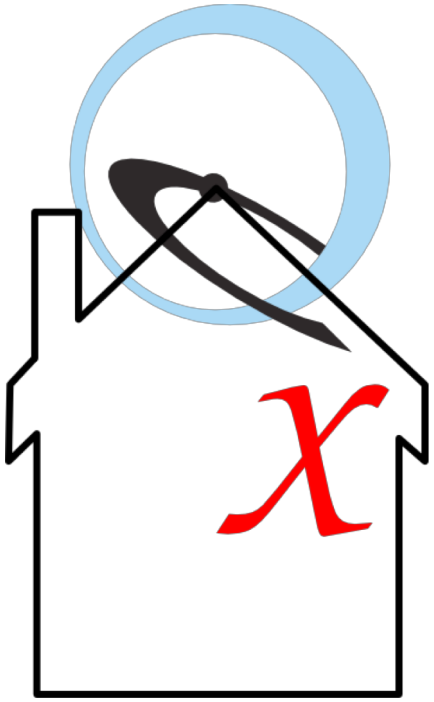


UCSF ChimeraX tutorial

Used version: 1.3.0 on MacOS Mojave 10.14.1

Made for 2022 spring ”Structural Biochemistry” course,
Institute of Biochemical Sciences,
National Taiwan University.

Kuen-Phon Wu
Institute of Biological Chemistry,
Academia Sinica

E-Mail:kpwulab@gmail.com
https://kpwulab.com
Twitter: @kpwu11

UCSF CHIMERA

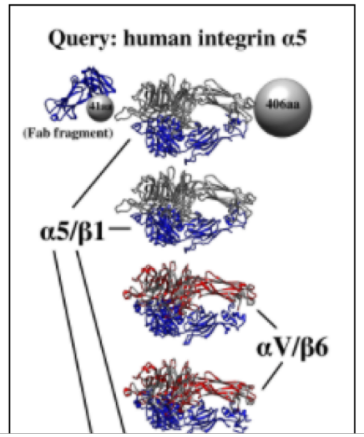
an Extensible Molecular Modeling System

UCSF Chimera is a program for the interactive visualization and analysis of molecular structures and related data, including density maps, trajectories, and sequence alignments. It is available free of charge for noncommercial use. Commercial users, please see Chimera commercial licensing.

We encourage Chimera users to try ChimeraX for much better performance with large structures, as well as other major advantages and completely new features. ChimeraX includes a significant subset of Chimera features (with more to come, see the missing features list) and is under active development. Users may choose to use both programs, and it is fine to have both installed.

Chimera is no longer under active development, and is only updated for critical maintenance. Chimera development was supported by a grant from the National Institutes of Health (P41-GM103311) that ended in 2018.

Feature Highlight



Find and Summarize Structures for a Sequence

One use of **Multidomain Assembler** is to set up comparative modeling and concatenation of existing structures to generate a full-length model of a multidomain protein. However, even without model-building, the byproduct is also useful: a visual summary of the structures available for a query sequence, optionally filtered by criteria such as BLAST score and % identity, laid out horizontally in approximate N→C order relative to the query. Overlapping hits are stacked vertically, and segments without structural coverage are indicated with spheres. By default, the multiple sequence alignment of the hits to the query is also displayed.

The figure shows the results of command:
mda p08648 ~/Desktop/MDA limit 4 percent 50
with sequence mismatches in red and molecules other than the hit chains in blue. Text and pointers have been added with **2D Labels**.

Multidomain Assembler is described in a paper.

(More features...)

Quick Links

Documentation
- Getting Started
- User's Guide
- Command Index
- Tutorials and Videos
- Guide to Volume Data
- Release Notes

Download
- What's New in Daily Builds
- Map of Download Locations

Galleries
- Image Gallery
- Animation Gallery

Publications and Talks

Related Databases and Software

Citing Chimera

Contact Us

Recent Citations

A structural basis for amylin receptor phenotype. Cao J, Belousoff MJ *et al. Science.* 2022 Mar 25;375(6587):eabm9609.

Chimera Search

Go

Google™ Search

News

December 20, 2021

The RBVI wishes you a safe and happy holiday season! See our 2021 card and the gallery of previous cards back to 1985.

December 17, 2021

Chimera production release 1.16 is now available. This will be the last release to support Windows 7. See the release notes for what's new.

December 18, 2020

Chimera production release 1.15 is now available. See the release notes for what's new.

(Previous news...)

Upcoming Events

https://www.cgl.ucsf.edu/chimera/

Quick Links

- UCSF ChimeraX Home
- Advantages
- Documentation
  - User Guide
  - Tutorials and Videos
  - Presentations
- Download
  - Toolshed
- Citing ChimeraX
- Contact Us
- Related Software

Featured Citations

Architecture and antigenicity of the Nipah virus attachment glycoprotein. Wang Z, Amaya M *et al. Science.* 2022 Mar 25;375(6587):1373-1378.

Altered TMPRSS2 usage by SARS-CoV-2 Omicron impacts infectivity and fusogenicity. Meng B, Abdullahi A *et al. Nature.* 2022 Mar 24;603(7902):706–714.

Recovery of particulate methane monooxygenase structure and activity in a lipid bilayer. Koo CW, Tucci FJ *et al. Science.* 2022 Mar 18;375(6586):1287-1291.

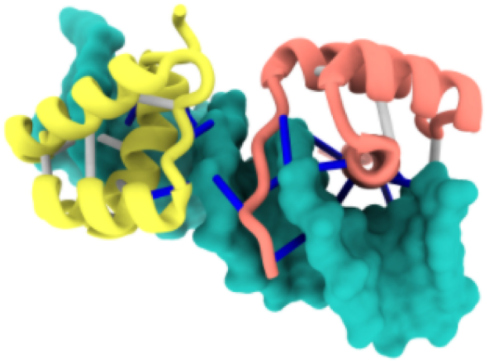
Ribosome collisions induce mRNA cleavage and ribosome rescue in bacteria. Saito K, Kratzat H *et al. Nature.* 2022 Mar 17;603(7901):503-508.

UCSF ChimeraX

UCSF ChimeraX (or simply ChimeraX) is the next-generation molecular visualization program from the Resource for Biocomputing, Visualization, and Informatics (RBVI), following UCSF Chimera. ChimeraX can be downloaded free of charge for academic, government, nonprofit, and personal use. Commercial users, please see ChimeraX commercial licensing.

ChimeraX is developed with support from National Institutes of Health R01-GM129325 and the Office of Cyber Infrastructure and Computational Biology, National Institute of Allergy and Infectious Diseases.

Feature Highlight



Struts for 3D Printing

Structures can be reinforced for 3D printing with pseudobonds. In this DNA-transcription factor complex (PDB 5ego), proteins are shown as ribbons and the DNA as a molecular surface. The pseudobonds in blue were read in from a manually created file, 5ego.pb, and further reinforcements in light gray were added automatically with the **struts** command. For image setup other than orientation, see the command file struts.cxc.

