

Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 04:03 PM JST

PDB ID	:	8YSA
Title	:	The co-crystal structure of SARS-CoV-2 Mpro in complex with compound
		H102
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Deposited on		
Resolution	:	1.50 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:

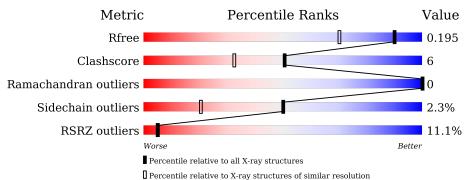
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.50 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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% 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	306	89%	10% •
2	В	4	75%	25%



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2689 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 nsp5.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	304	Total 2361	C 1495	N 400	0 444	S 22	0	4	0

• Molecule 2 is a protein called BOC-TBG-PHE-ELL.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	В	4	Total 37	C N 27 4	O 6	0	0	0

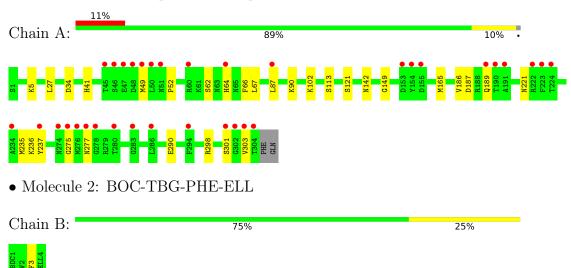
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	290	Total O 290 290	0	0
3	В	1	Total O 1 1	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: 3C-like proteinase nsp5



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	106.33Å 106.33Å 82.17Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.56 - 1.50	Depositor
Resolution (A)	26.56 - 1.50	EDS
% Data completeness	99.8 (26.56-1.50)	Depositor
(in resolution range)	99.8(26.56-1.50)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.86 (at 1.50 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.181 , 0.197	Depositor
R, R_{free}	0.180 , 0.195	DCC
R_{free} test set	2104 reflections $(4.76%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	13.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 42.6	EDS
L-test for twinning ²	$ L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2689	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: BOC, TBG, ELL

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		lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.30	0/2426	0.56	0/3299	
2	В	0.16	0/11	0.55	0/13	
All	All	0.30	0/2437	0.56	0/3312	

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	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2361	0	2317	27	0
2	В	37	0	28	1	0
3	А	290	0	0	13	3
3	В	1	0	0	0	0
All	All	2689	0	2345	27	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 6.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:303:VAL:N	3:A:402:HOH:O	2.16	0.79
1:A:49:MET:HG2	1:A:189:GLN:HG2	1.67	0.75
1:A:275:GLY:O	3:A:401:HOH:O	2.09	0.71
1:A:41:HIS:CE1	1:A:49:MET:SD	2.84	0.71
1:A:189:GLN:NE2	3:A:405:HOH:O	2.25	0.70
1:A:303:VAL:HG22	3:A:402:HOH:O	1.95	0.65
1:A:5:LYS:HD3	3:A:404:HOH:O	1.97	0.64
1:A:236:LYS:NZ	3:A:409:HOH:O	2.31	0.63
1:A:277:ASN:HB2	3:A:615:HOH:O	1.99	0.61
1:A:165:MET:HE1	1:A:187:ASP:HA	1.82	0.61
1:A:221:ASN:O	3:A:403:HOH:O	2.17	0.60
1:A:41:HIS:HE1	1:A:49:MET:SD	2.28	0.56
1:A:236:LYS:HD2	1:A:237:TYR:CE1	2.41	0.56
1:A:277:ASN:HB2	3:A:516:HOH:O	2.06	0.55
1:A:186:VAL:HG12	3:A:568:HOH:O	2.07	0.54
1:A:49:MET:O	1:A:52:PRO:HD3	2.13	0.49
1:A:142[A]:ASN:ND2	3:A:406:HOH:O	2.26	0.48
1:A:290:GLU:OE1	3:A:404:HOH:O	2.20	0.48
1:A:41:HIS:HE1	1:A:49:MET:CG	2.28	0.47
1:A:113:SER:O	1:A:149:GLY:HA2	2.17	0.45
1:A:41:HIS:HE1	1:A:49:MET:HG3	1.82	0.45
1:A:41:HIS:HB3	2:B:3:PHE:CZ	2.51	0.44
1:A:49:MET:CG	1:A:189:GLN:HG2	2.43	0.43
1:A:62:SER:OG	1:A:64:HIS:ND1	2.52	0.42
1:A:34:ASP:O	1:A:90:LYS:HD3	2.19	0.42
1:A:301:SER:C	3:A:402:HOH:O	2.57	0.42
1:A:66:PHE:CE1	1:A:87:LEU:HD21	2.55	0.41

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	Interatomic distance (Å)	Clash overlap (Å)
3:A:612:HOH:O	3:A:638:HOH:O[7_555]	1.67	0.53
3:A:473:HOH:O	3:A:473:HOH:O[10_664]	1.72	0.48
3:A:588:HOH:O	3:A:668:HOH:O[11_555]	1.74	0.46



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	Percer	ntiles
1	А	306/306~(100%)	299~(98%)	7(2%)	0	100	100
2	В	1/4~(25%)	1 (100%)	0	0	100	100
All	All	307/310~(99%)	300~(98%)	7(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	tameric Outliers		Percentiles		
1	А	265/263~(101%)	258~(97%)	7 (3%)	46	16		
2	В	1/1 (100%)	1 (100%)	0	100	100		
All	All	266/264~(101%)	259~(97%)	7 (3%)	50	16		

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	27	LEU
1	А	67	LEU
1	А	102	LYS
1	А	121[A]	SER
1	А	121[B]	SER
1	А	235	MET
1	А	298	ARG



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	41	HIS
1	А	244	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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).

Γ	Mol	ol Type Chain Res Lin		Link	Bond lengths			Bond angles			
	NIOI	Type	Chain	i nes	LIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
	2	TBG	В	2	2	6,7,8	0.52	0	$7,\!10,\!12$	0.52	0

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	TBG	В	2	2	-	0/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



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 >	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	А	304/306~(99%)	0.97	34 (11%) 5 5	6, 16, 44, 91	0
2	В	1/4~(25%)	1.42	0 100 100	15, 15, 15, 15	0
All	All	305/310~(98%)	0.97	34 (11%) 5 5	6, 16, 44, 91	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	277	ASN	11.2
1	А	154	TYR	11.0
1	А	47	GLU	9.8
1	А	46	SER	9.3
1	А	45	THR	7.5
1	А	278	GLY	7.1
1	А	50	LEU	5.9
1	А	49	MET	5.4
1	А	222	ARG	4.7
1	А	294	PHE	4.3
1	А	301	SER	4.2
1	А	223	PHE	4.1
1	А	276	MET	3.9
1	А	302	GLY	3.8
1	А	280	THR	3.8
1	А	51	ASN	3.7
1	А	237	TYR	3.7
1	А	48	ASP	3.7
1	А	303	VAL	3.4
1	А	274	ASN	3.4
1	А	275	GLY	3.4
1	А	283	GLY	3.1
1	А	60	ARG	3.1
1	А	191	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	А	153	ASP	2.7
1	А	234	ALA	2.7
1	А	189	GLN	2.5
1	А	304	THR	2.5
1	А	286	LEU	2.4
1	А	87	LEU	2.3
1	А	224	THR	2.2
1	А	190	THR	2.2
1	А	155	ASP	2.2
1	А	64	HIS	2.1

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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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	TBG	В	2	8/9	0.92	0.11	$13,\!16,\!18,\!22$	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.

