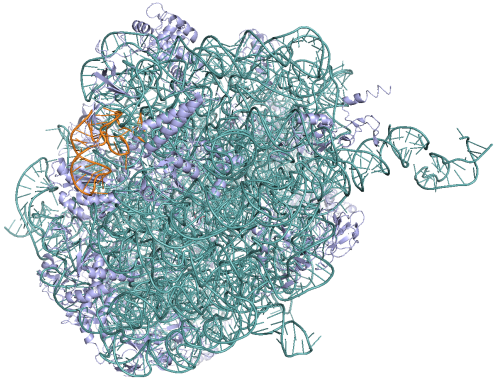
GEOMETRIC PROPERTIES OF RIBOSOMAL STRUCTURES

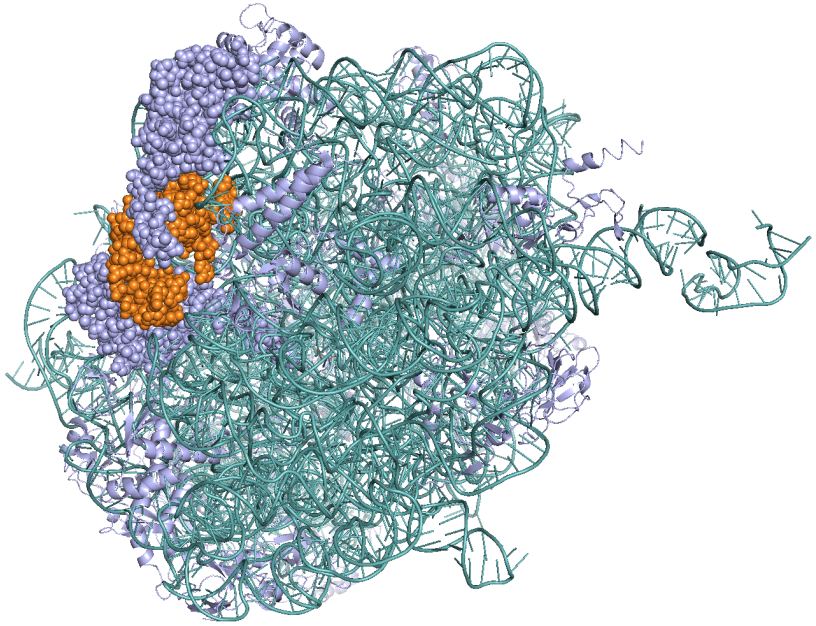
Caitlin Davis, 2019 DIMACS REU



E. Coli ribosome

Ribosomes

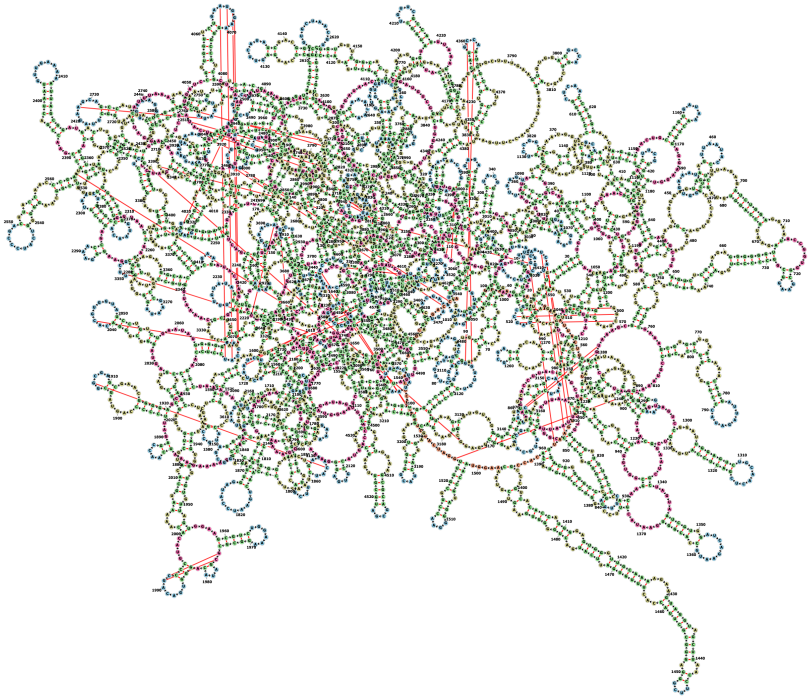
- Location of protein synthesis
- Relatively similar across all species
- Composed of RNA and proteins



