



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 17, 2022 – 12:09 PM JST

PDB ID : 7VK7  
Title : Crystal Structure of SARS-CoV-2 Mpro at 2.4 Å resolution-11  
Authors : DeMirici, H.; Dag, C.  
Deposited on : 2021-09-29  
Resolution : 2.40 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.25
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)	:	2.25

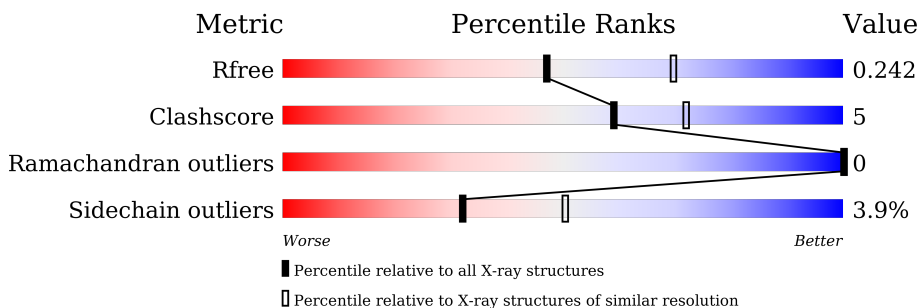
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	306	
1	B	306	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4772 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	300	Total	C	N	O	S	34	6	0
			2369	1498	404	444	23			
1	B	299	Total	C	N	O	S	0	3	0
			2342	1482	398	439	23			

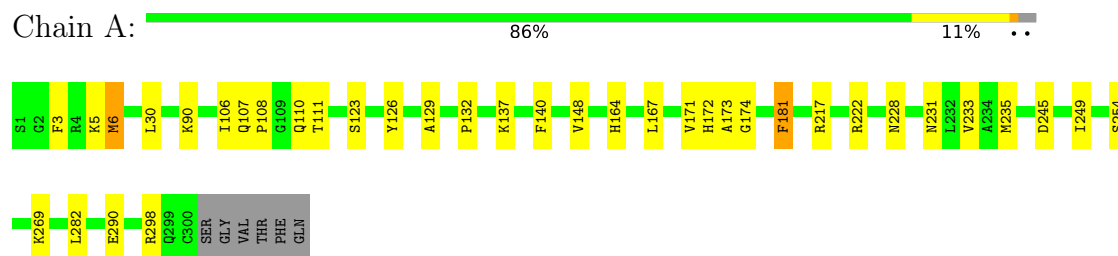
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	30	Total	O	0	0
			30	30		

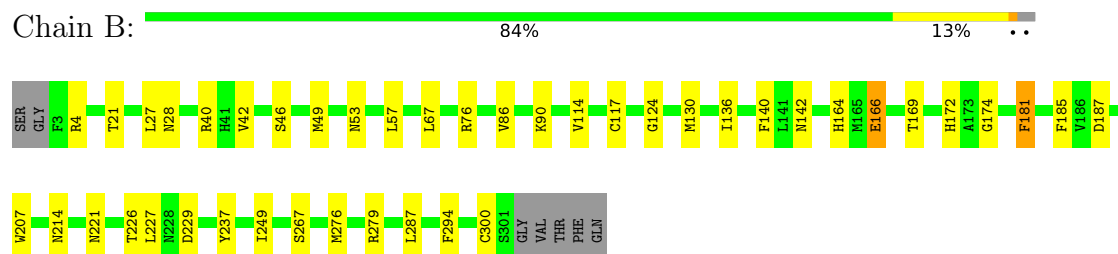
### 3 Residue-property plots [i](#)

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: 3C-like proteinase



- Molecule 1: 3C-like proteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.10Å 104.30Å 105.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.93 – 2.40 41.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.93-2.40) 97.0 (41.93-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.209 , 0.239 0.211 , 0.242	Depositor DCC
$R_{free}$ test set	1992 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.256 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/2422	0.48	0/3292
1	B	0.25	0/2394	0.47	0/3254
All	All	0.25	0/4816	0.48	0/6546

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	2369	0	2312	19	0
1	B	2342	0	2287	26	0
2	A	31	0	0	0	0
2	B	30	0	0	0	0
All	All	4772	0	4599	43	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 5.

