

Appendix A. Supplementary data

Molecular modelling of lactoferrin for food application: Insights from *in silico* techniques

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BLf	1	APRKNVRWCTISQPEWFKRRWQWRMKKLGAPSITCVRRFALECIIRAIA	50
HLf	1	RRRSRVQWCAVSNPEATKCFQWQRNMRKVRGPPVSCIKRDSPIQCIQAIA	50
	51	EKKADAVTLDGGMVFEAGRDPYKLRPVAAEYGTKEQPQTHYYAVAVVKK	100
	51	ENRADAVTLDGGFIYEAGLAPYKLRPVAAEVYGTQRPRTHYYAVAVVKK	100
	101	GSNFQLDQLQGRKSCHTGLGRSAGWIIPMGILRPYLSWTESLEPLQGAVA	150
	101	GGSFQLNELQGLKSCHTGLRRTAGWNVPIGTLRPF LNWTGPPEIEAAVA	150
	151	KFFSASCVPCIDRQAYPNLCQLCKGEGENQCACSSREPYFGYSGAFKCLQ	200
	151	RFFSASCVPGADKGFQPNLCRLCAGTGENKCAFSSQEPYFYSYSGAFKCLK	200
	201	DGAGDVAFVKETTTFENLPEKADRQYELLCNNRAPVDAFKECHLAQV	250
	201	DGAGDVAFIRESTVFEDLSDEAERDEYELLCPDNTRKPVDFKDCHLARV	250
	251	PSHAVVARSVDGKEDLIWKLKSKAQEKFGKNKSRSFQLFGSPPGQRDLF	300
	251	PSHAVVARSVNGKEDAIWNLLRQAQEKFGKDKSPKFQLFGSPSGQKDLF	300
	301	KDSALGFLRIPSKVDSALYLGSRYLTTLNKLNRETAEEVKARYTRVWCAV	350
	301	KDSAIIGFSRVPPRIDSGLYLGSYFTAIQNLKSEEEVAARRARVWCAV	350
	351	GPEEQKKCQQWSQSQGNVTCATASTTDDCIVLVLKGEADALNLDGGYIY	400
	351	GEQELRKCQWSGLSEGSVTCSSASTTEDCIALVLKGEADAMSLDGGYVY	400
	401	TAGKCGLVPVLAENRKSSKHSSLD--CVLRPTGYLAVAVVKKANEGLTW	448
	401	TAGKCGLVPVLAENYKSAQSSDPDPNCVDRPVEGYLAVAVVRRSDTSLTW	450
	449	NSLKDKKKSCHTAVDRTAGWNIIPMGLIVNQTGSCAFDEFFSQSCAPGADPK	498
	451	NSVKGKKSCHTAVDRTAGWNIIPMGLLNFNQTGSCKFDEYFSQSCAPGSDPA	500
	499	SRLCALCAGDDQGLDKCVPNSKEKYYGYTGAFRCLAEDVGDVAFVKNDTV	548
	501	SNLCALCIGDEEENKCVPNSEKYYGYTGAFRCLAENAGDVAFVKDVTV	550
	549	WENTNGESTADWAKNLNREDFRLCLDGTGRKPVTEAQSCHLAVAPNHAVV	598
	551	LQNTDGNNEAWAKDLKLDADFALLCLDGTGRKPVTEARSCHLAMAPNHAVV	600
	599	SRSRAAHVKQVLLHQQALFGKNGKNCPDKFCLFKSETKNLLFNDNTECL	648
	601	SRMDKVERLKQVLLHQQAKFGRNGSDCPDKFCLFQSETKNLLFNDNTECL	650
	649	AKLGGRPITYEYLGTEYVTAIANLKKCSTSPLEACEFLTR	689
	651	ARLHGKTTYEKYLGQYVAGITNLKKCSTSPLEACEFLRK	691

Figure S1. Comparison of the amino acid sequencing results for bovine lactoferrin (BLf) and human lactoferrin (HLf). Symbols adjoining the single-letter amino acid codes have following meanings: ‘|’ = identical residue; ‘:’ = BLOSUM matrix score > 0; and ‘.’ = BLOSUM matrix score ≤ 0.