E. Coli ribosome

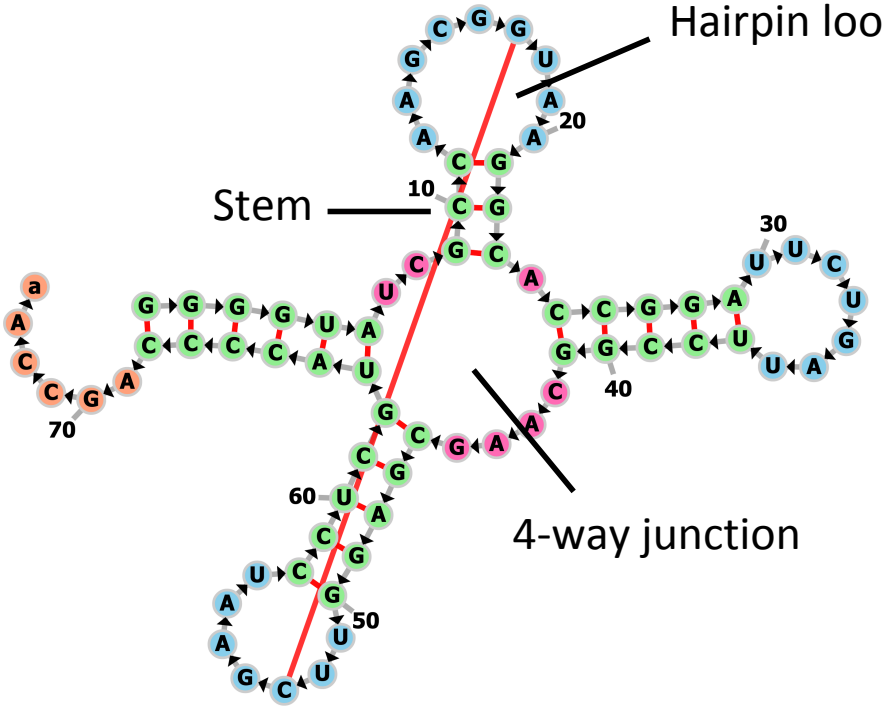
RNA secondary structure

- Typically single-stranded, but bases have some tendency to pair



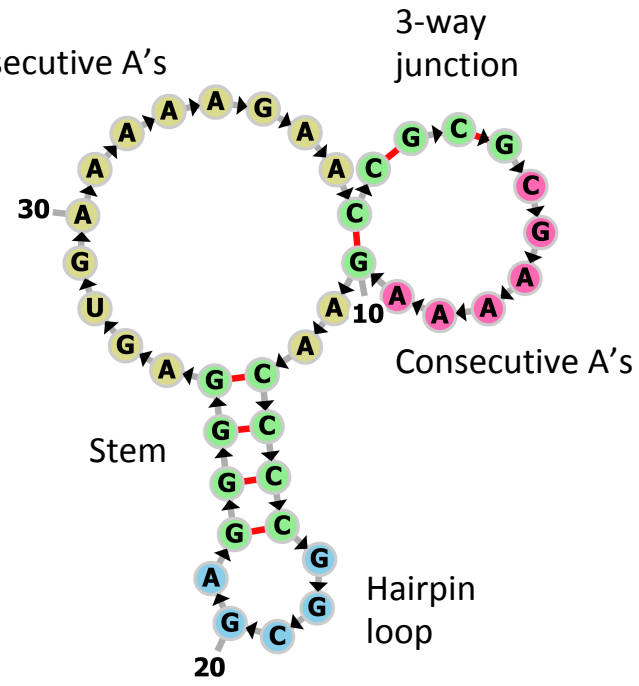
RNA secondary structure

- Often made up of simple, commonly occurring motifs



E. coli transfer RNA molecule

Motif from E. Coli ribosome



2D representation

3D representation

Questions

- In which ribosomes does this motif appear?
- How does the motif differ among ribosomes?

