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BE21B004

BT4110 – Computational Biology Lab

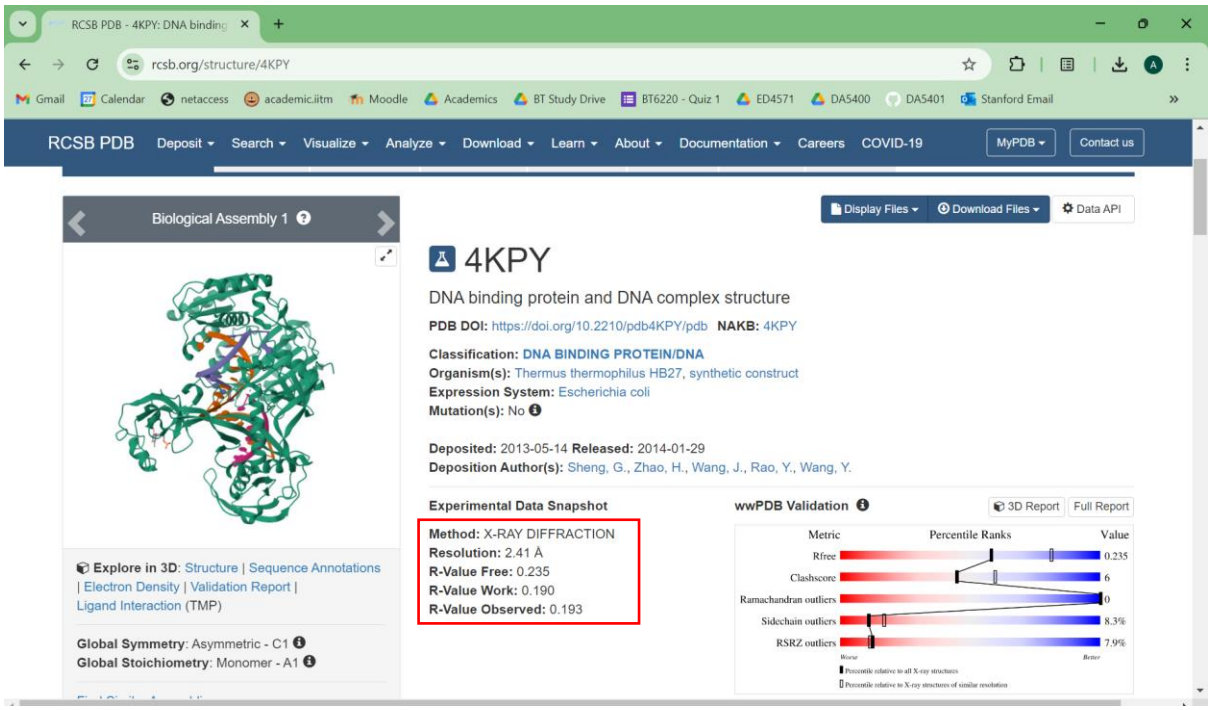
Practical 1

1

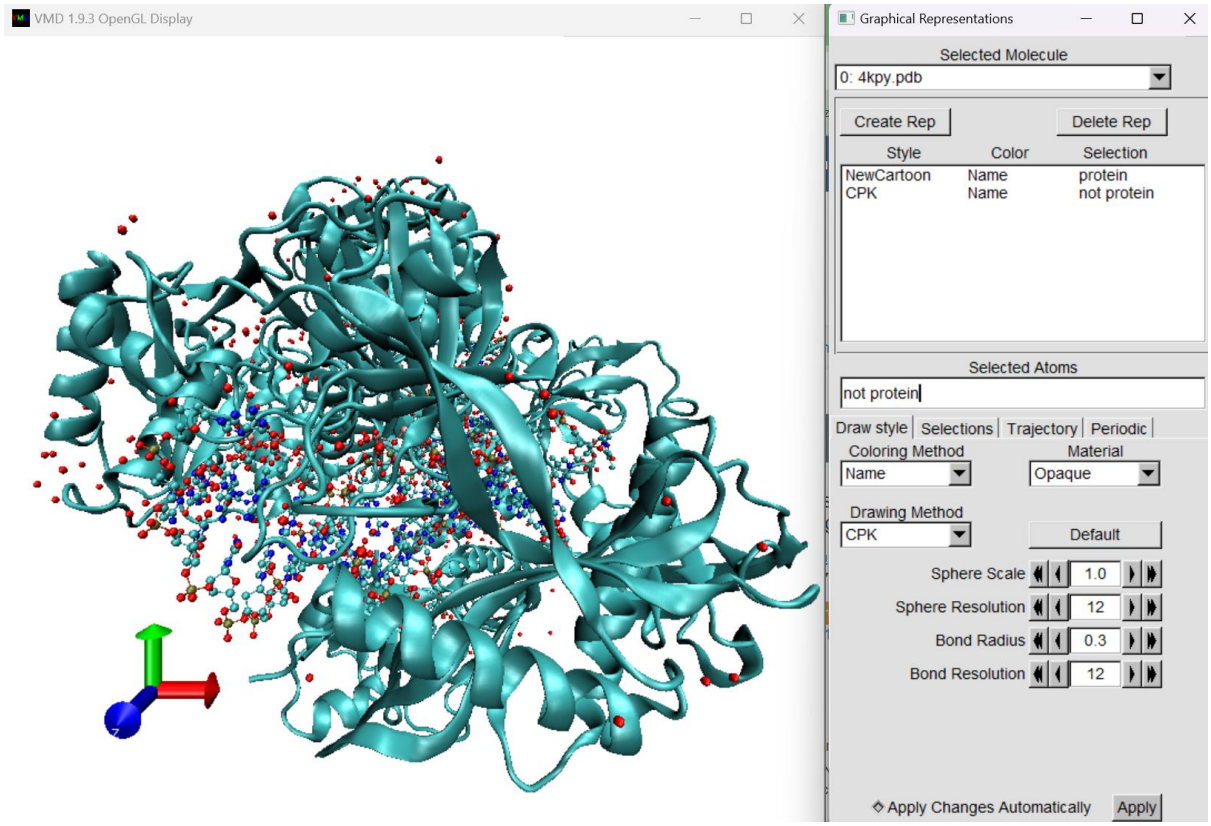
- The protein 4KPY is an uncharacterized DNA binding protein from *Thermus thermophilus* HB27.
- The structure contains the protein bound to DNA molecules.
- The protein has two chains, A and B, which are 685 residues long in total.
- The protein is an asymmetric monomer. The total weight of the structure is 178.94 kDa.
- The structure also contains two small molecule ligands – thymidine monophosphate and a manganese ion.

2