More features...

https://www.cgl.ucsf.edu/chimerax/

Example Image

The Human Ribosome

The architecture of the human ribosome has been determined at near-atomic resolution by electron microscopy (Anger *et al.*, *Nature* **497**:80 (2013)). The structure, comprising 82 proteins and five RNA molecules, is shown with shadows cast from all directions to accentuate depth. In the background are schematic representations of contacts between the

News

December 20, 2021

The RBVI wishes you a safe and happy holiday season! See our 2021 card and the gallery of previous cards back to 1985.

December 8, 2021

The ChimeraX 1.3 production release is available. See the change log for what's new.

October 22, 2021

The ChimeraX 1.3 release candidate is available. Please try it and report any issues. See the change log for what's new.

Previous news...

Upcoming Events

March 29, 2022

SBGrid webinar 9am PST Mar 29 (noon EST). Second speaker Tom Goddard (~9:30am) will show using AlphaFold-predicted structures for cryoEM modeling in ChimeraX [register for webinar].

About Chimera and ChimeraX

- Chimera and the successor ChimeraX are developed by the Resource for Biocomputing, Visualization, and Informatics (RBVI) at UC San Francisco. (https://www.cgl.ucsf.edu/index.html)

- ChimeraX can be downloaded free of charge for academic, government, nonprofit, and personal use. Commercial users, please see ChimeraX commercial licensing.

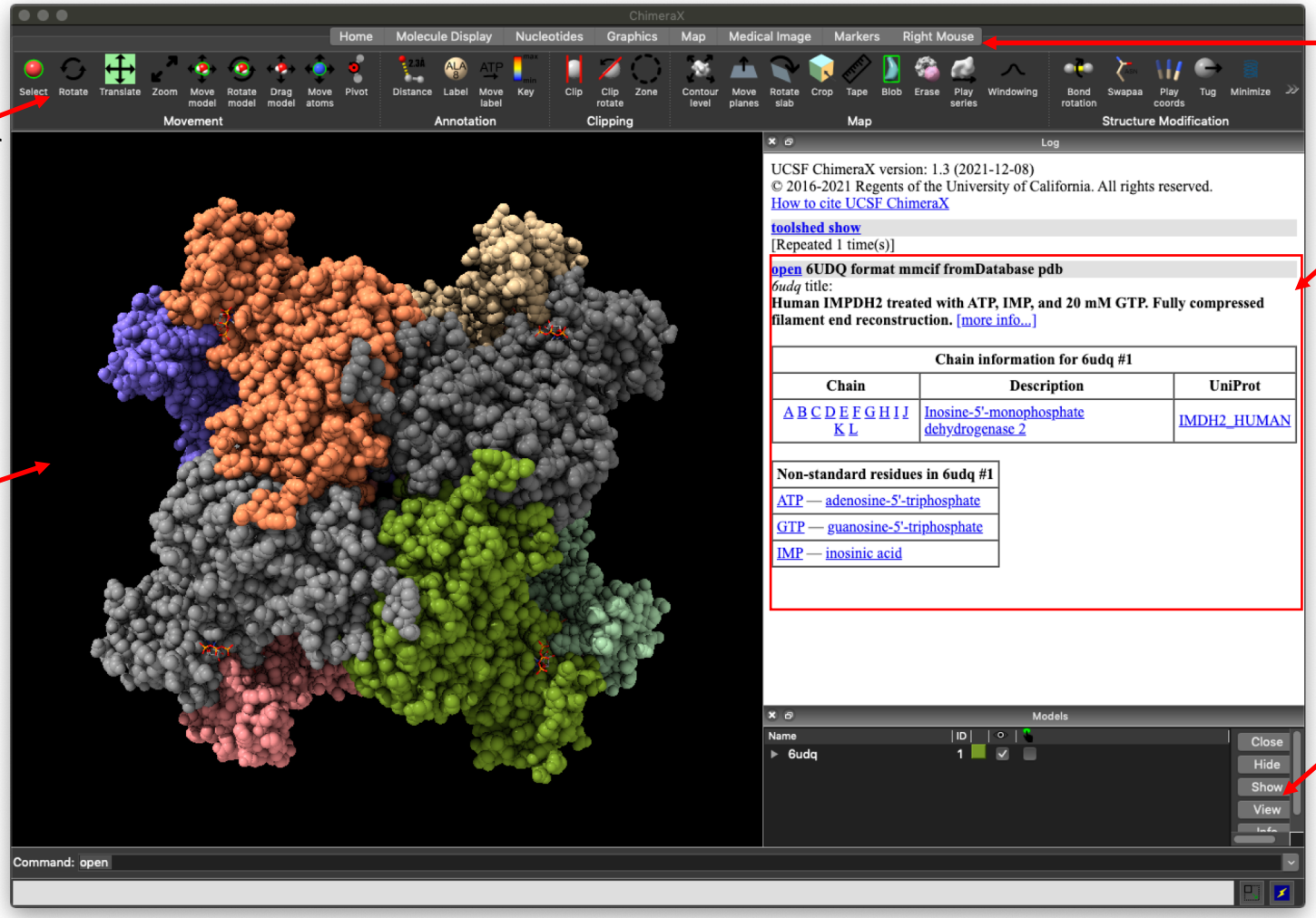
- Supporting OS: Windows, MacOS, Linux

- Download: https://www.cgl.ucsf.edu/chimerax/download.html

Why ChimeraX

- Active developement, current version: 1.3 as of March 30, 2022
- Free for nonprofit users
- Designed for handling large biomolecules and medical imaging system.
- Good documentation for users
  - Quick guide: https://www.rbvi.ucsf.edu/chimerax/docs/quickstart/index.html
  - Tutorials: https://www.rbvi.ucsf.edu/chimerax/tutorials.html
- Getting popular in the cryo-EM and crystallography circle.
- A hub for user-contributed plugin (called toolshed) https://cxtoolshed.rbvi.ucsf.edu/
- Connect to other good “tools”
  - Modeller
  - Alphafold
  - Autodock (viewDockX)

The GUI: exampled by a hetero 12meric IMPHD2



Function bar

Tool tabs

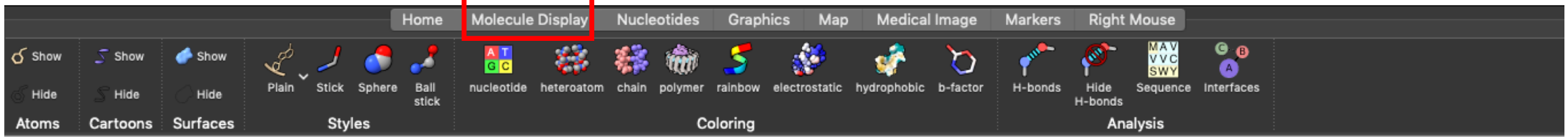
Log page

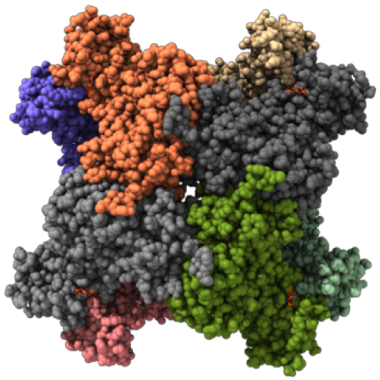
Protein information automatically displayed for user.

