Summary of integrative structure determination of integrative structure of the canonical human cop9 signalosome (PDBDEV00000037)

1. Model Composition	
Entry composition	- CSN1: Chain A (491 residues) - CSN6: Chain F (327 residues) - CSN8: Chain H (209 residues) - CSN3: Chain C (423 residues) - CSN7: Chain G (264 residues) - CSN2: Chain B (443 residues) - CSN4: Chain D (406 residues) - CSN5: Chain E (334 residues)
Datasets used for modeling	 Experimental model, PDB ID: Not listed Comparative model, template PDB ID: Not listed Experimental model, PDB ID: 4D10 Experimental model, PDB ID: Not listed Comparative model, template PDB ID: Not listed CX-MS data, Linker name and number of cross-links: DSSO, 74 cross-links CX-MS data, Linker name and number of cross-links: DSSO, 141 cross-links CX-MS data, Linker name and number of cross-links: BMSO, 40 cross-links CX-MS data, Linker name and number of cross-links: BMSO, 31 cross-links CX-MS data, Linker name and number of cross-links: BMSO, 91 cross-links CX-MS data, Linker name and number of cross-links: DHSO, 91 cross-links CX-MS data, Linker name and number of cross-links: DHSO, 79 cross-links
2. Representation	
Atomic structural coverage	85%
Number of <u>rigid bodies</u> , <u>flexible units</u>	23, 28

Flexible units	- A: 1-43, 108-127, 228-245, 427-430, 463-491. - B: 1-29, 180-191, 290-307, 398-416. - C: 1-2, 164-176, 362-367, 402-423. - D: 1-2, 132-138, 362-364. - E: 1-24, 284-295, 334-334. - F: 1-28, 208-214, 268-270, 317-327. - G: 1-7, 159-162, 213-264. - H: 1-10, 165-193.
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, 74 cross-links 1 unique CrossLinkRestraint: DSSO, 141 cross-links 1 unique CrossLinkRestraint: BMSO, 40 cross-links 1 unique CrossLinkRestraint: BMSO, 31 cross-links 1 unique CrossLinkRestraint: DHSO, 91 cross-links 1 unique CrossLinkRestraint: DHSO, 79 cross-links
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, dRMSD
Number of ensembles	7
Number of models in ensembles	54702, 132407, 98186, 87368, 243067, 312515, 357350
Model precision (uncertainty of models)	16.0Å, 22.0Å, 24.0Å, 27.0Å, 27.0Å, 29.0Å, 37.0Å
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Not applicable
Model quality: assessment of excluded volume	- Model-1: Number of violations-6767.0 - Model-2: Number of violations-6862.0 - Model-3: Number of violations-6769.0 - Model-4: Number of violations-6810.0 - Model-5: Number of violations-6831.0 - Model-6: Number of violations-6840.0 - Model-7: Number of violations-6830.0

Fit of the model to information used to compute it	- CX-MS Fit of medioid: model # 1, percentage satisfied 71.05% - CX-MS Fit of medioid: model # 2, percentage satisfied 71.93% - CX-MS Fit of medioid: model # 3, percentage satisfied 72.37% - CX-MS Fit of medioid: model # 4, percentage satisfied 67.76% - CX-MS Fit of medioid: model # 5, percentage satisfied 63.16% - CX-MS Fit of medioid: model # 6, percentage satisfied 65.79% - CX-MS Fit of medioid: model # 7, percentage satisfied 51.54%
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	
<u>Method</u>	Sampling
<u>Name</u>	Replica exchange Monte Carlo
<u>Name</u> <u>Details</u>	- Method details unspecified