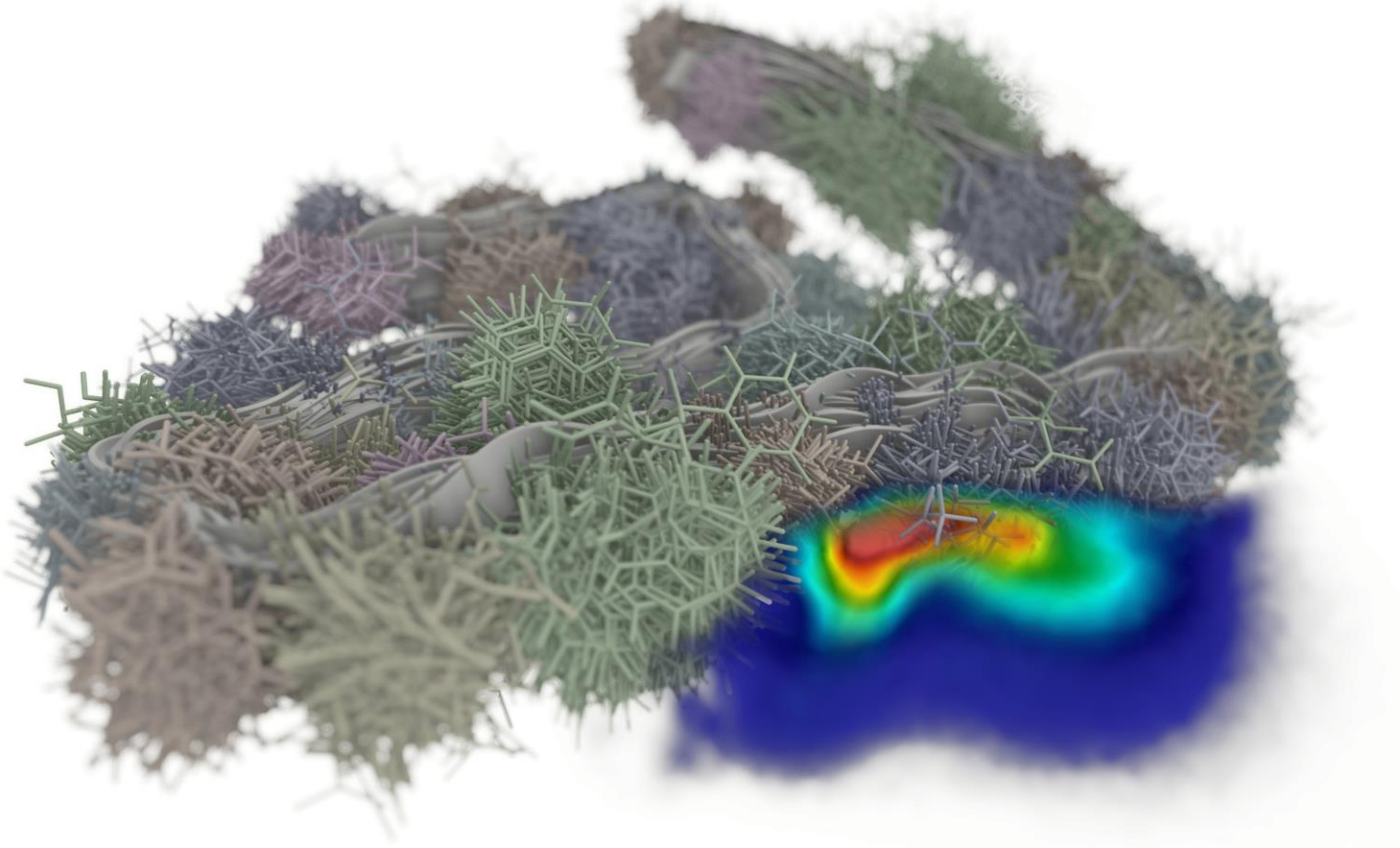
Visual Interactive Analysis of Molecular Dynamics



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(1) Scientific Visualization Group, Dept. of Science and Technology (LIU, Linköping, Sweden)
(2) PDC Supercomputer Center (KTH, Stockholm, Sweden)

LINKÖPINGS UNIVERSITET

bioexcel

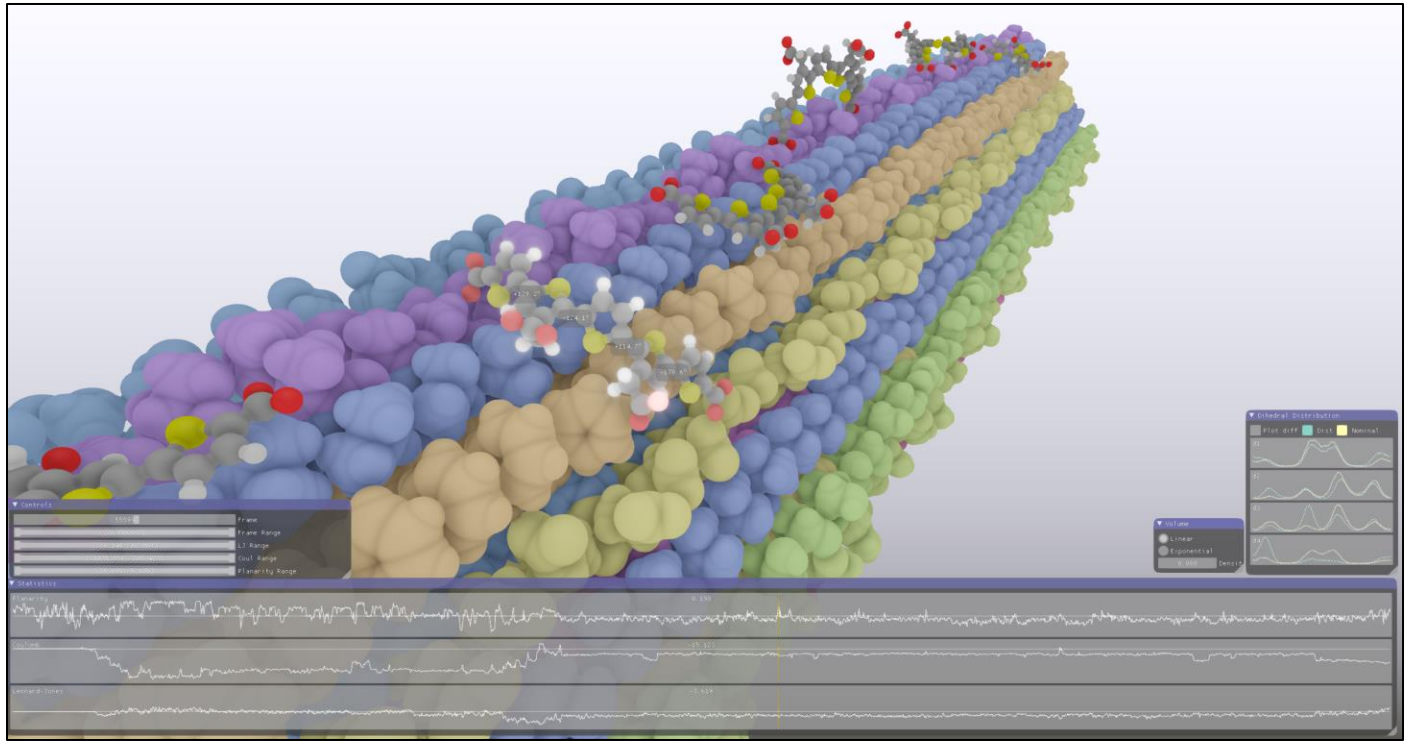
Webinar, 2024-02-06, 15:00 CET

linares@kth.se
robin.skanberg@liu.se

KTH VETENSKAP OCH KONST

History of VIAMD (Prototype 2018)[1]