Graphic display area

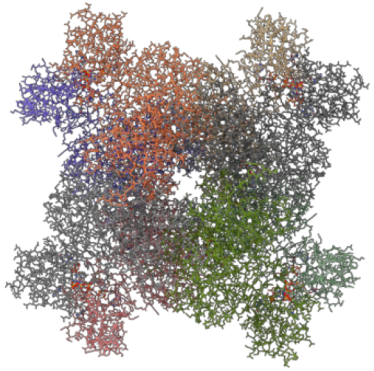
Model page

The “Molecule Display”

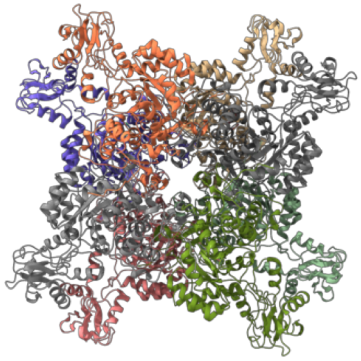




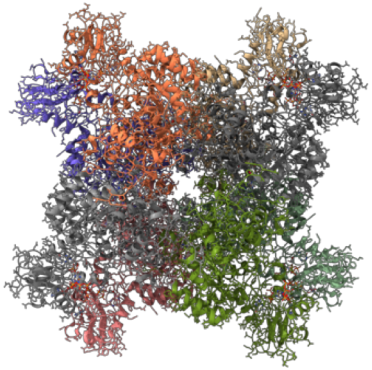
Default view
(Atoms: ball stick)



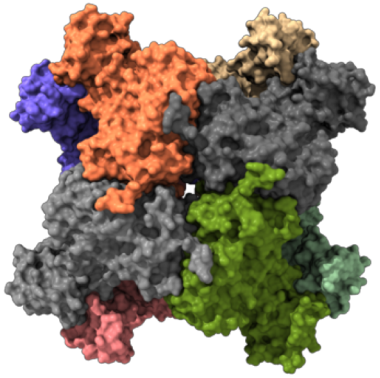
Atoms: Stick



Cartoons show
(Atoms hide)

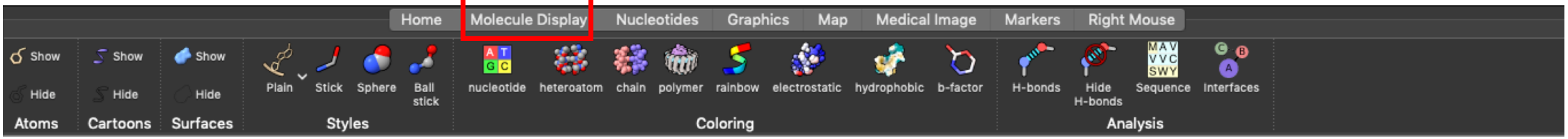


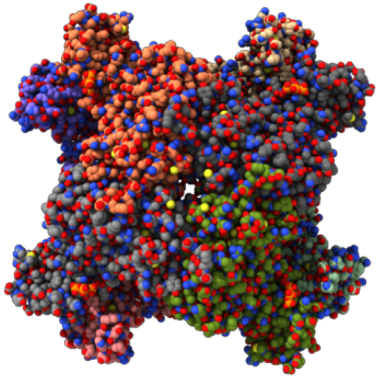
Cartoons show
+ Atoms show



Surface show
(others are hidden)

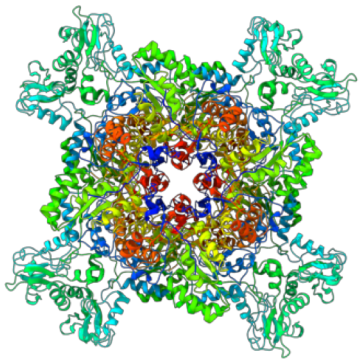
The “Molecule Display”





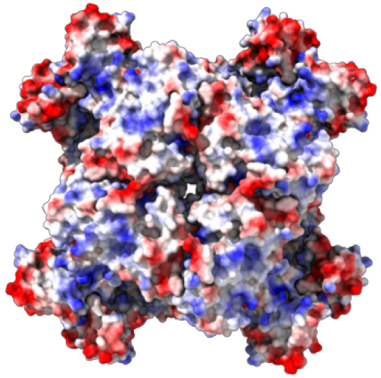
Heteroatom

Red: oxygen
Blue: nitrogen
Yellow: sulfur



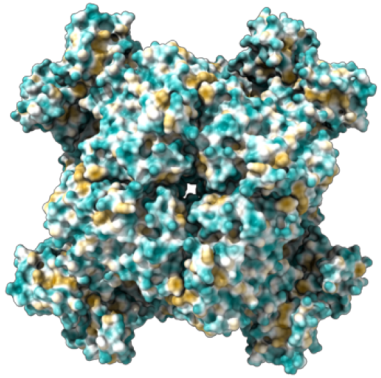
Rainbow color

N-term: blue
Middle: green
C-term: red



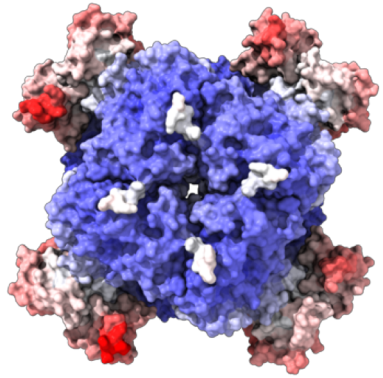
Electrostatic potential

Blue: positively charged
Red: negatively charged



Hydrophobicity

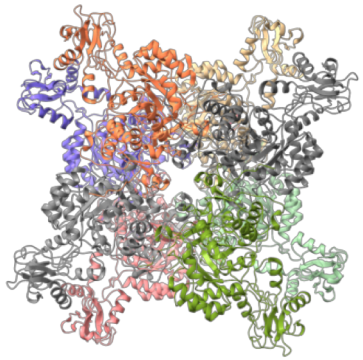
dark cyan (most hydrophilic) to white to dark goldenrod (most lipophilic)



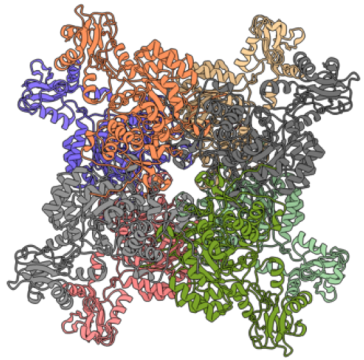
B-factor

Blue-white-red: Low to high b factor values

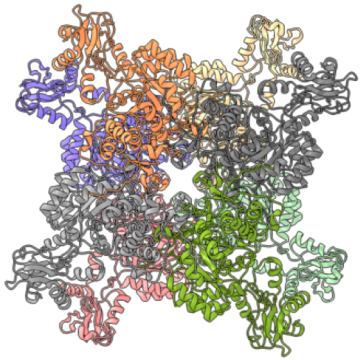
The “Graphics”



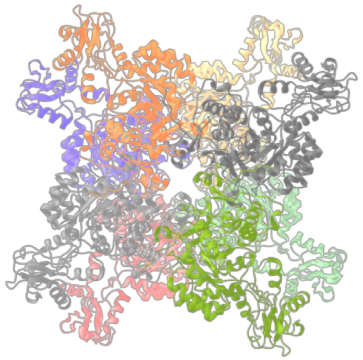
“Simple”



