



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:39 AM UTC

PDB ID : 5XMC / pdb_00005xmc
Title : Crystal structure of the auto-inhibited Nedd4 family E3 ligase Itch
Authors : Shan, Z.; Wen, W.
Deposited on : 2017-05-13
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

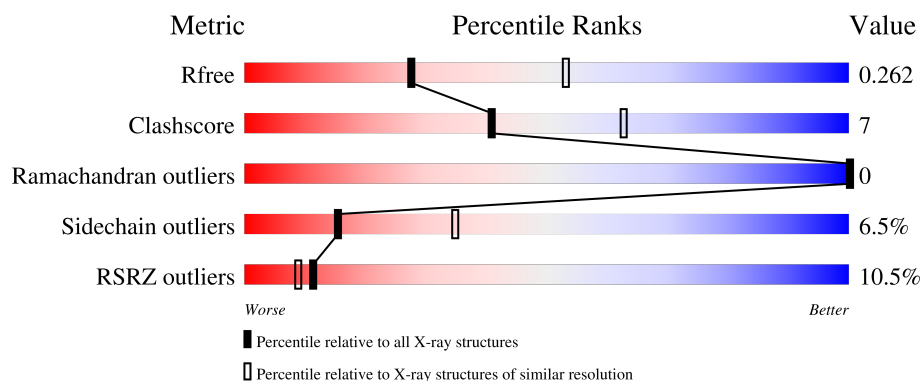
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	722	6% 45% 10% . 43%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3345 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	3	0
			3299	2151	555	577	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	46	Total	O	0	0
			46	46		

- Molecule 1: E3 ubiquitin-protein ligase Itchy



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.59Å 77.08Å 130.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.59 – 2.60 47.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.59-2.60) 97.0 (47.59-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.213 , 0.262 0.215 , 0.262	Depositor DCC
R_{free} test set	1122 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3345	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.51	0/3404	0.83	5/4621 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770	ILE	N-CA-C	-6.36	106.60	112.96
1	A	642	ASP	CA-C-N	5.57	125.41	119.28
1	A	642	ASP	C-N-CA	5.57	125.41	119.28
1	A	792	VAL	N-CA-C	5.24	115.90	110.82
1	A	839	PRO	O-C-N	5.19	123.59	121.15

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	3299	0	2976	41	0
2	A	46	0	0	2	0
All	All	3345	0	2976	41	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 7.

