

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

#### May 26, 2020 – 11:38 am BST

PDB ID	:	3SNA
Title	:	Crystal structure of SARS coronavirus main protease complexed with Ac-
		NSFSQ-H (soaking)
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Deposited on		
$\operatorname{Resolution}$	:	3.05  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:

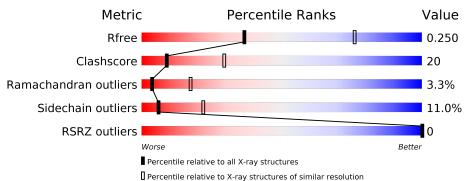
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
CCP4	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.05 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	А	301	61%	34%			
2	Н	6	50%	50%			



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2392 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	А	301	Total 2333	C 1474	N 399	O 438	S 22	0	0	0

• Molecule 2 is a protein called Peptide aldehyde inhibitor Ac-NSFSQ-H.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	Н	6	Total 45		N 7	0 11	0	1	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	14	Total         O           14         14	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.

Chain A:		61%	34% •	•
S1 K5 E14 Q19	124 125 126 126 132 133 133 133	733 733 744 745 745 745 745 745 745 745 745 745	N51 P52 P52 P52 P52 R60 N63 N63 R60 R65 R65 R65 R65 R65 R65 R65 R65 R65 R65	R88 193 193 195
T98 P99 X101 V104	4107 7109 6109 7111 1111 1111 1119 1129 4129	R130 P132 N133 H134 T136 T136 (149 (149 (149 (149 (149 (149) (153 (146) (153 (146) (153) (156)	C156 Y161 H164 H164 M165 M165 C170 C170 C170 C170 A191 A191 A191 A191 A191 A191 A191 A19	M207 A210 A211 V212
1213 N214 G215 D216 R217	M228 M228 M231 1233 M234 M235	D2 45 H2 46 12 49 0256 A260 M263 M264	12.68 12.68 12.68 12.73 12.75 12.86 12.78 12.86	D295 V296 C300 S301
• Molecule	e 2: Peptide alc	lehyde inhibitor A	Ac-NSFSQ-H	
Chain H:	Į	50%	50%	-
70 82 83 84 85 84 85				

• Molecule 1: 3C-like proteinase



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	107.87Å $82.09$ Å $53.08$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $104.30^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	42.25 - 3.05	Depositor
Resolution (A)	42.25 - 3.05	EDS
% Data completeness	99.9 (42.25-3.05)	Depositor
(in resolution range)	99.9(42.25 - 3.05)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.49 (at 3.06 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.0	Depositor
D D.	0.190 , $0.256$	Depositor
$R, R_{free}$	0.187 , $0.250$	DCC
$R_{free}$ test set	410 reflections $(4.74\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	76.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , $49.4$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2392	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.26% 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.



 $<sup>^1 {\</sup>rm Intensities}$  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: ECC, ACE

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		
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.71	0/2385	0.79	0/3239	
2	Н	0.90	0/32	0.72	0/42	
All	All	0.71	0/2417	0.79	0/3281	

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	<b>#Planarity outliers</b>
2	Н	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Group
2	Η	4	SER	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	А	2333	0	2285	95	1
2	Н	45	0	34	3	0
3	А	14	0	0	0	0
All	All	2392	0	2319	95	1

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 20.

The worst 5 of 95 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)
1:A:50:LEU:HD12	1:A:51:ASN:N	1.58	1.18
1:A:292:THR:HG22	1:A:294:PHE:H	1.04	1.15
1:A:50:LEU:HD11	1:A:51:ASN:HB3	1.17	1.14
1:A:50:LEU:HD12	1:A:50:LEU:C	1.67	1.12
1:A:50:LEU:CD1	1:A:51:ASN:HB3	1.81	1.09

All (1) 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	$\begin{array}{c} {\rm Interatomic}\\ {\rm distance}~({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:60:ARG:NH1	1:A:220:LEU:O[3_545]	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	А	299/301~(99%)	255~(85%)	35 (12%)	9~(3%)	4 19
2	Н	4/6~(67%)	1 (25%)	2 (50%)	1 (25%)	0 0
All	All	303/307~(99%)	256 (84%)	37 (12%)	10 (3%)	4 17

5 of 10 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	50	LEU
2	Н	2	SER
1	А	41	HIS
1	А	49	MET
1	А	80	HIS

#### 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	А	259/259~(100%)	230~(89%)	29 (11%)	6 21		
2	Н	4/4~(100%)	4 (100%)	0	100 100		
All	All	263/263~(100%)	234~(89%)	29 (11%)	6 22		

 $5~{\rm of}~29$  residues with a non-rotameric side chain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	153	ASP
1	А	171	VAL
1	А	268	LEU
1	А	165	MET
1	А	175	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	19	GLN
1	А	192	GLN
2	Н	1	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)

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	True	Chain	Res Link		B	ond leng	$\operatorname{gths}$	В	ond ang	gles
	Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ECC	Н	5[A]	1	8,8,8	0.33	0	$^{8,9,9}$	0.41	0
2	ECC	Н	5[B]	1	8,8,8	0.38	0	$^{8,9,9}$	0.78	1 (12%)

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	$\mathbf{Link}$	Chirals	Torsions	Rings
2	ECC	Н	5[A]	1	-	4/7/7/7	-
2	ECC	Н	5[B]	1	-	2/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	5[B]	ECC	CB-CA-C	-2.06	109.43	112.25

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	Н	5[A]	ECC	O-C-CA-N
2	Н	5[A]	ECC	C-CA-CB-CG
2	Н	5[A]	ECC	N-CA-CB-CG
2	Н	5[B]	ECC	C-CA-CB-CG
2	Н	5[B]	ECC	N-CA-CB-CG

There are no ring outliers.



No monomer is involved in short contacts.

#### 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)

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 $>$	$\# RSRZ {>}2$		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	301/301~(100%)	-0.50	0 100	100	39,68,90,105	0
2	Н	4/6~(66%)	0.76	0 100	100	107, 109, 111, 113	0
All	All	305/307~(99%)	-0.48	0 100	100	39, 68, 92, 113	0

There are no RSRZ outliers to report.

## 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
2	ECC	Н	5[A]	9/9	0.94	0.19	97,104,113,116	2
2	ECC	Н	5[B]	9/9	0.94	0.19	$97,\!104,\!113,\!115$	2

## 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.

