



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2024 – 10:12 am BST

PDB ID : 8ADC  
Title : Viral tegument-like DUBs  
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Deposited on : 2022-07-08  
Resolution : 1.70 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.

The types of validation reports are described at

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

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

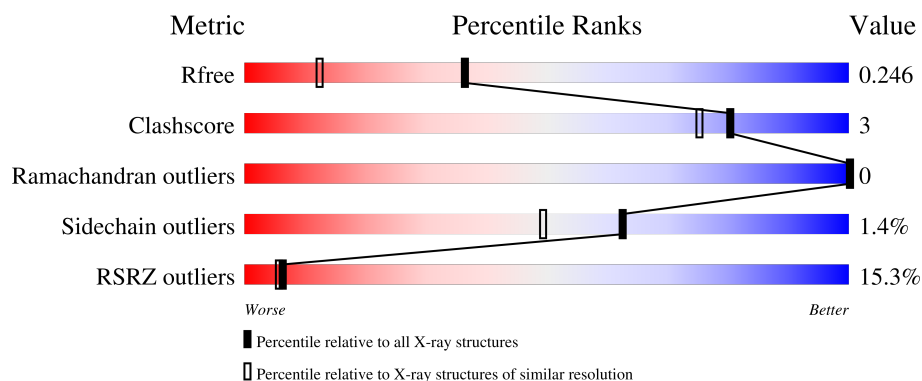
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	A	215	
1	B	215	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6530 atoms, of which 3143 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 Deubiquitinating enzyme.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	B	207	Total	C	H	N	O	S	Se		0	3	0
			3226	1030	1591	264	330	5	6				
1	A	203	Total	C	H	N	O	S	Se		0	1	0
			3143	1003	1552	258	319	5	6				

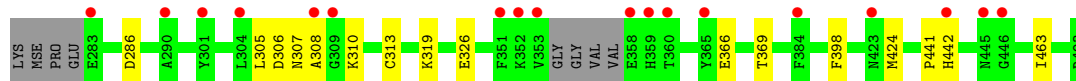
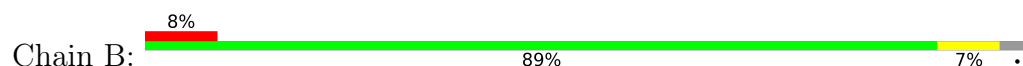
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	105	Total	O		
			105	105	0	0
2	A	56	Total	O		
			56	56	0	0

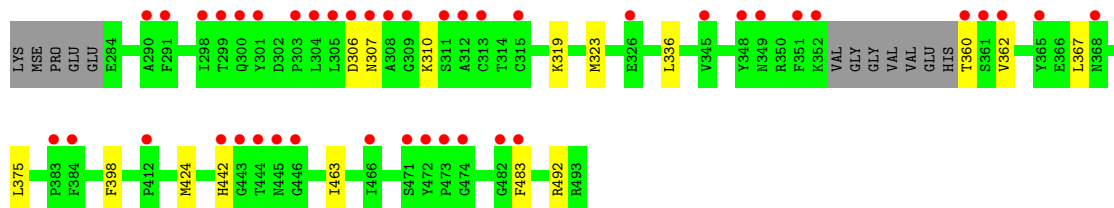
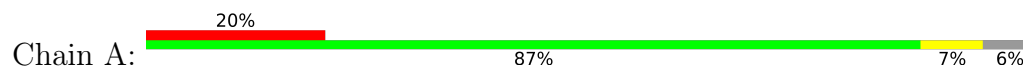
### 3 Residue-property plots [i](#)

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: Deubiquitinating enzyme



- Molecule 1: Deubiquitinating enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.12Å 70.30Å 75.89Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	51.06 – 1.70 51.06 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (51.06-1.70) 89.2 (51.06-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.25 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.20_4478, PHENIX 1.20_4478	Depositor
R, $R_{free}$	0.198 , 0.235 0.210 , 0.246	Depositor DCC
$R_{free}$ test set	39834 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.24% 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	A	0.36	0/1617	0.54	0/2174
1	B	0.42	0/1668	0.59	0/2243
All	All	0.39	0/3285	0.57	0/4417

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	A	1591	1552	1552	8	0
1	B	1635	1591	1591	10	1
2	A	56	0	0	1	0
2	B	105	0	0	1	0
All	All	3387	3143	3143	16	1

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 3.

