Structural Biology Syllabus

Department of Biochemistry & Molecular Biology and Department of Chemistry
BIOC 4703.03/5703.03 & CHEM 4603.03/5603.03
Winter 2026

Dalhousie University operates in the unceded territories of the Mi'kmaw, Wolastoqey, and Peskotomuhkati Peoples. These sovereign nations hold inherent rights as the original peoples of these lands, and we each carry collective obligations under the Peace and Friendship Treaties. Section 35 of the Constitution Act, 1982, recognizes and affirms Aboriginal and Treaty rights in Canada.

We recognize that African Nova Scotians are a distinct people whose histories, legacies, and contributions have enriched the part of Mi'kma'ki known as Nova Scotia for over 400 years.

Course Instructors

Name	Email	Office Hours
David N. Langelaan (coordinator)	dlangela@dal.ca	To be announced via Brightspace
James A. Davey	james.davey@dal.ca	To be announced via Brightspace
Jan K. Rainey	jan.rainey@dal.ca	To be announced via Brightspace

Course Description

This course covers theoretical and practical aspects of determining and assessing the quality of atomic-resolution biomolecular structures. The underlying theory and applications of X-ray diffraction, NMR spectroscopy, and cryo-electron microscopy are discussed in detail.

Course Prerequisites: BIOC 3700 or CHEM 3601, or instructor's consent

Learning Objectives

1) **Describe** crystallization experiments and the properties of protein crystals
2) **Understand** the basis of X-ray diffraction and the concept of reciprocal space
3) **Describe** the phase problem of X-ray diffraction and its solutions
4) **Understand** the basis of protein structure calculation via crystallography and cryo-electron microscopy
5) **Evaluate** the quality of published biomolecular structures
6) **Describe** and **apply** the principles of molecular dynamics simulations
7) **Discriminate** and **quantify** the components of the NMR energy function
8) **Use** vector diagrams to **explain** the major NMR experiments employed for protein NMR
9) **Describe** effects of spin-relaxation phenomena upon the experimental observable and the manner in which these are modulated by dynamic processes
10) **Assign** two-dimensional homonuclear and heteronuclear NMR data for a polypeptide and **apply** these assignments for structure determination

Course Structure

Under emergency circumstances that have a serious impact on the delivery of this class, there may be a need to alter the syllabus or course structure

Course Delivery: In person

Lectures: Tuesday/Thursday 10:05-11:25 – CHEB 150

Workshops: One workshop (see tentative schedule) will take place in Tupper 8J

Course Materials

All course materials will be posted on Brightspace:

Textbook: No required book; some good books are listed below and you may want to pick one or more up from the library, chapters/amazon etc. *You will also end up with copious course notes!*

Recommended books:

"Crystallography Made Crystal Clear" by Gale Rhodes ***– 2006 edition is available online from Dal library.*** Provides an in-depth overview of protein crystallography theory and practice.

"Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology" by Bernhard Rupp **–** Provides an in-depth overview of protein crystallography theory with an emphasis on practical aspects of the technique.

"Molecular Modeling: Principles and Applications" by Andrew R. Leach. **(1996)** An excellent primer for the theory and practice of molecular modelling.

"Nuclear Magnetic Resonance" by Peter J. Hore (2nd Ed., 2015). A relatively inexpensive, great introduction to NMR spectroscopy. (1st edition available from Dal library.)

Additional readily available NMR spectroscopy books:

"Spin Dynamics – Basics of Nuclear Magnetic Resonance" by Malcolm H. Levitt (2002 or 2008 editions, Wiley) – ***2nd edition available online from Dal library***. *Worth picking up if you are planning to do a lot of NMR in future.*

"Fundamentals of protein NMR spectroscopy" by Rule and Hitchens – ***2006 edition is available online from Dal library.*** Good source of more protein-specific discussion.

"Protein NMR Spectroscopy – Principles and Practice" by Cavanagh, Fairbrother, Palmer, Rance and Skelton – ***2nd edition is available online from Dal library.*** Highly referred to in the field, but of limited utility for this course since the level of the discussion is quite technical.

"Understanding NMR Spectroscopy" by Keeler – **1st ed. (2004) available free from Dr. James Keeler's website and on ResearchGate**; 2nd ed. (2010) available from Dal library. An excellent introduction to fundamentals of NMR spectroscopy both from practical and theoretical perspectives with a more "traditional" approach than Levitt.