- The structure was determined by X-ray diffraction.
- The resolution of the structure is 2.41 Å.



3


VMD 1.9.3 OpenGL Display
Graphical Representations
Selected Molecule
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Create Rep
Delete Rep
Style Color Selection
NewCartoon Name protein
CPK Name not protein
Selected Atoms
not protein
Draw style Selections Trajectory Periodic
Coloring Method
Name
Material
Opaque
Drawing Method
CPK
Default
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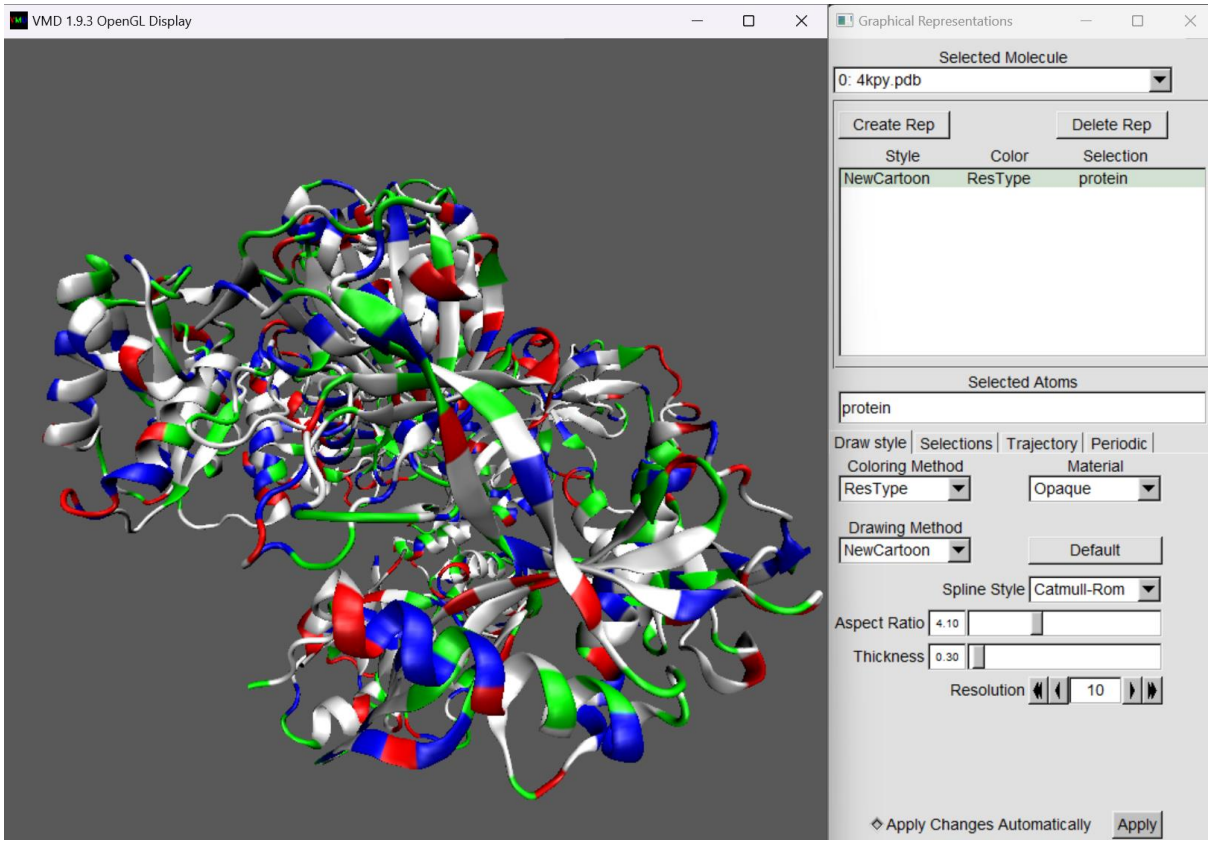
Sphere Resolution 12
Bond Radius 0.3
Bond Resolution 12
Apply Changes Automatically
Apply

