



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:08 pm BST

PDB ID : 3K8V  
Title : Crysatl structure of a bacterial cell-surface flagellin N20C20  
Authors : Maruyama, Y.; Momma, M.; Hashimoto, W.; Murata, K.  
Deposited on : 2009-10-15  
Resolution : 2.10 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.

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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	:	2.11
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)	:	2.11

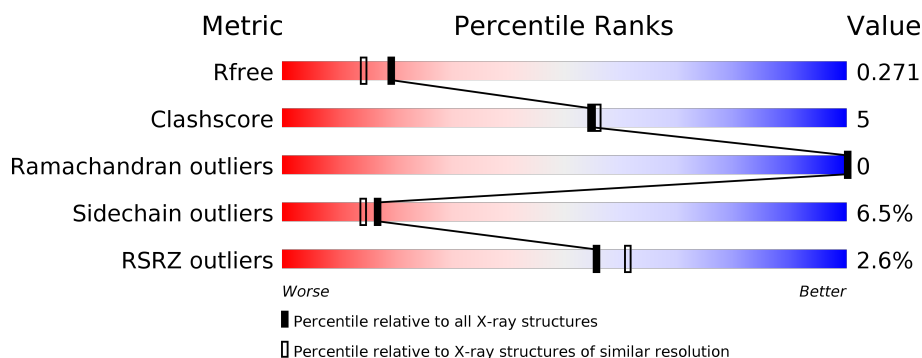
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	351	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>8%</div> </div> </div>
1	B	351	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4980 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 Flagellin homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	1	0
			2354	1410	428	512	4			
1	B	320	Total	C	N	O	S	0	1	0
			2327	1394	426	503	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	LEU	-	EXPRESSION TAG	UNP Q2PHB2
A	365	GLU	-	EXPRESSION TAG	UNP Q2PHB2
A	366	HIS	-	EXPRESSION TAG	UNP Q2PHB2
A	367	HIS	-	EXPRESSION TAG	UNP Q2PHB2
A	368	HIS	-	EXPRESSION TAG	UNP Q2PHB2
A	369	HIS	-	EXPRESSION TAG	UNP Q2PHB2
A	370	HIS	-	EXPRESSION TAG	UNP Q2PHB2
A	371	HIS	-	EXPRESSION TAG	UNP Q2PHB2
B	364	LEU	-	EXPRESSION TAG	UNP Q2PHB2
B	365	GLU	-	EXPRESSION TAG	UNP Q2PHB2
B	366	HIS	-	EXPRESSION TAG	UNP Q2PHB2
B	367	HIS	-	EXPRESSION TAG	UNP Q2PHB2
B	368	HIS	-	EXPRESSION TAG	UNP Q2PHB2
B	369	HIS	-	EXPRESSION TAG	UNP Q2PHB2
B	370	HIS	-	EXPRESSION TAG	UNP Q2PHB2
B	371	HIS	-	EXPRESSION TAG	UNP Q2PHB2

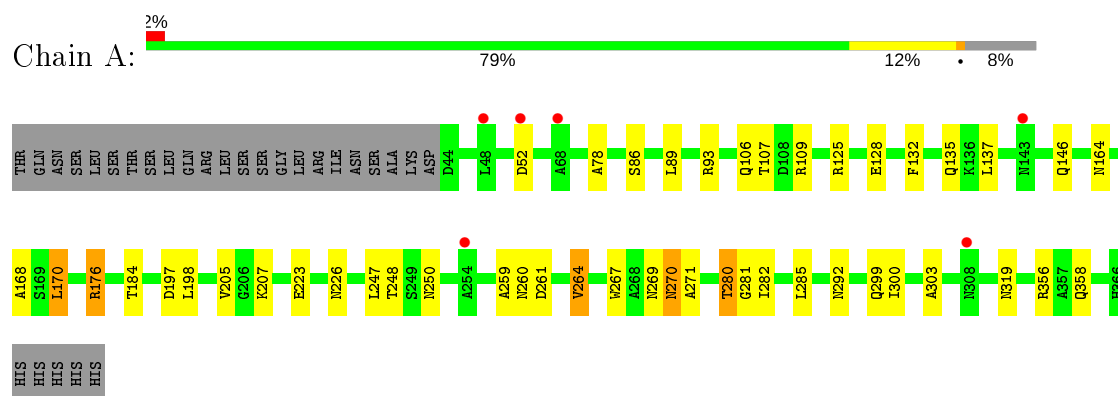
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		
2	B	139	Total	O	0	0
			139	139		