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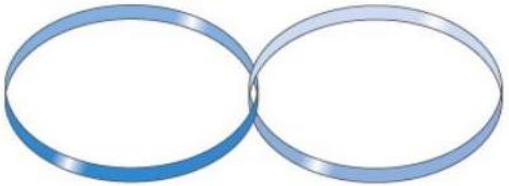
Motif from E. coli ribosome 3J5L

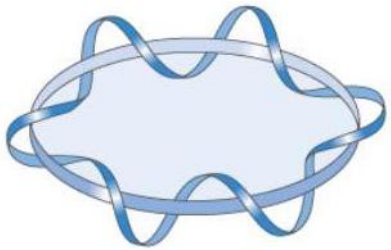
Motif from E. coli ribosome 3JA1

Topological and geometric properties

- Used to study circular DNA and other nucleic acid structures which are constrained at both ends
- Linking number—describes the number of times two curves wrap around each other



$Lk = 1$
(a)

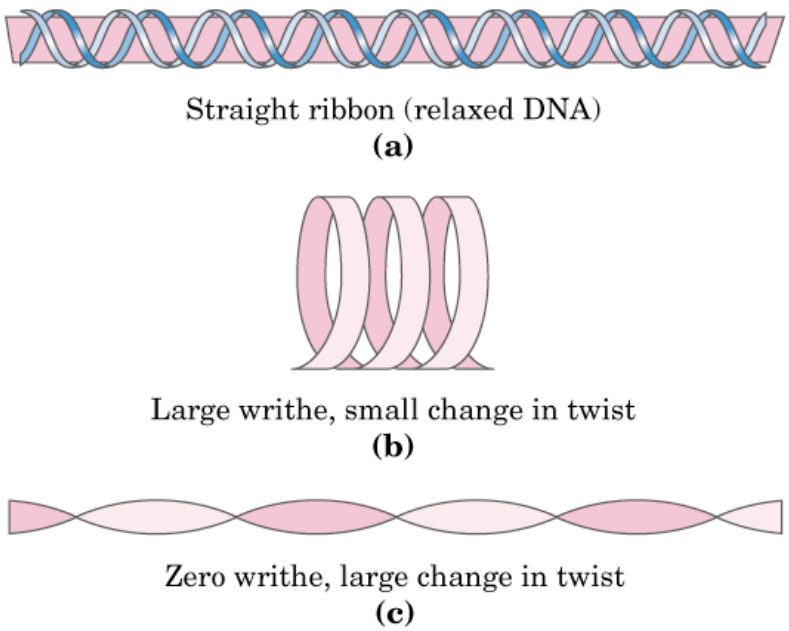


$Lk = 6$
(b)

Nelson, David L., Albert L. Lehninger, and Michael M. Cox. *Lehninger Principles of Biochemistry*. Macmillan, 2008.

Topological and geometric properties

- Twist—describes the rate of rotation of one curve about another
- Writhing number—describes the non-planarity and non-sphericity of a curve



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Writing number

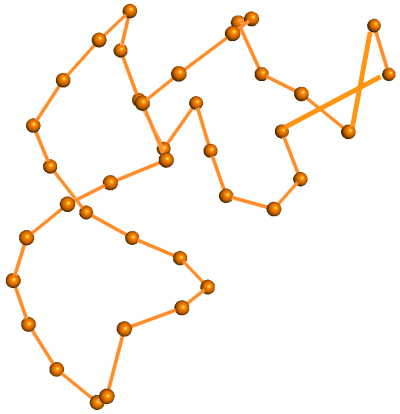
- The writing number of a smooth curve can be expressed as a Gauss integral:

$$\mathrm{Wr}(C) = \frac{1}{4\pi} \oint \oint \frac{t\left(s'\right) \times t(s) \cdot \left(\mathbf{r}\left(s'\right) - \mathbf{r}(s)\right)}{|\mathbf{r}(s') - \mathbf{r}(s)|^3} \mathrm{d}s \mathrm{d}s'$$

