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

| 1. Model Composition | |
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| Entry composition | - CSN7: Chain G (264 residues) - CSN8: Chain H (209 residues) - CSN3: Chain C (423 residues) - CSN5: Chain E (334 residues) - CSN4: Chain D (406 residues) - CSN6: Chain F (327 residues) - CSN1: Chain A (491 residues) - CSN2: Chain B (443 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: DHSO, 91 cross-links - CX-MS data, Linker name and number of cross-links: DHSO, 91 cross-links |
| 2. Representation | |
| Atomic structural coverage | 85% |
| Number of rigid bodies, flexible units | 23, 28 |
| | - A: 44-107:Comparative model/None, 128-227:Comparative model/None, 246-426:Comparative model/None, 431-462:Comparative model/None B: 30-179:Experimental model/4D10, 192-289:Experimental model/4D10, 308-397:Experimental model/4D10, 417-443:Experimental model/4D10 C: 3-163:Experimental model/4D10, 177-361:Experimental model/4D10, 368-401:Experimental model/4D10 D: 3-131:Experimental model/4D10, 139- |

| 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. |
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| 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 | - 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 | |
| <u>Method</u> | Sampling |

| <u>Name</u> | Replica exchange Monte Carlo |
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| <u>Details</u> | - Method details unspecified |
| <u>Software</u> | - IMP PMI module (version 20200514.develop.17be5981c6) - Integrative Modeling Platform (IMP) (version 20200514.develop.17be5981c6) - MODELLER (version SVN) - No location specified |