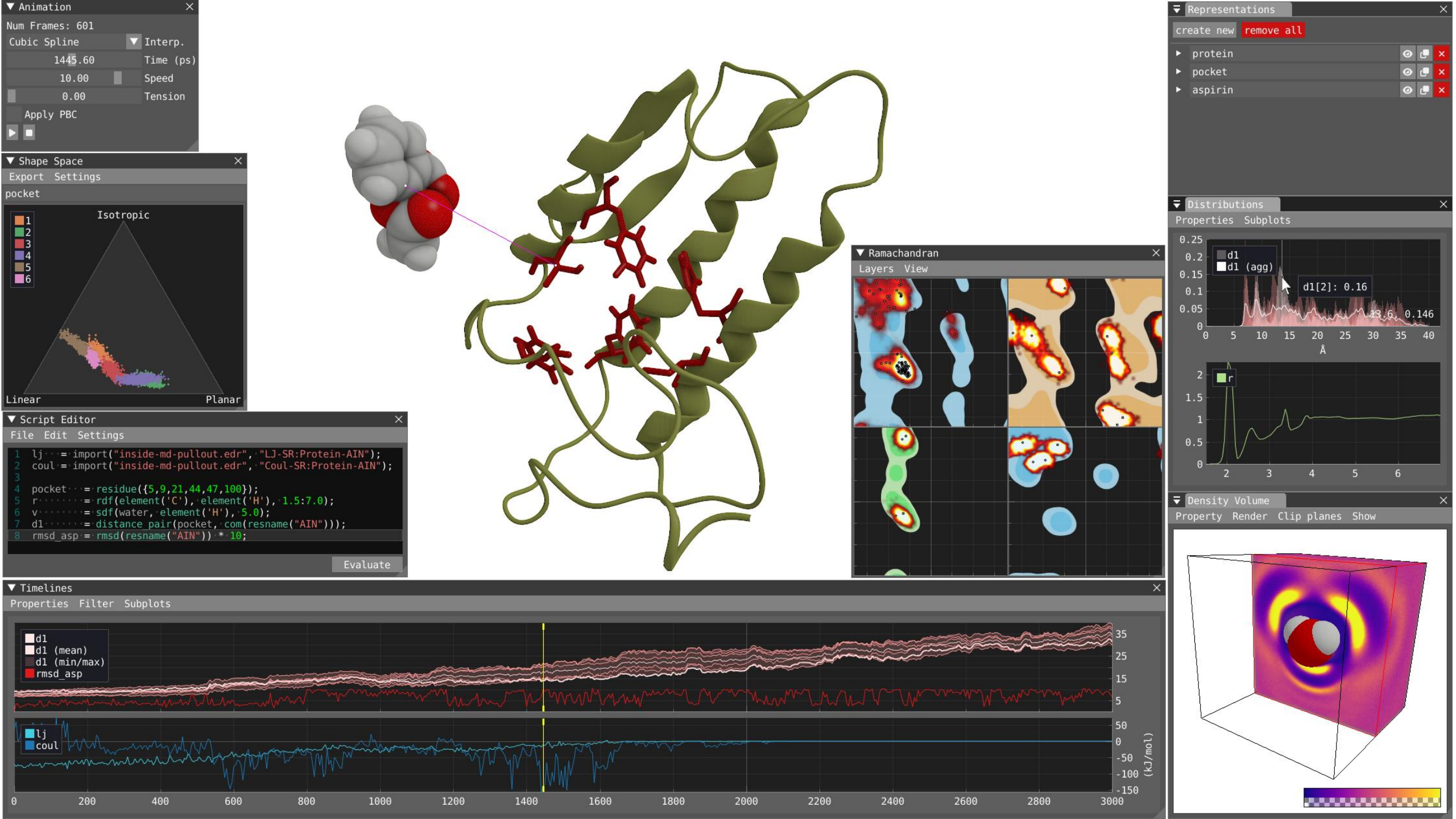
- Collaboration
  - KTH Theor. Chem. Bio. Group
  - LiU Scivis Group
- Specific Molecular System
  - Stacked amyloid fibrils
  - Fluorescent ligands
- Research Questions
  - Where do ligands bind
  - Favored conformation
  - Absorption spectra
- Implementation in Inviwo[2]



[1]: DOI: 10.2312/molva.20181102
[2]: https://inviwo.org/ (DOI: 10.1109/TVCG.2019.2920639)

Lessons Learned

- Generalize Core Principles
- Integrated Interactive Analysis
  - Visualize
  - Analyze / formulate hypothesis
  - Compute properties
- Expose in same Application
  - Minimize iteration time and friction
  - Exploit synnergies between components


