

# Contents

## Part I Foundations

1	An Overview of Bayesian Inference and Graphical Models .....	3
	Thomas Hamelryck	
2	Monte Carlo Methods for Inference in High-Dimensional Systems .....	49
	Jesper Ferkinghoff-Borg	

## Part II Energy Functions for Protein Structure Prediction

3	On the Physical Relevance and Statistical Interpretation of Knowledge-Based Potentials .....	97
	Mikael Borg, Thomas Hamelryck, and Jesper Ferkinghoff-Borg	
4	Towards a General Probabilistic Model of Protein Structure: The Reference Ratio Method .....	125
	Jes Frellsen, Kanti V. Mardia, Mikael Borg, Jesper Ferkinghoff-Borg, and Thomas Hamelryck	
5	Inferring Knowledge Based Potentials Using Contrastive Divergence .....	135
	Alexei A. Podtelezhnikov and David L. Wild	

## Part III Directional Statistics for Biomolecular Structure

6	Statistics of Bivariate von Mises Distributions .....	159
	Kanti V. Mardia and Jes Frellsen	
7	Statistical Modelling and Simulation Using the Fisher-Bingham Distribution .....	179
	John T. Kent	

**Part IV Shape Theory for Protein Structure Superposition**

- 8    **Likelihood and Empirical Bayes Superposition of Multiple Macromolecular Structures .....** 191  
Douglas L. Theobald
- 9    **Bayesian Hierarchical Alignment Methods.....** 209  
Kanti V. Mardia and Vysaul B. Nyirongo

**Part V Graphical Models for Structure Prediction**

- 10    **Probabilistic Models of Local Biomolecular Structure and Their Applications.....** 233  
Wouter Boomsma, Jes Frellsen, and Thomas Hamelryck
- 11    **Prediction of Low Energy Protein Side Chain Configurations Using Markov Random Fields .....** 255  
Chen Yanover and Menachem Fromer

**Part VI Inferring Structure from Experimental Data**

- 12    **Inferential Structure Determination from NMR Data .....** 287  
Michael Habeck
- 13    **Bayesian Methods in SAXS and SANS Structure Determination .....** 313  
Steen Hansen
- References.....** 343
- Index.....** 377