

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

#### Dec 17, 2023 – 12:44 AM EST

PDB ID : 2OP9

Title: Substrate Specificity Profiling and Identification of a New Class of Inhibitor

for the Major Protease of the SARS Coronavirus

Authors: Craik, C.S.; Goetz, D.H.

Deposited on : 2007-01-27

Resolution : 1.80 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
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: 4.02b-467

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

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

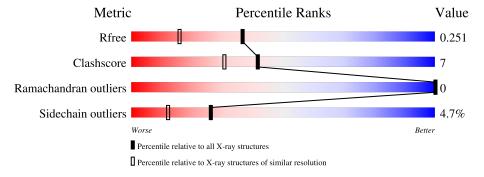
Validation Pipeline (wwPDB-VP) : 2.36

## 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 1.80 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}(\mathring{A}))$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 >=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%

$\mathbf{M}$	ol	Chain	Length	Quality of chain		
1		A	302	80%	18%	•
1		В	302	88%	11%	



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5198 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 Replicase polyprotein 1ab (pp1ab, ORF1AB) 3C-like proteinase (3CL-PRO, 3CLp).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	302	Total 2330	C 1472	N 400	O 436	S 22	0	0	0
1	В	299	Total 2319	C 1467	N 397	O 433	S 22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	cloning artifact	UNP P59641
В	0	ALA	-	cloning artifact	UNP P59641

• Molecule 2 is NALPHA-[(BENZYLOXY)CARBONYL]-N-[(1R)-4-HYDROXY-1-MET HYL-2-OXOBUTYL]-L-PHENYLALANINAMIDE (three-letter code: WR1) (formula:  $C_{22}H_{26}N_2O_5$ ).



Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf
2	A	1	Total 29	C 22			0	0
2	В	1	Total 29	C 22		O 5	0	0

## $\bullet\,$ Molecule 3 is water.

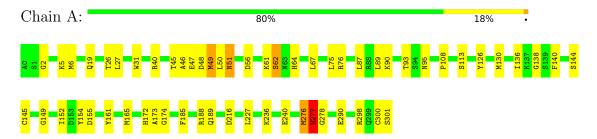
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	240	Total O 240 240	0	0
3	В	251	Total O 251 251	0	0



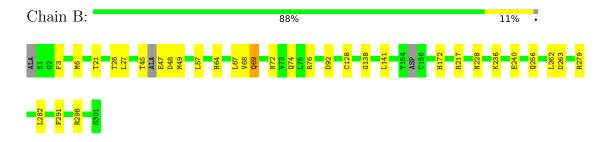
# 3 Residue-property plots (i)

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. 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. 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: Replicase polyprotein 1ab (pp1ab, ORF1AB) 3C-like proteinase (3CL-PRO, 3CLp)



• Molecule 1: Replicase polyprotein 1ab (pp1ab, ORF1AB) 3C-like proteinase (3CL-PRO, 3CLp)





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	52.31Å 96.80Å 67.88Å	Donositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 103.20° 90.00°	Depositor	
Resolution (Å)	20.00 - 1.80	Depositor	
Resolution (A)	54.58 - 1.80	EDS	
% Data completeness	98.6 (20.00-1.80)	Depositor	
(in resolution range)	98.6 (54.58-1.80)	EDS	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.99 (at 1.80Å)	Xtriage	
Refinement program	REFMAC 5.2.0019	Depositor	
$R, R_{free}$	0.170 , 0.207	Depositor	
it, it free	0.219 , $0.251$	DCC	
$R_{free}$ test set	2999 reflections $(5.00\%)$	wwPDB-VP	
Wilson B-factor $(A^2)$	25.9	Xtriage	
Anisotropy	0.360	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39, 61.2	EDS	
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.31$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o, F_c$ correlation	0.95	EDS	
Total number of atoms	5198	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.27% 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: WR1

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		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	RMSZ $\# Z  > 5$		# Z  > 5	
1	A	0.70	0/2382	0.76	3/3237 (0.1%)	
1	В	0.78	$2/2369 \ (0.1\%)$	0.81	4/3215 (0.1%)	
All	All	0.74	$2/4751 \ (0.0\%)$	0.79	7/6452 (0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(A)
1	В	128	CYS	CB-SG	-7.15	1.70	1.82
1	В	291	PHE	CB-CG	-5.87	1.41	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	В	217	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	В	217	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	62	SER	N-CA-C	6.59	128.78	111.00
1	В	298	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	277	ASN	N-CA-CB	-5.69	100.36	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	173	ALA	Peptide
1	A	277	ASN	Peptide
1	A	49	MET	Peptide
1	A	61	LYS	Peptide

