



# Full wwPDB X-ray Structure Validation Report

Apr 7, 2014 – 05:20 PM EDT

PDB ID : 1WLG  
Title : Crystal structure of FlgE31, a major fragment of the hook protein  
Authors : Samatey, F.A.; Matsunami, H.; Imada, K.; Nagashima, S.; Shaikh, T.R.;  
Thomas, D.R.; DeRosier, D.J.; Kitao, A.; Namba, K.  
Deposited on : 2004-06-25  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

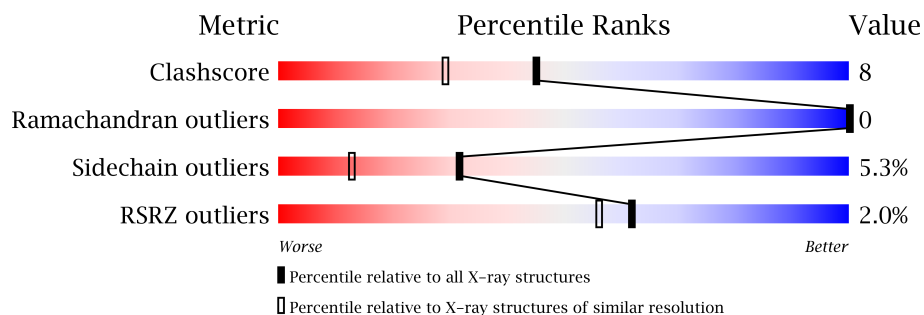
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	299	
1	B	299	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5063 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Flagellar hook protein flgE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2156	1327	369	454	6			
1	B	293	Total	C	N	O	S	0	0	0
			2156	1327	369	454	6			

- Molecule 2 is water.

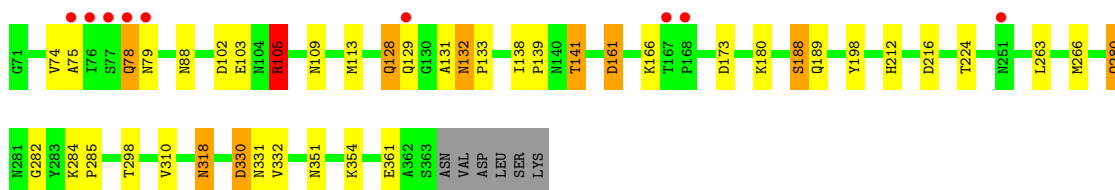
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	415	Total	O	0	0
			415	415		
2	B	336	Total	O	0	0
			336	336		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

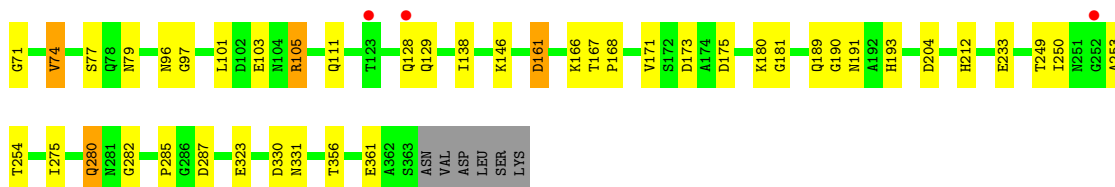
- Molecule 1: Flagellar hook protein flgE

Chain A: 



