



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2022 – 08:02 PM EDT

PDB ID : 7T2V  
Title : SARS CoV2 Mpro C145S mutant  
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Deposited on : 2021-12-06  
Resolution : 2.47 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](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.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.29
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)	:	2.29

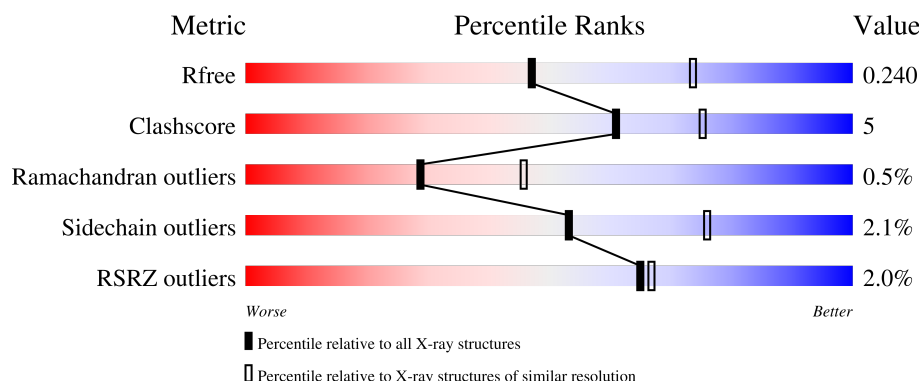
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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  $\leq 5\%$ . 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	A	319	
1	B	319	
1	C	319	
1	D	319	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9471 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 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2361	1495	400	445	21			
1	B	305	Total	C	N	O	S	0	0	0
			2345	1487	395	442	21			
1	C	305	Total	C	N	O	S	0	0	0
			2354	1491	399	443	21			
1	D	306	Total	C	N	O	S	0	0	0
			2365	1498	401	445	21			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP P0DTD1
A	-11	HIS	-	expression tag	UNP P0DTD1
A	-10	HIS	-	expression tag	UNP P0DTD1
A	-9	HIS	-	expression tag	UNP P0DTD1
A	-8	HIS	-	expression tag	UNP P0DTD1
A	-7	HIS	-	expression tag	UNP P0DTD1
A	-6	HIS	-	expression tag	UNP P0DTD1
A	-5	GLU	-	expression tag	UNP P0DTD1
A	-4	ASN	-	expression tag	UNP P0DTD1
A	-3	LEU	-	expression tag	UNP P0DTD1
A	-2	TYR	-	expression tag	UNP P0DTD1
A	-1	PHE	-	expression tag	UNP P0DTD1
A	145	SER	CYS	engineered mutation	UNP P0DTD1
B	-12	MET	-	initiating methionine	UNP P0DTD1
B	-11	HIS	-	expression tag	UNP P0DTD1
B	-10	HIS	-	expression tag	UNP P0DTD1
B	-9	HIS	-	expression tag	UNP P0DTD1
B	-8	HIS	-	expression tag	UNP P0DTD1
B	-7	HIS	-	expression tag	UNP P0DTD1
B	-6	HIS	-	expression tag	UNP P0DTD1
B	-5	GLU	-	expression tag	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASN	-	expression tag	UNP P0DTD1
B	-3	LEU	-	expression tag	UNP P0DTD1
B	-2	TYR	-	expression tag	UNP P0DTD1
B	-1	PHE	-	expression tag	UNP P0DTD1
B	145	SER	CYS	engineered mutation	UNP P0DTD1
C	-12	MET	-	initiating methionine	UNP P0DTD1
C	-11	HIS	-	expression tag	UNP P0DTD1
C	-10	HIS	-	expression tag	UNP P0DTD1
C	-9	HIS	-	expression tag	UNP P0DTD1
C	-8	HIS	-	expression tag	UNP P0DTD1
C	-7	HIS	-	expression tag	UNP P0DTD1
C	-6	HIS	-	expression tag	UNP P0DTD1
C	-5	GLU	-	expression tag	UNP P0DTD1
C	-4	ASN	-	expression tag	UNP P0DTD1
C	-3	LEU	-	expression tag	UNP P0DTD1
C	-2	TYR	-	expression tag	UNP P0DTD1
C	-1	PHE	-	expression tag	UNP P0DTD1
C	145	SER	CYS	engineered mutation	UNP P0DTD1
D	-12	MET	-	initiating methionine	UNP P0DTD1
D	-11	HIS	-	expression tag	UNP P0DTD1
D	-10	HIS	-	expression tag	UNP P0DTD1
D	-9	HIS	-	expression tag	UNP P0DTD1
D	-8	HIS	-	expression tag	UNP P0DTD1
D	-7	HIS	-	expression tag	UNP P0DTD1
D	-6	HIS	-	expression tag	UNP P0DTD1
D	-5	GLU	-	expression tag	UNP P0DTD1
D	-4	ASN	-	expression tag	UNP P0DTD1
D	-3	LEU	-	expression tag	UNP P0DTD1
D	-2	TYR	-	expression tag	UNP P0DTD1
D	-1	PHE	-	expression tag	UNP P0DTD1
D	145	SER	CYS	engineered mutation	UNP P0DTD1

