



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 7C2Q / pdb_00007c2q
Title : The crystal structure of COVID-19 main protease in the apo state
Authors : Zhou, X.L.; Zhong, F.L.; Lin, C.; Hu, X.H.; Zhou, H.; Wang, Q.S.; Li, j.; Zhang, J.
Deposited on : 2020-05-08
Resolution : 1.93 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

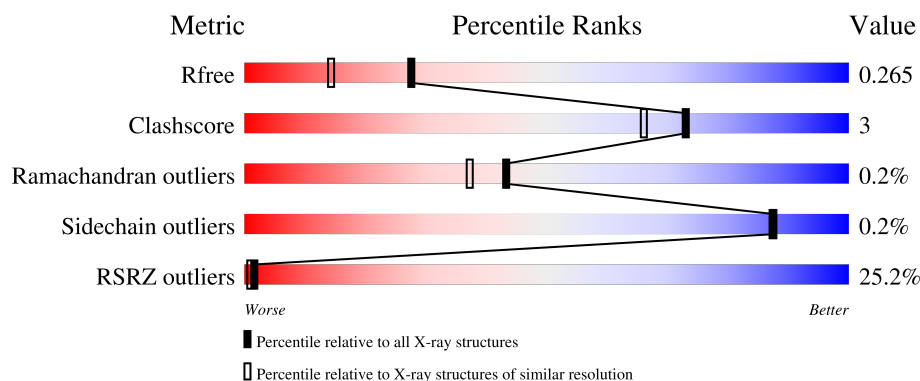
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 $\leq 5\%$. 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	296	20% 88% 9% .
1	B	296	29% 90% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4467 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	288	Total	C	N	O	S	0	0	0
			2206	1398	378	409	21			
1	B	284	Total	C	N	O	S	0	0	0
			2120	1347	365	390	18			

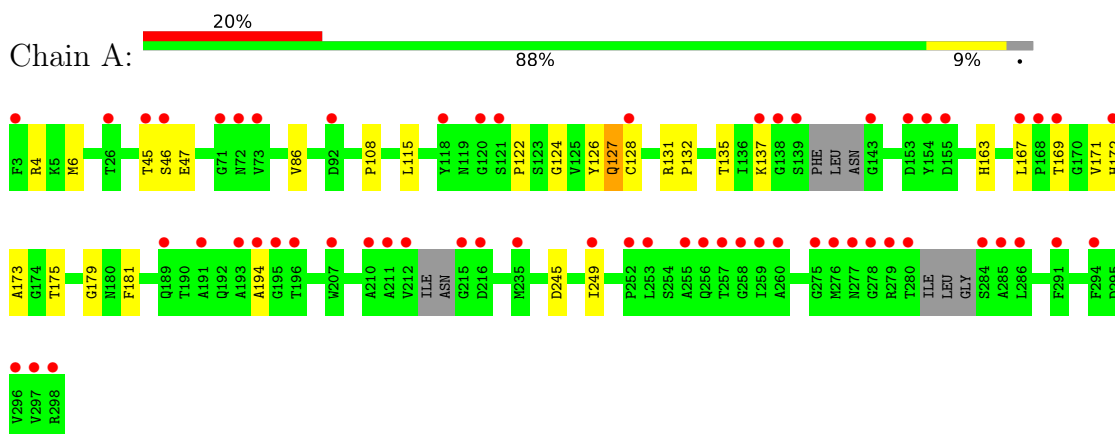
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	85	Total	O	0	0
			85	85		
2	B	56	Total	O	0	0
			56	56		

