# Full wwPDB Integrative Structure Validation Report

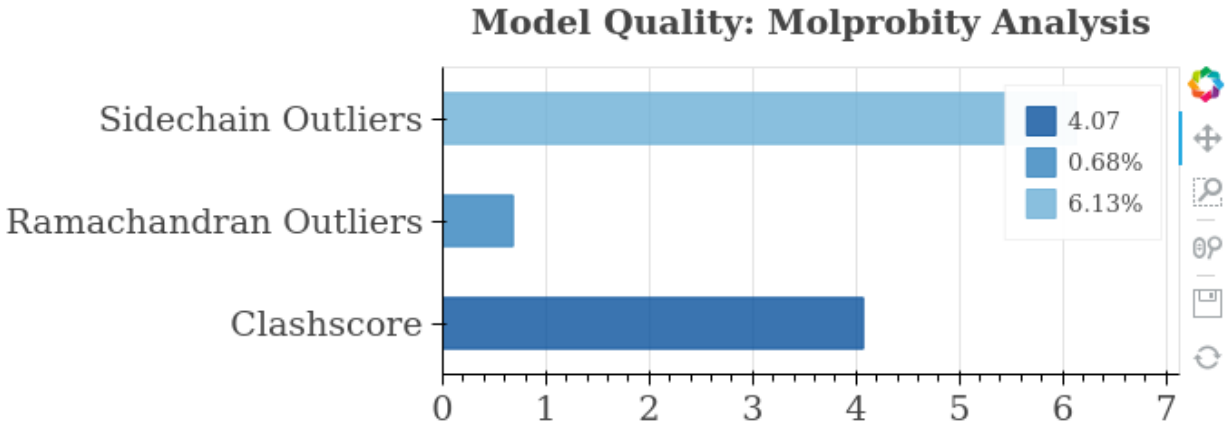
## December 11, 2019 -- 11:33 PM

| *PDB ID* | *PDBDEV00000004* |
|---|---|
| Molecule Name | Structure of K63-linked Diubiquitin |
| Title | Characterizing Protein Dynamics with Integrative Use of Bulk and Single-Molecule Techniques |
| Authors | Liu Z;Gong Z;Cao Y;Ding YH;Dong MQ;Lu YB;Zhang WP;Tang C |

**The following software were used in the production of this report:**

*Molprobity : Version 4.4*
*Integrative Modeling Validation Package : Version 1.0*

## 1. Overall quality at a glance




## 2. Ensemble information

*This entry consists of 0 distinct ensemble.*

## 3. Model composition

### 3.1 Summary

*This entry consists of 3 unique models, with 2 subunits in each model. A total of 5 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 2 flexible or non-rigid units.*

### 3.2 Entry composition

*There are 3 unique types of models in this entry.These models are titled None/Model 1, None/Model 2, None/Model 3 respectively.*

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Total residues |
|---|---|---|---|---|---|
| 1 | 1 | 1 | Ubiquitin | A | 76 |
| 1 | 2 | 1 | Ubiquitin | B | 76 |
| 2 | 1 | 1 | Ubiquitin | A | 76 |
| 2 | 2 | 1 | Ubiquitin | B | 76 |
| 3 | 1 | 1 | Ubiquitin | A | 76 |
| 3 | 2 | 1 | Ubiquitin | B | 76 |

### 3.3 Datasets used for modeling

*There are 5 unique datasets used to build the models in this entry.*

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 1 | SAS data | SASBDB | SASDCG7 |
| 2 | Experimental model | PDB | 1UBQ |
| 3 | Experimental model | PDB | 2N2K |
| 4 | CX-MS data | Not listed | None |
| 5 | Single molecule FRET data | Not listed | None |

## 4. Representation

*This entry has only one representation and includes 0 rigid bodies and 2 flexible units.*

| Chain ID | Rigid bodies | Non-rigid segments |
|---|---|---|
| A | - | 1-76. |

| | | |
|---|---|---|
| B | - | 1-76. |

## 5. Methodology and software

| Step number | Protocol ID | Method name | Method type | Number of computed models | Multi state modeling | Multi scale modeling |
|---|---|---|---|---|---|---|
| 1 | 1 | None | None | None | True | None |

