



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 PM UTC

PDB ID : 5ZQG / pdb_00005zqg
Title : Complex structure of PEDV 3CLpro mutant (C144A) with NEMO-231 peptide substrate
Authors : Gang, Y.; Chen, J.Y.; Dang, W.; Xiao, S.B.; Peng, G.Q.
Deposited on : 2018-04-18
Resolution : 1.60 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

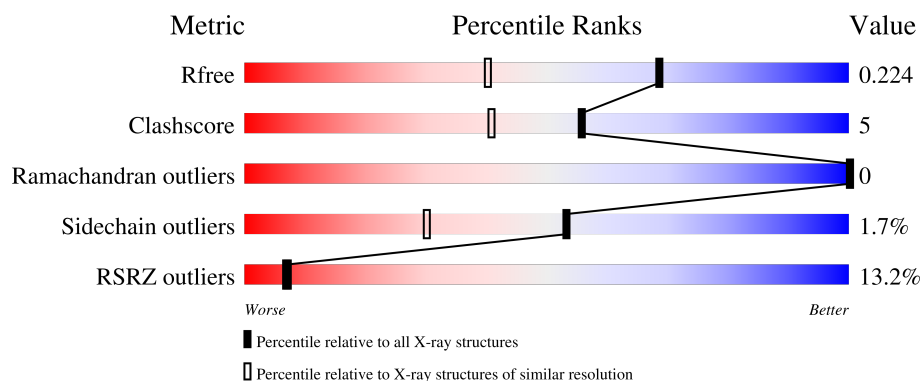
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	308	13% 85% 10% 5%
1	B	308	10% 87% 7% 5%
2	C	11	45% 27% 36% 36%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4880 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 Non-structural protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2230	1411	386	418	15			
1	B	294	Total	C	N	O	S	0	0	0
			2243	1418	388	422	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP R4JK63
A	144	ALA	CYS	engineered mutation	UNP R4JK63
A	300	LEU	-	expression tag	UNP R4JK63
A	301	GLU	-	expression tag	UNP R4JK63
A	302	HIS	-	expression tag	UNP R4JK63
A	303	HIS	-	expression tag	UNP R4JK63
A	304	HIS	-	expression tag	UNP R4JK63
A	305	HIS	-	expression tag	UNP R4JK63
A	306	HIS	-	expression tag	UNP R4JK63
A	307	HIS	-	expression tag	UNP R4JK63
B	0	MET	-	expression tag	UNP R4JK63
B	144	ALA	CYS	engineered mutation	UNP R4JK63
B	300	LEU	-	expression tag	UNP R4JK63
B	301	GLU	-	expression tag	UNP R4JK63
B	302	HIS	-	expression tag	UNP R4JK63
B	303	HIS	-	expression tag	UNP R4JK63
B	304	HIS	-	expression tag	UNP R4JK63
B	305	HIS	-	expression tag	UNP R4JK63
B	306	HIS	-	expression tag	UNP R4JK63
B	307	HIS	-	expression tag	UNP R4JK63

- Molecule 2 is a protein called PEPTIDE LEU-ALA-GLN-LEU-GLN-VAL-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			51	33	9	9			

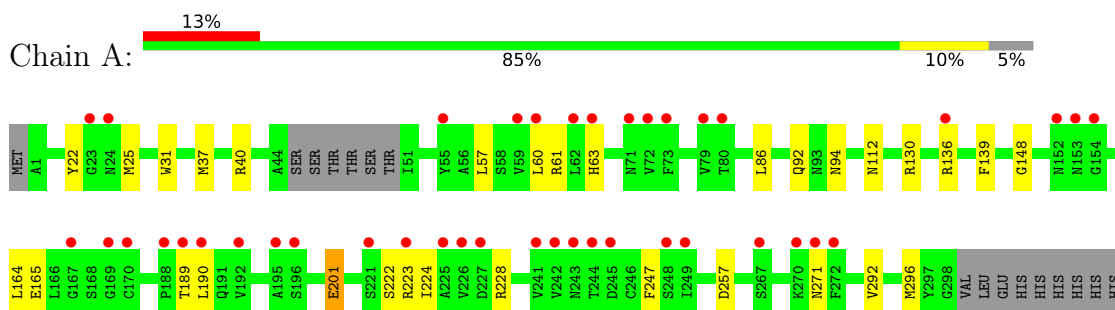
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total	O	0	0
			156	156		
3	B	199	Total	O	0	0
			199	199		
3	C	1	Total	O	0	0
			1	1		

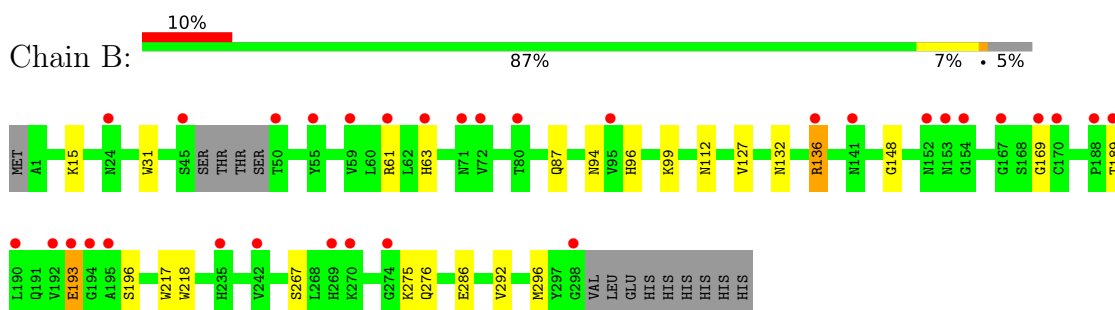
3 Residue-property plots [i](#)

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.

