README

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1 README

Run script `analyse.py` with no arguments to calculate RDF between oxygen-oxygen in the `example.pdb`. This will generate a plot of RDF, g_{ab}, and coordination number, N_{ab} as function of r in `rdf_and_coordination.png`.

Often by 'coordination number' people actually mean the value of N_{ab} at r where first peak of g_{ab} occurs. This you can either infer from the plot, or write code find the first maxima r_{max} and then get $N_{ab}(r_{max})$. Similarly, for second coordination shell, you can use the second peak and so on.