

Summary of integrative structure determination of Integrative structure of the canonical human COP9 Signalosome (PDB ID: 9A01, PDB-Dev ID: PDBDEV_00000037)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - CSN8: Chain H (209 residues) - CSN5: Chain E (334 residues) - CSN7: Chain G (264 residues) - CSN2: Chain B (443 residues) - CSN3: Chain C (423 residues) - CSN4: Chain D (406 residues) - CSN1: Chain A (491 residues) - CSN6: Chain F (327 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Experimental model, PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 4D10 - Experimental model, PDB ID: Not available - Comparative model, template PDB ID: Not available - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 74 cross-links - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 141 cross-links - Crosslinking-MS data, Linker name and number of cross-links: BMSO, 40 cross-links - Crosslinking-MS data, Linker name and number of cross-links: BMSO, 31 cross-links - Crosslinking-MS data, Linker name and number of cross-links: DHSO, 91 cross-links - Crosslinking-MS data, Linker name and number of cross-links: DHSO, 79 cross-links
2. Representation	
<u>Resolution</u>	Coarse-grained: 1, 2, 3, 5, 6 residue(s) per bead
<u>Number of rigid bodies, flexible units</u>	23, 28
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: 44-107, 128-227, 246-426, 431-462 - B: 30-179, 192-289, 308-397, 417-443 - C: 3-163, 177-361, 368-401 - D: 3-131, 139-361, 365-406 - E: 25-283, 296-333 - F: 29-207, 215-267, 271-316 - G: 8-158, 163-212 - H: 11-164, 194-209
<i>Flexible units</i>	<ul style="list-style-type: none"> - 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

<u>Structural coverage (rigid bodies)</u>	85%
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, 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	
<u>Number of ensembles</u>	7
<u>Number of models in ensembles</u>	54702, 132407, 98186, 87368, 243067, 312515, 357350
<u>Number of deposited models</u>	7
<u>Model precision (uncertainty of models)</u>	16.0, Å, 22.0, Å, 24.0, Å, 27.0, Å, 27.0, Å, 29.0, Å, 37.0, Å
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of excluded volume</u>	Satisfaction: 99.78-99.79%
<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	
<u>1. Method</u>	Sampling
<u>Name</u>	Replica exchange monte carlo
<u>Number of computed models</u>	5250000
<u>Software</u>	<ul style="list-style-type: none"> - IMP PMI module (version 20200514.develop.17be5981c6) - Integrative Modeling Platform (IMP) (version 20200514.develop.17be5981c6) - MODELLER (version SVN)