



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2021 – 06:18 AM EDT

PDB ID : 7MPM  
Title : Bartonella henselae NrnC bound to pAA  
Authors : Lormand, J.D.; Sondermann, H.  
Deposited on : 2021-05-04  
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

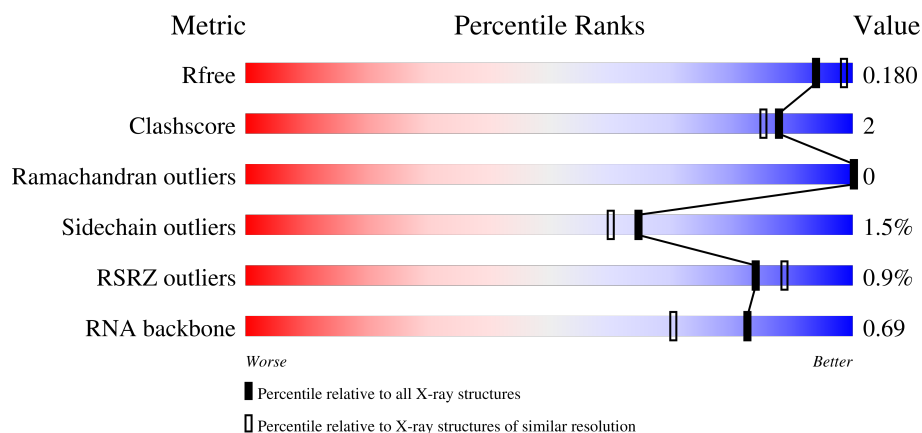
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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.



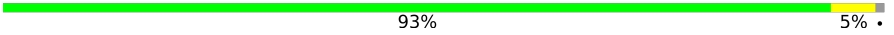
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)
RNA backbone	3102	1124 (2.50-1.42)

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	207	<div> <div>94%</div> <div>5%</div> </div>
1	C	207	<div> <div>%</div> <div>96%</div> <div>..</div> </div>
1	E	207	<div> <div>94%</div> <div>..</div> </div>
1	G	207	<div> <div>95%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	207	 93% 5% .
1	K	207	 96% . .
1	M	207	 2% 94% 5% .
1	O	207	 2% 95% . .
2	B	2	 50% 50%
2	D	2	 50% 50%
2	F	2	 50% 50%
2	H	2	 50% 50%
2	J	2	 50% 50%
2	L	2	 50% 50%
2	N	2	 50% 50%
2	P	2	 50% 50%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15812 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 NanoRNase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	8	0
			1676	1054	295	321	6			
1	C	205	Total	C	N	O	S	0	8	0
			1679	1057	298	317	7			
1	E	205	Total	C	N	O	S	0	4	0
			1658	1043	297	312	6			
1	G	205	Total	C	N	O	S	0	4	0
			1654	1040	293	315	6			
1	I	204	Total	C	N	O	S	0	2	0
			1637	1030	293	308	6			
1	K	205	Total	C	N	O	S	0	2	0
			1638	1031	290	311	6			
1	M	204	Total	C	N	O	S	0	3	0
			1646	1036	295	309	6			
1	O	204	Total	C	N	O	S	0	2	0
			1634	1028	291	309	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP X5MEI1
C	0	SER	-	expression tag	UNP X5MEI1
E	0	SER	-	expression tag	UNP X5MEI1
G	0	SER	-	expression tag	UNP X5MEI1
I	0	SER	-	expression tag	UNP X5MEI1
K	0	SER	-	expression tag	UNP X5MEI1
M	0	SER	-	expression tag	UNP X5MEI1
O	0	SER	-	expression tag	UNP X5MEI1

- Molecule 2 is a RNA chain called 5'-phosphorylated AA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	P	0	1	0
			68	30	15	20	3			
2	D	2	Total	C	N	O	P	0	1	0
			68	30	15	20	3			
2	F	2	Total	C	N	O	P	0	1	0
			68	30	15	20	3			
2	H	2	Total	C	N	O	P	0	1	0
			68	30	15	20	3			
2	J	2	Total	C	N	O	P	0	1	0
			68	30	15	20	3			
2	L	2	Total	C	N	O	P	0	1	0
			68	30	15	20	3			
2	N	2	Total	C	N	O	P	0	1	0
			68	30	15	20	3			
2	P	2	Total	C	N	O	P	0	1	0
			68	30	15	20	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	290	Total	O	0	1
			291	291		
3	B	9	Total	O	0	0
			9	9		
3	C	275	Total	O	0	0
			275	275		
3	D	9	Total	O	0	0
			9	9		
3	E	257	Total	O	0	0
			257	257		
3	F	6	Total	O	0	0
			6	6		
3	G	271	Total	O	0	1
			272	272		
3	H	9	Total	O	0	0
			9	9		
3	I	251	Total	O	0	1
			252	252		
3	J	7	Total	O	0	0
			7	7		
3	K	262	Total	O	0	0
			262	262		
3	L	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	199	Total 199	O 199	0	0
3	N	8	Total 8	O 8	0	0
3	O	174	Total 174	O 174	0	0
3	P	7	Total 7	O 7	0	0