- Molecule 1: Flagellar hook protein flgE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.71 Å   49.03 Å   96.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 1.80 32.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-1.80) 93.8 (32.29-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.190   ,   0.242 0.201   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 64196 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.63	0/2193	0.84	7/2993 (0.2%)
1	B	0.61	0/2193	0.80	4/2993 (0.1%)
All	All	0.62	0/4386	0.82	11/5986 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	105	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	204	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	330	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	161	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	330	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	287	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	161	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	102	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	173	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	216	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2156	0	2055	48	1
1	B	2156	0	2055	23	1
2	A	415	0	0	32	3
2	B	336	0	0	9	2
All	All	5063	0	4110	71	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (71) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:THR:HB	2:A:743:HOH:O	1.28	1.31
1:A:74:VAL:C	2:A:741:HOH:O	1.88	1.12
1:B:103:GLU:OE2	2:B:569:HOH:O	1.83	0.97
1:A:132:ASN:CG	2:A:655:HOH:O	2.13	0.86
1:B:173:ASP:OD1	2:B:673:HOH:O	1.94	0.85
1:B:96:ASN:CG	1:B:331:ASN:HD21	1.79	0.85
1:A:188:SER:CB	2:A:779:HOH:O	2.26	0.83
1:B:189:GLN:HE21	1:B:191:ASN:HD21	1.30	0.77
1:A:188:SER:HB2	2:A:779:HOH:O	1.85	0.76
1:B:323:GLU:OE2	2:B:674:HOH:O	2.04	0.75
1:B:171:VAL:HG11	1:B:212:HIS:HD2	1.53	0.73
1:A:128:GLN:H	1:A:128:GLN:HE21	1.35	0.72
1:A:330:ASP:CB	2:A:740:HOH:O	2.38	0.71
1:A:105:ARG:HD3	1:A:138:ILE:O	1.91	0.71
1:B:166:LYS:HD3	2:B:673:HOH:O	1.91	0.71
1:A:79:ASN:HB3	2:A:657:HOH:O	1.91	0.69
1:B:105:ARG:HD3	1:B:138:ILE:O	1.93	0.69
1:A:141:THR:HG21	2:A:529:HOH:O	1.93	0.68
1:A:330:ASP:HB2	2:A:740:HOH:O	1.94	0.68
1:A:74:VAL:CA	2:A:741:HOH:O	2.37	0.68
1:A:266:MET:CE	2:A:729:HOH:O	2.43	0.65
1:A:75:ALA:HB3	2:A:651:HOH:O	1.96	0.65
1:A:266:MET:HE2	2:A:729:HOH:O	1.95	0.64
1:A:318:ASN:OD1	1:A:351:ASN:ND2	2.30	0.64
1:B:175:ASP:OD1	2:B:673:HOH:O	2.16	0.63
1:A:331:ASN:N	2:A:740:HOH:O	2.11	0.62
1:A:128:GLN:HG3	2:A:649:HOH:O	2.00	0.61
1:B:171:VAL:HG11	1:B:212:HIS:CD2	2.35	0.61
1:B:77:SER:N	2:B:619:HOH:O	2.33	0.59
1:B:71:GLY:N	1:B:361:GLU:OE2	2.37	0.58
1:B:74:VAL:O	1:B:97:GLY:HA3	2.04	0.57
1:A:79:ASN:N	2:A:723:HOH:O	2.37	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:GLN:HB3	2:A:656:HOH:O	2.07	0.54
1:A:78:GLN:HG3	2:A:684:HOH:O	2.08	0.53
1:A:128:GLN:CG	1:A:131:ALA:HB2	2.40	0.52
1:A:132:ASN:HD22	1:A:133:PRO:HD2	1.75	0.51
1:A:103:GLU:OE1	2:A:736:HOH:O	2.19	0.51
1:A:266:MET:HB3	2:A:729:HOH:O	2.11	0.50
1:A:128:GLN:HG2	1:A:128:GLN:O	2.12	0.50
1:A:361:GLU:OE2	2:A:668:HOH:O	2.20	0.49
1:A:78:GLN:HB3	2:A:723:HOH:O	2.11	0.49
1:B:280:GLN:NE2	1:B:282:GLY:H	2.10	0.49
1:B:193:HIS:CE1	1:B:250:ILE:HD12	2.48	0.49
1:A:354:LYS:NZ	2:A:617:HOH:O	2.45	0.48
1:A:132:ASN:HD22	1:A:133:PRO:CD	2.26	0.48
1:A:109:ASN:HD21	1:A:113:MET:CE	2.26	0.47
1:B:146:LYS:NZ	2:B:534:HOH:O	2.34	0.47
1:B:181:GLY:HA3	1:B:275:ILE:CD1	2.44	0.47
1:A:330:ASP:HB3	2:A:740:HOH:O	2.07	0.47
1:B:180:LYS:HD3	2:B:660:HOH:O	2.13	0.47
1:A:139:PRO:HB2	1:A:141:THR:HG23	1.95	0.47
1:A:132:ASN:OD1	2:A:655:HOH:O	2.19	0.47
1:A:113:MET:HE1	1:A:332:VAL:HG21	1.97	0.46
1:A:284:LYS:HB2	1:A:285:PRO:HD2	1.97	0.46
1:A:132:ASN:ND2	2:A:561:HOH:O	2.47	0.45
1:A:78:GLN:NE2	2:A:723:HOH:O	2.38	0.44
1:B:167:THR:HB	1:B:168:PRO:HA	1.99	0.44
1:A:280:GLN:NE2	1:A:282:GLY:H	2.16	0.43
1:A:78:GLN:HB3	1:A:78:GLN:HE21	1.63	0.43
1:B:77:SER:HB3	1:B:356:THR:HG22	1.99	0.43
1:B:190:GLY:HA3	1:B:285:PRO:HD3	2.01	0.43
1:A:75:ALA:N	2:A:741:HOH:O	2.35	0.43
1:A:318:ASN:ND2	2:A:659:HOH:O	2.51	0.42
1:B:331:ASN:HB2	2:B:595:HOH:O	2.20	0.42
1:A:88:ASN:ND2	2:A:581:HOH:O	2.52	0.42
1:A:266:MET:HE3	2:A:729:HOH:O	2.12	0.41
1:A:128:GLN:NE2	1:A:128:GLN:H	2.11	0.41
1:A:310:VAL:HG23	2:A:743:HOH:O	2.19	0.41
1:A:109:ASN:HD21	1:A:113:MET:HE1	1.85	0.40
1:B:249:THR:HG23	1:B:253:ALA:O	2.21	0.40
1:A:180:LYS:HD2	1:A:198:TYR:CE2	2.57	0.40

