



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:33 PM UTC

PDB ID : 8WSK / pdb_00008wsk
Title : Crystal structure of SARS-Cov-2 main protease, pH=8.5
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Deposited on : 2023-10-17
Resolution : 1.88 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

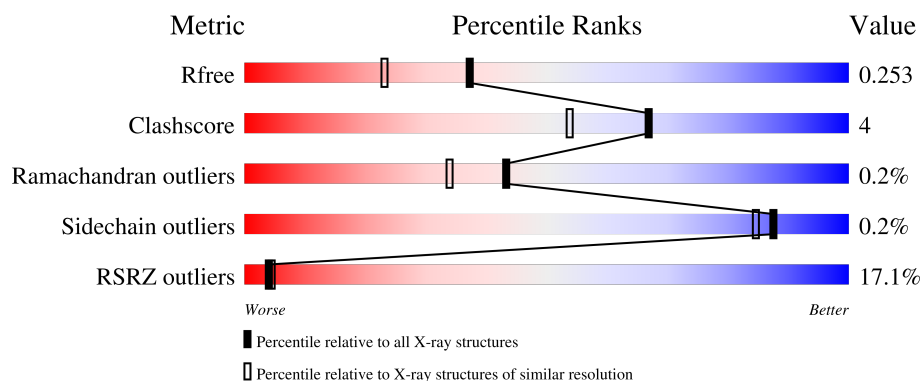
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	13% 92% 7%
1	B	296	21% 89% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4575 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	A	293	Total	C	N	O	S	0	0	0
			2219	1412	376	410	21			
1	B	292	Total	C	N	O	S	0	0	0
			2189	1389	370	409	21			

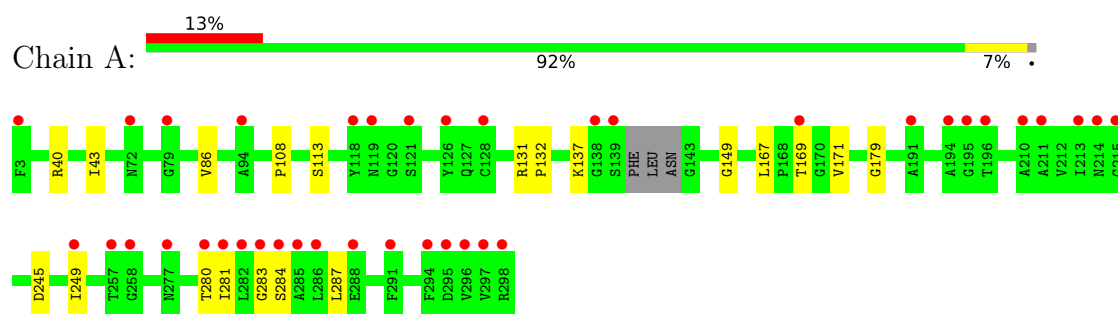
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		
2	B	57	Total	O	0	0
			57	57		

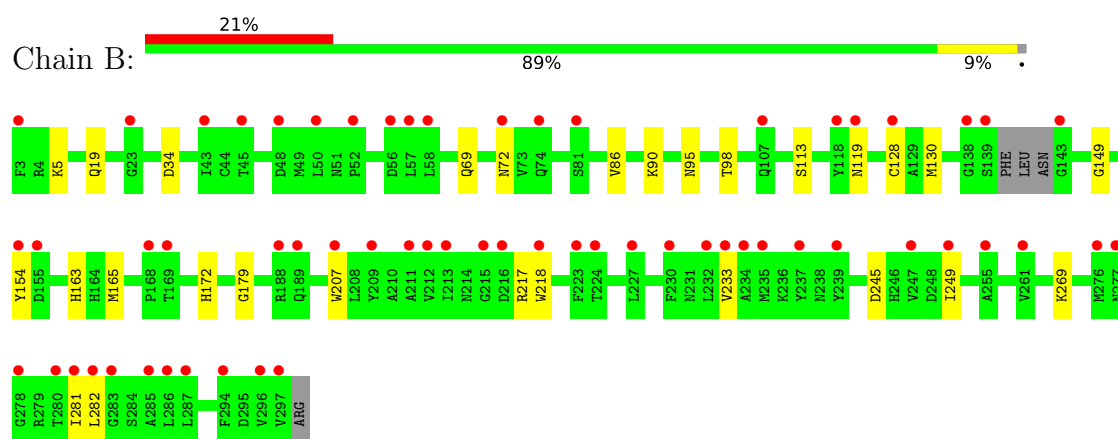
3 Residue-property plots [i](#)