Animation
Num Frames: 601
Cubic Spline
Interp.
1445.60
Time (ps)
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Speed
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Tension
Apply PBC
Shape Space
Export Settings
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Isotropic
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Linear
Planar
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Ramachandran
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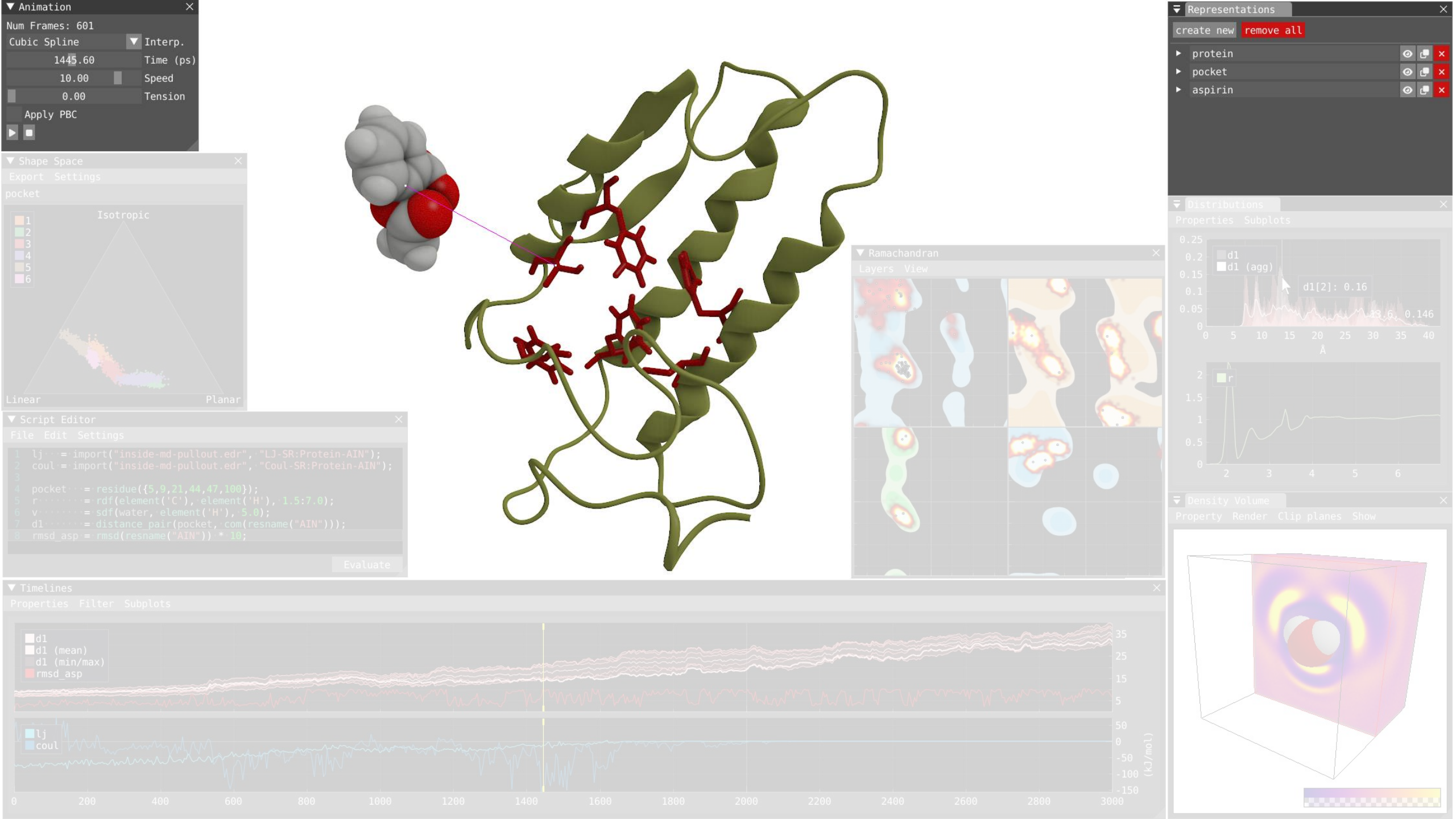
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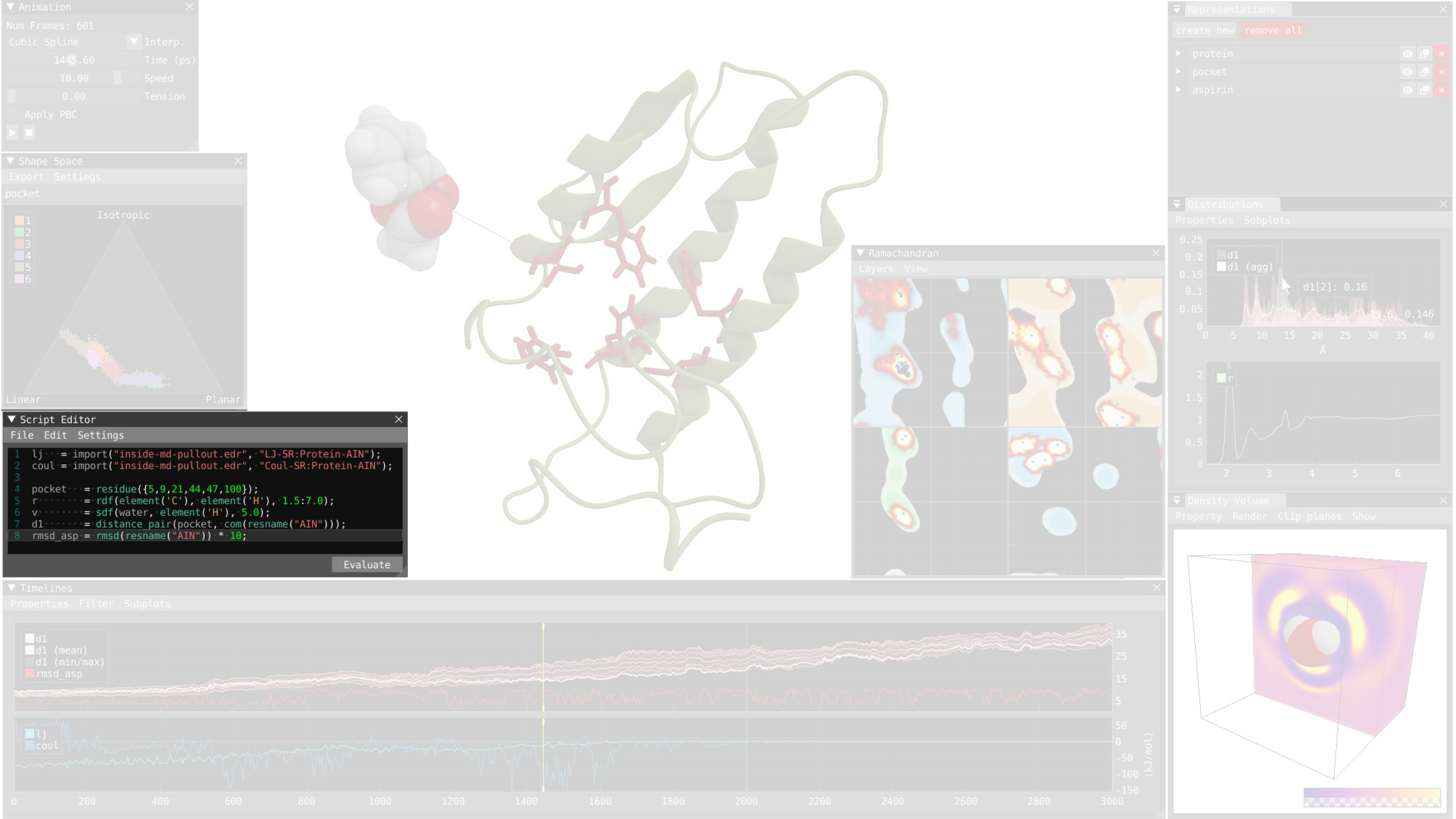
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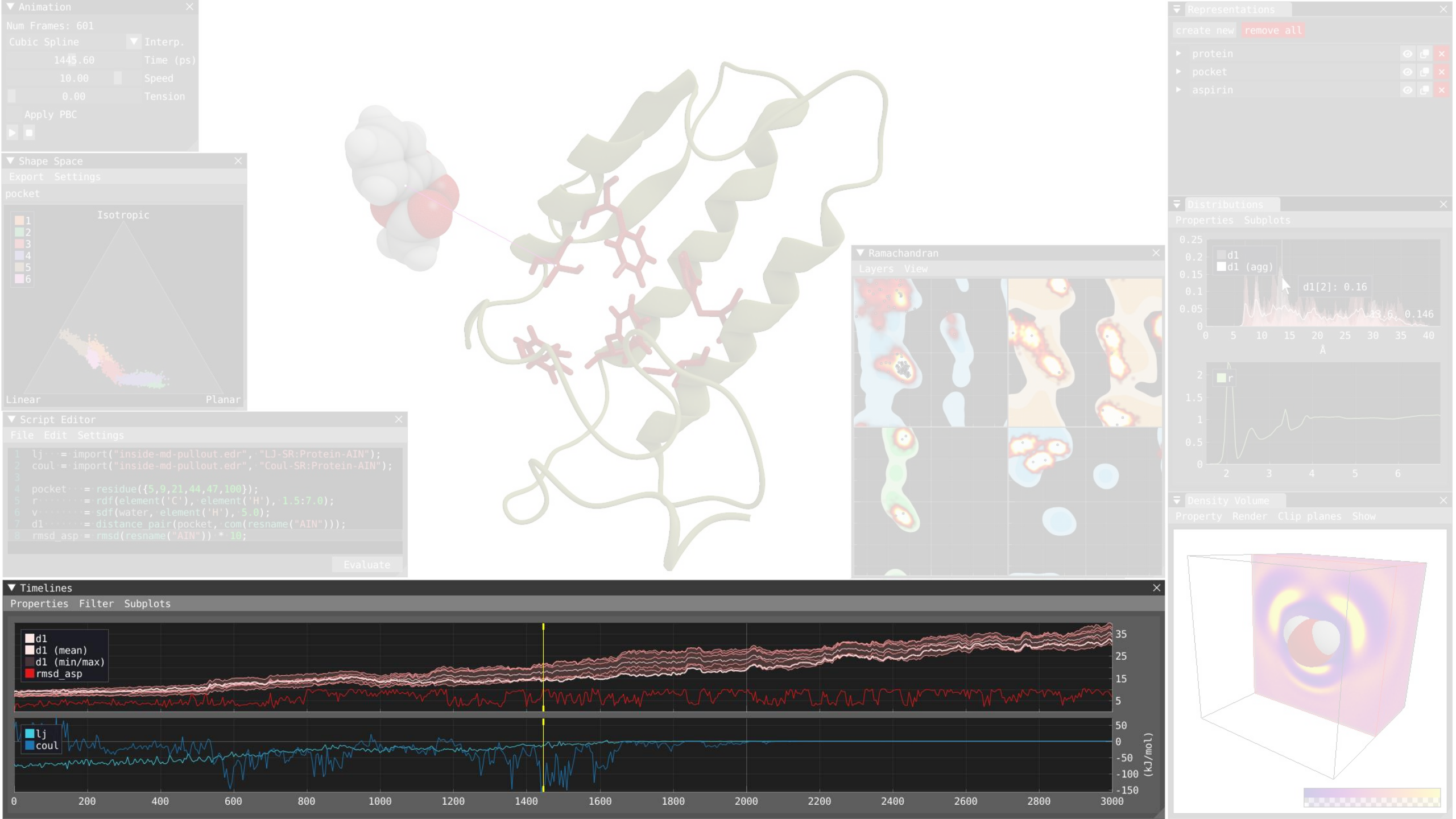
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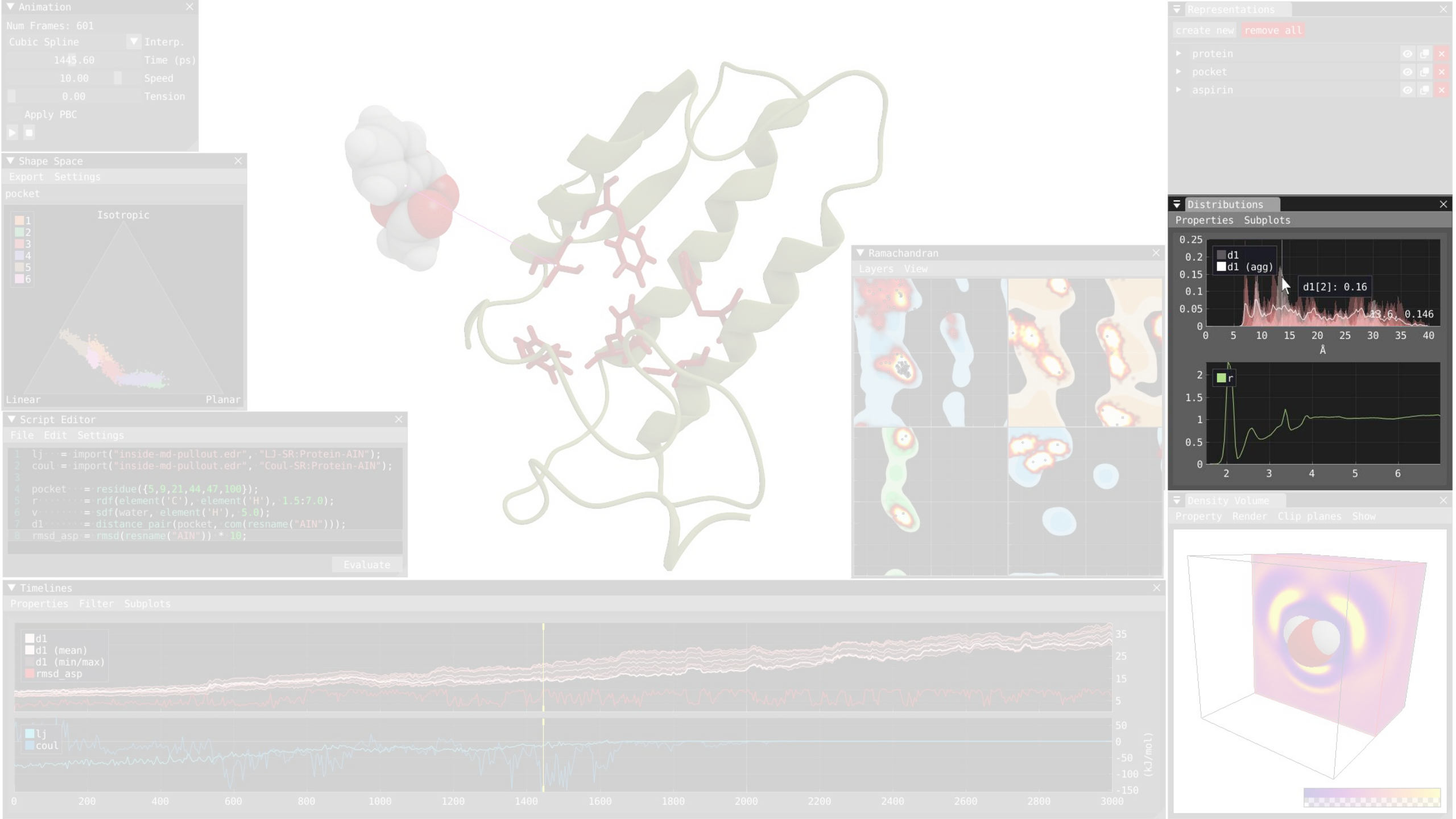
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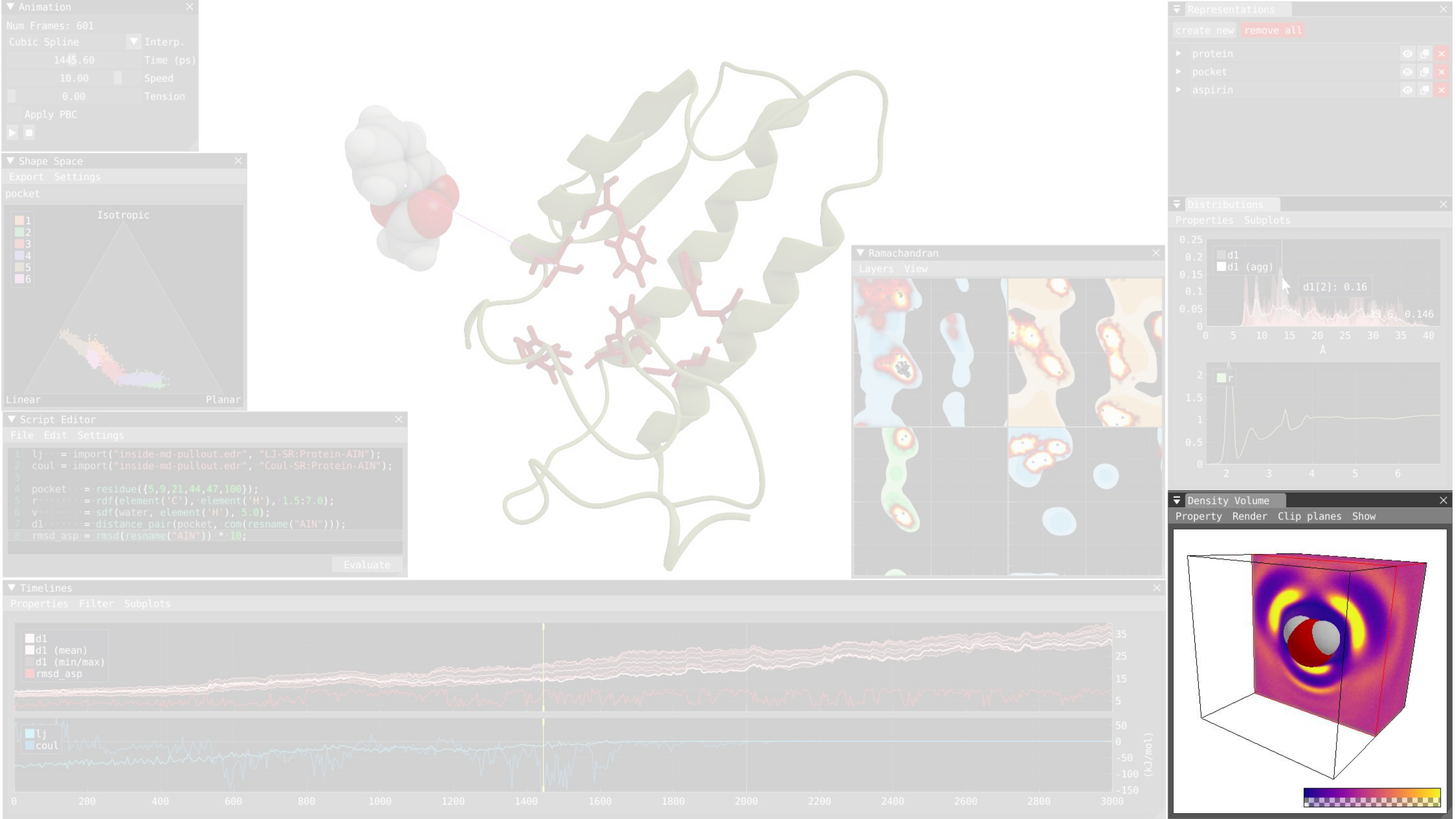
