



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 08:41 AM EDT

PDB ID : 3PRM  
Title : Structural analysis of a viral OTU domain protease from the Crimean-Congo Hemorrhagic Fever virus in complex with human ubiquitin  
Authors : Capodagli, G.C.; McKercher, M.A.; Baker, E.A.; Masters, E.M.; Brunzelle, J.S.; Pegan, S.D.  
Deposited on : 2010-11-30  
Resolution : 2.30 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

<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 : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

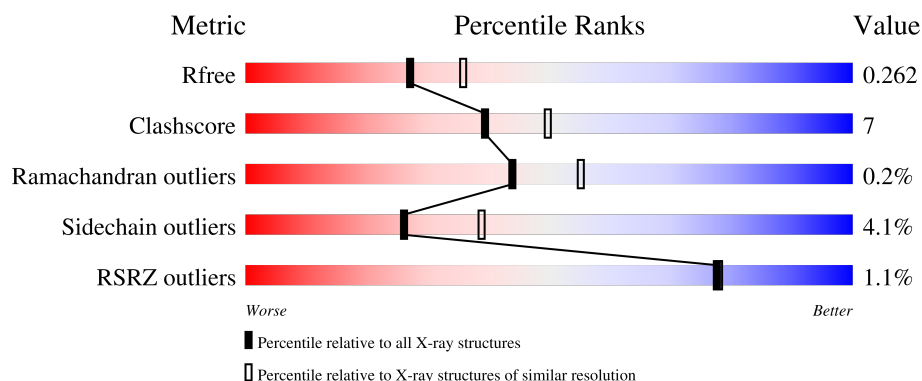
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	178	<div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
1	C	178	<div> <div>70%</div> <div>20%</div> <div>10%</div> </div>
2	B	76	<div> <div>88%</div> <div>12%</div> </div>
2	D	76	<div> <div>86%</div> <div>12%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4168 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	Se	0	9	0
			1367	869	232	261	1	4			
1	C	161	Total	C	N	O	S	Se	0	9	0
			1370	871	232	262	1	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q6TQR6
A	172	SER	-	expression tag	UNP Q6TQR6
A	173	HIS	-	expression tag	UNP Q6TQR6
A	174	HIS	-	expression tag	UNP Q6TQR6
A	175	HIS	-	expression tag	UNP Q6TQR6
A	176	HIS	-	expression tag	UNP Q6TQR6
A	177	HIS	-	expression tag	UNP Q6TQR6
A	178	HIS	-	expression tag	UNP Q6TQR6
C	171	GLY	-	expression tag	UNP Q6TQR6
C	172	SER	-	expression tag	UNP Q6TQR6
C	173	HIS	-	expression tag	UNP Q6TQR6
C	174	HIS	-	expression tag	UNP Q6TQR6
C	175	HIS	-	expression tag	UNP Q6TQR6
C	176	HIS	-	expression tag	UNP Q6TQR6
C	177	HIS	-	expression tag	UNP Q6TQR6
C	178	HIS	-	expression tag	UNP Q6TQR6

- Molecule 2 is a protein called Polyubiquitin-B (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	1	0
			610	384	107	118	1			
2	D	76	Total	C	N	O	S	0	0	0
			601	379	105	116	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	4LJ	-	insertion	UNP J3QS39
D	76	4LJ	-	insertion	UNP J3QS39

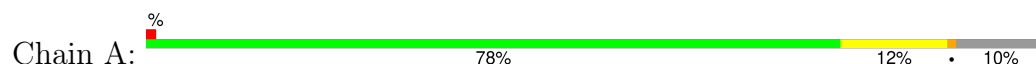
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total	O	0	0
			95	95		
3	B	31	Total	O	0	0
			31	31		
3	C	58	Total	O	0	0
			58	58		
3	D	36	Total	O	0	0
			36	36		

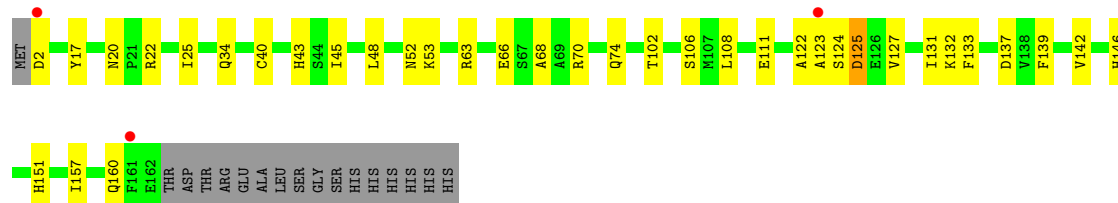
### 3 Residue-property plots [i](#)

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.