4


VMD 1.9.3 OpenGL Display
Graphical Representations
Selected Molecule
0: 4kpy.pdb
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Delete Rep
Style Color Selection
NewCartoon ResType protein
Selected Atoms
protein
Draw style Selections Trajectory Periodic
Coloring Method
ResType
Material
Opaque
Drawing Method
NewCartoon
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Thickness 0.30
Resolution 10
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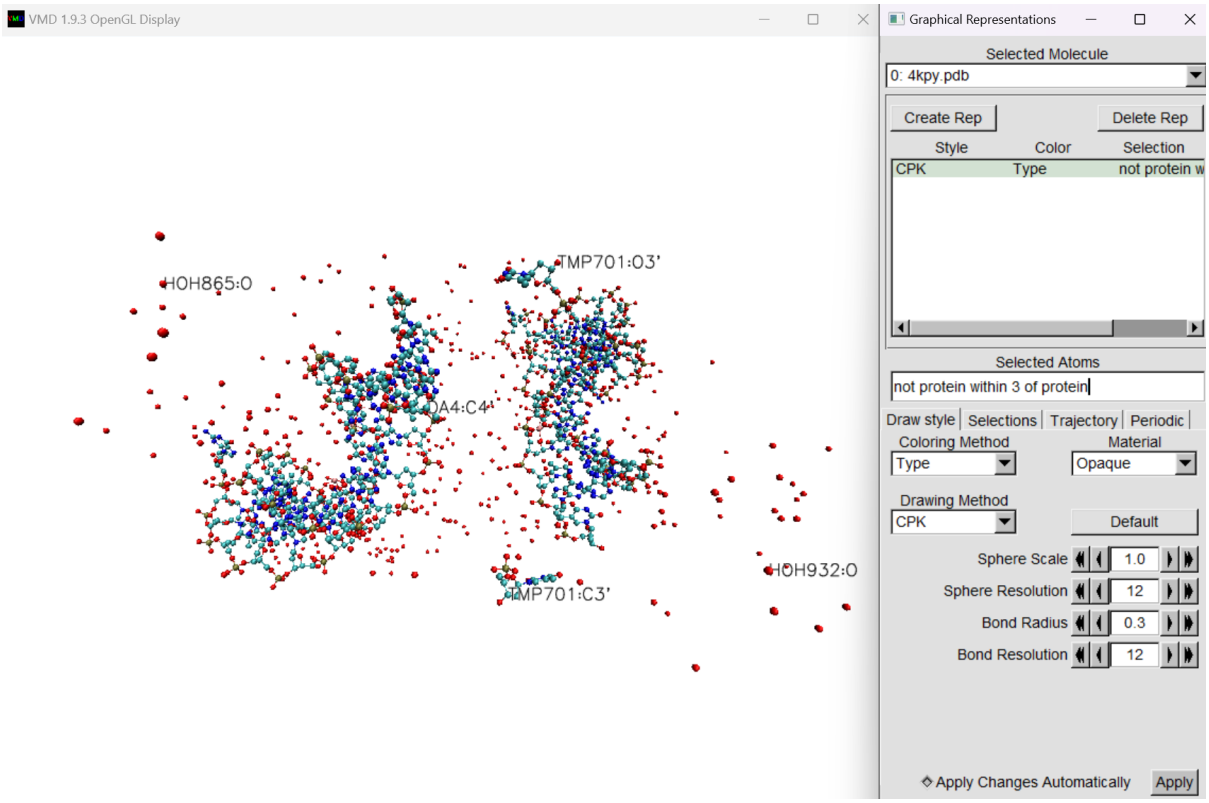
