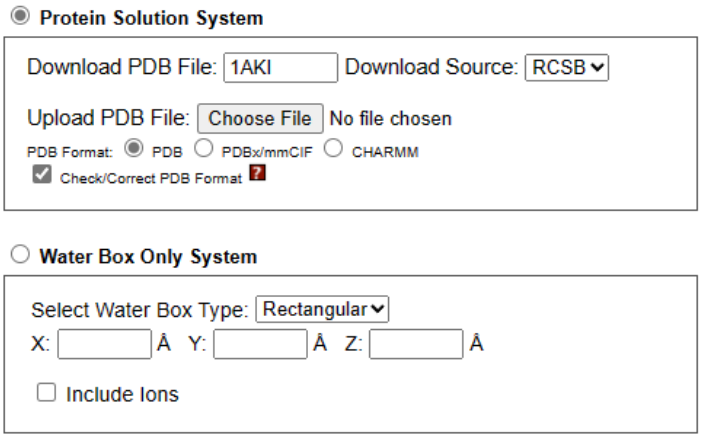
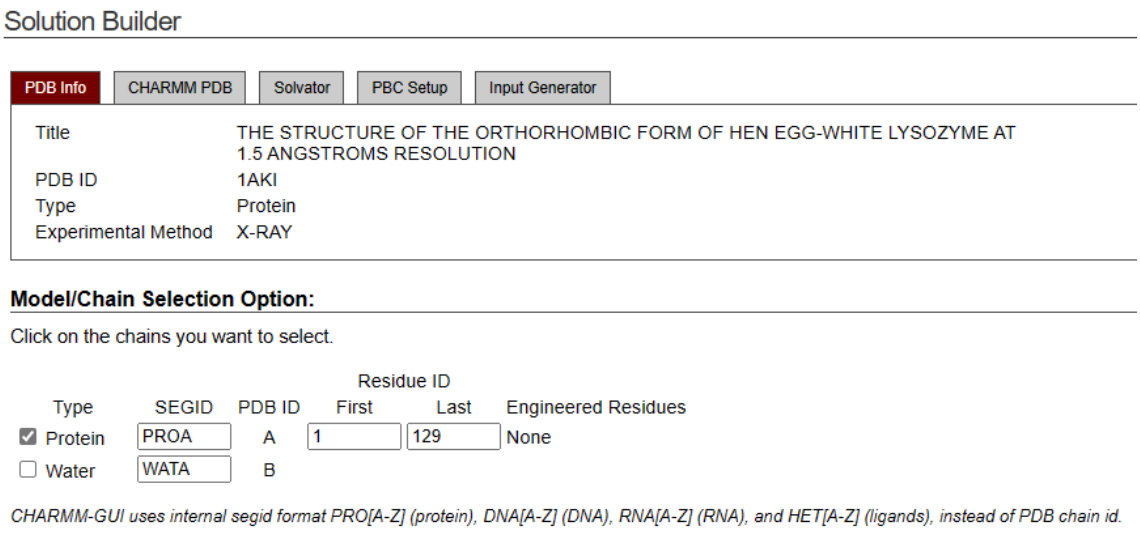
Configuración de la caja de modelación para la dinámica molecular de la lisozima solvatada utilizando CHARMM-GUI.

1



2



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PDB Manipulation Options:

Terminal group patching:

	First	Last	
PROA	NTER	CTER	Cyclic peptide?

Preserve hydrogen coordinates:

Mutation:

Protonation state:

Disulfide bonds:

Pair 1	Residue ID	Pair 2	Residue ID		
PROA	6	PROA	127	-	Add Bonds
PROA	30	PROA	115	-	
PROA	64	PROA	80	-	
PROA	76	PROA	94	-	

It is possible that a PDB file contains wrong disulfide bond information. Please double check when you get an error.

Phosphorylation:

Ubiquitylation / SUMOylation:

GPI anchor:

Glycosylation / Glycan Ligand(s):

Heme coordination

Add Lipid-tail

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Symmetry Operation Options:

Generation of Crystal Packing: Space Group P 21 21 21
(this is required for asymetric unit solvation)

Generation of Full Unit Cell: Space Group P 21 21 21

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PDB Info | CHARMM PDB | Solvator | PBC Setup | Input Generator

JOB ID: 9072747671

download.tgz

Original PDB File:	1AKI.cif (view structure)
Individual Chains:	1aki_proa.pdb
CHARMM Input:	step1_pdbreader.inp
CHARMM Output:	step1_pdbreader.out
CHARMM PDB:	step1_pdbreader.pdb (view structure)
CHARMM CRD:	step1_pdbreader.crd
CHARMM PSF:	step1_pdbreader.psf
Unitcell:	step1_unitcell.str
Unitcell Info:	step1_unitcell.info

Computed Energy:

Please beware of that the computed energy is CHARMM single-point energy and is displayed to make sure all the coordinates are defined.

