Representations/visualization of Macromolecular Structure

Biophysical Chemistry/Physical Chemistry of Biological Systems
An Introduction to Biomolecular Structure and Interactions
Fall 2009

Professor Wilma K. Olson

RCSB Protein Data Bank

http://www.rcsb.org

PDB file 3e7l

Batchelor JD, Doucleff M, Lee CJ, Matsubara K, De Carlo S, Heideker J, Lamers MH, Pelton JG, Wemmer DE.

Structure and regulatory mechanism of *Aquifex aeolicus* NtrC4: variability and evolution in bacterial transcriptional regulation.

J Mol Biol (2008) **384**(5), 1058-1075.

NtrC4: (nitrogen regulatory protein C4) an activator protein that stimulates gene expression by binding sigma-54
sigma-54 (σ^{54})**:** protein subunit of the RNA polymerase assembly of molecular weight 54 kDa, which is required for the expression of a wide variety of genes
***Aquifex aeolicus*:** thermophilic (heat-loving) bacterium

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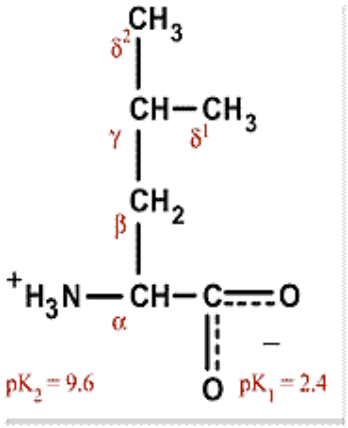
```
ATOM     19  N   LEU A  22      13.495  17.685  -7.418  1.00 107.88           N
ATOM     20  CA  LEU A  22      12.855  16.698  -6.555  1.00 100.06           C
ATOM     21  C   LEU A  22      11.626  16.031  -7.172  1.00  97.04           C
ATOM     22  O   LEU A  22      11.508  14.807  -7.158  1.00  94.39           O
ATOM     23  CB  LEU A  22      12.487  17.336  -5.213  1.00  95.81           C
ATOM     24  CG  LEU A  22      13.669  17.846  -4.385  1.00  91.39           C
ATOM     25  CD1 LEU A  22      13.197  18.737  -3.246  1.00  88.32           C
ATOM     26  CD2 LEU A  22      14.492  16.681  -3.861  1.00  88.80           C
```

ATOM 'card':
ATOM, atom #, atom name, res name, chain ID, res #, x, y, z, occupancy, B-factor, atom type



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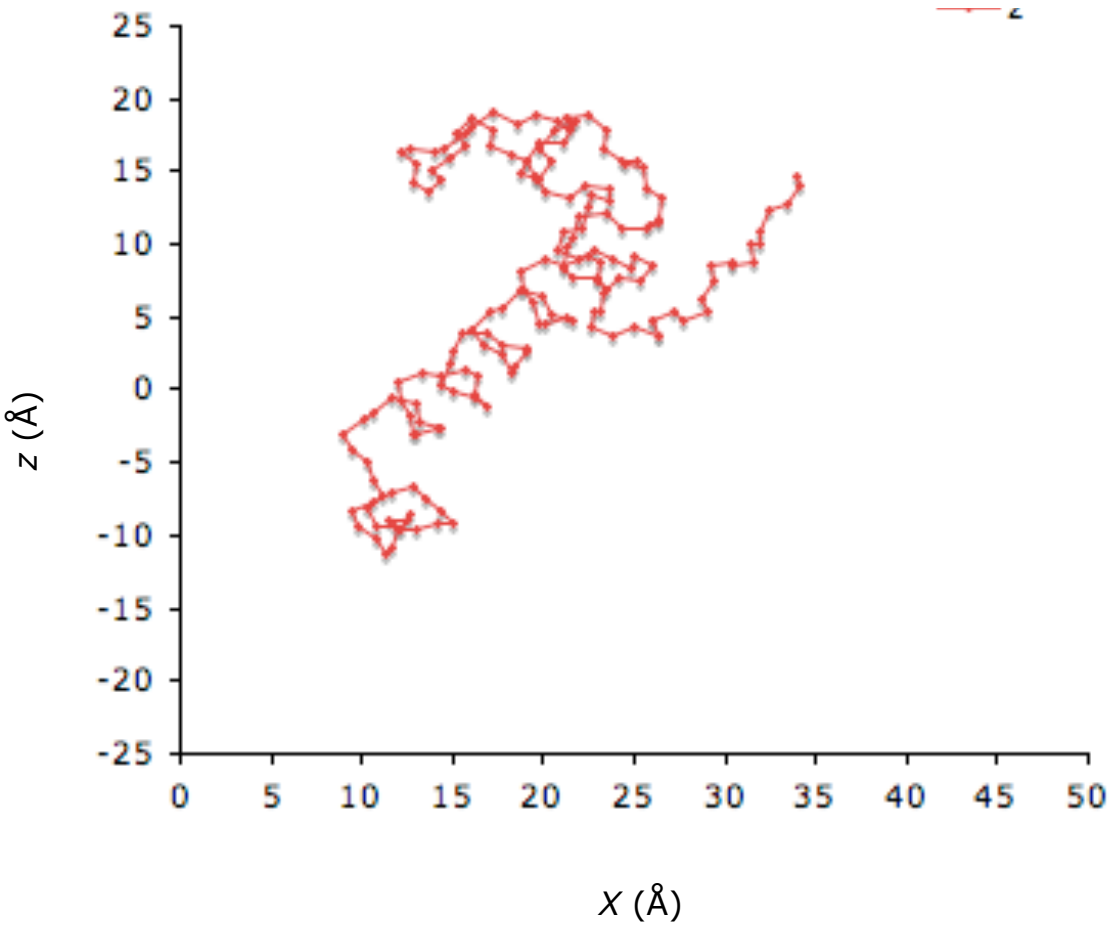
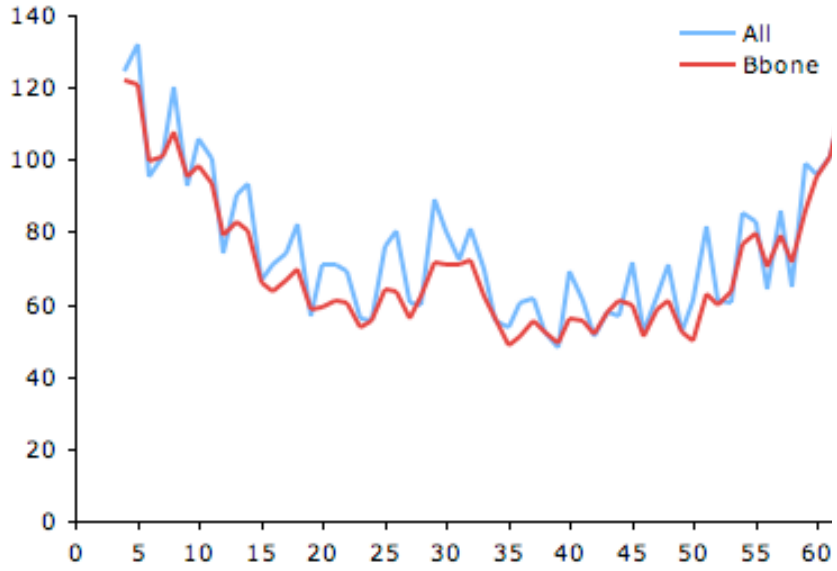
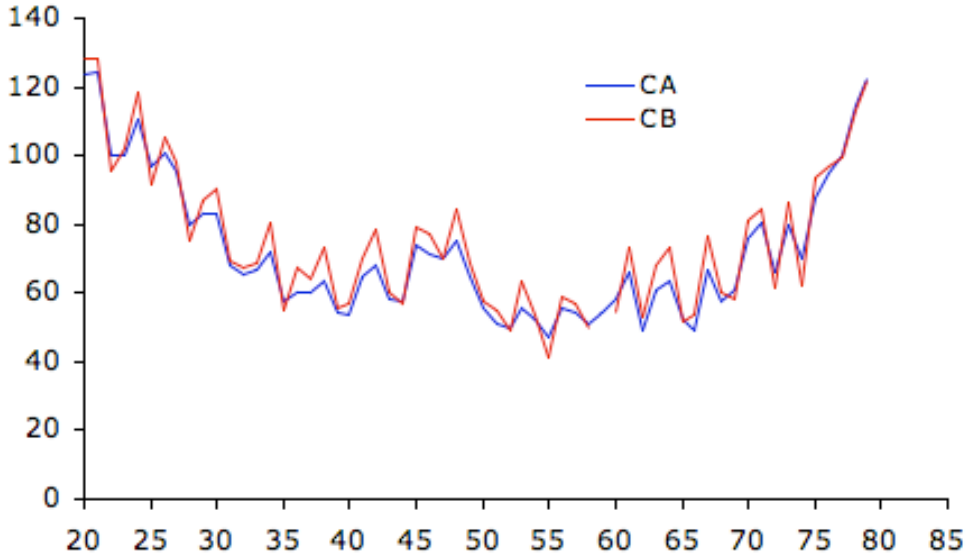
Cartesian coordinates: N, CA, C (Chain A)



