wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2024 – 05:57 PM EST

PDB ID	:	3K1I
Title	:	Crystal strcture of FliS-HP1076 complex in H. pylori
Authors	:	Lam, W.W.L.; Kotaka, M.; Ling, T.K.W.; Au, S.W.N.
Deposited on	:	2009-09-28
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

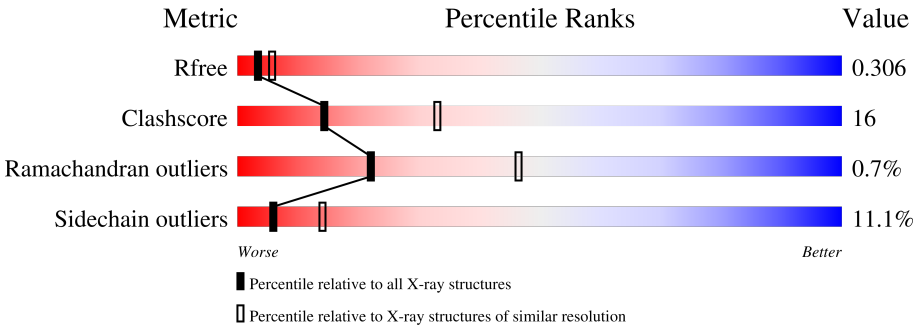
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	131	50% 27% . 19%
1	B	131	47% 27% 5% 21%
2	C	178	47% 18% . 33%
2	D	178	40% 24% .. 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3603 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			859	548	142	167	2			
1	B	104	Total	C	N	O	S	0	0	0
			842	539	140	161	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP O25448
A	-3	PRO	-	expression tag	UNP O25448
A	-2	LEU	-	expression tag	UNP O25448
A	-1	GLY	-	expression tag	UNP O25448
A	0	SER	-	expression tag	UNP O25448
B	-4	GLY	-	expression tag	UNP O25448
B	-3	PRO	-	expression tag	UNP O25448
B	-2	LEU	-	expression tag	UNP O25448
B	-1	GLY	-	expression tag	UNP O25448
B	0	SER	-	expression tag	UNP O25448

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	119	Total	C	N	O	S	0	0	0
			938	599	150	184	5			
2	D	120	Total	C	N	O	S	0	0	0
			948	604	152	187	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP O25709
C	-5	HIS	-	expression tag	UNP O25709

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP O25709
C	-3	HIS	-	expression tag	UNP O25709
C	-2	HIS	-	expression tag	UNP O25709
C	-1	HIS	-	expression tag	UNP O25709
C	0	MET	-	expression tag	UNP O25709
D	-6	HIS	-	expression tag	UNP O25709
D	-5	HIS	-	expression tag	UNP O25709
D	-4	HIS	-	expression tag	UNP O25709
D	-3	HIS	-	expression tag	UNP O25709
D	-2	HIS	-	expression tag	UNP O25709
D	-1	HIS	-	expression tag	UNP O25709
D	0	MET	-	expression tag	UNP O25709

- Molecule 3 is water.

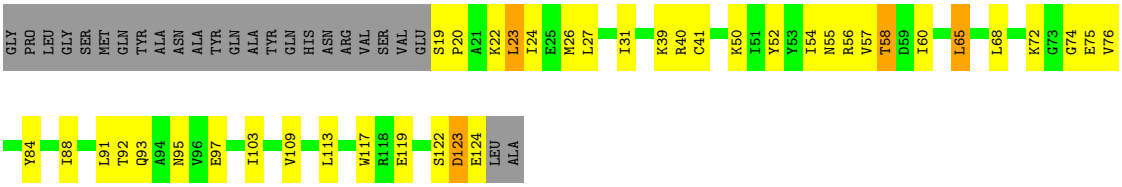
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	3	Total O 3 3	0	0
3	C	3	Total O 3 3	0	0
3	D	6	Total O 6 6	0	0

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. 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. 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.

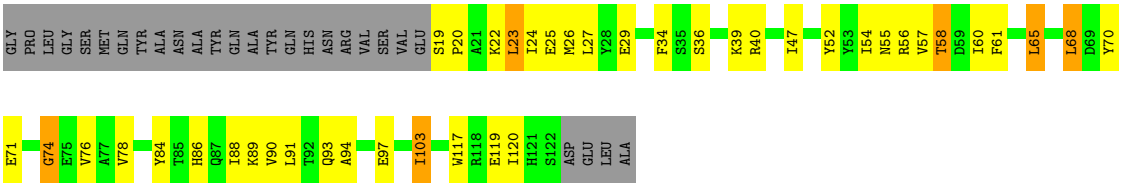
• Molecule 1: Flagellar protein

Chain A:



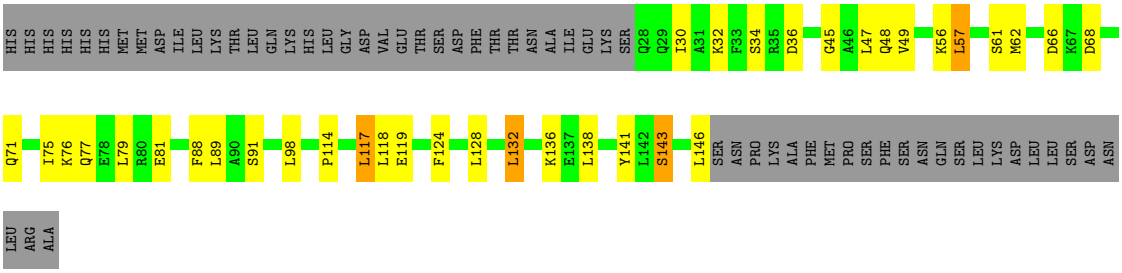
• Molecule 1: Flagellar protein

Chain B:



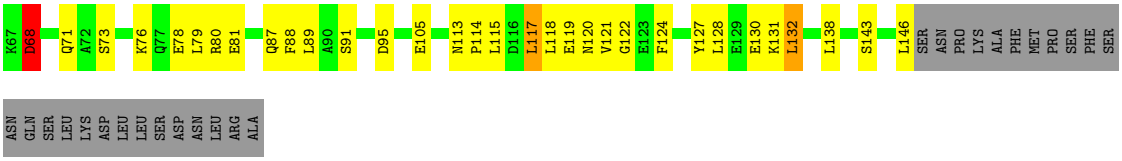
• Molecule 2: Putative uncharacterized protein

Chain C:



• Molecule 2: Putative uncharacterized protein

Chain D:


K67
D68
Q71
A72
S73
K76
Q77
E78
L79
R80
E81
Q87
F88
L89
A90
S91
D95
E105
N113
P114
L115
D116
L117
L118
E119
N120
V121
G122
E123
F124
Y127
L128
E129
E130
K131
L132
L138
S143
L146
SER
ASN
PRO
LYS
ALA
PHE
MET
PRO
SER
PHE
SER
ASN
GLN
SER
LEU
LYS
ASP
LEU
LEU
SER
ASP
ASN
LEU
ARG
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	50.25Å 50.25Å 242.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.33 – 2.70 19.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.33-2.70) 95.7 (19.33-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.70Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.258 , 0.299 0.258 , 0.306	Depositor DCC
R_{free} test set	771 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 4.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3603	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.74	1/871 (0.1%)	0.74	0/1177
1	B	0.69	0/854	0.74	0/1154
2	C	0.69	0/947	0.72	0/1274
2	D	0.70	0/957	0.75	1/1287 (0.1%)
All	All	0.70	1/3629 (0.0%)	0.74	1/4892 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	LYS	CE-NZ	5.77	1.63	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	68	ASP	CB-CG-OD2	-5.17	113.65	118.30

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	859	0	865	33	0
1	B	842	0	855	37	0
2	C	938	0	953	21	0
2	D	948	0	964	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	6	0	0	1	0
All	All	3603	0	3637	112	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 16.

The worst 5 of 112 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:65:LEU:CD2	2:D:30:ILE:HD11	1.82	1.10
2:D:76:LYS:HG2	2:D:118:LEU:HD13	1.39	1.02
2:C:76:LYS:HG2	2:C:118:LEU:HD13	1.37	1.02
1:A:65:LEU:HD23	2:D:30:ILE:HD11	1.43	0.96
2:C:32:LYS:HG2	2:C:36:ASP:OD2	1.85	0.76

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	104/131 (79%)	97 (93%)	6 (6%)	1 (1%)	15	37
1	B	102/131 (78%)	96 (94%)	5 (5%)	1 (1%)	15	37
2	C	117/178 (66%)	102 (87%)	15 (13%)	0	100	100
2	D	118/178 (66%)	108 (92%)	9 (8%)	1 (1%)	19	43
All	All	441/618 (71%)	403 (91%)	35 (8%)	3 (1%)	22	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	GLY
1	B	74	GLY
2	D	121	VAL

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	94/113 (83%)	85 (90%)	9 (10%)	8 19
1	B	92/113 (81%)	84 (91%)	8 (9%)	10 23
2	C	105/162 (65%)	92 (88%)	13 (12%)	4 11
2	D	107/162 (66%)	93 (87%)	14 (13%)	4 10
All	All	398/550 (72%)	354 (89%)	44 (11%)	6 14

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	141	TYR
2	D	66	ASP
2	C	143	SER
2	D	57	LEU
2	D	73	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	48	GLN
2	D	87	GLN
2	D	125	GLN
2	D	97	GLN
2	C	48	GLN

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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.