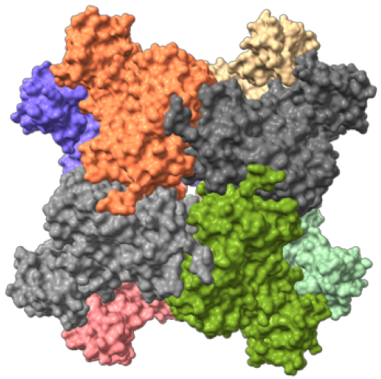
“Flat”

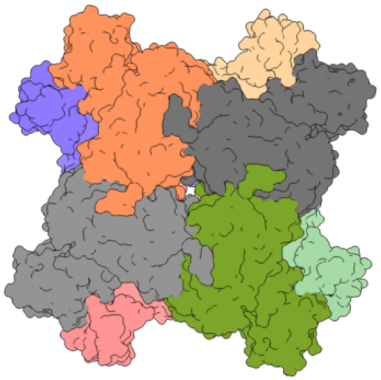


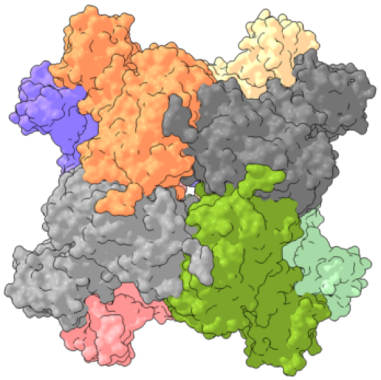
“Flat” “no shadow”

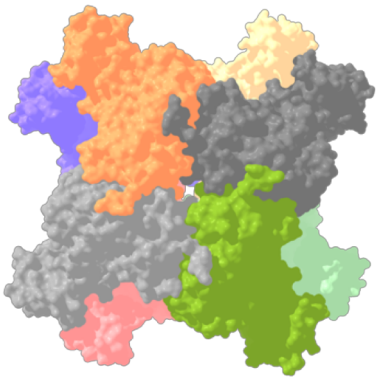


“Flat”, no shadow, no silhouettes









The ”selection” arguments in ChimeraX

- Select an object using “#”: select #1
- Select chain B in object 1: select #1/B
- Select residue 10-30 of chain C in object 2: select #2/C:10-30
- Select residue 10-30 of chain A and C in object 2: select #2/A,C:10-30
- Select all atoms CA of lysine in object 3: select #3:lys@CA

Cheating signs:

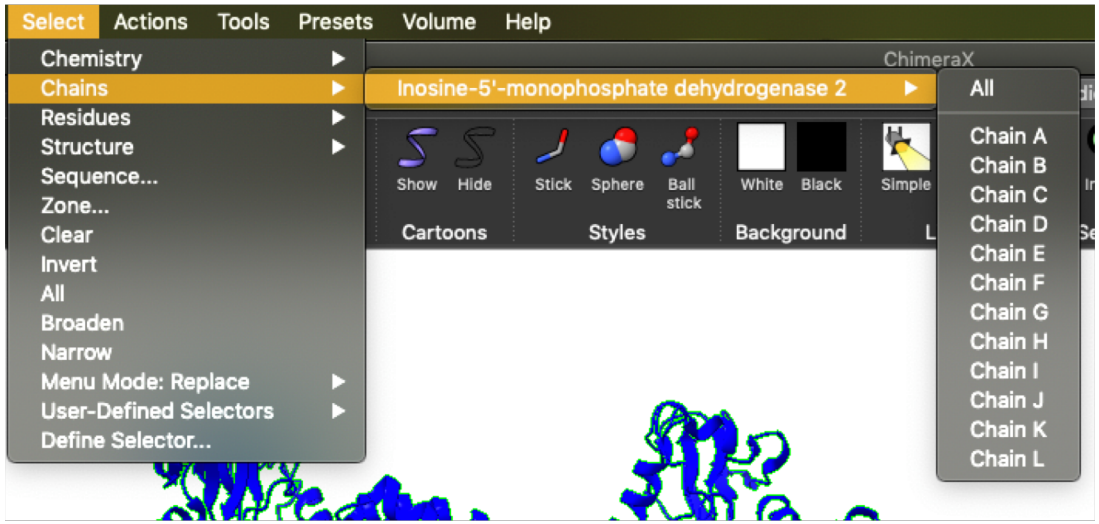
Object: #

Chain: /

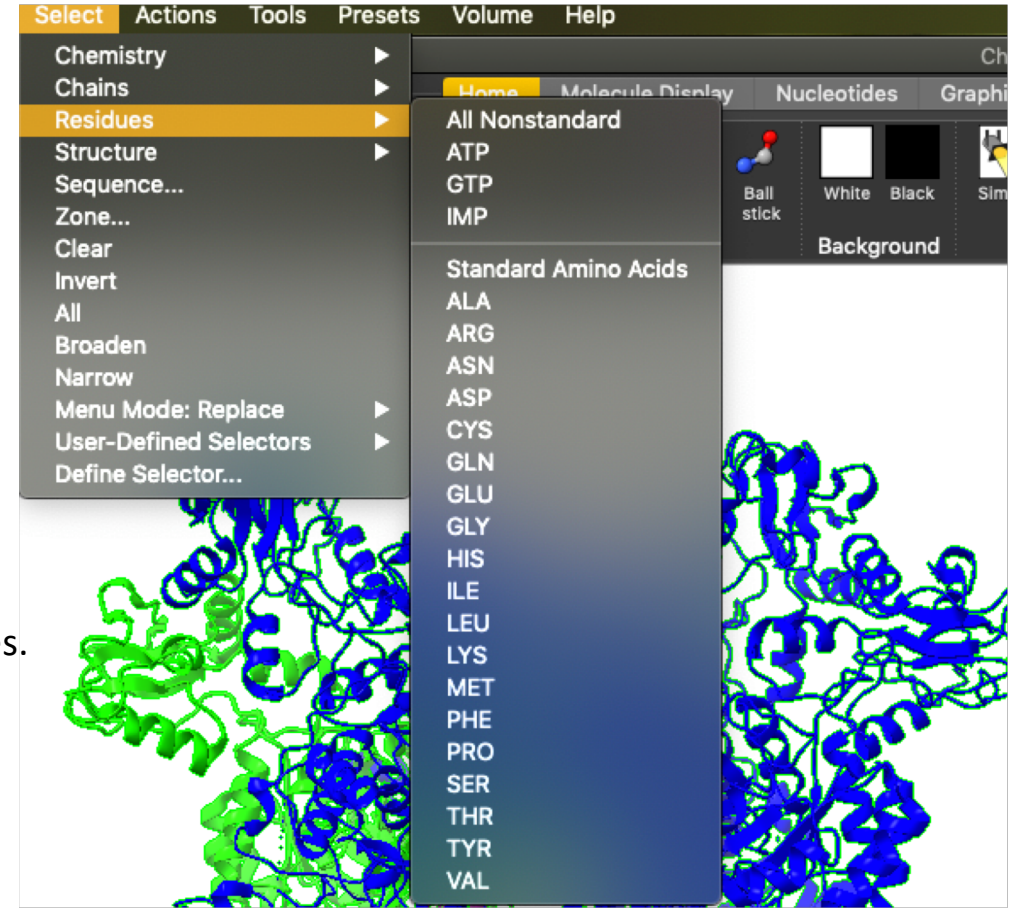
Residues: :

Atoms: @

The ”selection” function



Simple selections for chain, residues, atoms or other available types.



