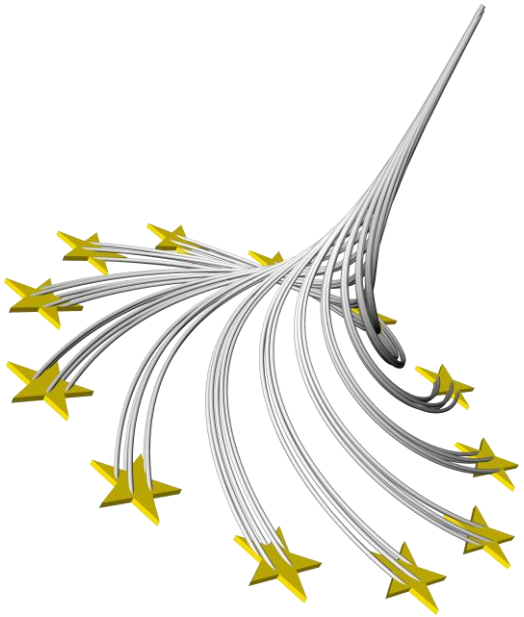
EuroVis 2011

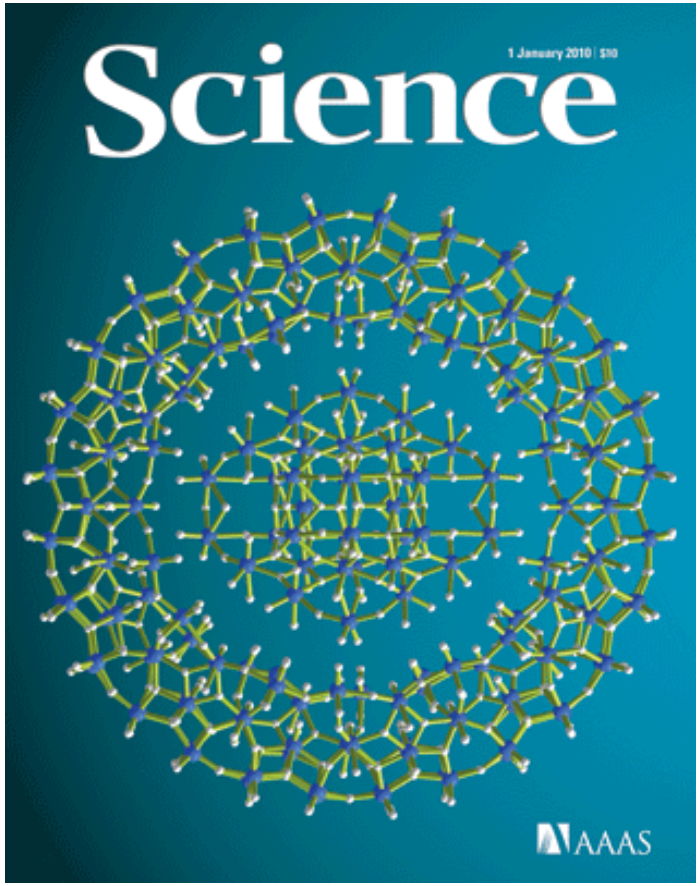
Illustrative Molecular Visualization with Continuous Abstraction

Matthew van der Zwan
Wouter Lueks
Henk Bekker
Tobias Isenberg



university of groningen

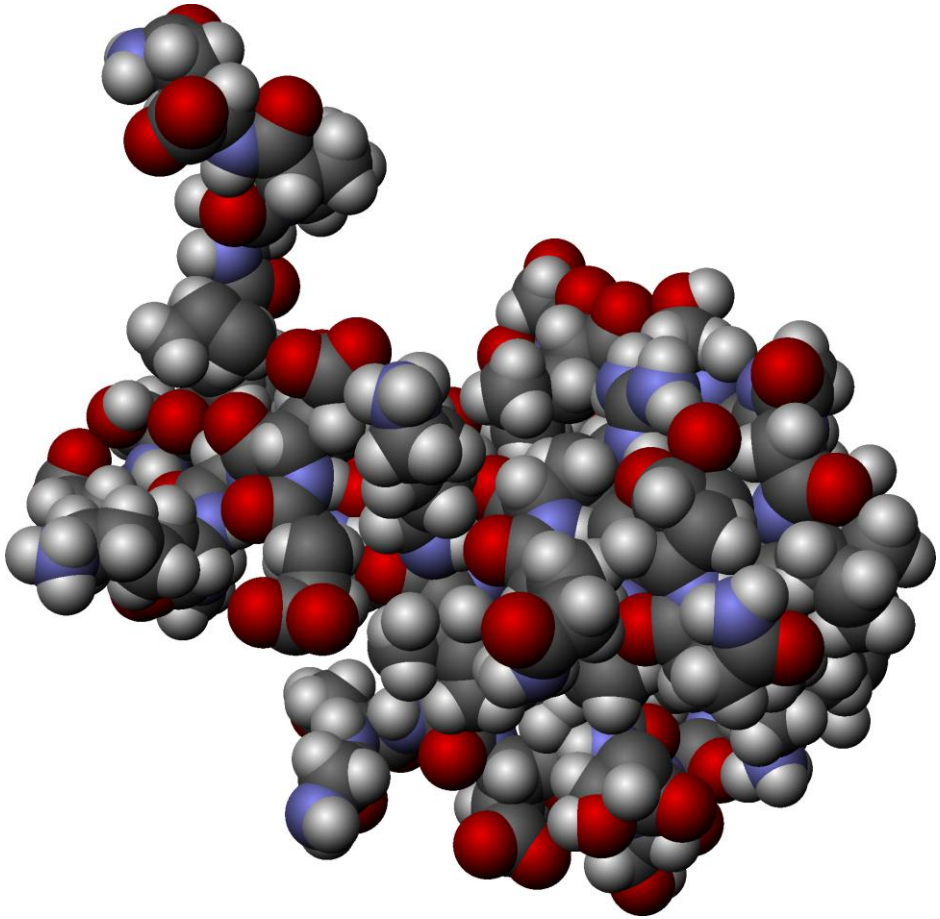
Molecular Visualization



Crystal structure of a molybdenum oxide nanowheel.
Science 327(1), January 2010

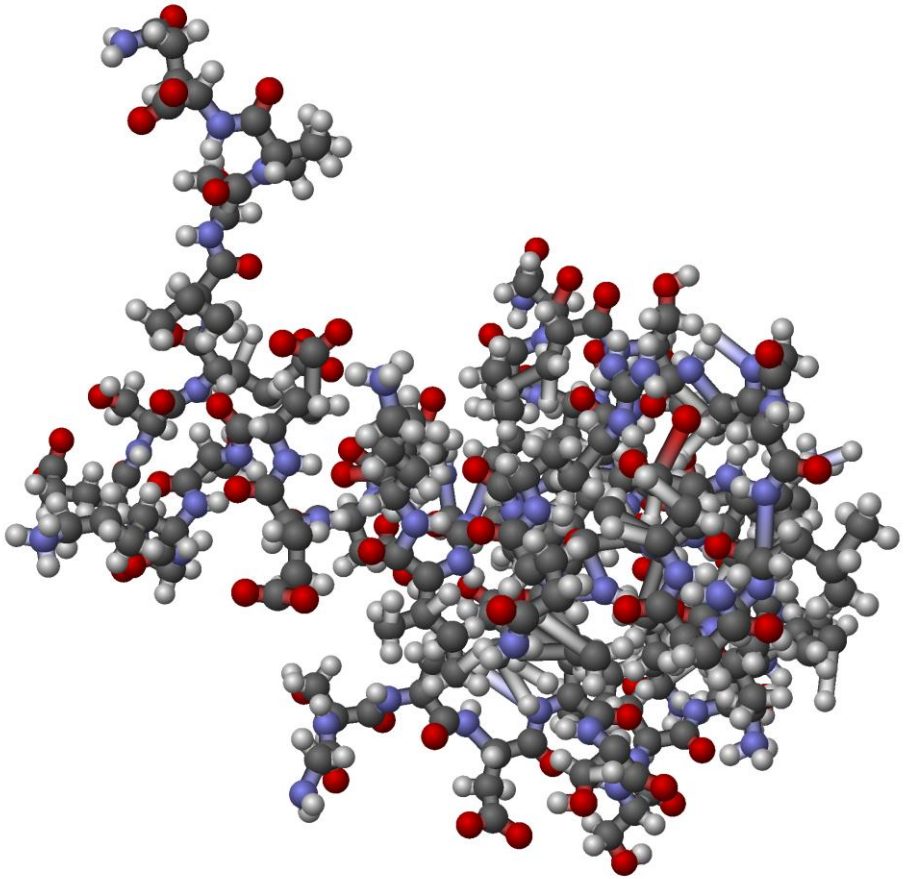
Ribbon diagram of the EspG structure.
Biochemistry 50(21)