### 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.

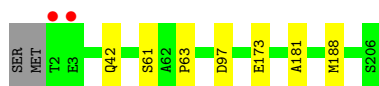
- Molecule 1: NanoRNase C

Chain A: 

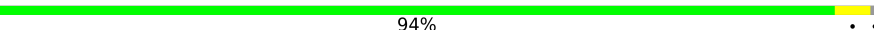


- Molecule 1: NanoRNase C

Chain C: 



- Molecule 1: NanoRNase C

Chain E: 



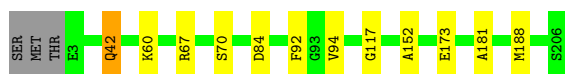
- Molecule 1: NanoRNase C

Chain G: 



- Molecule 1: NanoRNase C

Chain I: 



- Molecule 1: NanoRNase C

Chain K:  96% ..



- Molecule 1: NanoRNase C

Chain M:  94% 5% ..



- Molecule 1: NanoRNase C

Chain O:  95% ..



- Molecule 2: 5'-phosphorylated AA

Chain B:  50% 50%



- Molecule 2: 5'-phosphorylated AA

Chain D:  50% 50%



- Molecule 2: 5'-phosphorylated AA

Chain F:  50% 50%



- Molecule 2: 5'-phosphorylated AA

Chain H:  50% 50%



- Molecule 2: 5'-phosphorylated AA

Chain J:  50% 50%



A603  
A604

- Molecule 2: 5'-phosphorylated AA

Chain L:  50% 50%

A603  
A604

- Molecule 2: 5'-phosphorylated AA

Chain N:  50% 50%

A603  
A604

- Molecule 2: 5'-phosphorylated AA

Chain P:  50% 50%

A603  
A604

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.78Å 127.47Å 128.59Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	43.48 – 1.95 49.72 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.48-1.95) 96.5 (49.72-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.145 , 0.180 0.146 , 0.180	Depositor DCC
$R_{free}$ test set	2000 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 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	0.37	0/1728	0.53	0/2335
1	C	0.38	0/1731	0.54	0/2337
1	E	0.36	0/1698	0.52	0/2293
1	G	0.37	0/1694	0.54	0/2289
1	I	0.35	0/1671	0.52	0/2257
1	K	0.34	0/1672	0.53	0/2260
1	M	0.32	0/1683	0.49	0/2272
1	O	0.32	0/1668	0.50	0/2253
2	B	1.69	2/76 (2.6%)	0.88	0/113
2	D	1.80	2/76 (2.6%)	1.01	0/113
2	F	1.84	2/76 (2.6%)	1.13	0/113
2	H	1.77	2/76 (2.6%)	0.78	0/113
2	J	1.74	2/76 (2.6%)	0.75	0/113
2	L	1.79	2/76 (2.6%)	0.88	0/113
2	N	1.81	2/76 (2.6%)	0.83	0/113
2	P	1.81	2/76 (2.6%)	1.25	0/113
All	All	0.51	16/14153 (0.1%)	0.55	0/19200

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	603[A]	A	OP3-P	-10.80	1.48	1.61
2	F	603[B]	A	OP3-P	-10.80	1.48	1.61
2	N	603[A]	A	OP3-P	-10.69	1.48	1.61
2	N	603[B]	A	OP3-P	-10.69	1.48	1.61
2	L	603[A]	A	OP3-P	-10.66	1.48	1.61

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	1676	0	1678	9	0
1	C	1679	0	1689	4	0
1	E	1658	0	1664	9	0
1	G	1654	0	1651	4	0
1	I	1637	0	1638	8	0
1	K	1638	0	1632	5	0
1	M	1646	0	1651	9	0
1	O	1634	0	1633	5	0
2	B	68	0	34	3	0
2	D	68	0	34	2	0
2	F	68	0	34	1	0
2	H	68	0	34	1	0
2	J	68	0	34	2	0
2	L	68	0	34	0	0
2	N	68	0	34	5	0
2	P	68	0	34	3	0
3	A	291	0	0	4	0
3	B	9	0	0	2	0
3	C	275	0	0	0	0
3	D	9	0	0	2	0
3	E	257	0	0	6	0
3	F	6	0	0	1	0
3	G	272	0	0	2	0
3	H	9	0	0	1	0
3	I	252	0	0	3	0
3	J	7	0	0	1	0
3	K	262	0	0	1	0
3	L	9	0	0	0	0
3	M	199	0	0	2	0
3	N	8	0	0	1	0
3	O	174	0	0	1	0
3	P	7	0	0	2	0
All	All	15812	0	13508	54	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 2.