Non-smooth curves

- Geometric information about a molecule consists of the coordinates of all atoms in the molecule
- Instead of fitting a smooth curve to these points, we can study the molecule as a piecewise linear curve

Motif from E. coli ribosome 3J5L



Discrete curve representation of motif

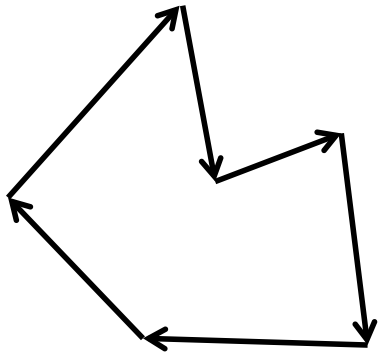
Discrete writhing number

- We compute the discrete writhing number by summing the contribution of each pair of edges in the curve

$$Wr\left(\{\mathbf{v}_i\}\right) = \frac{1}{2\pi}\sum_{p,q} w^{pq}$$

- Each pair of edges contributes a quantity involving four dihedral angles:

$$w^{pq} = \xi^{pq}(1,0) + \xi^{pq}(0,1) - \xi^{pq}(1,1) - \xi^{pq}(0,0)$$



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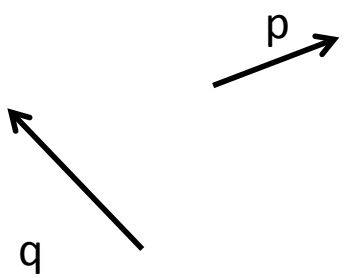

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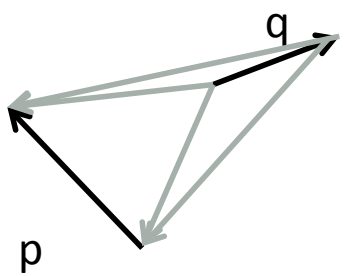

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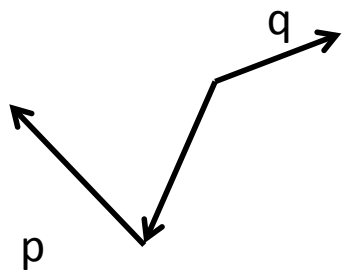

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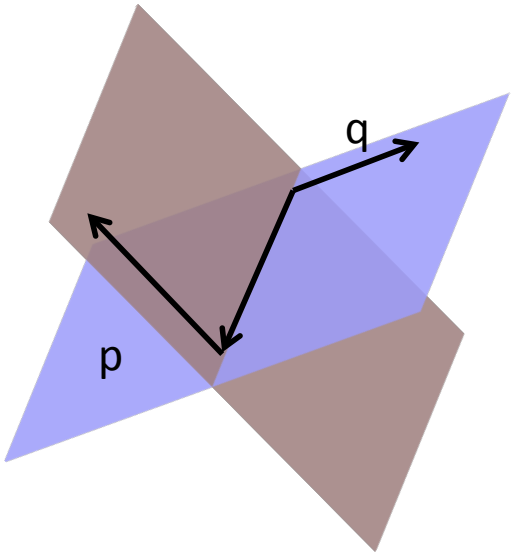
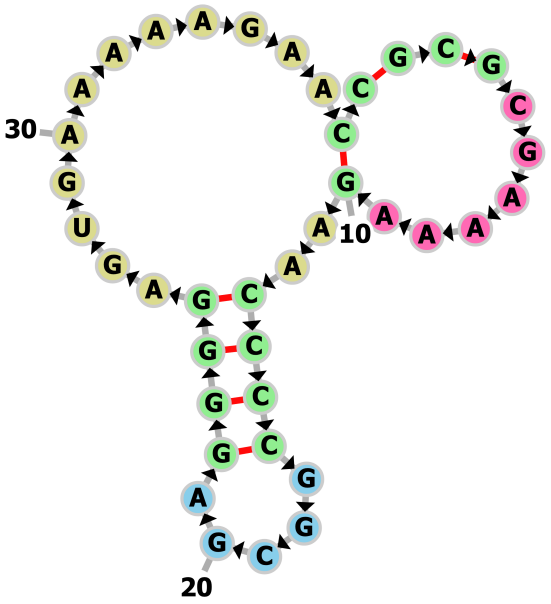