All (41) 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:505:MET:HB3	1:A:536:ARG:HG2	1.71	0.72
1:A:494[B]:GLN:NE2	2:A:901:HOH:O	2.24	0.69
1:A:631:LYS:NZ	2:A:903:HOH:O	2.31	0.60
1:A:287:ALA:O	1:A:317:ARG:NH1	2.34	0.60
1:A:617:ASP:OD1	1:A:797:ARG:NH1	2.36	0.58
1:A:505:MET:HG3	1:A:506:PRO:HD2	1.86	0.58
1:A:827:PRO:HG2	1:A:851:LEU:HD23	1.86	0.58
1:A:294:GLU:OE1	1:A:308:HIS:NE2	2.37	0.53
1:A:378:ARG:NH1	1:A:745:GLY:O	2.43	0.52
1:A:778:LYS:HA	1:A:785:ARG:HH21	1.75	0.51
1:A:848:LYS:O	1:A:852:LEU:HB2	2.13	0.49
1:A:305:TYR:CZ	1:A:317:ARG:HB2	2.47	0.49
1:A:536:ARG:O	1:A:612:HIS:HE1	1.96	0.49
1:A:294:GLU:CD	1:A:296:ARG:HE	2.21	0.48
1:A:493:VAL:O	1:A:497:ARG:HG2	2.12	0.48
1:A:841:TYR:HD2	1:A:847:LEU:HD12	1.78	0.48
1:A:748:GLU:OE2	1:A:782:ASN:ND2	2.45	0.47
1:A:826:LEU:HD12	1:A:826:LEU:HA	1.81	0.47
1:A:514:THR:OG1	1:A:517:THR:OG1	2.33	0.46
1:A:347:TRP:CG	1:A:593:PRO:HD2	2.51	0.46
1:A:792:VAL:HG11	1:A:815:PHE:CE1	2.50	0.46
1:A:347:TRP:CD1	1:A:593:PRO:HD2	2.52	0.45
1:A:575:TYR:CG	1:A:580:ASN:HA	2.52	0.45
1:A:358:TYR:HA	1:A:568:PRO:HG2	1.99	0.44
1:A:847:LEU:O	1:A:851:LEU:HB2	2.17	0.44
1:A:621:SER:O	1:A:624:PHE:HB3	2.18	0.44
1:A:380:ILE:HG22	1:A:381:TYR:CD2	2.53	0.44
1:A:293:TRP:CD2	1:A:318:PRO:HG3	2.53	0.43
1:A:641:ILE:HG23	1:A:642:ASP:H	1.82	0.43
1:A:822:LYS:O	1:A:825:TRP:HB2	2.18	0.43
1:A:757:HIS:CD2	1:A:804:ALA:HB2	2.52	0.43
1:A:527:MET:SD	1:A:604:ARG:HD2	2.58	0.43
1:A:622:LEU:HD12	1:A:622:LEU:HA	1.79	0.43
1:A:567:ASN:HB3	1:A:570:TYR:CD2	2.54	0.42
1:A:489:PHE:CD1	1:A:738:GLU:HG2	2.55	0.42
1:A:625:TYR:HE1	1:A:743:LEU:HD12	1.84	0.42
1:A:565:VAL:HG12	1:A:566:LEU:HD23	2.01	0.41
1:A:827:PRO:HD2	1:A:854:ALA:HB2	2.01	0.41
1:A:737:LYS:NZ	1:A:857:GLU:OE1	2.43	0.41
1:A:610:LEU:HD21	1:A:743:LEU:HG	2.02	0.41
1:A:378:ARG:HD3	1:A:744:CYS:O	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	398/722 (55%)	381 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	311/644 (48%)	290 (93%)	21 (7%)	14	32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	THR
1	A	363	LEU
1	A	365	ARG
1	A	367	GLN
1	A	377	GLN
1	A	378	ARG
1	A	555	ARG
1	A	565	VAL
1	A	622	LEU
1	A	707	LEU
1	A	726	LEU
1	A	729[A]	GLN
1	A	729[B]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	731	LEU
1	A	748	GLU
1	A	786	MET
1	A	810	ASN
1	A	820	VAL
1	A	826	LEU
1	A	851	LEU
1	A	852	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	502	GLN
1	A	716	GLN

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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	409/722 (56%)	0.28	43 (10%) 11 9	16, 42, 89, 110	3 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	766	THR	5.7
1	A	642	ASP	4.5
1	A	705	TRP	4.1
1	A	484	ALA	4.0
1	A	645	PHE	4.0
1	A	842	LYS	3.9
1	A	485	TYR	3.8
1	A	824	ASN	3.8
1	A	652	VAL	3.8
1	A	641	ILE	3.7
1	A	841	TYR	3.5
1	A	773	PHE	3.5
1	A	762	HIS	3.5
1	A	772	TRP	3.4
1	A	765	ARG	3.3
1	A	709	ARG	3.1
1	A	843	SER	2.9
1	A	770	ILE	2.9
1	A	769	GLN	2.8
1	A	706	ARG	2.8
1	A	579	ASP	2.7
1	A	507	GLN	2.6
1	A	810	ASN	2.5
1	A	813	GLN	2.5
1	A	640	SER	2.4
1	A	648	SER	2.4
1	A	549	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	576	ALA	2.4
1	A	542	PHE	2.4
1	A	840	PRO	2.4
1	A	800	VAL	2.4
1	A	752	ASN	2.3
1	A	650	ILE	2.3
1	A	590	TYR	2.3
1	A	580	ASN	2.2
1	A	651	TRP	2.2
1	A	816	CYS	2.1
1	A	815	PHE	2.1
1	A	634	GLY	2.1
1	A	776	PHE	2.1
1	A	846	GLN	2.0
1	A	820	VAL	2.0
1	A	646	TYR	2.0

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 oligosaccharides 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.