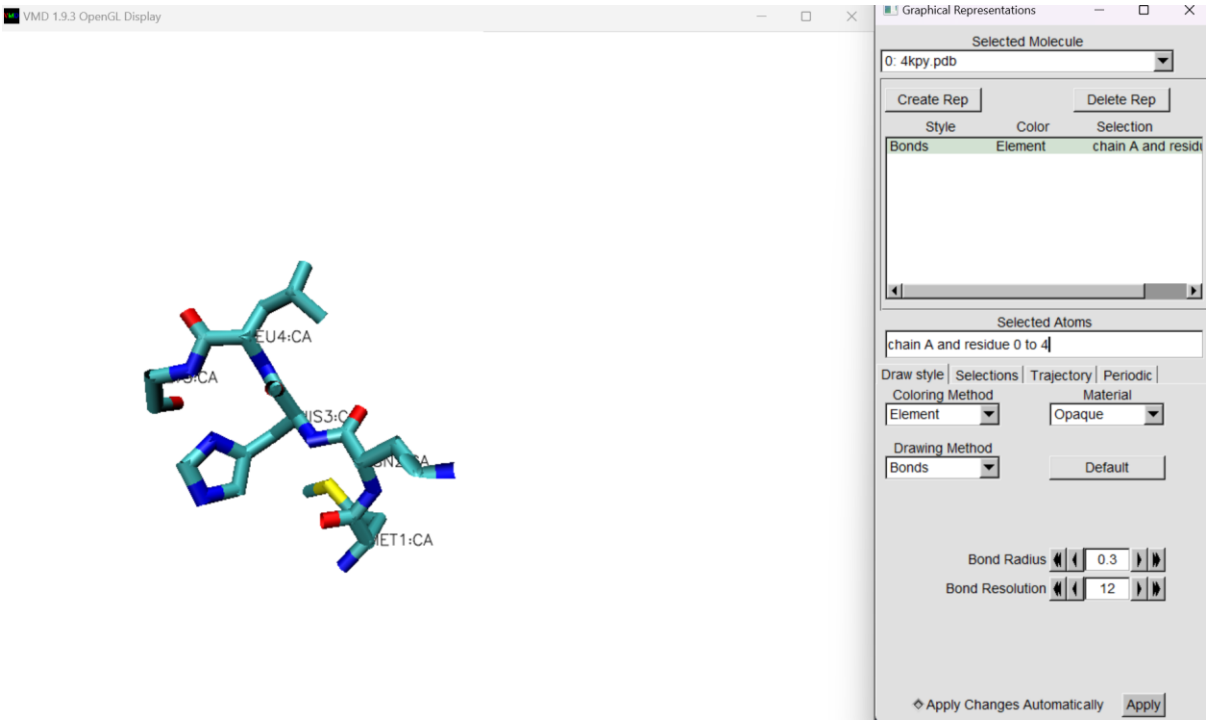
Apply

5



This includes 2 DNA molecules, waters, and 2 thymidine monophosphate molecules. There are too many atoms to list individually.

6



The first five residues are Met1, Asn2, His3, Leu4, and Gly5.

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The molecule status flags in VMD are:

- T – Top
  If more than one molecule is loaded, the "T" toggle appears for the molecule at the top of the stack.