Colors in ChimeraX

- ChimeraX has predefined color codes (https://www.cgl.ucsf.edu/chimerax/docs/user/commands/colornames.html#builtin)
- Command: “color”
- Usage: color name color-spec

Examples:
color #1 blue

color #1/A,B purple (predefined color code)

color #1/A 50,50,90 (the “rgb” color)

color #1/A #17FF00 (the “rgb” color in HEX number)

Name	Hex	RGB (%)
misty rose	#FFE4E1	100,89,88
pink	#FFC0CB	100,75,80
light pink	#FFB6C1	100,71,76
hot pink	#FF69B4	100,41,71
deep pink	#FF1493	100,8,58
medium violet red	#C71585	78,8,52
pale violet red	#DB7093	86,44,58
light coral	#F08080	94,50,50
salmon	#FA8072	98,50,45
light salmon	#FFA07A	100,63,48
dark salmon	#E9967A	91,59,48
indian red	#CD5C5C	80,36,36
crimson	#DC143C	86,8,24
firebrick	#B22222	70,13,13
brown	#A52A2A	65,17,17
dark red	#8B0000	54,0,0
maroon	#800000	50,0,0
red	#FF0000	100,0,0
orange red	#FF4500	100,27,0
tomato	#FF6347	100,39,28
coral	#FF7F50	100,50,31
dark orange	#FF8C00	100,55,0
orange	#FFA500	100,65,0
gold	#FFD700	100,84,0
yellow	#FFFF00	100,100,0

Name	Hex	RGB (%)
khaki	#F0E68C	94,90,55
goldenrod	#DAA520	86,65,12
dark goldenrod	#B8860B	72,52,4
lemon chiffon	#FFFACD	100,98,80
light goldenrod yellow	#FAFAD2	98,98,82
light yellow	#FFFFE0	100,100,88
cornsilk	#FFF8DC	100,97,86
papaya whip	#FFEFD5	100,94,84
blanched almond	#FFEBCD	100,92,80
peach puff	#FFDAB9	100,86,72
bisque	#FFE4C4	100,89,77
moccasin	#FFE4B5	100,89,71
navajo white	#FFDEAD	100,87,68
wheat	#F5DEB3	96,87,70
burly wood	#DEB887	87,72,53
tan	#D2B48C	82,71,55
sandy brown	#F4A460	96,64,38
peru	#CD853F	80,52,25
chocolate	#D2691E	82,41,12
saddle brown	#8B4513	54,27,8
sienna	#A0522D	63,32,18
rosy brown	#BC8F8F	74,56,56

Name	Hex	RGB (%)
beige	#F5F5DC	96,96,86
pale goldenrod	#EEE8AA	93,91,67
dark khaki	#BDB76B	74,72,42
dark olive green	#556B2F	33,42,18
olive	#808000	50,50,0
olive drab	#6B8E23	42,56,14
yellow green	#9ACD32	60,80,20
green yellow	#ADFF2F	68,100,18
chartreuse	#7FFF00	50,100,0
lawn green	#7CFC00	49,99,0
lime	#00FF00	0,100,0
lime green	#32CD32	20,80,20
forest green	#228B22	13,54,13
green	#008000	0,50,0
dark green	#006400	0,39,0
pale green	#98FB98	60,98,60
light green	#90EE90	56,93,56
spring green	#00FF7F	0,100,50
medium spring green	#00FA9A	0,98,60
medium sea green	#3CB371	24,70,44
sea green	#2E8B57	18,54,34
dark sea green	#8FBC8F	56,74,56
medium aquamarine	#66CDAA	40,80,67
aquamarine	#7FFFD4	50,100,83

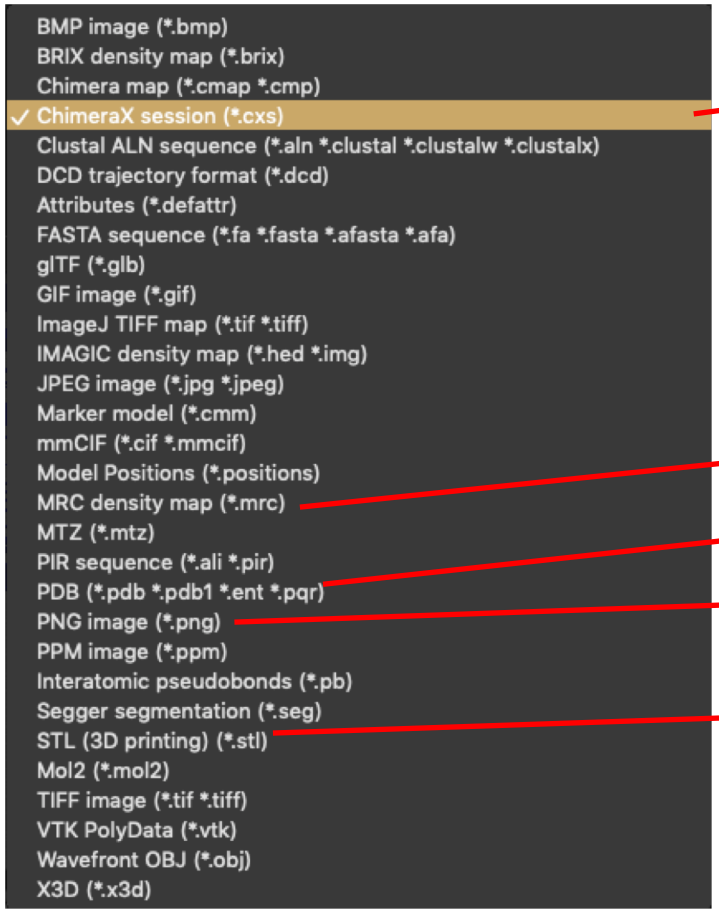
Name	Hex	RGB (%)
turquoise	#40E0D0	25,88,82
medium turquoise	#48D1CC	28,82,80
light sea green	#20B2AA	12,70,67
cyan (aqua)	#00FFFF	0,100,100
dark turquoise	#00CED1	0,81,82
cadet blue	#5F9EA0	34,62,63
dark cyan	#008B8B	0,54,54
teal	#008080	0,50,50
pale turquoise	#AFEEEE	69,93,93
powder blue	#B0E0E6	69,88,90
light blue	#ADD8E6	68,85,90
light steel blue	#B0C4DE	69,77,87
steel blue	#4682B4	28,51,71
sky blue	#87CEEB	53,81,92
light sky blue	#87CEFA	53,81,98
deep sky blue	#00BFFF	0,75,100
dodger blue	#1E90FF	12,56,100
cornflower blue	#6495ED	39,58,93
royal blue	#4169E1	26,41,88
blue	#0000FF	0,0,100
medium blue	#0000CD	0,0,80
dark blue	#00008B	0,0,54
navy	#000080	0,0,50