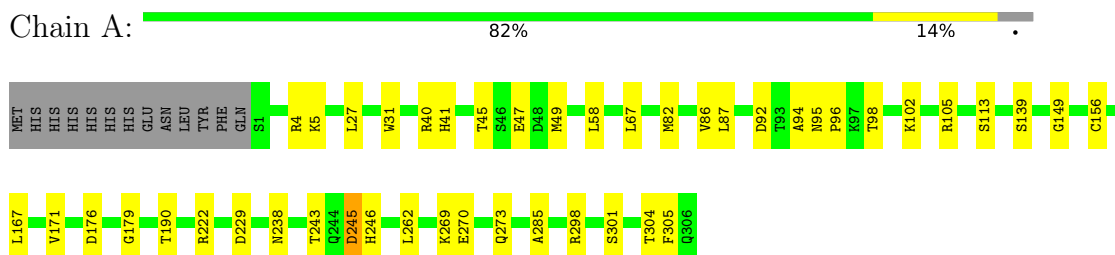
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	9	Total O 9 9	0	0
2	C	10	Total O 10 10	0	0
2	D	17	Total O 17 17	0	0

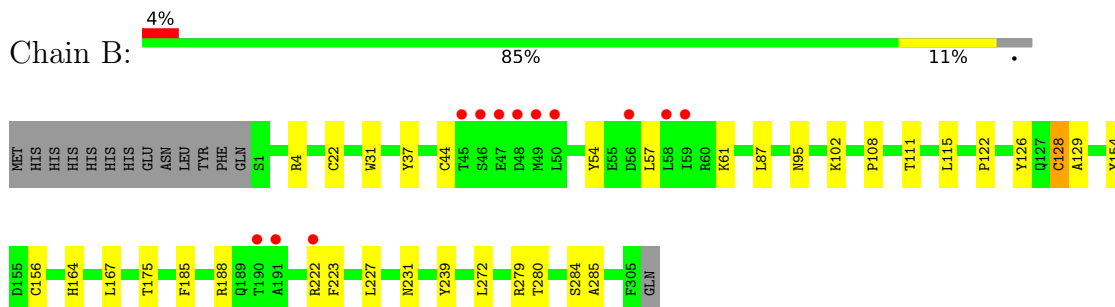
### 3 Residue-property plots [i](#)

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.