Assessment

Course Assessment – BIOC 4703/CHEM 4603

Component	***Weight (% of final grade)***	***Date***
Tests (2x80 min)	*2x15%[1]*	*Feb. 10th and Mar. 19th*
Final exam (3 h)	*30%[2]*	*(Scheduled by Registrar)*
Assignments[3]	*40%[2]*	*Throughout term*

Course Assessment – BIOC 5703/CHEM 5603

Component	***Weight (% of final grade)***	***Date***
Tests (2x80 min)	*2x12.5%[1]*	*Feb. 10th and Mar. 19th*
Final exam (3 h)	*25%[2]*	*(Scheduled by Registrar)*
Assignments[3]	*30%[2]*	*Throughout term*
Term project – seminar	*10%*	*Apr. 7th*
Term project – report	*10%*	*Apr. 7th*

Notes applicable to grading:

[1.] If your final exam mark is higher than the mark on a written test (i.e., you cannot simply skip a test), your lowest test mark will be replaced with the final exam mark.

[2.] Students must receive passing grades for the final exam and assignment components of the final mark to pass the course.

[3.] There will be approximately 6 assignments throughout the term (due dates TBD).

Conversion of numerical grades to final letter grades follows the
Dalhousie Grade Scale

A+ (90-100)	B+ (77-79)	C+ (65-69)	D (50-54)
A (85-89)	B (73-76)	C (60-64)	F (0-49)
A- (80-84)	B- (70-72)	C- (55-59)	

Notes: Letter grade assignment in BIOC 4703/CHEM 4603 and in BIOC 5703/CHEM 5603 will follow the Faculty of Science recommendation that numbers falling in the interval between letter grades be rounded up if the fraction is 0.5 or greater. Students in BIOC 5703/CHEM 5603 should note that the Faculty of Graduate Studies requires that students must achieve a letter grade of B- or higher to pass. Any numerical grade below 69.5 for BIOC 5703/CHEM 5603 will therefore result in an F.

Course Content

Approximate timeline: Winter 2026 (may be subject to change)

Class	Lecture	Date	Topic
1 – DL	1	08-Jan	Syllabus review and introduction (Rh2,10 & Ru1,2)
2 – DL	2	13-Jan	Protein crystallization, crystal symmetry, reciprocal lattice (Rh3 & Ru3,5)
3 – DL	3	15-Jan	**Workshop:** Visualizing protein structure using pymol
4 – DL	4	20-Jan	X-ray diffraction, Bragg's law, data collection and analysis (Rh4 & Ru6,8)
5 – DL	5	22-Jan	**Workshop:** Setting up a crystallization experiment (**Tupper 8J**)
6 – DL	6	27-Jan	The Fourier Transform, electron density, and the phase problem (Rh5 & Ru9)
7 – DL	7	29-Jan	Solving the phase problem, model building, and model validation (Rh6,7 & Ru10,11,12,13)
8 – DL	8	03-Feb	**Workshop:** Molecular replacement and model building
9 – JD	9	05-Feb	Introduction to statistical mechanics
10 – DL		10-Feb	***Test 1 – X-ray diffraction (Lectures 1-8)***
11 – JD	10	12-Feb	**Workshop:** QM/MM calculation of functions
		17-Feb	Winter break
		19-Feb	Winter break
12 – JD	11	24-Feb	Molecular dynamics simulation I (theory)
13 – JD	12	26-Feb	Molecular dynamics simulation II (method)
14 – JD	13	03-Mar	**Workshop:** Molecular dynamics simulation III (application)
15 – JR	14	05-Mar	Spectroscopy, NMR Hamiltonian, nuclear spin & the observable *(Le1,2,*5,8*)*
16 – JR	15	10-Mar	Anatomy of NMR spectrometer, quadrature detection, components of the Hamiltonian *(Le4,*5,9*)*
17 – JR	16	12-Mar	FT NMR, 2D NMR & apodization - lecture & **workshop**
18 – JR	17	17-Mar	TOCSY, nOe and NOESY, triple-resonance experiments & backbone walk (Le20)
19		19-Mar	***Test 2 – Simulations & NMR spectroscopy (Lectures 9-16)***
20 – JR	18	24-Mar	**Workshop:** Sequential assignment of homonuclear and heteronuclear data sets
21 – JR	19	26-Mar	Protein NMR restraints & structure calculation
22 – JR	20	31-Mar	Solid-state NMR: Experimental considerations & application to biomacromolecules
23 – DL	21	02-Apr	Cryo EM
24	22	07-Apr	***Grad student presentations***

Note: DL = David Langelaan; JD = James Davey (guest instructor); JR = Jan Rainey. Literature references are starting points for background reading, which may not cover all topics of a given lecture. Ho = Hore; Lh = Leach; Rh = Rhodes; Ru = Rupp. Number = chapter (or section).