- A – Active
  This is used to toggle molecules between their active state and inactive state. If the molecule is active, VMD commands have an affect on the molecule. Inactive molecules are unaffected by these commands.

- D – Drawn
  This toggle is used to show (draw) or hide a molecule.

- F – Fixed
  This toggle is used to "fix" or "unfix" a molecule. Fixed molecules are unaffected by mouse operations like rotation and translation.

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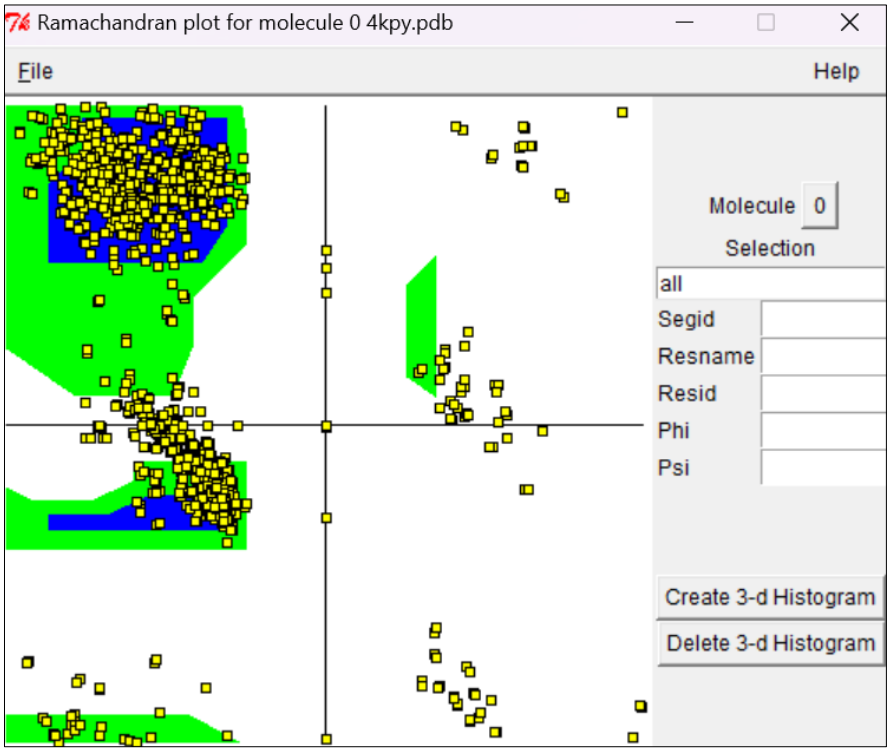
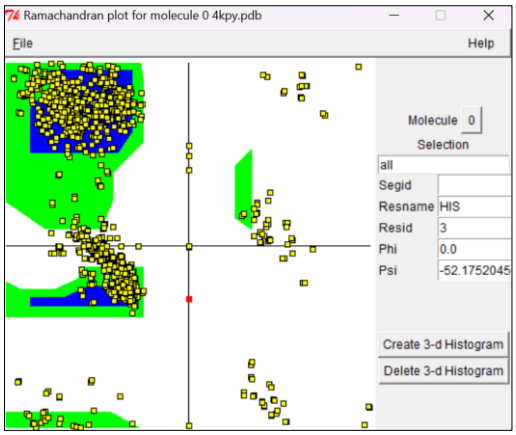


His3 and Gly235 are two residues in the disallowed region of the plot.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File
Help
Molecule 0
Selection
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Segid
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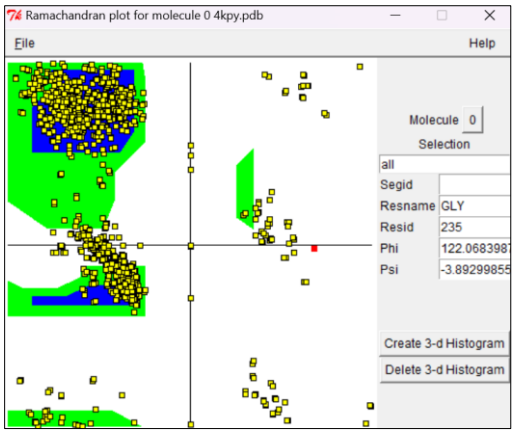
Resid 3
Phi 0.0
Psi -52.1752045
Create 3-d Histogram
Delete 3-d Histogram


