

Summary of integrative structure determination of structure of k63-linked diubiquitin (PDBDEV00000004)

| 1. Model Composition | |
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| Entry composition | <ul style="list-style-type: none"> - Ubiquitin: Chain B (76 residues) - Ubiquitin: Chain A (76 residues) |
| Datasets used for modeling | <ul style="list-style-type: none"> - SAS data, SASDCG7 - Experimental model, PDB ID: 1UBQ - Experimental model, PDB ID: 2N2K - CX-MS data, Linker name and number of cross-links: EGS, 1 cross-links - Single molecule FRET data, Not listed |
| 2. Representation | |
| Atomic structural coverage | 100% |
| Number of rigid bodies, flexible units | 0, 2 |
| Rigid bodies | <ul style="list-style-type: none"> - A: - - B: - |
| Flexible units | <ul style="list-style-type: none"> - A: 1-76. - B: 1-76. |
| Resolution | <ul style="list-style-type: none"> - Rigid bodies: 1 residue per bead. - Flexible regions: N/A |
| 3. Restraints | |
| Physical principles | Information about physical principles was not provided |
| Experimental data | <ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: EGS, 1 cross-links - 1 unique CrossLinkRestraint: BS3, 1 cross-links - 1 unique CrossLinkRestraint: BS2G, 1 cross-links - 1 unique CrossLinkRestraint: DST, 1 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, 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 | <ul style="list-style-type: none"> - SASDCG7: Rg from Guinier is 2.1nm and Rg from p(r) is 2.0nm |

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| <i>Model quality: assessment of atomic segments</i> | Clashscore: 4.07, Ramachandran outliers: 0.68% , Sidechain outliers: 6.13% |
| <i>Model quality: assessment of excluded volume</i> | - Not applicable |
| <i>Fit of the model to information used to compute it</i> | - Fit of model to data has not been deposited |
| <i>Fit of the model to information not used to compute it</i> | - Fit of model to information not used to compute it has not been determined |
| 5. Methodology and Software | |
| <i>Method</i> | None |
| <i>Name</i> | None |
| <i>Details</i> | - Method details unspecified |
| <i>Software</i> | - Software details not provided - No location specified |