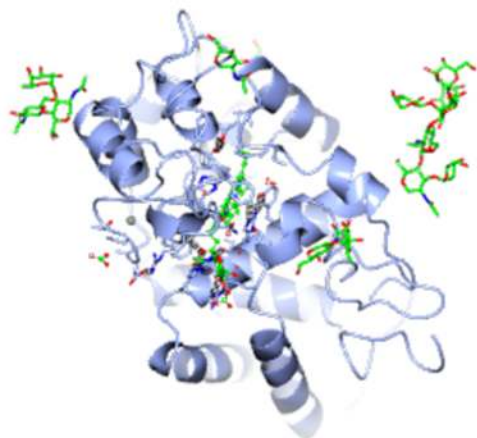
CCP4MG and Mr Bump

- CCP4MG uses initial steps of the Mr Bump to interactively edit molecular replacement models.
- Scheme:
 - Mr Bump is sent a sequence from CCP4MG
 - uses the hmmer tool to search for 70% homologous structures,
 - selects just the relevant chains from the structures,
 - prunes side chains,
 - structurally aligns the pruned structures (gesamt).
 - CCP4MG loads the structures.

CCP4MG and Mr Bump

- 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 ...
- And then everything visible can be saved into one ensemble coordinate file for use in a molecular replacement calculation.

CCP4MG version 2.10.5



Display Table

Create object Tools

4cuo

Display Table

Simplified Display Table

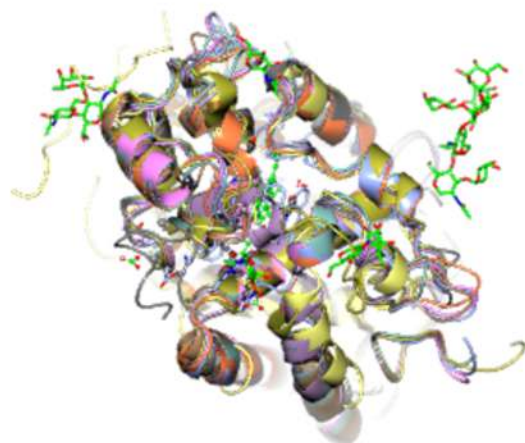
Sequence Viewer

4cuo_A

10 20 30 40 50 60 70 80 90 100 110

QLTPTFY STCPNVTISIV GVIQDALQTDL IPASLI LHPHCFVNGCGLSLLDNSDTIESEQAAPNNNSA GFDVVONI TAVENACPGVVSCADILTIAAEQSVMLSGGPSW

Run blastp on this sequence locally
Run blastp on this sequence on EBI server
Run mrbump to find search models



Display Table

Create object Tools

- 4cuo
- 1bgp_A_SCLPTR
- 1gwu_A_SCLPTR
- 1iyn_A_SCLPTR
- 1pa2_A_SCLPTR
- 1qgj_A_SCLPTR
- 1sch_A_SCLPTR
- 2vcn_A_SCLPTR
- 3fmu_A_SCLPTR

Display Table Simplified Display Table

Sequence Viewer

			10	20	30	40	50	60	70	80	90	100						
4cuo_A	☐			QLTPTFY	STCPNVT	SIV	GVIQDAL	QTDL	IPASLI	LHFHDC	FVNGC	GSLLD	NSDTIESE	QAAPNNNSA	GFDVVNI	TAVENAC	GVVSCAD	ILTIAN
1bgp_A_SCLPTR_A	☐			QLTPTFY	STCPNVT	SIV	GVIQDAL	QTDL	IPASLI	LHFHDC	FVNGC	GSLLD	NSDTIESE	QAAPNNNSA	GFDVVNI	TAVENAC	GVVSCAD	ILTIAN
1gwu_A_SCLPTR_A	☐			QLTPTFY	STCPNVT	SIV	GVIQDAL	QTDL	IPASLI	LHFHDC	FVNGC	GSLLD	NSDTIESE	QAAPNNNSA	GFDVVNI	TAVENAC	GVVSCAD	ILTIAN
1iyn_A_SCLPTR_A	☐			TSIV	GVIQDAL	QTDL	IPASLI	LHFHDC	FVNGC	GSLLD	NSDTIESE	QAAPNNNSA	GFDVVNI	TAVEVVS	CADILTIAA	QSVML	SGGPS	NPVPLG
1pa2_A_SCLPTR_A	☐			QLTPTFY	STCPNVT	SIV	GVIQDAL	QTDL	IPASLI	LHFHDC	FVNGC	GSLLD	NSDTIESE	QAAPNNNSA	GFDVVNI	TAVENAC	GVVSCAD	ILTIAN

Simplified Display Table

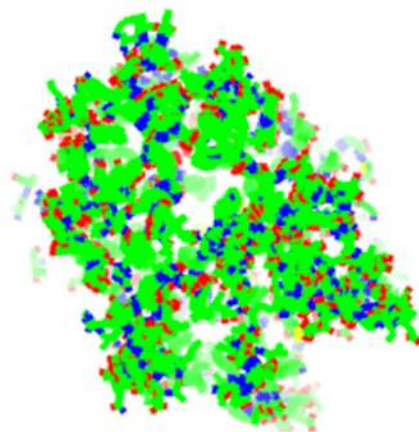
	R	L	Nb	W	Su	BS	MS	NA	M	G	B
All											
4cuo											
1bgp											
1gwu											
1lyn											
1pa2											
1qgj											
1sch											
2vcn											
3fmw											
4cuo											