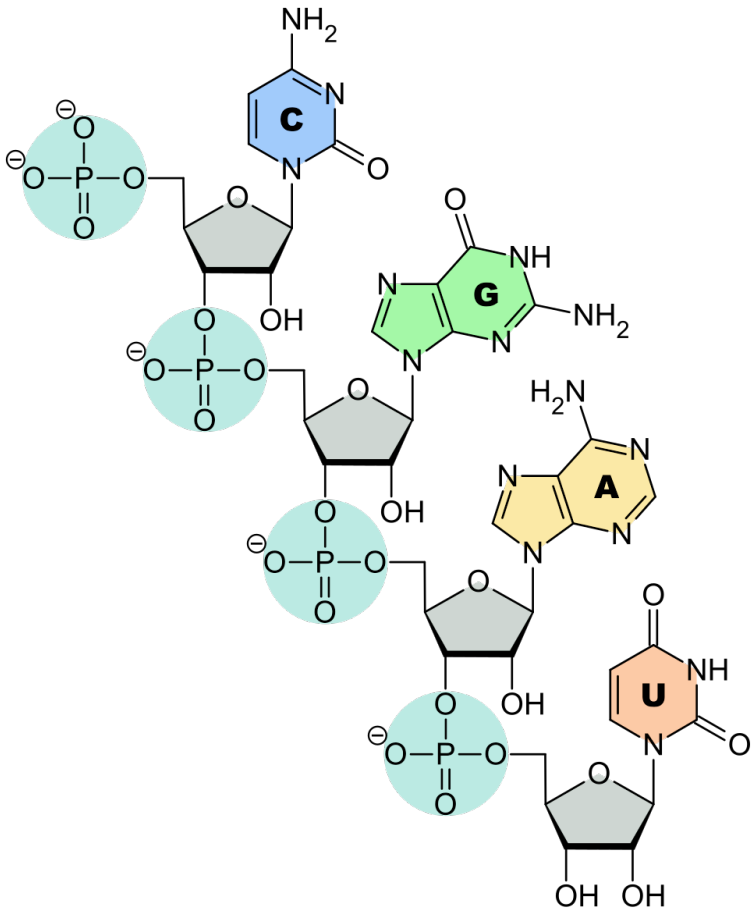
Motif from E. Coli ribosome



2D representation

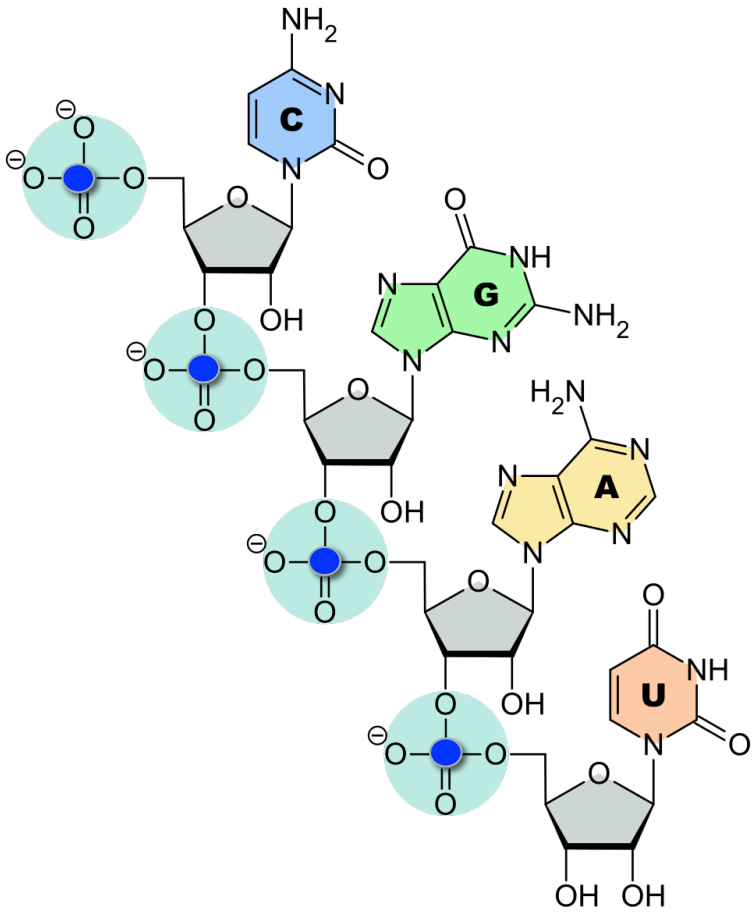
3D representation

RNA structure



