



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2016 – 10:24 PM EDT

PDB ID : 5JG6  
Title : APC11-Ubv shows role of noncovalent RING-Ubiquitin interactions in processive multiubiquitination and Ubiquitin chain elongation by APC/C  
Authors : Brown, N.G.; Zhang, W.; Yu, S.; Miller, D.J.; Sidhu, S.S.; Schulman, B.A.  
Deposited on : 2016-04-19  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : **FAILED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

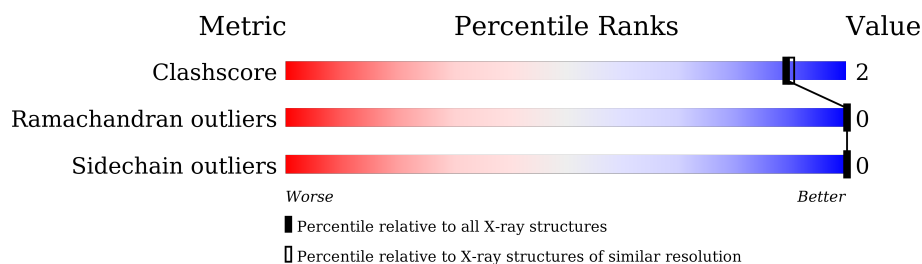
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	70	
1	D	70	
2	B	84	
2	C	84	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2279 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	61	Total	C	N	O	S	0	0	0
			469	293	89	74	13			
1	D	66	Total	C	N	O	S	0	0	0
			503	311	94	84	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP Q9NYG5
A	16	SER	-	expression tag	UNP Q9NYG5
D	15	GLY	-	expression tag	UNP Q9NYG5
D	16	SER	-	expression tag	UNP Q9NYG5

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	S	0	2	0
			606	383	104	117	2			
2	C	75	Total	C	N	O	S	0	1	0
			579	368	97	112	2			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP P0CG47
B	-4	SER	-	expression tag	UNP P0CG47
B	-3	GLY	-	expression tag	UNP P0CG47
B	-2	GLY	-	expression tag	UNP P0CG47
B	-1	SER	-	expression tag	UNP P0CG47
B	4	LEU	PHE	conflict	UNP P0CG47
B	8	PRO	LEU	conflict	UNP P0CG47
B	9	ARG	THR	conflict	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
B	42	ILE	ARG	conflict	UNP P0CG47
B	44	PHE	ILE	conflict	UNP P0CG47
B	47	VAL	GLY	conflict	UNP P0CG47
B	49	ARG	GLN	conflict	UNP P0CG47
B	64	LYS	GLU	conflict	UNP P0CG47
B	66	SER	THR	conflict	UNP P0CG47
B	68	LEU	HIS	conflict	UNP P0CG47
B	70	ALA	VAL	conflict	UNP P0CG47
B	71	MET	LEU	conflict	UNP P0CG47
B	73	VAL	LEU	conflict	UNP P0CG47
B	74	PRO	ARG	conflict	UNP P0CG47
B	76	LYS	GLY	conflict	UNP P0CG47
B	78	LYS	GLN	conflict	UNP P0CG47
C	-5	GLY	-	expression tag	UNP P0CG47
C	-4	SER	-	expression tag	UNP P0CG47
C	-3	GLY	-	expression tag	UNP P0CG47
C	-2	GLY	-	expression tag	UNP P0CG47
C	-1	SER	-	expression tag	UNP P0CG47
C	4	LEU	PHE	conflict	UNP P0CG47
C	8	PRO	LEU	conflict	UNP P0CG47
C	9	ARG	THR	conflict	UNP P0CG47
C	42	ILE	ARG	conflict	UNP P0CG47
C	44	PHE	ILE	conflict	UNP P0CG47
C	47	VAL	GLY	conflict	UNP P0CG47
C	49	ARG	GLN	conflict	UNP P0CG47
C	64	LYS	GLU	conflict	UNP P0CG47
C	66	SER	THR	conflict	UNP P0CG47
C	68	LEU	HIS	conflict	UNP P0CG47
C	70	ALA	VAL	conflict	UNP P0CG47
C	71	MET	LEU	conflict	UNP P0CG47
C	73	VAL	LEU	conflict	UNP P0CG47
C	74	PRO	ARG	conflict	UNP P0CG47
C	76	LYS	GLY	conflict	UNP P0CG47
C	78	LYS	GLN	conflict	UNP P0CG47

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Zn 3 3	0	0
3	D	3	Total Zn 3 3	0	0

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	B	41	Total 41	O 41	0	0
4	C	33	Total 33	O 33	0	0
4	D	22	Total 22	O 22	0	0

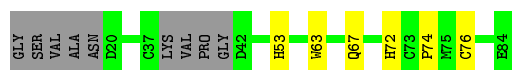
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

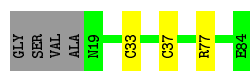
- Molecule 1: Anaphase-promoting complex subunit 11

Chain A: 




- Molecule 1: Anaphase-promoting complex subunit 11

Chain D: 



- Molecule 2: Polyubiquitin-B

Chain B: 



- Molecule 2: Polyubiquitin-B

Chain C: 



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.07Å 35.19Å 72.77Å 90.00° 120.42° 90.00°	Depositor
Resolution (Å)	36.33 – 2.00	Depositor
% Data completeness (in resolution range)	98.3 (36.33-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.185 , 0.220	Depositor
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.063	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/484	0.46	0/652
1	D	0.30	0/520	0.48	0/705
2	B	0.29	0/619	0.48	0/834
2	C	0.30	0/589	0.48	0/797
All	All	0.30	0/2212	0.48	0/2988

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	469	0	399	5	0
1	D	503	0	423	2	0
2	B	606	0	640	3	0
2	C	579	0	599	1	0
3	A	3	0	0	0	0
3	D	3	0	0	0	0
4	A	20	0	0	0	0
4	B	41	0	0	0	0
4	C	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	22	0	0	0	0
All	All	2279	0	2061	10	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 10 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:HE22	1:A:72:HIS:H	1.40	0.69
1:A:67:GLN:O	2:B:6:LYS:NZ	2.36	0.58
2:C:1:MET:HB2	2:C:63:LYS:HD3	1.96	0.48
1:A:63:TRP:CD1	1:A:74:PRO:HG3	2.49	0.48
1:D:77:ARG:HG3	1:D:77:ARG:HH11	1.80	0.46

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	57/70 (81%)	56 (98%)	1 (2%)	0	100	100
1	D	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
2	B	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
2	C	74/84 (88%)	73 (99%)	1 (1%)	0	100	100
All	All	272/308 (88%)	268 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	47/62 (76%)	47 (100%)	0	100	100
1	D	52/62 (84%)	52 (100%)	0	100	100
2	B	70/73 (96%)	70 (100%)	0	100	100
2	C	65/73 (89%)	65 (100%)	0	100	100
All	All	234/270 (87%)	234 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.