



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:50 PM UTC

PDB ID : 8WSJ / pdb_00008wsj
Title : Crystal structure of SARS-Cov-2 main protease, pH=6.5
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Deposited on : 2023-10-17
Resolution : 1.74 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

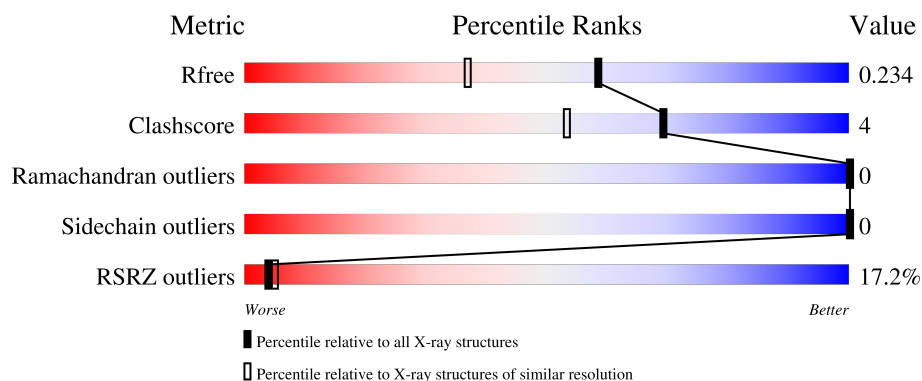
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	295	12% 93% 7%
2	B	299	22% 92% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4617 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	295	Total	C	N	O	S	0	0	0
			2217	1403	378	415	21			

- Molecule 2 is a protein called 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	299	Total	C	N	O	S	0	0	0
			2176	1383	372	402	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	140	LEU	PHE	conflict	UNP P0DTC1
B	141	PHE	LEU	conflict	UNP P0DTC1

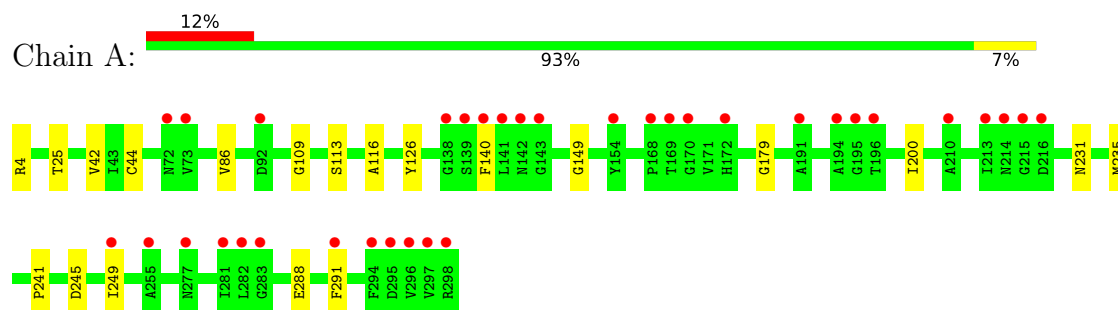
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total	O	0	0
			137	137		
3	B	87	Total	O	0	0
			87	87		

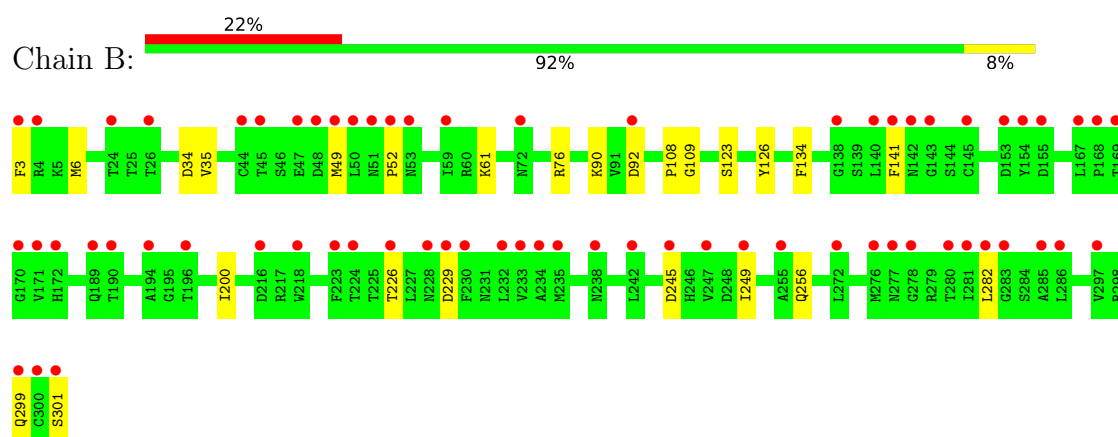
3 Residue-property plots [i](#)

