Full wwPDB Integrative Structure Validation Report

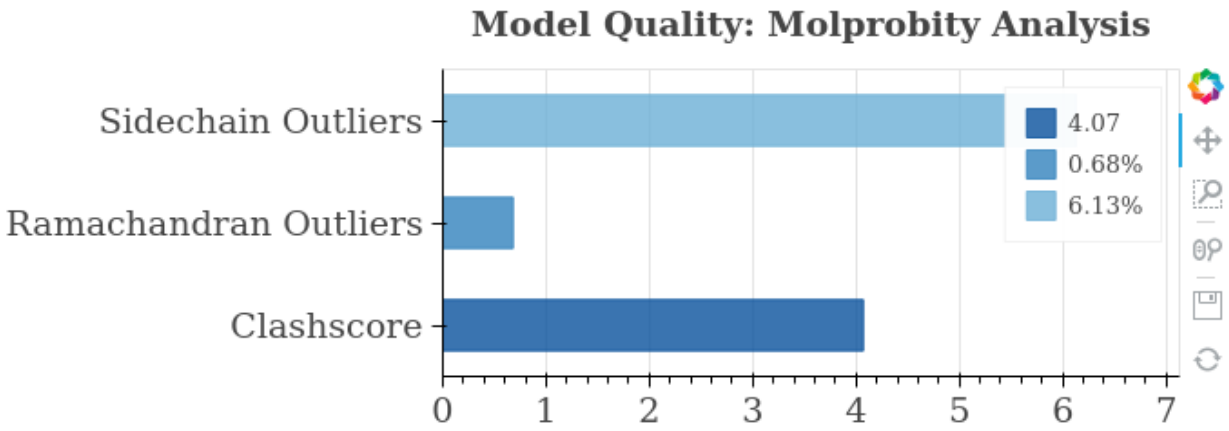
December 10, 2019 -- 10:49 AM

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

NaN

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.

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

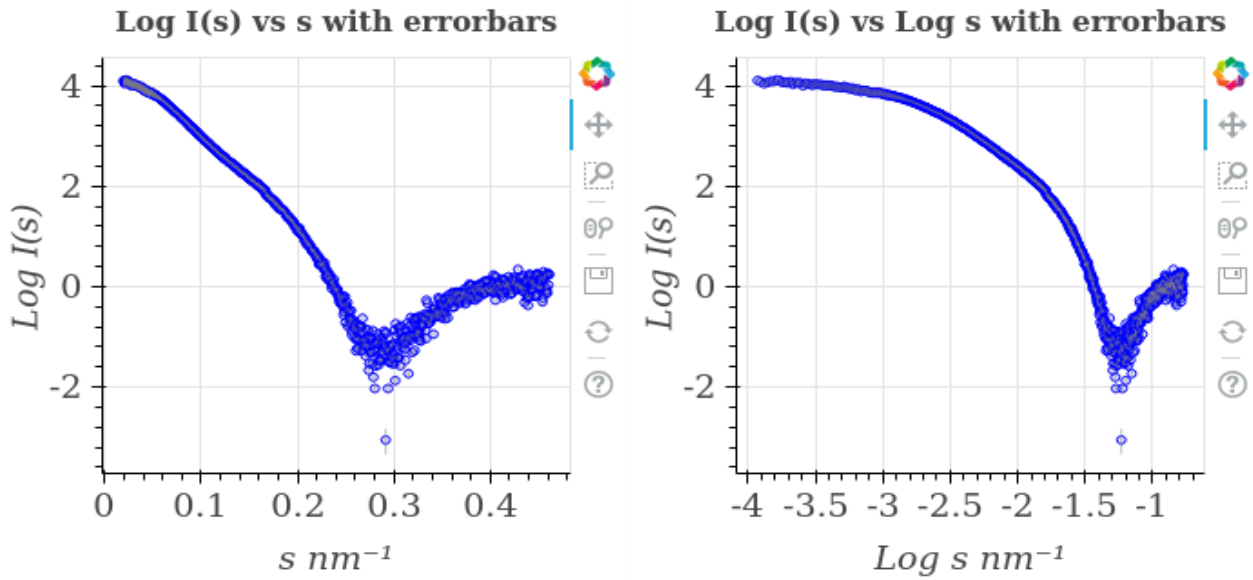
3	A:74	ARG
3	B:13	ILE
3	B:15	LEU
3	B:39	ASP
3	B:71	LEU

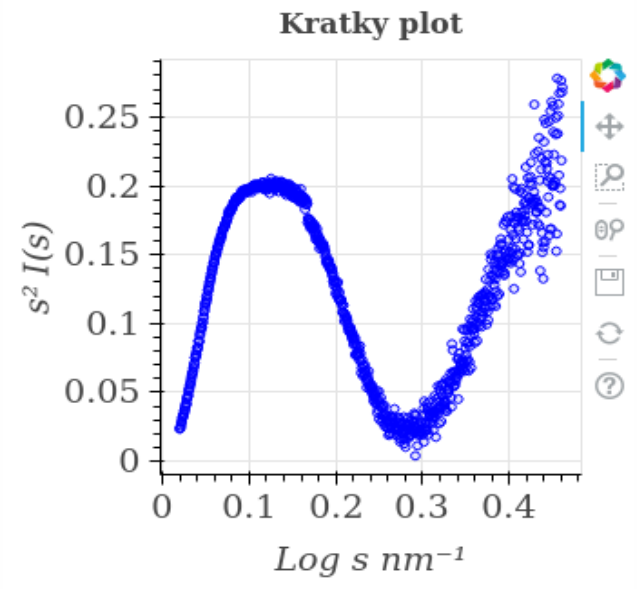
8. Fit of model to data used for modeling

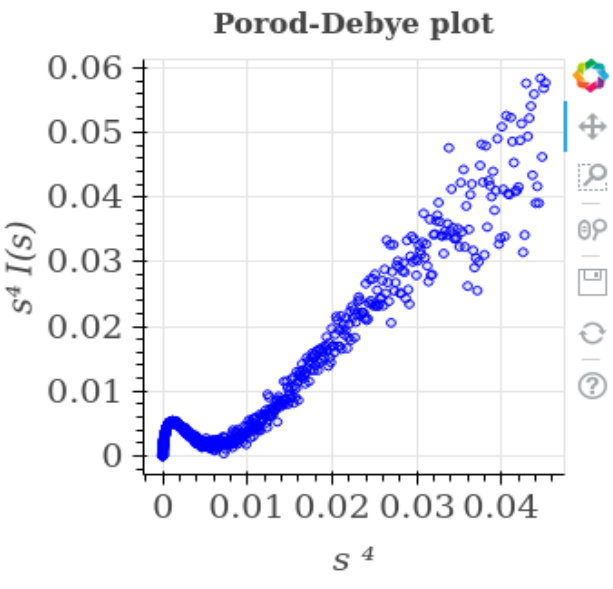
8.1 Fit of model to SAS data

9. Fit of model to data not used for modeling

10. Uncertainty of model




Kratky plot
0.25
0.2
0.15
0.1
0.05
0
0
0.1
0.2
0.3
0.4
$s^2 I(s)$
$Log\ s\ nm^{-1}$


Porod-Debye plot
0.06
0.05
0.04
0.03
0.02
0.01
0
0
0.01
0.02
0.03
0.04
$s^4 I(s)$
s^4