All (4) 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	Distance(Å)	Clash(Å)
2:A:778:HOH:O	2:B:569:HOH:O[1_556]	1.18	1.02
1:A:212:HIS:NE2	2:B:569:HOH:O[1_556]	1.91	0.29
1:B:103:GLU:OE2	2:A:778:HOH:O[1_554]	2.07	0.13
2:A:649:HOH:O	2:A:739:HOH:O[2_655]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	291/299 (97%)	287 (99%)	4 (1%)	0	100	100
1	B	291/299 (97%)	286 (98%)	5 (2%)	0	100	100
All	All	582/598 (97%)	573 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	235/241 (98%)	221 (94%)	14 (6%)	27	10
1	B	235/241 (98%)	224 (95%)	11 (5%)	36	16
All	All	470/482 (98%)	445 (95%)	25 (5%)	32	13

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	105	ARG
1	A	128	GLN
1	A	129	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	132	ASN
1	A	141	THR
1	A	161	ASP
1	A	166	LYS
1	A	188	SER
1	A	189	GLN
1	A	224	THR
1	A	263	LEU
1	A	280	GLN
1	A	318	ASN
1	B	74	VAL
1	B	79	ASN
1	B	101	LEU
1	B	105	ARG
1	B	111	GLN
1	B	128	GLN
1	B	129	GLN
1	B	161	ASP
1	B	233	GLU
1	B	254	THR
1	B	280	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	88	ASN
1	A	109	ASN
1	A	111	GLN
1	A	128	GLN
1	A	132	ASN
1	A	196	ASN
1	A	244	ASN
1	A	280	GLN
1	A	318	ASN
1	A	322	ASN
1	A	351	ASN
1	B	78	GLN
1	B	79	ASN
1	B	88	ASN
1	B	109	ASN
1	B	132	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	154	GLN
1	B	156	ASN
1	B	189	GLN
1	B	196	ASN
1	B	280	GLN
1	B	331	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 ⓘ

### 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	293/299 (97%)	-0.07	9 (3%)	47 39	11, 21, 36, 45	0
1	B	293/299 (97%)	-0.17	3 (1%)	79 76	13, 22, 35, 43	0
All	All	586/598 (97%)	-0.12	12 (2%)	62 56	11, 22, 36, 45	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	ILE	7.2
1	A	75	ALA	4.5
1	B	252	GLY	4.3
1	A	78	GLN	3.0
1	A	168	PRO	3.0
1	A	79	ASN	2.7
1	A	77	SER	2.6
1	A	129	GLN	2.5
1	A	167	THR	2.5
1	B	123	THR	2.4
1	B	128	GLN	2.3
1	A	251	ASN	2.1

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.