



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2025 – 12:32 PM EST

PDB ID : 9YHI / pdb\_00009yhi  
Title : Crystal structure of Chikungunya virus nsP3 macrodomain N24A mutant (P31 crystal form)  
Authors : Correy, G.J.; Fraser, J.S.  
Deposited on : 2025-09-30  
Resolution : 1.43 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](mailto: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>.

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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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

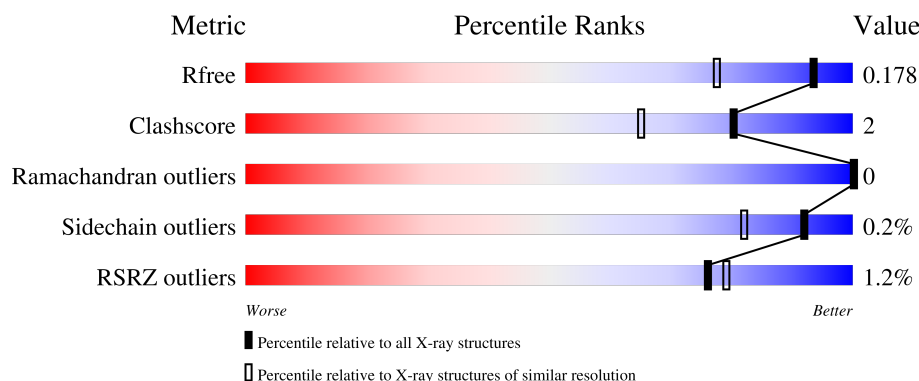
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.43 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))
$R_{free}$	164625	2809 (1.46-1.42)
Clashscore	180529	3008 (1.46-1.42)
Ramachandran outliers	177936	2971 (1.46-1.42)
Sidechain outliers	177891	2971 (1.46-1.42)
RSRZ outliers	164620	2809 (1.46-1.42)

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  $\geq 3$ , 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	168	
1	B	168	
1	C	168	
1	D	168	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	202[B]	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10837 atoms, of which 5036 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 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	160	Total	C	H	N	O	S	0	10	0
			2576	802	1284	230	252	8			
1	B	160	Total	C	H	N	O	S	0	5	0
			2517	788	1258	219	244	8			
1	C	162	Total	C	H	N	O	S	0	3	0
			2508	786	1247	223	244	8			
1	D	160	Total	C	H	N	O	S	0	5	0
			2498	780	1247	221	242	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q8JUX6
A	-6	LYS	-	expression tag	UNP Q8JUX6
A	-5	HIS	-	expression tag	UNP Q8JUX6
A	-4	HIS	-	expression tag	UNP Q8JUX6
A	-3	HIS	-	expression tag	UNP Q8JUX6
A	-2	HIS	-	expression tag	UNP Q8JUX6
A	-1	HIS	-	expression tag	UNP Q8JUX6
A	0	HIS	-	expression tag	UNP Q8JUX6
A	24	ALA	ASN	engineered mutation	UNP Q8JUX6
B	-7	MET	-	initiating methionine	UNP Q8JUX6
B	-6	LYS	-	expression tag	UNP Q8JUX6
B	-5	HIS	-	expression tag	UNP Q8JUX6
B	-4	HIS	-	expression tag	UNP Q8JUX6
B	-3	HIS	-	expression tag	UNP Q8JUX6
B	-2	HIS	-	expression tag	UNP Q8JUX6
B	-1	HIS	-	expression tag	UNP Q8JUX6
B	0	HIS	-	expression tag	UNP Q8JUX6
B	24	ALA	ASN	engineered mutation	UNP Q8JUX6
C	-7	MET	-	initiating methionine	UNP Q8JUX6
C	-6	LYS	-	expression tag	UNP Q8JUX6
C	-5	HIS	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP Q8JUX6
C	-3	HIS	-	expression tag	UNP Q8JUX6
C	-2	HIS	-	expression tag	UNP Q8JUX6
C	-1	HIS	-	expression tag	UNP Q8JUX6
C	0	HIS	-	expression tag	UNP Q8JUX6
C	24	ALA	ASN	engineered mutation	UNP Q8JUX6
D	-7	MET	-	initiating methionine	UNP Q8JUX6
D	-6	LYS	-	expression tag	UNP Q8JUX6
D	-5	HIS	-	expression tag	UNP Q8JUX6
D	-4	HIS	-	expression tag	UNP Q8JUX6
D	-3	HIS	-	expression tag	UNP Q8JUX6
D	-2	HIS	-	expression tag	UNP Q8JUX6
D	-1	HIS	-	expression tag	UNP Q8JUX6
D	0	HIS	-	expression tag	UNP Q8JUX6
D	24	ALA	ASN	engineered mutation	UNP Q8JUX6

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	2	Total Cl 2 2	0	1
2	C	2	Total Cl 2 2	0	0
2	D	2	Total Cl 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	207	Total O 208 208	0	5
3	B	166	Total O 166 166	0	1
3	C	199	Total O 200 200	0	3
3	D	156	Total O 157 157	0	2

### 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 3

Chain A: 



- Molecule 1: Non-structural protein 3

Chain B: 



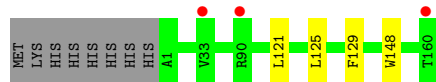
- Molecule 1: Non-structural protein 3

Chain C: 



