



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 12, 2016 – 08:16 PM EDT

PDB ID : 5C7M  
Title : CRYSTAL STRUCTURE OF E3 LIGASE ITCH WITH A UB VARIANT  
Authors : Walker, J.R.; Hu, J.; Dong, A.; Wernimont, A.; Zhang, W.; Sidhu, S.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.H.; Tong, Y.; Structural Genomics Consortium (SGC)  
Deposited on : 2015-06-24  
Resolution : 3.03 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.

---

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	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

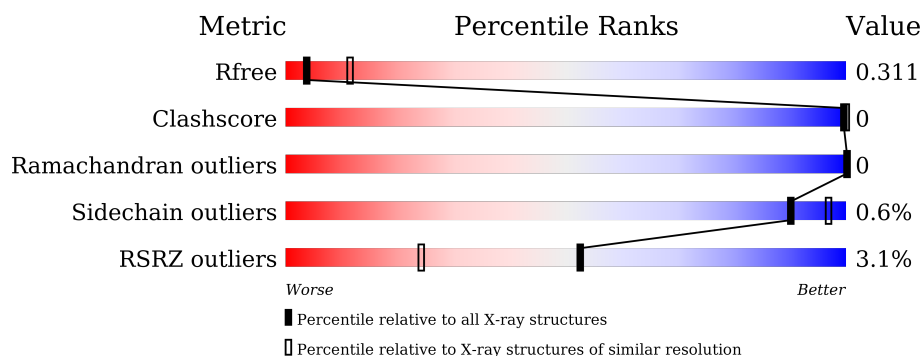
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.03 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))
$R_{free}$	91344	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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.

Mol	Chain	Length	Quality of chain
1	A	394	 8% 93% 6%
2	B	84	 8% 86% 13%
2	C	84	 8% 85% 15%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3871 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 E3 ubiquitin-protein ligase Itchy homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	2	0
			2862	1853	477	518	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	MET	-	expression tag	UNP Q96J02
A	507	HIS	-	expression tag	UNP Q96J02
A	508	HIS	-	expression tag	UNP Q96J02
A	509	HIS	-	expression tag	UNP Q96J02
A	510	HIS	-	expression tag	UNP Q96J02
A	511	HIS	-	expression tag	UNP Q96J02
A	512	HIS	-	expression tag	UNP Q96J02
A	513	SER	-	expression tag	UNP Q96J02
A	514	SER	-	expression tag	UNP Q96J02
A	515	GLY	-	expression tag	UNP Q96J02
A	516	ARG	-	expression tag	UNP Q96J02
A	517	GLU	-	expression tag	UNP Q96J02
A	518	ASN	-	expression tag	UNP Q96J02
A	519	LEU	-	expression tag	UNP Q96J02
A	520	TYR	-	expression tag	UNP Q96J02
A	521	PHE	-	expression tag	UNP Q96J02
A	522	GLN	-	expression tag	UNP Q96J02
A	523	GLY	-	expression tag	UNP Q96J02
A	605	SER	LEU	conflict	UNP Q96J02
A	801	ARG	HIS	conflict	UNP Q96J02

- Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			554	348	96	109	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	71	Total	C	N	O	0	0	0
			452	276	84	92			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	HIS	GLN	engineered mutation	UNP P0CG48
B	4	LEU	PHE	engineered mutation	UNP P0CG48
B	9	ARG	THR	engineered mutation	UNP P0CG48
B	44	LEU	ILE	engineered mutation	UNP P0CG48
B	46	GLY	ALA	engineered mutation	UNP P0CG48
B	48	ASN	LYS	engineered mutation	UNP P0CG48
B	49	LYS	GLN	engineered mutation	UNP P0CG48
B	66	ASN	THR	engineered mutation	UNP P0CG48
B	68	TYR	HIS	engineered mutation	UNP P0CG48
B	70	LEU	VAL	engineered mutation	UNP P0CG48
B	73	ARG	LEU	engineered mutation	UNP P0CG48
B	74	LEU	ARG	engineered mutation	UNP P0CG48
B	76	SER	-	expression tag	UNP P0CG48
B	77	LYS	-	expression tag	UNP P0CG48
B	78	PHE	-	expression tag	UNP P0CG48
B	79	HIS	-	expression tag	UNP P0CG48
B	80	HIS	-	expression tag	UNP P0CG48
B	81	HIS	-	expression tag	UNP P0CG48
B	82	HIS	-	expression tag	UNP P0CG48
B	83	HIS	-	expression tag	UNP P0CG48
B	84	HIS	-	expression tag	UNP P0CG48
C	2	HIS	GLN	engineered mutation	UNP P0CG48
C	4	LEU	PHE	engineered mutation	UNP P0CG48
C	9	ARG	THR	engineered mutation	UNP P0CG48
C	44	LEU	ILE	engineered mutation	UNP P0CG48
C	46	GLY	ALA	engineered mutation	UNP P0CG48
C	48	ASN	LYS	engineered mutation	UNP P0CG48
C	49	LYS	GLN	engineered mutation	UNP P0CG48
C	66	ASN	THR	engineered mutation	UNP P0CG48
C	68	TYR	HIS	engineered mutation	UNP P0CG48
C	70	LEU	VAL	engineered mutation	UNP P0CG48
C	73	ARG	LEU	engineered mutation	UNP P0CG48
C	74	LEU	ARG	engineered mutation	UNP P0CG48
C	76	SER	-	expression tag	UNP P0CG48
C	77	LYS	-	expression tag	UNP P0CG48
C	78	PHE	-	expression tag	UNP P0CG48

