

wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2023 – 12:09 PM JST

PDB ID : 8GWJ

Title: SARS CoV-2 Mpro 1-302 C145A in complex with peptide 7

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Deposited on : 2022-09-17

Resolution : 2.90 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:

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

EDS : 2.35.1

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)

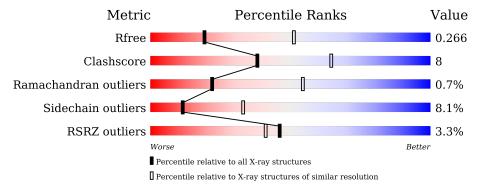
Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.90 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 chai	$\overline{\mathbf{n}}$	
1	A	302	73%		20% • 6%
1	В	302	76%		21% •
2	С	8	62%	25%	12%
2	D	8	62%	25%	12%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4594 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	283	Total 2145	C 1355	N 367	O 404	S 19	0	0	0
1	В	302	Total 2315	C 1462	N 397	O 435	S 21	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	CYS	$\operatorname{conflict}$	UNP P0DTD1
В	145	ALA	CYS	$\operatorname{conflict}$	UNP P0DTD1

• Molecule 2 is a protein called VAL-LYS-LEU-GLN-ALA-VAL-PHE-ARG.

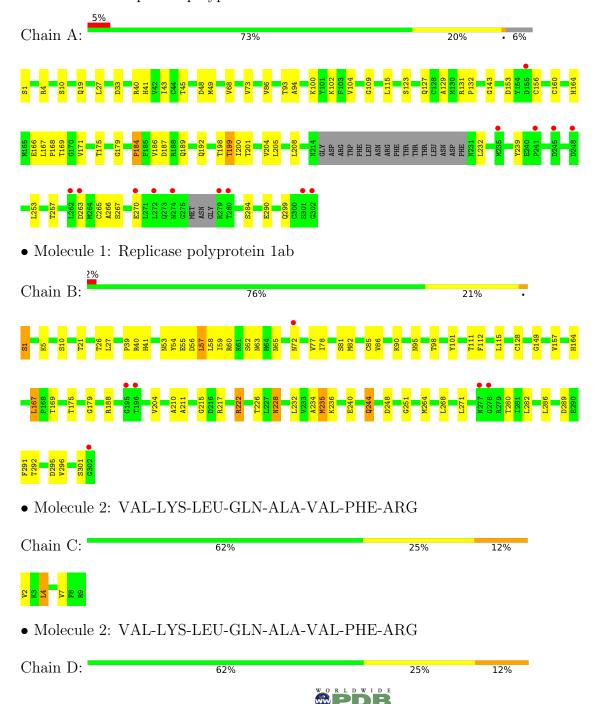
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	С	8	Total 67			O 0	0	0	0	
2	D	8	Total			O	0	0	0	
	2 D			45	13	9	0	U		



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: Replicase polyprotein 1ab







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	66.89Å 66.89Å 240.66Å	D: t
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.38 - 2.90	Depositor
Resolution (A)	22.37 - 2.90	EDS
% Data completeness	98.2 (22.38-2.90)	Depositor
(in resolution range)	98.5 (22.37-2.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sum}	(Not available)	Depositor
$< I/\sigma(I) > 1$	11.03 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
Ρ. Р.	0.211 , 0.271	Depositor
R, R_{free}	0.215 , 0.266	DCC
R_{free} test set	640 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 32.0	EDS
L-test for twinning ²	$< L > = 0.43, < L^2> = 0.25$	Xtriage
Estimated twinning fraction	0.068 for -h,-k,l	Xtriage
Reported twinning fraction	0.140 for -h,-k,l	Depositor
Outliers	0 of 14335 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4594	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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	Bond	lengths	Bond angles			
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	A	0.73	0/2189	0.89	0/2976		
1	В	0.71	0/2365	0.89	0/3215		
2	С	0.68	0/67	0.94	0/88		
2	D	0.68	0/67	0.92	0/88		
All	All	0.72	0/4688	0.89	0/6367		

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	A	2145	0	2090	31	0
1	В	2315	0	2263	38	0
2	С	67	0	76	6	0
2	D	67	0	76	3	0
All	All	4594	0	4505	69	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 8.

The worst 5 of 69 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:A:40:ARG:O	1:A:43:ILE:HG12	1.87	0.74
1:B:222:ARG:HD2	1:B:222:ARG:H	1.56	0.70
1:B:56:ASP:OD2	1:B:60:ARG:NH2	2.27	0.67
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.77	0.67
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.78	0.64

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	entiles
1	A	277/302~(92%)	243 (88%)	32 (12%)	2 (1%)	22	54
1	В	300/302 (99%)	280 (93%)	18 (6%)	2 (1%)	22	54
2	С	6/8 (75%)	6 (100%)	0	0	100	100
2	D	6/8 (75%)	6 (100%)	0	0	100	100
All	All	589/620 (95%)	535 (91%)	50 (8%)	4 (1%)	22	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
1	В	235	MET
1	A	184	PRO
1	В	251	GLY

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	${\rm sidechain}$	conformation	was
analysed, and the total	number of	residues	S.						

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	235/258~(91%)	217 (92%)	18 (8%)	13 35
1	В	255/258~(99%)	235 (92%)	20 (8%)	12 34
2	С	7/7 (100%)	6 (86%)	1 (14%)	3 10
2	D	7/7 (100%)	5 (71%)	2 (29%)	0 1
All	All	504/530 (95%)	463 (92%)	41 (8%)	11 33

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	226	THR
1	В	280	THR
1	В	228	ASN
1	В	240	GLU
1	В	301	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	164	HIS
1	В	189	GLN
2	С	5	GLN
1	A	180	ASN
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)

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	283/302 (93%)	-0.03	14 (4%) 29 26	9, 26, 68, 85	0
1	В	302/302 (100%)	-0.21	6 (1%) 65 63	5, 21, 55, 78	0
2	С	8/8 (100%)	-0.48	0 100 100	18, 22, 37, 37	0
2	D	8/8 (100%)	-0.16	0 100 100	18, 24, 29, 56	0
All	All	601/620 (96%)	-0.13	20 (3%) 46 41	5, 24, 62, 85	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	302	GLY	4.7
1	В	196	THR	3.8
1	A	302	GLY	3.6
1	В	277	ASN	3.5
1	A	155	ASP	3.3

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 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.