PDB file 3e7l

B factors: (averages all chains; CA, CB Chain A)



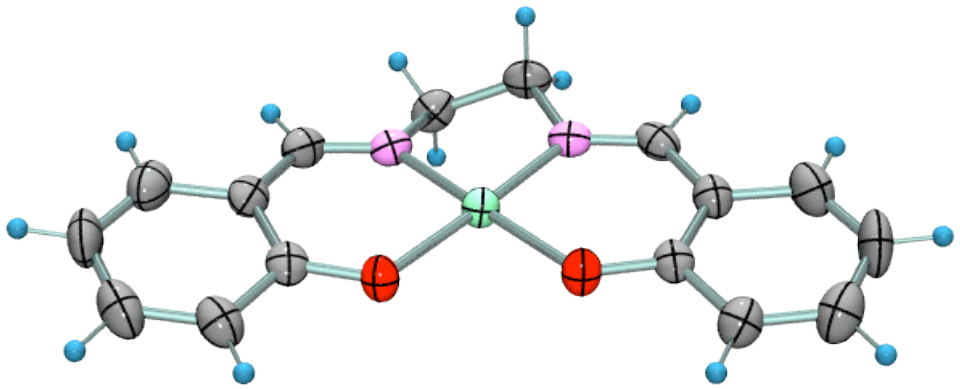


PDB file 3e7l

```
ANISOU   19  N   LEU A  22    14100  17318   9571    573   -137  -1512       N
ANISOU   20  CA  LEU A  22    13114  15959   8944    721   -260  -1765       C
ANISOU   21  C   LEU A  22    12724  15723   8423    731   -434  -1914       C
ANISOU   22  O   LEU A  22    12299  15338   8226    800   -463  -2338       O
ANISOU   23  CB  LEU A  22    12686  14934   8782    809   -337  -1457       C
ANISOU   24  CG  LEU A  22    12130  14162   8432    811   -200  -1368       C
ANISOU   25  CD1 LEU A  22    11863  13382   8313    859   -275  -1035       C
ANISOU   26  CD2 LEU A  22    11691  13692   8358    884   -129  -1767       C
```

ANISOU 'card':
ANISOU, atom #, atom name, res name, chain ID, res#, U11, U22, U33, U12, U13, U23, atom type

$$\begin{bmatrix} U11 & U12 & U13 \\ U12 & U22 & U23 \\ U13 & U23 & U33 \end{bmatrix}$$



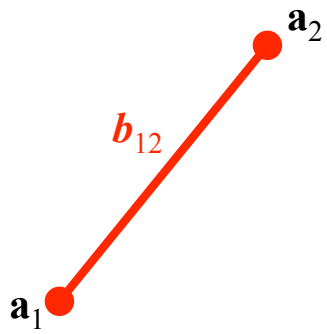
Internal coordinates: bond lengths
(distance between bonded atoms)

Atomic coordinates

$$\mathbf{a}_1 = (a_{1x},\ a_{1y},\ a_{1z}) \qquad \mathbf{a}_2 = (a_{2x},\ a_{2y},\ a_{2z})$$