Ramachandran plot for molecule 0 4kpy.pdb
File
Help
Molecule 0
Selection
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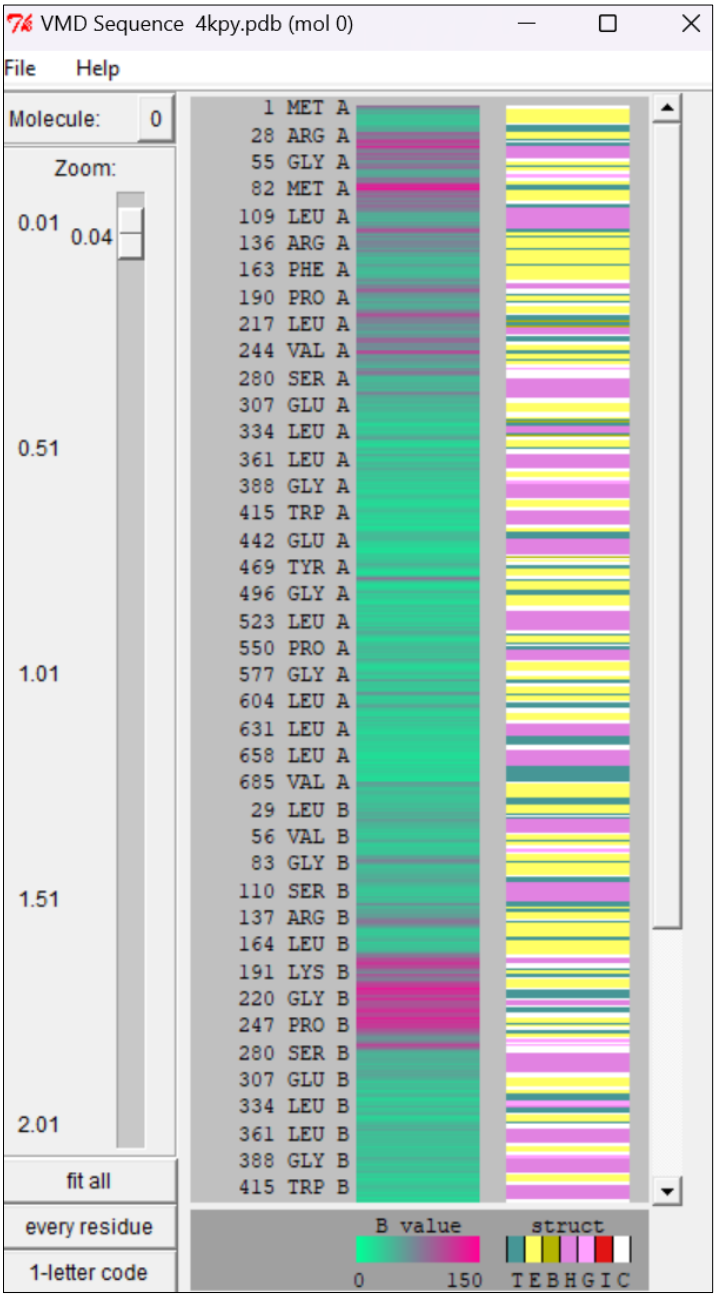
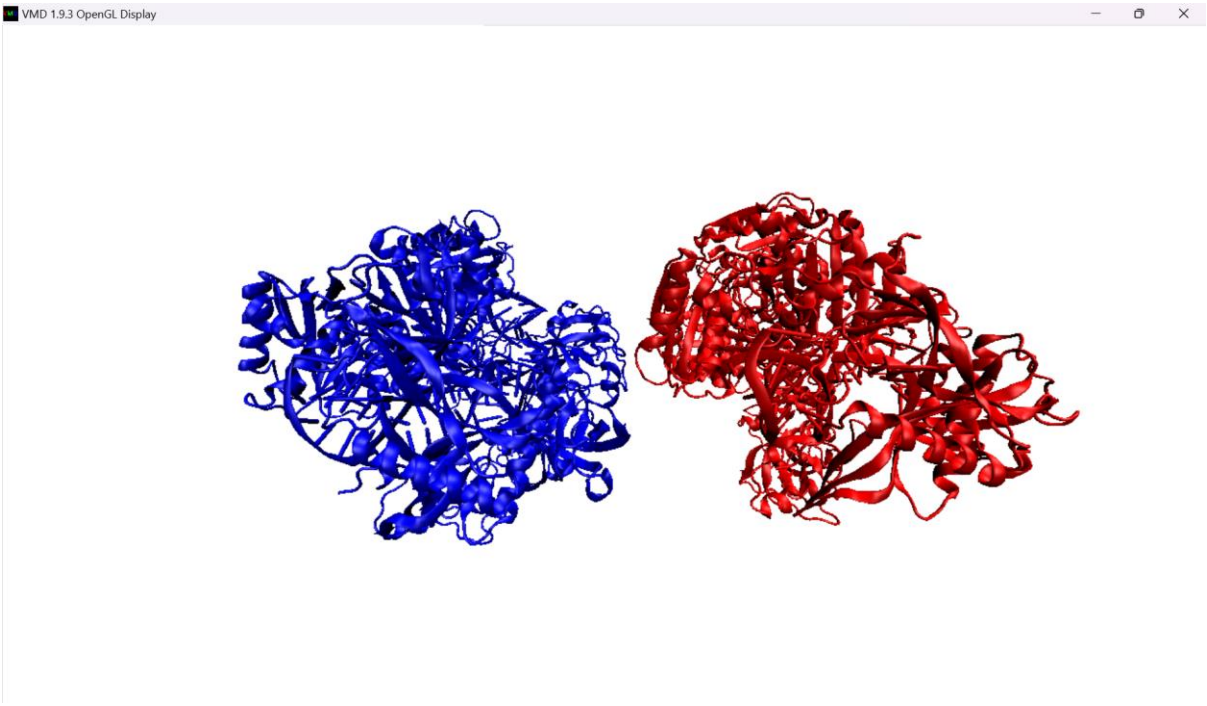
Segid
Resname GLY
Resid 235
Phi 122.068398
Psi -3.89299855
Create 3-d Histogram
Delete 3-d Histogram

