Summary of integrative structure determination of integrative modeling of a sin3/hdac complex sub-structure (PDBDEV00000043)

1. Model Composition	
Entry composition	- SAP30L C terminal: Chain A (90 residues) - HDAC1: Chain D (369 residues) - SAP30L N terminal: Chain B (68 residues) - SIN3A: Chain C (122 residues)
Datasets used for modeling	- Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - CX-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, Not listed
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies, flexible units	4, 0
Rigid bodies	- A: 1-90:Comparative model/None. - B: 1-68:Comparative model/None. - C: 1-122:Comparative model/None. - D: 1-369:Comparative model/None.
Flexible units	- A: - - B: - - C: - - D: -
Resolution	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSSO, 12 cross-links - 16 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
4. Validation	
Sampling validation	- Information related to sampling validation has not been provided
Clustering algorithm ,clustering feature	Distance threshold-based clustering used if ensembles are deposited, Not applicable
Number of ensembles	0

Number of models in ensembles	Not applicable
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Clashscore: 6.09, Ramachandran outliers: 0.47% , Sidechain outliers: 8.2%
Model quality: assessment of excluded volume	- Not applicable
Fit of the model to information used to compute it	- Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	?
Name	comparative modeling
Details	- Method details unspecified
Software	- HADDOCK (version None) - SWISS-MODEL (version None) - No location specified