



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:02 am GMT

PDB ID : 1IO1  
Title : CRYSTAL STRUCTURE OF F41 FRAGMENT OF FLAGELLIN  
Authors : Samatey, F.A.; Imada, K.; Nagashima, S.; Vondervisz, F.; Kumasaka, T.; Yamamoto, M.; Namba, K.  
Deposited on : 2000-12-28  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

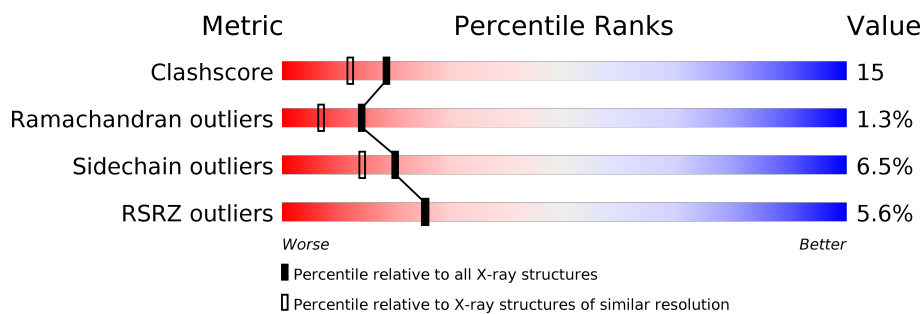
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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	398	<div> <div>6%</div> <div>75%</div> <div>21%</div> <div>••</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3234 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 PHASE 1 FLAGELLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2880	1747	501	631	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	ALA	GLY	CONFLICT	UNP P06179

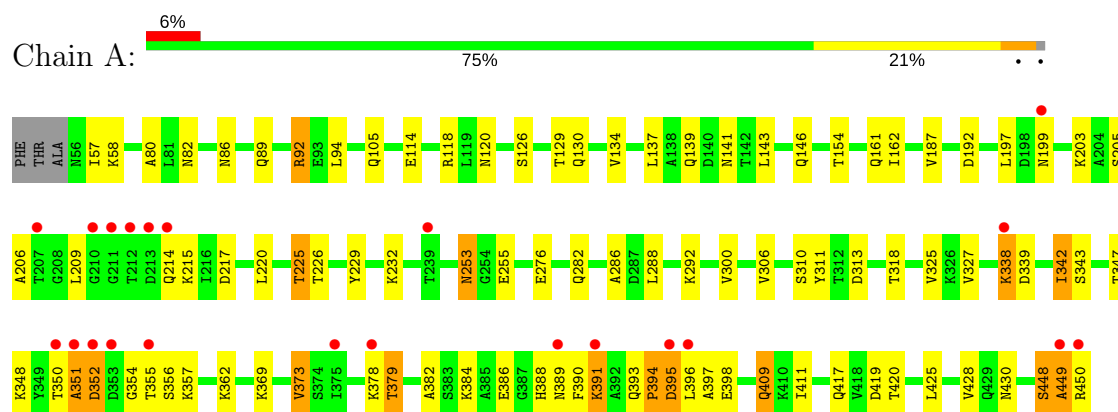
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	354	Total	O	0	0
			354	354		

### 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: PHASE 1 FLAGELLIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.75Å 36.44Å 118.35Å 90.00° 91.15° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 31.07 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 98.8 (31.07-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 1.91Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.234 , 0.266 0.231 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3234	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 7.21% 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	0.47	0/2900	0.73	0/3938

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	2880	0	2831	85	0
2	A	354	0	0	26	0
All	All	3234	0	2831	85	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 15.