ENER ENR:	Eval#	ENERgy	Delta-E	GRMS		
ENER INTERN:		BONDs	ANGLes	UREY-b	DIHEdrals	IMPRopers
ENER CROSS:		CMAPs	PMF1D	PMF2D	PRIMO	
ENER EXTERN:		VDWaals	ELEC	HBONds	ASP	USER
ENER>	0	-580.36804	0.00000	19.64395		
ENER INTERN>		246.76446	522.90638	44.49137	1211.35778	84.13497
ENER CROSS>		-76.61089	0.00000	0.00000	0.00000	
ENER EXTERN>		-202.27749	-2411.13462	0.00000	0.00000	0.00000

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Waterbox Size Options:

- ○ Unitcell Solvation
- ○ Specify Waterbox Size
- ◉ Fit Waterbox Size to Protein Size

Waterbox type: Rectangular (Currently, the octahedral box is supported only for CHARMM and NAMD)
Enter Edge Distance: 10.0

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Add Ions:

☑ Include Ions

Ion Placing Method: Monte-Carlo

☑ Basic Ion Types

$MgCl_2$ Add Simple Ion Type

☐ More Ion Types

Formula	Cation	Anion	Concentration	Neutralizing	
KCl	K^+	Cl^-	0.15	◉	-
$MgCl_2$	Mg^{2+}	Cl^-	0.15	○	-

Calculate Solvent Composition

Ion	Count
K^+	175
Mg^{2+}	175
Cl^-	557

Please note that the ion count is an approximation based on geometry. The real number will be calculated in the next step.

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PDB Info | CHARMM PDB | Solvator | PBC Setup | Input Generator

JOB ID: 9072747671

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CHARMM PDB:	step1_pdbreader.pdb (view structure)	
Solvator Input:	step2_solvator.inp	
Solvator Output:	step2_solvator.out	
Solvator PDB:	step2_solvator.pdb (view structure)	
Solvator CRD:	step2_solvator.crd	
Solvator Stream:	step2_solvator.str	
Waterbox Info:	step2.1_waterbox.prm	
Water Box:	step2.1_waterbox.inp	Input file for water box
	step2.1_waterbox.out	Output file for water box
	step2.1_waterbox.str	Stream file for water box reading
	step2.1_waterbox.pdb (view structure)	water box PDB file
	step2.1_waterbox.crd	water box CRD file
	step2.1_waterbox.prm	
Ions:	step2.2_ions.inp	Input file for ions
	step2.2_ions.out	Output file for ions
	step2.2_ions.str	Ion Information
	step2.2_ions.pdb	ions PDB file

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PDB Info | CHARMM PDB | Solvator | PBC Setup | Input Generator | JOB ID: 9072747671

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Solvator PDB:	step2_solvator.pdb (view structure)
PBC Setup Input:	step3_pbcsetup.inp
PBC Setup Output:	step3_pbcsetup.out
PBC Setup Stream:	step3_pbcsetup.str
PBC Setup CRD:	step3_pbcsetup.crd
PBC Setup PSF:	step3_pbcsetup.psf
PBC Setup PDB:	step3_pbcsetup.pdb (view structure)
FFT Calculation:	checkfft.py

Force Field Options:

CHARMM36m

- [ ] WYF parameter for cation-pi interactions
- [ ] Hydrogen mass repartitioning

Y. Gao, J. Lee, I.P.S. Smith, H. Lee, S. Kim, Y. Qi, J.B. Klauda, G. Widmalm, S. Khalid, and W. Im *Journal of Chemical Information and Modeling* 2021 61 (2), 831-839. DOI.

- [ ] Multi-site Ca^{2+}

Currently only available for CHARMM, NAMD, GROMACS, and OpenMM

Zhang, A., Yu, H., Liu, C. *et al.* The Ca^{2+} permeation mechanism of the ryanodine receptor revealed by a multi-site ion model. *Nat. Commun.* 11, 922 (2020). DOI.

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Input Generation Options:

The input generation scheme has been changed recently. Please check your system, input, and restraint files carefully. Let us know if you see any issue.

- [x] NAMD
- [x] GROMACS
- [x] AMBER
- [x] OpenMM
- [x] CHARMM/OpenMM
- [ ] GENESIS
- [ ] Desmond
- [x] LAMMPS
- [ ] Tinker

Equilibration Input Generation Options:

- (•) NVT Ensemble

Dynamics Input Generation Options:

- (•) NPT Ensemble
- ( ) NVT Ensemble

Temperature: 303.15 K

Next Step:
Generate Equilibration and Dynamics inputs