



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:40 PM GMT

PDB ID : 4FQ0
Title : Crystal structure of FliG-FliM complex from H. pylori
Authors : Lam, K.H.; Au, S.W.N.
Deposited on : 2012-06-24
Resolution : 2.82 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

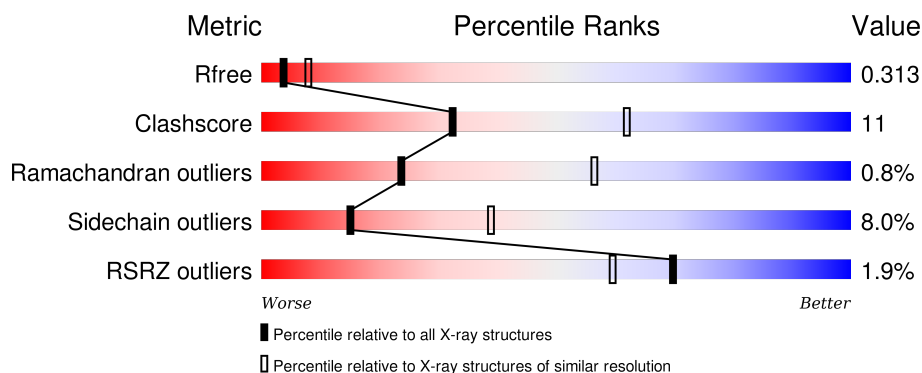
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 ≥ 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	210	<div> <div>2%</div> <div>61% 21% • 14%</div> </div>
1	B	210	<div> <div>2%</div> <div>66% 20% 13%</div> </div>
2	C	111	<div> <div>%</div> <div>50% 23% 28%</div> </div>
2	D	111	<div> <div></div> <div>42% 28% • 28%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3974 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 Flagellar motor switch protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	182	Total	C	N	O	S	0	0	0
			1377	874	224	267	12			
1	A	180	Total	C	N	O	S	0	0	0
			1376	873	229	262	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	GLY	-	EXPRESSION TAG	UNP O25675
B	29	PRO	-	EXPRESSION TAG	UNP O25675
B	30	LEU	-	EXPRESSION TAG	UNP O25675
B	31	GLY	-	EXPRESSION TAG	UNP O25675
B	32	SER	-	EXPRESSION TAG	UNP O25675
A	28	GLY	-	EXPRESSION TAG	UNP O25675
A	29	PRO	-	EXPRESSION TAG	UNP O25675
A	30	LEU	-	EXPRESSION TAG	UNP O25675
A	31	GLY	-	EXPRESSION TAG	UNP O25675
A	32	SER	-	EXPRESSION TAG	UNP O25675

- Molecule 2 is a protein called Flagellar motor switch protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total	C	N	O	S	0	0	0
			606	389	100	114	3			
2	D	80	Total	C	N	O	S	0	0	0
			606	389	100	114	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	95	HIS	-	EXPRESSION TAG	UNP O25119
C	96	HIS	-	EXPRESSION TAG	UNP O25119

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Chain	Residue	Modelled	Actual	Comment	Reference
C	97	HIS	-	EXPRESSION TAG	UNP O25119
C	98	HIS	-	EXPRESSION TAG	UNP O25119
C	99	HIS	-	EXPRESSION TAG	UNP O25119
C	100	HIS	-	EXPRESSION TAG	UNP O25119
C	101	HIS	-	EXPRESSION TAG	UNP O25119
C	102	MET	-	EXPRESSION TAG	UNP O25119
C	103	ALA	-	EXPRESSION TAG	UNP O25119
C	104	SER	-	EXPRESSION TAG	UNP O25119
C	105	MET	-	EXPRESSION TAG	UNP O25119
C	106	THR	-	EXPRESSION TAG	UNP O25119
C	107	GLY	-	EXPRESSION TAG	UNP O25119
C	108	GLY	-	EXPRESSION TAG	UNP O25119
C	109	GLN	-	EXPRESSION TAG	UNP O25119
C	110	GLN	-	EXPRESSION TAG	UNP O25119
C	111	MET	-	EXPRESSION TAG	UNP O25119
C	112	GLY	-	EXPRESSION TAG	UNP O25119
C	113	ARG	-	EXPRESSION TAG	UNP O25119
C	114	GLY	-	EXPRESSION TAG	UNP O25119
C	115	SER	-	EXPRESSION TAG	UNP O25119
D	95	HIS	-	EXPRESSION TAG	UNP O25119
D	96	HIS	-	EXPRESSION TAG	UNP O25119
D	97	HIS	-	EXPRESSION TAG	UNP O25119
D	98	HIS	-	EXPRESSION TAG	UNP O25119
D	99	HIS	-	EXPRESSION TAG	UNP O25119
D	100	HIS	-	EXPRESSION TAG	UNP O25119
D	101	HIS	-	EXPRESSION TAG	UNP O25119
D	102	MET	-	EXPRESSION TAG	UNP O25119
D	103	ALA	-	EXPRESSION TAG	UNP O25119
D	104	SER	-	EXPRESSION TAG	UNP O25119
D	105	MET	-	EXPRESSION TAG	UNP O25119
D	106	THR	-	EXPRESSION TAG	UNP O25119
D	107	GLY	-	EXPRESSION TAG	UNP O25119
D	108	GLY	-	EXPRESSION TAG	UNP O25119
D	109	GLN	-	EXPRESSION TAG	UNP O25119
D	110	GLN	-	EXPRESSION TAG	UNP O25119
D	111	MET	-	EXPRESSION TAG	UNP O25119
D	112	GLY	-	EXPRESSION TAG	UNP O25119
D	113	ARG	-	EXPRESSION TAG	UNP O25119
D	114	GLY	-	EXPRESSION TAG	UNP O25119
D	115	SER	-	EXPRESSION TAG	UNP O25119