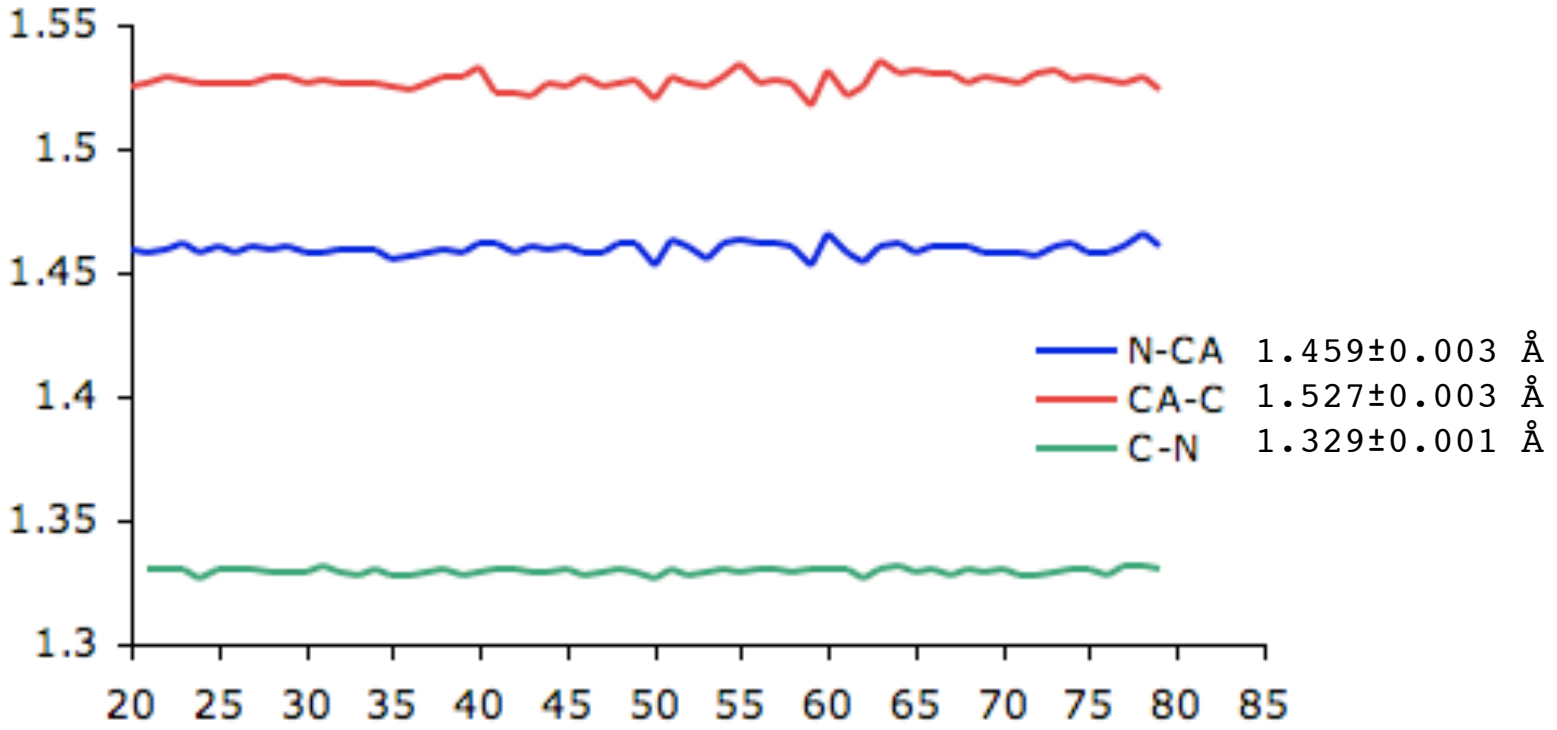
Bond length

$$b_{12} = ((a_{2x}-a_{1x})^2+(a_{2y}-a_{1y})^2+(a_{2z}-a_{1z})^2)^{1/2}$$



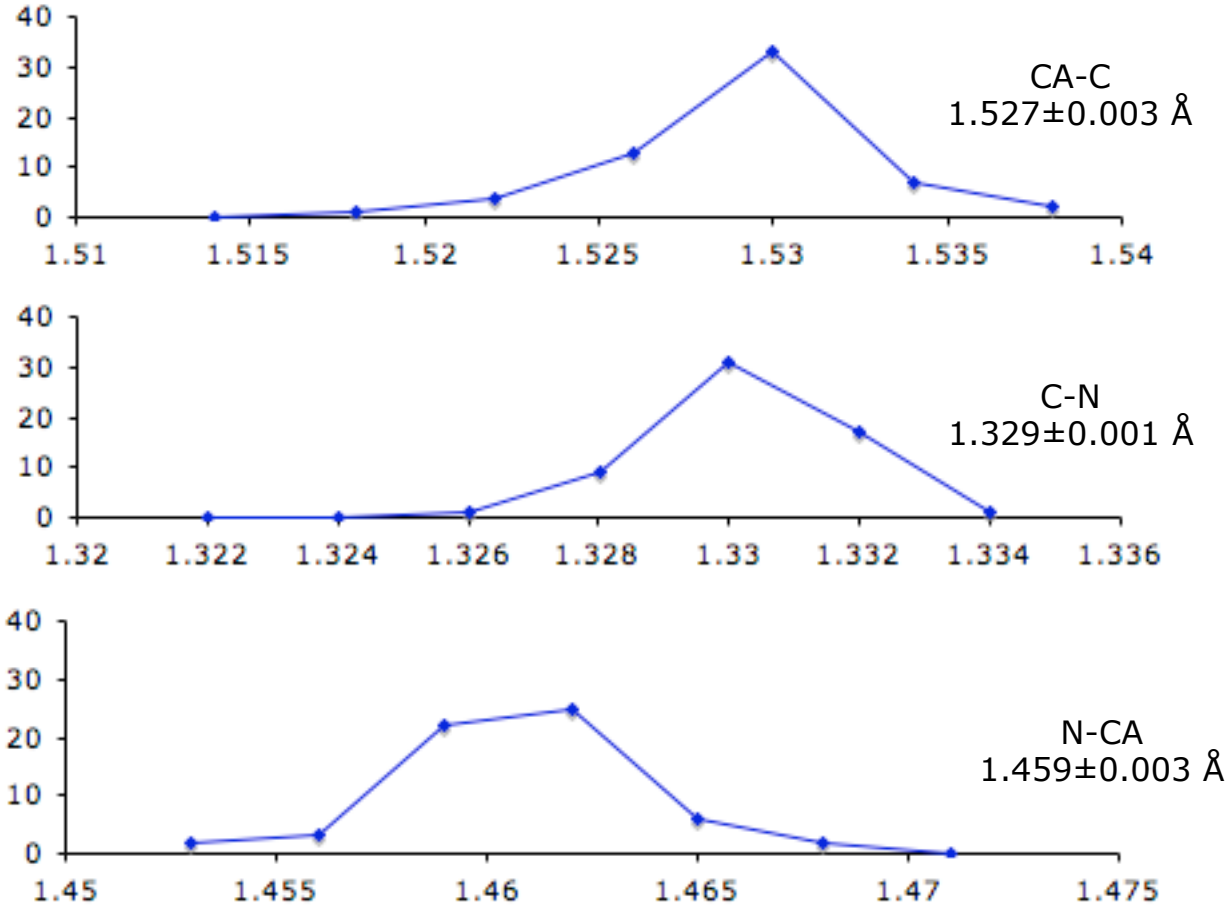
PDB file 3e7l

Bond lengths: Chain A backbone



PDB file 3e7l

Bond length histograms: Chain A backbone



Internal coordinates: valence angles
(complement of angle formed by successive chemical bonds)

Atomic coordinates

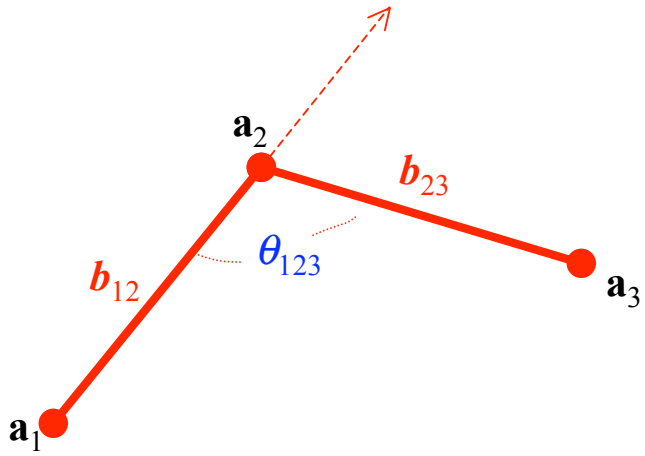
$\mathbf{a}_1 = (a_{1x}, a_{1y}, a_{1z})$ $\mathbf{a}_2 = (a_{2x}, a_{2y}, a_{2z})$ $\mathbf{a}_3 = (a_{3x}, a_{3y}, a_{3z})$

Bond vectors

$\mathbf{b}_{12} = (a_{2x}-a_{1x}, a_{2y}-a_{1y}, a_{2z}-a_{1z})$ $\mathbf{b}_{23} = (a_{3x}-a_{2x}, a_{3y}-a_{2y}, a_{3z}-a_{2z})$

Scalar product

$$\mathbf{b}_{12}\cdot\mathbf{b}_{23} = (a_{2x}-a_{1x})(a_{3x}-a_{2x})+(a_{2y}-a_{1y})(a_{3y}-a_{2y})+(a_{2z}-a_{1z})(a_{3z}-a_{2z})$$



$$\mathbf{b}_{12}\cdot\mathbf{b}_{23} = b_{12}b_{23}\cos(\pi-\theta_{123})$$

$$\cos\theta_{123} = -\mathbf{b}_{12}\cdot\mathbf{b}_{23}/(b_{12}b_{23})$$

$$\cos(\pi-\theta_{123}) = \cos\pi\cos\theta_{123} + \sin\pi\sin\theta_{123} = -\cos\theta_{123}$$

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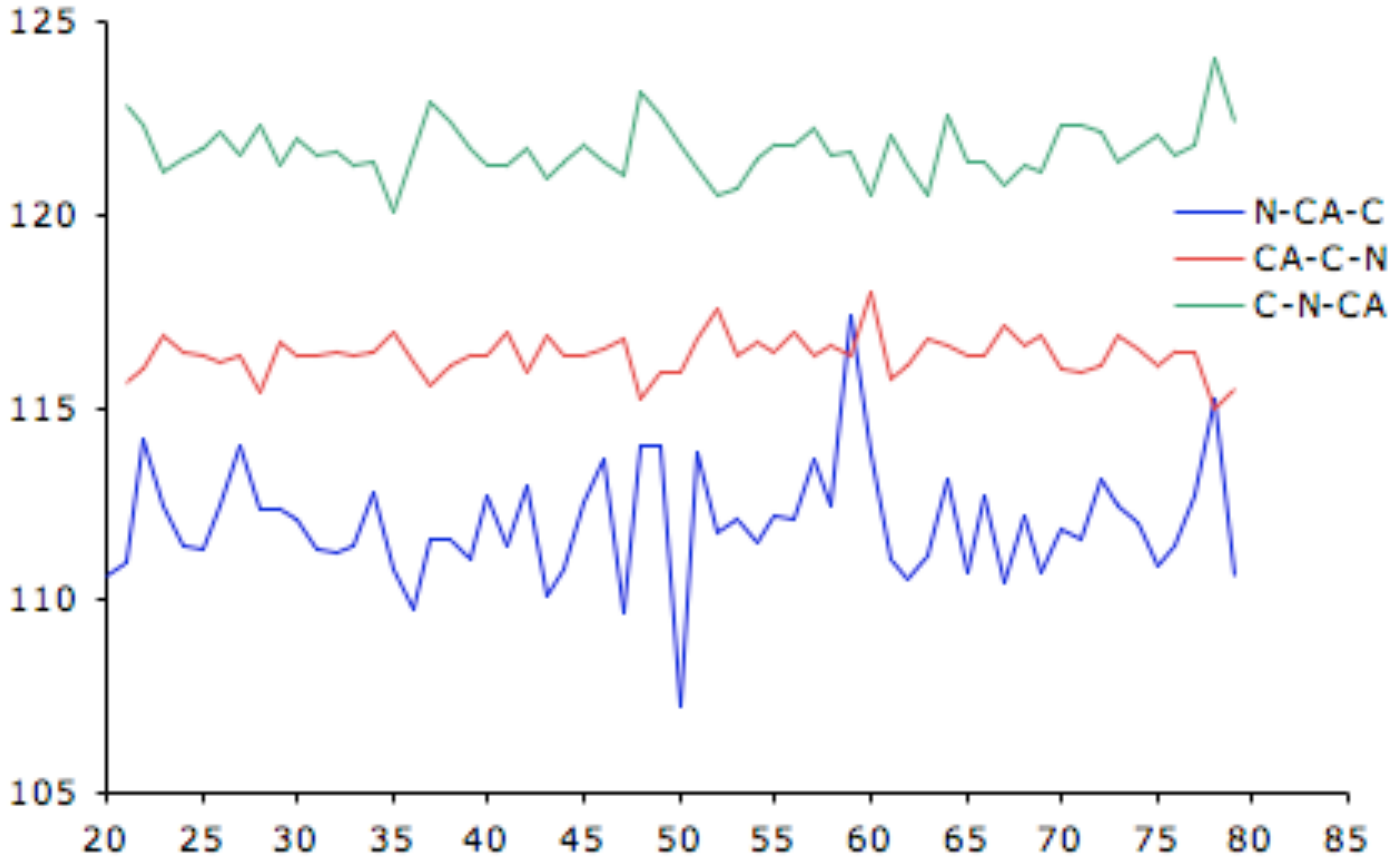
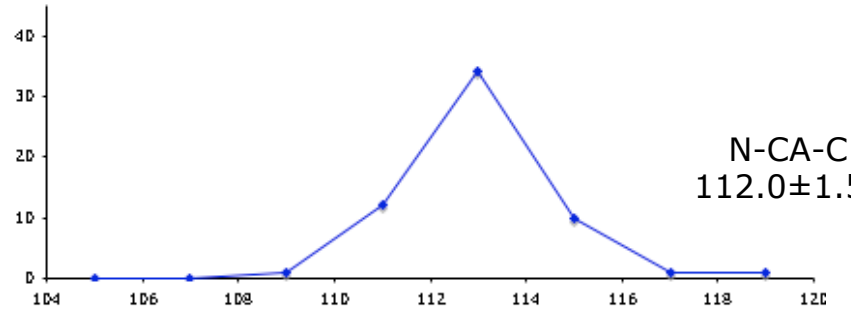
Valence angles: Chain A backbone