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



- Molecule 1: 3C-like proteinase nsp5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.01Å 102.90Å 103.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.48 – 1.88 36.48 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.48-1.88) 98.9 (36.48-1.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.222 , 0.251 0.222 , 0.253	Depositor DCC
R_{free} test set	2870 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4575	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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 [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	0.35	0/2268	0.59	0/3087
1	B	0.29	0/2237	0.52	1/3049 (0.0%)
All	All	0.32	0/4505	0.56	1/6136 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	CYS	CB-CA-C	-5.45	99.99	110.24

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	2219	0	2151	12	0
1	B	2189	0	2097	20	0
2	A	110	0	0	0	0
2	B	57	0	0	0	0
All	All	4575	0	4248	32	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 4.

All (32) 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:281:ILE:H	1:A:284:SER:H	1.39	0.71
1:B:218:TRP:CZ2	1:B:281:ILE:HD11	2.30	0.67
1:A:280:THR:HB	1:A:284:SER:N	2.13	0.64
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.81	0.63
1:B:282:LEU:O	1:B:282:LEU:HD12	1.98	0.62
1:A:245:ASP:O	1:A:249:ILE:HG12	1.99	0.62
1:A:169:THR:HG23	1:A:171:VAL:HG22	1.81	0.62
1:B:218:TRP:CZ2	1:B:281:ILE:CD1	2.87	0.57
1:A:281:ILE:N	1:A:284:SER:H	2.02	0.55
1:B:233:VAL:HG21	1:B:269:LYS:HE2	1.90	0.54
1:B:207:TRP:HE1	1:B:282:LEU:HD11	1.75	0.50
1:B:233:VAL:HG11	1:B:269:LYS:HG3	1.93	0.50
1:B:19:GLN:OE1	1:B:119:ASN:HB3	2.12	0.50
1:B:245:ASP:O	1:B:249:ILE:HG12	2.12	0.50
1:B:69:GLN:NE2	1:B:72:ASN:O	2.47	0.48
1:A:280:THR:HB	1:A:283:GLY:C	2.41	0.45
1:A:108:PRO:HB3	1:A:132:PRO:HA	1.98	0.44
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.76	0.44
1:B:217:ARG:HE	1:B:217:ARG:HB3	1.66	0.44
1:B:34:ASP:CG	1:B:90:LYS:HE2	2.43	0.44
1:B:207:TRP:NE1	1:B:282:LEU:HD11	2.33	0.44
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.98	0.43
1:B:165:MET:HE2	1:B:165:MET:HB2	1.74	0.43
1:A:40:ARG:O	1:A:43:ILE:HG12	2.18	0.43
1:B:5:LYS:HE3	1:B:5:LYS:HB2	1.87	0.43
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.19	0.42
1:B:207:TRP:NE1	1:B:282:LEU:HD21	2.35	0.42
1:A:131:ARG:HD3	1:A:137:LYS:HE3	2.01	0.42
1:B:113:SER:O	1:B:149:GLY:HA2	2.20	0.41
1:A:113:SER:O	1:A:149:GLY:HA2	2.20	0.41
1:B:130:MET:HE2	1:B:130:MET:HB2	1.88	0.41
1:B:163:HIS:CD2	1:B:172:HIS:HB3	2.56	0.41

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	289/296 (98%)	281 (97%)	8 (3%)	0	100	100
1	B	288/296 (97%)	280 (97%)	7 (2%)	1 (0%)	36	26
All	All	577/592 (98%)	561 (97%)	15 (3%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	239/255 (94%)	238 (100%)	1 (0%)	84	79
1	B	234/255 (92%)	234 (100%)	0	100	100
All	All	473/510 (93%)	472 (100%)	1 (0%)	87	84

