



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:15 PM UTC

PDB ID : 8WSH / pdb_00008wsh
Title : Crystal structure of SARS-Cov-2 main protease, pH=4.0
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Deposited on : 2023-10-17
Resolution : 1.80 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

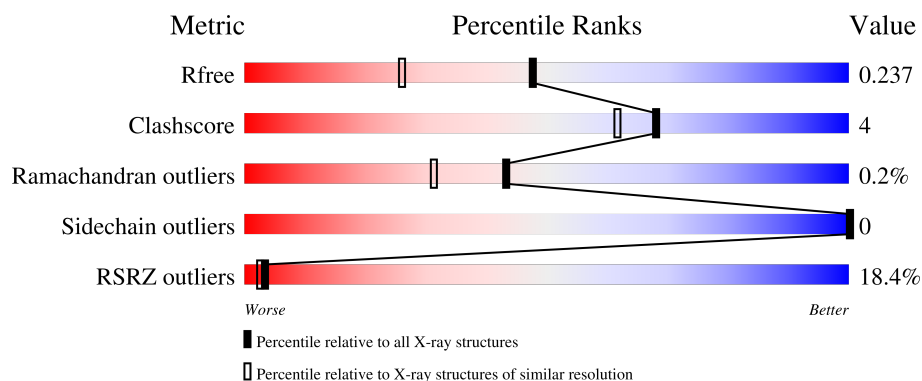
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	298	14% 94% ..
1	B	298	23% 94% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4500 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 polypeptide 1ab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2190	1389	370	410	21			
1	B	298	Total	C	N	O	S	0	0	0
			2150	1366	365	399	20			

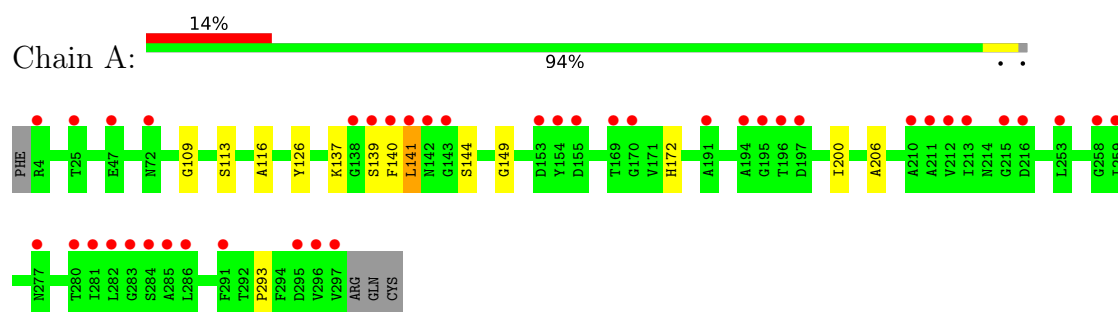
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	66	Total	O	0	0
			66	66		