Name	Hex	RGB (%)
lavender	#E6E6FA	90,90,98
thistle	#D8BFD8	85,75,85
plum	#DDA0DD	87,63,87
violet	#EE82EE	93,51,93
orchid	#DA70D6	86,44,84
magenta (fuchsia)	#FF00FF	100,0,100
dark magenta	#8B008B	54,0,54
purple	#800080	50,0,50
medium orchid	#BA55D3	73,33,83
dark orchid	#9932CC	60,20,80
dark violet	#9400D3	58,0,83
blue violet	#8A2BE2	54,17,89
medium purple	#9370DB	58,44,86
rebecca purple	#663399	40,20,60
indigo	#4B0082	29,0,51
medium slate blue	#7B68EE	48,41,93
slate blue	#6A5ACD	42,35,80
dark slate blue	#483D8B	28,24,54
midnight blue	#191970	10,10,44
white	#FFFFFF	100,100,100
snow	#FFFAFA	100,98,98
mint cream	#F5FFFA	96,100,98
honeydew	#F0FFF0	94,100,94
azure	#F0FFFF	94,100,100
light cyan	#E0FFFF	88,100,100

Name	Hex	RGB (%)
alice blue	#F0F8FF	94,97,100
ghost white	#F8F8FF	97,97,100
white smoke	#F5F5F5	96,96,96
lavender blush	#FFF0F5	100,94,96
seashell	#FFF5EE	100,96,93
old lace	#FDF5E6	99,96,90
floral white	#FFFAF0	100,98,94
ivory	#FFFFF0	100,100,94
linen	#FAF0E6	98,94,90
antique white	#FAEBD7	98,92,84
gainsboro	#DCDCDC	86,86,86
light gray	#D3D3D3	83,83,83
silver	#C0C0C0	75,75,75
dark gray	#A9A9A9	66,66,66
gray	#808080	50,50,50
dim gray	#696969	41,41,41
light slate gray	#778899	47,53,60
slate gray	#708090	44,50,56
dark slate gray	#2F4F4F	18,31,31
black	#000000	0,0,0

The “save” function in ChimeraX

Save as ”image”, “map”, “sequence”, “3D printing”, “session”



CXS: ChimeraX session (like PyMOL session “pse”)