Help

Display Table Simplified Display Table

Sequence Viewer

				10	20	30	40	50	60	70	80	90	100																																								
4cuo_A	☒			QL	IP	TF	YR	ST	CP	NV	TS	IV	RG	VI	QD	AL	QT	DL	RI	PA	SL	IR	LF	HD	CF	VG	NC	DG	SL	LL	DN	SD	TI	ES	EK	QA	AP	NN	SA	RG	FD	VD	NI	KT	AV	EA	CP	GV	VS	CA	DI	LT	IA
1bgp_A_SCLPTR_A	☒			QL	IP	TF	YR	ST	CP	NV	TS	IV	RG	VI	QD	AL	QT	DL	RI	PA	SL	IR	LF	HD	CF	VG	NC	DG	SL	LL	DN	SD	TI	ES	EK	QA	AP	NN	SA	RG	FD	VD	NI	KT	AV	EA	CP	GV	VS	CA	DI	LT	IA
1gwu_A_SCLPTR_A	☒			QL	IP	TF	YR	ST	CP	NV	TS	IV	RG	VI	QD	AL	QT	DL	RI	PA	SL	IR	LF	HD	CF	VG	NC	DG	SL	LL	DN	SD	TI	ES	EK	QA	AP	NN	SA	RG	FD	VD	NI	KT	AV	EA	CP	GV	VS	CA	DI	LT	IA
1lyn_A_SCLPTR_A	☒			-----	TS	IV	RG	VI	QD	AL	QT	DL	RI	PA	SL	IR	LF	HD	CF	VG	NC	DG	SL	LL	DN	SD	TI	ES	EK	QA	AP	NN	SA	RG	FD	VD	NI	KT	AV	EA	CP	GV	VS	CA	DI	LT	IA						
1pa2_A_SCLPTR_A	☒			QL	IP	TF	YR	ST	CP	NV	TS	IV	RG	VI	QD	AL	QT	DL	RI	PA	SL	IR	LF	HD	CF	VG	NC	DG	SL	LL	DN	SD	TI	ES	EK	QA	AP	NN	SA	RG	FD	VD	NI	KT	AV	EA	CP	GV	VS	CA	DI	LT	IA



Display Table

Create object Tools

	HBon..	Nhoo..	comp..
	Nhoo..	Nhoo..	comp..
	{sol..	{sol..	comp..
	meta..	Atom..	Sphe..
	sacc..	Atom..	Cyli..
	Solv..	Atom..	Cyli..
	Solute	Atom..	Cyli..
	A/13..	Same..	elec..
	Nhoo..	All ..	elec..

Display Table Simplified Display Table

Sequence Viewer

		10	20	30	40	50	60	70	80	90	100
4cuo_A	☐		QLIPTFYRSTCPNV	TSIVRGVIQDALQ	TDLRIPASLIRL	HFHDCFVNGC	IGSLLLDNSD	TIESEKQAAPNNN	SARGFDVVDNIKTAVE	NACPCVVSCADILTIAA	
1bgp_A_SCLPTR_A	☐		QLIPTFYRSTCPNV	TSIVRGVIQDALQ	TDLRIPASLIRL	HFHDCFVNGC	IGSLLLDNSD	TIESEKQAAPNNN	SARGFDVVDNIKTAVE	NACPCVVSCADILTIAA	
1gwu_A_SCLPTR_A	☐		QLIPTFYRSTCPNV	TSIVRGVIQDALQ	TDLRIPASLIRL	HFHDCFVNGC	IGSLLLDNSD	TIESEKQAAPNNN	SARGFDVVDNIKTAVE	NACPCVVSCADILTIAA	
1iyn_A_SCLPTR_A	☐		-----	TSIVRGVIQDALQ	TDLRIPASLIRL	HFHDCFVNGC	IGSLLLDNSD	TIESEKQAAPNNN	SARGFDVVDNIKTAVE	-----	VVSCADILTIAA
1pa2_A_SCLPTR_A	☐		QLIPTFYRSTCPNV	TSIVRGVIQDALQ	TDLRIPASLIRL	HFHDCFVNGC	IGSLLLDNSD	TIESEKQAAPNNN	SARGFDVVDNIKTAVE	NACPCVVSCADILTIAA	

QtMG File Edit View Display Applications Windows Tools Help CCP4i2

CCP4MG version 2.10.5

Display Table

Create object Tools

HBon..	Nhoo..	comp..
Nhoo..	Nhoo..	comp..
{sol..	{sol..	comp..
meta..	Atom..	Sphe..
sacc..	Atom..	Cyli..
Solv..	Atom..	Cyli..
Solute	Atom..	Cyli..
A/13..	Same..	elec..
Nhoo..	All ..	elec..

Display Table Simplified Display Table

Sequence Viewer

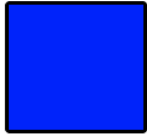
	10	20	30	40	50	60	70	80	90	100
4cuo_A	QLTPFIRSTCPNV	TSIVRGVIQDALQTDLRIPASLIRLHFHDCPVNGC	EGSLLLDNSD	TIES	EKQAAPNNN	SARGFDV	VDNIKTAVE	NACPG	VVSCADILTIA	
1bgp_A_SCLPTR_A	QLTPFIRSTCPNV	TSIVRGVIQDALQTDLRIPASLIRLHFHDCPVNGC	EGSLLLDNSD	TIES	EKQAAPNNN	SARGFDV	VDNIKTAVE	NACPG	VVSCADILTIA	
1gwu_A_SCLPTR_A	QLTPFIRSTCPNV	TSIVRGVIQDALQTDLRIPASLIRLHFHDCPVNGC	EGSLLLDNSD	TIES	EKQAAPNNN	SARGFDV	VDNIKTAVE	NACPG	VVSCADILTIA	
1iyn_A_SCLPTR_A	-----	TSIVRGVIQDALQTDLRIPASLIRLHFHDCPVNGC	EGSLLLDNSD	TIES	EKQAAPNNN	SARGFDV	VDNIKTAVE	-----	VVSCADILTIA	
1pa2_A_SCLPTR_A	QLTPFIRSTCPNV	TSIVRGVIQDALQTDLRIPASLIRLHFHDCPVNGC	EGSLLLDNSD	TIES	EKQAAPNNN	SARGFDV	VDNIKTAVE	NACPG	VVSCADILTIA	

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.
- With eukaryotic expression systems ramping up the production of glycoproteins and thus the deposition rate of their three-dimensional structures, the need for a clear way of depicting these interactions is more pressing than ever.
- CCP4MG brings the familiar two-dimensional identification convention used by the glycobiology community into three dimensions.
- All Jon's genius, insight, encouragement, etc.