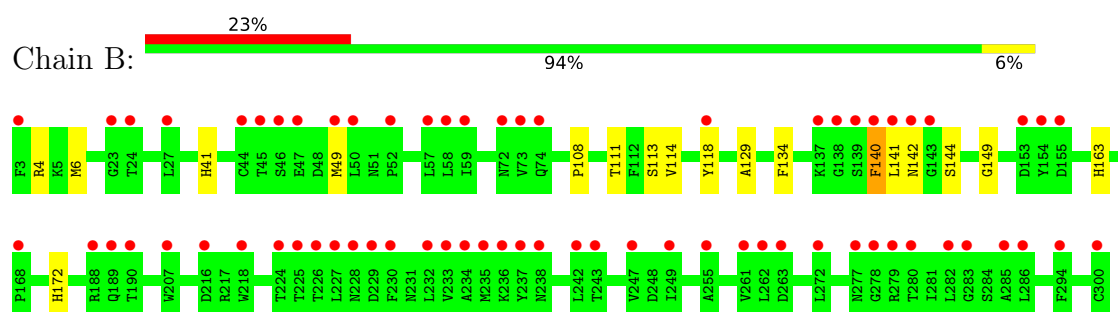
3 Residue-property plots

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: Replicase polypeptide 1ab



• Molecule 1: Replicase polypeptide 1ab



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.06Å 102.60Å 103.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.31 – 1.80 51.31 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (51.31-1.80) 97.8 (51.31-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.213 , 0.236 0.213 , 0.237	Depositor DCC
R_{free} test set	3365 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4500	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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	0.31	0/2239	0.52	0/3055
1	B	0.27	0/2200	0.50	0/3011
All	All	0.29	0/4439	0.51	0/6066

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	PHE	Peptide

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	2190	0	2074	13	0
1	B	2150	0	1973	22	0
2	A	94	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	66	0	0	0	0
All	All	4500	0	4047	30	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 (30) 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:B:141:LEU:H	1:B:142:ASN:HA	1.33	0.92
1:B:41:HIS:HB2	1:B:49:MET:HE1	1.52	0.87
1:A:126:TYR:HD2	1:B:6:MET:HE3	1.53	0.74
1:B:141:LEU:N	1:B:142:ASN:HA	2.02	0.73
1:B:141:LEU:HB2	1:B:144:SER:HB2	1.73	0.69
1:B:114:VAL:HG11	1:B:140:PHE:CZ	2.27	0.69
1:A:140:PHE:HD2	1:A:172:HIS:CG	2.14	0.65
1:B:114:VAL:HG11	1:B:140:PHE:HZ	1.63	0.61
1:A:141:LEU:H	1:A:141:LEU:HD23	1.66	0.60
1:B:118:TYR:HB2	1:B:141:LEU:HD21	1.82	0.60
1:B:141:LEU:H	1:B:142:ASN:CA	2.13	0.58
1:B:141:LEU:CB	1:B:144:SER:HB2	2.35	0.55
1:A:126:TYR:CD2	1:B:6:MET:HE3	2.40	0.54
1:A:139:SER:OG	1:B:4:ARG:HB2	2.09	0.53
1:A:141:LEU:HG	1:A:144:SER:HB3	1.91	0.51
1:A:137:LYS:O	1:B:4:ARG:NE	2.35	0.49
1:A:140:PHE:HB2	1:A:172:HIS:NE2	2.29	0.48
1:B:140:PHE:HB3	1:B:163:HIS:CE1	2.50	0.47
1:A:206:ALA:HB2	1:A:293:PRO:HG3	1.98	0.46
1:B:140:PHE:HB2	1:B:172:HIS:CD2	2.51	0.45
1:A:140:PHE:CD2	1:A:172:HIS:CG	3.02	0.45
1:B:140:PHE:HB2	1:B:172:HIS:NE2	2.32	0.45
1:B:111:THR:HG22	1:B:129:ALA:HB2	1.99	0.45
1:B:113:SER:O	1:B:149:GLY:HA2	2.18	0.44
1:A:109:GLY:HA2	1:A:200:ILE:HD13	2.00	0.43
1:B:108:PRO:HG3	1:B:134:PHE:CE1	2.53	0.42
1:B:114:VAL:HG11	1:B:140:PHE:CE1	2.55	0.42
1:B:140:PHE:HD2	1:B:172:HIS:CG	2.39	0.41
1:A:116:ALA:HB3	1:B:6:MET:HE1	2.02	0.41
1:A:113:SER:O	1:A:149:GLY:HA2	2.22	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	292/298 (98%)	288 (99%)	3 (1%)	1 (0%)	36	25
1	B	296/298 (99%)	293 (99%)	3 (1%)	0	100	100
All	All	588/596 (99%)	581 (99%)	6 (1%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LEU