mrc: EM density map

pdb: biomolecule 3D coordinates

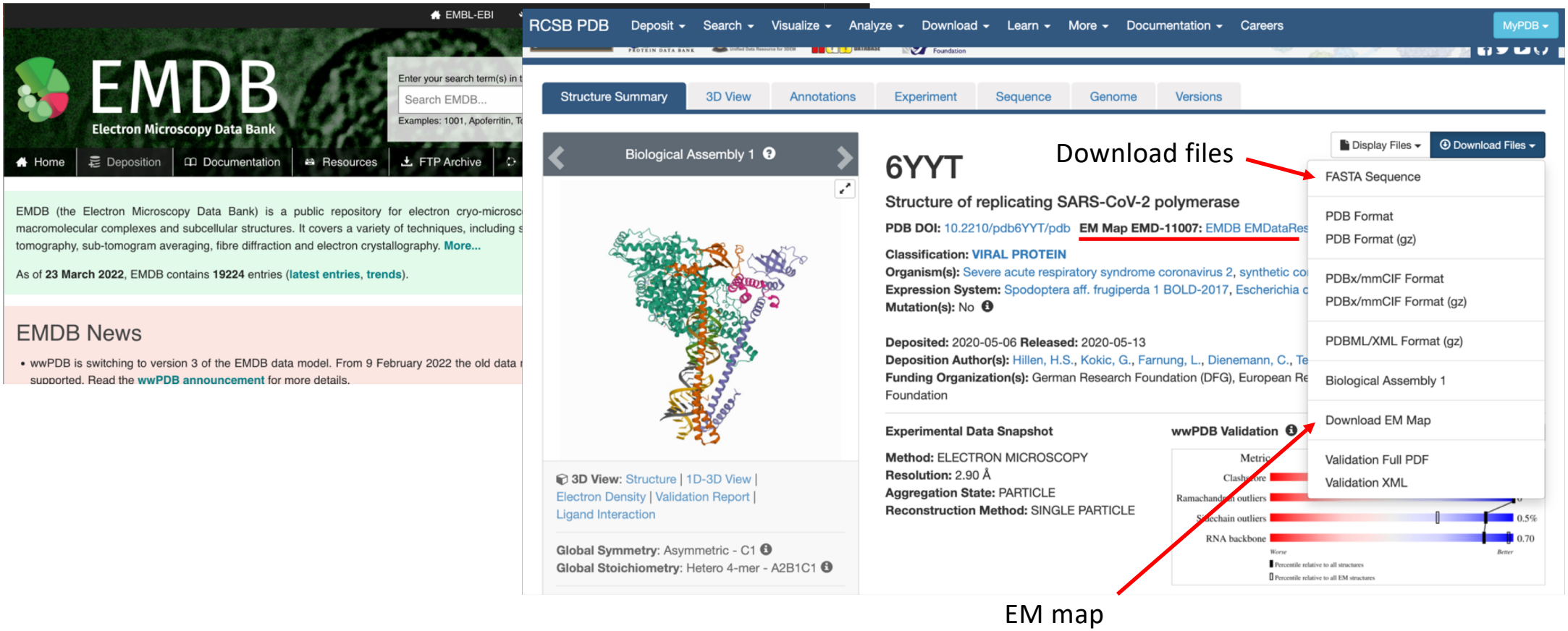
png: image with transparency option

stl: 3D printing file

Analyze structure+ EM map by Chimerax

Electron Microscopy Data Bank (EMDB)
https://www.ebi.ac.uk/emdb/

Protein Data Bank (PDB)
https://www.rcsb.org/

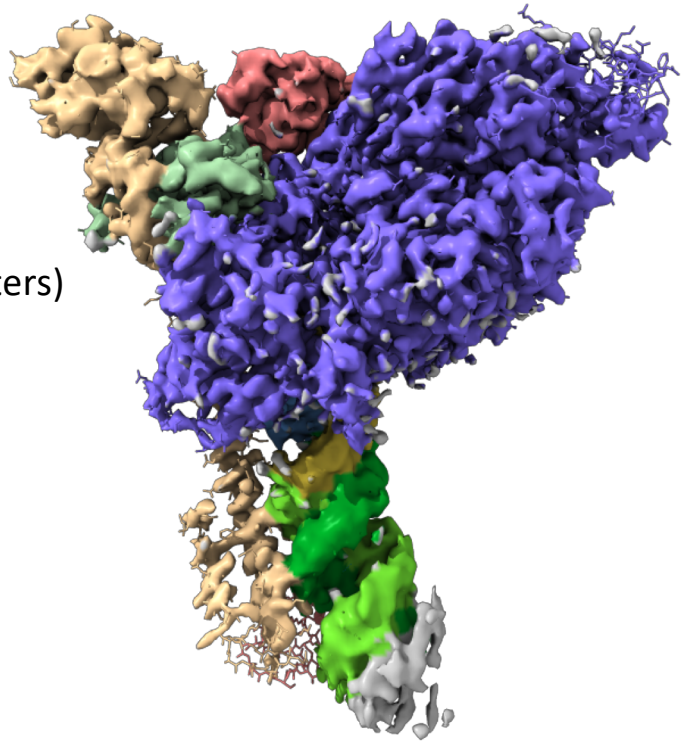


Analyze structure+ EM map by Chimerax – SARS-CoV2 RdRp example

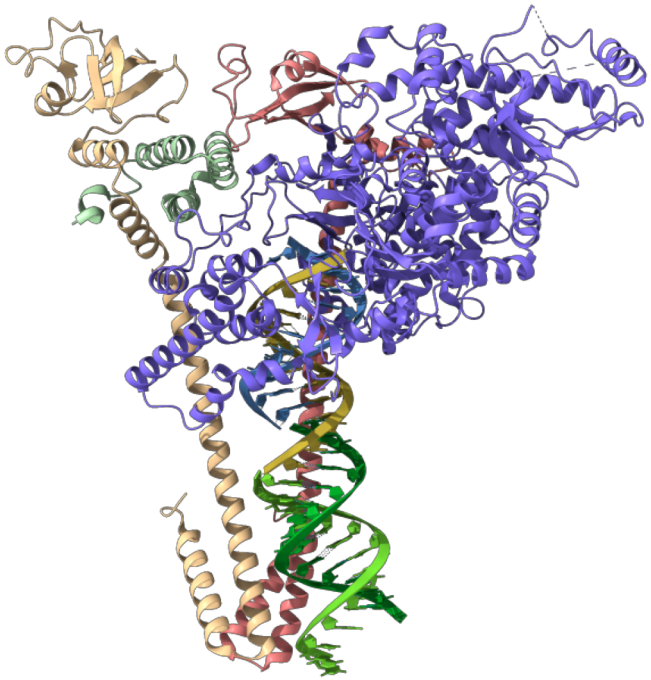
PDB: 6YYT EMDB: 11007

In ChimeraX command line:

- open 6YYT
- open emdb:11007
  (NOTE: emdb must be lower case letters)
- style #1 stick
- volume #2 level 3
- color bychain
- color zone #2 near #1 dist 3.5
- surface dust #2 size 3



Map overlays structure (shown in atoms stick style)



DNA chain IDs: Q and U

Structure shown in cartoon but the nucleic acid is additionally shown with atoms and “filled plan”.

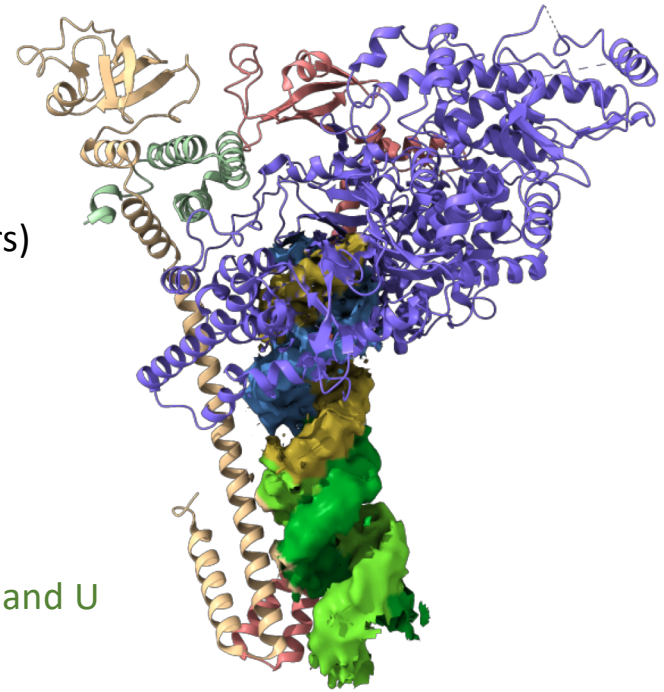
Analyze structure+ EM map by Chimerax – SARS-CoV2 RdRp example

PDB: 6YYT EMDB: 11007

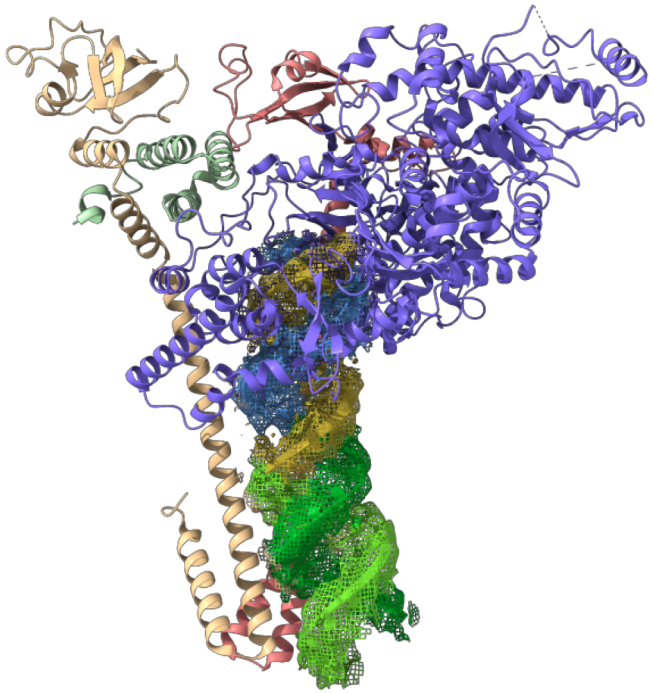
In ChimeraX command line:

- open 6YYT
- open emdb:11007
  (NOTE: emdb must be lower case letters)
- style #1 stick
- volume #2 level 3
- color bychain
- color zone #2 near #1 dist 3.5
- surface dust #2 size 3
- vol zone #2 near #1/P,T,U,Q range 3.5