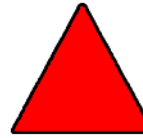
Saccharide display in 2D



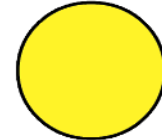
N-Acetyl-glucosamine
(NAG)



Mannose
(BMA, MAN)



Fucose
(FCA, FCB, FUC)



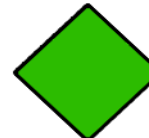
Galactose
(GAL)



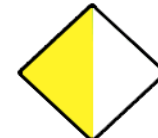
N-Acetyl-galactosamine
(NGA)



Glucose
(GLC, BGC)



2-keto-3-deoxynononic acid
(KDN)



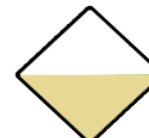
Galacturonic acid
(ADA, GTR)



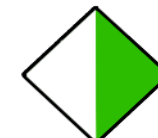
Glucosamine
(GCS)



Xylose
(XYS, XYP)

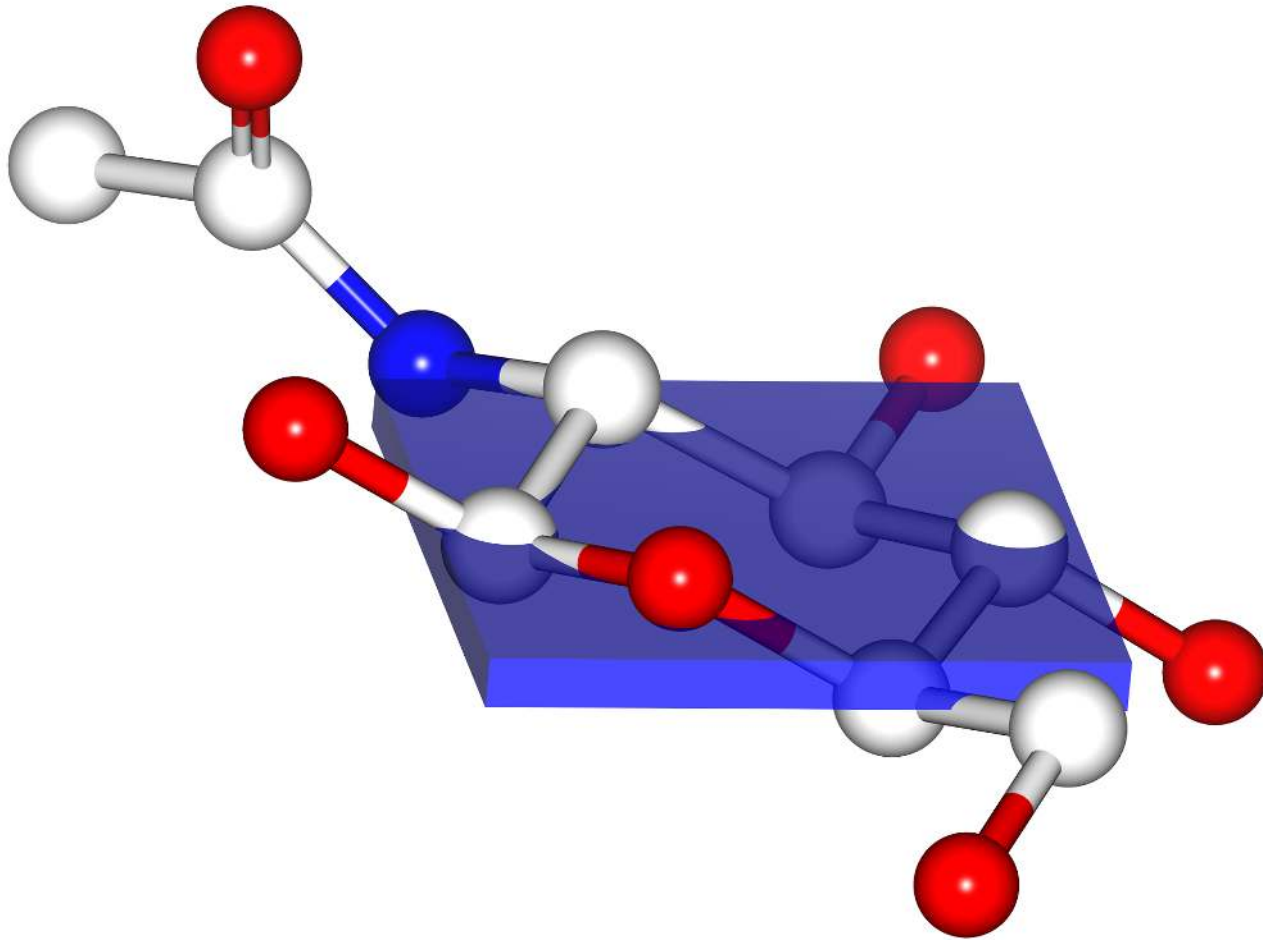


Iduronic acid
(IDR)

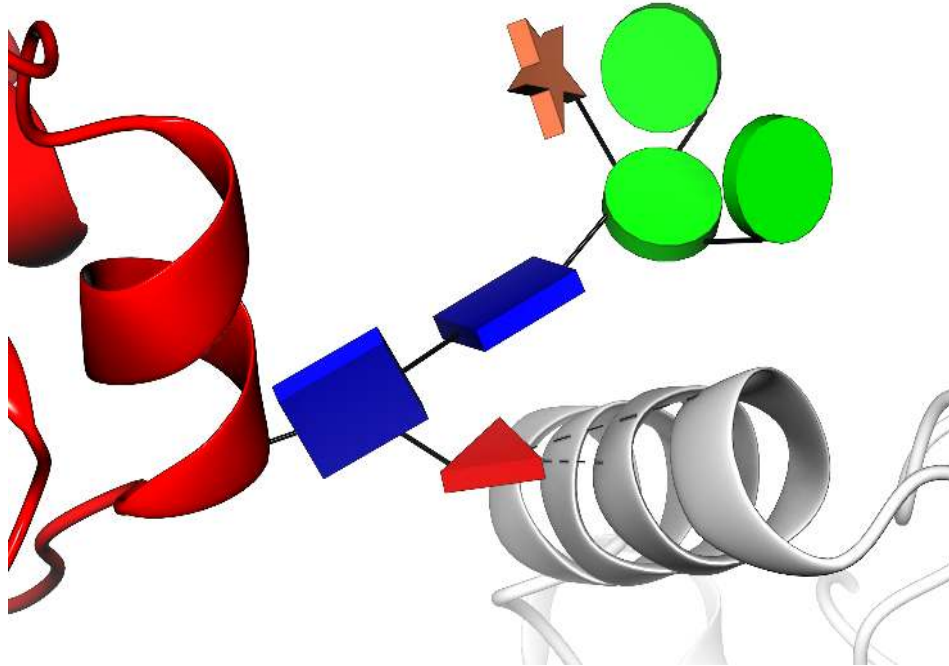


Mannuronic acid
(BEM)