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

Mol	Chain	Res	Type
1	A	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	163	HIS
1	A	172	HIS
1	A	273	GLN
1	B	151	ASN
1	B	163	HIS

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Mol	Chain	Res	Type
1	B	214	ASN
1	B	273	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](#)

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	293/296 (98%)	0.76	39 (13%) 7 7	20, 30, 50, 61	0
1	B	292/296 (98%)	1.11	61 (20%) 2 2	21, 39, 60, 68	0
All	All	585/592 (98%)	0.94	100 (17%) 4 4	20, 34, 56, 68	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	LEU	6.0
1	A	283	GLY	5.4
1	A	296	VAL	5.3
1	B	118	TYR	5.2
1	B	215	GLY	5.2
1	A	118	TYR	4.6
1	B	223	PHE	4.2
1	A	282	LEU	4.2
1	B	139	SER	4.1
1	B	297	VAL	4.1
1	A	297	VAL	4.0
1	B	285	ALA	4.0
1	A	215	GLY	4.0
1	A	210	ALA	3.9
1	B	283	GLY	3.7
1	B	255	ALA	3.7
1	A	286	LEU	3.6
1	A	213	ILE	3.6
1	A	191	ALA	3.6
1	A	3	PHE	3.6
1	A	214	ASN	3.5
1	B	235	MET	3.4
1	B	281	ILE	3.4
1	B	72	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	168	PRO	3.4
1	B	280	THR	3.3
1	B	276	MET	3.2
1	A	280	THR	3.2
1	B	278	GLY	3.2
1	A	138	GLY	3.1
1	A	258	GLY	3.0
1	B	286	LEU	3.0
1	B	128	CYS	3.0
1	B	277	ASN	3.0
1	B	45	THR	2.9
1	B	143	GLY	2.9
1	A	291	PHE	2.9
1	B	230	PHE	2.9
1	A	298	ARG	2.9
1	A	139	SER	2.9
1	A	281	ILE	2.9
1	B	50	LEU	2.9
1	B	224	THR	2.8
1	B	189	GLN	2.8
1	B	138	GLY	2.8
1	B	56	ASP	2.8
1	A	284	SER	2.7
1	A	277	ASN	2.7
1	B	48	ASP	2.7
1	B	57	LEU	2.7
1	B	232	LEU	2.7
1	B	216	ASP	2.6
1	B	234	ALA	2.6
1	B	154	TYR	2.6
1	A	128	CYS	2.5
1	B	237	TYR	2.5
1	B	249	ILE	2.5
1	B	119	ASN	2.5
1	A	196	THR	2.5
1	A	169	THR	2.5
1	A	119	ASN	2.4
1	A	94	ALA	2.4
1	A	195	GLY	2.4
1	B	3	PHE	2.4
1	B	218	TRP	2.4
1	A	294	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	211	ALA	2.3
1	B	58	LEU	2.3
1	A	72	ASN	2.3
1	B	74	GLN	2.3
1	A	79	GLY	2.3
1	B	296	VAL	2.3
1	B	207	TRP	2.2
1	A	285	ALA	2.2
1	A	194	ALA	2.2
1	A	126	TYR	2.2
1	B	294	PHE	2.2
1	B	188	ARG	2.2
1	B	212	VAL	2.2
1	B	239	TYR	2.2
1	A	249	ILE	2.2
1	A	288	GLU	2.2
1	B	107	GLN	2.2
1	B	233	VAL	2.2
1	B	52	PRO	2.2
1	B	209	TYR	2.1
1	B	213	ILE	2.1
1	B	169	THR	2.1
1	B	23	GLY	2.1
1	B	247	VAL	2.1
1	B	227	LEU	2.1
1	B	43	ILE	2.1
1	B	155	ASP	2.1
1	B	81	SER	2.1
1	A	257	THR	2.1
1	B	287	LEU	2.1
1	A	121	SER	2.0
1	B	211	ALA	2.0
1	A	295	ASP	2.0
1	B	261	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.