

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 4, 2023 – 11:27 PM EDT

PDB ID	:	6VGY
Title	:	2.05 A resolution structure of MERS 3CL protease in complex with inhibitor
		6b
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Deposited on	:	2020-01-09
Resolution	:	2.05  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 (i) 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 (1)) were used in the production of this report:

MolProbity Mogul		FAILED 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\hbox{-}RAY\,DIFFRACTION$ 

The reported resolution of this entry is 2.05 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



#### 6VGY

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4722 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	297	Total	С	N O S	0	3	0		
	A	297	2217	1416	360	417	24	0	5	0
1	В	298	Total	С	Ν	0	S	0	4	0
	D	290	2250	1439	365	420	26	0	4	U

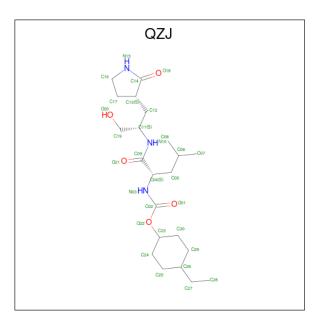
• Molecule 1 is a protein called Orf1a protein.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-6	MET	-	expression tag	UNP A0A1L2E0X0
А	-5	HIS	-	expression tag	UNP A0A1L2E0X0
А	-4	HIS	-	expression tag	UNP A0A1L2E0X0
А	-3	HIS	-	expression tag	UNP A0A1L2E0X0
А	-2	HIS	-	expression tag	UNP A0A1L2E0X0
А	-1	HIS	-	expression tag	UNP A0A1L2E0X0
А	0	HIS	-	expression tag	UNP A0A1L2E0X0
В	-6	MET	-	expression tag	UNP A0A1L2E0X0
В	-5	HIS	-	expression tag	UNP A0A1L2E0X0
В	-4	HIS	-	expression tag	UNP A0A1L2E0X0
В	-3	HIS	-	expression tag	UNP A0A1L2E0X0
В	-2	HIS	-	expression tag	UNP A0A1L2E0X0
В	-1	HIS	-	expression tag	UNP A0A1L2E0X0
В	0	HIS	-	expression tag	UNP A0A1L2E0X0

There are 14 discrepancies between the modelled and reference sequences:

• Molecule 2 is N 2 -{[(trans-4-ethylcyclohexyl)oxy]carbonyl}-N-{(2S)-1-hydroxy-3-[( 3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-leucinamide (three-letter code: QZJ) (formula:  $C_{22}H_{39}N_3O_5$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C N O   30 22 3 5	0	0
2	В	1	Total C N O   30 22 3 5	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	66	Total O 66 66	0	0
3	В	129	Total O 129 129	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	76.14Å 91.67Å 100.70Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	38.18 - 2.05	Depositor
% Data completeness	98.9 (38.18-2.05)	Depositor
(in resolution range)		-
R <sub>merge</sub>	0.08	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.00 (at 2.05 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_ $3587$	Depositor
$R, R_{free}$	0.192 , $0.239$	Depositor
Wilson B-factor $(Å^2)$	40.0	Xtriage
Anisotropy	0.386	Xtriage
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4722	wwPDB-VP
Average B, all atoms $(Å^2)$	46.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 4 Model quality (i)

## 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  > 2$	is considered an	ı outlier wor	th inspection	
RMSZ is the root-mean-square	of all Z scores of the bo	nd lengths (or a	ngles).		
		- ,	- ,		
			-		

Mol Type	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	B	ond leng	gths	B	Sond ang	gles
10101	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2				
2	QZJ	В	401	1	31,31,31	3.07	15 (48%)	39,41,41	2.02	9 (23%)				
2	QZJ	А	401	1	31,31,31	3.19	16 (51%)	39,41,41	2.11	11 (28%)				

