

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

#### Aug 9, 2020 – 04:27 PM BST

PDB ID : 6LU7

Title: The crystal structure of COVID-19 main protease in complex with an inhibitor

N3

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Deposited on : 2020-01-26

Resolution : 2.16 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.13.1

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)

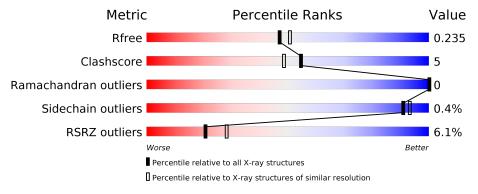
Validation Pipeline (wwPDB-VP) : 2.13.1

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.16 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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 <=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	306	90% 10%					
2	С	6	33%	50%	17%			



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2500 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 main protease.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	306	Total 2367	C 1499	N 402	O 444	S 22	0	0	0

• Molecule 2 is a protein called N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	С	6	Total 49	C 35	N 6	O 8	0	0	0

• Molecule 3 is water.

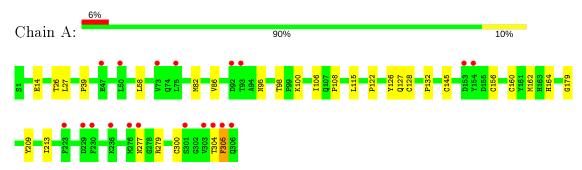
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	84	Total O 84 84	0	0



## 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: main protease



• Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE

Chain C: 33% 50% 17%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	97.93Å 79.48Å 51.80Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $114.55^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	27.81 - 2.16	Depositor
resolution (A)	42.31 - 2.16	EDS
% Data completeness	99.5 (27.81-2.16)	Depositor
(in resolution range)	99.6 (42.31-2.16)	EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.09 \; ({\rm at} \; 2.16 {\rm \AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
P. P.	0.202 , $0.235$	Depositor
$R, R_{free}$	0.204 , $0.235$	DCC
$R_{free}$ test set	998 reflections $(5.13\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 45.9	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.47, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2500	wwPDB-VP
Average B, all atoms $(Å^2)$	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.73% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  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.

## 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: 010, PJE, 02J

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		
IVIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.25	0/2420	0.44	0/3289	
2	С	1.59	0/19	0.65	0/25	
All	All	0.29	0/2439	0.44	0/3314	

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 (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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2367	0	2313	24	0
2	С	49	0	45	6	0
3	A	84	0	0	1	0
All	All	2500	0	2358	25	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 5.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



A + a ma 1	A 4 a ma 2	Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f \AA})$	overlap (Å)
1:A:26:THR:H	2:C:6:010:H4	1.41	0.85
1:A:106:ILE:C	1:A:106:ILE:HD12	2.10	0.71
1:A:115:LEU:HD11	1:A:122:PRO:HB3	1.83	0.61
1:A:100:LYS:HD3	1:A:156:CYS:HB2	1.85	0.59
1:A:26:THR:N	2:C:6:010:H4	2.19	0.54
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.94	0.49
1:A:126:TYR:HE2	1:A:128:CYS:HG	1.61	0.48
1:A:26:THR:H	2:C:6:010:C4	2.20	0.48
1:A:27:LEU:HD13	1:A:39:PRO:HD2	1.96	0.48
1:A:108:PRO:HB3	1:A:132:PRO:HA	1.95	0.48
1:A:213:ILE:HG21	1:A:300:CYS:HB3	1.96	0.47
1:A:106:ILE:C	1:A:106:ILE:CD1	2.80	0.47
1:A:127:GLN:NE2	3:A:408:HOH:O	2.48	0.47
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.14	0.47
1:A:277:ASN:OD1	1:A:279:ARG:NH2	2.48	0.46
1:A:106:ILE:O	1:A:106:ILE:HD12	2.16	0.45
1:A:58:LEU:HD22	1:A:82:MET:HB2	1.99	0.45
1:A:26:THR:O	2:C:6:010:H4	2.17	0.44
1:A:145:CYS:HB2	2:C:5:PJE:H4	1.36	0.43
1:A:304:THR:HG23	1:A:305:PHE:H	1.83	0.43
1:A:106:ILE:HG23	1:A:160:CYS:HB2	2.01	0.42
1:A:14:GLU:HG2	1:A:122:PRO:HG2	2.01	0.42
1:A:209:TYR:O	1:A:213:ILE:HG13	2.21	0.41
2:C:4:LEU:HA	2:C:4:LEU:HD23	1.88	0.41
1:A:162:MET:O	1:A:164:HIS:HD2	2.03	0.41

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.

