

Marking schema - 2025 - (50 total)

- Average should be 31 pts (62%)
- Below 25 pts (50%) is a fail

Abstract (5 pts)

- more than 150 words: -1 pt per 50 words over
- summarises the project clearly: +1 pt
- understandable as a standalone piece: +1 pt
- describes the problem under investigation: +1 pt
- describes approach taken: +1 pt
- highlights key observations, conclusions: +1 pt

Introduction (5 pts)

- more than 150 words: -1 pt per 50 words over
- gives a motivation of the project: +1 pt
- mentions the objective of the experiment: +1 pt
- mentions MD simulation: +1 pt
- mentions composition and/or conditions(e.g., pH>5) of the investigation: +1 pt
- good comprehensive writing style: +1 pt

Methodology (15 pts total)

- more than 600 words: -1 pt per 50 words over
- every key step of the setup is described:

- mention forcefield: +1 pt
- mention how the system was manipulated: +1 pt
- mentions setup, energy minimisation & equilibration: +1 pt each (+3 pts total)
- mentions time step, temperature, pressure, simulation length: +1 pt each (+4 pts total)
- justification for specific set up (e.g., semi-isotropic P-scaling to ensure independent scaling f xy and z) +1 pt
- states how equilibration was checked +1 pt
- states what part of trajectory used for further analysis +1 pt
- mentions software used (i.e, gromacs 2024.4, VMD, XMgrace) +1 pt
- colours of atoms must be mentioned either here or in captions of the figure (else - 1 pt)
- points: barostat, thermostat not mentioned -½ pt each (-1 pt total)
- points: analysis incl. plotting described: +1 pt
- points: visualisation described: +1 pt

Results (10 pts total)

- more than 600 words: -1 pt per 50 words over
- good comprehensive writing style: +2 pts
- all figures/tables are mentioned in the text and discussed: +2 pts
- observations are clearly stated: +2 pts
- systems compared to each other: +1 pt
- comparison to literature: +1 pt
- reflection on the quality of simulations WRT literature +1 pt
- discusses relevant interactions/alingsments: +1 pt

Figures/Tables (5 pts total)

- Plots are included: +1 pt
- Correct axis and legend labels: +1 pt

- Plot displays the relevant section of the data / illustrates the result: +1 pt
- Rendering is included: +1 pt
- Rendering demonstrates result: +1 pt

Captions (2 pts total)

- Captions included: +½ pt each (+1 pts total)
- Captions are clear and allow to understand the figure/table w/o the need to read the main text: +½ pt each (+1 pt total)
- Captions for VMD do not include colours: -1 pt (make sure not to mark/penalise twice if also done in the Methods)

Conclusions (3 pts total)

- more than 150 words: -1 pt per 50 words over
- clear summary of the findings of the study: +1 pt
- abstract and conclusions should give same info on the results, but are not the same: +1 pt
- indication of future work/directions: +1 pt

References

- absent: -2 pt
- poor/inconsistent format: -1 pt

Quality of the study (5 points total)

- extra marks are reserved for the study of high quality, where the simulation set-up and analysis are of publishable quality (+3 pts total)
- extra marks for the production quality (visual appeal, ease of reading, logical flow) of the report being of publishable standard (+2 pts total).