



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:46 PM UTC

PDB ID : 7E6N / pdb_00007e6n
Title : Crystal structure of HCoV-NL63 3C-like protease,pH5.2
Authors : Gao, H.X.; Zhang, Y.T.; Zhou, X.L.; Zhong, F.L.; Li, J.; Zhang, J.
Deposited on : 2021-02-22
Resolution : 1.84 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

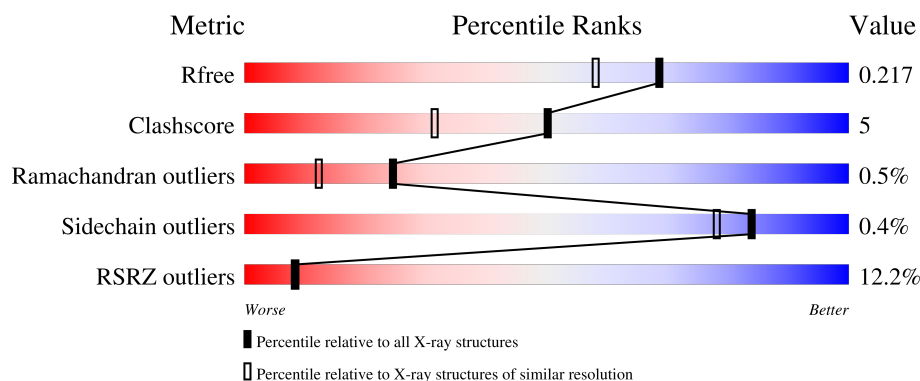
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	303	
1	B	303	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4817 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	299	Total	C	N	O	S	0	0	0
			2251	1427	381	426	17			
1	B	297	Total	C	N	O	S	0	2	0
			2247	1426	380	423	18			

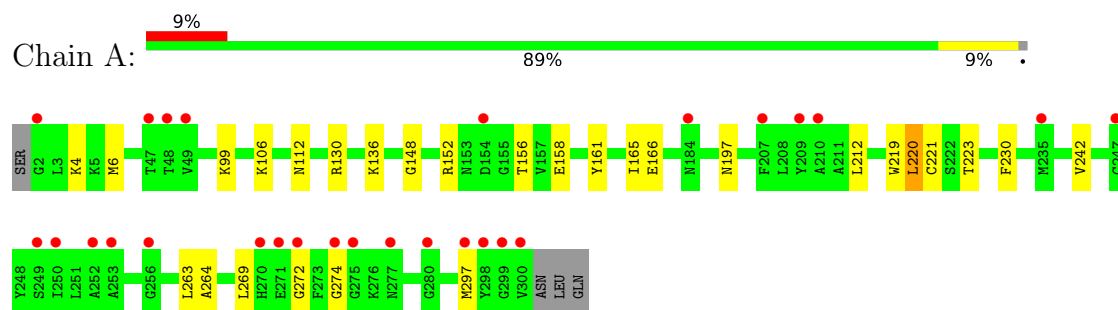
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	170	Total	O	0	0
			170	170		
2	B	149	Total	O	0	0
			149	149		

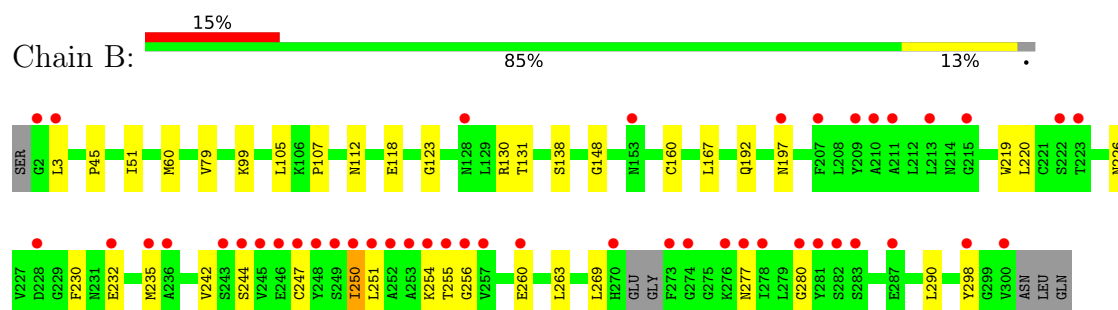
3 Residue-property plots [i](#)