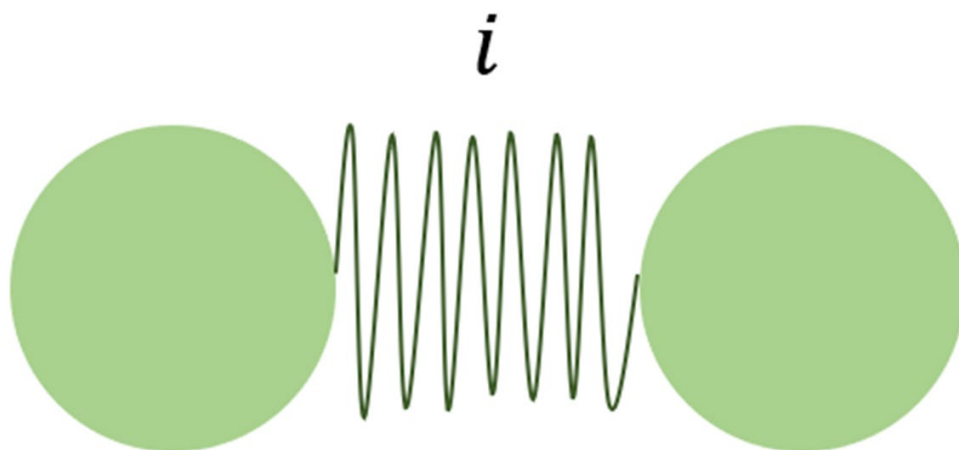


Figure S2. A cartoon representation of the stretching of bonds

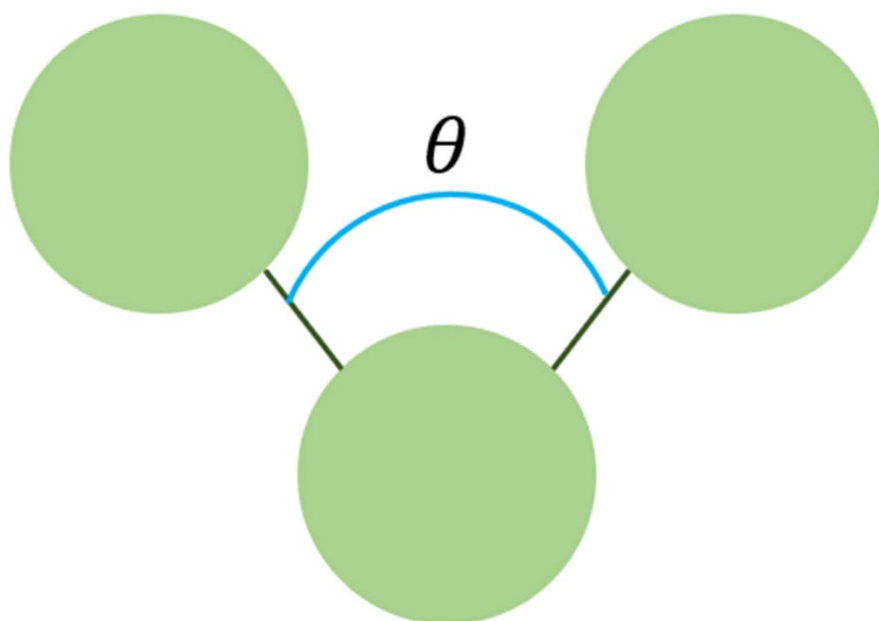


Figure S3. A cartoon representation of the bond angle calculation

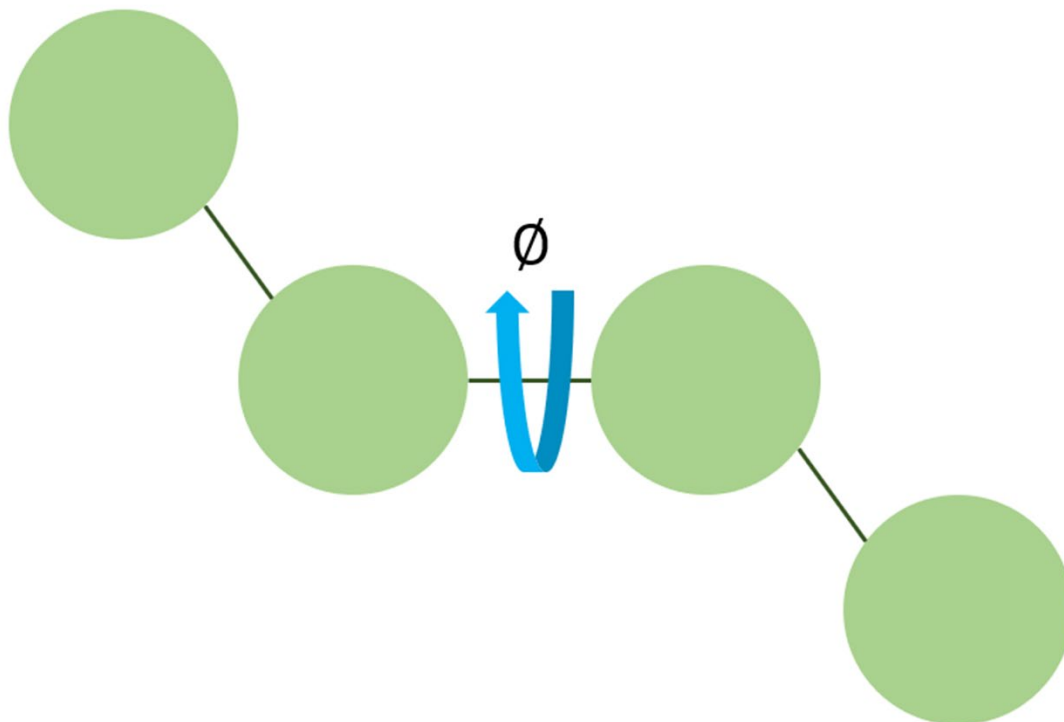