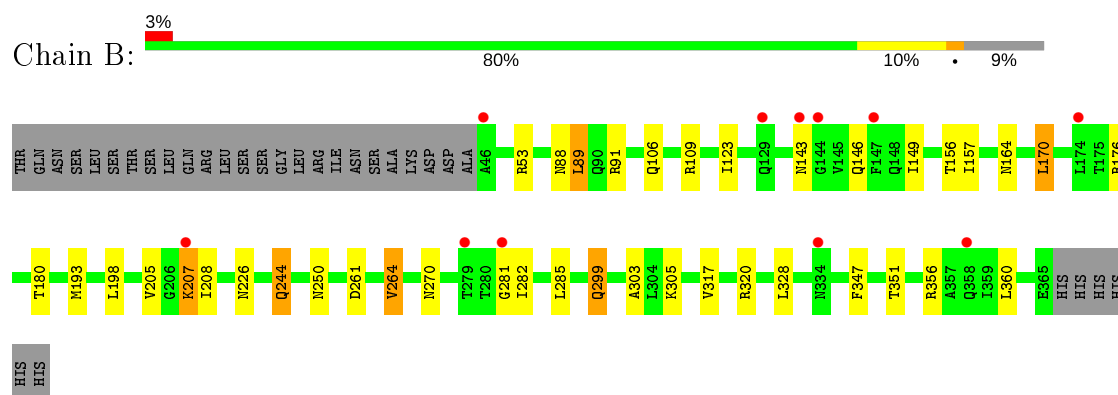
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Flagellin homolog



#### • Molecule 1: Flagellin homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.68Å 52.62Å 64.83Å 100.32° 109.54° 111.62°	Depositor
Resolution (Å)	29.58 – 2.10 29.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.58-2.10) 95.7 (29.58-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.212 , 0.268 0.212 , 0.271	Depositor DCC
$R_{free}$ test set	1614 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 19.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.457 for k,h,-h-k-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4980	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.68% 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 [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	0.40	0/2370	0.54	0/3220
1	B	0.40	0/2339	0.55	0/3177
All	All	0.40	0/4709	0.55	0/6397

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	2354	0	2309	26	0
1	B	2327	0	2294	22	0
2	A	160	0	0	2	0
2	B	139	0	0	1	0
All	All	4980	0	4603	48	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 (48) 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:282:ILE:HA	1:B:285:LEU:HD23	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:O	1:A:281:GLY:HA2	1.82	0.80
1:A:260:ASN:HD22	1:A:269:ASN:H	1.31	0.76
1:B:106:GLN:HE22	1:B:226:ASN:HD22	1.34	0.75
1:B:282:ILE:CA	1:B:285:LEU:HD23	2.18	0.73
1:A:106:GLN:HE22	1:A:226:ASN:HD22	1.35	0.73
1:B:282:ILE:HA	1:B:285:LEU:CD2	2.22	0.67
1:B:261:ASP:HB3	1:B:264:VAL:HG13	1.76	0.67
1:A:260:ASN:ND2	1:A:269:ASN:H	1.92	0.66
1:B:299:GLN:HE21	1:B:299:GLN:HA	1.65	0.61
1:B:170:LEU:O	1:B:281:GLY:HA2	2.00	0.61
1:A:184:THR:HG22	2:A:488:HOH:O	2.02	0.59
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.66	0.59
1:B:146:GLN:HG3	1:B:156:THR:HB	1.86	0.56
1:B:106:GLN:NE2	1:B:226:ASN:HD22	2.02	0.56
1:B:180:THR:CG2	1:B:244:GLN:HG2	2.37	0.55
1:B:285:LEU:HD21	1:B:299:GLN:HG2	1.88	0.55
1:A:106:GLN:NE2	1:A:226:ASN:HD22	2.02	0.55
1:B:91[A]:ARG:HH11	1:B:91[A]:ARG:HG3	1.72	0.54
1:B:143:ASN:HA	2:B:389:HOH:O	2.07	0.53
1:A:106:GLN:NE2	1:A:109:ARG:HH21	2.09	0.50
1:A:198:LEU:HD23	1:A:205:VAL:HG21	1.93	0.50
1:B:193:MET:HB2	1:B:208:ILE:HB	1.93	0.50
1:A:106:GLN:HB2	1:A:223:GLU:HG2	1.93	0.50
1:A:261:ASP:HB3	1:A:264:VAL:HG13	1.93	0.49
1:A:132:PHE:O	1:A:135:GLN:HG2	2.12	0.49
1:A:170:LEU:HD22	1:A:303:ALA:HB1	1.96	0.48
1:B:170:LEU:HD22	1:B:303:ALA:HB1	1.95	0.48
1:B:157:ILE:HD12	1:B:320:ARG:HG2	1.96	0.47
1:A:93:ARG:HB2	1:A:300:ILE:HG21	1.97	0.47
1:B:207:LYS:H	1:B:207:LYS:HD2	1.79	0.47
1:A:299:GLN:NE2	1:A:299:GLN:HA	2.31	0.46
1:B:106:GLN:NE2	1:B:109:ARG:HH21	2.14	0.46
1:A:247:LEU:HG	1:A:267:TRP:CZ2	2.53	0.43
1:A:125:ARG:HA	1:A:128:GLU:HG2	2.01	0.43
1:A:248:THR:HG21	1:A:292:ASN:ND2	2.34	0.43
1:B:347:PHE:O	1:B:351:THR:HG23	2.20	0.42
1:A:168:ALA:O	1:A:280:THR:HB	2.20	0.42
1:A:270:ASN:HD22	1:A:271:ALA:N	2.18	0.41
1:A:107:THR:HG23	2:A:2:HOH:O	2.21	0.41
1:A:285:LEU:HD21	1:A:299:GLN:HB3	2.02	0.41
1:A:78:ALA:HB2	1:A:137:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LEU:O	1:B:205:VAL:HG22	2.21	0.41
1:B:89:LEU:HD13	1:B:123:ILE:HD13	2.02	0.41
1:A:282:ILE:O	1:A:285:LEU:HB2	2.21	0.40
1:A:197:ASP:HB3	1:A:259:ALA:HB2	2.02	0.40
1:B:88:ASN:HA	1:B:91[A]:ARG:HD2	2.02	0.40
1:A:176:ARG:HG3	1:A:248:THR:OG1	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	323/351 (92%)	316 (98%)	7 (2%)	0	100	100
1	B	319/351 (91%)	315 (99%)	4 (1%)	0	100	100
All	All	642/702 (92%)	631 (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	248/272 (91%)	233 (94%)	15 (6%)	19	16
1	B	245/272 (90%)	228 (93%)	17 (7%)	15	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	493/544 (91%)	461 (94%)	32 (6%)	17	14