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 2: 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	67.84Å 102.73Å 102.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.49 – 1.74 32.49 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.4 (32.49-1.74) 97.3 (32.49-1.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.209 , 0.233 0.209 , 0.234	Depositor DCC
R_{free} test set	3540 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4617	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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	0.29	0/2266	0.54	0/3089
2	B	0.27	0/2226	0.51	0/3044
All	All	0.28	0/4492	0.52	0/6133

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	2217	0	2113	15	0
2	B	2176	0	2022	20	0
3	A	137	0	0	0	0
3	B	87	0	0	1	0
All	All	4617	0	4135	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:A:25:THR:HG21	1:A:44:CYS:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:THR:HG23	2:B:229:ASP:H	1.61	0.66
1:A:126:TYR:HD2	2:B:6:MET:HE3	1.61	0.64
2:B:245:ASP:O	2:B:249:ILE:HG13	1.97	0.63
2:B:3:PHE:HB2	2:B:282:LEU:HD22	1.84	0.59
1:A:126:TYR:CD2	2:B:6:MET:HE3	2.43	0.53
2:B:108:PRO:HG3	2:B:134:PHE:CE1	2.44	0.53
2:B:61:LYS:NZ	3:B:402:HOH:O	2.41	0.53
1:A:245:ASP:O	1:A:249:ILE:HD13	2.08	0.52
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.92	0.52
2:B:35:VAL:HG22	2:B:90:LYS:HE2	1.91	0.52
2:B:109:GLY:HA2	2:B:200:ILE:HD13	1.93	0.50
2:B:76:ARG:CB	2:B:92:ASP:OD2	2.60	0.50
2:B:226:THR:CG2	2:B:229:ASP:H	2.25	0.49
1:A:25:THR:OG1	1:A:42:VAL:O	2.31	0.47
2:B:256:GLN:OE1	2:B:301:SER:HB3	2.16	0.46
2:B:34:ASP:O	2:B:90:LYS:HD3	2.15	0.46
1:A:86:VAL:HG23	1:A:179:GLY:HA2	1.97	0.46
1:A:116:ALA:HB3	2:B:6:MET:HE1	1.98	0.46
1:A:235:MET:HE2	1:A:241:PRO:HB3	1.98	0.45
1:A:231:ASN:HB3	1:A:235:MET:HE3	1.98	0.45
2:B:123:SER:OG	2:B:141:PHE:HZ	1.99	0.45
2:B:49:MET:HA	2:B:52:PRO:HG3	1.99	0.45
1:A:288:GLU:HG2	1:A:291:PHE:CE1	2.52	0.44
1:A:140:PHE:CD2	2:B:299:GLN:O	2.70	0.44
2:B:34:ASP:OD1	2:B:90:LYS:NZ	2.50	0.43
1:A:140:PHE:CD2	1:A:140:PHE:C	2.97	0.43
2:B:6:MET:HB3	2:B:6:MET:HE2	1.81	0.42
1:A:113:SER:O	1:A:149:GLY:HA2	2.19	0.42
1:A:4:ARG:HD2	2:B:126:TYR:CD2	2.56	0.41