Molecular Visualization - Structure



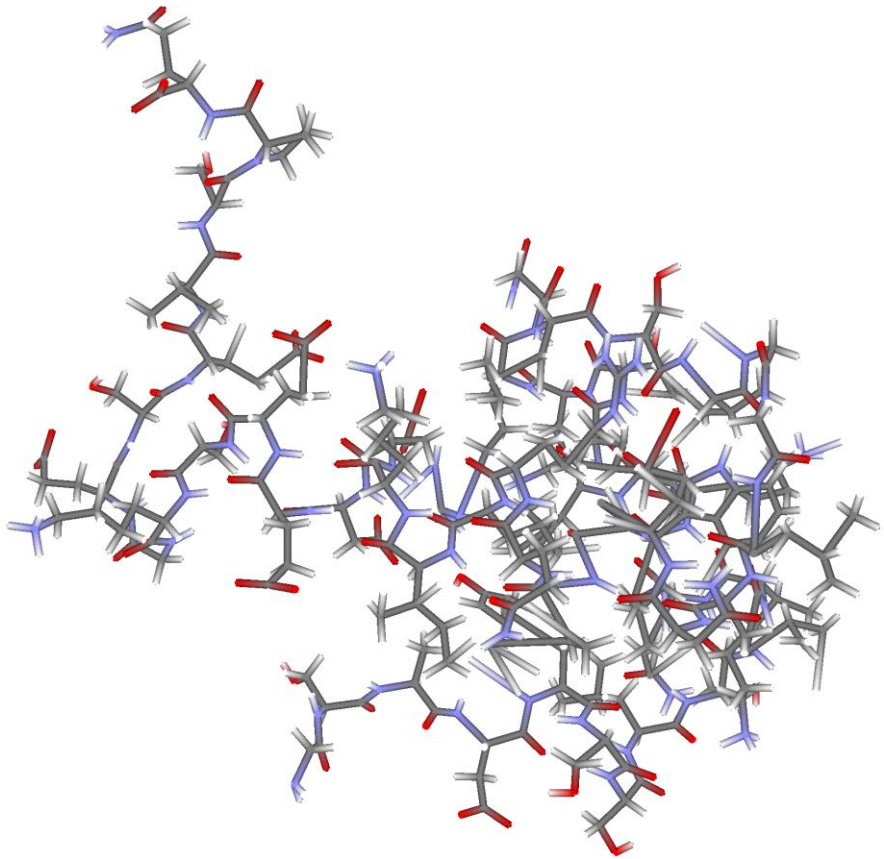
Space-fill

Molecular Visualization - Structure



Balls-and-sticks

Molecular Visualization - Structure



Licorice

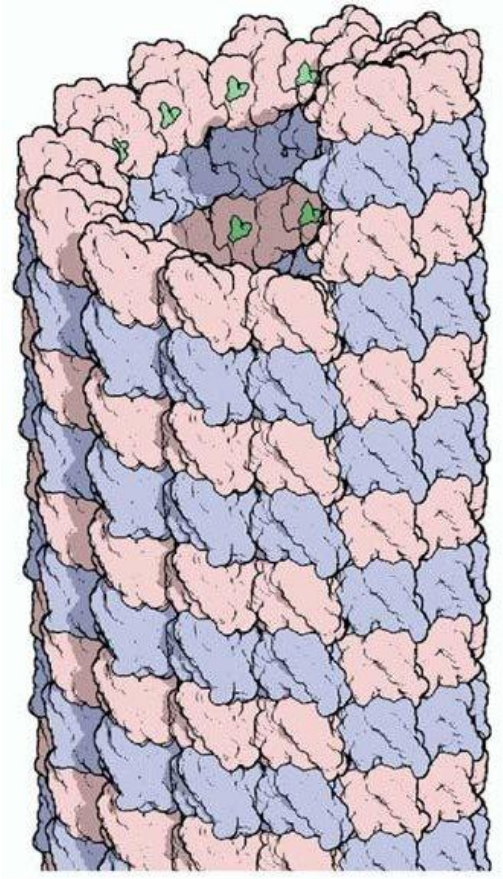
Molecular Visualization - Structure

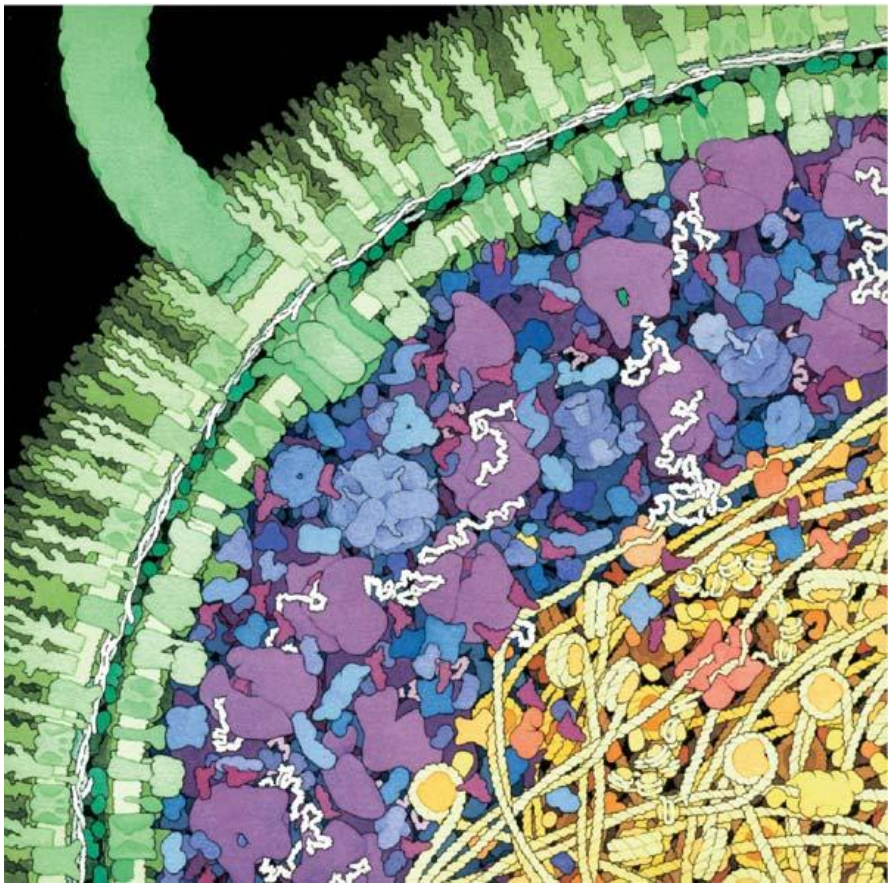
Backbone

Molecular Visualization - Structure

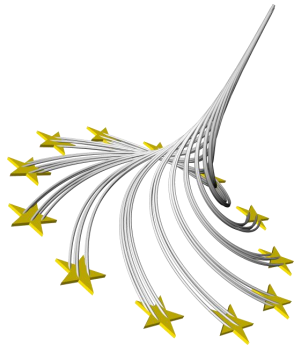
Ribbon

Molecular Visualization

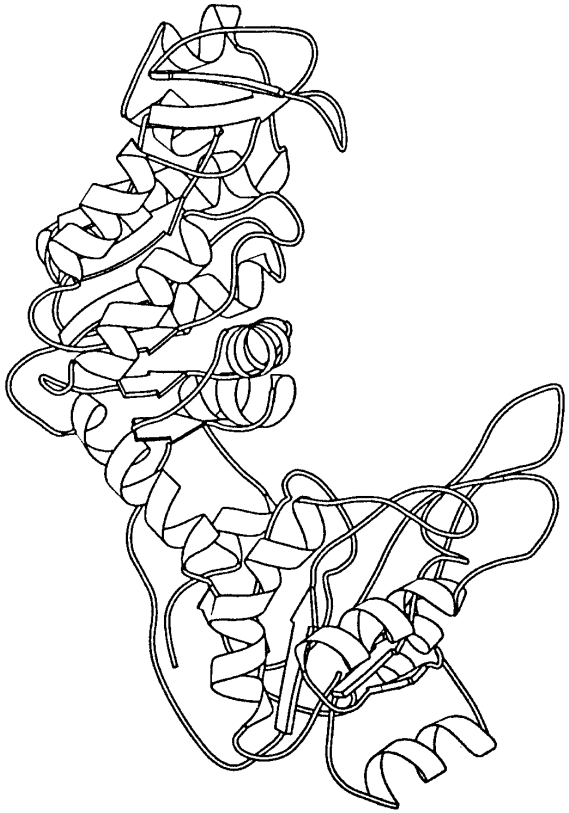




Goodsell, 2005

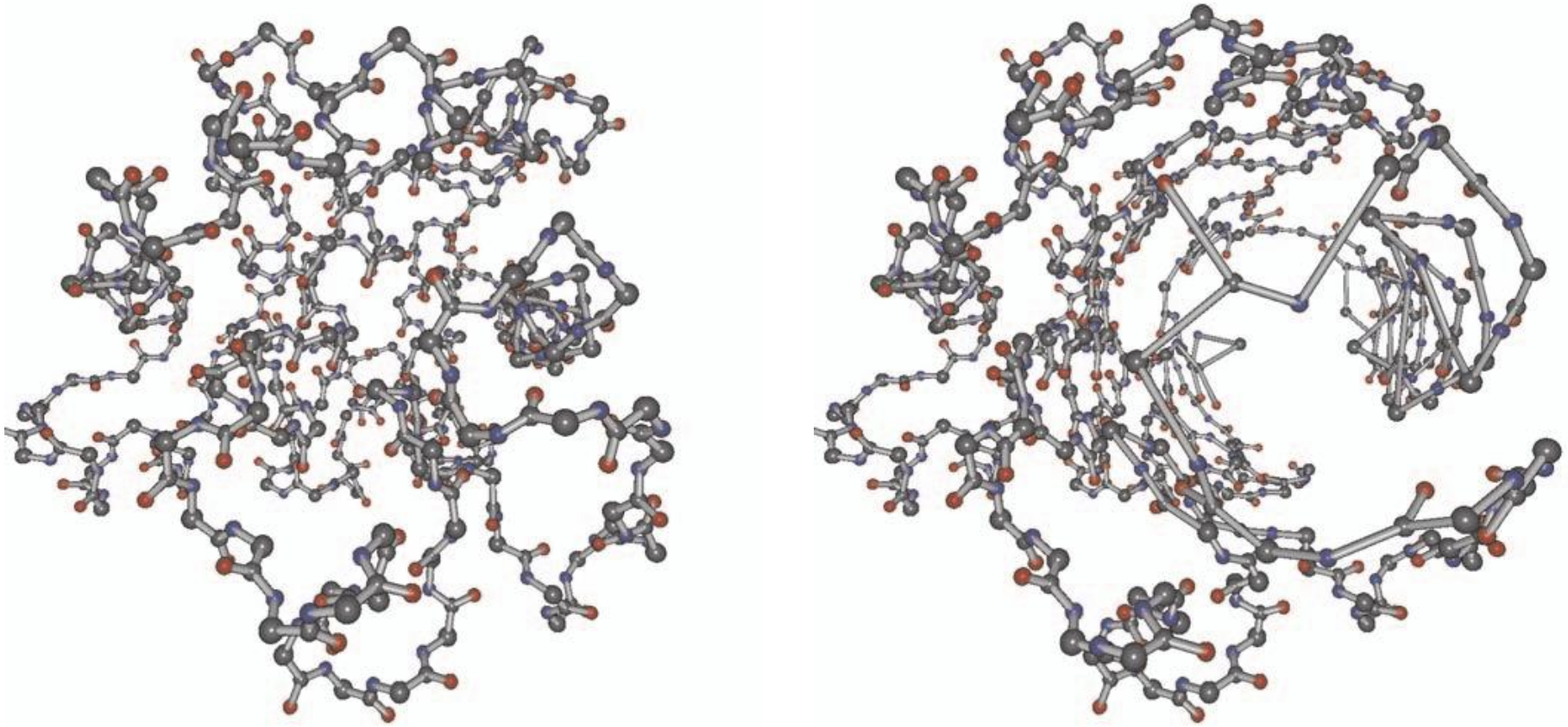


Molecular Visualization



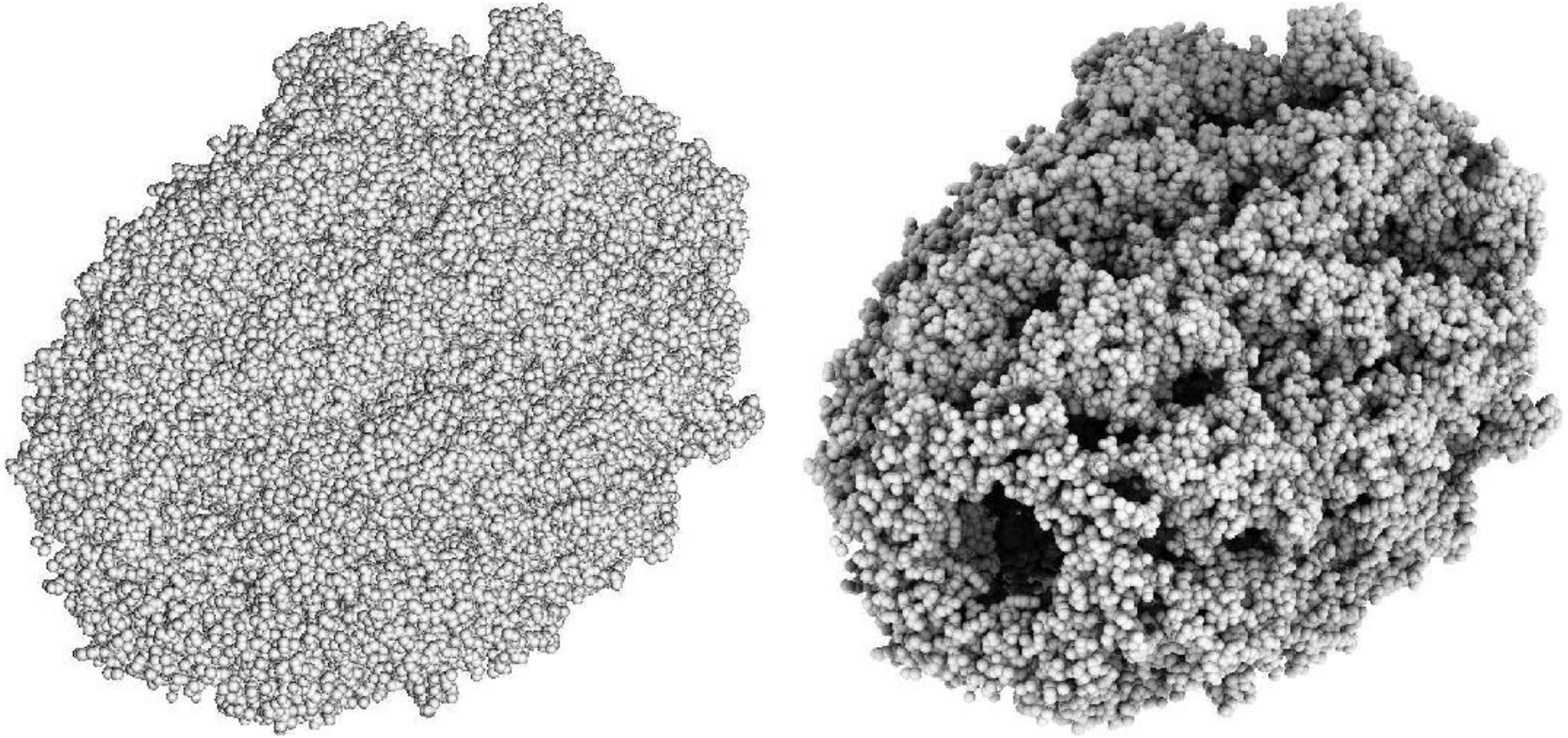
Goodsell, 2003

Structural abstraction

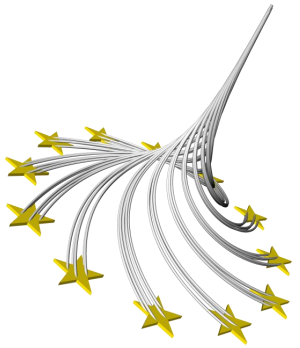


Lampe et al., 2007