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



• Molecule 1: 3C-like proteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.35Å 83.21Å 64.05Å 90.00° 108.65° 90.00°	Depositor
Resolution (Å)	60.69 – 1.84 60.69 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (60.69-1.84) 99.0 (60.69-1.84)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.184 , 0.217 0.185 , 0.217	Depositor DCC
R_{free} test set	2693 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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	0.32	0/2302	0.55	0/3131
1	B	0.30	0/2303	0.52	0/3131
All	All	0.31	0/4605	0.53	0/6262

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	2251	0	2175	19	0
1	B	2247	0	2178	30	0
2	A	170	0	0	1	0
2	B	149	0	0	2	0
All	All	4817	0	4353	47	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.

All (47) 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:244:SER:OG	1:B:247:CYS:SG	2.47	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:OE1	2:B:401:HOH:O	2.08	0.71
1:B:251:LEU:HD22	1:B:251:LEU:H	1.61	0.63
1:A:223:THR:HG23	1:A:264:ALA:HB1	1.80	0.63
1:B:118:GLU:OE1	2:B:402:HOH:O	2.17	0.59
1:B:45:PRO:HD2	1:B:51:ILE:HD12	1.84	0.59
1:B:250:ILE:HG22	1:B:254:LYS:HE2	1.84	0.59
1:B:219:TRP:HB2	1:B:269:LEU:HD11	1.85	0.58
1:A:106:LYS:NZ	2:A:403:HOH:O	2.35	0.58
1:B:60:MET:HE1	1:B:79:VAL:HB	1.91	0.53
1:B:251:LEU:CD2	1:B:290:LEU:HD11	2.38	0.53
1:A:6:MET:HE3	1:B:123:GLY:HA3	1.92	0.52
1:A:165:ILE:HD12	1:A:166:GLU:H	1.76	0.51
1:B:226:ASN:HA	1:B:260:GLU:HG2	1.94	0.49
1:A:221:CYS:HB3	1:A:223:THR:HG22	1.93	0.49
1:B:254:LYS:HE3	1:B:298:TYR:CE1	2.48	0.49
1:A:219:TRP:HB2	1:A:269:LEU:HD11	1.94	0.48
1:A:242:VAL:HG21	1:A:263:LEU:HD21	1.95	0.48
1:B:251:LEU:HD23	1:B:290:LEU:HD11	1.95	0.48
1:B:99:LYS:HB3	1:B:99:LYS:HE3	1.74	0.47
1:A:136:LYS:HD3	1:A:136:LYS:H	1.79	0.47
1:A:130:ARG:HB3	1:A:197:ASN:OD1	2.16	0.46
1:A:112:ASN:O	1:A:148:GLY:HA2	2.16	0.45
1:A:230:PHE:CE2	1:A:242:VAL:HG23	2.51	0.45
1:B:112:ASN:O	1:B:148:GLY:HA2	2.16	0.45
1:B:235:MET:HE3	1:B:235:MET:HB2	1.68	0.45
1:B:105:LEU:HG	1:B:160[A]:CYS:HB2	1.98	0.45
1:A:4:LYS:HB3	1:B:138:SER:HB2	2.00	0.44
1:B:277:ASN:HD21	1:B:280:GLY:CA	2.30	0.44
1:B:167:LEU:HD22	1:B:192[B]:GLN:HG3	2.00	0.44
1:A:148:GLY:HA3	1:A:161:TYR:HB3	1.99	0.43
1:A:297:MET:HB2	1:A:297:MET:HE2	1.58	0.43
1:B:219:TRP:CD1	1:B:219:TRP:H	2.36	0.43
1:B:230:PHE:CE2	1:B:242:VAL:HG23	2.54	0.43
1:B:130:ARG:HB3	1:B:197:ASN:OD1	2.19	0.43
1:A:99:LYS:HD2	1:A:156:THR:OG1	2.19	0.43
1:A:242:VAL:HG21	1:A:263:LEU:CD2	2.49	0.42
1:B:242:VAL:HG21	1:B:263:LEU:HD21	2.01	0.42
1:B:255:THR:N	1:B:256:GLY:HA2	2.35	0.42
1:B:251:LEU:HD21	1:B:290:LEU:HD11	2.02	0.42
1:B:3:LEU:HD23	1:B:3:LEU:HA	1.94	0.41
1:A:212:LEU:HD21	1:A:220:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HD22	1:B:251:LEU:N	2.33	0.41
1:A:219:TRP:CD1	1:A:219:TRP:H	2.35	0.41
1:B:107:PRO:HB3	1:B:131:THR:HA	2.03	0.41
1:B:277:ASN:HD21	1:B:280:GLY:C	2.28	0.41
1:A:152:ARG:HD3	1:A:158:GLU:OE2	2.21	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	297/303 (98%)	289 (97%)	6 (2%)	2 (1%)	18	7
1	B	295/303 (97%)	286 (97%)	8 (3%)	1 (0%)	36	25
All	All	592/606 (98%)	575 (97%)	14 (2%)	3 (0%)	24	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLY
1	A	274	GLY
1	B	250	ILE