### 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	2330	0	2278	40	0
1	В	2319	0	2274	26	0
2	A	29	0	26	4	0
2	В	29	0	25	0	0
3	A	240	0	0	9	0
3	В	251	0	0	11	0
All	All	5198	0	4603	65	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 65 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:47:GLU:O	1:A:50:LEU:CB	2.01	1.08
1:A:19:GLN:HE21	1:A:26:THR:HG21	1.29	0.96
1:B:45:THR:HG22	3:B:830:HOH:O	1.69	0.93
1:A:161:TYR:CE1	1:A:174:GLY:HA3	2.07	0.90
1:A:145:CYS:SG	2:A:601:WR1:C3	2.72	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	Perce	ntiles
1	A	300/302~(99%)	294 (98%)	6 (2%)	0	100	100
1	В	293/302 (97%)	287 (98%)	6 (2%)	0	100	100
All	All	593/604 (98%)	581 (98%)	12 (2%)	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	257/259 (99%)	242 (94%)	15 (6%)	20 7		
1	В	258/259 (100%)	249 (96%)	9 (4%)	36 21		
All	All	515/518 (99%)	491 (95%)	24 (5%)	26 12		

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	SER
1	В	67	LEU
1	В	57	LEU
1	В	68	VAL
1	A	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	72	ASN
1	В	164	HIS
1	В	246	HIS
1	В	172	HIS

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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)

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)

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 outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Trme	Chain Res		Link	Bo	ond leng	$ ag{ths}$	В	ond ang	les
MOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	WR1	A	601	-	29,30,30	1.24	2 (6%)	33,38,38	1.20	4 (12%)
2	WR1	В	602	1	29,30,30	1.19	1 (3%)	33,38,38	1.00	2 (6%)

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	WR1	A	601	-	-	7/27/28/28	0/2/2/2
2	WR1	В	602	1	-	4/27/28/28	0/2/2/2



All (3) bond length outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
2	В	602	WR1	O5-C15	5.52	1.45	1.35
2	A	601	WR1	O5-C15	5.46	1.45	1.35
2	A	601	WR1	C2-C3	2.31	1.54	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
2	A	601	WR1	C16-O5-C15	3.56	123.88	115.93
2	В	602	WR1	C8-C7-N2	-2.67	105.17	110.79
2	A	601	WR1	O5-C15-O4	-2.52	119.42	124.25
2	A	601	WR1	O5-C16-C17	2.49	115.37	109.39
2	A	601	WR1	C7-N2-C15	2.43	126.83	120.90

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	WR1	O1-C1-C2-C3
2	A	601	WR1	C17-C16-O5-C15
2	В	602	WR1	O1-C1-C2-C3
2	A	601	WR1	O3-C6-C7-N2
2	В	602	WR1	O3-C6-C7-N2

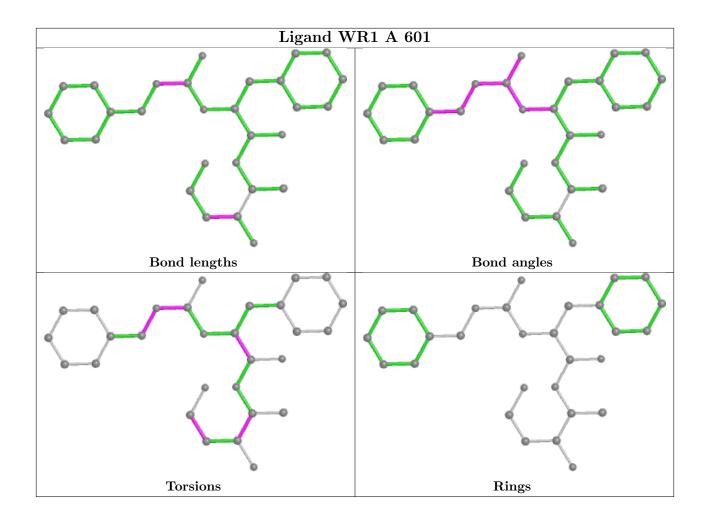
There are no ring outliers.