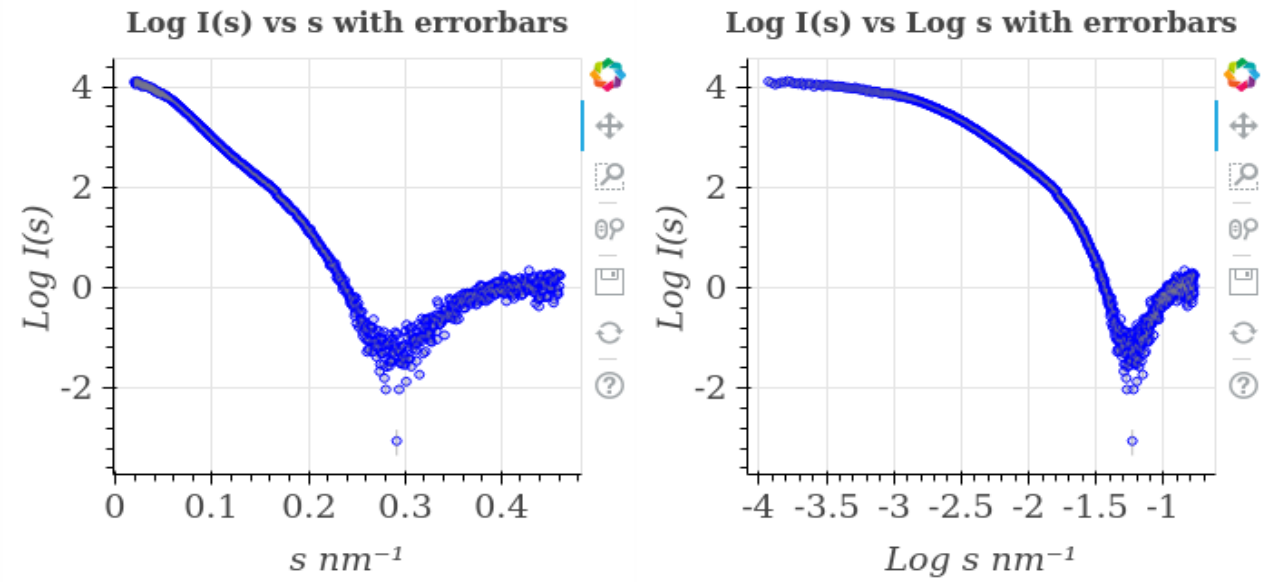
*Software packages used for modeling were either not reported or not used.*

## 6. Data quality

### 6.1 Analysis of SAXS data used in this entry

#### 6.1.1 Intensity plots

*SAXS data was obtained from deposited SASBDB entry: SASDCG7. Below are plots of intentisities, for further information, refer to entry on SASBDB.*




#### 6.1.2. Key experimental estimates

*Molecular weight (MW) estimates from experiments and analysis.*

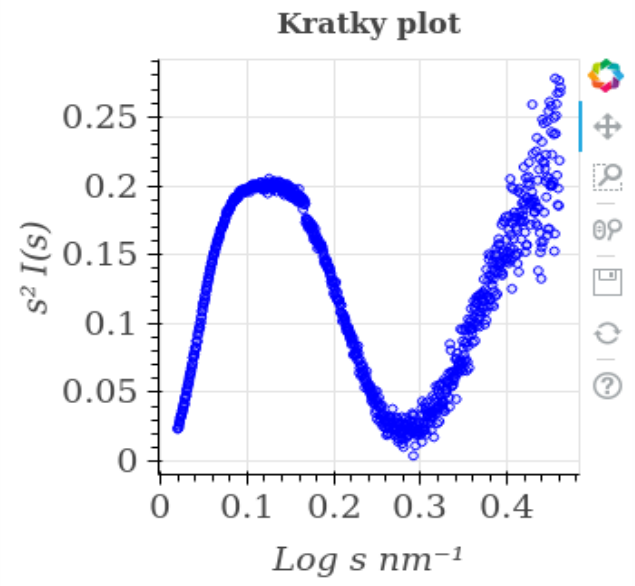
| Molecule MW | Experimental MW | Porod MW | Guinier MW |
|---|---|---|---|
| 17.130 | 13.000 | 13.000 | None |