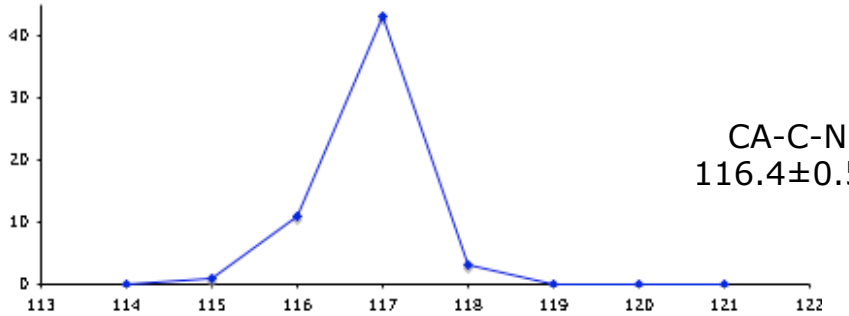
112.0±1.5°
116.4±0.5°
121.7±0.7°

PDB file 3e7l

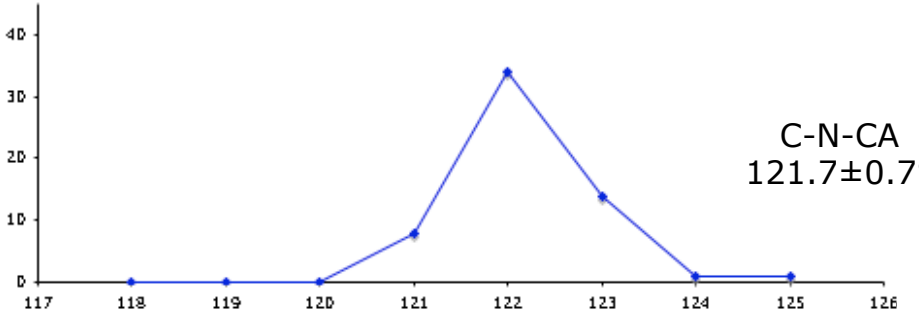
Valence angle histograms: Chain A backbone



N-CA-C
112.0±1.5°



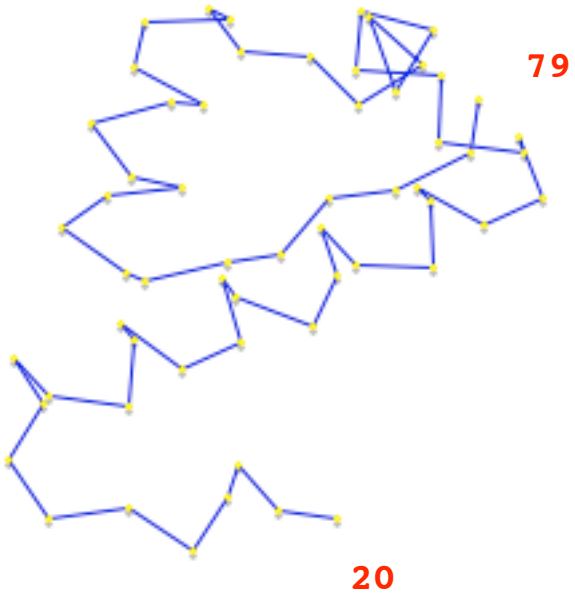
CA-C-N
116.4±0.5°



C-N-CA
121.7±0.7°

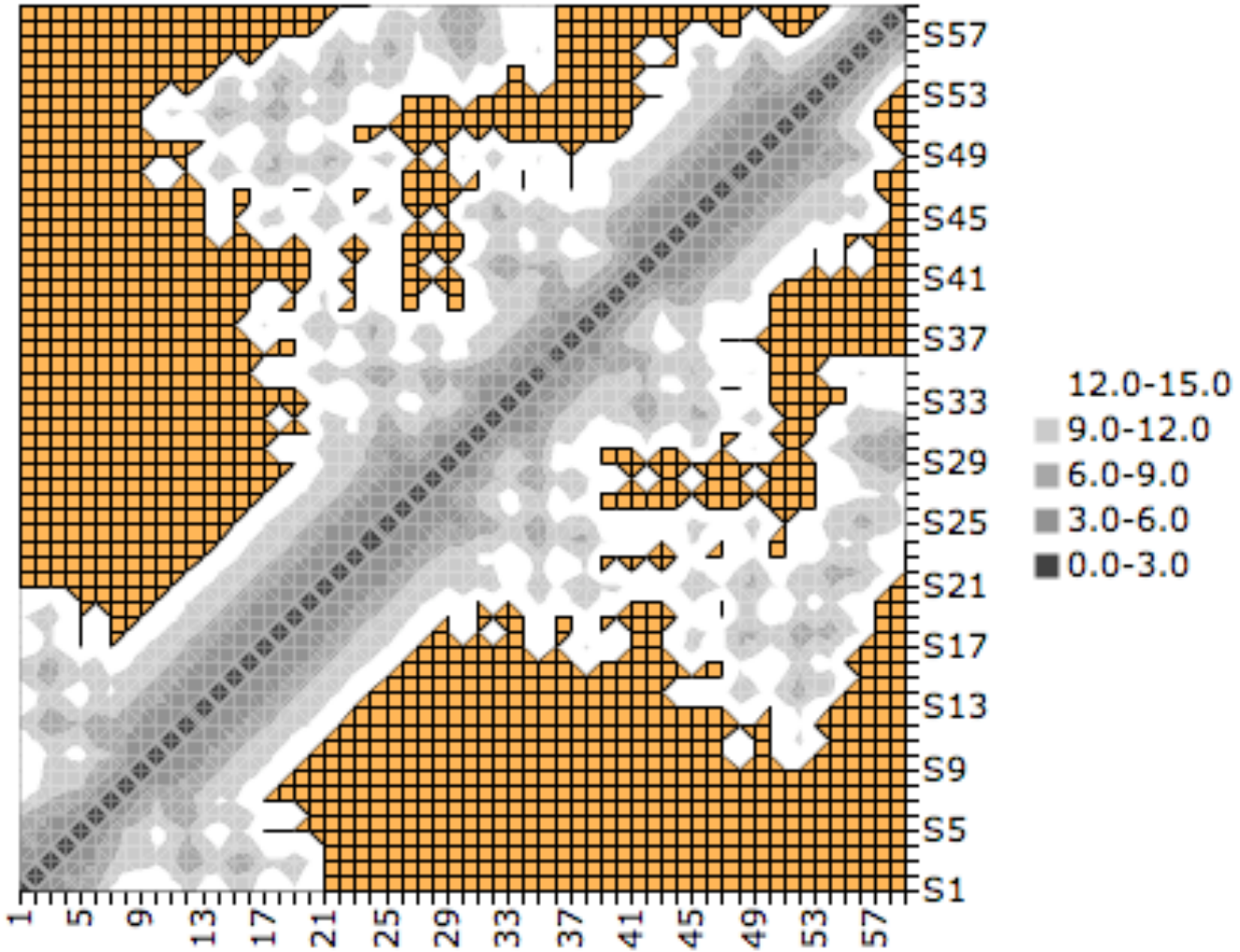
PDB file 3e7l

Exercise:
Compare the long-range folding of chains A and B (in terms of CA···CA distances).