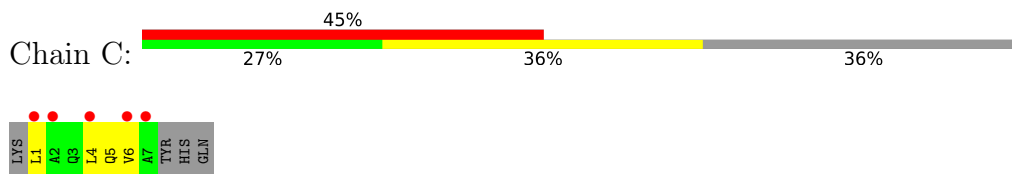
- Molecule 1: Non-structural protein



- Molecule 1: Non-structural protein



- Molecule 2: PEPTIDE LEU-ALA-GLN-LEU-GLN-VAL-ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.58Å 92.43Å 58.03Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	35.56 – 1.60 35.56 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.56-1.60) 99.0 (35.56-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.47 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.194 , 0.224 0.195 , 0.224	Depositor DCC
R_{free} test set	2008 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4880	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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	0.39	0/2275	0.72	0/3087
1	B	0.40	0/2288	0.70	0/3105
2	C	0.39	0/50	0.75	0/67
All	All	0.39	0/4613	0.71	0/6259

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 [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	2230	0	2186	21	0
1	B	2243	0	2198	21	0
2	C	51	0	59	5	0
3	A	156	0	0	2	2
3	B	199	0	0	4	2
3	C	1	0	0	0	0
All	All	4880	0	4443	42	2

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 (42) 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:136:ARG:HD3	1:B:136:ARG:H	1.45	0.81
1:A:139:PHE:HB3	2:C:5:GLN:HE22	1.49	0.77
1:A:92:GLN:OE1	3:A:401:HOH:O	2.05	0.74
1:B:276:GLN:NE2	3:B:405:HOH:O	2.23	0.71
1:B:136:ARG:HH12	1:B:286:GLU:HB3	1.59	0.68
1:B:87:GLN:NE2	3:B:406:HOH:O	2.26	0.67
1:A:164:LEU:HB3	2:C:4:LEU:HD23	1.79	0.64
1:B:136:ARG:HD3	1:B:136:ARG:N	2.12	0.64
1:A:61:ARG:HD2	1:A:63:HIS:CE1	2.34	0.62
1:B:15:LYS:HE3	1:B:96:HIS:HB3	1.84	0.58
1:B:169:GLY:O	3:B:402:HOH:O	2.18	0.55
1:A:201:GLU:HG3	1:A:247:PHE:CZ	2.43	0.53
1:A:139:PHE:CB	2:C:5:GLN:HE22	2.22	0.51
1:A:61:ARG:HD2	1:A:63:HIS:HE1	1.76	0.51
1:A:165:GLU:HB2	2:C:5:GLN:OE1	2.12	0.49
1:B:136:ARG:H	1:B:136:ARG:CD	2.19	0.49
1:A:292:VAL:O	1:A:296:MET:HG2	2.13	0.49
1:A:22:TYR:CZ	1:A:60:LEU:HD22	2.48	0.48
1:A:112:ASN:O	1:A:148:GLY:HA2	2.14	0.48
1:B:112:ASN:O	1:B:148:GLY:HA2	2.15	0.47
1:A:223:ARG:NH2	1:A:257:ASP:OD2	2.29	0.46
1:B:31:TRP:CE2	1:B:94:ASN:HB2	2.50	0.46
1:A:201:GLU:HG3	1:A:247:PHE:HZ	1.81	0.46
1:B:136:ARG:HH22	1:B:286:GLU:HB2	1.80	0.46
1:A:130:ARG:NH1	1:A:136:ARG:HB2	2.32	0.45
1:B:61:ARG:HH21	1:B:63:HIS:CE1	2.35	0.45
1:B:132:ASN:ND2	1:B:196:SER:HB3	2.31	0.45
1:B:217:TRP:CD2	1:B:275:LYS:HD3	2.51	0.45
1:A:25:MET:HB3	2:C:6:VAL:HG21	1.97	0.44
1:B:127:VAL:HA	1:B:136:ARG:HH21	1.83	0.44
1:A:40:ARG:HA	1:A:86:LEU:HG	1.99	0.44
1:A:224:ILE:HD11	1:A:228:ARG:HG3	2.00	0.43
1:A:57:LEU:HA	1:A:60:LEU:HG	2.00	0.43
1:B:267:SER:OG	3:B:401:HOH:O	2.12	0.43
1:A:31:TRP:CE2	1:A:94:ASN:HB2	2.54	0.43
1:B:61:ARG:HD2	1:B:63:HIS:NE2	2.34	0.42
1:B:193:GLU:H	1:B:193:GLU:HG3	1.38	0.42
1:B:292:VAL:O	1:B:296:MET:HG2	2.20	0.42
1:B:136:ARG:HH12	1:B:286:GLU:CB	2.32	0.41
1:A:37:MET:HG2	3:A:501:HOH:O	2.19	0.41
1:B:218:TRP:CD1	1:B:218:TRP:H	2.38	0.40
1:A:189:THR:HG22	1:A:190:LEU:N	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:401:HOH:O	3:B:477:HOH:O[1_655]	1.97	0.23
3:A:502:HOH:O	3:B:401:HOH:O[1_655]	2.15	0.05