- Molecule 1: Non-structural protein 3

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.82Å 87.82Å 85.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.06 – 1.43 39.06 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.06-1.43) 99.9 (39.06-1.43)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 1.43Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.136 , 0.177 0.141 , 0.178	Depositor DCC
$R_{free}$ test set	7016 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.027 for h,-h-k,-l 0.013 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9107e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
CL

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	0.30	0/1333	0.49	0/1803
1	B	0.28	0/1282	0.44	0/1737
1	C	0.32	0/1297	0.50	0/1757
1	D	0.33	0/1294	0.50	0/1753
All	All	0.31	0/5206	0.48	0/7050

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	1292	1284	1260	7	1
1	B	1259	1258	1256	9	0
1	C	1261	1247	1241	5	0
1	D	1251	1247	1234	4	0
2	A	1	0	0	0	0
2	B	2	0	0	2	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	208	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	166	0	0	0	0
3	C	200	0	0	2	0
3	D	157	0	0	0	0
All	All	5801	5036	4991	25	1

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 2.

All (25) 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:133:ASP:OD2	1:A:159[A]:ARG:NH2	2.26	0.69
1:B:114:TYR:HD2	2:B:202[B]:CL:CL	2.14	0.68
1:A:80[A]:GLU:OE1	1:A:83:ARG:NH1	2.39	0.56
1:B:31:ASP:OD2	1:B:113:VAL:HG11	2.06	0.55
1:D:121:LEU:C	1:D:121:LEU:HD23	2.32	0.55
1:A:121:LEU:C	1:A:121:LEU:HD23	2.36	0.51
1:B:121[A]:LEU:C	1:B:121[A]:LEU:HD23	2.38	0.49
1:B:121[A]:LEU:HD12	1:B:148:TRP:CG	2.49	0.48
1:D:125:LEU:HG	1:D:129:PHE:CE2	2.49	0.47
1:C:121:LEU:C	1:C:121:LEU:HD23	2.41	0.46
1:C:15:ASP:O	1:C:15:ASP:CG	2.59	0.46
1:B:114:TYR:CD2	2:B:202[B]:CL:CL	3.03	0.44
1:B:125[A]:LEU:HG	1:B:129:PHE:CE2	2.52	0.44
1:B:108[B]:LEU:HB3	1:B:111[B]:THR:HG21	2.00	0.44
1:C:44:SER:HB3	1:C:60:CYS:SG	2.58	0.43
1:A:121:LEU:HD12	1:A:148:TRP:CG	2.53	0.43
1:C:159:ARG:HD3	3:C:417:HOH:O	2.18	0.42
1:D:121:LEU:HD23	1:D:121:LEU:O	2.20	0.42
1:B:55:ALA:HA	1:B:67:HIS:O	2.20	0.41
1:C:7:LYS:HE2	1:C:9:MET:SD	2.59	0.41
1:A:13:LYS:HE3	3:C:391:HOH:O	2.21	0.41
1:B:109:LEU:O	1:B:111[B]:THR:HG23	2.20	0.41
1:A:55:ALA:HA	1:A:67:HIS:O	2.21	0.40
1:D:121:LEU:HD12	1:D:148:TRP:CG	2.56	0.40
1:A:128:LEU:C	1:A:128:LEU:HD23	2.47	0.40

All (1) 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)
1:A:75:ASN:OD1	1:A:90[B]:ARG:HH22[3_554]	1.59	0.01

## 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	168/168 (100%)	167 (99%)	1 (1%)	0	100	100
1	B	163/168 (97%)	161 (99%)	2 (1%)	0	100	100
1	C	163/168 (97%)	162 (99%)	1 (1%)	0	100	100
1	D	163/168 (97%)	162 (99%)	1 (1%)	0	100	100
All	All	657/672 (98%)	652 (99%)	5 (1%)	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	141/140 (101%)	141 (100%)	0	100	100
1	B	136/140 (97%)	136 (100%)	0	100	100
1	C	137/140 (98%)	136 (99%)	1 (1%)	81	61
1	D	137/140 (98%)	137 (100%)	0	100	100
All	All	551/560 (98%)	550 (100%)	1 (0%)	92	82

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

Mol	Chain	Res	Type
1	C	146	LYS

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

Mol	Chain	Res	Type
1	C	0	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	160/168 (95%)	-0.51	0 <b>100</b> <b>100</b>	10, 25, 45, 66	7 (4%)
1	B	160/168 (95%)	-0.34	4 (2%) 58 59	17, 29, 64, 96	5 (3%)
1	C	162/168 (96%)	-0.47	1 (0%) 85 88	12, 27, 47, 72	2 (1%)
1	D	160/168 (95%)	-0.33	3 (1%) 66 68	11, 27, 52, 75	3 (1%)
All	All	642/672 (95%)	-0.41	8 (1%) 76 79	10, 27, 53, 96	17 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	MET	3.3
1	D	160	THR	3.3
1	B	1	ALA	3.2
1	B	146	LYS	2.8
1	B	160	THR	2.5
1	C	160	THR	2.2
1	D	33	VAL	2.1
1	D	90[A]	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	B	202[B]	1/1	0.93	0.18	39,39,39,39	1
2	CL	C	202	1/1	0.96	0.08	47,47,47,47	0
2	CL	D	202	1/1	0.98	0.07	44,44,44,44	0
2	CL	B	201	1/1	0.99	0.08	52,52,52,52	0
2	CL	D	201	1/1	0.99	0.04	39,39,39,39	1
2	CL	A	201	1/1	0.99	0.07	38,38,38,38	0
2	CL	C	201	1/1	1.00	0.04	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.