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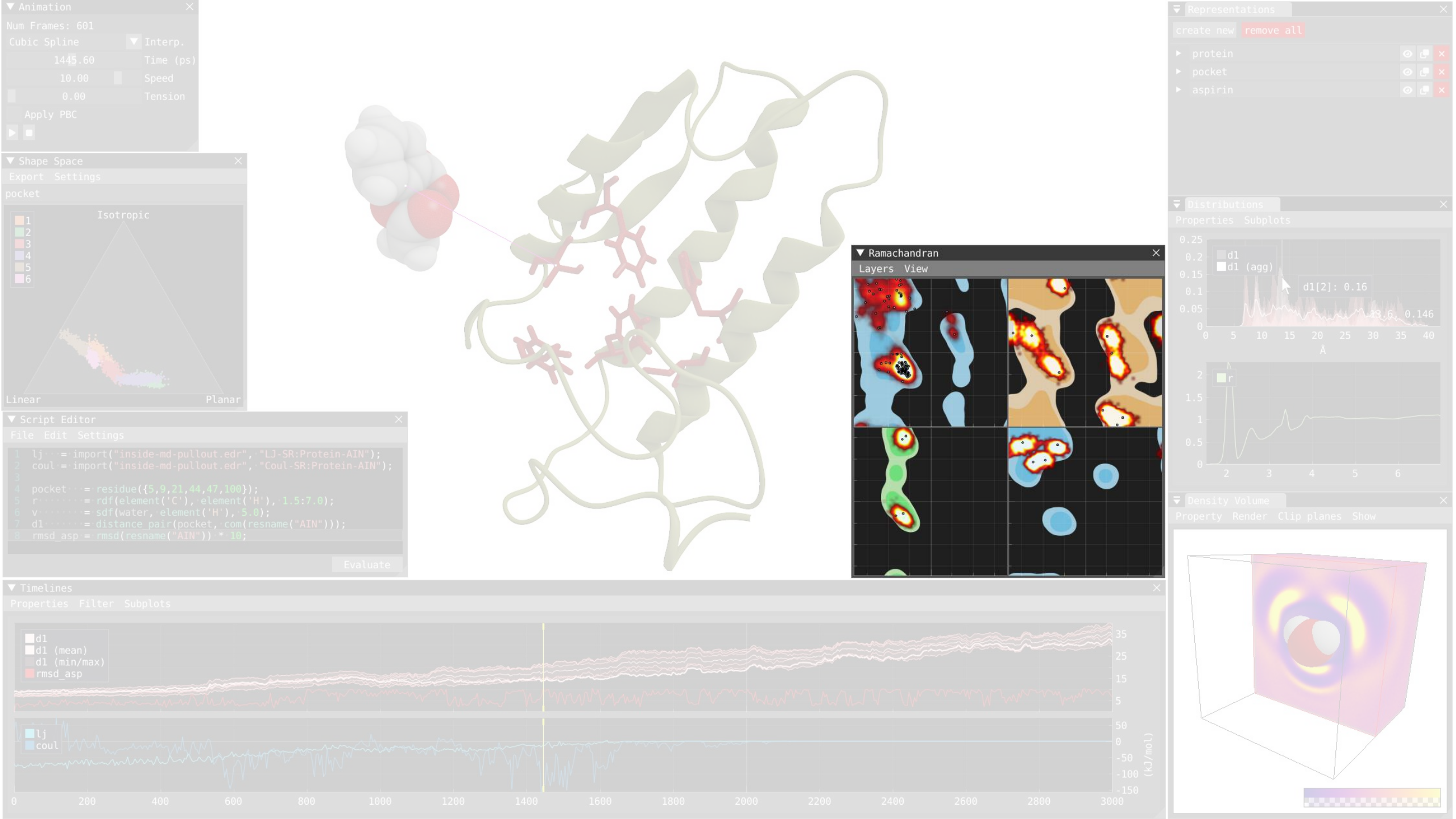
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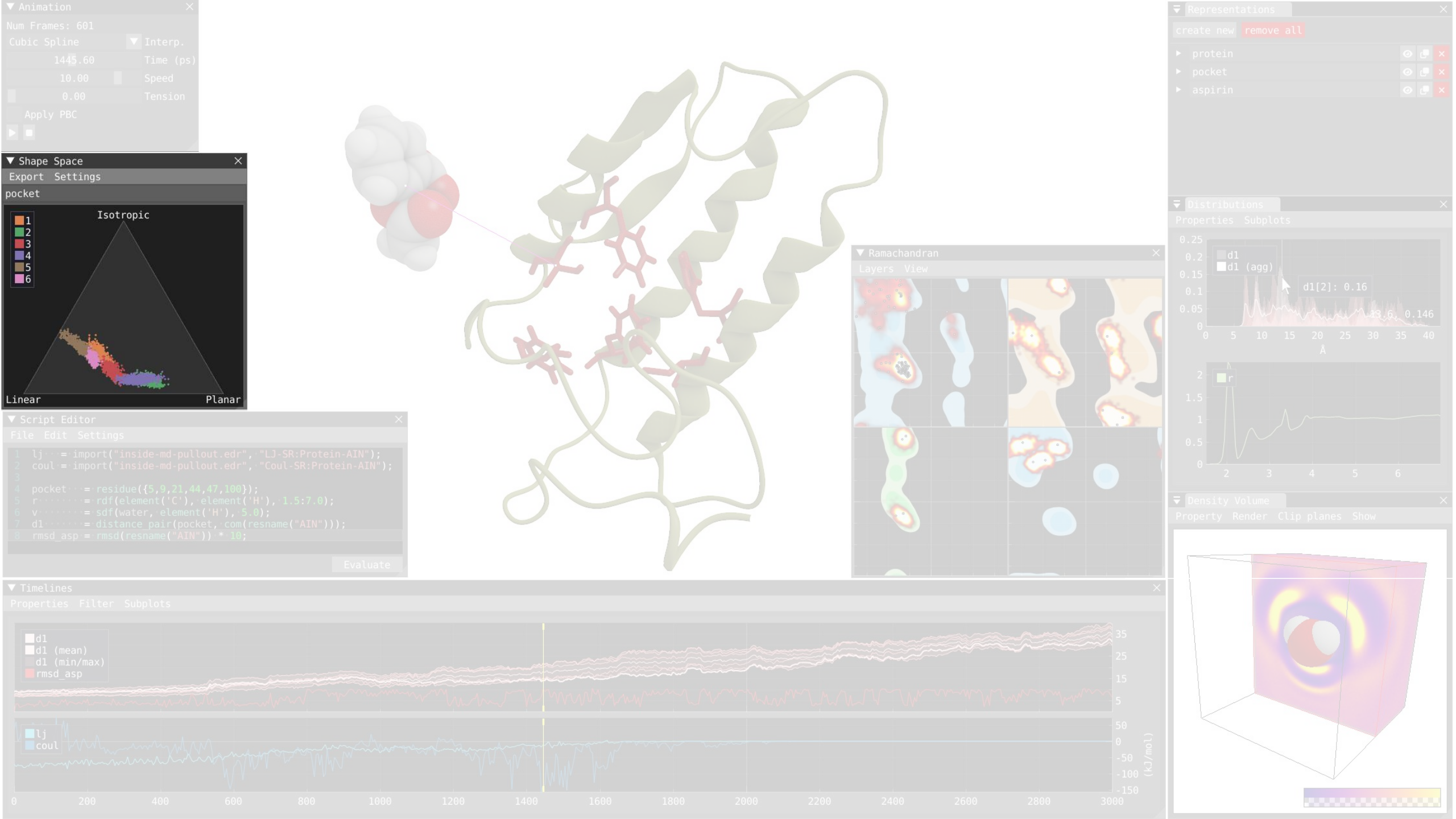
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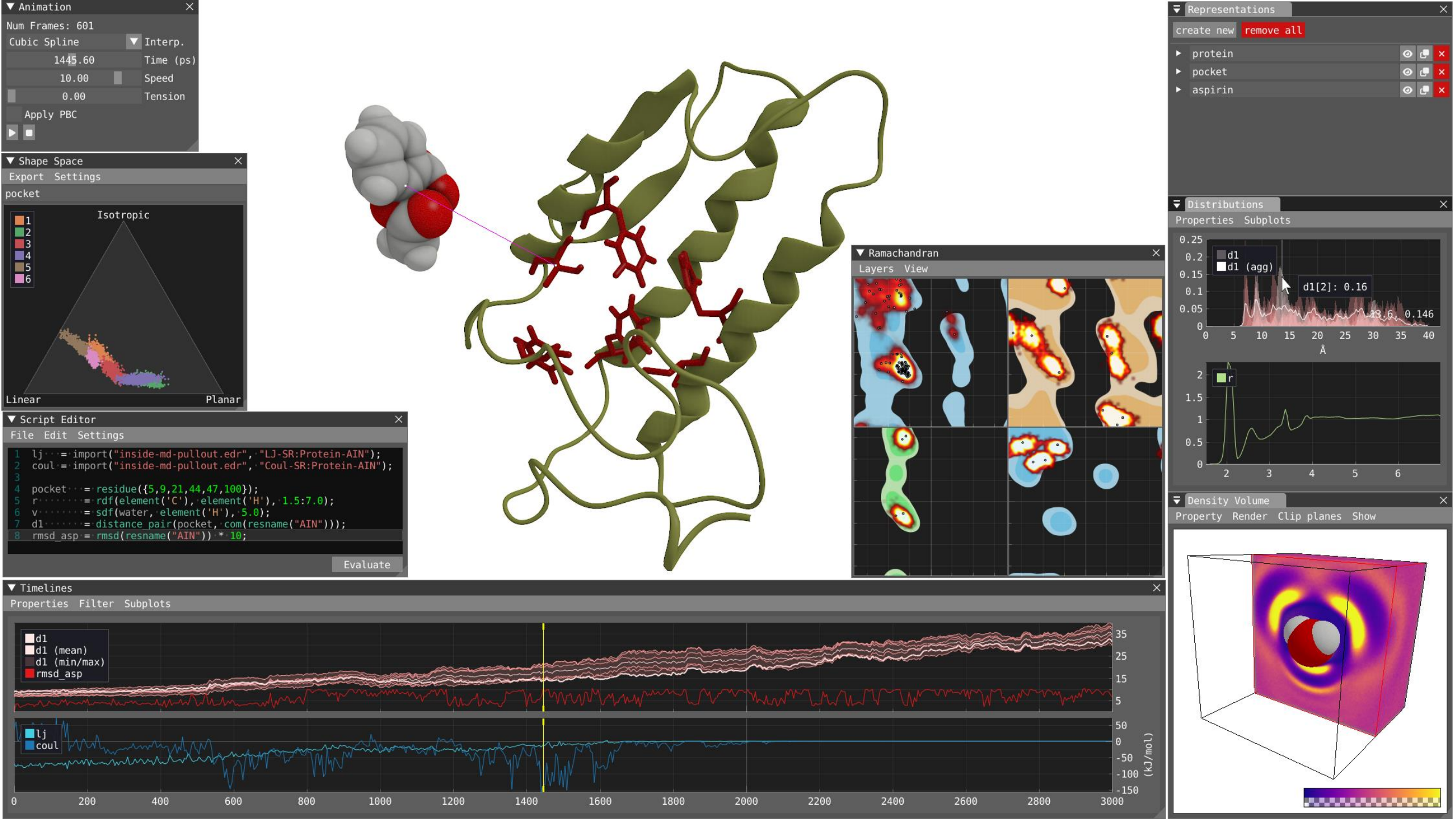
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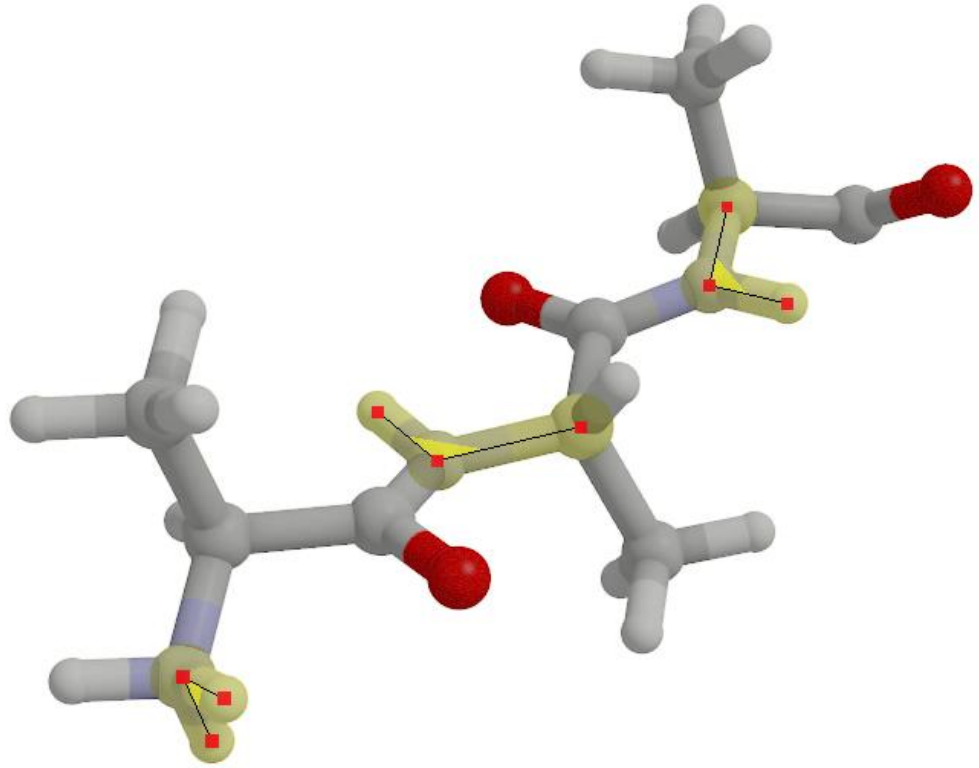
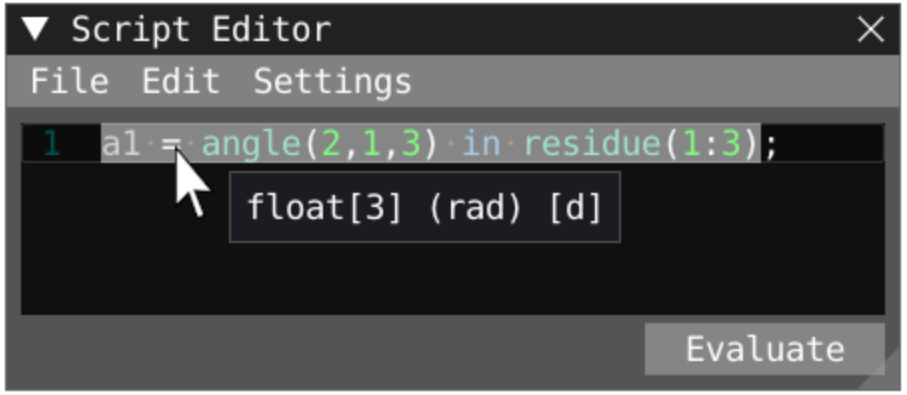
2800
3000