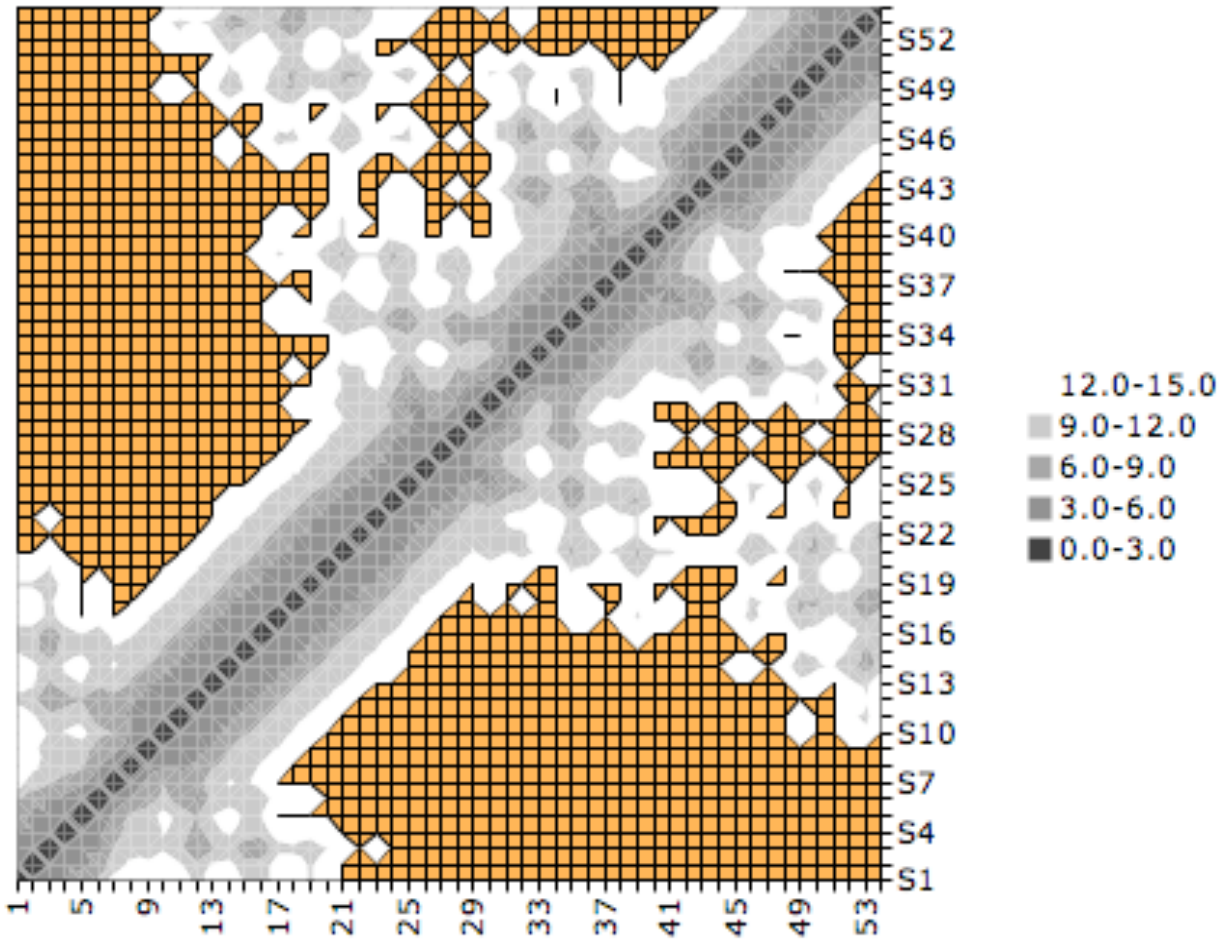
PDB file 3e7l

Distance plot: Chain A, 60 CA atoms



PDB file 3e7l

Distance plot: Chain B, 54 CA atoms



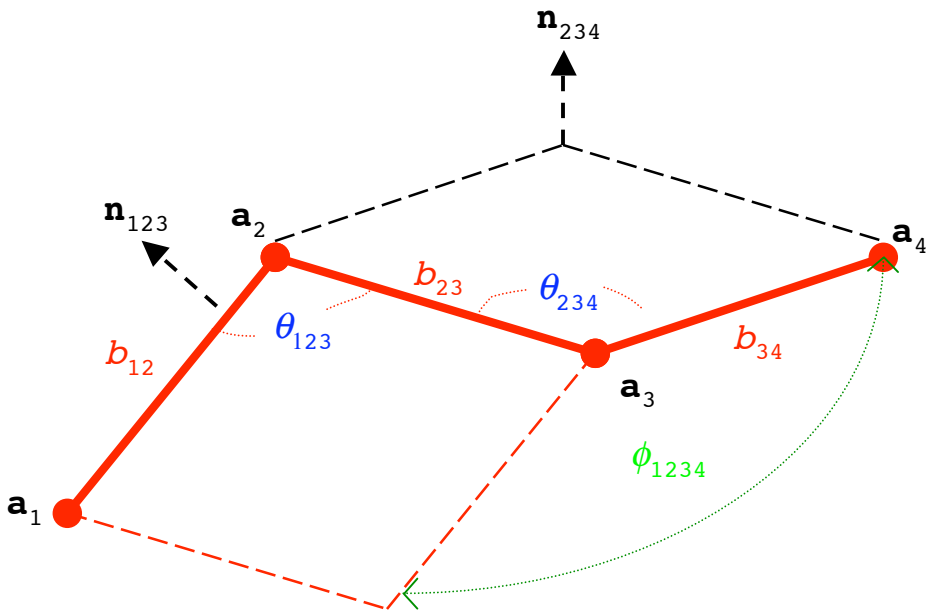
Internal coordinates: torsion/dihedral angles
(angle between planes containing successive pairs of chemical bonds)

Atomic coordinates

$\mathbf{a}_1 = (a_{1x}, a_{1y}, a_{1z})$ $\mathbf{a}_2 = (a_{2x}, a_{2y}, a_{2z})$ $\mathbf{a}_3 = (a_{3x}, a_{3y}, a_{3z})$ $\mathbf{a}_3 = (a_{4x}, a_{4y}, a_{4z})$

Bond vectors

$\mathbf{b}_{12}=(a_{2x}-a_{1x}, a_{2y}-a_{1y}, a_{2z}-a_{1z})$ $\mathbf{b}_{23}=(a_{3x}-a_{2x}, a_{3y}-a_{2y}, a_{3z}-a_{2z})$ $\mathbf{b}_{34}=(a_{4x}-a_{3x}, a_{4y}-a_{3y}, a_{4z}-a_{3z})$



$\mathbf{n}_{123} = \mathbf{b}_{12} \times \mathbf{b}_{23}$

$\mathbf{n}_{234} = \mathbf{b}_{23} \times \mathbf{b}_{34}$

$\mathbf{n}_{123} \cdot \mathbf{n}_{234} = \cos\phi_{1234}$

$(\mathbf{n}_{123} \times \mathbf{n}_{234}) \cdot \mathbf{b}_{23} > 0 \Rightarrow \phi_{1234} > 0$

$(\mathbf{n}_{123} \times \mathbf{n}_{234}) \cdot \mathbf{b}_{23} < 0 \Rightarrow \phi_{1234} < 0$

Vector/cross product

$$\mathbf{v}_1 \times \mathbf{v}_2 = \begin{vmatrix} i & j & k \\ v_{1x} & v_{1y} & v_{1z} \\ v_{2x} & v_{2y} & v_{2z} \end{vmatrix}$$

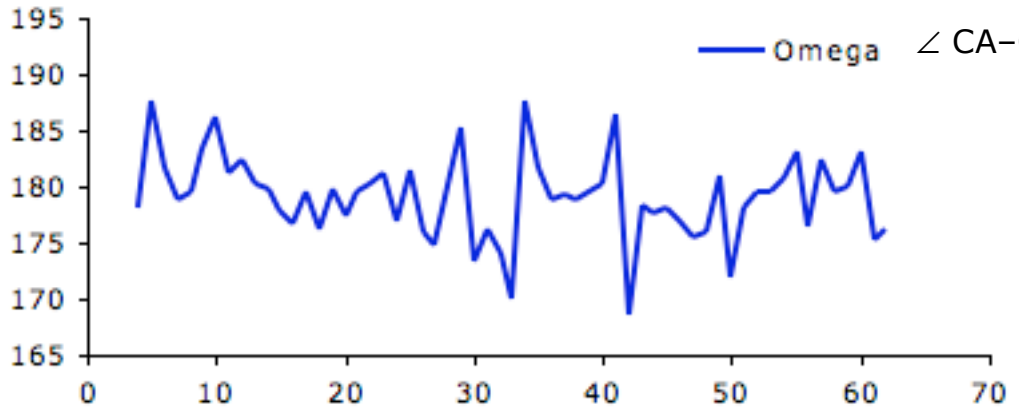
$$= \left(v_{1y}v_{2z} - v_{2y}v_{1z}\right) i + \left(v_{1z}v_{2x} - v_{2z}v_{1x}\right) j + \left(v_{1x}v_{2y} - v_{2x}v_{1y}\right) k$$

