

Summary of integrative structure determination of Molecular architecture of the endocytic TPLATE/TSET complex (PDB ID: 9A0T, PDB-Dev ID: PDBDEV_0000065)

| 1. Model Composition | |
|---------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p>Entry composition</p> | <ul style="list-style-type: none"> - tash3: Chain B (1198 residues) - tplate: Chain C (1176 residues) - lol: Chain A (147 residues) - wd2: Chain F (1376 residues) - eh1: Chain G (1019 residues) - eh2: Chain H (1218 residues) - tml: Chain D (646 residues) - wd1: Chain E (1592 residues) |
| <p>Datasets used for modeling</p> | <ul style="list-style-type: none"> - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Crosslinking-MS data, Linker name and number of cross-links: BS3, 119 cross-links - Experimental model, PDB ID: 5NZR - Experimental model, PDB ID: 5MU7 - Experimental model, PDB ID: 6OWT - Experimental model, PDB ID: 2KYM - Experimental model, PDB ID: 2JKR - Experimental model, PDB ID: 5JP2 - Experimental model, PDB ID: 5AWS - Experimental model, PDB ID: 3G9H - Experimental model, PDB ID: 3MKQ - Experimental model, PDB ID: 3MKR - Experimental model, PDB ID: 2YNP - Experimental model, PDB ID: 6YEU - Experimental model, PDB ID: 6YET |
| 2. Representation | |

| | |
|--------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Resolution | Coarse-grained: 1, 2, 3, 5, 6, 7, 12, 15 residue(s) per bead |
| Number of rigid bodies, flexible units | 26, 24 |
| Rigid bodies | <ul style="list-style-type: none"> - A: 1-147 - B: 104-171, 205-258, 281-419, 464-499, 551-686, 716-734, 766-812, 1131-1198 - C: 1-467, 771-1045 - D: 1-40, 96-191, 407-646 - E: 18-349, 450-1002, 1303-1592 - F: 1-52, 125-534, 676-752, 771-974, 1012-1167 - G: 1-110, 346-449 - H: 1-112, 400-512 |
| Flexible units | <ul style="list-style-type: none"> - A: - - B: 1-103, 172-204, 259-280, 420-463, 500-550, 687-715, 735-765, 813-1130 - C: 468-770, 1046-1176 - D: 41-95, 192-406 - E: 1-17, 350-449, 1003-1302 - F: 53-124, 535-675, 753-770, 975-1011, 1168-1376 - G: 111-345, 450-1019 - H: 113-399, 513-1218 |
| Structural coverage (rigid bodies) | 52% |
| 3. Restraints | |
| Physical principles | Information about physical principles was not provided |
| Experimental data | - 1 unique CrossLinkRestraint: BS3, 119 cross-links |
| 4. Validation | |
| Number of ensembles | 1 |
| Number of models in ensembles | 3981 |
| Number of deposited models | 1 |
| Model precision (uncertainty of models) | 39.4, Å |
| Data quality | Data quality has not been assessed |
| Model quality: assessment of excluded volume | Satisfaction: 99.89-99.89% |
| Fit to data used for modeling | Fit of model to information used to compute it has not been determined |
| Fit to data used for validation | Fit of model to information not used to compute it has not been determined |
| 5. Methodology and Software | |

| | |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| <i>1. Method</i> | Sampling |
| <i>Name</i> | Replica exchange monte carlo |
| <i>Number of computed models</i> | 1000000 |
| <i>Software</i> | - IMP PMI module (version 2.12.0) - Integrative Modeling Platform (IMP) (version 2.12.0) |