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	79	HIS	-	expression tag	UNP P0CG48
C	80	HIS	-	expression tag	UNP P0CG48
C	81	HIS	-	expression tag	UNP P0CG48
C	82	HIS	-	expression tag	UNP P0CG48
C	83	HIS	-	expression tag	UNP P0CG48
C	84	HIS	-	expression tag	UNP P0CG48

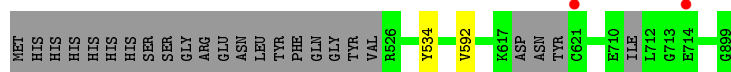
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0

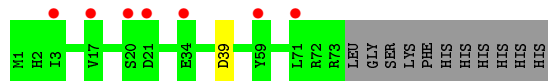
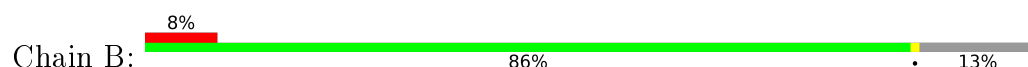
### 3 Residue-property plots [i](#)

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.

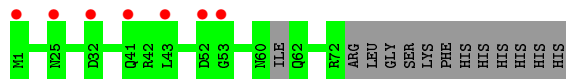
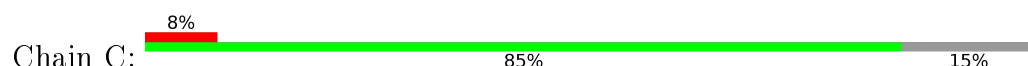
- Molecule 1: E3 ubiquitin-protein ligase Itchy homolog



- Molecule 2: Polyubiquitin-C



- Molecule 2: Polyubiquitin-C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.11Å 121.11Å 85.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.43 – 3.03 49.43 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.43-3.03) 99.5 (49.43-3.03)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.254 , 0.297 0.252 , 0.311	Depositor DCC
$R_{free}$ test set	583 reflections (4.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.5	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 88.5	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 14277 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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](#)

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	0.41	0/2943	0.52	0/4006
2	B	0.37	0/560	0.48	0/760
2	C	0.41	0/456	0.46	0/628
All	All	0.40	0/3959	0.50	0/5394

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	2862	0	2477	1	0
2	B	554	0	536	0	0
2	C	452	0	342	0	0
3	A	3	0	0	0	0
All	All	3871	0	3355	1	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 0.

All (1) 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:592:VAL:HG12	1:A:592:VAL:O	2.17	0.44

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	366/394 (93%)	353 (96%)	13 (4%)	0	100	100
2	B	71/84 (84%)	70 (99%)	1 (1%)	0	100	100
2	C	67/84 (80%)	66 (98%)	1 (2%)	0	100	100
All	All	504/562 (90%)	489 (97%)	15 (3%)	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	253/356 (71%)	252 (100%)	1 (0%)	93	98
2	B	57/77 (74%)	56 (98%)	1 (2%)	66	90
2	C	31/77 (40%)	31 (100%)	0	100	100
All	All	341/510 (67%)	339 (99%)	2 (1%)	90	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	TYR
2	B	39	ASP

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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	370/394 (93%)	-0.07	2 (0%) 91 77	59, 97, 127, 155	0
2	B	73/84 (86%)	0.55	7 (9%) 10 4	89, 131, 155, 160	0
2	C	71/84 (84%)	0.25	7 (9%) 9 3	85, 140, 156, 172	0
All	All	514/562 (91%)	0.06	16 (3%) 52 24	59, 103, 150, 172	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	21	ASP	4.0
2	B	20	SER	3.3
2	B	17	VAL	3.3
2	C	52	ASP	3.1
1	A	621	CYS	3.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.