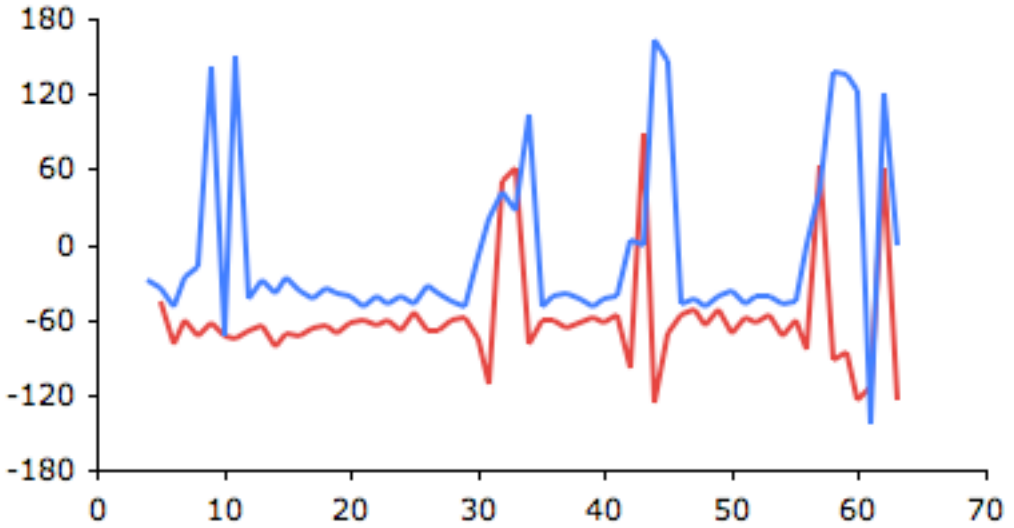
$$= \left[\left(v_{1y}v_{2z} - v_{2y}v_{1z}\right), \left(v_{1z}v_{2x} - v_{2z}v_{1x}\right), \left(v_{1x}v_{2y} - v_{2x}v_{1y}\right)\right]$$