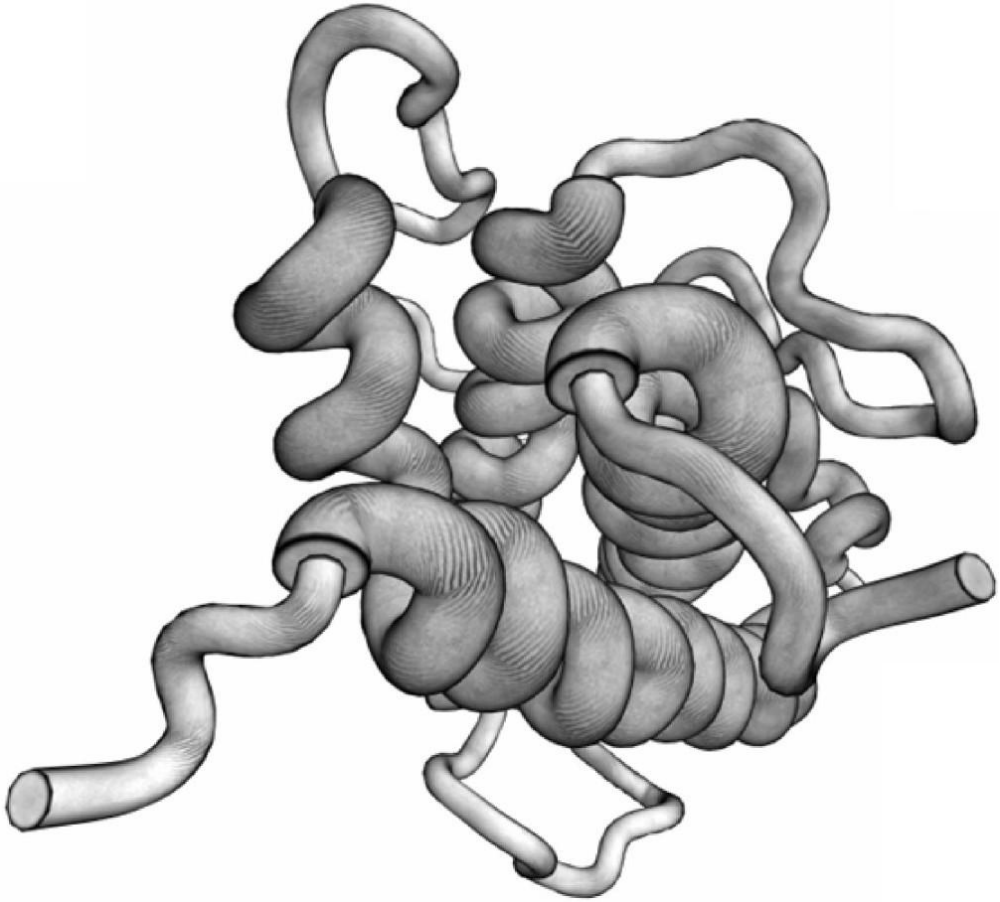
Support of spatial perception



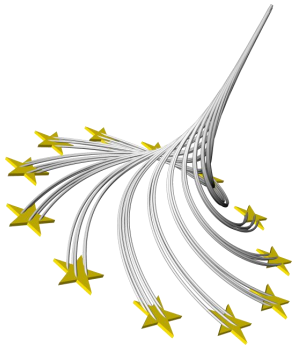
Tarini et al., 2006



Illustrative rendering



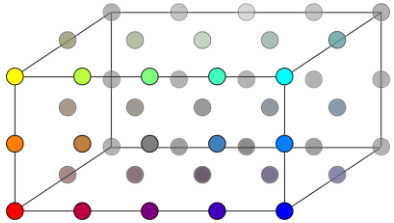
Weber, 2009

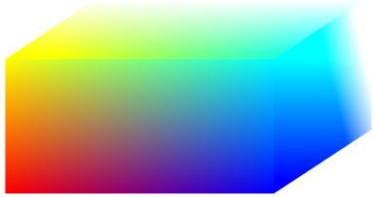


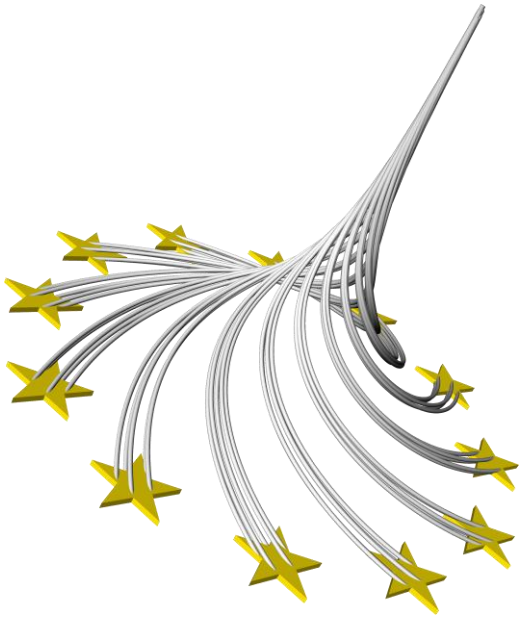
Challenges

- ***Continuous*** transition from volumetric primitives to line primitives
- Choice and order of depth cueing techniques
- Large datasets (≥ 10^4 atoms)

Abstraction Space

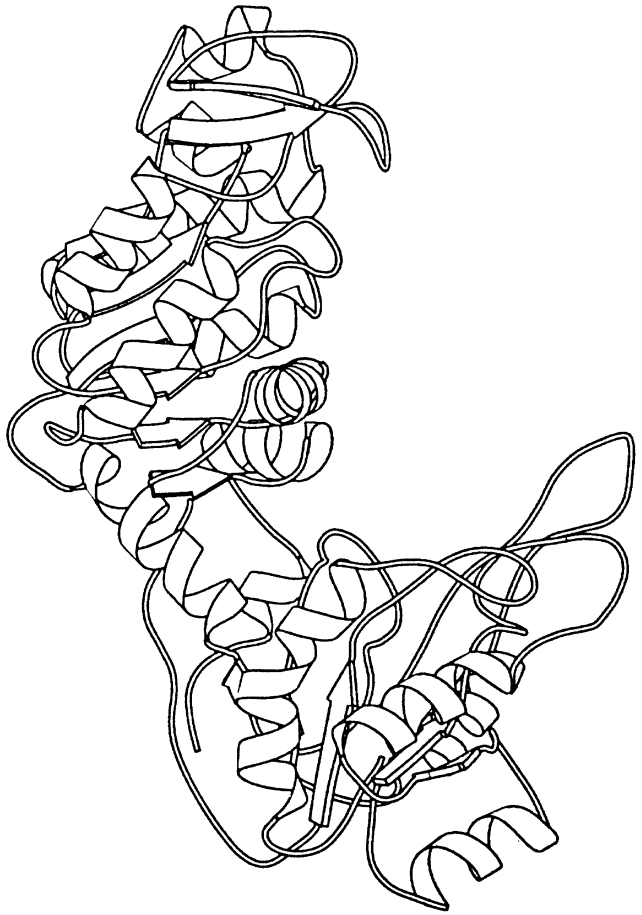






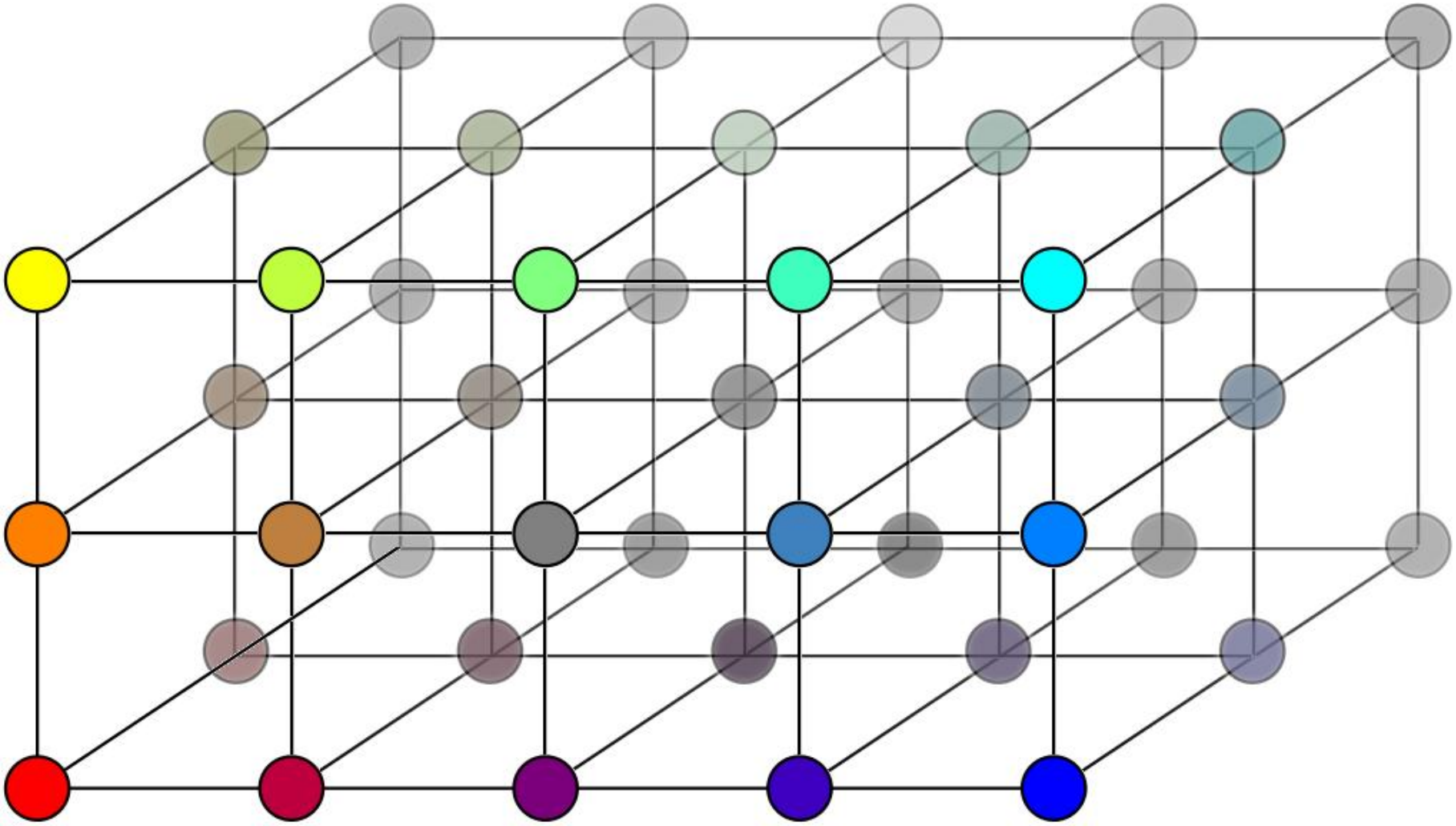
Abstraction Space

- Structural abstraction
- Abstraction through the visual style
  - Support of spatial perception
  - Illustrativeness