Course Policies on Missed or Late Academic Requirements

Assignments must be submitted either in class (preferably) or in person to the indicated professor no later than 5:00 pm on the designated due date. Extension of the due date may be granted upon submission of a Student Declaration of Absence Form (protocol detailed below) or by consulting with the instructors. Extension of the due date will not normally exceed 7 calendar days. **In all other cases, a grade of 0 will be received for that assignment.**

Department of Biochemistry & Molecular Biology Policy on missed examinations/mid-terms and assignments

A student who misses an evaluation component of the course (midterm test, assignment, presentation, lab, etc.) due to illness should, if possible, notify the instructor, course coordinator, or department office either prior to, or within 48 h of the scheduled time or due date for that component. The student must also submit a **Student Declaration of Absence Form** (through the course Brightspace page) within three **(3) calendar days** following the last day of absence. Special 'make-up' tests (if offered) will normally be written within 7 calendar days after the missed test. A missed evaluation component for which no satisfactory arrangement has been made will be given a mark of zero. The Student Declaration of Absence form can only be submitted up to two (2) separate times per course during a term. Students who exceed this limit must inform their course instructor(s) and will be required to register with an Advisor at Student Academic Success (SAS). If students have recurring short-term absences and do not register with SAS, it is at the instructor(s)' discretion to disallow any further Student Declarations and deny alternate coursework
arrangements.

Course Policies related to Academic Integrity

Students are encouraged to work collaboratively with others to complete workshops and assignments; However, students are still expected to complete and submit their own work. The use of generative language artificial intelligence (e.g., Chat GPT) is not permitted in this course.

Department of Biochemistry & Molecular Biology Statement on Plagiarism

What is plagiarism?

"Dalhousie University defines plagiarism as the submission or presentation of the work of another as if it were one's own†." The Department of Biochemistry & Molecular Biology is committed to protecting honest students against the devaluation of their work by students who resort to plagiarism.

Some examples of plagiarism include (but are not restricted to):

> Submitting as your own work any material created, in whole or in part, by someone else, including **material created in collaboration with other students**, unless specifically allowed by the class instructor and credited appropriately.

> Paraphrasing extensively or copying from sources such as the Internet, journal articles, or books (including textbooks) without crediting the original author or source.

> Using another student's laboratory data, unless specifically allowed by the lab instructor and credited appropriately.

> Submitting, in whole or in part, any work that has been submitted in another class, or re-submitting the same work in different years of the same class.

How can plagiarism be detected?

If required by the Instructor, work submitted for credit must be submitted in electronic as well as hard copy form. Submissions may be screened by one or both of the following methods:

> A pattern recognition program that compares all submissions with one another as well as submissions from previous years. Every individual has a unique pattern of writing. This program will detect submissions that are derived from a common source, even if words or phrases have been changed.

> A third-party computer-based assessment system that compares submissions against a large database including previous submissions and Internet sources.

What are the consequences of plagiarism?
"Plagiarism is considered a serious academic offence that may lead to the assignment of a failing grade, suspension or expulsion from the University. If a penalty results in a student no longer meeting the requirements of a degree that has been awarded, the University may rescind that degree.†" At Dalhousie University, the Department is obligated to refer any cases of suspected plagiarism to an Academic Integrity Officer, who will then conduct a hearing to evaluate the innocence or guilt of students alleged to have committed an act of plagiarism.

How can accusations of plagiarism be avoided?
You can avoid accusations of plagiarism by:

> Preparing all submissions independently and ensuring that they are expressed in your own unique writing style.

> Never sharing any written or electronic material with other students. You may not work with another student while preparing materials you are planning to hand in.

> Acknowledging any material paraphrased extensively or copied from sources such as the Internet, journal articles or textbooks. Paraphrasing of short phrases from the class textbook need not be acknowledged.

> Guarding all your work, both drafts and final submissions, to ensure that no one else can copy it. If you provide access to your work and someone (including a student taking the same class in a future year) copies it, then you may be aiding in the commission of an academic offence. If you suspect that someone has taken any of your work, notify your class instructor immediately.

> Using only laboratory data that you actually collected in the lab. Altering laboratory data is not permitted. If your data are unusable, you must still report your own data along with any explanation as

to why the data are unusable. You may then use data supplied by the lab instructor for analysis, but you must acknowledge such use.

† Dalhousie University Undergraduate Calendar, 2022/2023, University Regulations, Intellectual Honesty.