Figure S4. A cartoon representation of the dihedral angle

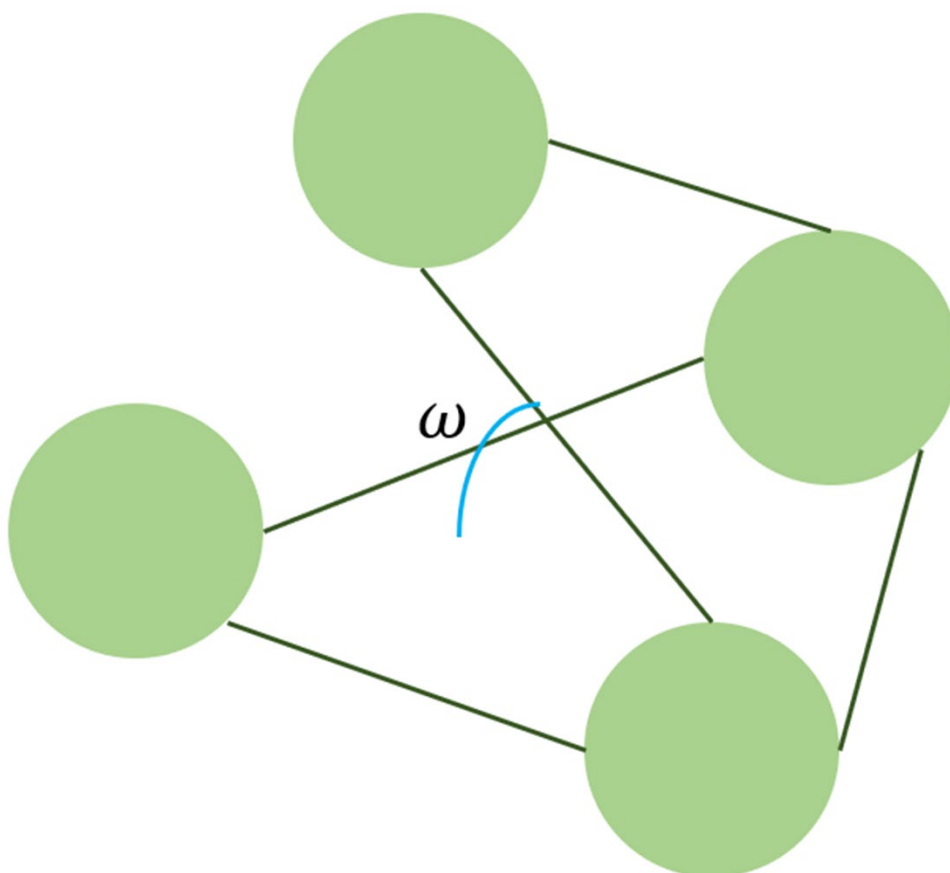


Figure S5. A cartoon representation of the improper dihedral angle

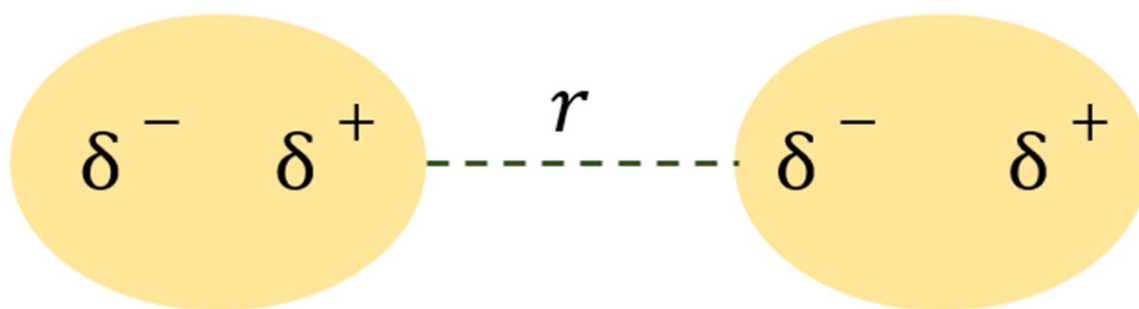