https://commons.wikimedia.org/wiki/File:RNA-Nucleobases.svg

RNA structure



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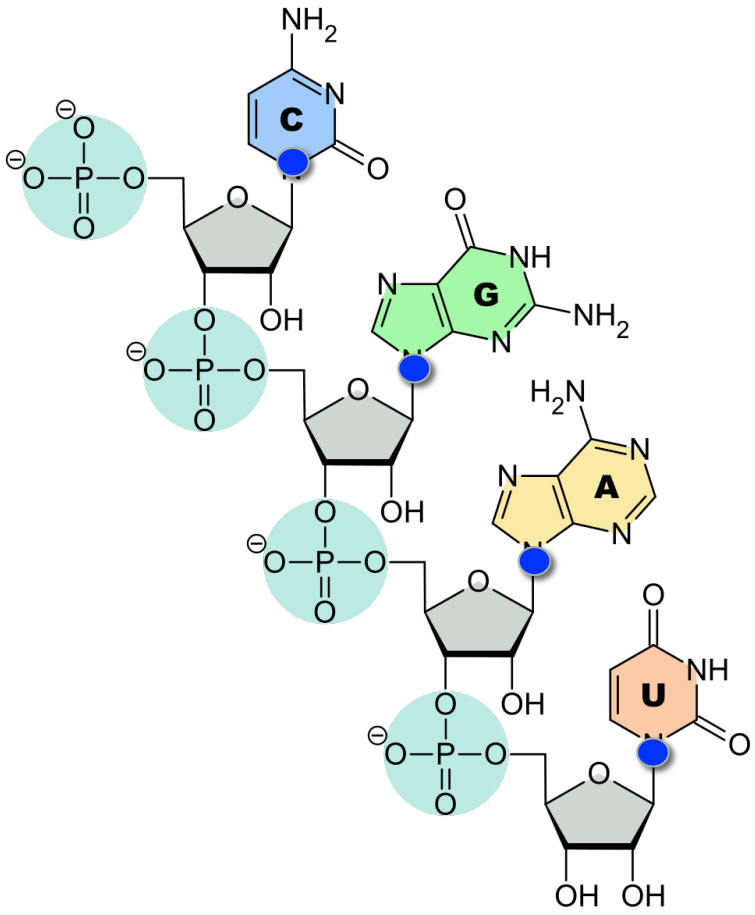
RNA structure