$\mathbf{Mol}$	Chain	Analysed	Favoured	Allowed	Outliers	$\mid$ Percentiles	
1	A	304/306 (99%)	295 (97%)	9 (3%)	0	100 100	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	С	1/6 (17%)	1 (100%)	0	0	100	100
All	All	305/312 (98%)	296 (97%)	9 (3%)	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	$263/263 \; (100\%)$	262 (100%)	1 (0%)	91 93		
2	С	2/2~(100%)	2 (100%)	0	100 100		
All	All	$265/265 \; (100\%)$	264 (100%)	1 (0%)	91 93		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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 outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type Chain		n Pos	Dog	Dog	Dog	Pos	Pos	Pos	Pos	Dog	Dag	Dag	Dog	Dag	Dag	Dog	Res	T in le	Bo	nd leng	ths	В	ond ang	les
MIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2															
2	PJE	С	5	1,2	12,13,14	2.79	5 (41%)	12,16,18	1.84	3 (25%)															
2	02J	С	1	2	6,8,9	2.81	3 (50%)	4,10,12	2.65	2 (50%)															

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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PJE	С	5	1,2	_	1/7/18/19	0/1/1/1
2	02J	С	1	2	-	0/0/2/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	С	5	PJE	C29-N6	7.55	1.41	1.33
2	С	1	02J	C3-C41	5.25	1.54	1.48
2	С	1	02J	C6-C5	3.52	1.52	1.48
2	С	5	PJE	O8-C29	-3.04	1.17	1.23
2	С	5	PJE	C21-C22	3.02	1.53	1.44
2	С	5	PJE	C19-C20	2.44	1.53	1.50
2	С	5	PJE	C19-N5	-2.08	1.41	1.48
2	С	1	02J	C4-C3	2.04	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
2	С	1	02J	O42-C41-C3	-4.62	119.84	124.22
2	С	5	PJE	C19-C20-C21	-3.25	119.76	124.41
2	С	5	PJE	C27-C26-C29	2.62	106.28	102.88
2	С	5	PJE	C28-N6-C29	-2.35	109.23	113.84
2	С	1	02J	C4-C3-N2	-2.23	105.92	109.94

There are no chirality outliers.

All (1) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	С	5	PJE	C20-C21-C22-O7

There are no ring outliers.

1 monomer is involved in 1 short contact:

$\mathbf{Mol}$	Chain	${f Res}$	Type	Clashes	Symm-Clashes
2	С	5	PJE	1	0

## 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q<0.9
1	A	306/306 (100%)	0.51	19 (6%) 20 27	23, 42, 62, 81	0
2	С	3/6 (50%)	0.22	0 100 100	39, 39, 41, 42	0
All	All	309/312 (99%)	0.51	19 (6%) 21 28	23, 42, 62, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	PHE	8.0
1	A	304	THR	6.4
1	A	306	GLN	5.0
1	A	277	ASN	4.4
1	A	73	VAL	4.0
1	A	154	TYR	4.0
1	A	92	ASP	3.7
1	A	93	THR	3.6
1	A	303	VAL	3.6
1	A	153	ASP	2.9
1	A	301	SER	2.9
1	A	276	MET	2.5
1	A	50	LEU	2.3
1	A	236	LYS	2.3
1	A	230	PHE	2.3
1	A	229	ASP	2.1
1	A	47	GLU	2.1
1	A	75	LEU	2.0
1	A	223	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	PJE	С	5	13/14	0.79	0.16	20,20,20,20	0
2	02J	С	1	8/9	0.84	0.29	47,54,63,64	0

### 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.