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	288/308 (94%)	283 (98%)	5 (2%)	0	100	100
1	B	290/308 (94%)	285 (98%)	5 (2%)	0	100	100
2	C	5/11 (46%)	4 (80%)	1 (20%)	0	100	100
All	All	583/627 (93%)	572 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	238/254 (94%)	235 (99%)	3 (1%)	61	40
1	B	240/254 (94%)	236 (98%)	4 (2%)	53	30
2	C	5/9 (56%)	4 (80%)	1 (20%)	1	0
All	All	483/517 (93%)	475 (98%)	8 (2%)	53	30

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	GLU
1	A	222	SER
1	A	271	ASN
1	B	99	LYS
1	B	136	ARG
1	B	189	THR
1	B	193	GLU
2	C	1	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	92	GLN
1	B	87	GLN
1	B	243	ASN
1	B	276	GLN
2	C	5	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 ⓘ

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	292/308 (94%)	0.72	41 (14%) 6 6	7, 17, 34, 43	0
1	B	294/308 (95%)	0.51	32 (10%) 10 10	7, 15, 30, 41	1 (0%)
2	C	7/11 (63%)	2.94	5 (71%) 0 0	25, 30, 36, 44	0
All	All	593/627 (94%)	0.64	78 (13%) 7 7	7, 16, 33, 44	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	LEU	5.2
1	A	242	VAL	4.9
1	A	189	THR	4.8
1	A	243	ASN	4.8
2	C	1	LEU	4.7
1	A	153	ASN	4.6
1	B	50	THR	4.3
1	A	63	HIS	4.2
1	A	271	ASN	4.1
1	B	170	CYS	4.0
1	B	188	PRO	3.9
1	A	167	GLY	3.9
1	A	272	PHE	3.7
1	B	167	GLY	3.7
1	B	136	ARG	3.6
1	B	189	THR	3.6
1	B	72	VAL	3.6
1	A	221	SER	3.6
1	A	60	LEU	3.6
1	A	227	ASP	3.5
2	C	6	VAL	3.5
1	B	269	HIS	3.5
1	B	153	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	4	LEU	3.3
2	C	2	ALA	3.3
1	A	267	SER	3.2
1	A	244	THR	3.2
1	A	195	ALA	3.1
1	B	235	HIS	3.1
1	B	169	GLY	3.0
1	B	80	THR	3.0
1	A	71	ASN	3.0
1	B	195	ALA	2.9
1	A	80	THR	2.9
1	A	241	VAL	2.9
1	B	61	ARG	2.8
1	A	190	LEU	2.8
1	A	270	LYS	2.8
1	B	63	HIS	2.8
1	A	192	VAL	2.7
1	A	24	ASN	2.7
2	C	7	ALA	2.6
1	A	249	ILE	2.6
1	B	45	SER	2.6
1	B	270	LYS	2.5
1	B	24	ASN	2.5
1	A	154	GLY	2.5
1	B	192	VAL	2.5
1	A	226	VAL	2.5
1	B	59	VAL	2.5
1	A	73	PHE	2.4
1	A	225	ALA	2.4
1	A	59	VAL	2.4
1	A	72	VAL	2.4
1	B	193	GLU	2.4
1	B	152	ASN	2.4
1	B	242	VAL	2.4
1	A	196	SER	2.3
1	A	245	ASP	2.3
1	B	71	ASN	2.3
1	A	223	ARG	2.3
1	B	154	GLY	2.3
1	A	152	ASN	2.3
1	B	141	ASN	2.3
1	A	55	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	274	GLY	2.3
1	A	62	LEU	2.2
1	A	79	VAL	2.2
1	A	248	SER	2.2
1	A	170	CYS	2.2
1	B	194	GLY	2.2
1	B	298	GLY	2.2
1	A	23	GLY	2.1
1	A	136	ARG	2.1
1	A	188	PRO	2.1
1	A	169	GLY	2.1
1	B	95	VAL	2.1
1	B	55	TYR	2.1

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.