

Summary of integrative structure determination of Integrative Modeling of a Sin3/HDAC Complex Sub-structure (PDB ID: 9A07, PDB-Dev ID: PDBDEV_00000043)

| 1. Model Composition | |
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| <u>Entry composition</u> | <ul style="list-style-type: none"> - SAP30L N terminal: Chain B (68 residues) - HDAC1: Chain D (369 residues) - SIN3A: Chain C (122 residues) - SAP30L C terminal: Chain A (90 residues) |
| <u>Datasets used for modeling</u> | <ul style="list-style-type: none"> - Comparative model, template PDB ID: Not available - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 12 cross-links - Experimental model, PDB ID: 2LD7 - Experimental model, PDB ID: 2N1U - Experimental model, PDB ID: 2N2H - Experimental model, PDB ID: 5IX0 - Mutagenesis data, File: 10.1074/jbc.RA119.009780 |
| 2. Representation | |
| <u>Resolution</u> | Atomic |
| <u>Number of rigid bodies, flexible units</u> | 4, 0 |
| <u>Rigid bodies</u> | <ul style="list-style-type: none"> - A: 1-90 - B: 1-68 - C: 1-122 - D: 1-369 |
| <u>Structural coverage (rigid bodies)</u> | 100% |
| 3. Restraints | |
| <u>Physical principles</u> | Information about physical principles was not provided |
| <u>Experimental data</u> | <ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 12 cross-links - 16 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0 |
| 4. Validation | |
| <u>Number of ensembles</u> | 0 |
| <u>Number of models in ensembles</u> | Not applicable |
| <u>Number of deposited models</u> | 1 |

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| <u>Model precision (uncertainty of models)</u> | Model precision can not be calculated with one structure |
| <u>Data quality</u> | Data quality has not been assessed |
| <u>Model quality: assessment of atomic segments</u> | Model-1: Clashscore = 5.99, Number of Ramachandran outliers = 3, Number of sidechain outliers = 47 |
| <u>Model quality: assessment of excluded volume</u> | Not applicable |
| <u>Fit to data used for modeling</u> | Fit of model to information used to compute it has not been determined |
| <u>Fit to data used for validation</u> | Fit of model to information not used to compute it has not been determined |
| 5. Methodology and Software | |
| 1. <u>Method</u> | ? |
| <u>Name</u> | comparative modeling |
| <u>Number of computed models</u> | ? |
| 2. <u>Method</u> | ? |
| <u>Name</u> | docking |
| <u>Number of computed models</u> | 200 |
| <u>Software</u> | - <u>HADDOCK</u> (version Not available) - <u>SWISS-MODEL</u> (version Not available) |