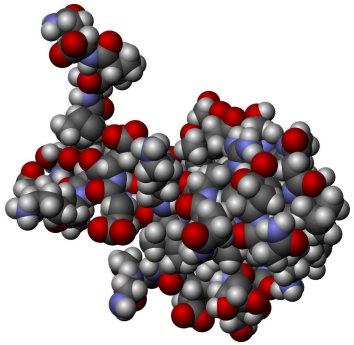


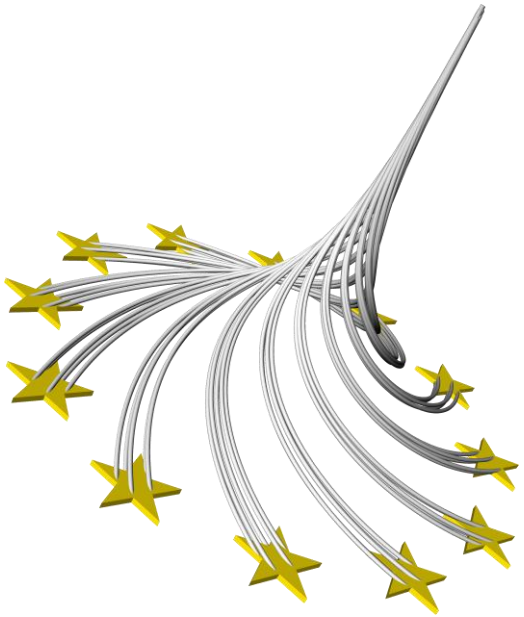
Goodsell, 2003

Continuous Abstraction Space

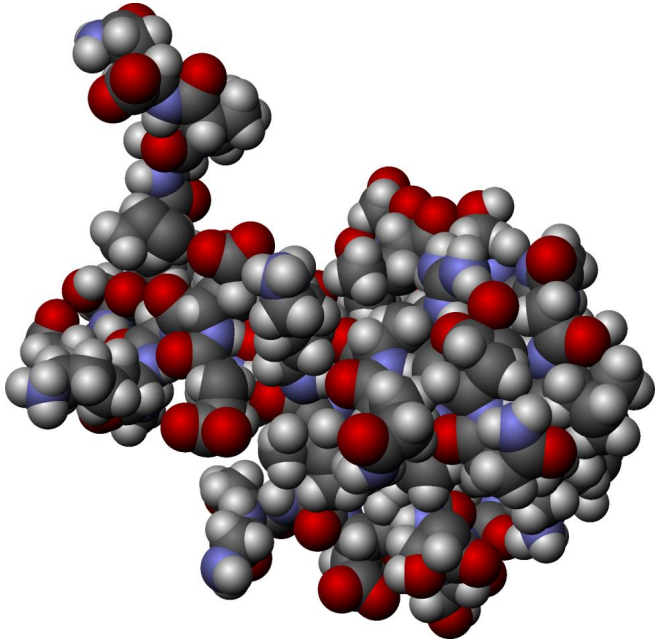


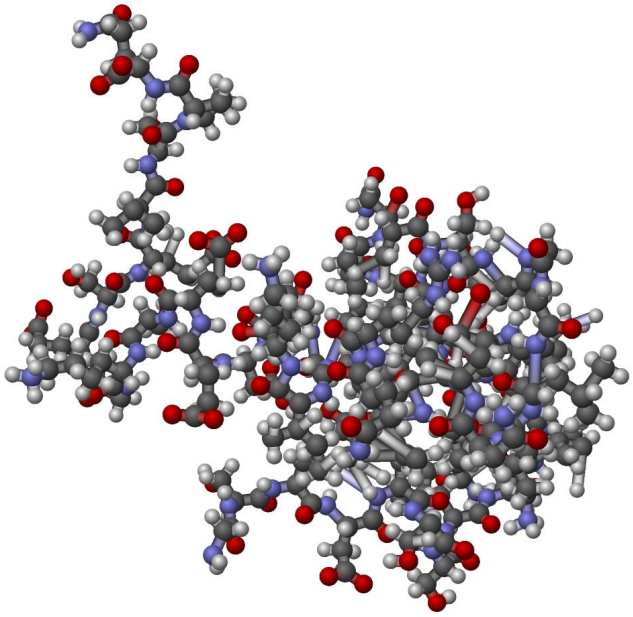
Structural abstraction



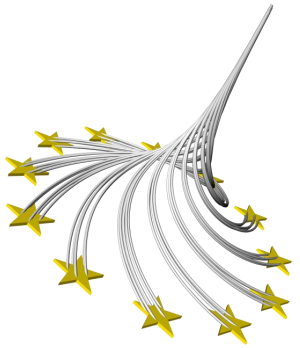


Structural Abstraction

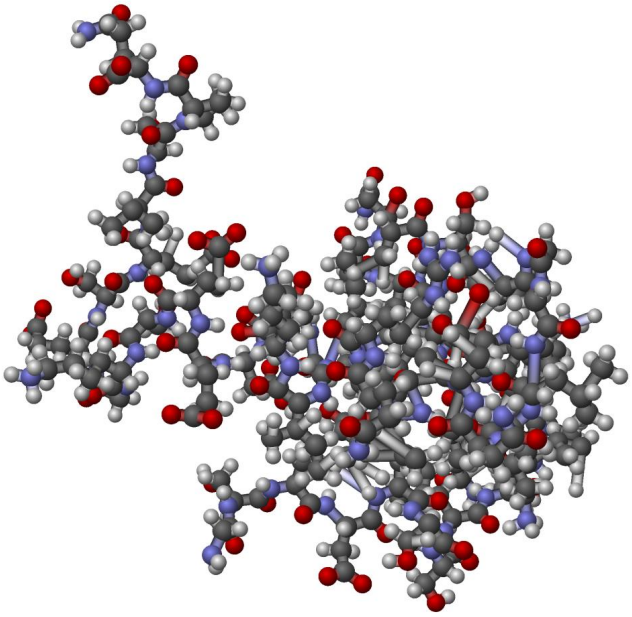


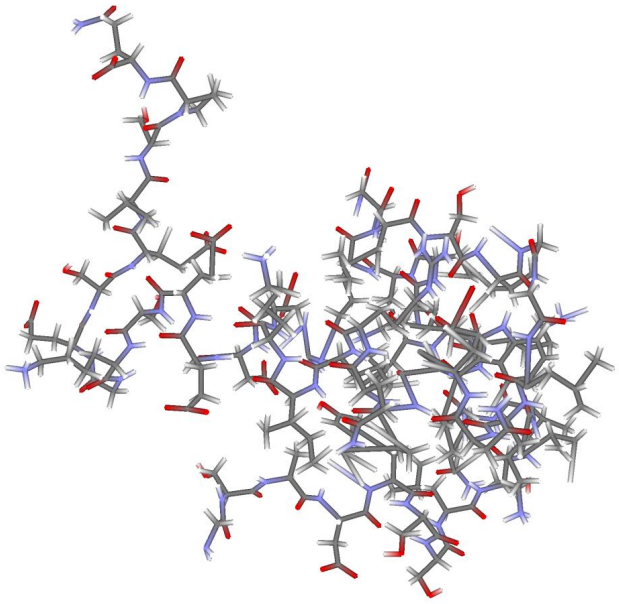


- Transition from Space-fill to balls-and-sticks
  - Reduce atom radii



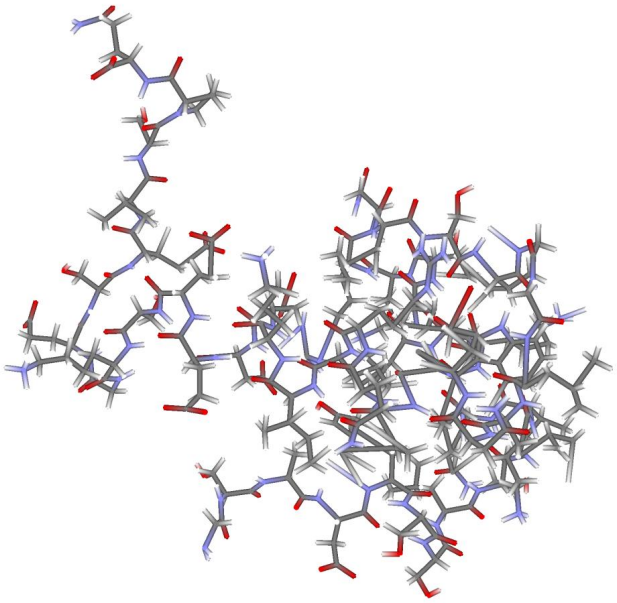
Structural Abstraction





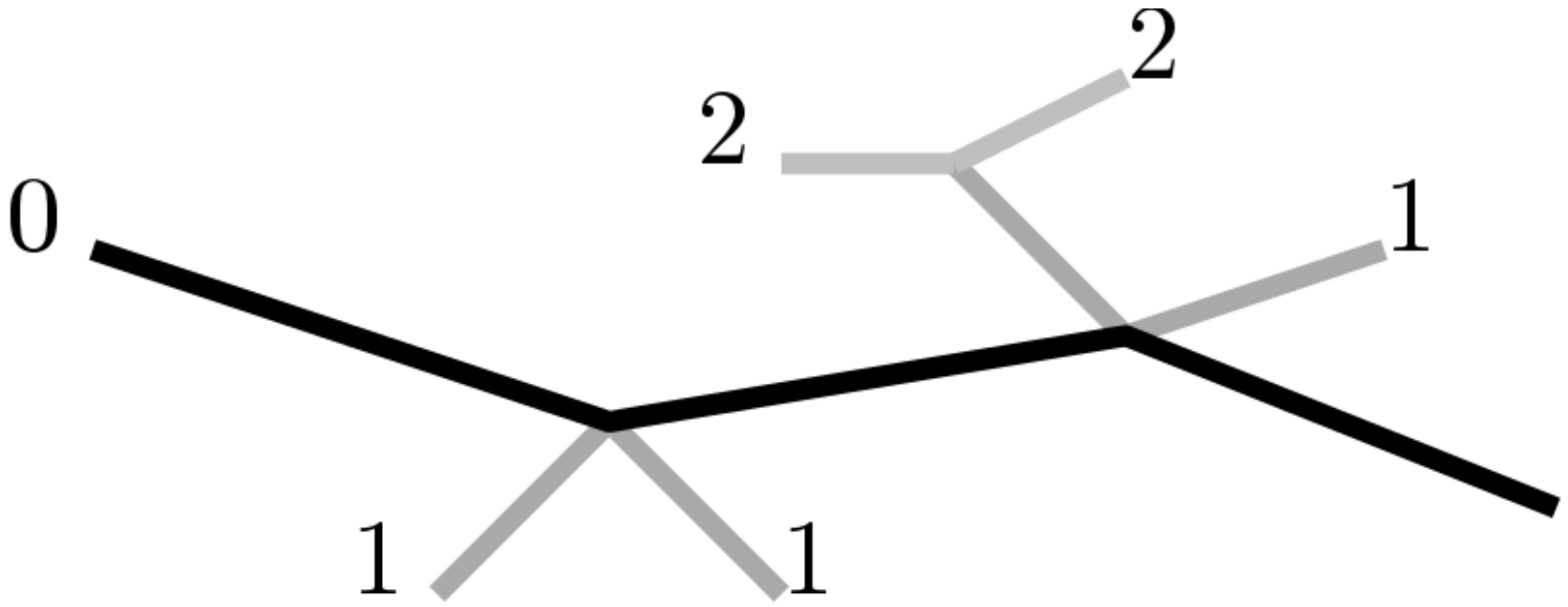
- Transition from balls-and-sticks to licorice
  - Reduce atom radii to zero and remove atoms

Structural Abstraction



- Transition from licorice to backbone
  - Remove bonds which are not part of the backbone
  - Start with bonds which are furthest away
  - Shorten bonds and remove when length is zero

Atom rank



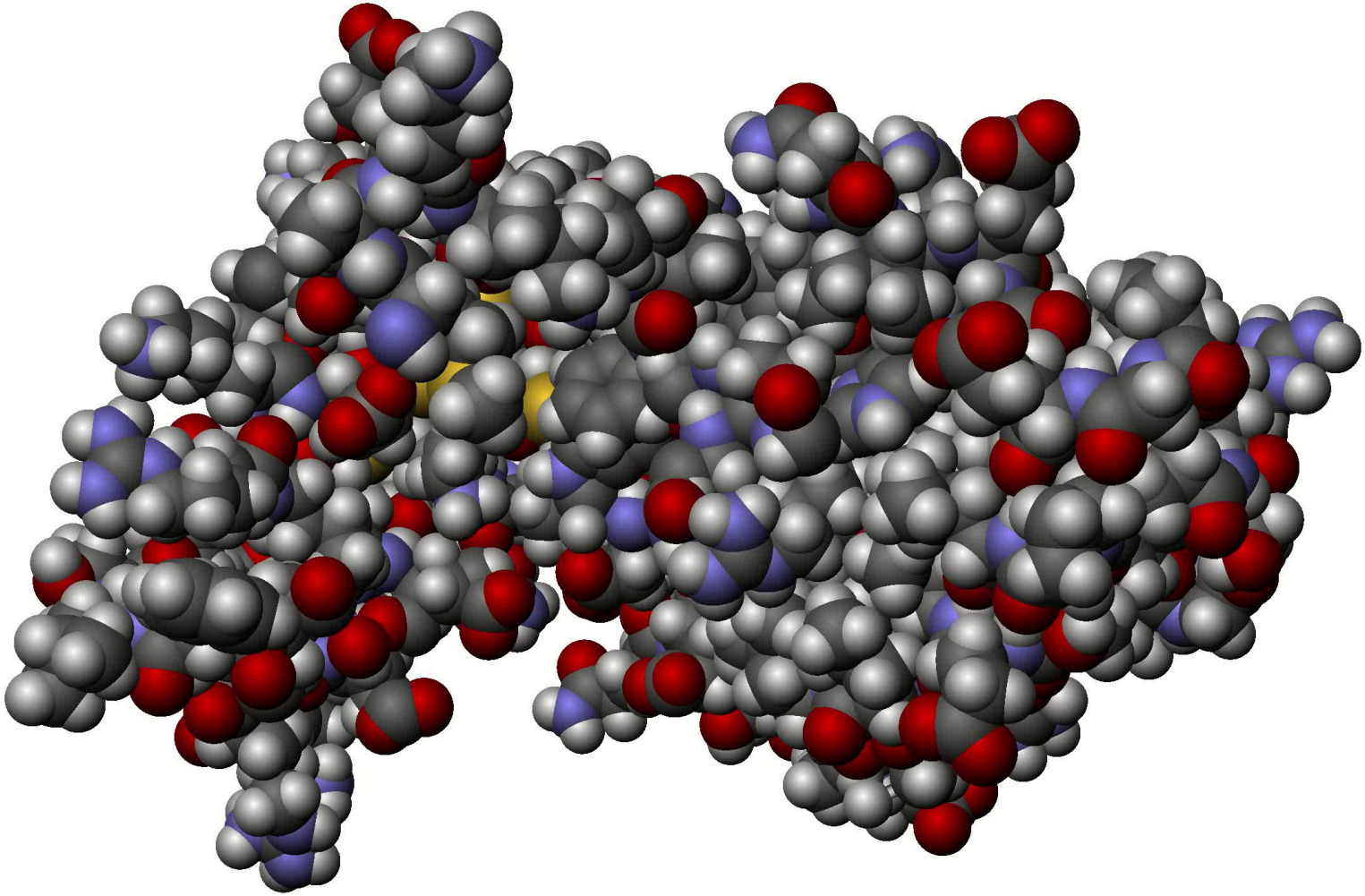
$$\text{rank}(a) = \begin{cases} 0 & \text{if } a \in \text{backbone} \\ 1 + \min_{b \in \text{conn}(a)}\{rank(b)\} & \text{else} \end{cases}$$

