

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

May 23, 2020 – 05:14 pm BST

PDB ID : 1Z1I

Title : Crystal structure of native SARS CLpro

Authors: Liang, P.H.; Wang, A.H.

Deposited on : 2005-03-04

Resolution : 2.80 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 following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} Mol Probity & : & 4.02b\text{-}467 \\ Xtriage (Phenix) & : & 1.13 \end{array}$ 

EDS : 2.11

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)

al geometry (DNA, RNA) : Parkinson et al. (1996)

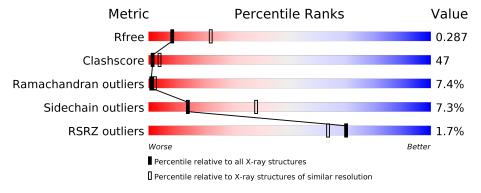
Ideal geometry (DNA, RNA) : Parkinson Validation Pipeline (wwPDB-VP) : 2.11

### 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 2.80 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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				
			2%				
1	A	306	35%	51%	9% • •		



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2472 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 3C-like proteinase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	301	Total 2332	C 1474	N 399	O 437	S 22	0	0	0

• Molecule 2 is water.

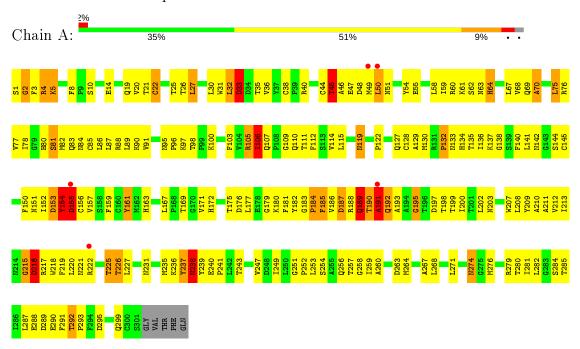
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	140	Total O 140 140	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: 3C-like proteinase





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	107.19Å 45.06Å 53.99Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 2.80	Depositor
resolution (A)	24.85 - 2.30	EDS
% Data completeness	(Not available) (30.00-2.80)	Depositor
(in resolution range)	97.5 (24.85-2.30)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.55 (at 2.31Å)	Xtriage
Refinement program	unknown	Depositor
P. P.	0.241 , 0.288	Depositor
$R, R_{free}$	0.245 , $0.287$	DCC
$R_{free}$ test set	695  reflections  (5.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31,67.5	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.61% 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)

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	Bo	Bond lengths		ond angles
MIOI	$oxed{ ext{Nol}} egin{array}{c c}  ext{Chain} & & & \ & & \ \end{array}$		# Z  > 5	RMSZ	# Z >5
1	A	0.97	$12/2384 \ (0.5\%)$	1.06	$27/3239 \ (0.8\%)$

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	1	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
1	A	191	ALA	C-O	19.04	1.59	1.23
1	A	154	TYR	C-N	16.72	1.72	1.34
1	A	50	LEU	C-N	15.30	1.69	1.34
1	A	216	ASP	C-N	14.84	1.68	1.34
1	A	238	ASN	C-N	13.28	1.64	1.34

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
1	A	238	ASN	CA-CB-CG	13.90	143.97	113.40
1	A	33	ASP	N-CA-CB	-12.55	88.00	110.60
1	A	33	ASP	CB-CA-C	11.15	132.71	110.40
1	A	238	ASN	CA-C-N	-10.54	94.01	117.20
1	A	154	TYR	CA-CB-CG	10.36	133.09	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	106	ILE	СВ



All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ALA	Mainchain
1	A	238	ASN	Mainchain
1	A	32	LEU	Mainchain
1	A	45	THR	Mainchain

#### 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	2332	0	2284	219	2
2	A	140	0	0	14	2
All	All	2472	0	2284	219	3

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 47.

The worst 5 of 219 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:50:LEU:C	1:A:51:ASN:N	1.69	1.46
1:A:216:ASP:C	1:A:217:ARG:N	1.68	1.45
1:A:154:TYR:C	1:A:155:ASP:N	1.72	1.42
1:A:64:HIS:CD2	2:A:655:HOH:O	1.96	1.14
1:A:154:TYR:O	1:A:155:ASP:HB2	1.50	1.11

All (3) 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	$egin{array}{c}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	Clash overlap (Å)
1:A:154:TYR:OH	2:A:536:HOH:O[2_655]	1.96	0.24
1:A:285:THR:OG1	1:A:285:THR:OG1[2_655]	1.99	0.21
2:A:652:HOH:O	2:A:652:HOH:O[2_655]	2.19	0.01



### 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	299/306 (98%)	228 (76%)	49 (16%)	22 (7%)	1 2

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLY
1	A	33	ASP
1	A	106	ILE
1	A	154	TYR
1	A	184	PRO

#### 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	Analysed Rotameric		Percentiles	
1	A	259/263 (98%)	240 (93%)	19 (7%)	14 38	

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	189	GLN
1	A	274	ASN
1	A	75	LEU
1	A	290	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	172	HIS
1	A	256	GLN
1	A	110	GLN
1	A	238	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 carbohydrates 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
1	A	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	154:TYR	С	155:ASP	N	1.72

Continued on next page...



#### $Continued\ from\ previous\ page...$

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	50:LEU	С	51:ASN	N	1.69
1	A	216:ASP	С	217:ARG	N	1.68
1	A	238:ASN	С	239:TYR	N	1.64
1	A	106:ILE	С	107:GLN	N	1.62



### 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 $>$	#RS	$\mathrm{RZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	301/306 (98%)	-0.15	5 (1%)	70 63	21, 55, 77, 88	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	MET	4.6
1	A	155	ASP	3.3
1	A	50	LEU	3.0
1	A	222	ARG	2.6
1	A	191	ALA	2.2

#### 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 carbohydrates 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.