Figure S6. A cartoon representation of Lennard-Jones interactions

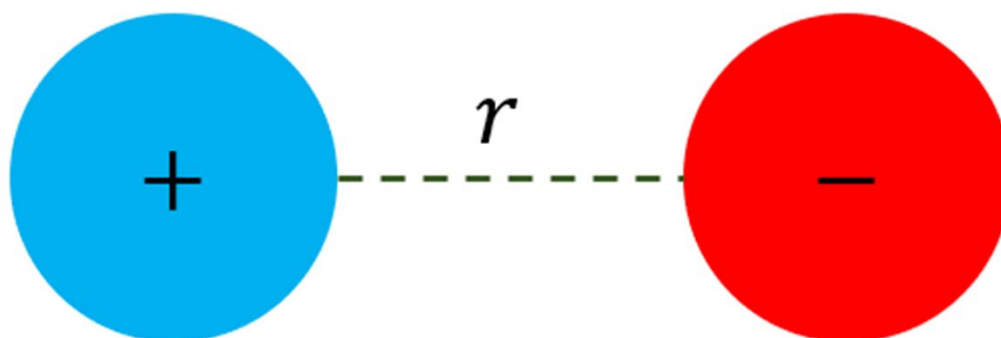


Figure S7. A cartoon representation of electrostatic interactions

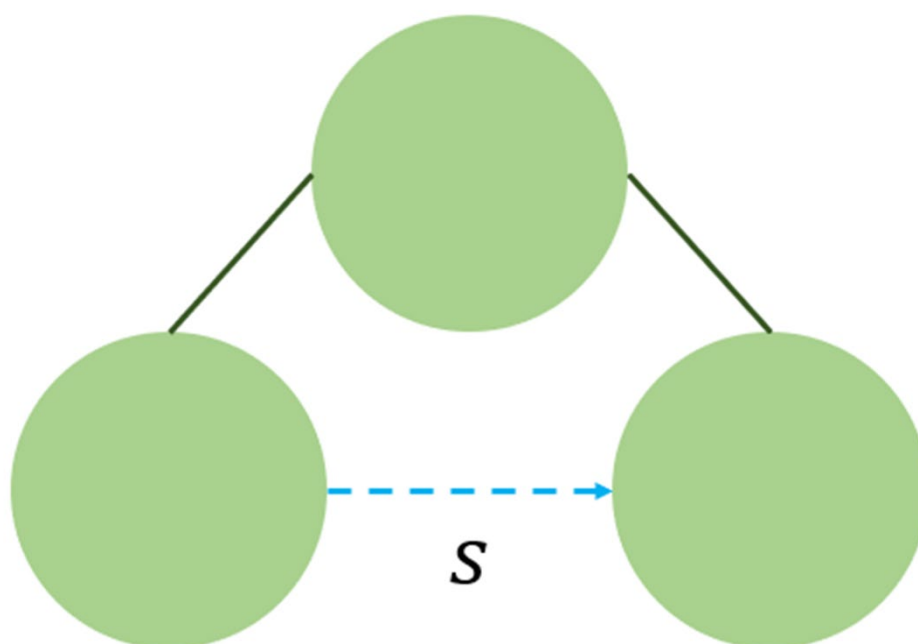