All (16) 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:483:PHE:O	2:A:501:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:MSE:HE2	1:B:442:HIS:HB2	1.82	0.62
1:A:398:PHE:CZ	1:A:463:ILE:HG13	2.38	0.59
1:B:398:PHE:CZ	1:B:463:ILE:HG13	2.40	0.56
1:A:424:MSE:HE2	1:A:442:HIS:HB2	1.88	0.56
1:B:310:LYS:NZ	1:A:306:ASP:OD2	2.39	0.56
1:B:424:MSE:HE1	1:B:441:PRO:HD2	1.91	0.53
1:B:306:ASP:OD1	1:A:310:LYS:NZ	2.44	0.51
1:B:326:GLU:OE2	2:B:501:HOH:O	2.20	0.49
1:A:375:LEU:HD11	1:A:492:ARG:HD2	1.95	0.48
1:A:323:MSE:HE2	1:A:336:LEU:HD11	1.96	0.48
1:B:313[A]:CYS:SG	1:B:424:MSE:SE	3.23	0.47
1:B:305:LEU:O	1:B:308:ALA:O	2.34	0.44
1:A:362:VAL:HG13	1:A:367:LEU:HD21	1.99	0.43
1:B:366[B]:GLU:HG3	1:B:369:THR:HG23	2.02	0.41
1:B:313[A]:CYS:SG	1:B:441:PRO:HG2	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASP:H	1:B:366[B]:GLU:OE1[1_455]	1.56	0.04

## 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	200/215 (93%)	199 (100%)	1 (0%)	0	100	100
1	B	206/215 (96%)	203 (98%)	3 (2%)	0	100	100
All	All	406/430 (94%)	402 (99%)	4 (1%)	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	175/177 (99%)	172 (98%)	3 (2%)	56	41
1	B	181/177 (102%)	179 (99%)	2 (1%)	70	60
All	All	356/354 (101%)	351 (99%)	5 (1%)	62	49

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	307	ASN
1	B	319	LYS
1	A	307	ASN
1	A	319	LYS
1	A	360	THR

Sometimes 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 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 [i](#)

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, 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	197/215 (91%)	1.36	43 (21%) <b>3</b> <b>2</b>	31, 50, 94, 117	1 (0%)
1	B	201/215 (93%)	0.58	18 (8%) <b>17</b> <b>16</b>	18, 37, 73, 118	3 (1%)
All	All	398/430 (92%)	0.96	61 (15%) <b>6</b> <b>6</b>	18, 44, 88, 118	4 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	VAL	6.4
1	A	309	GLY	4.6
1	A	351	PHE	4.6
1	A	308	ALA	4.5
1	A	305	LEU	4.4
1	B	301	TYR	4.1
1	A	301	TYR	4.1
1	A	298	ILE	4.1
1	A	303	PRO	3.8
1	A	384	PHE	3.8
1	A	442	HIS	3.8
1	A	291	PHE	3.8
1	A	299	THR	3.7
1	B	359	HIS	3.7
1	A	312	ALA	3.7
1	A	304	LEU	3.7
1	A	352	LYS	3.6
1	A	446	GLY	3.4
1	A	348	TYR	3.4
1	A	307	ASN	3.4
1	B	304	LEU	3.3
1	A	472	TYR	3.3
1	A	360	THR	3.2
1	B	309	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	306	ASP	3.2
1	A	383	PRO	3.1
1	A	311	SER	3.1
1	A	290	ALA	3.0
1	A	313[A]	CYS	2.8
1	A	349	ASN	2.8
1	B	290	ALA	2.8
1	B	358	GLU	2.8
1	A	443	GLY	2.8
1	A	365	TYR	2.6
1	B	351	PHE	2.6
1	A	445	ASN	2.6
1	A	473	PRO	2.6
1	B	308	ALA	2.5
1	A	483	PHE	2.5
1	B	445	ASN	2.5
1	B	446	GLY	2.4
1	B	365	TYR	2.4
1	A	315	CYS	2.4
1	A	444	THR	2.4
1	A	466	ILE	2.4
1	A	474	GLY	2.4
1	A	368	ASN	2.3
1	A	362	VAL	2.3
1	A	471	SER	2.2
1	B	360	THR	2.2
1	B	423	ASN	2.2
1	A	326	GLU	2.1
1	A	345	VAL	2.1
1	B	352	LYS	2.1
1	A	300	GLN	2.1
1	A	361	SER	2.1
1	B	442	HIS	2.0
1	A	482	GLY	2.0
1	B	384	PHE	2.0
1	B	283	GLU	2.0
1	A	412	PRO	2.0

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

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.