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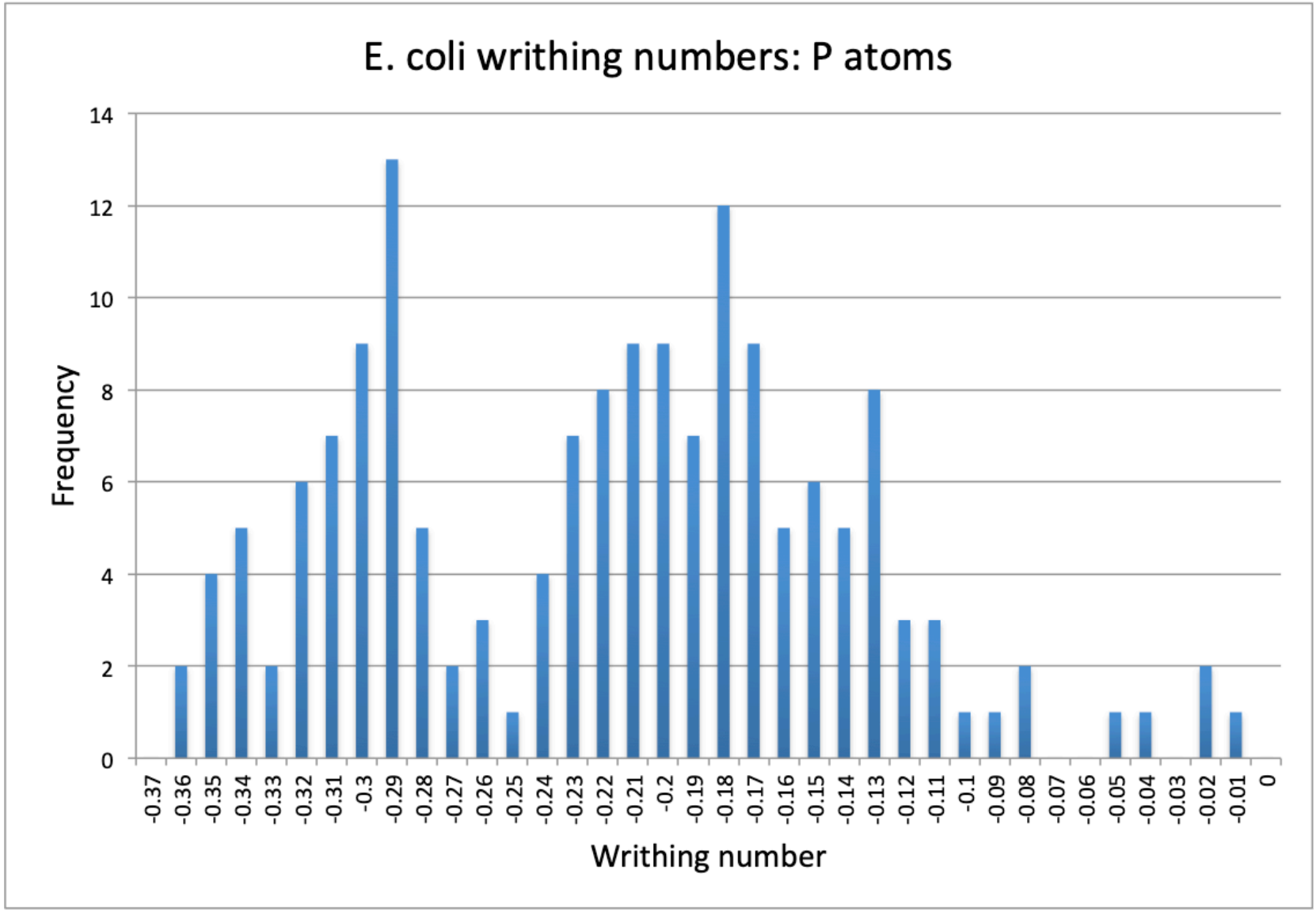
Questions

- How does the choice of vertices affect the writhing number of the motif?
- How does the writhing number of the motif vary across species?
- How does the writhing number of the motif vary across ribosomes of the same species?