Saccharide display in 3D

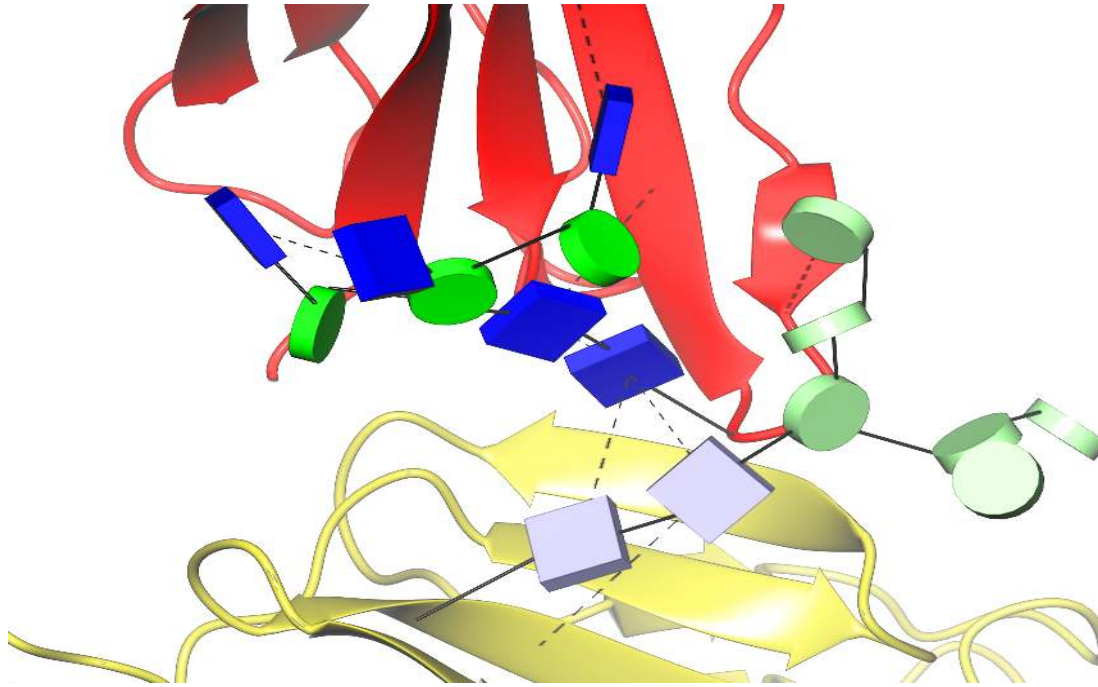


Saccharide display in 3D



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



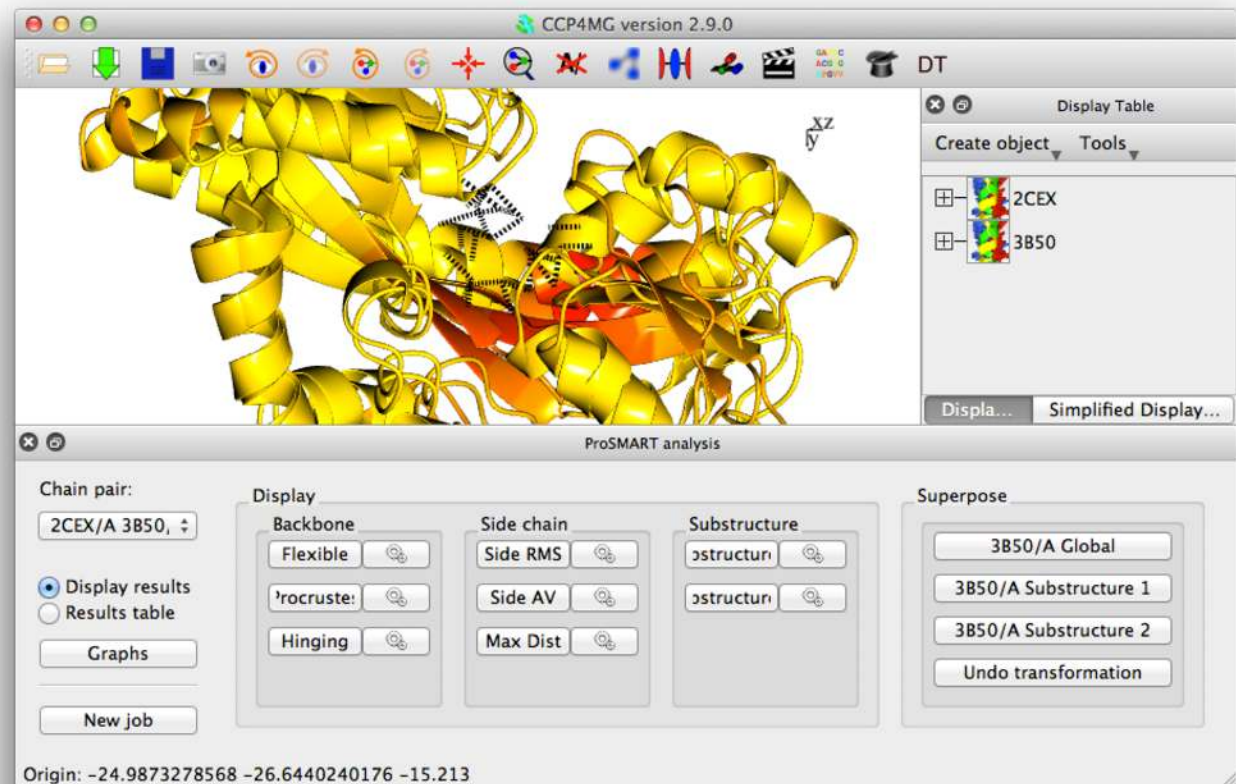
Glycoblocks view of carbohydrate-carbohydrate interactions (PDB 3SGK). Two N-glycans attached to two separate Fc fragments (depicted in red and gold) establish hydrogen bonds with each other and the protein part. These interactions, along with others that are described in Ferrara et al. (2011), make 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.