Script Language: Motivation

- Simple, Task Specific
- Good, specific feedback
  - Error messages
- Inspect Expressions
  - Type, Length
  - Provide Visualizations





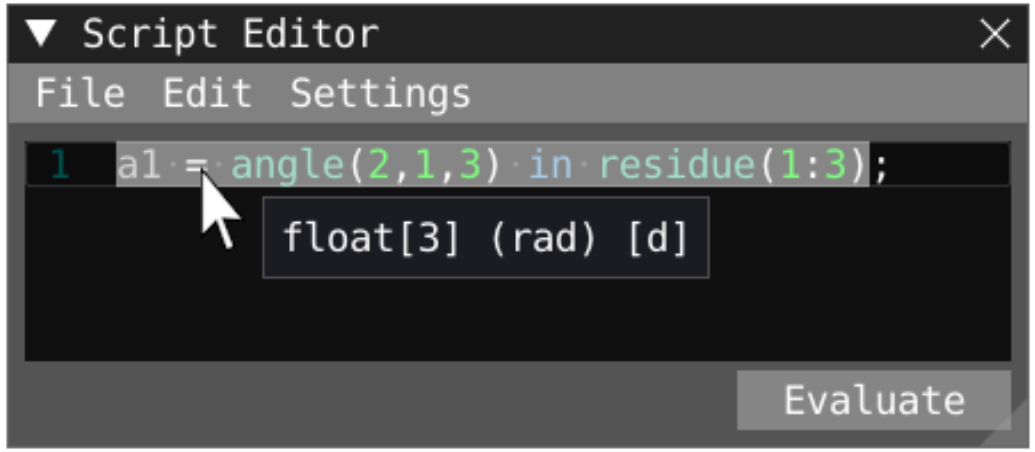
Script Language: Syntax

- Declarative Syntax
  - State what should be accomplished without specifying how (Imperative)
  - Control flow is implicit
  - Tie results of expressions into variables

```
s1 = resname("ALA")[5:];
d1 = distance(10,30);
a1 = angle(2,1,3) in resname("ALA");
r  = rdf(element('C'), element('H'), 10.0);
v  = sdf(s1, element('H'), 10.0);
```