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	86	SER
1	A	89	LEU
1	A	146	GLN
1	A	164	ASN
1	A	170	LEU
1	A	176	ARG
1	A	207	LYS
1	A	250	ASN
1	A	264	VAL
1	A	270	ASN
1	A	280	THR
1	A	319	ASN
1	A	356	ARG
1	A	358	GLN
1	B	53	ARG
1	B	89	LEU
1	B	149	ILE
1	B	164	ASN
1	B	170	LEU
1	B	176	ARG
1	B	207	LYS
1	B	244	GLN
1	B	250	ASN
1	B	264	VAL
1	B	270	ASN
1	B	299	GLN
1	B	305	LYS
1	B	317	VAL
1	B	328	LEU
1	B	356	ARG
1	B	360	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	69	ASN
1	A	76	GLN
1	A	87	ASN
1	A	90	GLN
1	A	98	GLN
1	A	104	ASN
1	A	106	GLN
1	A	124	GLN
1	A	133	ASN
1	A	135	GLN
1	A	164	ASN
1	A	166	GLN
1	A	250	ASN
1	A	260	ASN
1	A	269	ASN
1	A	270	ASN
1	A	299	GLN
1	A	302	ASN
1	A	327	ASN
1	A	329	GLN
1	B	63	GLN
1	B	67	ASN
1	B	87	ASN
1	B	98	GLN
1	B	104	ASN
1	B	106	GLN
1	B	124	GLN
1	B	133	ASN
1	B	143	ASN
1	B	164	ASN
1	B	166	GLN
1	B	250	ASN
1	B	269	ASN
1	B	270	ASN
1	B	299	GLN
1	B	302	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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	323/351 (92%)	0.45	6 (1%) 66 71	18, 28, 39, 49	1 (0%)
1	B	320/351 (91%)	0.51	11 (3%) 45 51	18, 27, 38, 48	2 (0%)
All	All	643/702 (91%)	0.48	17 (2%) 56 61	18, 28, 38, 49	3 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	3.0
1	B	144	GLY	2.8
1	A	254	ALA	2.5
1	B	129	GLN	2.5
1	B	207	LYS	2.4
1	B	46	ALA	2.4
1	A	52	ASP	2.4
1	B	334	ASN	2.4
1	B	147	PHE	2.3
1	B	358	GLN	2.3
1	A	68	ALA	2.2
1	A	308	ASN	2.2
1	B	279	THR	2.1
1	B	281	GLY	2.1
1	B	143	ASN	2.1
1	A	143	ASN	2.0
1	B	174	LEU	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 carbohydrates 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.