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

- 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' panel is open, showing a search for 'cyclotide'. The search results are listed in a table with checkboxes next to the PDB IDs. The following table represents the data shown in the image:

PDB ID	Description
☒ 2lam	Three-dimensional str
☒ 1r1f	Solution Structure of t
☒ 3e4h	Crystal structure of the
☒ 1vp8	Solution structure of t
☒ 1pt4	Solution structure
☐ 1vb8	solution structure
☐ 2knn	Solution structure
☐ 1znu	Structure of cyclotide
☐ 2knn	Solution structure
☐ 2kux	Solution structure of t
☐ 1za8	NMR solution structure
☐ 2qi0	Cycloviolacin O14
☐ 2kuk	Solution structure of
☐ 2k7g	Solution Structure of
☐ 1nb1	High resolution sol
☐ 1nbi	High-resolution soluti

At the bottom of the panel, there is a 'Save to folder' field with the path '/Users/stuart' and a 'Browse' button. Below this is a 'Download selected files' button. At the very bottom, there are 'Display Table' and 'Ebeye search' buttons.

Type search string here

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.

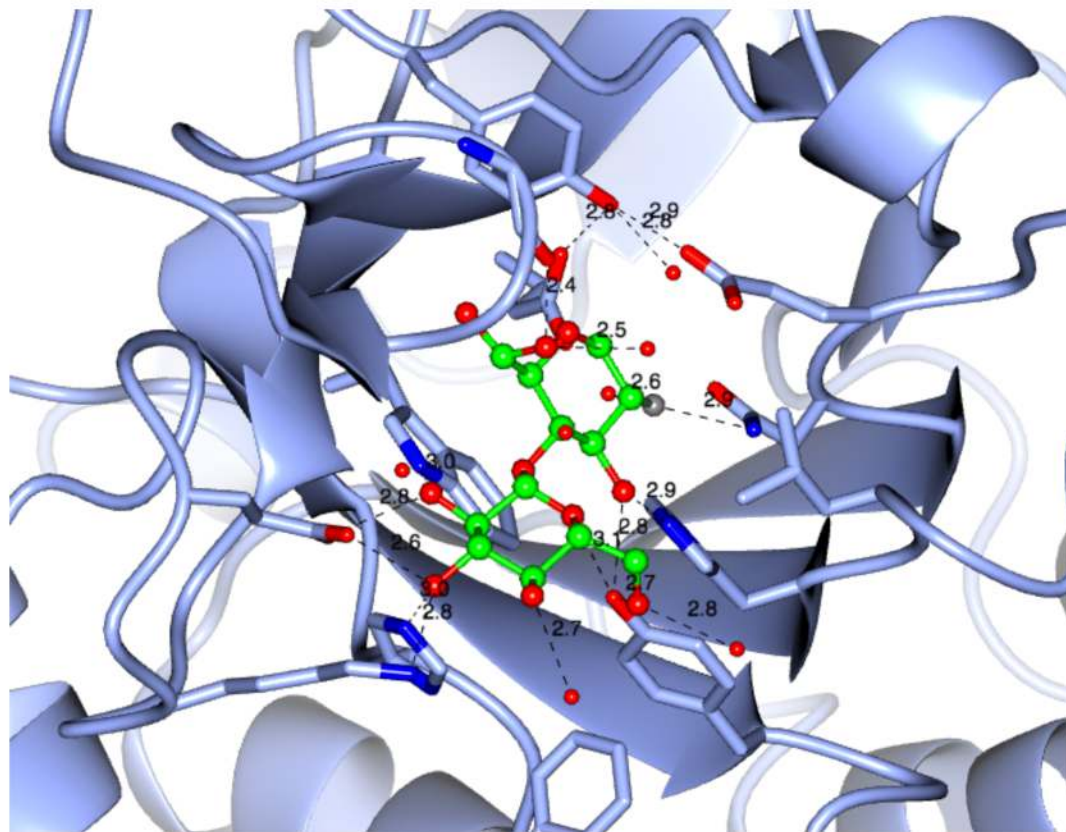
CCP4MG on the Web

Web GL

- WebGL is a JavaScript technology for displaying 3D (and 2D) graphics in a web browser.
- WebGL is very similar to OpenGL ES, a technology which is very similar to OpenGL which is what CCP4MG uses for its graphics.
- Should be reasonably straightforward to write a WebGL application which uses existing CCP4MG code/expertise to do molecular graphics.

WebGL

- Most of the hard work in CCP4MG is done in a mixture of Python and C++ programming languages. This is not *trivially* portable to JavaScript.
- However if the hard work (converting macromolecular coordinates to picture elements – lines, triangles) was done on a server, the WebGL application (browser) could just draw the triangles which are computed.