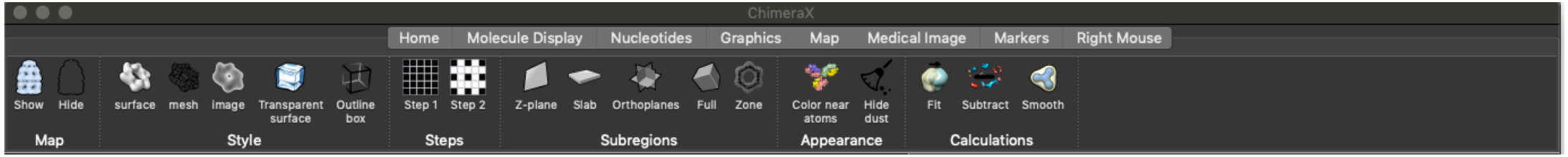
DNA chain IDs: P,Q,T and U

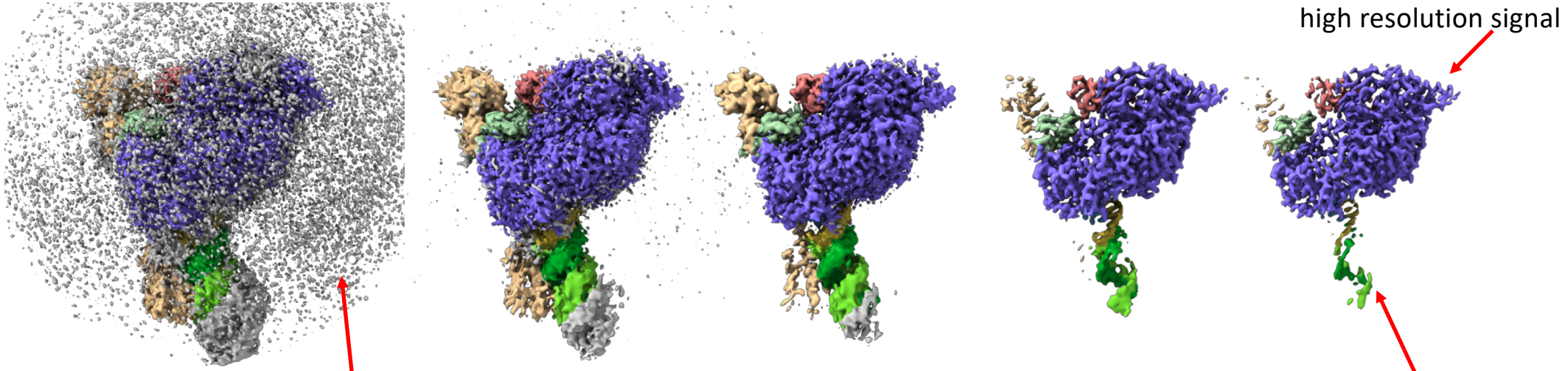


Only display maps of DNA in a range of 3.5 Å



Map shown in “mesh” stype





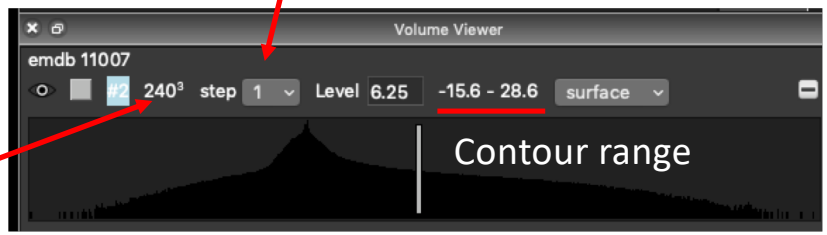
high resolution signal

Contour level 1.3 2 3 6.25 8

Display steps (1 for high quality)

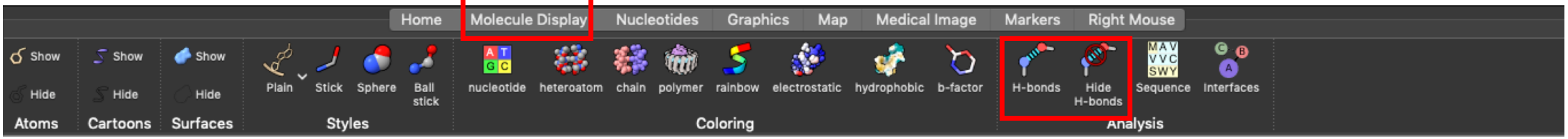
noises

Box size = 240 Å^3

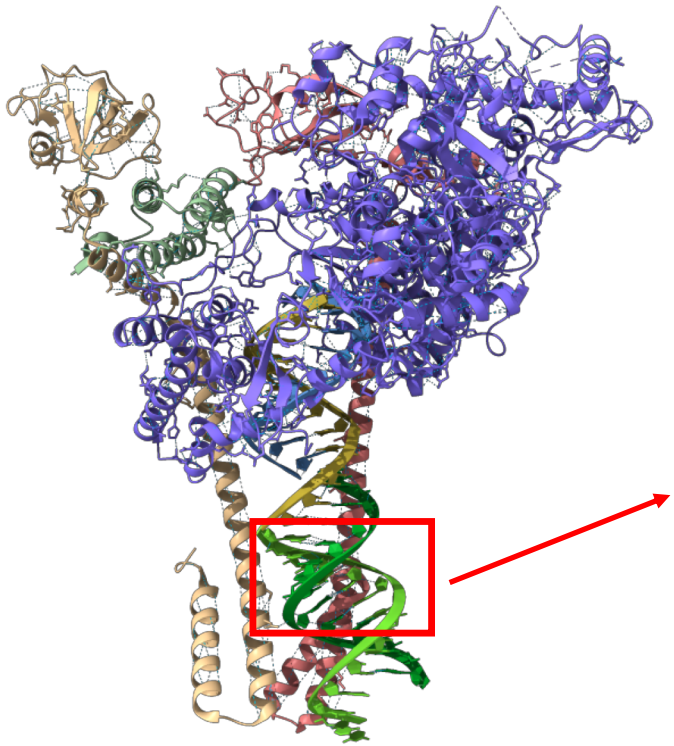


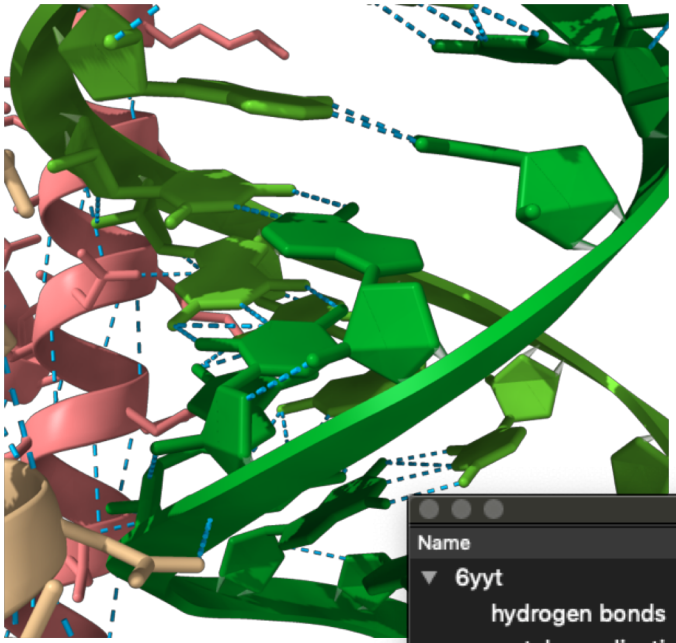
Low resolution signal

The “Molecule Display”

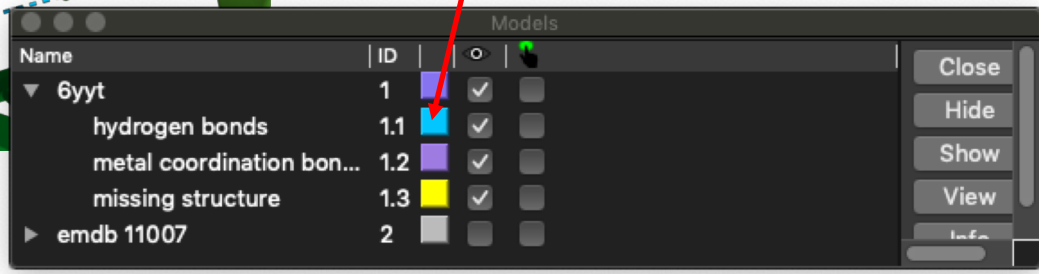


on off





Click square to change desired color



The “Right Mouse tab”