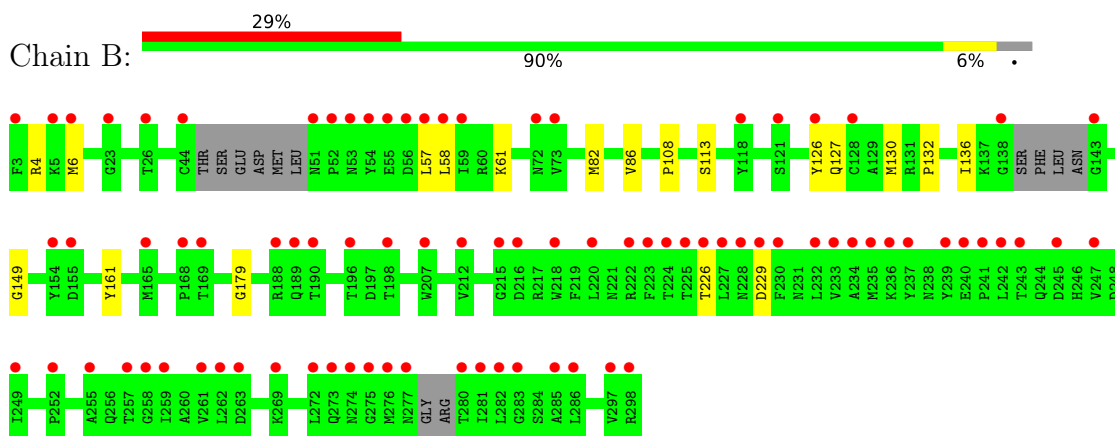
3 Residue-property plots

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



• 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, α , β , γ	67.95Å 102.66Å 103.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.90 – 1.93 72.90 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.90-1.93) 92.0 (72.90-1.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.226 , 0.265 0.226 , 0.265	Depositor DCC
R_{free} test set	2003 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4467	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.35	0/2253	0.55	0/3061
1	B	0.32	0/2163	0.51	0/2946
All	All	0.33	0/4416	0.53	0/6007

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

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	2206	0	2142	17	0
1	B	2120	0	2042	14	0
2	A	85	0	0	0	0
2	B	56	0	0	0	0
All	All	4467	0	4184	27	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 3.

All (27) 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:6:MET:O	1:A:127:GLN:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:HG23	1:A:171:VAL:HG22	1.78	0.65
1:A:245:ASP:O	1:A:249:ILE:HG12	1.97	0.64
1:A:45:THR:O	1:A:47:GLU:N	2.34	0.61
1:A:131:ARG:HD3	1:A:137:LYS:HE3	1.85	0.58
1:A:124:GLY:HA3	1:B:6:MET:HG2	1.88	0.55
1:A:167:LEU:HD21	1:A:173:ALA:HB2	1.87	0.55
1:B:6:MET:O	1:B:127:GLN:HG2	2.07	0.54
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.91	0.53
1:B:58:LEU:HD22	1:B:82:MET:HE3	1.92	0.51
1:B:136:ILE:HD12	1:B:161:TYR:CZ	2.49	0.48
1:A:163:HIS:CD2	1:A:172:HIS:HB3	2.49	0.47
1:B:226:THR:OG1	1:B:229:ASP:HB2	2.15	0.46
1:B:113:SER:O	1:B:149:GLY:HA2	2.16	0.46
1:A:126:TYR:CD1	1:B:4:ARG:HD2	2.51	0.46
1:A:135:THR:HG21	1:A:194:ALA:HB2	1.98	0.45
1:B:57:LEU:O	1:B:61:LYS:HG2	2.18	0.43
1:A:108:PRO:HB3	1:A:132:PRO:HA	2.00	0.43
1:A:126:TYR:HE1	1:A:128:CYS:SG	2.41	0.43
1:A:4:ARG:HD2	1:B:126:TYR:CD2	2.54	0.42
1:A:175:THR:HG22	1:A:181:PHE:HA	2.01	0.42
1:B:6:MET:HE3	1:B:6:MET:HB2	1.62	0.42
1:B:108:PRO:HB3	1:B:132:PRO:HA	2.02	0.41
1:A:137:LYS:O	1:B:4:ARG:NE	2.47	0.41
1:B:86:VAL:HG13	1:B:179:GLY:HA2	2.01	0.41
1:A:115:LEU:HD21	1:A:122:PRO:HB3	2.03	0.41
1:B:130:MET:HE2	1:B:130:MET:HB2	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	280/296 (95%)	270 (96%)	9 (3%)	1 (0%)	30	22
1	B	276/296 (93%)	271 (98%)	5 (2%)	0	100	100
All	All	556/592 (94%)	541 (97%)	14 (2%)	1 (0%)	43	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	SER