Clip

5A3H

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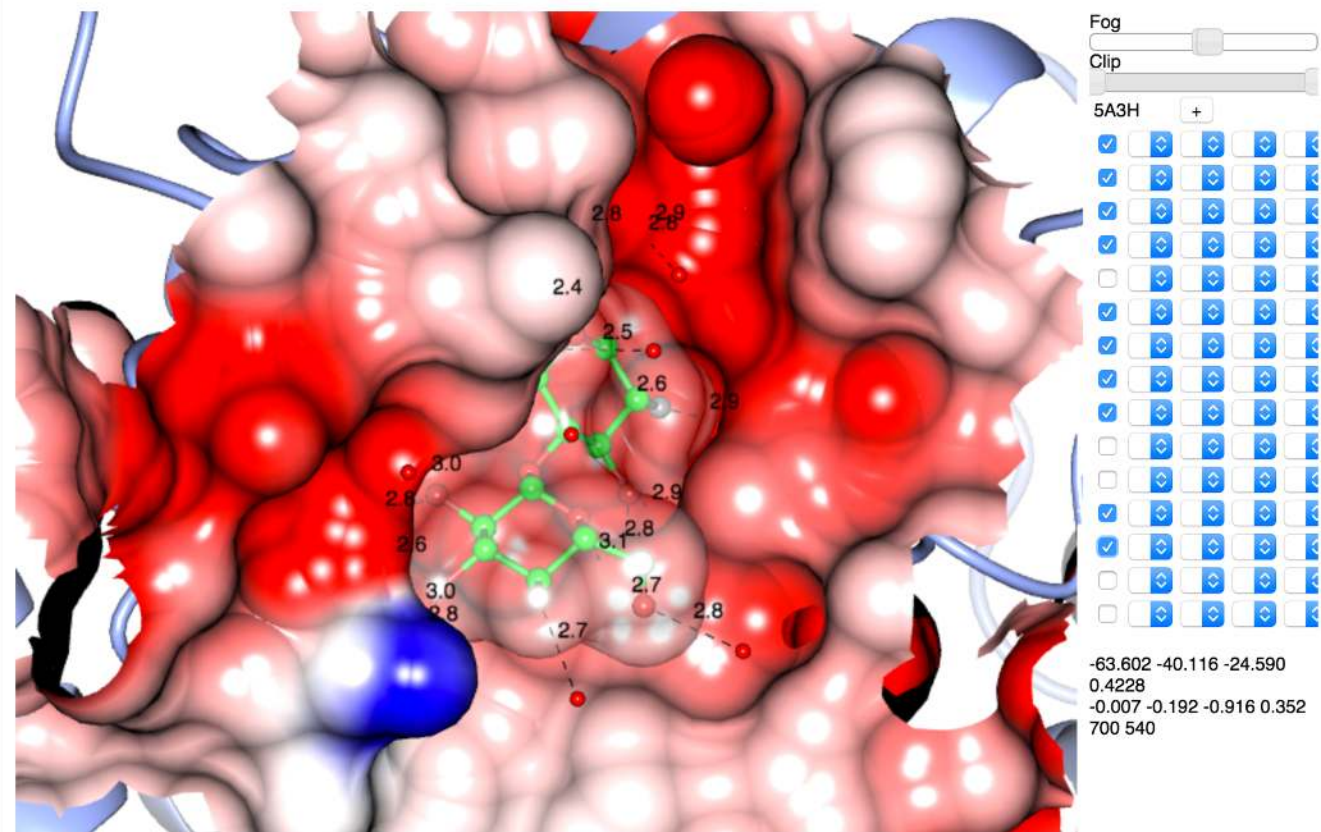
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Choose File ascene.scene.xml

Load file

Load PDB code

Stuart's client server WebGL



Fog

Clip

5A3H +

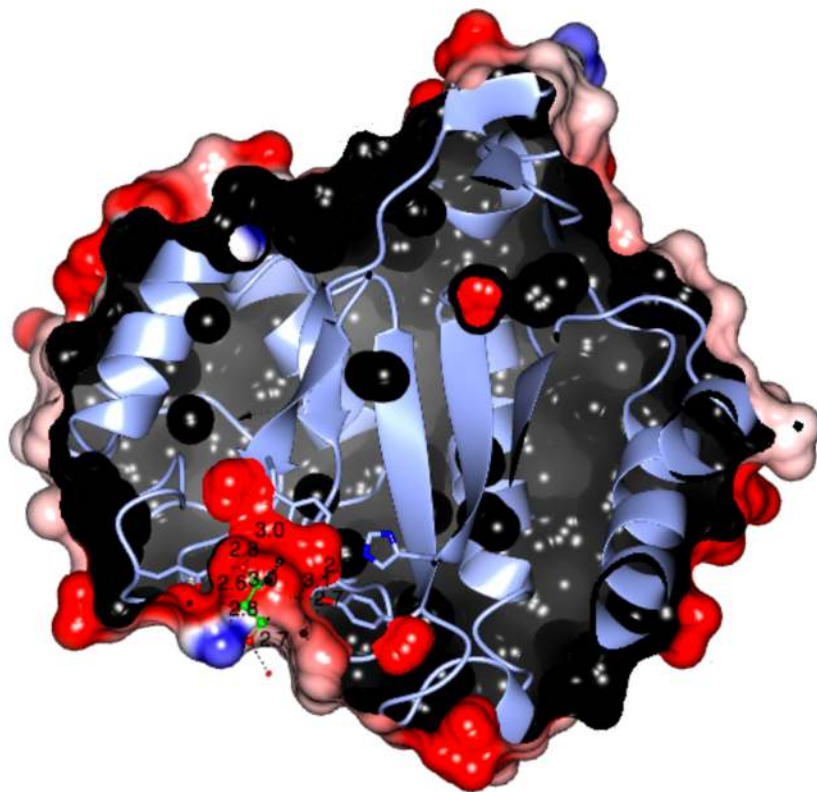
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Choose File ascene.scene.xml Load file