Script Language: Contextual Operations

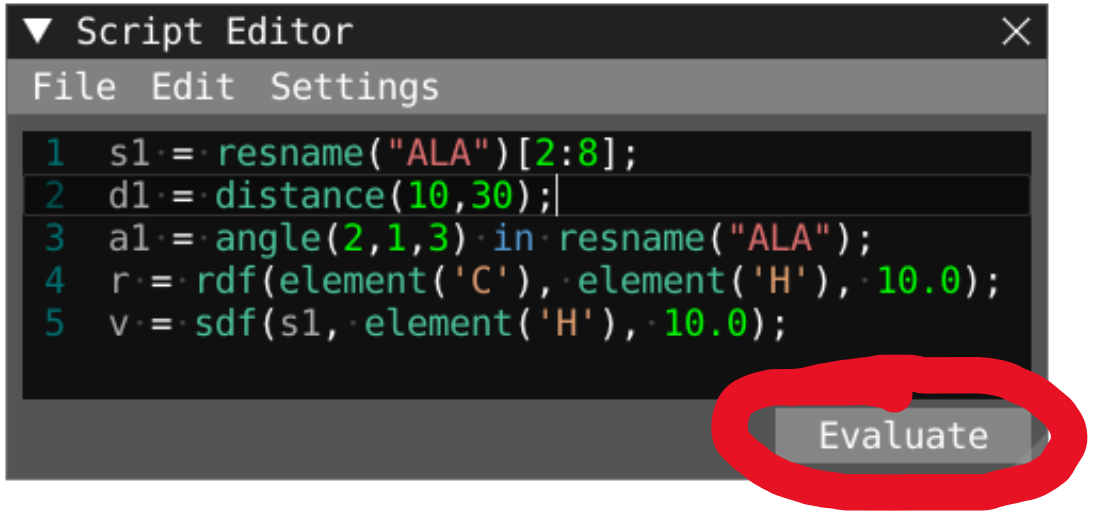
- The keyword ***in*** declares the context(s) for operations
- LHS = Operation, RHS = Context(s)
- For N contexts, resulting type will have length N
- Replaces traditional for-loop

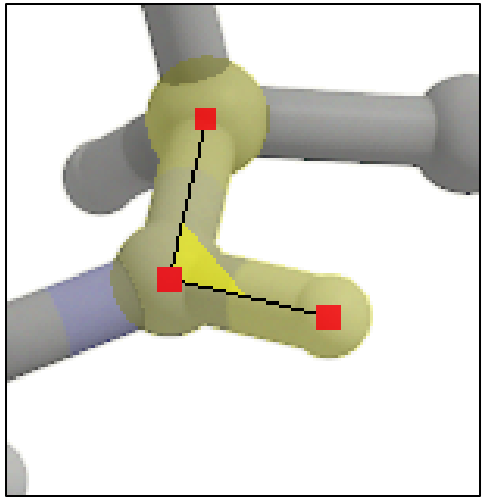


Script Evaluation: Three Scenarios

1. Static Validation
   - Occurs during compilation
   - Validates the script against topology
2. Data Evaluation
   - Computes and outputs a value
3. Visualization
   - When user hovers expression
   - Can output Rendering primitives
     - Points / Lines / Spheres / Triangles
     - Sets of Atoms to highlight

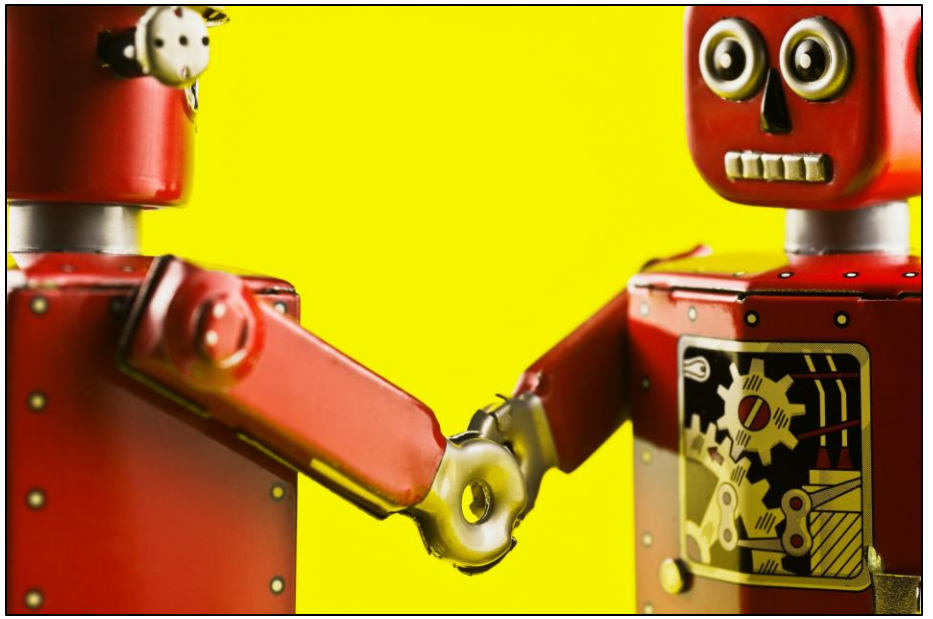
- Implemented Procedures
  - Must support 2
  - Optionally support 1,3