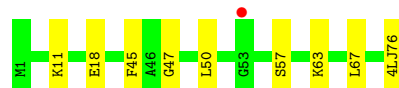
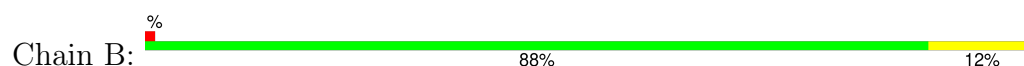
- Molecule 1: RNA-directed RNA polymerase L



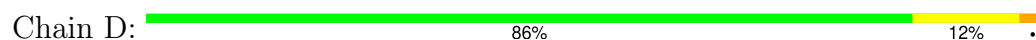
- Molecule 1: RNA-directed RNA polymerase L



- Molecule 2: Polyubiquitin-B (Fragment)



- Molecule 2: Polyubiquitin-B (Fragment)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.46Å 65.65Å 133.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.30 29.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.48-2.30) 98.4 (29.48-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.80 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204 , 0.267 0.200 , 0.262	Depositor DCC
$R_{free}$ test set	1212 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.17% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 4LJ

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	0.92	0/1397	0.83	2/1884 (0.1%)
1	C	0.84	0/1397	0.78	0/1884
2	B	0.84	0/612	0.86	0/823
2	D	0.82	0/603	0.91	2/811 (0.2%)
All	All	0.87	0/4009	0.83	4/5402 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	22	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	D	42	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	D	15	LEU	CB-CG-CD1	-5.40	101.82	111.00

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	1367	0	1315	16	0
1	C	1370	0	1316	27	0
2	B	610	0	637	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	601	0	632	11	0
3	A	95	0	0	1	0
3	B	31	0	0	0	0
3	C	58	0	0	2	0
3	D	36	0	0	1	0
All	All	4168	0	3900	50	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.

The worst 5 of 50 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)
2:D:75:GLY:C	2:D:76:4LJ:H8	1.29	1.33
1:A:40:CYS:SG	2:B:76:4LJ:C1	2.26	1.24
1:C:40:CYS:SG	2:D:76:4LJ:C1	2.49	1.00
1:C:34:GLN:HE21	1:C:43:HIS:HB3	1.43	0.83
1:C:160:GLN:HG3	3:C:220:HOH:O	1.84	0.77

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	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
1	C	168/178 (94%)	159 (95%)	8 (5%)	1 (1%)	22	27
2	B	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	D	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
All	All	483/508 (95%)	468 (97%)	14 (3%)	1 (0%)	44	55



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	ALA

### 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	148/150 (99%)	142 (96%)	6 (4%)	26	39
1	C	148/150 (99%)	143 (97%)	5 (3%)	32	47
2	B	69/68 (102%)	66 (96%)	3 (4%)	25	36
2	D	68/68 (100%)	65 (96%)	3 (4%)	24	35
All	All	433/436 (99%)	416 (96%)	17 (4%)	26	41

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	2	GLN
2	D	62	GLN
2	B	57	SER
2	B	63	LYS
1	C	52	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	34	GLN
1	C	74	GLN
2	D	25	ASN
1	C	160	GLN
2	B	25	ASN

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	75:GLY	C	76:4LJ	N1	1.91
1	B	75:GLY	C	76:4LJ	N1	1.68

## 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	157/178 (88%)	-0.03	1 (0%) 85 86	9, 28, 47, 67	9 (5%)
1	C	157/178 (88%)	0.25	3 (1%) 66 67	12, 36, 59, 80	9 (5%)
2	B	75/76 (98%)	-0.16	1 (1%) 74 75	14, 29, 42, 50	1 (1%)
2	D	75/76 (98%)	0.03	0 100 100	23, 33, 45, 49	0
All	All	464/508 (91%)	0.05	5 (1%) 77 78	9, 31, 51, 80	19 (4%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	PHE	2.9
1	C	123	ALA	2.4
1	A	75	GLU	2.2
2	B	53	GLY	2.1
1	C	2	ASP	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.