$$= \left(c_1, c_2, c_3\right)$$

PDB file 3e7l

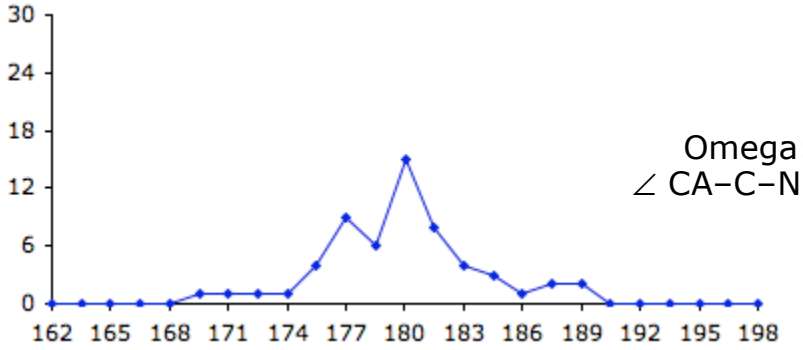
Torsion angle vs. PDB#
Chain A



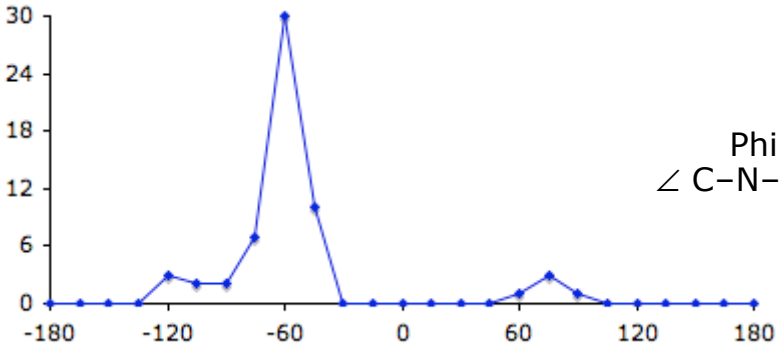


PDB file 3e7l

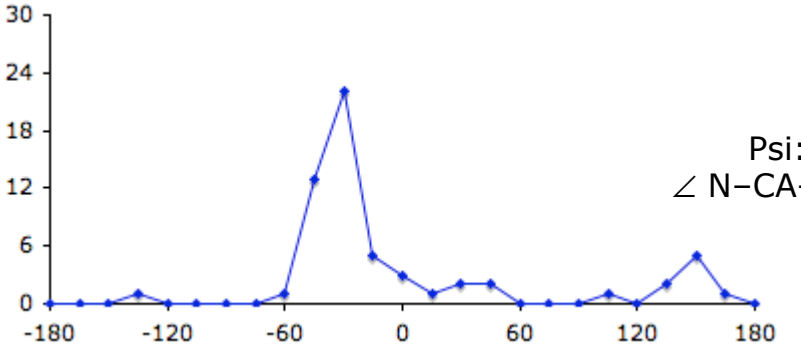
Torsion angle histograms
Chain A



Omega:
∠ CA–C–N–CA



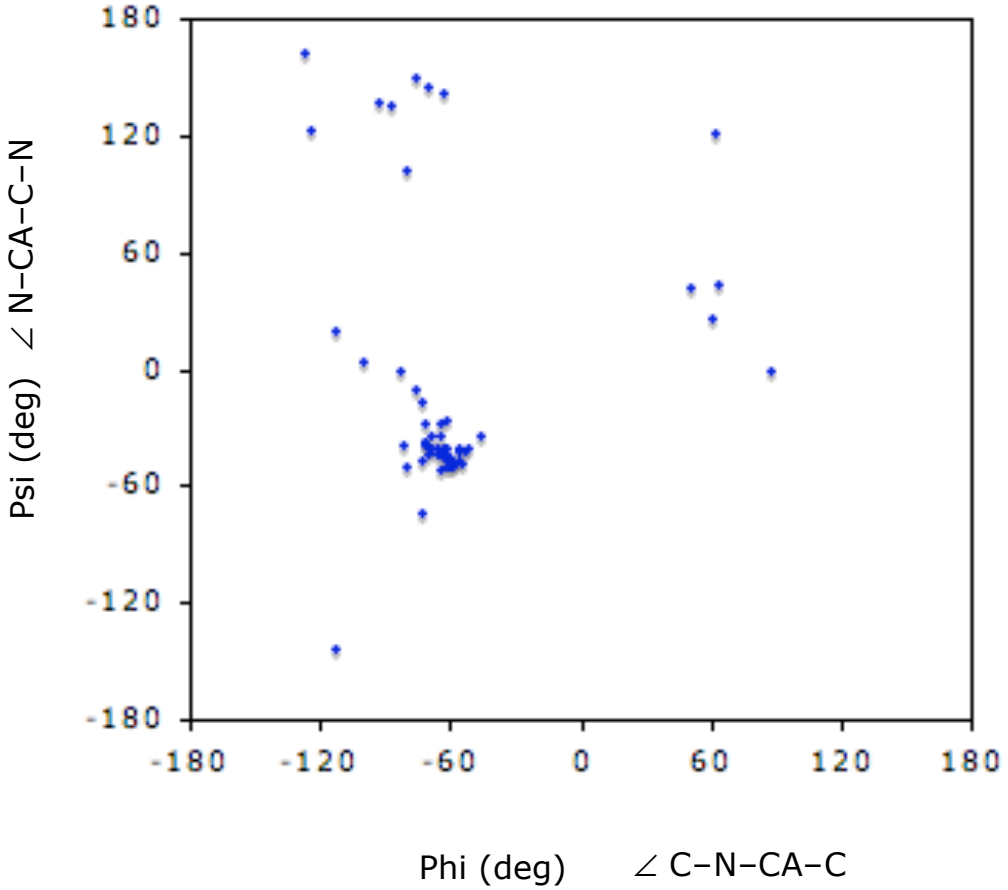
Phi:
∠ C–N–CA–C



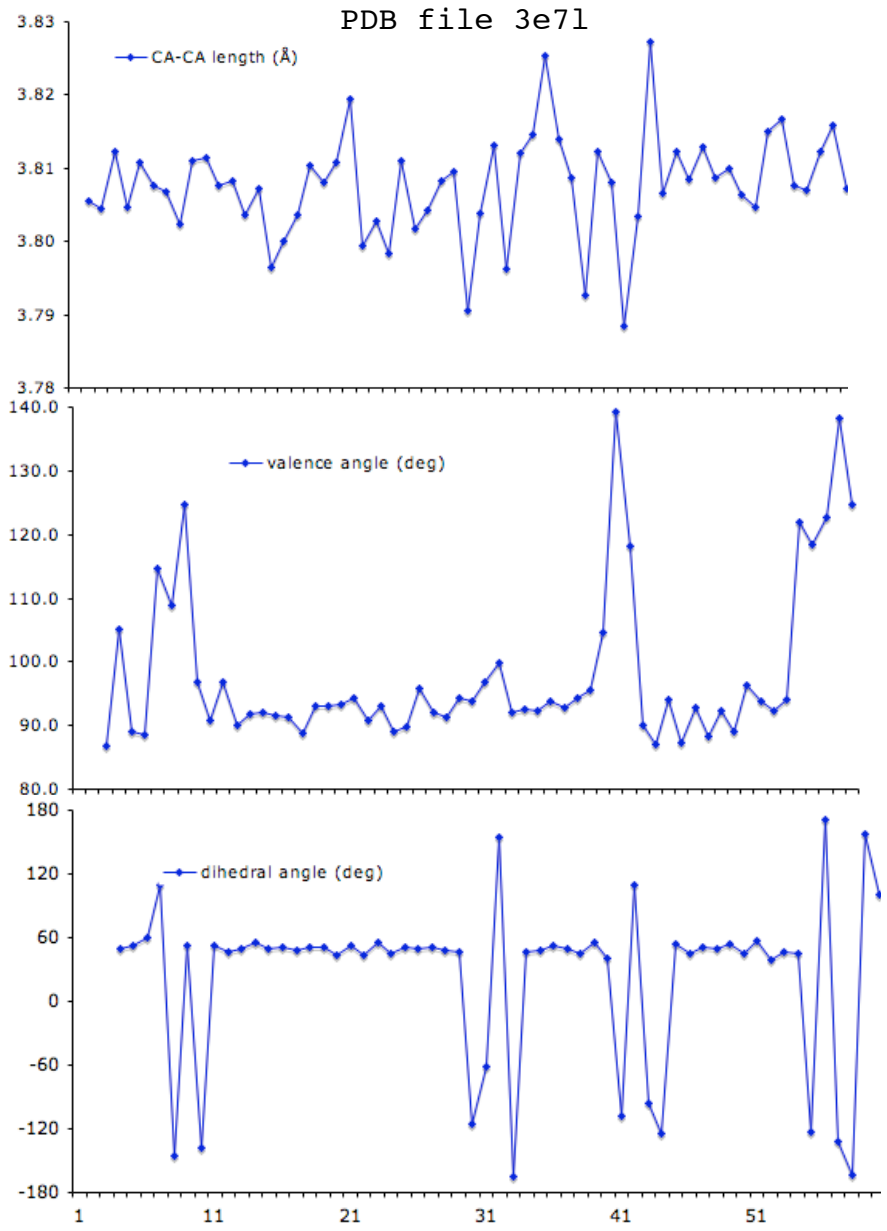
Psi:
∠ N–CA–C–N

PDB file 3e7l

Phi-Psi scatter plot
Chain A



CA internal parameters
Chain A



59 CA-CA lengths (Å)

58 ∠ CA–CA–CA angles (deg)

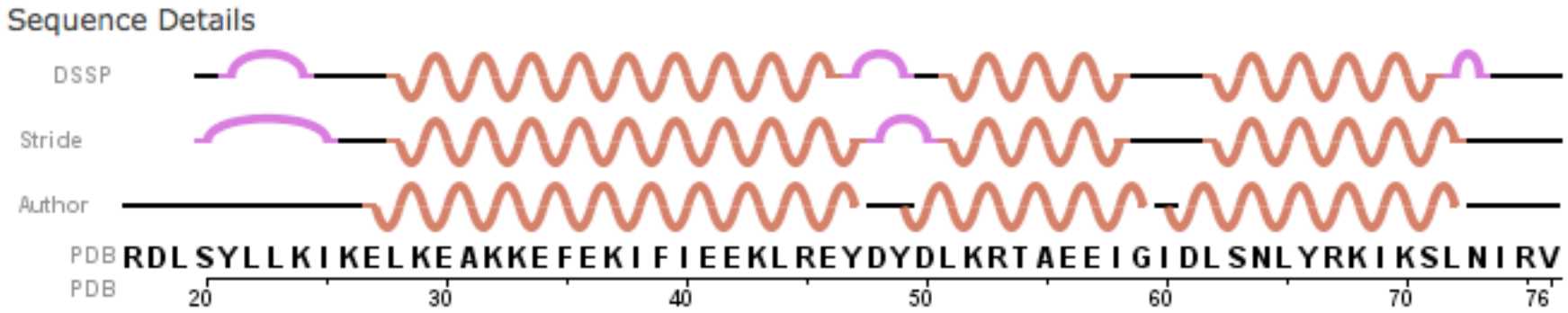
57 ∠ CA–CA–CA–CA dihedrals (deg)

The repetition of local chemical parameters in successive residues generates a regular helical structure.

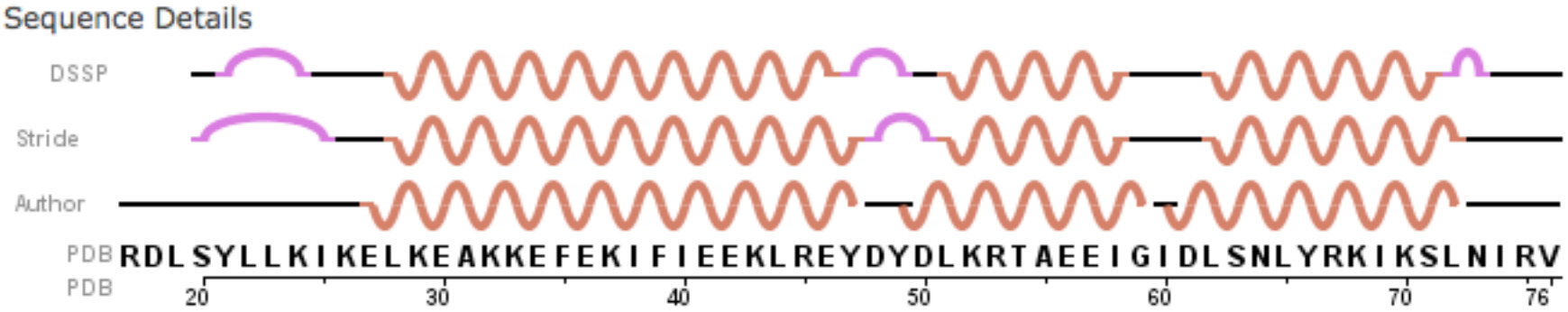
Three segments of chain A (involving residues 28-49, 54-60, and 62-74) show such repeating patterns:

CA-CA bond lengths ~3.81 Å
CA-CA-CA valence angles ~90°
CA-CA-CA-CA dihedral angles ~50°

The PDB includes the following helical residue assignments for `3e7l`:



The PDB image reflects the helical assignments.



Color-coded ribbons are drawn through the helical fragments: chain A **h1**, **h2**, **h3**; chain B **h1**, **h2**, **h3**.

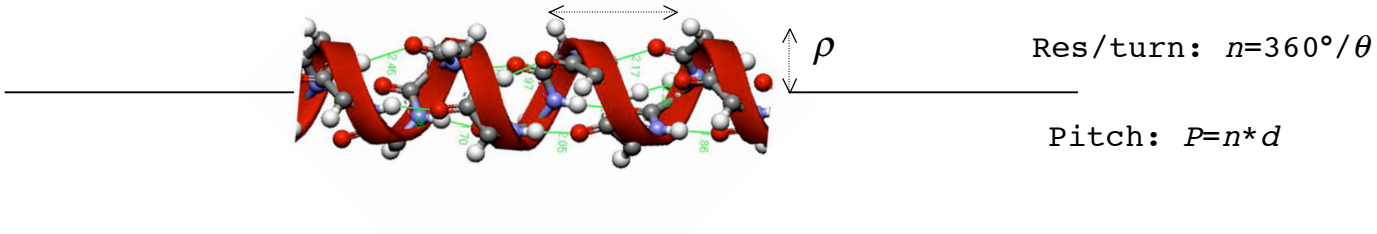
The values of the repeated bond lengths r, valence angles ϕ, and dihedral angles τ determine the radius ρ, cylindrical angle θ, and displacement d of the helix.