$\text{conn}(a)$ are all the atoms which are connected to atom a

Structural Abstraction

- Transition from backbone to ribbons
  - Interpolate between (linear) bond position and smooth ribbons
  - Also modify orientation for helices

Structural Abstraction



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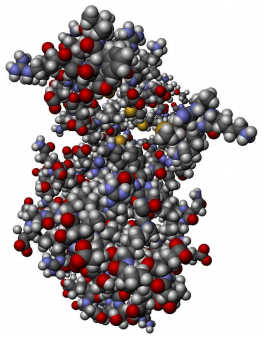
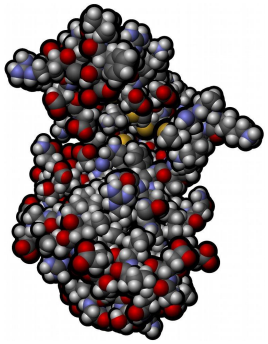
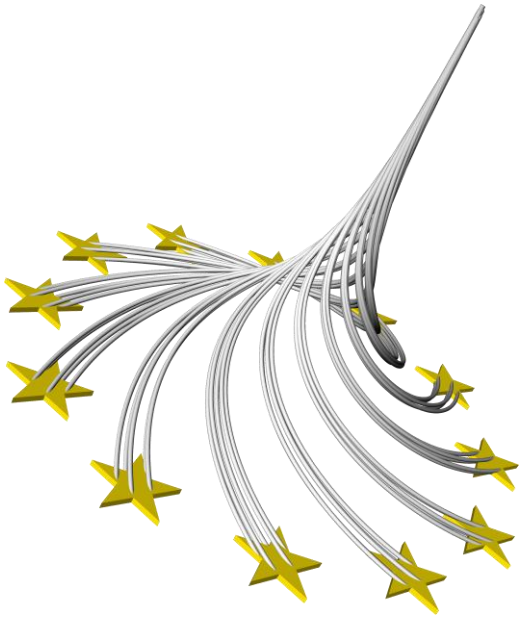
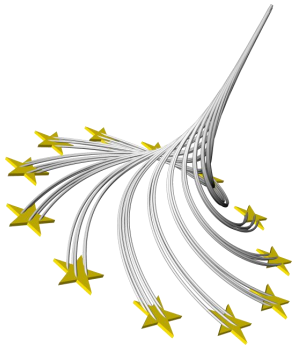
Support of spatial perception