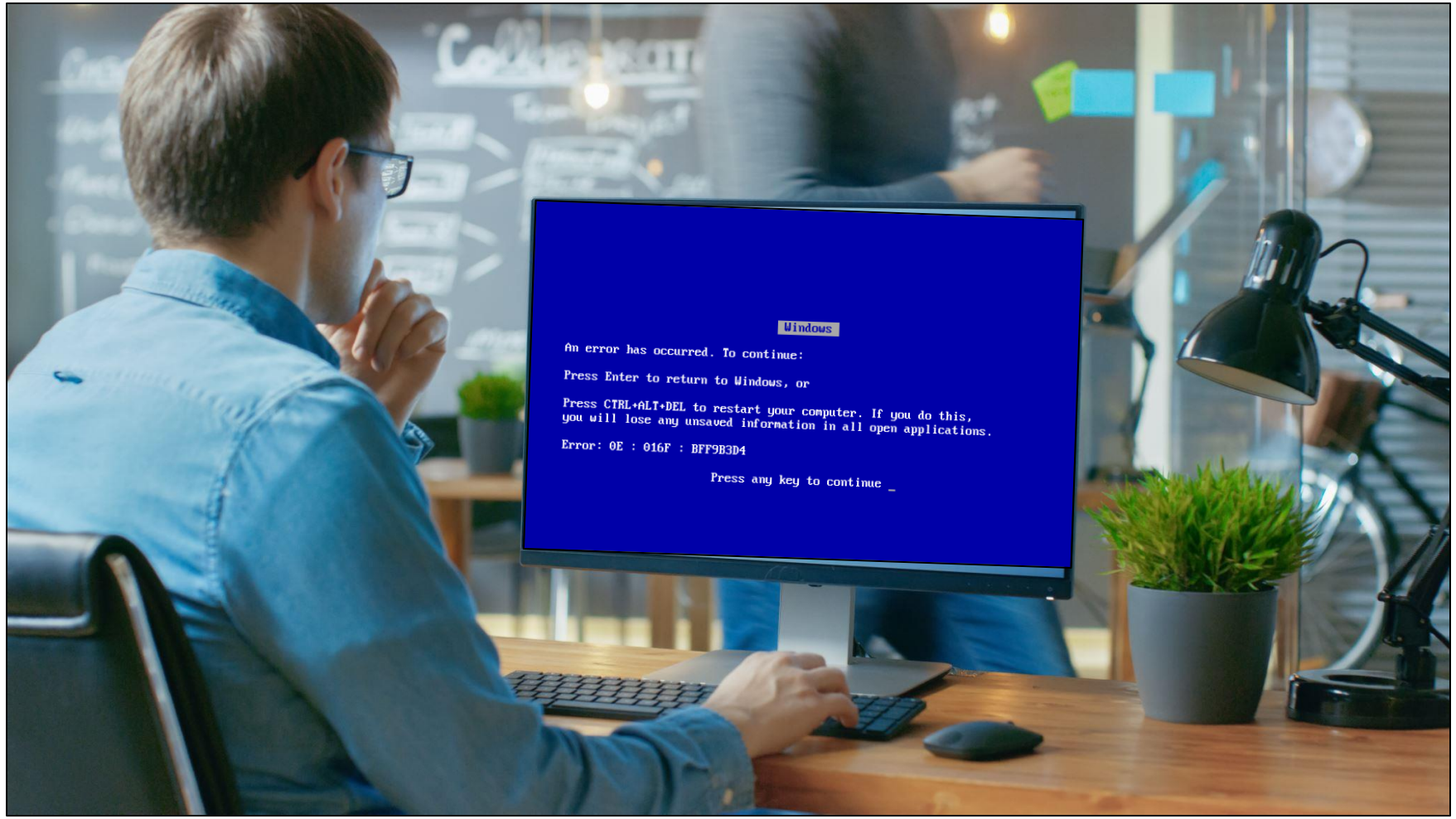


Script Evaluation: Properties

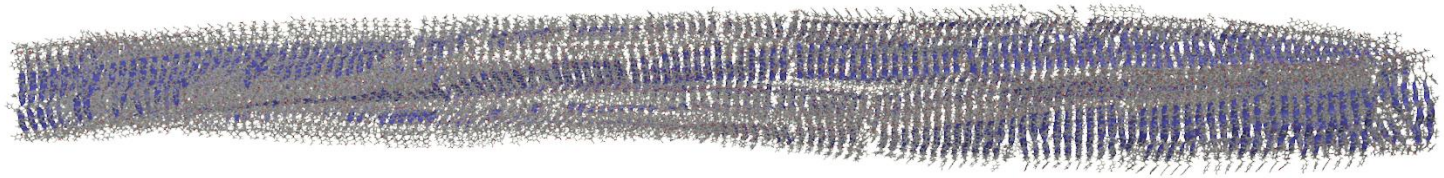
- Variables of particular types are promoted into *properties*
  - Dynamic (Value changes over frames)
    - Floats [1:N]
    - Distributions (Float[M])
    - Volumes (Float[L][L][L])
- Properties are exposed
  - Timeline Window
  - Distribution Window
  - Volume Window
  - …

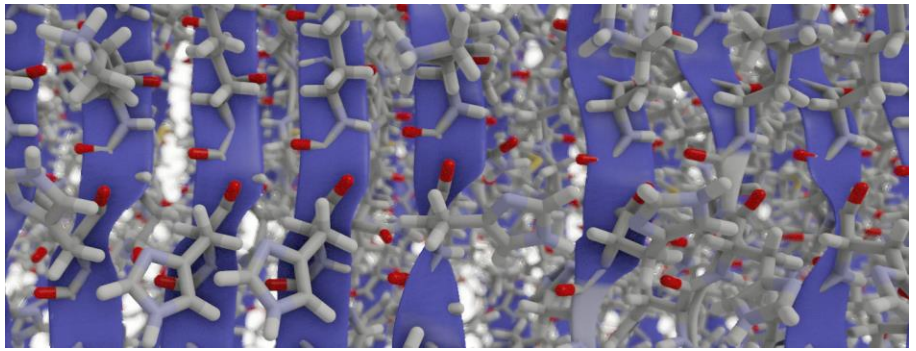


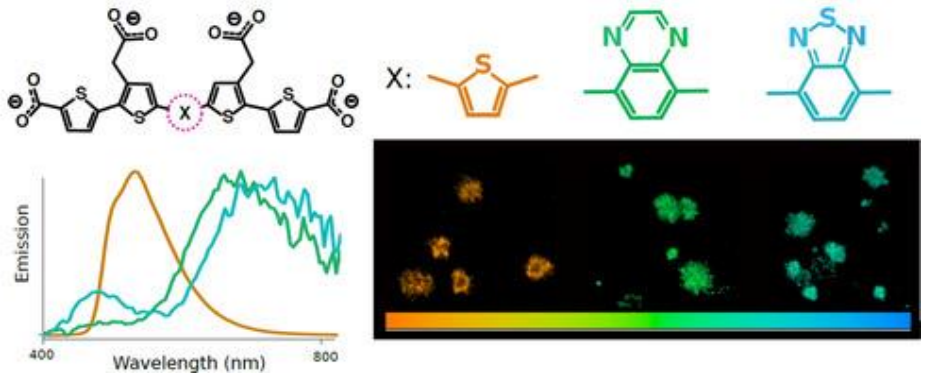
Demo Time


Windows
An error has occurred. To continue:
Press Enter to return to Windows, or
Press CTRL+ALT+DEL to restart your computer. If you do this,
you will lose any unsaved information in all open applications.
Error: 0E : 016F : BFF9B3D4
Press any key to continue _

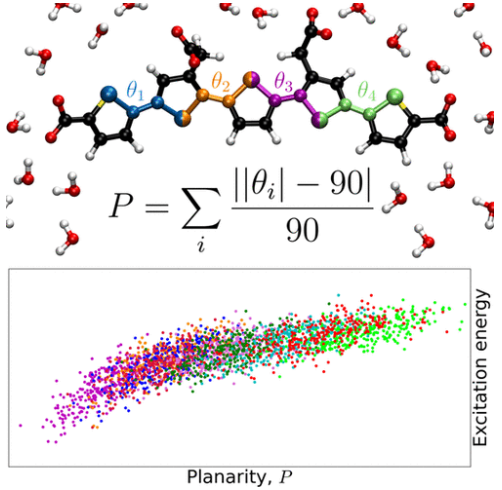
Amyloid Fibril detection



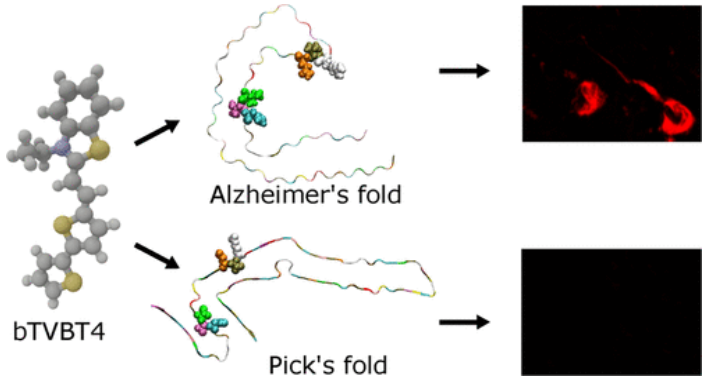




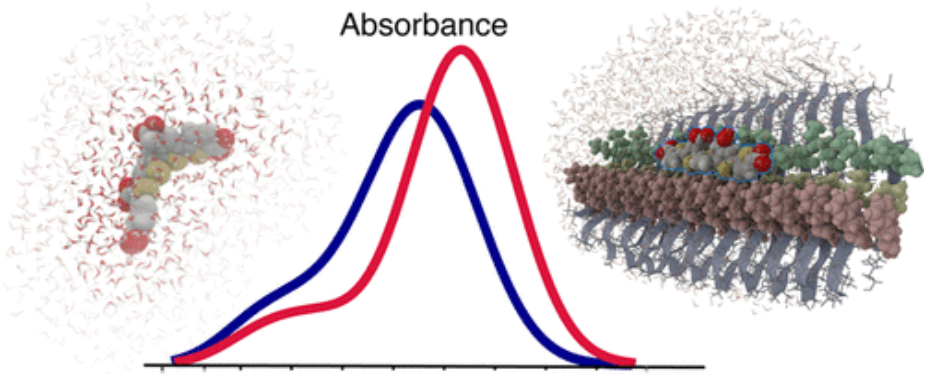
ChemPhysChem 2021, 22 (3), 323-335



J. Phys. Chem. A 2014, 118, 42, 9820–9827



J. Phys. Chem. B 2021, 125, 42, 11628–11636



J. Phys. Chem. A 2020, 124, 5, 875–888

Future of VIAMD

- Support analysis of multiple systems
  - Compare properties from multiple trajectories
- Transition to next gen. Graphics APIs
- Support more Script Operations
- Support more file formats
  - Gromacs (tpr)
  - Amber
  - NAMD

Resources

https://github.com/scanberg/viamd

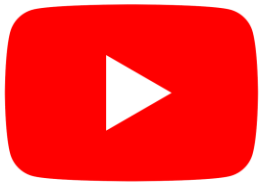
Wiki and Tutorials

Issues

Discussions

Robin Skånberg, Ingrid Hotz, Anders Ynnerman, Mathieu Linares
"VIAMD: a software for Visual Interactive Analysis of Molecular Dynamics",
JCIM, 2023, 63, 23, 7382–7391
https://pubs.acs.org/doi/10.1021/acs.jcim.3c01033

We encourage the users to publish their VIAMD script in ESI (together with the trajectory on Zenodo)



https://bit.ly/4aRsPrh

@VIAMD_

Acknowledgements

Martin Falk
Ingrid Hotz
Talha Bin Masood
Anders Ynnerman
Gustav Eriksson
Carolin König
Patrick Norman

People sharing their data with us...
on Zenodo and Others...

Thanks!