$$\cos\left(\theta/2\right) = \cos\left(\tau/2\right)\sin\left(\phi/2\right)$$

$$d\sin\left(\theta/2\right) = r\sin\left(\tau/2\right)\sin\left(\phi/2\right)$$

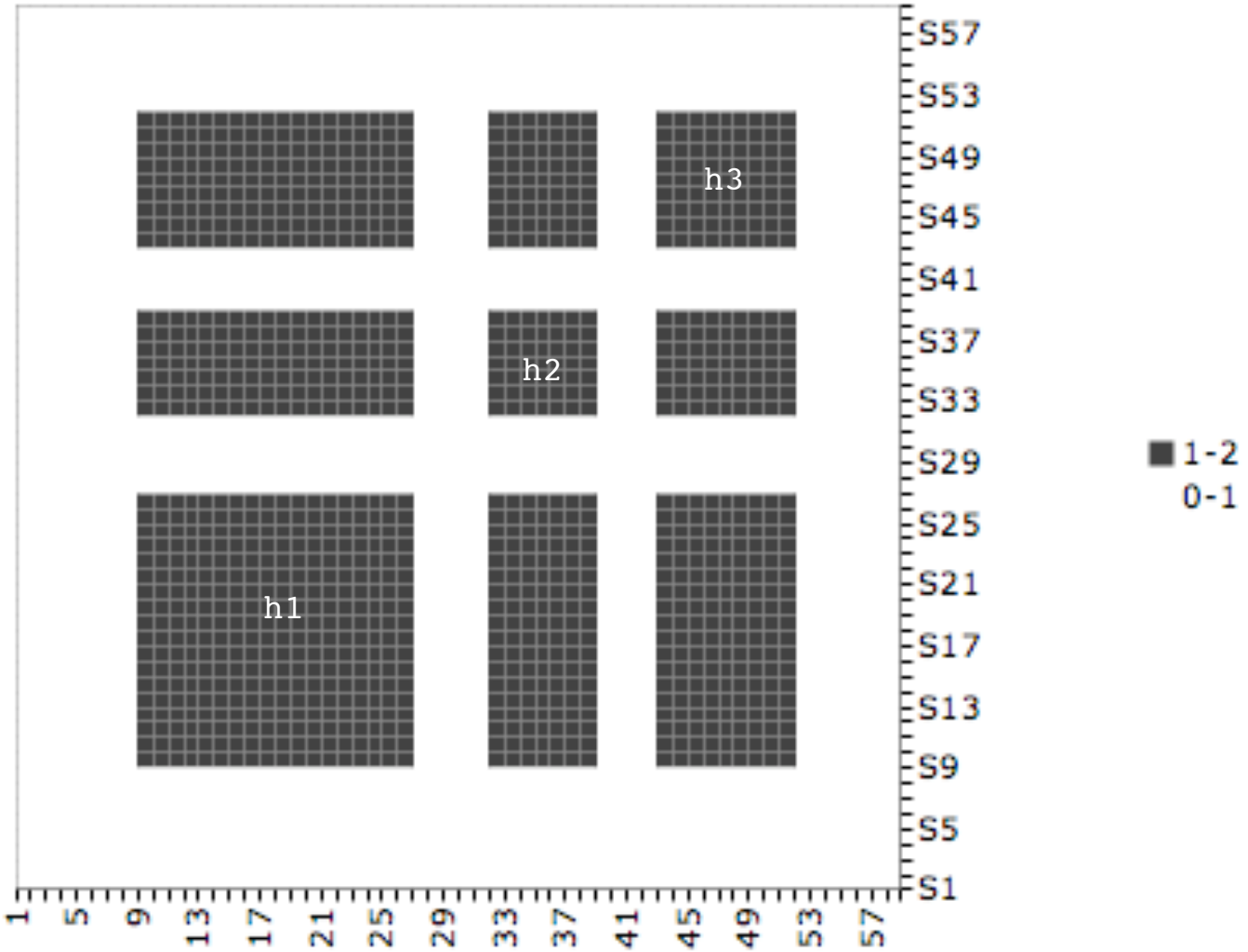
$$2\rho^2\left(1 - \cos\theta\right) + d^2 = r^2$$

Miyazawa, T. (1961) Molecular vibrations and structure of high polymers. II. Helical parameters of infinite polymer chains as functions of bond lengths, bond angles, and internal rotation angles. *J. Poly. Sci.*, **55**, 215-231.



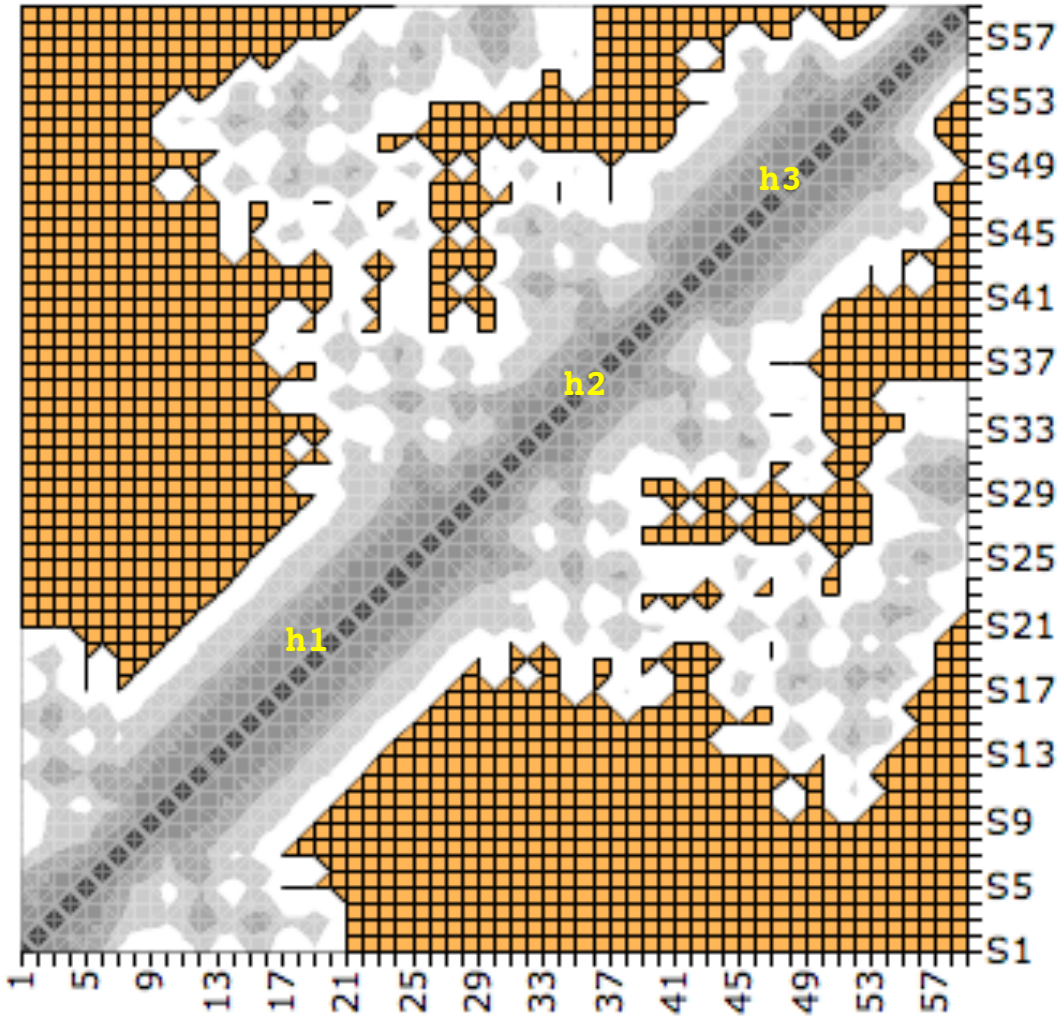
PDB file 3e7l

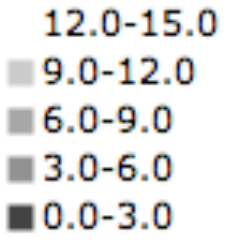
Helix plot: Chain A



PDB file 3e7l

Distance plot: Chain A, CA atoms





The three helices show characteristic patterns along the diagonal.

The image also reveals the long-range contacts between h1 and h3 and between h1 and the chain termini.

Use the Jmol viewer to explore the features of the structure.

3E7L_CA_A.pdb is a smaller pdb-formatted file with only the CA atoms of chain A of 3E7L.
The Jena website allows the user to upload pdb-formatted files like this:
http://www.fli-leibniz.de/cgi-bin/ImgLib.pl?CODE=3E7L

PDB file 3e7l

Exercise (due September 10, 2009):
Find the pseudo 'valence' angles between successive helical fragments in chains A, B, C, D (*i.e.*, h1, h2 and h2, h3 in each chain)