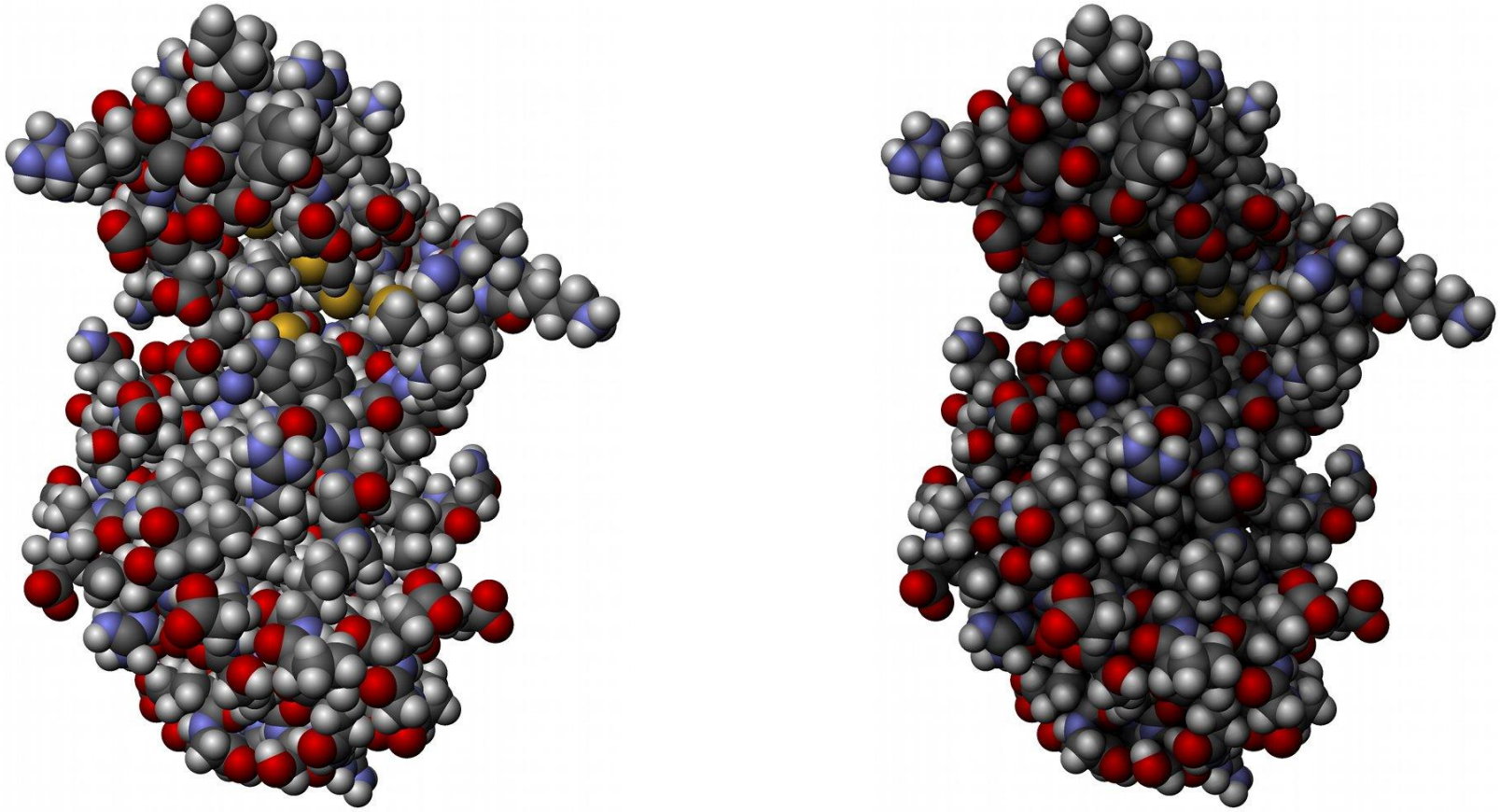






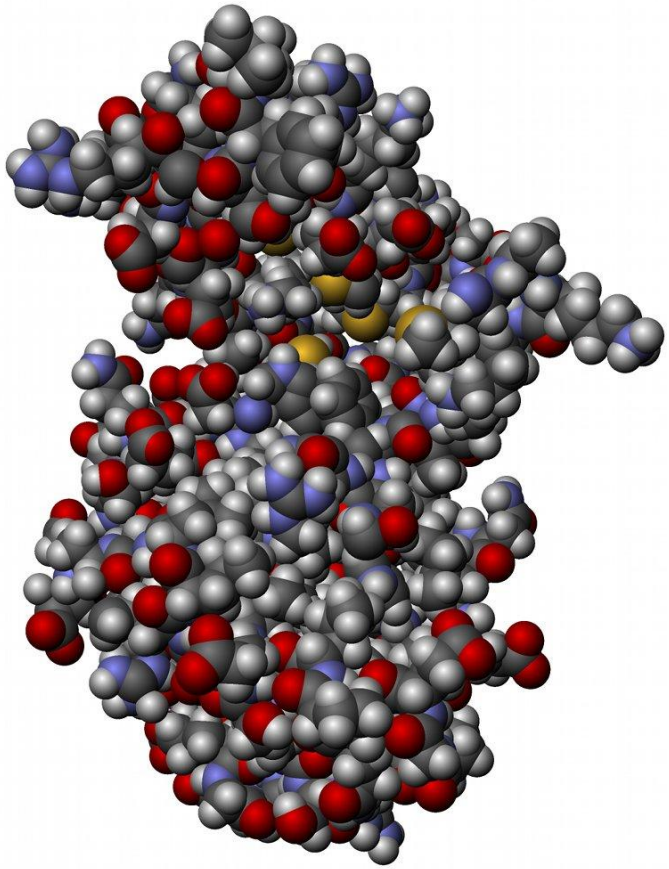


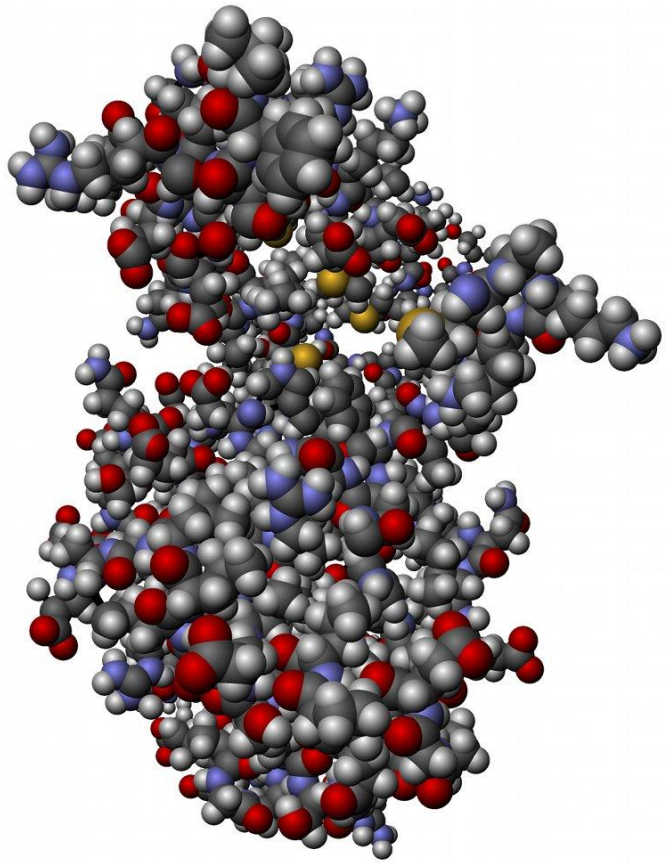
Ambient Occlusion



Following Tarini et al., 2006

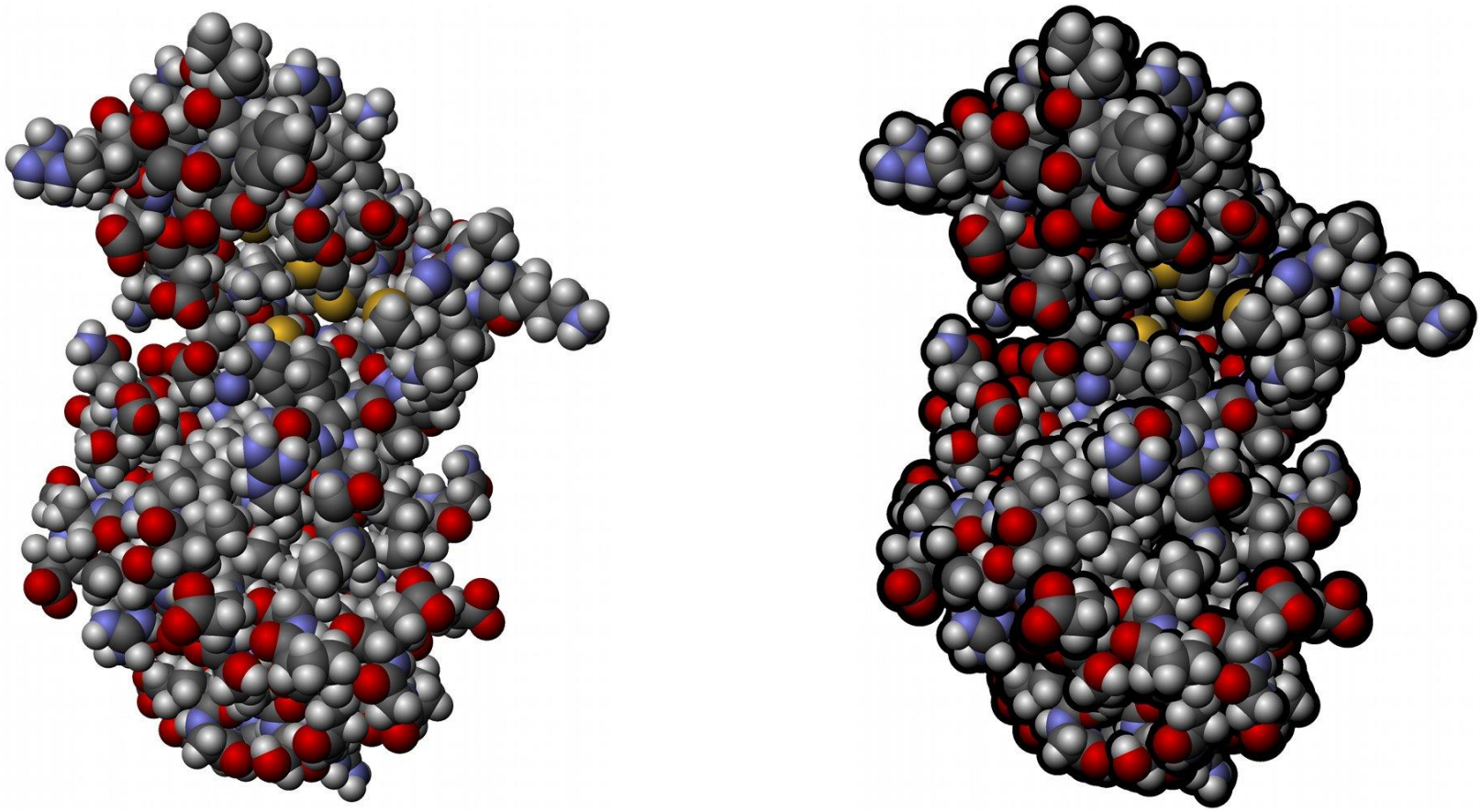
Object attenuation / Dolly zoom





Following Everts et al., 2009

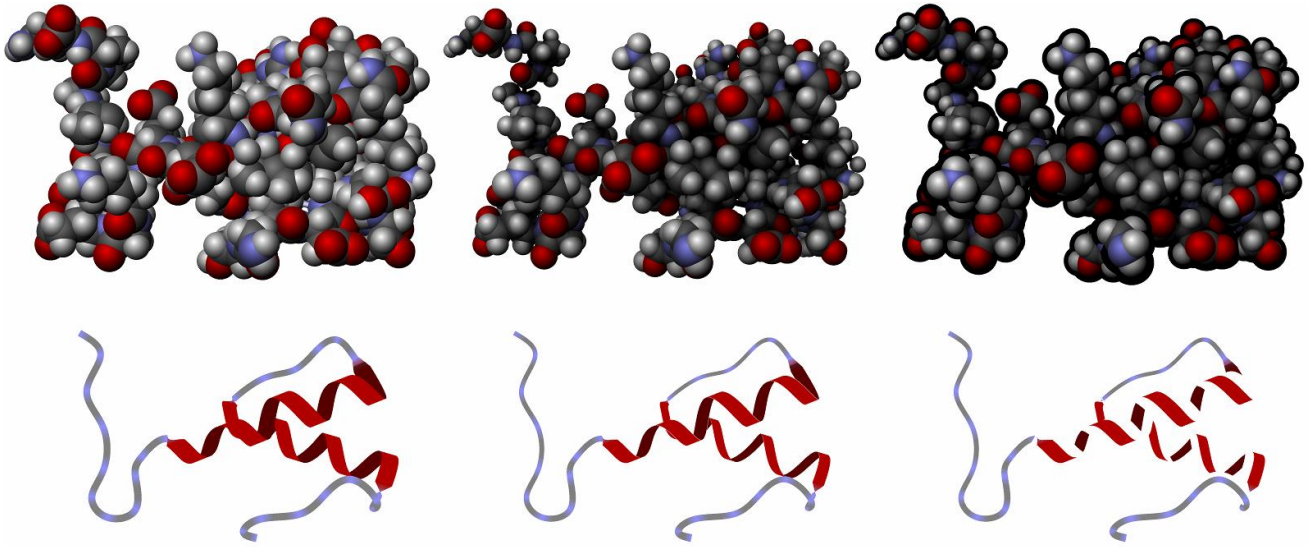
Halos



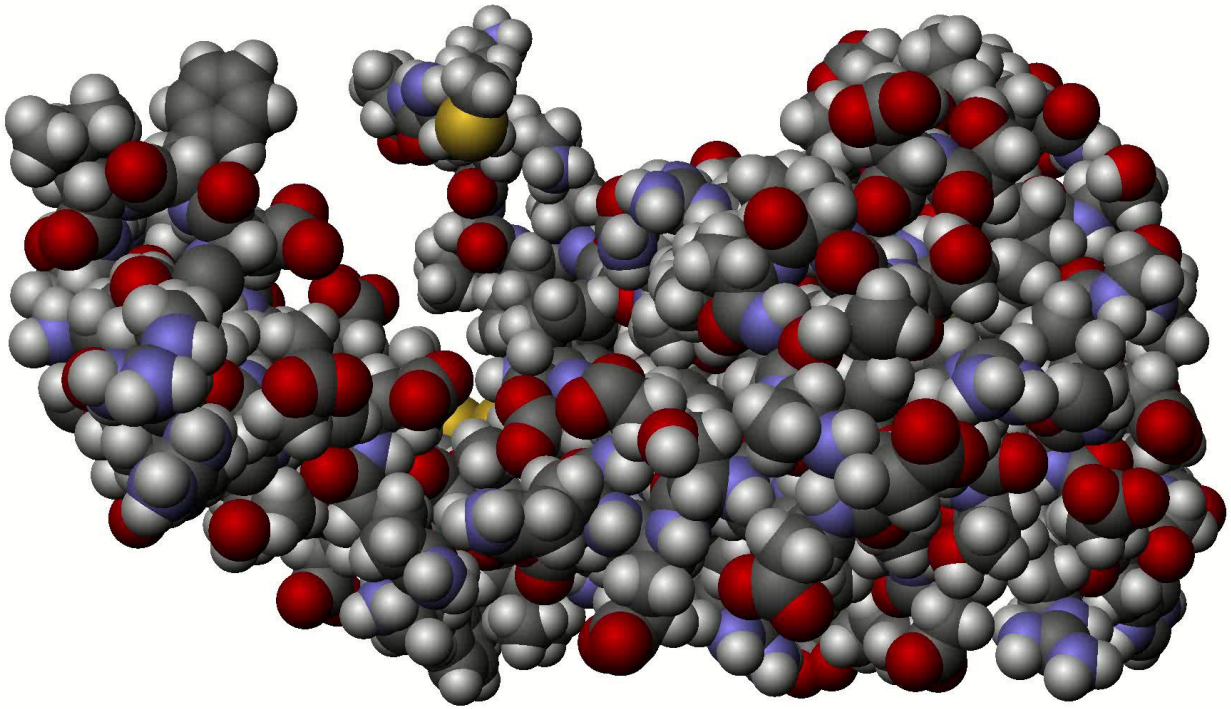
Following Tarini et al., 2006 and Everts et al., 2009

Ordering of effects

- Apply halos last, because of blocking effect
- Combine ambient occlusion and object attenuation/dolly zoom to avoid gaps in the abstraction space



Support of spatial perception



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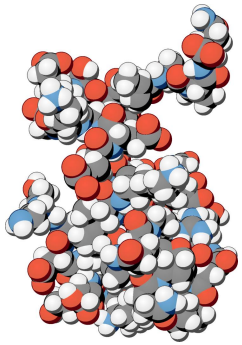
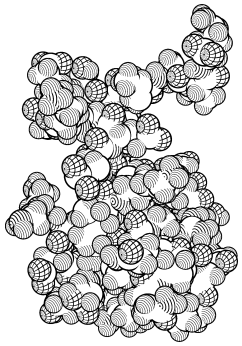
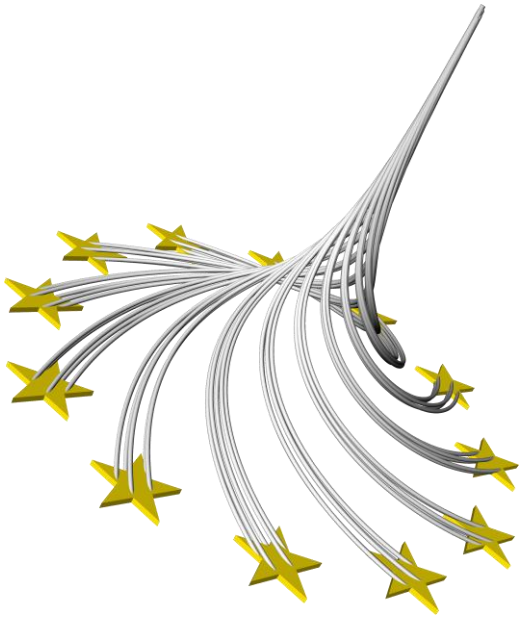
‘Illustrativeness’