Outline your policies on missed or late academic requirements, including late or missed assignments, labs, tests, or exams. Indicate what students should do if they miss or are late with an assessment (e.g., exam, assignment, lab), and the consequence(s) of missing or being late (e.g., late penalties, alternate evaluation schemes). Indicate if students are expected to use the Student Declaration of Absence form for late or missed requirements during the term, and if so, how many times they may use the form in your course.

University Policies and Statements

Recognition of Mi'kmaq Territory

Dalhousie University would like to acknowledge that the University is on Traditional Mi'kmaq Territory. The Elders in Residence program provides students with access to First Nations elders for guidance, counsel, and support. Visit or e-mail the Indigenous Student Centre at 1321 Edward St or elders@dal.ca. Additional information regarding Mi'kmaq and Indigenous Relations (including the Elders in Residence program, Land Acknowledgements, Understanding Our Roots, and much more) can be found at: https://www.dal.ca/about/mission-vision-values/mikmaq-indigenous-relations.html

Internationalization

At Dalhousie, 'thinking and acting globally' enhances the quality and impact of education, supporting learning that is "interdisciplinary, cross-cultural, global in reach, and orientated toward solving problems that extend across national borders." Additional internationalization information can be found at: https://www.dal.ca/about/mission-vision-values/global-relations.html

Academic Integrity

At Dalhousie University, we are guided in all our work by the values of academic integrity: honesty, trust, fairness, responsibility, and respect. As a student, you are required to demonstrate these values in all the work you do. The University provides policies and procedures that every member of the university community is required to follow to ensure academic integrity. Additional academic integrity information can be found at: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Student Accessibility Centre is Dalhousie's centre of expertise for matters related to student accessibility and accommodation. If there are aspects of the design, instruction, and/or experiences within this course (online or in-person) that result in barriers to your inclusion, please contact the Student Accessibility Centre (https://www.dal.ca/campus_life/academic-support/accessibility.html) for all courses offered by Dalhousie with the exception of Truro. For courses offered by the Faculty of Agriculture, please contact the Student Success Centre in Truro (https://www.dal.ca/campus_life/ssc.html).

Conduct in the Classroom – Culture of Respect

Substantial and constructive dialogue on challenging issues is an important part of academic inquiry and exchange. It requires willingness to listen and tolerance of opposing points of view. Consideration of individual differences and alternative viewpoints is required of all class members, towards each other, towards instructors, and towards guest speakers. While expressions of differing perspectives are welcome and encouraged, the words and language used should remain within acceptable bounds of civility and respect.

Diversity and Inclusion – Culture of Respect

Every person at Dalhousie has a right to be respected and safe. We believe inclusiveness is fundamental to education. We stand for equality. Dalhousie is strengthened in our diversity. We are a respectful and inclusive community. We are committed to being a place where everyone feels welcome and supported, which is why our Strategic Direction prioritizes fostering a culture of diversity and inclusiveness (Strategic Priority 5.2). Additional diversity and inclusion information can be found at: https://www.dal.ca/about/mission-vision-values/equity-diversity-inclusion-and-accessibility/about-office-equity-inclusion.html

Student Code of Conduct

Everyone at Dalhousie is expected to treat others with dignity and respect. The Code of Student Conduct allows Dalhousie to take disciplinary action if students don't follow this community expectation. When appropriate, violations of the code can be resolved in a reasonable and informal manner - perhaps through a restorative justice process. If an informal resolution can't be reached, or would be inappropriate, procedures exist for formal dispute resolution. The full Code of Student Conduct can be found at: https://www.dal.ca/content/dam/www/about/leadership-and-governance/governing-bodies/code-student-conduct.pdf

Fair Dealing Policy

The Dalhousie University Fair Dealing Policy provides guidance for the limited use of copyright protected material without the risk of infringement and without having to seek the permission of copyright owners. It is intended to provide a balance between the rights of creators and the rights of users at Dalhousie. Additional information regarding the Fair Dealing Policy can be found at: https://www.dal.ca/content/dam/www/about/leadership-and-governance/university-policies/fair-dealing-policy.pdf

Student Use of Course Materials

Course materials are designed for use as part of this course at Dalhousie University and are the property of the instructor unless otherwise stated. Third party copyrighted materials (such as books, journal articles, music, videos, etc.) have either been licensed for use in this course or fall under an exception or limitation in Canadian Copyright law. Copying this course material for distribution (e.g. uploading to a commercial third-party website) may lead to a violation of Copyright law.