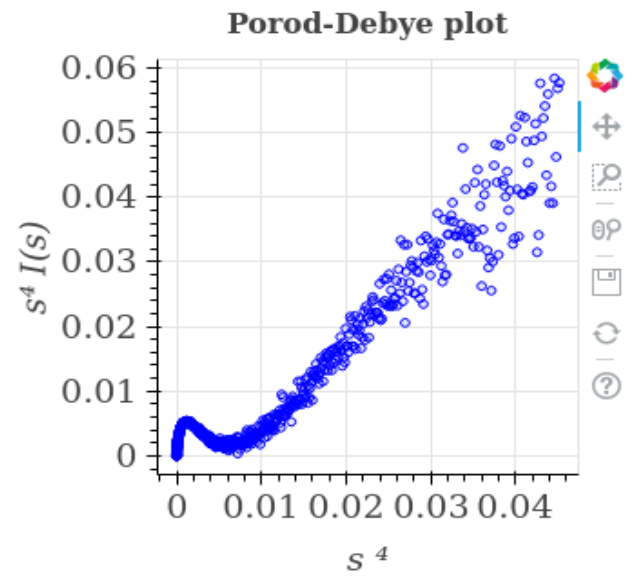
*Volume estimates from experiments and analysis.*

| Estimated volume | Estimated volume method | Porod volume |
|---|---|---|
| None | None | 22.00 nmÂ³ |

#### 6.1.3. Flexibility analysis

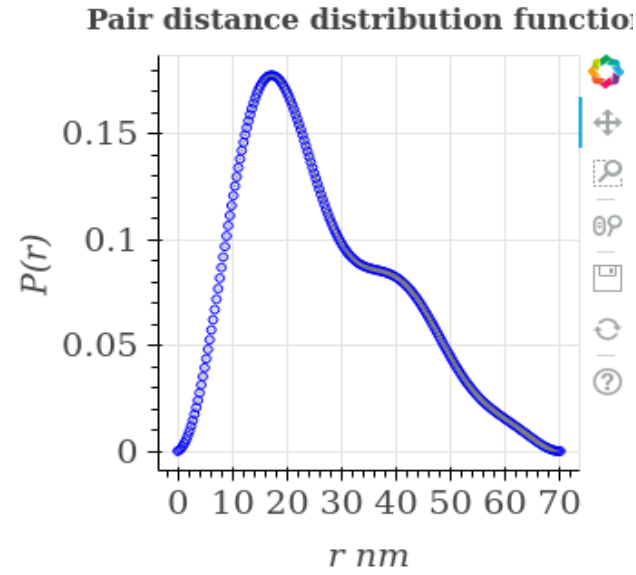
*Flexibility is assessed by Kratky and Porod-Debye plots. For details, refer to Rambo and Tainer,2011.*




#### 6.1.4. Pair-distance distribution analysis

*Pair-distance distribution was evaluated using ATSAS software. The analysis resulted in a $D_{max}$ of 7nm and a radius of gyration of 2.1nm*




## 7. Model quality

### 7.1 Standard geometry

*There are 3774 bond outliers in this entry.*

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| NH1--HH12 | 0.999 | 0.86 | 23 |
| NZ--HZ2 | 1.039 | 0.89 | 38 |
| NZ--HZ1 | 1.038 | 0.89 | 41 |
| NE--HE | 1.008 | 0.86 | 23 |
| N--H2 | 1.04 | 0.89 | 5 |
| CE1--HE1 | 1.078 | 0.93 | 23 |
| CD1--HD1 | 1.079 | 0.93 | 17 |
| CZ--HZ | 1.078 | 0.93 | 11 |
| CD2--HD2 | 1.078 | 0.93 | 23 |
| CE2--HE2 | 1.078 | 0.93 | 17 |
| NZ--HZ3 | 1.038 | 0.89 | 38 |
| N--H3 | 1.038 | 0.89 | 5 |
| NH2--HH22 | 0.999 | 0.86 | 23 |
| N--H1 | 1.039 | 0.89 | 5 |
| NH2--HH21 | 0.985 | 0.86 | 23 |
| NH1--HH11 | 0.977 | 0.86 | 23 |
| ND2--HD22 | 0.979 | 0.86 | 11 |
| NE2--HE22 | 0.979 | 0.86 | 35 |
| CD--HD2 | 1.077 | 0.97 | 83 |
| OG1--HG1 | 0.959 | 0.84 | 41 |
| N--H | 0.978 | 0.86 | 431 |
| NE2--HE21 | 0.958 | 0.86 | 35 |
| OG--HG | 0.959 | 0.84 | 17 |
| ND1--HD1 | 0.979 | 0.86 | 5 |
| ND2--HD21 | 0.956 | 0.86 | 11 |
| OH--HH | 0.958 | 0.84 | 5 |