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	241/255 (94%)	240 (100%)	1 (0%)	84	84
1	B	224/255 (88%)	224 (100%)	0	100	100
All	All	465/510 (91%)	464 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	172	HIS
1	A	273	GLN
1	B	180	ASN
1	B	214	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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, 95th 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	A	288/296 (97%)	1.00	59 (20%) 2 2	22, 32, 54, 60	0
1	B	284/296 (95%)	1.31	85 (29%) 1 1	22, 38, 58, 71	0
All	All	572/592 (96%)	1.15	144 (25%) 1 1	22, 35, 57, 71	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	GLY	5.6
1	B	233	VAL	5.3
1	A	280	THR	5.3
1	A	286	LEU	5.2
1	A	296	VAL	5.1
1	A	3	PHE	4.9
1	A	255	ALA	4.8
1	B	280	THR	4.8
1	A	191	ALA	4.5
1	B	285	ALA	4.5
1	B	286	LEU	4.4
1	B	276	MET	4.4
1	B	189	GLN	4.4
1	A	284	SER	4.3
1	B	143	GLY	4.2
1	A	278	GLY	3.9
1	A	139	SER	3.9
1	B	277	ASN	3.9
1	B	234	ALA	3.9
1	B	232	LEU	3.8
1	A	298	ARG	3.8
1	A	143	GLY	3.8
1	A	194	ALA	3.8
1	B	237	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	128	CYS	3.7
1	A	258	GLY	3.7
1	B	216	ASP	3.6
1	B	138	GLY	3.6
1	A	128	CYS	3.6
1	A	118	TYR	3.5
1	A	45	THR	3.5
1	B	228	ASN	3.5
1	B	155	ASP	3.3
1	A	138	GLY	3.3
1	B	255	ALA	3.3
1	A	277	ASN	3.2
1	B	227	LEU	3.2
1	A	212	VAL	3.1
1	A	253	LEU	3.1
1	A	169	THR	3.1
1	B	57	LEU	3.0
1	B	235	MET	3.0
1	A	256	GLN	3.0
1	B	51	ASN	3.0
1	A	167	LEU	2.9
1	B	298	ARG	2.9
1	B	168	PRO	2.9
1	B	282	LEU	2.9
1	A	249	ILE	2.9
1	B	56	ASP	2.9
1	B	247	VAL	2.9
1	B	261	VAL	2.9
1	A	257	THR	2.9
1	A	210	ALA	2.8
1	B	245	ASP	2.8
1	B	258	GLY	2.8
1	B	226	THR	2.8
1	A	92	ASP	2.8
1	A	279	ARG	2.8
1	B	229	ASP	2.8
1	B	154	TYR	2.7
1	B	230	PHE	2.7
1	B	236	LYS	2.7
1	B	249	ILE	2.7
1	A	252	PRO	2.7
1	B	52	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	297	VAL	2.7
1	B	188	ARG	2.7
1	A	121	SER	2.7
1	B	274	ASN	2.7
1	A	285	ALA	2.7
1	A	168	PRO	2.7
1	B	59	ILE	2.7
1	B	281	ILE	2.6
1	B	118	TYR	2.6
1	B	207	TRP	2.6
1	B	58	LEU	2.6
1	A	155	ASP	2.6
1	B	263	ASP	2.6
1	A	193	ALA	2.6
1	A	153	ASP	2.6
1	B	215	GLY	2.6
1	A	46	SER	2.5
1	B	224	THR	2.5
1	B	225	THR	2.5
1	B	55	GLU	2.5
1	A	294	PHE	2.5
1	A	154	TYR	2.5
1	B	23	GLY	2.5
1	B	273	GLN	2.5
1	A	260	ALA	2.5
1	A	196	THR	2.5
1	B	169	THR	2.5
1	A	195	GLY	2.4
1	A	73	VAL	2.4
1	B	6	MET	2.4
1	B	252	PRO	2.4
1	A	189	GLN	2.4
1	B	198	THR	2.4
1	B	223	PHE	2.3
1	B	72	ASN	2.3
1	B	241	PRO	2.3
1	A	276	MET	2.3
1	A	207	TRP	2.3
1	B	272	LEU	2.3
1	B	3	PHE	2.3
1	B	53	ASN	2.3
1	A	120	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	243	THR	2.3
1	A	211	ALA	2.2
1	B	73	VAL	2.2
1	B	190	THR	2.2
1	B	240	GLU	2.2
1	A	71	GLY	2.2
1	B	218	TRP	2.2
1	A	259	ILE	2.2
1	B	5	LYS	2.2
1	B	126	TYR	2.2
1	A	172	HIS	2.2
1	A	216	ASP	2.2
1	B	275	GLY	2.2
1	B	196	THR	2.1
1	B	297	VAL	2.1
1	B	121	SER	2.1
1	A	275	GLY	2.1
1	B	283	GLY	2.1
1	B	242	LEU	2.1
1	B	262	LEU	2.1
1	A	72	ASN	2.1
1	B	239	TYR	2.1
1	B	269	LYS	2.1
1	B	165	MET	2.1
1	B	26	THR	2.1
1	A	235	MET	2.1
1	B	44	CYS	2.1
1	B	220	LEU	2.1
1	B	222	ARG	2.1
1	A	291	PHE	2.0
1	B	54	TYR	2.0
1	A	26	THR	2.0
1	B	257	THR	2.0
1	A	137	LYS	2.0
1	B	259	ILE	2.0
1	B	212	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.