All (43) 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:137:LYS:HB2	1:B:4:ARG:HH21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:OG1	1:B:229:ASP:OD2	2.04	0.73
1:A:140:PHE:HB2	1:A:172:HIS:CE1	2.22	0.73
1:A:233:VAL:HG21	1:A:269:LYS:HE2	1.84	0.59
1:A:231:ASN:O	1:A:235:MET:HG2	2.06	0.55
1:B:166:GLU:HG2	1:B:172:HIS:CE1	2.41	0.55
1:A:140:PHE:HB2	1:A:172:HIS:HE1	1.71	0.54
1:A:167:LEU:HD12	1:A:171:VAL:HG23	1.89	0.54
1:B:276:MET:HG2	1:B:279:ARG:H	1.74	0.52
1:B:140:PHE:HB2	1:B:172:HIS:CD2	2.44	0.52
1:A:245:ASP:O	1:A:249:ILE:HG13	2.10	0.51
1:B:28:ASN:ND2	1:B:117:CYS:O	2.43	0.51
1:A:3:PHE:HB2	1:A:282:LEU:HD23	1.93	0.50
1:A:107:GLN:H	1:A:110:GLN:NE2	2.09	0.49
1:A:5:LYS:NZ	1:A:290:GLU:OE1	2.36	0.48
1:B:221:ASN:HD21	1:B:267:SER:HA	1.80	0.47
1:B:142:ASN:OD1	1:B:142:ASN:N	2.47	0.46
1:A:106:ILE:HB	1:A:110:GLN:HE21	1.80	0.46
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.98	0.45
1:B:40:ARG:NE	1:B:187:ASP:OD2	2.43	0.45
1:B:114:VAL:HG11	1:B:140:PHE:HZ	1.83	0.44
1:B:140:PHE:HD2	1:B:172:HIS:CD2	2.36	0.44
1:A:108:PRO:HB3	1:A:132:PRO:HA	2.00	0.44
1:B:130:MET:HE3	1:B:136:ILE:HG23	2.00	0.44
1:B:140:PHE:HB2	1:B:172:HIS:NE2	2.33	0.44
1:A:6:MET:HG2	1:B:124:GLY:HA3	1.99	0.44
1:B:164:HIS:HB2	1:B:174:GLY:HA2	1.99	0.44
1:B:181:PHE:CE1	1:B:185:PHE:HB2	2.54	0.43
1:B:249:ILE:HD13	1:B:249:ILE:HA	1.89	0.43
1:B:76:ARG:CZ	1:B:76:ARG:HB2	2.49	0.43
1:A:30:LEU:HD22	1:A:148:VAL:HG11	2.00	0.42
1:A:126:TYR:HE1	1:A:140:PHE:HE1	1.65	0.42
1:A:173:ALA:HB1	1:A:181:PHE:HE1	1.84	0.42
1:A:164:HIS:HB2	1:A:174:GLY:HA2	2.02	0.42
1:A:111:THR:HG22	1:A:129:ALA:HB2	2.01	0.41
1:A:106:ILE:HB	1:A:110:GLN:NE2	2.35	0.41
1:B:207:TRP:CZ3	1:B:287:LEU:HA	2.55	0.41
1:B:53:ASN:O	1:B:57:LEU:HD12	2.21	0.41
1:B:140:PHE:HD2	1:B:172:HIS:HD2	1.68	0.41
1:B:21:THR:HB	1:B:67:LEU:HB2	2.02	0.41
1:B:140:PHE:CD2	1:B:172:HIS:HD2	2.39	0.41
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:PHE:HB2	1:B:172:HIS:HE2	1.87	0.40

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	Percentiles	
1	A	303/306 (99%)	297 (98%)	6 (2%)	0	100	100
1	B	300/306 (98%)	294 (98%)	6 (2%)	0	100	100
All	All	603/612 (98%)	591 (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	263/263 (100%)	253 (96%)	10 (4%)	33	51
1	B	261/263 (99%)	249 (95%)	12 (5%)	27	43
All	All	524/526 (100%)	502 (96%)	22 (4%)	32	47

All (22) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	6	MET
1	A	90	LYS
1	A	123	SER
1	A	181	PHE
1	A	217	ARG
1	A	222[A]	ARG
1	A	222[B]	ARG
1	A	228	ASN
1	A	254	SER
1	A	298	ARG
1	B	46[A]	SER
1	B	46[B]	SER
1	B	49	MET
1	B	86	VAL
1	B	90	LYS
1	B	166	GLU
1	B	169	THR
1	B	181	PHE
1	B	214	ASN
1	B	237	TYR
1	B	294	PHE
1	B	300	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	172	HIS
1	A	277	ASN
1	B	119	ASN
1	B	221	ASN
1	B	238	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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.

### 6.5 Other polymers [i](#)

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