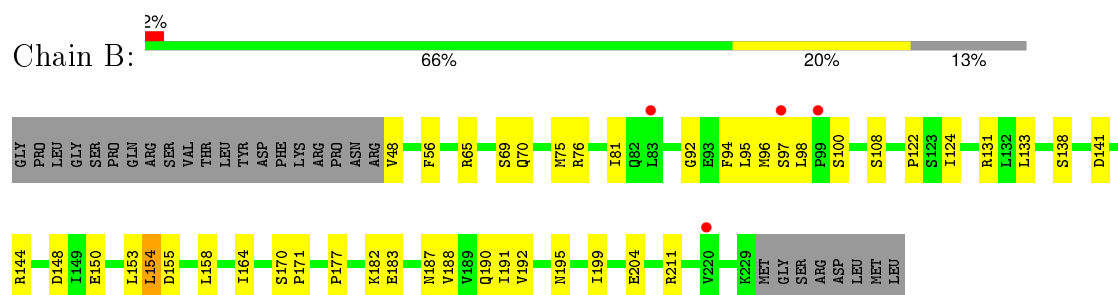
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	O 1	0	0
3	A	2	Total 2	O 2	0	0
3	C	5	Total 5	O 5	0	0
3	D	1	Total 1	O 1	0	0

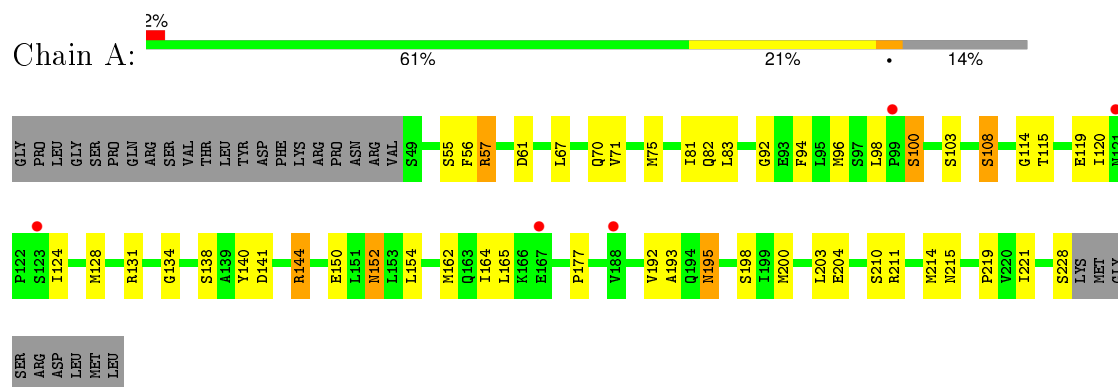
3 Residue-property plots

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.