Initial observations: E. coli



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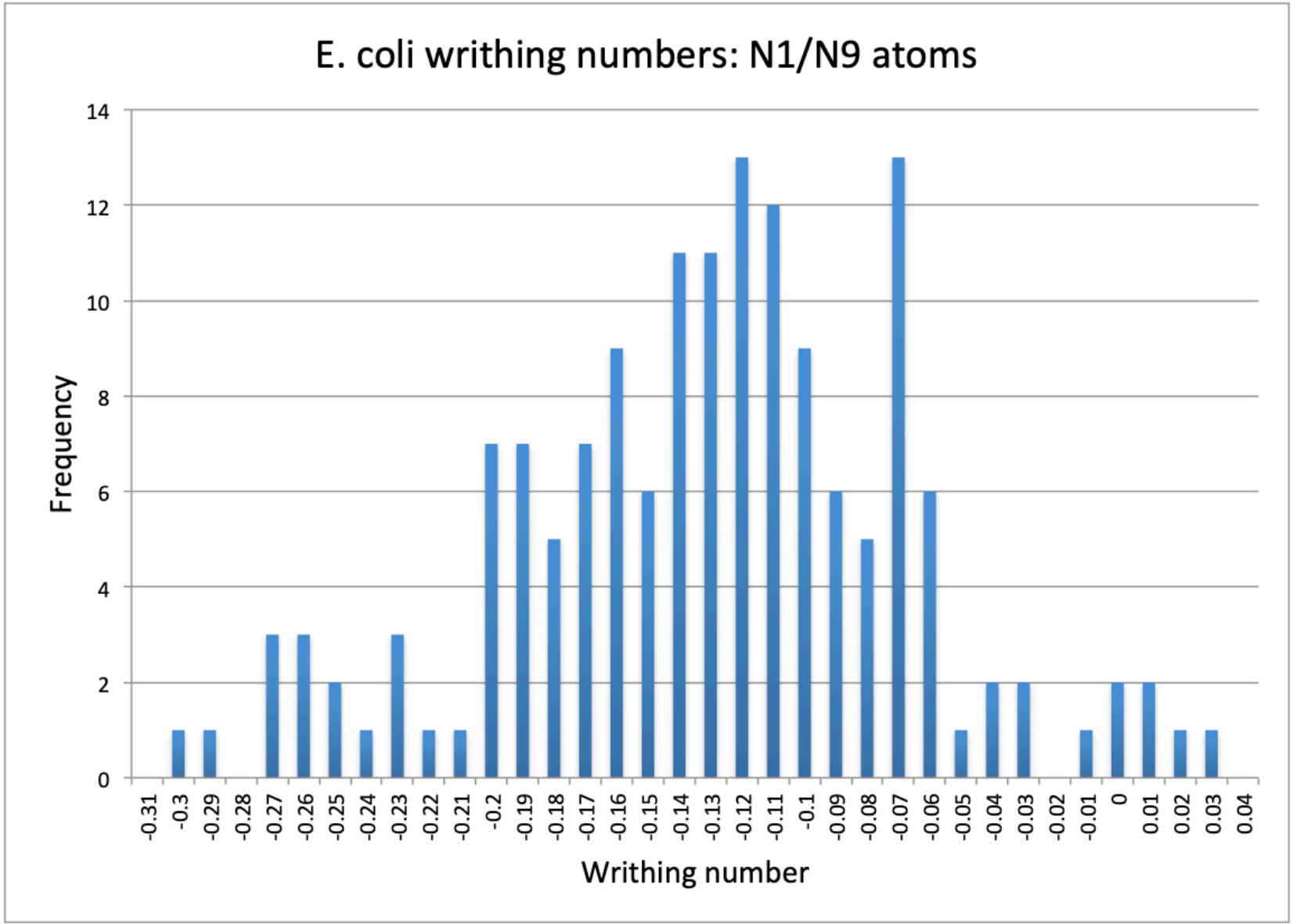

Next steps

- Study characteristics of different E. coli ribosomes in order to understand variations in writhing numbers
- Study writhing numbers computed for structures from other species
- Compare results from E. coli to those from other species

Acknowledgements

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References

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