Figure S8. A cartoon representation of the Urey-Bradley potential

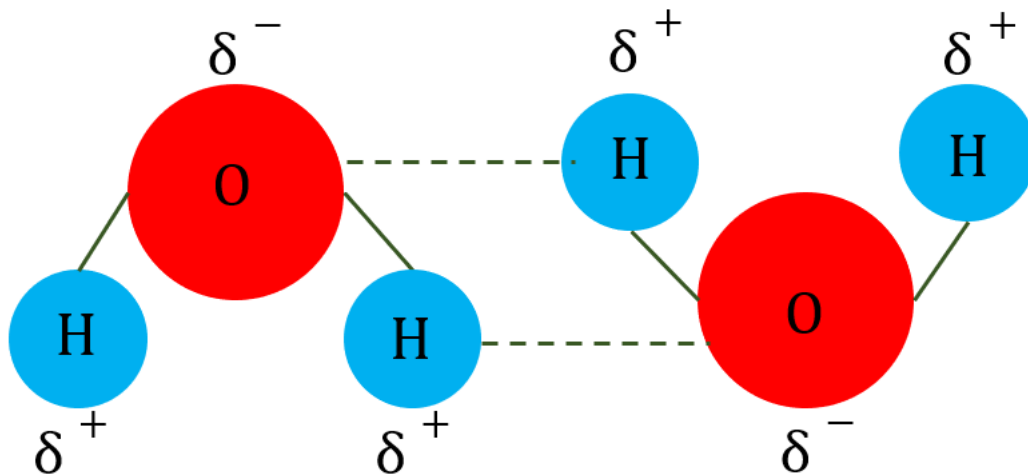


Figure S9. A cartoon representation of hydrogen bonds

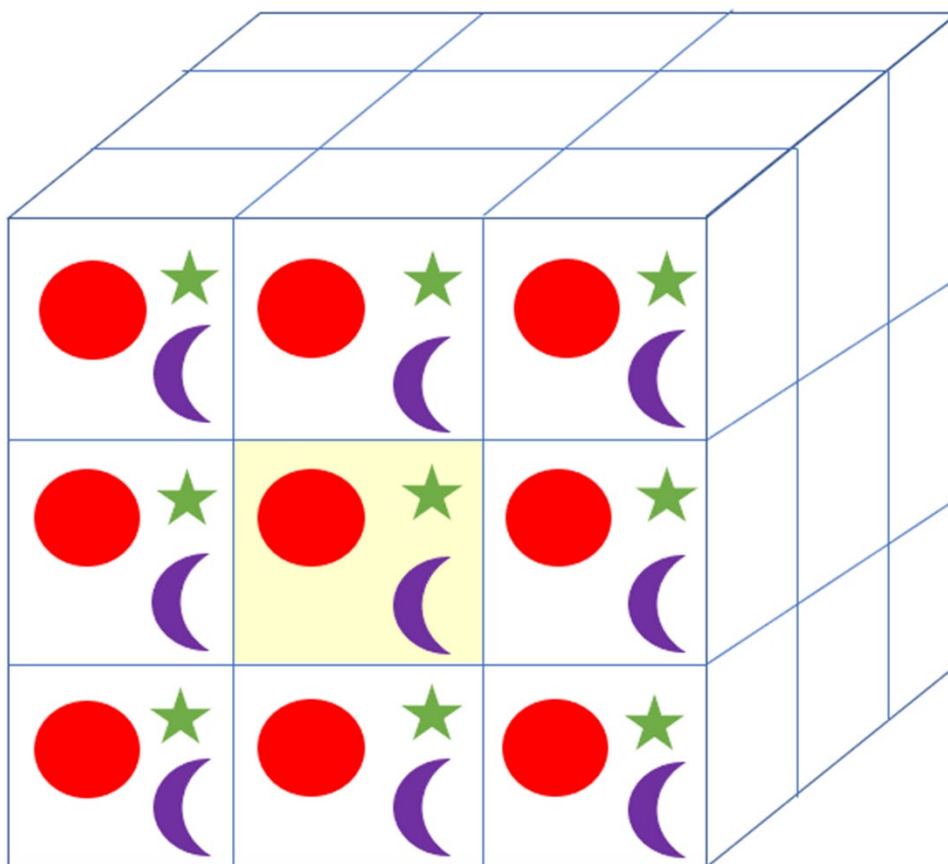


Figure S10. A 3D illustration of a periodic boundary condition