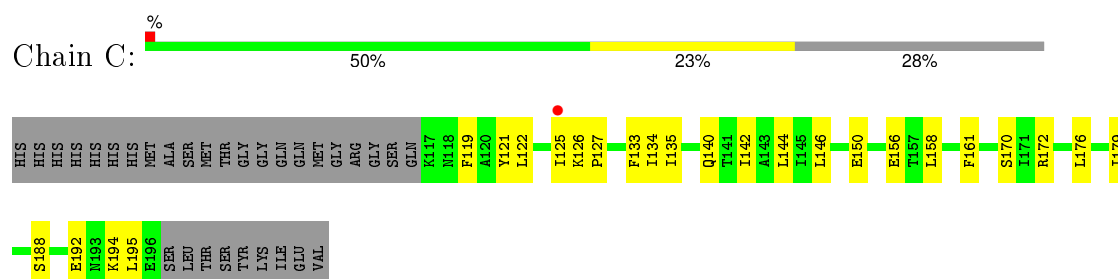
- Molecule 1: Flagellar motor switch protein



- Molecule 1: Flagellar motor switch protein



- Molecule 2: Flagellar motor switch protein



- Molecule 2: Flagellar motor switch protein



P181	Q182	V183	V184	K185	R186	W187	S188	L191	E192	W193	K194	L195	E196	SER	LEU	THR	SER	ARG	GLY	LYS	SER	ILE	GLU	VAL	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	SER	MET	THR	GLY	GLY	GLN	SER	GLN	K117	Y121	K124	F133	I134	I135	Q140	T141	I142	I145	M149	E150	A151	P152	M153	A154	T157	L158	F161	M165	I169	S170	I171	R172	L176	S180
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.09Å 124.54Å 137.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.77 – 2.82 36.77 – 2.82	Depositor EDS
% Data completeness (in resolution range)	96.9 (36.77-2.82) 97.0 (36.77-2.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.237 , 0.308 0.239 , 0.313	Depositor DCC
R_{free} test set	880 reflections (5.51%)	DCC
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 16833 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3974	wwPDB-VP
Average B, all atoms (Å ²)	91.0	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 65.20 % 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 7.3534e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.60	0/1398	0.80	0/1893
1	B	0.60	0/1399	0.74	0/1898
2	C	0.62	0/617	0.82	0/840
2	D	0.58	0/617	0.83	0/840
All	All	0.60	0/4031	0.79	0/5471

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	1376	0	1376	33	0
1	B	1377	0	1361	24	0
2	C	606	0	597	13	0
2	D	606	0	597	23	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	5	0	0	0	0
3	D	1	0	0	0	0
All	All	3974	0	3931	83	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 11.

The worst 5 of 83 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:70:GLN:HG3	1:A:164:ILE:HD11	1.55	0.89
1:B:100:SER:HB3	1:A:100:SER:HB2	1.59	0.84
2:D:140:GLN:HG2	2:D:172:ARG:HH11	1.45	0.82
2:D:140:GLN:HG2	2:D:172:ARG:NH1	1.98	0.79
2:D:121:TYR:CE2	2:D:192:GLU:HG3	2.24	0.73

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	178/210 (85%)	164 (92%)	13 (7%)	1 (1%)	30	63
1	B	180/210 (86%)	171 (95%)	8 (4%)	1 (1%)	30	63
2	C	78/111 (70%)	69 (88%)	9 (12%)	0	100	100
2	D	78/111 (70%)	67 (86%)	9 (12%)	2 (3%)	7	21
All	All	514/642 (80%)	471 (92%)	39 (8%)	4 (1%)	24	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	96	MET
1	A	114	GLY
2	D	124	LYS
2	D	182	GLN

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	157/192 (82%)	141 (90%)	16 (10%)	9	26
1	B	157/192 (82%)	148 (94%)	9 (6%)	25	57
2	C	63/95 (66%)	58 (92%)	5 (8%)	15	39
2	D	63/95 (66%)	58 (92%)	5 (8%)	15	39
All	All	440/574 (77%)	405 (92%)	35 (8%)	15	39

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	THR
1	A	154	LEU
2	D	170	SER
1	A	138	SER
1	A	144	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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 [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, 95th 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 ²)	Q<0.9
1	A	180/210 (85%)	0.05	5 (2%) 56 44	69, 94, 112, 126	0
1	B	182/210 (86%)	0.06	4 (2%) 65 54	70, 90, 110, 126	0
2	C	80/111 (72%)	-0.17	1 (1%) 79 71	62, 89, 104, 108	0
2	D	80/111 (72%)	-0.16	0 100 100	62, 88, 107, 117	0
All	All	522/642 (81%)	-0.01	10 (1%) 70 59	62, 91, 110, 126	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	VAL	3.5
1	B	99	PRO	3.2
2	C	125	ILE	2.8
1	A	99	PRO	2.8
1	A	121	ASN	2.7

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.