The worst 5 of 54 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:C:188[B]:MET:HE1	1:K:178:VAL:HG22	1.58	0.83
1:E:184[B]:GLN:NE2	3:E:305:HOH:O	2.28	0.67
1:E:181:ALA:HB3	1:M:188:MET:HG2	1.76	0.65
1:I:67:ARG:NH2	3:I:303:HOH:O	2.31	0.62
1:C:181:ALA:HB3	1:K:188:MET:HG2	1.84	0.60

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	212/207 (102%)	211 (100%)	1 (0%)	0	100	100
1	C	211/207 (102%)	210 (100%)	1 (0%)	0	100	100
1	E	207/207 (100%)	206 (100%)	1 (0%)	0	100	100
1	G	207/207 (100%)	206 (100%)	1 (0%)	0	100	100
1	I	204/207 (99%)	203 (100%)	1 (0%)	0	100	100
1	K	205/207 (99%)	204 (100%)	1 (0%)	0	100	100
1	M	205/207 (99%)	204 (100%)	1 (0%)	0	100	100
1	O	204/207 (99%)	203 (100%)	1 (0%)	0	100	100
All	All	1655/1656 (100%)	1647 (100%)	8 (0%)	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	186/180 (103%)	184 (99%)	2 (1%)	73	71
1	C	186/180 (103%)	183 (98%)	3 (2%)	62	58
1	E	182/180 (101%)	180 (99%)	2 (1%)	73	71
1	G	182/180 (101%)	178 (98%)	4 (2%)	52	44
1	I	179/180 (99%)	176 (98%)	3 (2%)	60	55
1	K	179/180 (99%)	177 (99%)	2 (1%)	73	71
1	M	180/180 (100%)	178 (99%)	2 (1%)	73	71
1	O	179/180 (99%)	176 (98%)	3 (2%)	60	55
All	All	1453/1440 (101%)	1432 (99%)	21 (1%)	65	62

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	42	GLN
1	M	173	GLU
1	O	173	GLU
1	O	42	GLN
1	M	42	GLN

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

Mol	Chain	Res	Type
1	M	16	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	1/2 (50%)	0	0
2	D	1/2 (50%)	0	0
2	F	1/2 (50%)	0	0
2	H	1/2 (50%)	0	0
2	J	1/2 (50%)	0	0
2	L	1/2 (50%)	0	0
2	N	1/2 (50%)	0	0
2	P	1/2 (50%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8/16 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 monosaccharides 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, 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	206/207 (99%)	-0.34	1 (0%) 91 94	16, 23, 40, 73	0
1	C	205/207 (99%)	-0.31	2 (0%) 82 87	17, 23, 39, 77	0
1	E	205/207 (99%)	-0.33	1 (0%) 91 94	19, 26, 43, 61	0
1	G	205/207 (99%)	-0.35	1 (0%) 91 94	17, 25, 40, 51	0
1	I	204/207 (98%)	-0.41	0 100 100	19, 26, 42, 51	0
1	K	205/207 (99%)	-0.36	1 (0%) 91 94	18, 27, 42, 60	0
1	M	204/207 (98%)	-0.11	5 (2%) 57 66	20, 34, 54, 76	0
1	O	204/207 (98%)	-0.07	4 (1%) 65 73	21, 34, 54, 68	0
2	B	2/2 (100%)	-0.62	0 100 100	26, 26, 26, 30	0
2	D	2/2 (100%)	-0.60	0 100 100	25, 25, 25, 31	0
2	F	2/2 (100%)	-0.66	0 100 100	29, 29, 29, 30	0
2	H	2/2 (100%)	-0.70	0 100 100	25, 25, 25, 31	0
2	J	2/2 (100%)	-0.70	0 100 100	28, 28, 28, 31	0
2	L	2/2 (100%)	-0.66	0 100 100	29, 29, 29, 31	0
2	N	2/2 (100%)	-0.55	0 100 100	29, 29, 29, 36	0
2	P	2/2 (100%)	-0.56	0 100 100	32, 32, 32, 34	0
All	All	1654/1672 (98%)	-0.29	15 (0%) 84 89	16, 27, 46, 77	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.1
1	C	3	GLU	3.4
1	E	2	THR	3.2
1	A	1	MET	3.1
1	O	15	ASP	3.0



## 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 monosaccharides 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.