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	231/257 (90%)	231 (100%)	0	100	100
1	B	214/257 (83%)	214 (100%)	0	100	100
All	All	445/514 (87%)	445 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	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 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	294/298 (98%)	0.77	41 (13%) 6 5	19, 29, 47, 67	0
1	B	298/298 (100%)	1.15	68 (22%) 2 1	19, 35, 55, 68	0
All	All	592/596 (99%)	0.96	109 (18%) 3 2	19, 33, 52, 68	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	PHE	9.2
1	A	141	LEU	7.9
1	A	140	PHE	7.6
1	B	141	LEU	6.0
1	A	213	ILE	5.4
1	B	142	ASN	4.8
1	A	282	LEU	4.5
1	B	24	THR	4.3
1	A	215	GLY	4.3
1	A	142	ASN	4.2
1	B	277	ASN	4.2
1	B	139	SER	4.1
1	B	249	ILE	4.1
1	B	228	ASN	4.1
1	A	296	VAL	4.1
1	B	138	GLY	3.9
1	B	233	VAL	3.8
1	A	139	SER	3.7
1	B	278	GLY	3.7
1	B	232	LEU	3.6
1	A	280	THR	3.6
1	A	297	VAL	3.5
1	A	210	ALA	3.5
1	B	255	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	227	LEU	3.5
1	B	247	VAL	3.4
1	A	143	GLY	3.4
1	B	50	LEU	3.3
1	B	285	ALA	3.3
1	B	300	CYS	3.2
1	B	118	TYR	3.2
1	B	237	TYR	3.2
1	B	3	PHE	3.2
1	B	72	ASN	3.1
1	A	154	TYR	3.1
1	B	45	THR	3.1
1	B	154	TYR	3.1
1	B	286	LEU	3.1
1	B	189	GLN	3.0
1	A	138	GLY	3.0
1	B	143	GLY	3.0
1	A	194	ALA	2.9
1	B	153	ASP	2.9
1	A	284	SER	2.9
1	A	169	THR	2.9
1	B	225	THR	2.9
1	B	238	ASN	2.9
1	B	230	PHE	2.9
1	A	291	PHE	2.8
1	B	282	LEU	2.8
1	B	229	ASP	2.7
1	B	235	MET	2.7
1	A	277	ASN	2.7
1	A	170	GLY	2.6
1	B	49	MET	2.6
1	B	155	ASP	2.6
1	A	196	THR	2.6
1	A	295	ASP	2.6
1	B	137	LYS	2.6
1	B	190	THR	2.6
1	B	224	THR	2.6
1	A	72	ASN	2.5
1	B	234	ALA	2.5
1	B	59	ILE	2.5
1	A	212	VAL	2.5
1	B	47	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	188	ARG	2.5
1	B	226	THR	2.4
1	A	216	ASP	2.4
1	B	74	GLN	2.4
1	B	57	LEU	2.4
1	B	261	VAL	2.4
1	B	294	PHE	2.4
1	B	23	GLY	2.4
1	A	253	LEU	2.3
1	A	191	ALA	2.3
1	A	4	ARG	2.3
1	B	168	PRO	2.3
1	A	281	ILE	2.3
1	A	153	ASP	2.3
1	B	218	TRP	2.2
1	B	279	ARG	2.2
1	B	73	VAL	2.2
1	B	243	THR	2.2
1	B	283	GLY	2.2
1	B	216	ASP	2.2
1	A	195	GLY	2.2
1	A	259	ILE	2.2
1	B	236	LYS	2.2
1	A	47	GLU	2.2
1	B	207	TRP	2.1
1	B	44	CYS	2.1
1	A	25	THR	2.1
1	A	197	ASP	2.1
1	B	280	THR	2.1
1	A	283	GLY	2.1
1	B	27	LEU	2.1
1	B	58	LEU	2.1
1	B	242	LEU	2.1
1	B	262	LEU	2.1
1	B	272	LEU	2.1
1	A	285	ALA	2.1
1	A	155	ASP	2.1
1	B	46	SER	2.0
1	A	286	LEU	2.0
1	A	211	ALA	2.0
1	B	263	ASP	2.0
1	A	258	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	52	PRO	2.0

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 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.