All (85) 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:82:ASN:OD1	2:A:846:HOH:O	1.76	1.02
1:A:205:SER:O	2:A:849:HOH:O	1.79	0.99
1:A:347:THR:HG21	1:A:382:ALA:HB1	1.47	0.97
1:A:384:LYS:CE	2:A:789:HOH:O	2.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:HG22	2:A:705:HOH:O	1.74	0.86
1:A:89:GLN:OE1	2:A:848:HOH:O	1.94	0.84
1:A:187:VAL:HG12	2:A:729:HOH:O	1.79	0.82
1:A:217:ASP:HB2	1:A:232:LYS:HD3	1.62	0.82
1:A:338:LYS:HD3	1:A:339:ASP:H	1.46	0.80
1:A:114:GLU:OE1	2:A:847:HOH:O	2.00	0.78
1:A:409:GLN:HG2	2:A:803:HOH:O	1.85	0.76
1:A:354:GLY:HA2	1:A:391:LYS:NZ	2.01	0.75
1:A:357:LYS:HB3	2:A:812:HOH:O	1.89	0.71
1:A:338:LYS:HG3	2:A:698:HOH:O	1.90	0.70
1:A:225:THR:HG22	1:A:226:THR:HG23	1.72	0.70
1:A:384:LYS:HG3	2:A:708:HOH:O	1.92	0.70
1:A:354:GLY:HA2	1:A:391:LYS:HZ1	1.56	0.69
1:A:396:LEU:HD12	1:A:397:ALA:H	1.57	0.68
1:A:92:ARG:HG3	1:A:411:ILE:HG21	1.75	0.66
1:A:197:LEU:HD13	1:A:220:LEU:HD22	1.79	0.65
1:A:310:SER:OG	2:A:854:HOH:O	1.93	0.63
1:A:352:ASP:HA	1:A:390:PHE:HB2	1.81	0.62
1:A:57:ILE:HG13	1:A:58:LYS:N	2.15	0.62
1:A:357:LYS:HD3	2:A:812:HOH:O	2.01	0.60
1:A:352:ASP:HB3	1:A:357:LYS:NZ	2.17	0.60
1:A:384:LYS:HD2	2:A:789:HOH:O	2.02	0.59
1:A:325:VAL:HG22	1:A:342:ILE:HD11	1.84	0.59
1:A:192:ASP:HB3	1:A:282:GLN:HE22	1.68	0.59
1:A:187:VAL:CG1	2:A:729:HOH:O	2.47	0.57
1:A:94:LEU:HD11	1:A:114:GLU:HG3	1.86	0.56
1:A:92:ARG:HG3	1:A:411:ILE:CG2	2.36	0.56
1:A:300:VAL:CG1	1:A:327:VAL:HG11	2.36	0.56
1:A:288:LEU:HB2	1:A:292:LYS:HG3	1.87	0.55
1:A:300:VAL:HG12	1:A:327:VAL:HG11	1.88	0.55
1:A:357:LYS:CG	2:A:812:HOH:O	2.55	0.54
1:A:378:LYS:HB3	1:A:398:GLU:HG2	1.89	0.54
1:A:343:SER:HB3	2:A:561:HOH:O	2.08	0.53
1:A:311:TYR:CE2	1:A:369:LYS:HB3	2.45	0.52
1:A:86:ASN:ND2	2:A:826:HOH:O	2.43	0.52
1:A:396:LEU:HD12	1:A:397:ALA:N	2.25	0.52
1:A:357:LYS:CB	2:A:812:HOH:O	2.51	0.51
1:A:384:LYS:HE3	2:A:789:HOH:O	1.97	0.51
1:A:187:VAL:CG1	1:A:286:ALA:HA	2.41	0.51
1:A:379:THR:HG23	1:A:398:GLU:OE1	2.10	0.51
1:A:338:LYS:HD3	1:A:339:ASP:N	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:OD1	1:A:255:GLU:HG3	2.11	0.51
1:A:120:ASN:HD21	1:A:384:LYS:HE3	1.76	0.50
1:A:389:ASN:OD1	1:A:391:LYS:HB3	2.12	0.50
1:A:306:VAL:HG22	1:A:342:ILE:HD13	1.93	0.49
1:A:105:GLN:HG3	1:A:313:ASP:HB2	1.93	0.49
1:A:384:LYS:HE2	2:A:789:HOH:O	2.00	0.49
1:A:137:LEU:HD22	1:A:162:ILE:HB	1.94	0.48
1:A:146:GLN:HA	1:A:154:THR:HG22	1.96	0.48
1:A:338:LYS:CD	1:A:339:ASP:H	2.23	0.47
1:A:354:GLY:HA2	1:A:391:LYS:HZ2	1.78	0.47
1:A:356:SER:O	1:A:357:LYS:HG3	2.15	0.47
1:A:352:ASP:HB3	1:A:357:LYS:HZ2	1.79	0.47
1:A:379:THR:O	1:A:398:GLU:HB3	2.14	0.47
1:A:425:LEU:O	1:A:428:VAL:HG12	2.14	0.47
1:A:276:GLU:HG2	2:A:682:HOH:O	2.14	0.46
1:A:141:ASN:HD21	1:A:143:LEU:CD1	2.28	0.46
1:A:384:LYS:CD	2:A:789:HOH:O	2.52	0.46
1:A:450:ARG:NH2	2:A:751:HOH:O	2.48	0.46
1:A:373:VAL:O	1:A:379:THR:HA	2.17	0.45
1:A:388:HIS:HE1	1:A:393:GLN:O	2.00	0.45
1:A:449:ALA:O	1:A:450:ARG:OXT	2.33	0.45
1:A:325:VAL:CG2	1:A:342:ILE:HD11	2.46	0.45
1:A:206:ALA:HB1	1:A:209:LEU:HD12	2.00	0.44
1:A:199:ASN:HD22	1:A:199:ASN:N	2.15	0.44
1:A:352:ASP:HB3	1:A:357:LYS:HZ3	1.83	0.44
1:A:187:VAL:HG11	1:A:286:ALA:HA	2.00	0.43
1:A:80:ALA:HB2	1:A:129:THR:HG21	2.00	0.43
1:A:139:GLN:HA	1:A:161:GLN:HB2	2.01	0.43
1:A:448:SER:O	1:A:449:ALA:HB2	2.18	0.42
1:A:114:GLU:O	1:A:118:ARG:HG2	2.20	0.42
1:A:187:VAL:HG13	1:A:286:ALA:HA	2.02	0.42
1:A:351:ALA:HB2	1:A:391:LYS:NZ	2.35	0.41
1:A:351:ALA:HA	1:A:355:THR:O	2.20	0.41
1:A:394:PRO:HB2	1:A:395:ASP:H	1.74	0.41
1:A:126:SER:HB2	1:A:162:ILE:O	2.21	0.41
1:A:130:GLN:HA	1:A:134:VAL:O	2.20	0.41
1:A:417:GLN:NE2	2:A:529:HOH:O	2.53	0.41
1:A:362:LYS:HD2	2:A:687:HOH:O	2.21	0.40
1:A:351:ALA:HB2	1:A:391:LYS:HZ3	1.86	0.40
1:A:203:LYS:HB2	1:A:203:LYS:HE3	1.94	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	393/398 (99%)	374 (95%)	14 (4%)	5 (1%)	14 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	ASP
1	A	395	ASP
1	A	394	PRO
1	A	449	ALA
1	A	351	ALA