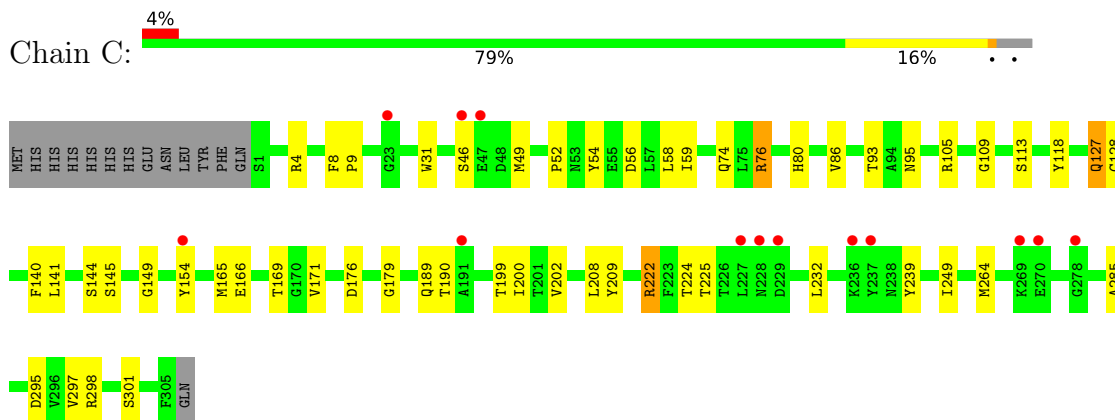
- Molecule 1: 3C-Like Protease



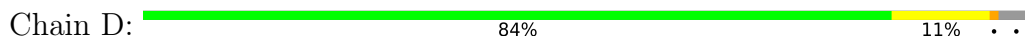
- Molecule 1: 3C-Like Protease

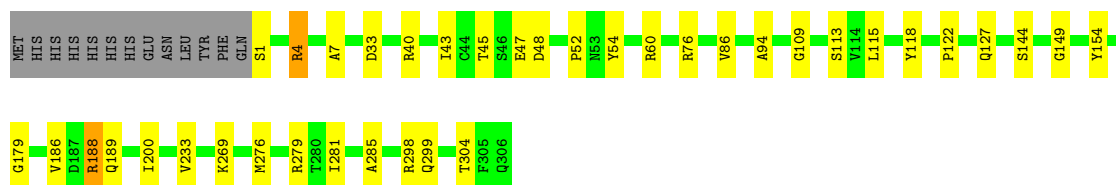


- Molecule 1: 3C-Like Protease



- Molecule 1: 3C-Like Protease





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.59Å 67.51Å 77.65Å 102.11° 89.30° 106.41°	Depositor
Resolution (Å)	38.05 – 2.47 38.05 – 2.47	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.05-2.47) 96.9 (38.05-2.47)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, $R_{free}$	0.196 , 0.237 0.202 , 0.240	Depositor DCC
$R_{free}$ test set	2037 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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

### 5.1 Standard geometry

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	0.33	0/2414	0.62	0/3281
1	B	0.32	0/2398	0.59	0/3262
1	C	0.33	0/2407	0.61	0/3273
1	D	0.35	0/2418	0.63	0/3285
All	All	0.33	0/9637	0.61	0/13101

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	0	3
1	B	0	1
1	C	0	3
1	D	0	6
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ARG	Sidechain
1	A	298	ARG	Sidechain
1	A	4	ARG	Sidechain
1	B	279	ARG	Sidechain
1	C	4	ARG	Sidechain



## 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	2361	0	2299	22	0
1	B	2345	0	2280	16	0
1	C	2354	0	2295	32	0
1	D	2365	0	2310	22	0
2	A	10	0	0	0	0
2	B	9	0	0	0	0
2	C	10	0	0	0	0
2	D	17	0	0	0	0
All	All	9471	0	9184	84	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.

The worst 5 of 84 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:C:166:GLU:OE2	1:D:1:SER:HB3	1.85	0.76
1:A:269:LYS:O	1:A:273:GLN:HG3	1.96	0.65
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.79	0.65
1:D:113:SER:O	1:D:149:GLY:HA2	1.99	0.63
1:A:285:ALA:HB3	1:B:285:ALA:HB3	1.81	0.62

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	304/319 (95%)	286 (94%)	17 (6%)	1 (0%)	41	59
1	B	303/319 (95%)	283 (93%)	18 (6%)	2 (1%)	22	36
1	C	303/319 (95%)	287 (95%)	14 (5%)	2 (1%)	22	36
1	D	304/319 (95%)	291 (96%)	12 (4%)	1 (0%)	41	59
All	All	1214/1276 (95%)	1147 (94%)	61 (5%)	6 (0%)	29	46

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	46	SER
1	A	238	ASN
1	B	223	PHE
1	D	154	TYR
1	B	154	TYR

### 5.3.2 Protein sidechains ⓘ

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	261/276 (95%)	252 (97%)	9 (3%)	37	61
1	B	259/276 (94%)	254 (98%)	5 (2%)	57	78
1	C	261/276 (95%)	255 (98%)	6 (2%)	50	74
1	D	262/276 (95%)	260 (99%)	2 (1%)	81	92
All	All	1043/1104 (94%)	1021 (98%)	22 (2%)	53	76

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	93	THR
1	C	145	SER
1	C	128	CYS
1	C	165	MET
1	A	270	GLU

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	C	142	ASN
1	D	127	GLN
1	D	151	ASN
1	A	273	GLN
1	A	231	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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	306/319 (95%)	-0.16	0 <span>100</span> <span>100</span>	27, 47, 77, 95	0
1	B	305/319 (95%)	0.02	12 (3%) <span>39</span> <span>41</span>	27, 51, 87, 147	0
1	C	305/319 (95%)	0.01	13 (4%) <span>35</span> <span>37</span>	29, 50, 93, 110	0
1	D	306/319 (95%)	-0.33	0 <span>100</span> <span>100</span>	25, 39, 62, 102	0
All	All	1222/1276 (95%)	-0.12	25 (2%) <span>65</span> <span>67</span>	25, 46, 85, 147	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	LEU	9.7
1	B	49	MET	5.0
1	B	222	ARG	3.5
1	C	23	GLY	3.3
1	B	56	ASP	3.2

### 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 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.