

Summary of integrative structure determination of Structure of human myr-Arf1-GTP bound to MSPdH5 nanodisc (PDB ID: 9A8S)

1. Model Composition	
<p>Entry composition</p>	<ul style="list-style-type: none"> - Membrane Scaffold Protein (MSP) Apolipoprotein A-I: chain(s) A, B (167 residues) - [(2R)-2-[(E)-octadec-9-enoyl]oxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] (E)-octadec-9-enoate: chain(s) AD [A], AF [A], AU [B], AV [B], AX [P], AY [P] - [(2R)-2-[(E)-octadec-9-enoyl]oxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] (E)-octadec-9-enoate: chain(s) AU [B], BE [A], BF [B], BG [B], BH [B], BJ [P], BK [P] - ADP-ribosylation factor 1: chain(s) C [P] (180 residues) - 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine: chain(s) D [A], E [A], F [A], G [A], H [A], I [A], J [A], K [A], L [A], M [A], N [A], O [A], Q [A], R [A], S [A], T [A], U [A], V [A], W [A], X [A], Y [A], Z [A], AA [A], AC [B], BA [A], BB [B], BC [B], CA [A], CB [B], CC [B], DB [B], DC [P], EA [A], EB [B], EC [P], FA [A], FB [B], FC [P], GA [A], GB [B], GC [P], HA [A], HB [B], HC [P], IA [B], IB [B], IC [P], JA [B], JB [B], JC [P], KA [B], KB [B], KC [P], LA [B], LB [B], LC [P], MB [B], MC [P], NA [B], NB [B], NC [P], OA [B], OB [B], OC [P], PA [B], PB [B], PC [P], QA [B], QB [B], QC [P], RA [B], RB [B], RC [P], SA [B], SB [B], TA [B], TB [B], UA [B], UB [B], UC [P], VA [B], VB [B], VC [P], WA [B], WB [B], WC [P], XA [B], XC [P], YA [B], YB [B], YC [P], ZA [B], ZB [B] - 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine: chain(s) D [A], E [A], F [A], G [A], H [A], I [A], J [A], K [A], M [A], N [A], O [A], Q [A], R [A], S [A], T [A], V [A], W [A], X [A], Y [A], Z [A], AA [A], AE [A], AG [A], AH [A], AI [A], AJ [A], AK [A], AL [A], AM [A], AN [A], AO [A], AP [A], AQ [A], AR [A], AS [A], AT [B], AW [B], AZ [P], BA [A], BB [B], BD [P], CA [A], CB [B], DB [B], DC [P], EA [A], EB [B], EC [P], FA [A], FB [B], FC [P], GA [A], GB [B], GC [P], HA [A], HB [B], HC [P], IA [B], IB [B], IC [P], JA [B], JB [B], KA [B], KB [B], LA [B], LB [B], LC [P], MB [B], MC [P], NB [B], NC [P], OA [B], OB [B], OC [P], PA [B], PB [B], PC [P], QA [B], QB [B], QC [P], RA [B], RB [B], RC [P], SA [B], TA [B], UA [B], UC [P], VA [B], VC [P], WA [B], WC [P], XA [B], XC [P], YA [B] - 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine: chain(s) D [A], E [A], F [A], G [A], H [A], I [A], J [A], L [A], M [A], N [A], O [A], Q [A], R [A], S [A], T [A], U [A], V [A], W [A], X [A], Y [A], Z [A], AA [A], AE [A], AG [A], AT [B],

	<p>AW [B], AZ [P], BA [A], BB [B], BD [P], BI [B], BL [P], BM [P], BN [P], BO [P], CA [A], CB [B], DC [P], EA [A], EB [B], EC [P], FA [A], FB [B], FC [P], GA [A], GB [B], GC [P], HA [A], HB [B], HC [P], IA [B], IB [B], IC [P], JA [B], JB [B], JC [P], KA [B], KB [B], KC [P], LA [B], LB [B], LC [P], MB [B], MC [P], NB [B], NC [P], OA [B], OB [B], OC [P], PA [B], PB [B], QA [B], QB [B], QC [P], RB [B], RC [P], SA [B], SB [B], TA [B], TB [B], UA [B], UB [B], UC [P], VA [B], VC [P], WA [B], WB [B], WC [P], XA [B], XC [P], YA [B], YB [B], ZA [B]</p> <p>- [(2R)-2-[(E)-octadec-9-enoyl]oxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] (E)-octadec-9-enoate: chain(s) P [A], AB [B], DA [A], MA [B], SC [P], TC [P], XB [B]</p>
Datasets used for modeling	<ul style="list-style-type: none"> - NMR data, BMRB: 27726 - Experimental model, PDB: 3LVO - NMR data, BMRbig: BMRbig101 - Experimental model, PDB: 2N5E - Comparative model, Not available - Experimental model, PDB: 2KSQ
2. Representation	
Number of representations	3
Scale	<ul style="list-style-type: none"> - Atomic - Atomic - Atomic
<i>Number of rigid and flexible segments</i>	<ul style="list-style-type: none"> - 0, 3 - 0, 3 - 0, 3
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	3
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 0.00-0.00 - Ramachandran outliers: 3-6 - Sidechain outliers: 36-38
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Name</i>	None
<i>Description</i>	NAMD multi-state modeling
2. <i>Name</i>	None
<i>Description</i>	NAMD multi-state modeling
3. <i>Name</i>	None
<i>Description</i>	NAMD multi-state modeling
<i>Software</i>	<ul style="list-style-type: none"> - NAMD2 (version Not available) - CHARMM-GUI (version Not available) - Swiss-Model (version Not available) - Visual Molecular Dynamics (VMD) (version Not available)