### 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	309/311 (99%)	289 (94%)	20 (6%)	20 14

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	A	214	GLN
1	A	215	LYS
1	A	225	THR
1	A	229	TYR
1	A	253	ASN

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Mol	Chain	Res	Type
1	A	318	THR
1	A	338	LYS
1	A	342	ILE
1	A	348	LYS
1	A	350	THR
1	A	373	VAL
1	A	379	THR
1	A	386	GLU
1	A	391	LYS
1	A	409	GLN
1	A	419	ASP
1	A	420	THR
1	A	430	ASN
1	A	448	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	68	ASN
1	A	86	ASN
1	A	105	GLN
1	A	120	ASN
1	A	141	ASN
1	A	282	GLN
1	A	337	ASN
1	A	388	HIS
1	A	417	GLN
1	A	445	ASN

### 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 [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 [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	395/398 (99%)	0.41	22 (5%) 25 25	7, 27, 54, 66	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	ASP	4.6
1	A	450	ARG	4.1
1	A	355	THR	3.8
1	A	210	GLY	3.8
1	A	353	ASP	3.7
1	A	396	LEU	3.2
1	A	391	LYS	3.1
1	A	207	THR	3.0
1	A	449	ALA	2.8
1	A	212	THR	2.7
1	A	338	LYS	2.7
1	A	350	THR	2.6
1	A	239	THR	2.5
1	A	214	GLN	2.5
1	A	378	LYS	2.5
1	A	199	ASN	2.4
1	A	352	ASP	2.4
1	A	213	ASP	2.4
1	A	389	ASN	2.3
1	A	351	ALA	2.2
1	A	375	ILE	2.1
1	A	211	GLY	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 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.