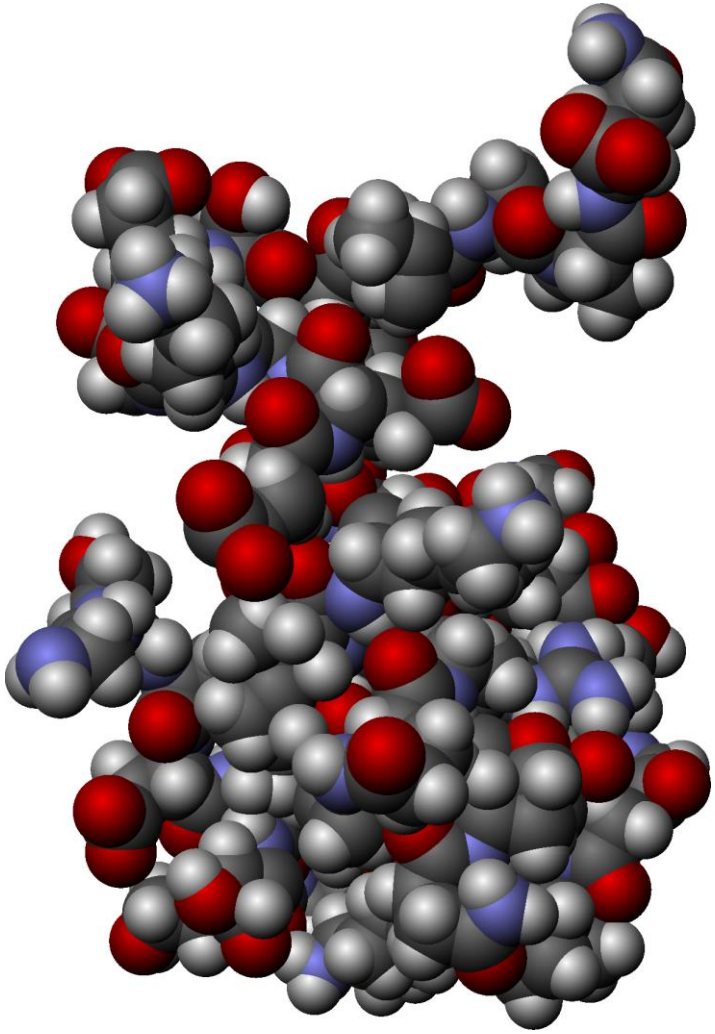






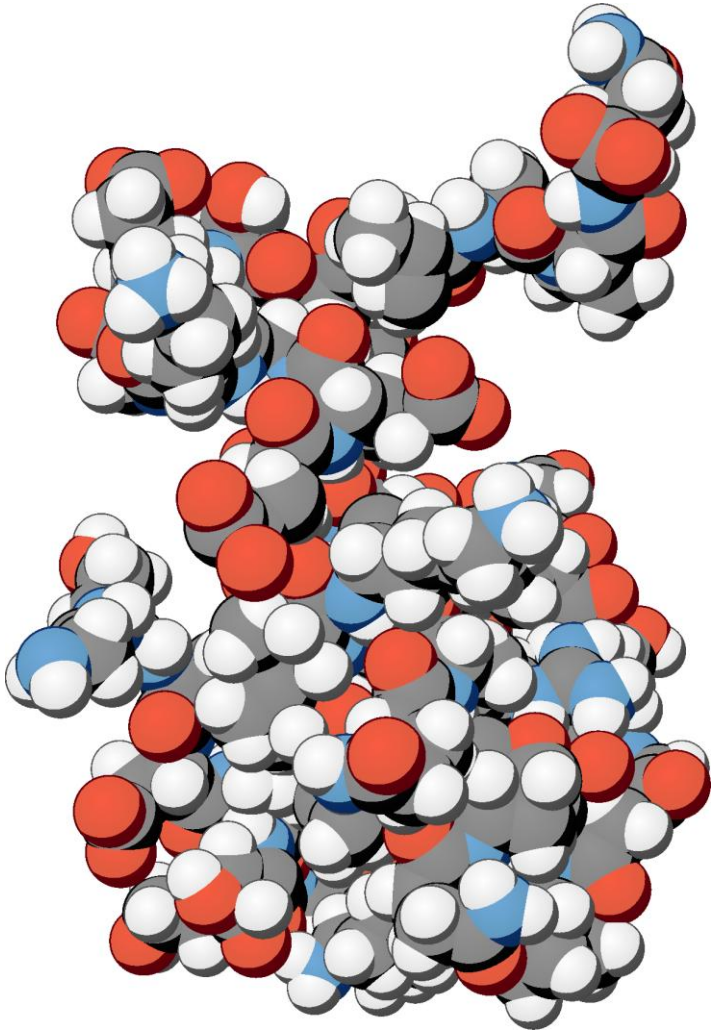
Photorealistic

- Realistic shading
- Colors indicate atom type
- *“Normal” visualization*



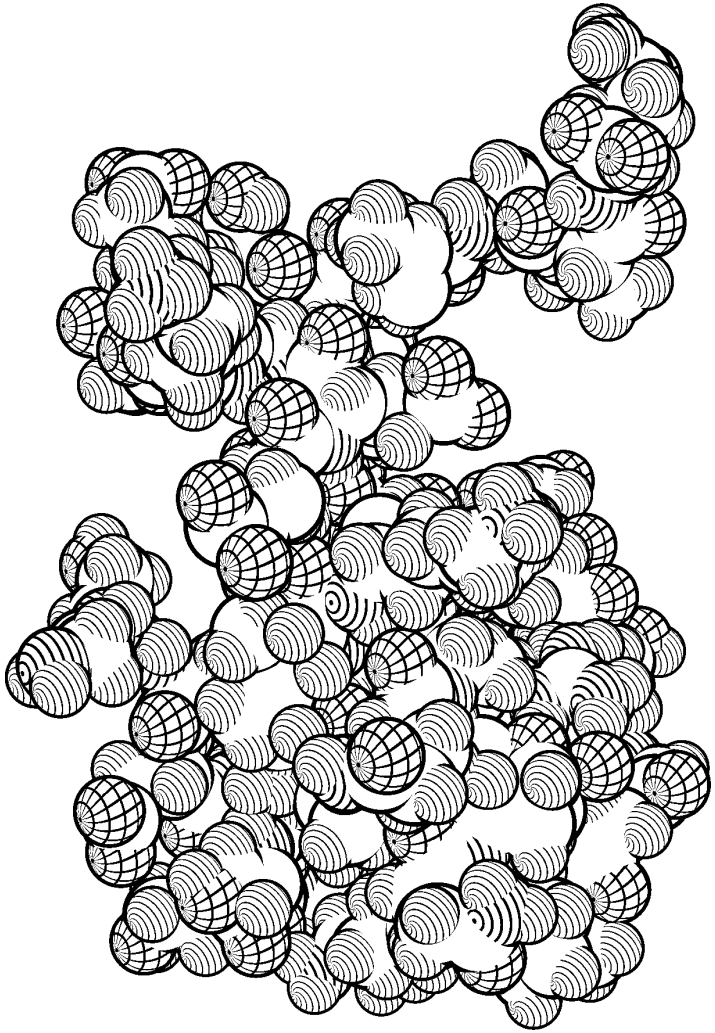
Cartoon

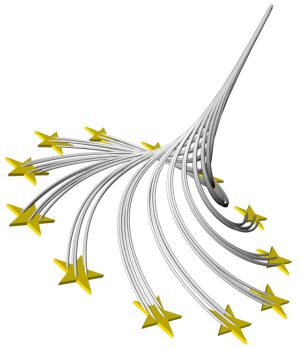
- Cel shading
- Pastel colors based on the photorealistic colors
- Colors indicate atom types
- *Shows less details*
- *Flattens the image, shows overall shape of molecule*



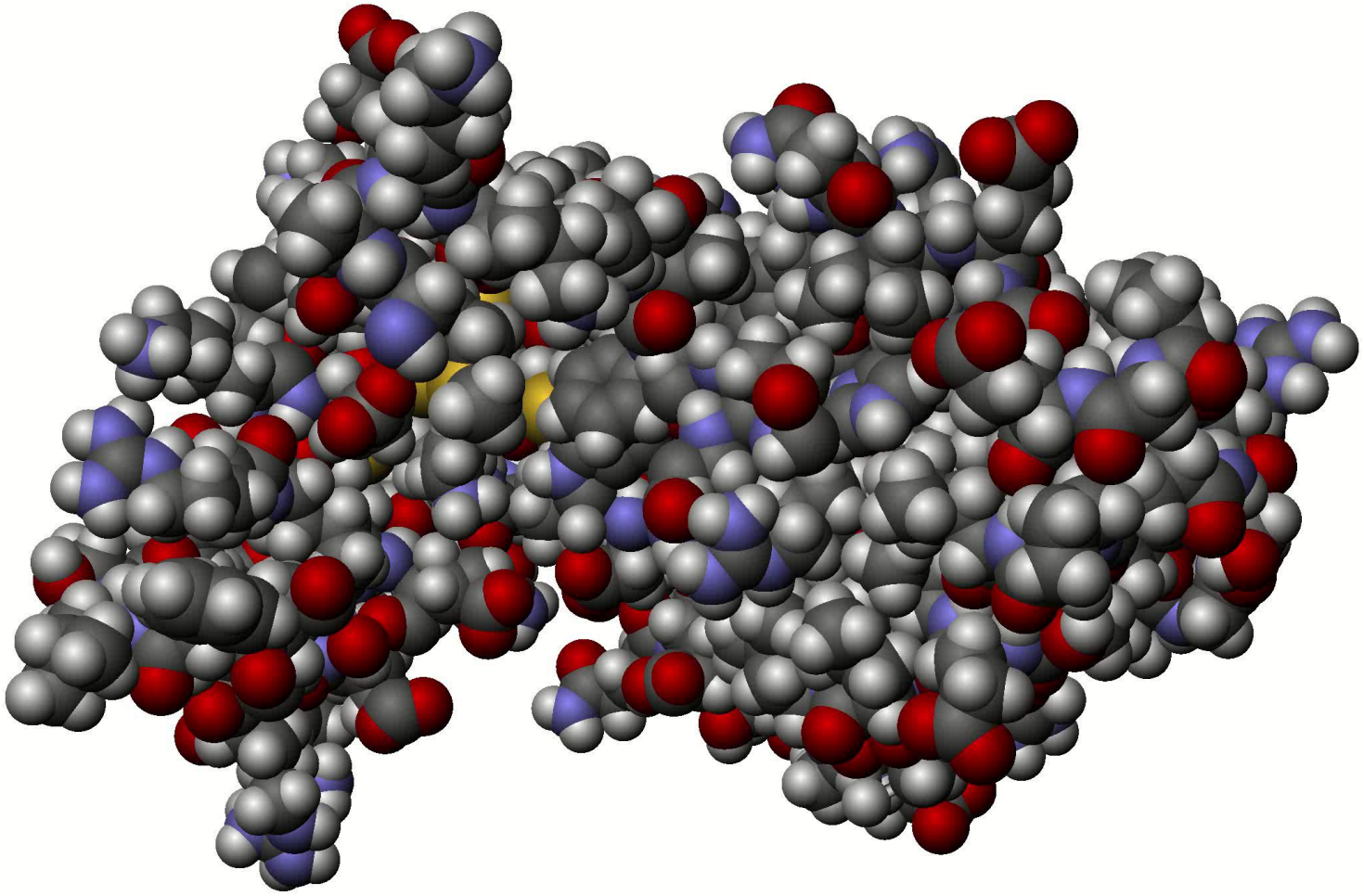
Black-and-white

- Flat shading
- Hatching patterns indicate atom types
- *For black-and-white printing*
- *Black-and-white and intermediate stages for visual de-emphasis*





Visual Style - Illustrativeness



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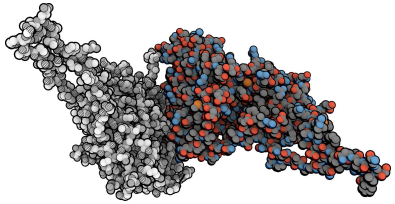
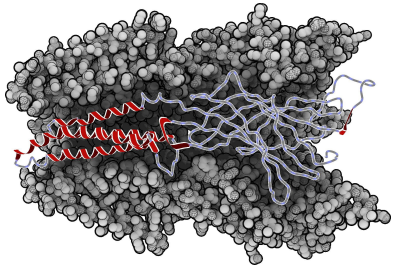
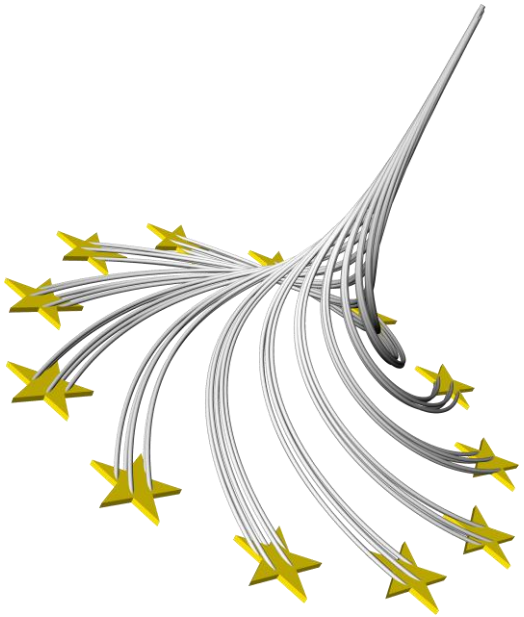
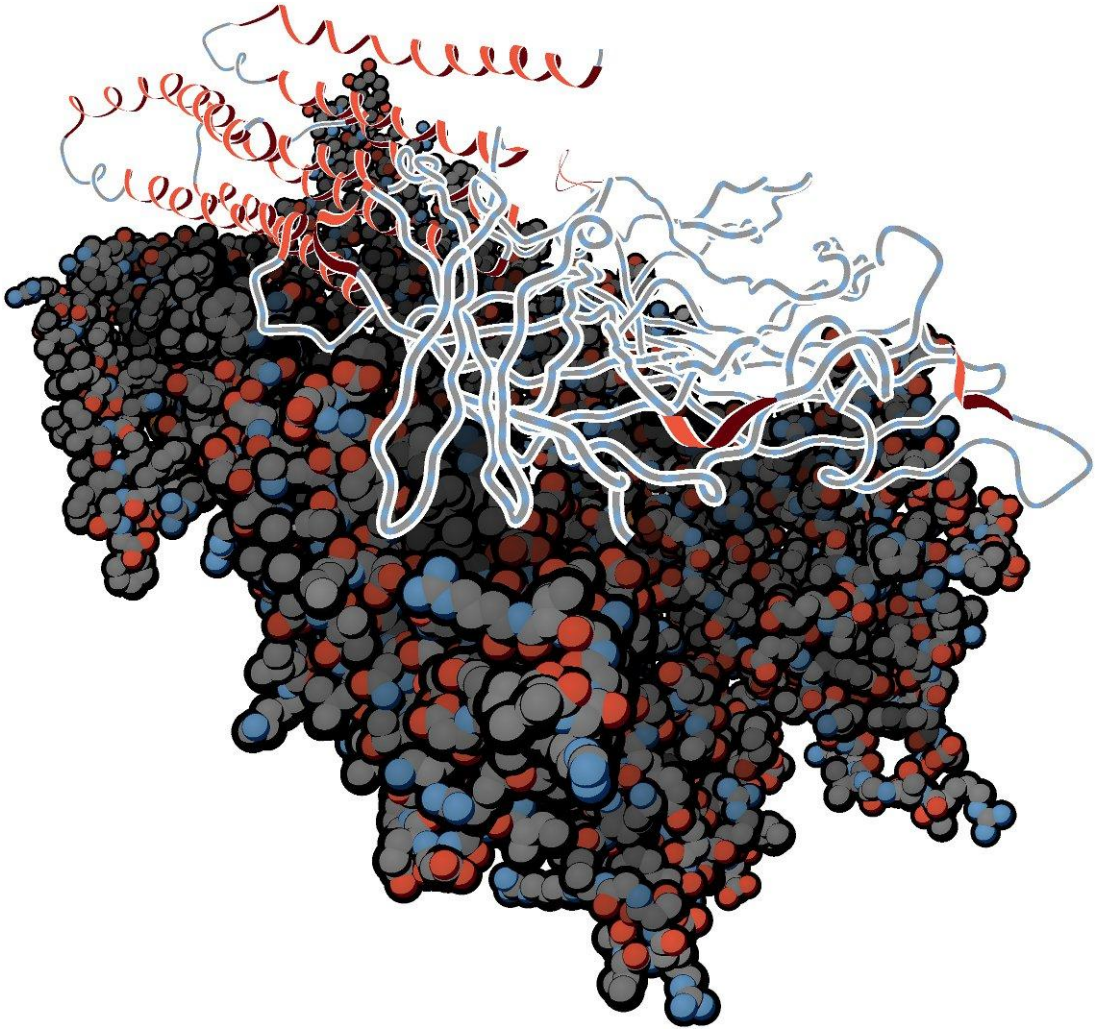
Beyond global abstraction



