

# Marking schema (30 pts total)

- Average should be 19 pts (63%)
- Below 15 pts (50%) is a fail

## Overview (5 pts)

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- more than 100 words: -1 pt per 50 words over
- mention MD simulation: +1 pt
- mention composition of the system: +1 pt
- mention objective of the experiment: +1 pt
- mention key findings: +1 pt
- good comprehensive writing style: +1 pt

## Methodology (12 pts total)

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- more than 500 words: -1 pt per 50 words over
- every key step of the setup is described:
  - mention source of structure: +1 pt
  - mention forcefield: +1 pt
  - mention how the system was manipulated: +1 pts
- mention setup, energy minimisation & equilibration: 1 pt each (3 pts total)
- mention time step, temperature, pressure, simulation length: +1 pt each (4 pts total)
- points: barostat, thermostat not mentioned -1/2 pt each (1 pts total)
- points: analysis incl. plotting described: +1 pt
- points: visualisation described: +1 pt

## Results (5 pts total)

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- more than 400 words: -1 pt per 50 words over
- good comprehensive writing style: +2 pt
- Figures are mentioned in the text: +1 pt
- Observations are clearly stated: +2 pt

## Figures (5 pts total)

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- Plot is included: +1 pt
- Correct axis 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 (3 pts total)

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- Captions included: +½ pt each (1 pts total)
- Captions are descriptive: +½ pt each (1 pts total)
- Captions for VMD include colours: +1 pt

## References

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- absent: -2 pt
- poor: -1 pt