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mo	l Type	Chain	Res	Link	Chirals	Torsions	Rings
2	QZJ	В	401	1	-	3/28/48/48	0/2/2/2
2	QZJ	А	401	1	-	0/28/48/48	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	В	401	QZJ	C14-N15	7.55	1.41	1.33
2	А	401	QZJ	C13-C14	-7.33	1.43	1.52
2	В	401	QZJ	C17-C16	-6.88	1.42	1.53
2	А	401	QZJ	C17-C16	-6.32	1.43	1.53
2	В	401	QZJ	O22-C23	-6.21	1.31	1.46
2	А	401	QZJ	C16-N15	-5.95	1.33	1.46
2	В	401	QZJ	C19-C11	5.61	1.61	1.52
2	А	401	QZJ	C14-N15	4.87	1.38	1.33
2	А	401	QZJ	C12-C13	-4.80	1.42	1.53
2	А	401	QZJ	C17-C13	-4.64	1.41	1.54
2	А	401	QZJ	C19-C11	4.59	1.60	1.52
2	А	401	QZJ	O22-C23	-4.15	1.36	1.46
2	В	401	QZJ	C13-C14	-4.14	1.47	1.52
2	В	401	QZJ	C16-N15	-4.04	1.37	1.46
2	В	401	QZJ	C12-C11	3.85	1.63	1.53
2	А	401	QZJ	C04-N03	-3.37	1.38	1.45
2	В	401	QZJ	C12-C13	-3.15	1.46	1.53
2	В	401	QZJ	C24-C23	-3.12	1.42	1.51
2	А	401	QZJ	O22-C02	-3.10	1.30	1.35
2	А	401	QZJ	C12-C11	3.10	1.61	1.53
2	В	401	QZJ	C25-C24	-3.08	1.45	1.52
2	В	401	QZJ	O21-C09	-3.00	1.17	1.23
2	А	401	QZJ	C25-C24	-2.89	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	401	QZJ	O21-C09	-2.83	1.17	1.23
2	А	401	QZJ	O18-C14	-2.82	1.17	1.23
2	В	401	QZJ	O18-C14	-2.52	1.18	1.23
2	А	401	QZJ	C30-C29	-2.49	1.46	1.52
2	В	401	QZJ	C04-N03	-2.37	1.40	1.45
2	А	401	QZJ	C11-N10	-2.23	1.42	1.46
2	В	401	QZJ	O01-C02	-2.04	1.18	1.21
2	В	401	QZJ	C17-C13	-2.00	1.48	1.54

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All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	401	QZJ	O22-C02-N03	7.32	119.82	110.32
2	А	401	QZJ	O22-C02-N03	6.87	119.23	110.32
2	А	401	QZJ	C12-C11-C19	5.84	119.78	111.65
2	В	401	QZJ	C12-C11-C19	4.15	117.42	111.65
2	А	401	QZJ	C23-O22-C02	4.13	122.40	116.48
2	В	401	QZJ	C23-O22-C02	4.09	122.35	116.48
2	А	401	QZJ	C04-C09-N10	3.45	124.27	116.70
2	В	401	QZJ	C04-C09-N10	3.26	123.85	116.70
2	А	401	QZJ	O22-C02-O01	-3.05	119.94	124.53
2	В	401	QZJ	O22-C02-O01	-3.03	119.96	124.53
2	А	401	QZJ	O21-C09-N10	-2.86	117.64	122.93
2	В	401	QZJ	O01-C02-N03	-2.83	120.21	124.85
2	В	401	QZJ	O21-C09-N10	-2.80	117.74	122.93
2	В	401	QZJ	O18-C14-N15	2.72	129.31	125.54
2	А	401	QZJ	O01-C02-N03	-2.49	120.77	124.85
2	А	401	QZJ	O18-C14-N15	2.45	128.94	125.54
2	В	401	QZJ	C29-C30-C23	2.43	114.56	110.82
2	А	401	QZJ	C17-C13-C14	2.41	106.01	102.88
2	А	401	QZJ	C12-C13-C14	-2.38	107.65	112.89
2	А	401	QZJ	C25-C24-C23	2.22	114.24	110.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

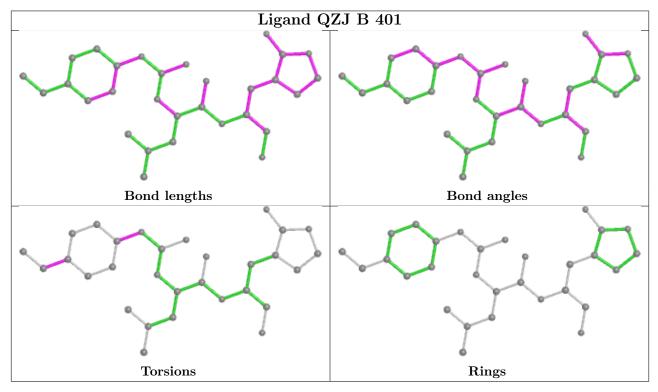
Mol	Chain	Res	Type	Atoms
2	В	401	QZJ	C25-C26-C27-C28
2	В	401	QZJ	C29-C26-C27-C28
2	В	401	QZJ	C30-C23-O22-C02

There are no ring outliers.

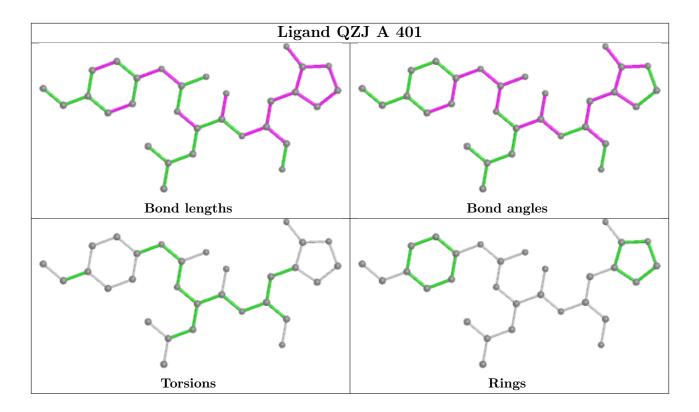


No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 5 Fit of model and data (i)

## 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

## 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