Load PDB code

Stuart's client server WebGL



Fog

Clip

5A3H +

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700 540

Choose File

ascene.scene.xml

Load file

Load PDB code

Stuart's client server WebGL

Fog

Clip

5A3H +

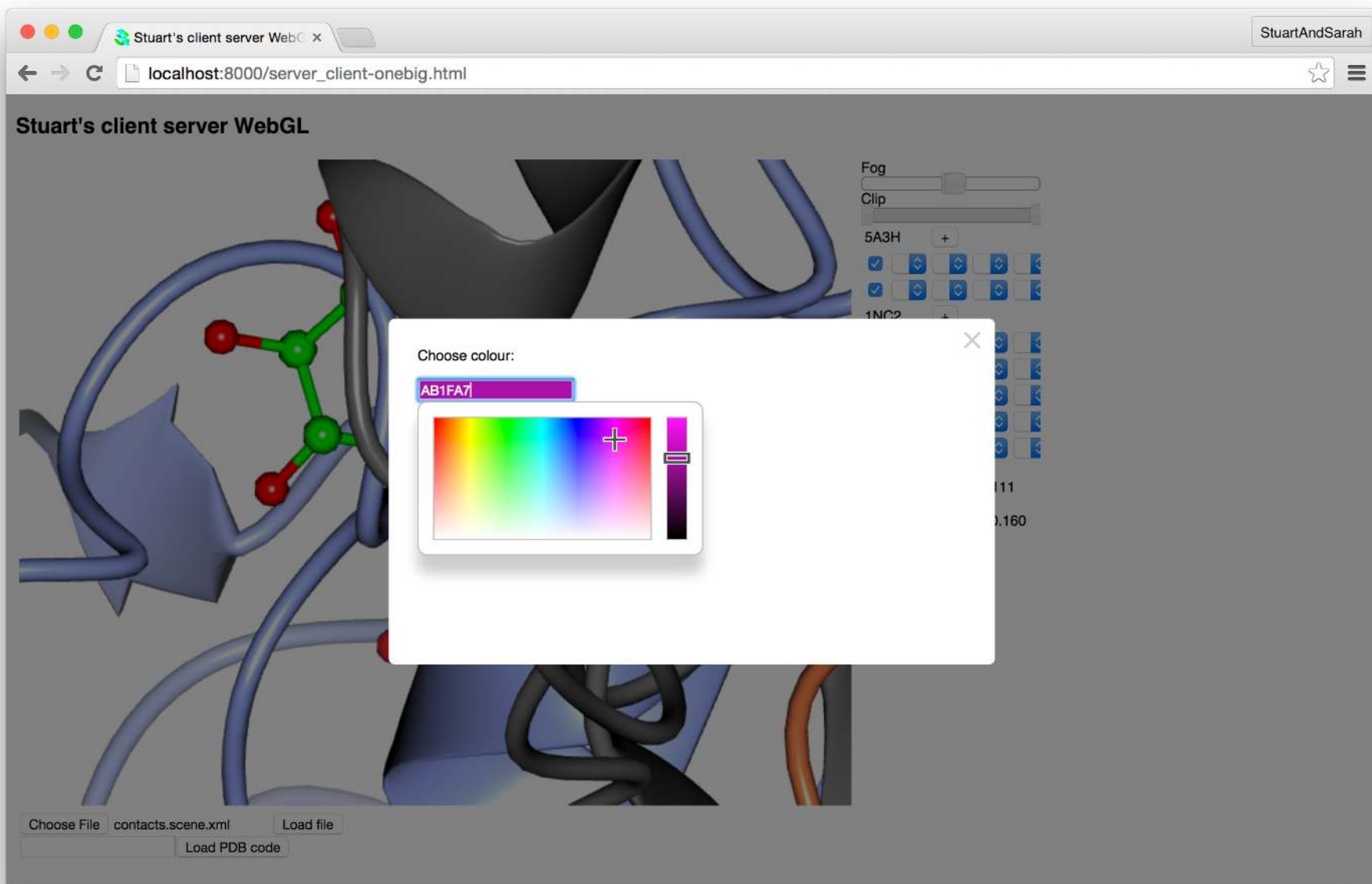
- | ☒ | ☒ | ☒ | ☒ | Atom type |
|-------------------------------------|-------------------------------------|-------------------------------------|-------------------------------------|------------------------|
| ☒ | ☒ | ☒ | ☒ | By chain |
| ☒ | ☒ | ☒ | ☒ | By model |
| ☒ | ☒ | ☒ | ☒ | Main/side chain |
| ☒ | ☒ | ☒ | ☒ | Secondary structure |
| ☐ | ☒ | ☒ | ☒ | Blend through model |
| ☐ | ☒ | ☒ | ☒ | Residue property |
| ☒ | ☒ | ☒ | ☒ | Residue type |
| ☒ | ☒ | ☒ | ☒ | Residue solvent access |
| ☒ | ☒ | ☒ | ☒ | Atom property |
| ☒ | ☒ | ☒ | ☒ | Temperature factor |
| ☒ | ☒ | ☒ | ☒ | Occupancy |
| ☐ | ☒ | ☒ | ☒ | Alternate location |
| ☐ | ☒ | ☒ | ☒ | Charge |
| ☐ | ☒ | ☒ | ☒ | Atom solvent access |
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700 540