9


VMD Sequence 4kpy.pdb (mol 0)
File
Help
Molecule: 0
Zoom:
0.01
0.04
0.51
1.01
1.51
2.01
fit all
every residue
1-letter code
1 MET A
28 ARG A
55 GLY A
82 MET A
109 LEU A
136 ARG A
163 PHE A
190 PRO A
217 LEU A
244 VAL A
280 SER A
307 GLU A
334 LEU A
361 LEU A
388 GLY A
415 TRP A
442 GLU A
469 TYR A
496 GLY A
523 LEU A
550 PRO A
577 GLY A
604 LEU A
631 LEU A
658 LEU A
685 VAL A
29 LEU B
56 VAL B
83 GLY B
110 SER B
137 ARG B
164 LEU B
191 LYS B
220 GLY B
247 PRO B
280 SER B
307 GLU B
334 LEU B
361 LEU B
388 GLY B
415 TRP B
B value
0
150
struct
T E B H G I C

Helices are found at multiple locations in the protein. From the .pdb file, we can find that there are 39 helices in the protein.

Helix No.	Chain	Helix Start	Helix End	Helix Length
1	A	GLU41	GLY54	14
2	A	PRO69	LEU73	5
3	A	ASP102	ARG123	22
4	A	SER178	ALA184	7
5	A	SER222	LYS230	9
6	A	THR266	LEU270	5
7	A	PRO282	LEU301	20
8	A	LYS329	ALA331	3
9	A	ASP332	GLY337	6
10	A	PRO358	GLY373	16
11	A	HIS384	GLN387	4
12	A	GLY388	GLU401	14
13	A	ALA414	GLU428	15
14	A	GLU443	ALA458	16
15	A	PRO515	GLY535	21
16	A	PHE554	GLY565	12
17	A	ARG608	GLY612	5
18	A	PRO627	THR639	13
19	A	PRO653	GLY670	18
20	A	ILE671	LEU674	4
21	B	GLU41	ALA53	13
22	B	PRO69	LEU73	5
23	B	ASP102	ARG123	22
24	B	SER178	ALA184	7
25	B	SER222	SER229	8
26	B	THR266	GLU274	9
27	B	PRO282	LEU301	20
28	B	LYS329	ALA331	3
29	B	ASP332	GLY337	6
30	B	PRO358	GLY373	16
31	B	HIS384	GLN387	4
32	B	GLY388	GLU401	14
33	B	ALA414	GLU428	15
34	B	GLU443	GLY459	17
35	B	PRO515	GLY535	21
36	B	PHE554	GLY565	12
37	B	PRO627	THR639	13
38	B	PRO653	GLY670	18
39	B	ILE671	LEU674	4


VMD 1.9.3 OpenGL Display