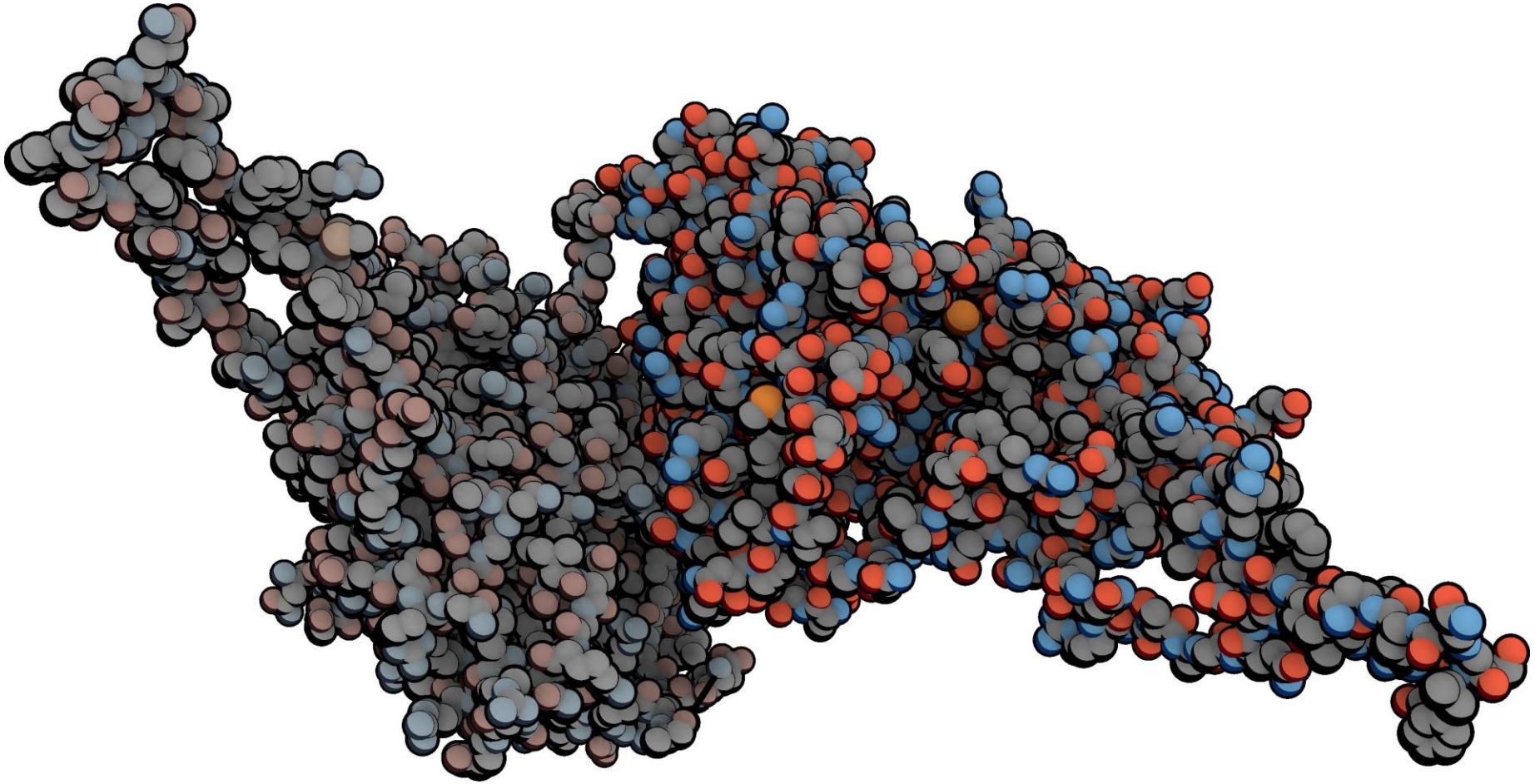




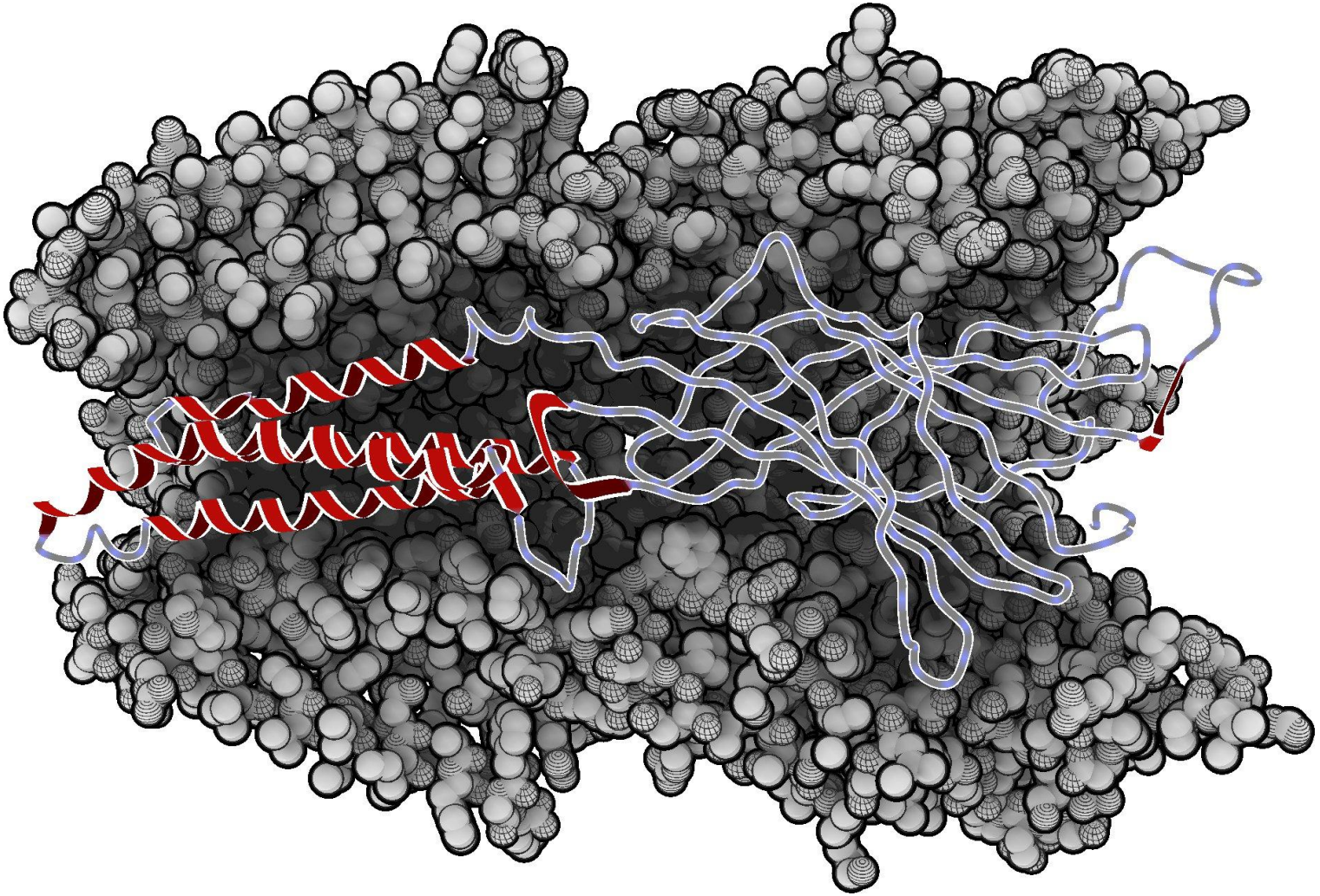
Local structural abstraction

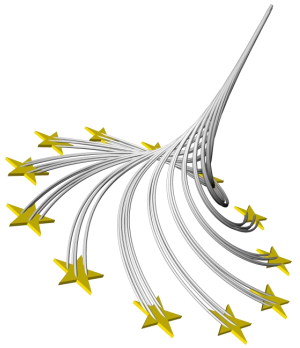


Local ‘illustrativeness’



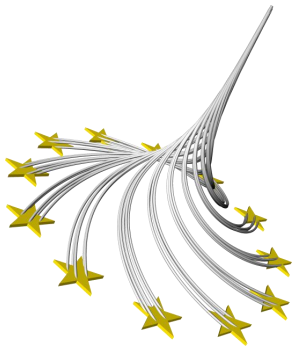
Focus and context





Feedback

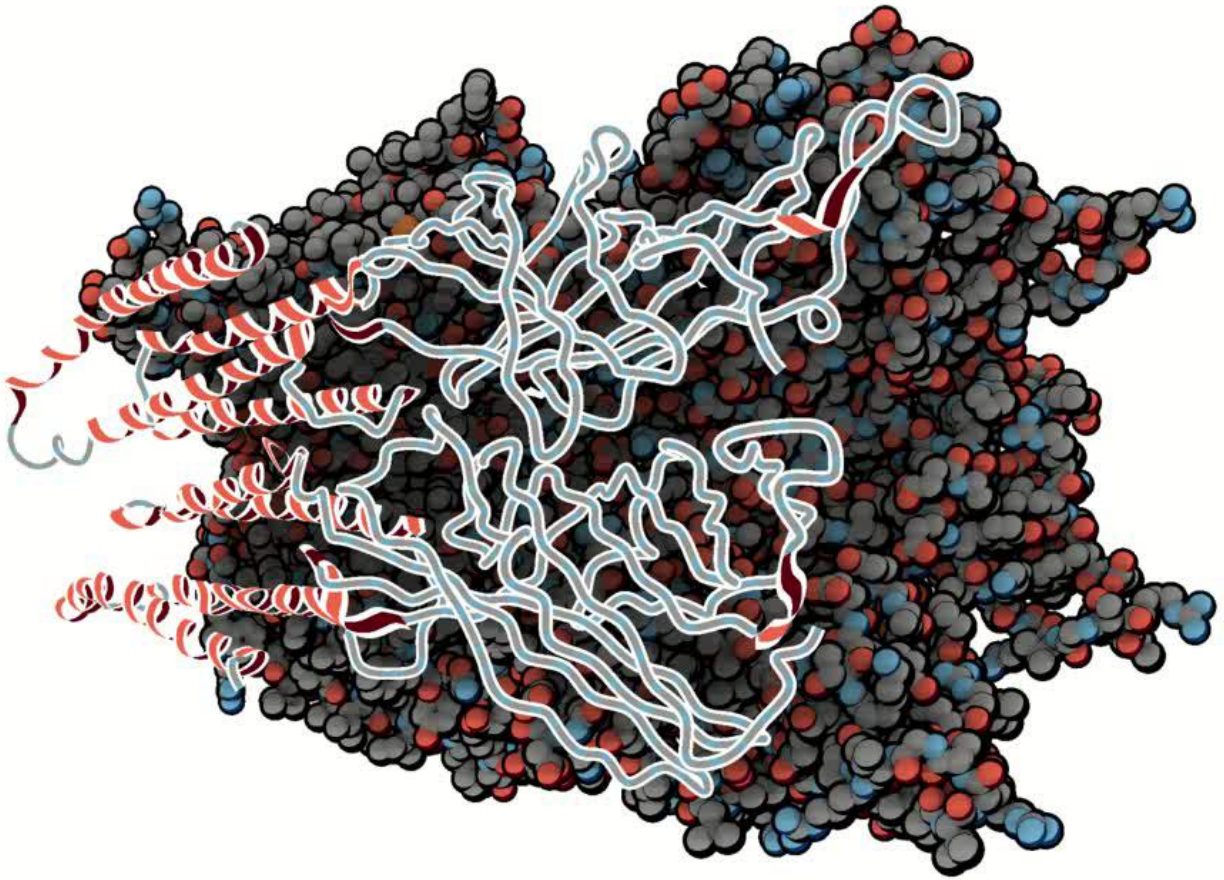
- Combining styles prefered over blending
- Continuity is useful for teaching
- Intermediate stages might provide new inside
- Easier than PyMol



Contributions

- Abstraction space for molecular visualization
- Seamless transformation of
  - Structural abstraction
  - Support of spatial perception
  - ‘Illustrativeness’
- GPU shader implementation of transitions
- Dedicated interactive control of abstraction in illustrative visualization

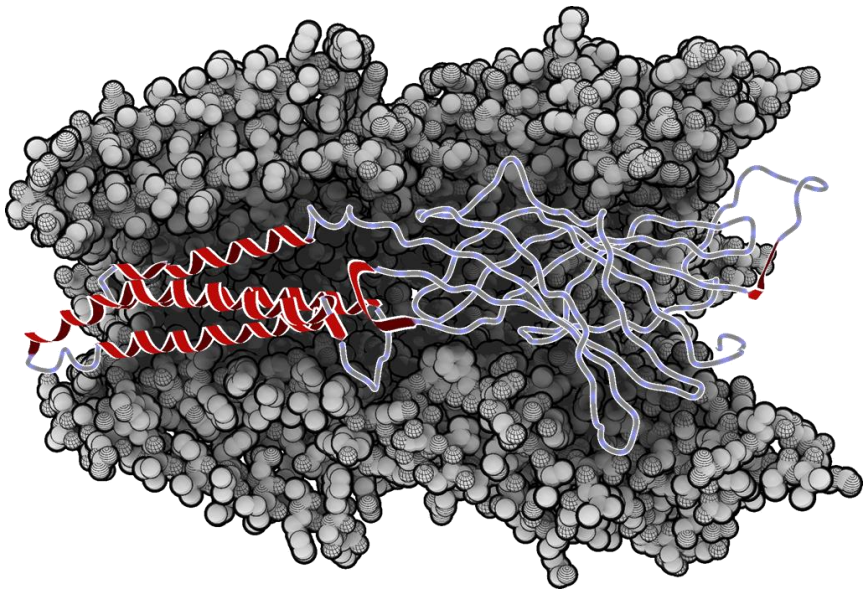
Result



EuroVis 2011

Illustrative Molecular Visualization with Continuous Abstraction

Matthew van der Zwan
Wouter Lueks
Henk Bekker
Tobias Isenberg



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