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	293/295 (99%)	285 (97%)	8 (3%)	0	100	100
2	B	297/299 (99%)	292 (98%)	5 (2%)	0	100	100
All	All	590/594 (99%)	577 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	236/254 (93%)	236 (100%)	0	100	100
2	B	220/258 (85%)	220 (100%)	0	100	100
All	All	456/512 (89%)	456 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	228	ASN
1	A	273	GLN
2	B	163	HIS

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 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	295/295 (100%)	0.72	35 (11%)  	21, 30, 49, 65	0
2	B	299/299 (100%)	1.09	67 (22%)  	22, 36, 55, 68	0
All	All	594/594 (100%)	0.90	102 (17%)  	21, 33, 54, 68	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	PHE	6.4
2	B	141	PHE	5.9
1	A	281	ILE	5.8
1	A	297	VAL	5.8
1	A	282	LEU	5.8
2	B	140	LEU	5.4
1	A	141	LEU	4.9
2	B	50	LEU	4.7
2	B	281	ILE	4.6
2	B	3	PHE	4.4
2	B	45	THR	4.2
2	B	234	ALA	4.1
1	A	296	VAL	4.0
2	B	282	LEU	4.0
2	B	300	CYS	3.8
2	B	277	ASN	3.7
2	B	242	LEU	3.6
2	B	286	LEU	3.6
2	B	226	THR	3.4
1	A	72	ASN	3.4
1	A	298	ARG	3.3
2	B	255	ALA	3.3
2	B	168	PRO	3.2
2	B	92	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	51	ASN	3.2
1	A	213	ILE	3.1
2	B	72	ASN	3.1
2	B	172	HIS	3.1
2	B	233	VAL	3.0
2	B	24	THR	3.0
1	A	142	ASN	3.0
2	B	49	MET	3.0
1	A	92	ASP	2.9
1	A	216	ASP	2.9
2	B	245	ASP	2.9
2	B	230	PHE	2.9
2	B	142	ASN	2.9
2	B	189	GLN	2.9
1	A	196	THR	2.8
2	B	224	THR	2.8
2	B	229	ASP	2.8
1	A	154	TYR	2.8
2	B	154	TYR	2.8
1	A	194	ALA	2.8
2	B	278	GLY	2.8
1	A	210	ALA	2.7
2	B	47	GLU	2.7
2	B	228	ASN	2.7
1	A	169	THR	2.7
2	B	285	ALA	2.7
2	B	59	ILE	2.7
1	A	195	GLY	2.7
2	B	283	GLY	2.7
2	B	48	ASP	2.7
2	B	196	THR	2.6
2	B	280	THR	2.6
2	B	44	CYS	2.6
2	B	216	ASP	2.6
2	B	223	PHE	2.6
2	B	190	THR	2.5
1	A	168	PRO	2.5
1	A	143	GLY	2.5
1	A	283	GLY	2.5
2	B	232	LEU	2.5
2	B	247	VAL	2.5
2	B	138	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	171	VAL	2.5
2	B	235	MET	2.5
1	A	295	ASP	2.4
2	B	145	CYS	2.4
2	B	52	PRO	2.4
1	A	214	ASN	2.4
1	A	255	ALA	2.4
2	B	297	VAL	2.4
2	B	153	ASP	2.4
2	B	276	MET	2.4
1	A	215	GLY	2.4
1	A	191	ALA	2.4
2	B	143	GLY	2.3
2	B	238	ASN	2.3
2	B	299	GLN	2.3
1	A	172	HIS	2.3
1	A	277	ASN	2.3
1	A	138	GLY	2.3
2	B	170	GLY	2.3
2	B	169	THR	2.2
1	A	294	PHE	2.2
1	A	249	ILE	2.2
2	B	4	ARG	2.2
2	B	26	THR	2.2
1	A	139	SER	2.2
2	B	301	SER	2.2
1	A	170	GLY	2.2
2	B	249	ILE	2.2
2	B	167	LEU	2.1
2	B	53	ASN	2.1
1	A	73	VAL	2.1
2	B	272	LEU	2.1
1	A	291	PHE	2.1
2	B	194	ALA	2.0
2	B	218	TRP	2.0
2	B	155	ASP	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.