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	247/254 (97%)	246 (100%)	1 (0%)	84	78
1	B	248/254 (98%)	247 (100%)	1 (0%)	84	78
All	All	495/508 (97%)	493 (100%)	2 (0%)	84	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	LEU
1	B	220	LEU

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	63	HIS
1	A	96	HIS
1	A	214	ASN
1	B	270	HIS
1	B	277	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 ⓘ

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	299/303 (98%)	0.41	27 (9%) 15 16	17, 27, 46, 62	0
1	B	297/303 (98%)	0.75	46 (15%) 5 5	16, 31, 57, 69	2 (0%)
All	All	596/606 (98%)	0.58	73 (12%) 8 8	16, 28, 54, 69	2 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	ALA	7.4
1	B	244	SER	6.8
1	B	250	ILE	6.5
1	A	2	GLY	5.9
1	A	250	ILE	5.8
1	B	300	VAL	5.7
1	B	248	TYR	5.7
1	B	255	THR	5.3
1	A	247	CYS	5.3
1	B	2	GLY	5.2
1	B	252	ALA	5.2
1	B	245	VAL	5.0
1	B	251	LEU	4.4
1	B	256	GLY	4.4
1	B	249	SER	4.3
1	A	297	MET	4.2
1	B	247	CYS	4.1
1	A	274	GLY	3.7
1	B	254	LYS	3.5
1	A	298	TYR	3.5
1	A	280	GLY	3.4
1	B	215	GLY	3.4
1	B	270	HIS	3.3
1	A	48	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLY	3.2
1	B	210	ALA	3.1
1	A	256	GLY	3.1
1	B	243	SER	3.0
1	A	210	ALA	3.0
1	B	274	GLY	3.0
1	B	280	GLY	3.0
1	A	207	PHE	3.0
1	A	47	THR	2.9
1	B	246	GLU	2.8
1	B	281	TYR	2.8
1	B	287	GLU	2.7
1	B	298	TYR	2.7
1	B	277	ASN	2.7
1	B	232	GLU	2.6
1	B	223	THR	2.6
1	A	249	SER	2.6
1	A	270	HIS	2.6
1	A	235	MET	2.6
1	A	49	VAL	2.6
1	B	209	TYR	2.6
1	B	228	ASP	2.6
1	B	276	LYS	2.6
1	A	300	VAL	2.6
1	B	278	ILE	2.5
1	B	235	MET	2.5
1	B	222	SER	2.5
1	B	282	SER	2.5
1	B	283	SER	2.4
1	B	257	VAL	2.4
1	B	207	PHE	2.4
1	A	253	ALA	2.3
1	B	128	ASN	2.3
1	B	153	ASN	2.3
1	B	211	ALA	2.3
1	B	273	PHE	2.3
1	A	275	GLY	2.3
1	A	184	ASN	2.2
1	B	213	LEU	2.2
1	B	236	ALA	2.2
1	B	197	ASN	2.2
1	A	271	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	277	ASN	2.1
1	A	209	TYR	2.1
1	B	260	GLU	2.1
1	A	299	GLY	2.1
1	B	3	LEU	2.1
1	A	154	ASP	2.1
1	A	252	ALA	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.