



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2021 – 04:01 pm BST

PDB ID : 7NVK  
Title : Crystal structure of UBA5 fragment fused to the N-terminus of UFC1  
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Deposited on : 2021-03-15  
Resolution : 2.65 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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

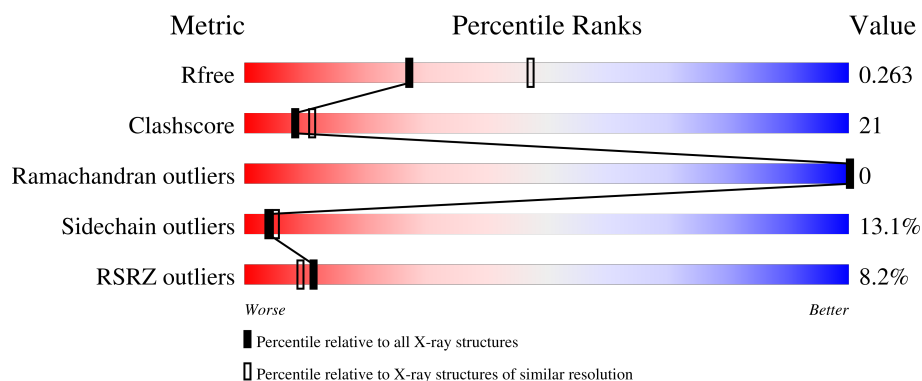
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	AAA	226	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1488 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 Ubiquitin-like modifier-activating enzyme 5, Ubiquitin-fold modifier-conjugating enzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	183	Total	C	N	O	S	0	0	0
			1488	955	251	274	8			

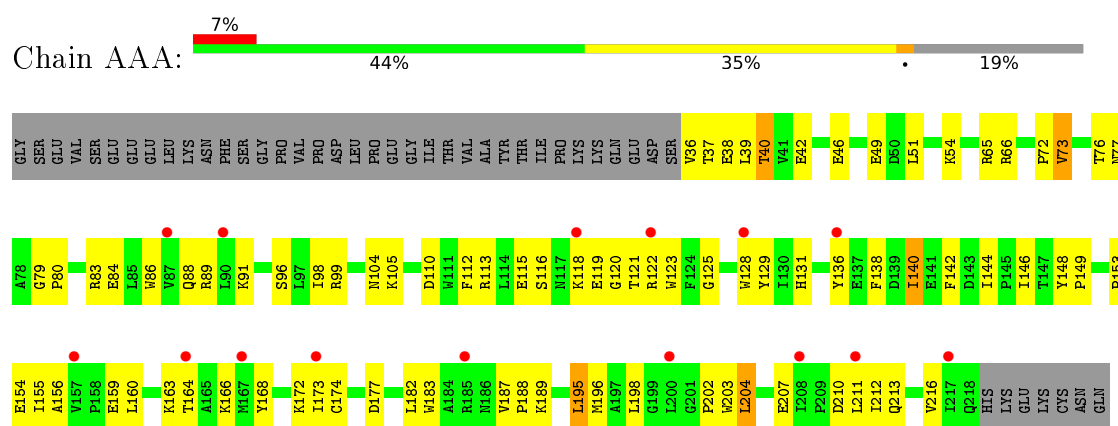
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	GLY	-	expression tag	UNP Q9GZZ9

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Ubiquitin-like modifier-activating enzyme 5, Ubiquitin-fold modifier-conjugating enzyme 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.63 Å 84.63 Å 60.77 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.78 – 2.65 46.78 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.78-2.65) 100.0 (46.78-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.65 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.216 , 0.264 0.216 , 0.263	Depositor DCC
$R_{free}$ test set	373 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.2	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 125.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	AAA	0.31	0/1524	0.74	0/2065

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 ⓘ

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	AAA	1488	0	1481	62	0
All	All	1488	0	1481	62	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 21.