| | | | |
|---|---|---|---|
| NE2--HE2 | 0.978 | 0.86 | 5 |
| CB--HB2 | 1.073 | 0.97 | 311 |
| CA--HA | 1.076 | 0.97 | 419 |
| CB--HB | 1.079 | 0.97 | 107 |
| CB--HB3 | 1.069 | 0.97 | 311 |
| CG--HG3 | 1.076 | 0.97 | 161 |
| CG--HG2 | 1.074 | 0.97 | 161 |
| CG--HG | 1.077 | 0.97 | 53 |
| CA--HA2 | 1.076 | 0.97 | 35 |
| CA--HA3 | 1.076 | 0.97 | 35 |
| CG1--HG13 | 1.078 | 0.97 | 65 |
| CE--HE2 | 1.077 | 0.97 | 47 |
| CD--HD3 | 1.057 | 0.97 | 83 |
| CD1--HD13 | 1.078 | 0.97 | 95 |
| CG1--HG12 | 1.077 | 0.97 | 65 |
| CE--HE3 | 1.078 | 0.97 | 47 |
| CG2--HG23 | 1.078 | 0.97 | 107 |
| CD2--HD21 | 1.077 | 0.97 | 53 |
| CD1--HD12 | 1.077 | 0.97 | 95 |
| CD2--HD22 | 1.079 | 0.97 | 53 |
| CG2--HG21 | 1.077 | 0.97 | 107 |
| CG2--HG22 | 1.078 | 0.97 | 107 |
| CD1--HD11 | 1.078 | 0.97 | 95 |
| CD2--HD23 | 1.078 | 0.97 | 53 |
| CE--HE1 | 1.081 | 0.97 | 5 |
| CG1--HG11 | 1.079 | 0.97 | 23 |
| CB--HB1 | 1.079 | 0.97 | 11 |

*There are 0 angle outliers in this entry.*

## 7.2 Too-close contacts

*The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.*

| Model ID | Clash score | Number of clashes |
|---|---|---|
| Model 1 | 4.07 | 10 |
| Model 2 | 0.00 | 0 |
| Model 3 | 0.00 | 0 |

*All 10 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.*

## 7.3 Torsion angles

### 7.3.1 Protein backbone

*In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation wasanalysed.*

| Model ID | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|
| 1 | 148 | 144 | 3 | 1 |
| 2 | 148 | 146 | 1 | 1 |
| 3 | 148 | 145 | 2 | 1 |

*Detailed list of outliers are tabulated below.*

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 1 | B:73 | LEU |
| 2 | B:73 | LEU |
| 3 | B:75 | GLY |

### 7.3.2 Protein sidechains

*In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.*

| Model ID | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 136 | 116 | 12 | 8 |
| 2 | 136 | 116 | 12 | 8 |
| 3 | 136 | 114 | 13 | 9 |

*Detailed list of outliers are tabulated below.*

| Model ID | Chain and res ID | Residue type |
|---|---|---|
| 1 | A:13 | ILE |
| 1 | A:15 | LEU |
| 1 | A:39 | ASP |
| 1 | A:71 | LEU |
| 1 | B:13 | ILE |
| 1 | B:15 | LEU |
| 1 | B:39 | ASP |
| 1 | B:71 | LEU |
| 2 | A:13 | ILE |
| 2 | A:15 | LEU |
| 2 | A:39 | ASP |
| 2 | A:71 | LEU |
| 2 | B:13 | ILE |
| 2 | B:15 | LEU |
| 2 | B:39 | ASP |
| 2 | B:71 | LEU |
| 3 | A:13 | ILE |
| 3 | A:15 | LEU |
| 3 | A:39 | ASP |
| 3 | A:71 | LEU |
| 3 | A:74 | ARG |

| | | |
|---|---|---|
| 3 | B:13 | ILE |
| 3 | B:15 | LEU |
| 3 | B:39 | ASP |
| 3 | B:71 | LEU |

## 8. Fit of model to data used for modeling

### 8.1 Fit of model to SAS data

*Model fit for this entry has not been deposited.*

## 9. Fit of model to data not used for modeling

## 10. Uncertainty of model