1 monomer is involved in 4 short contacts:

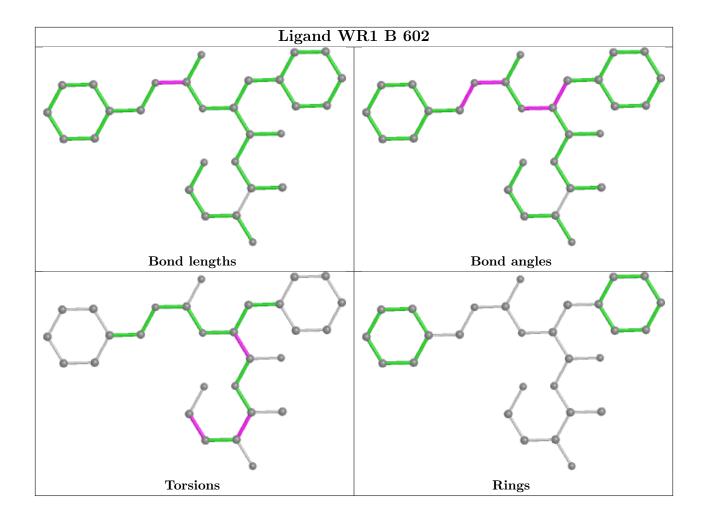
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	WR1	4	0

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.









## 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

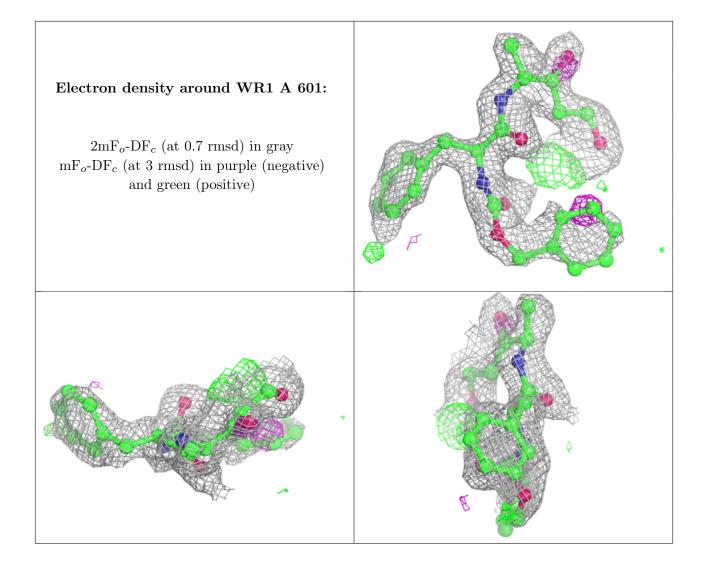
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands (i)

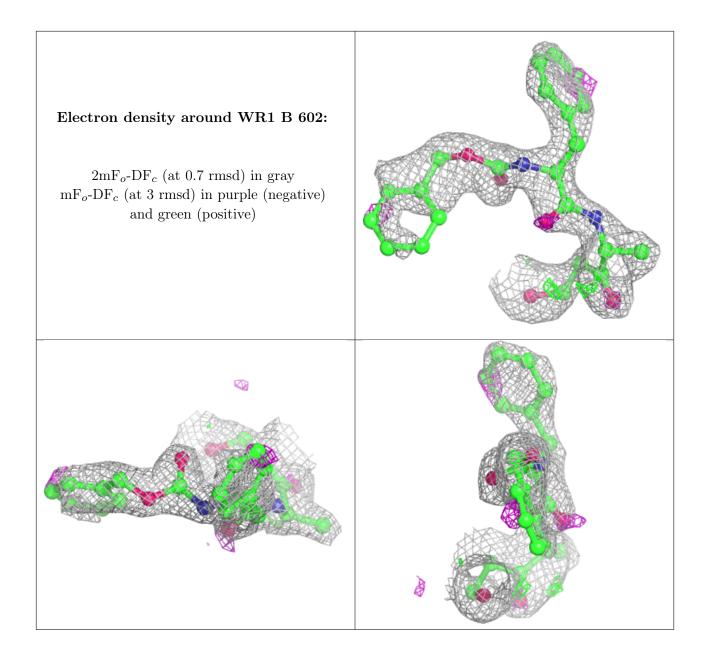
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









## 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