Choose File ascene.scene.xml

Load file

Load PDB code



Stuart's client server WebGL

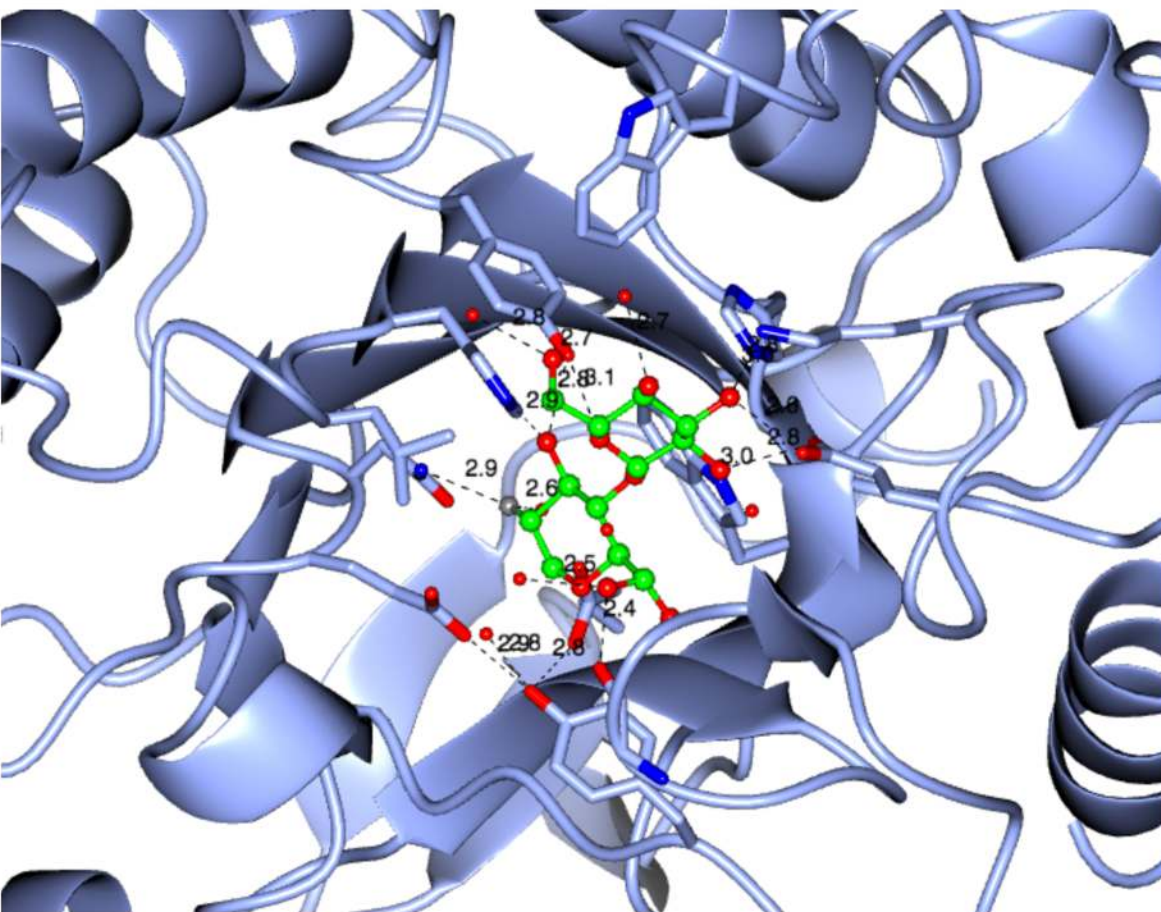
Fog

Clip

5A3H +

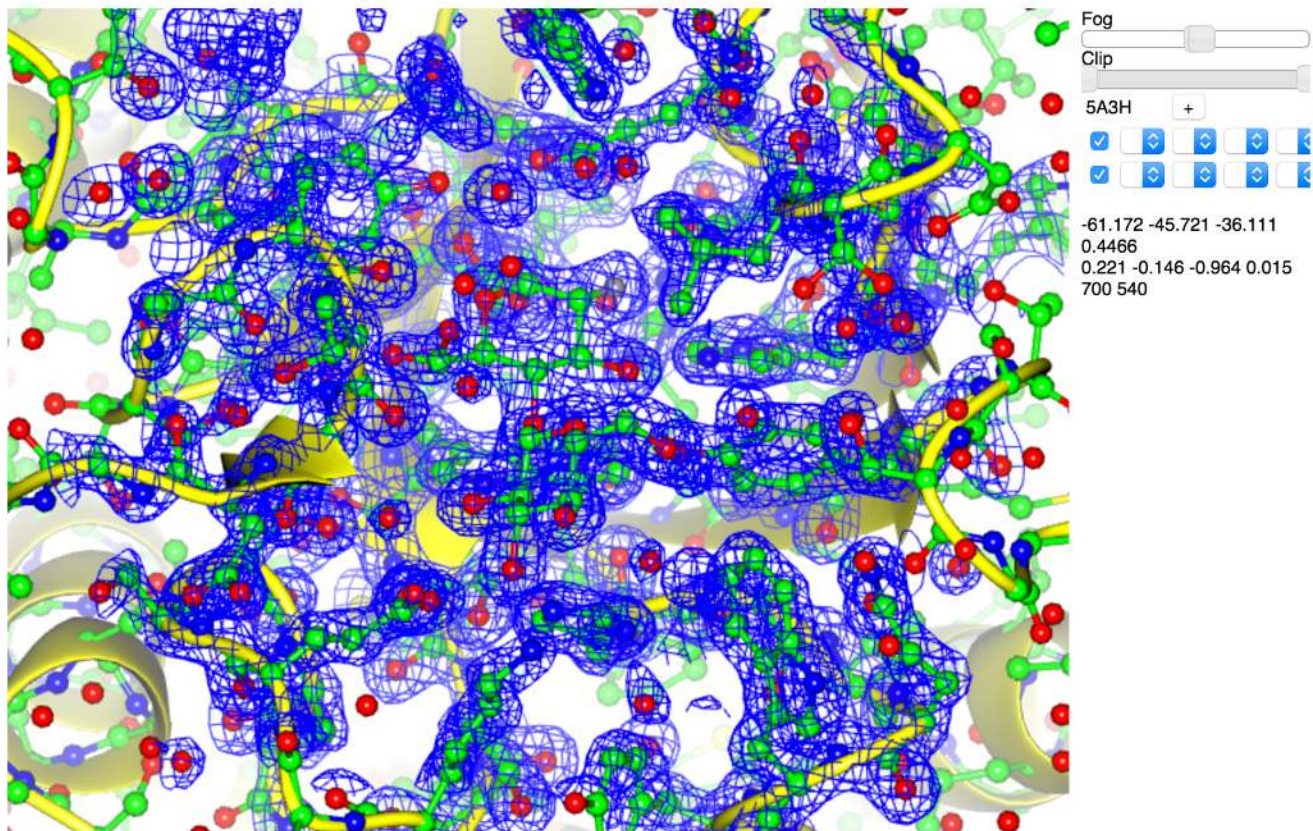
- ☒ ☐ ✓ All atoms
- ☒ ☐ All non-solvent
- ☒ ☐ Peptide
- ☒ ☐ All peptide
- ☒ ☐ CA trace
- ☐ ☐ Main chain
- ☐ ☐ Side chains
- ☒ ☐ SS bridges
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- ☒ ☐ Saccharides
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- ☐ ☐ NUC
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- ☐ ☐ Saccharides
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0.5299
-0.235 -0.035 0.406 0.882
700 540



Choose File ascene.scene.xml Load file
Load PDB code

Stuart's client server WebGL



Choose File ascene2.scene.xml Load file

Load PDB code

WebGL and CCP4MG

- “Client” is a web page on which user can load a CCP4MG status file. e.g. saved status from CCP4MG, but **not** currently .pkl), or a hand crafted one (from a template hopefully).
- The client sends the status file to a server. The server runs a “headless” version of CCP4MG which interprets status file, generates CCP4MG “data and display objects” and transforms the display objects into collections of triangles/lines.
- The server sends back the triangles and lines (plus other information) to the client which draws them.

WebGL and CCP4MG

- Advantages:
 - Absolutely rock solid (sort of); server can currently be confused by dodgy uploaded files; but client is fairly indestructible – JavaScript is hard to crash browser with or to cause other unwelcome behaviour with.
 - User interface is currently quite simple (it will get more complicated), requires very little to no interaction with internal complexities of CCP4MG and is thus very fast.
 - Extremely similar programming language (OpenGL ES) as required for Android/iOS 3D graphics. So Android port of this should be easy. iOS client which just draws without connecting to server already exists.

WebGL and CCP4MG

- Disadvantages:
 - Client/server communication is by plain text (json). Although the packing of triangle data is pretty efficient, the server side packing is slower than ideal.
 - Requires server to be running, so not as simple to install as most applications. However a centralized server at institution would make this a non-issue. *Care would be required to avoid accidental transmission of sensitive data.*

Acknowledgements

- Programming:

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

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- 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