All (62) 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:AAA:168:TYR:HD2	1:AAA:172:LYS:O	1.67	0.76
1:AAA:125:GLY:O	1:AAA:140:ILE:HG13	1.89	0.72
1:AAA:183:TRP:O	1:AAA:187:VAL:HG23	1.92	0.69
1:AAA:182:LEU:HD12	1:AAA:182:LEU:O	1.94	0.67
1:AAA:73:VAL:HG22	1:AAA:189:LYS:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:120:GLY:O	1:AAA:123:TRP:NE1	2.32	0.62
1:AAA:168:TYR:CD2	1:AAA:172:LYS:O	2.50	0.61
1:AAA:129:TYR:CE2	1:AAA:131:HIS:HB2	2.36	0.61
1:AAA:136:TYR:HB3	1:AAA:138:PHE:CZ	2.36	0.60
1:AAA:79:GLY:O	1:AAA:86:TRP:HB2	2.03	0.57
1:AAA:198:LEU:O	1:AAA:202:PRO:HG2	2.06	0.56
1:AAA:159:GLU:HG2	1:AAA:160:LEU:HD23	1.86	0.56
1:AAA:163:LYS:O	1:AAA:211:LEU:HD22	2.07	0.55
1:AAA:148:TYR:CG	1:AAA:149:PRO:HA	2.42	0.55
1:AAA:110:ASP:OD1	1:AAA:113:ARG:NH1	2.34	0.54
1:AAA:73:VAL:CG2	1:AAA:189:LYS:HB3	2.37	0.54
1:AAA:116:SER:HB3	1:AAA:123:TRP:CD2	2.42	0.54
1:AAA:159:GLU:HG2	1:AAA:160:LEU:N	2.22	0.54
1:AAA:38:GLU:O	1:AAA:40:THR:HG23	2.10	0.52
1:AAA:113:ARG:HG2	1:AAA:128:TRP:CH2	2.45	0.51
1:AAA:76:THR:OG1	1:AAA:88:GLN:NE2	2.43	0.51
1:AAA:83:ARG:HB2	1:AAA:83:ARG:HH11	1.76	0.51
1:AAA:113:ARG:HG2	1:AAA:128:TRP:CZ3	2.46	0.51
1:AAA:146:ILE:HD13	1:AAA:146:ILE:N	2.26	0.50
1:AAA:121:THR:O	1:AAA:122:ARG:HG3	2.11	0.50
1:AAA:112:PHE:O	1:AAA:113:ARG:NH1	2.45	0.50
1:AAA:84:GLU:H	1:AAA:84:GLU:CD	2.15	0.50
1:AAA:110:ASP:CG	1:AAA:113:ARG:HH12	2.15	0.50
1:AAA:80:PRO:HG3	1:AAA:144:ILE:HG22	1.94	0.49
1:AAA:155:ILE:O	1:AAA:172:LYS:HA	2.12	0.49
1:AAA:129:TYR:HE2	1:AAA:131:HIS:HB2	1.77	0.49
1:AAA:119:GLU:H	1:AAA:119:GLU:CD	2.15	0.49
1:AAA:195:LEU:O	1:AAA:195:LEU:HG	2.13	0.49
1:AAA:113:ARG:O	1:AAA:125:GLY:HA3	2.14	0.48
1:AAA:104:ASN:HB3	1:AAA:110:ASP:HA	1.95	0.48
1:AAA:153:PRO:HD2	1:AAA:195:LEU:HD13	1.96	0.47
1:AAA:105:LYS:HE3	1:AAA:110:ASP:OD2	2.14	0.47
1:AAA:203:TRP:CZ2	1:AAA:207:GLU:HG3	2.50	0.46
1:AAA:113:ARG:CG	1:AAA:128:TRP:HH2	2.28	0.46
1:AAA:204:LEU:HD22	1:AAA:204:LEU:HA	1.80	0.45
1:AAA:182:LEU:HD12	1:AAA:182:LEU:C	2.37	0.45
1:AAA:77:ASN:HB2	1:AAA:188:PRO:HG3	1.99	0.45
1:AAA:168:TYR:CZ	1:AAA:174:CYS:SG	3.07	0.45
1:AAA:173:ILE:HG22	1:AAA:203:TRP:CZ2	2.51	0.44
1:AAA:166:LYS:HA	1:AAA:166:LYS:HD3	1.87	0.44
1:AAA:131:HIS:ND1	1:AAA:212:ILE:HD13	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:164:THR:HB	1:AAA:211:LEU:HD11	1.98	0.44
1:AAA:37:THR:O	1:AAA:37:THR:HG22	2.18	0.44
1:AAA:80:PRO:HB3	1:AAA:121:THR:HG22	2.00	0.44
1:AAA:155:ILE:HG22	1:AAA:156:ALA:N	2.32	0.44
1:AAA:76:THR:O	1:AAA:89:ARG:HD3	2.19	0.43
1:AAA:164:THR:HB	1:AAA:211:LEU:HD21	2.00	0.43
1:AAA:113:ARG:HG3	1:AAA:128:TRP:HH2	1.84	0.42
1:AAA:51:LEU:O	1:AAA:54:LYS:N	2.52	0.42
1:AAA:49:GLU:C	1:AAA:51:LEU:N	2.72	0.42
1:AAA:142:PHE:HB3	1:AAA:155:ILE:HA	2.01	0.42
1:AAA:113:ARG:O	1:AAA:125:GLY:CA	2.68	0.41
1:AAA:173:ILE:HB	1:AAA:203:TRP:NE1	2.35	0.41
1:AAA:72:PRO:HG2	1:AAA:96:SER:HA	2.02	0.41
1:AAA:116:SER:HA	1:AAA:122:ARG:O	2.21	0.41
1:AAA:119:GLU:CD	1:AAA:119:GLU:N	2.74	0.41
1:AAA:118:LYS:HD2	1:AAA:118:LYS:HA	1.95	0.40

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	AAA	181/226 (80%)	157 (87%)	24 (13%)	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	AAA	160/199 (80%)	139 (87%)	21 (13%)	<b>4</b> <b>5</b>

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

Mol	Chain	Res	Type
1	AAA	36	VAL
1	AAA	39	LEU
1	AAA	40	THR
1	AAA	42	GLU
1	AAA	46	GLU
1	AAA	65	ARG
1	AAA	66	ARG
1	AAA	73	VAL
1	AAA	91	LYS
1	AAA	98	ILE
1	AAA	99	ARG
1	AAA	115	GLU
1	AAA	140	ILE
1	AAA	154	GLU
1	AAA	177	ASP
1	AAA	195	LEU
1	AAA	196	MET
1	AAA	204	LEU
1	AAA	210	ASP
1	AAA	213	GLN
1	AAA	216	VAL

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	AAA	183/226 (80%)	0.56	15 (8%) 11 9	88, 149, 252, 301	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	208	ILE	5.0
1	AAA	164	THR	4.2
1	AAA	217	ILE	3.7
1	AAA	157	VAL	3.5
1	AAA	128	TRP	3.0
1	AAA	90	LEU	2.8
1	AAA	173	ILE	2.7
1	AAA	167	MET	2.7
1	AAA	136	TYR	2.6
1	AAA	118	LYS	2.4
1	AAA	185	ARG	2.4
1	AAA	200	LEU	2.3
1	AAA	122	ARG	2.1
1	AAA	211	LEU	2.1
1	AAA	87	VAL	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 monosaccharides 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.