



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 01:18 AM GMT

PDB ID : 2E2L
Title : Helicobacter pylori formamidase AmiF contains a fine-tuned cysteine-glutamate-lysine catalytic triad
Authors : Wang, W.C.; Hung, C.L.
Deposited on : 2006-11-14
Resolution : 2.29 Å (reported)

This is a wwPDB 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/ValidationPDFNotes.html>

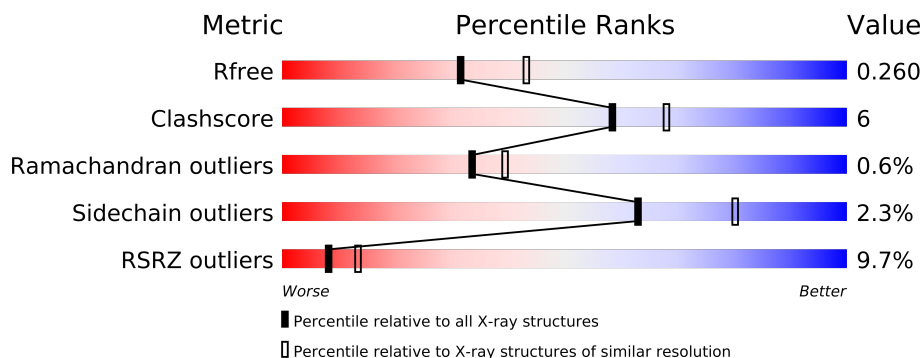
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.29 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. 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	334	
1	B	334	
1	C	334	
1	D	334	
1	E	334	
1	F	334	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15751 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.

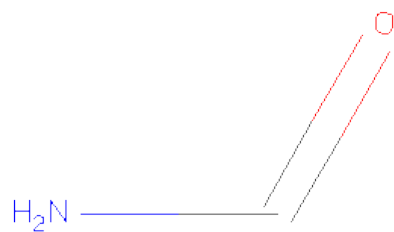
- Molecule 1 is a protein called Formamidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			
1	B	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			
1	C	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			
1	D	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			
1	E	316	Total	C	N	O	S	0	0	0
			2492	1604	417	460	11			
1	F	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	SER	CYS	ENGINEERED	UNP O25836
B	166	SER	CYS	ENGINEERED	UNP O25836
C	166	SER	CYS	ENGINEERED	UNP O25836
D	166	SER	CYS	ENGINEERED	UNP O25836
E	166	SER	CYS	ENGINEERED	UNP O25836
F	166	SER	CYS	ENGINEERED	UNP O25836

- Molecule 2 is FORMAMIDE (three-letter code: ARF) (formula: CH₃NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			3	1	1	1		
2	C	1	Total	C	N	O	0	0
			3	1	1	1		
2	F	1	Total	C	N	O	0	0
			3	1	1	1		

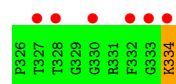
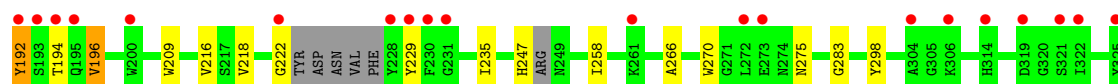
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		
3	B	131	Total	O	0	0
			131	131		
3	C	143	Total	O	0	0
			143	143		
3	D	102	Total	O	0	0
			102	102		
3	E	114	Total	O	0	0
			114	114		
3	F	112	Total	O	0	0
			112	112		



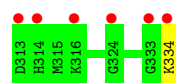
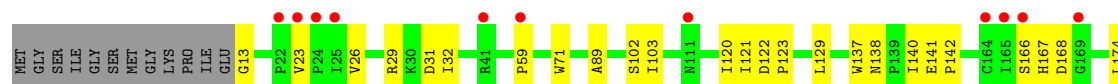
• Molecule 1: Formamidase

Chain E:



• Molecule 1: Formamidase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.09Å 151.79Å 89.08Å 90.00° 114.99° 90.00°	Depositor
Resolution (Å)	30.00 – 2.29 29.62 – 2.29	Depositor EDS
% Data completeness (in resolution range)	90.9 (30.00-2.29) 90.9 (29.62-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.253 , 0.285 0.253 , 0.260	Depositor DCC
R_{free} test set	4091 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.8	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 81861 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15751	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ARF

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	0.33	0/2574	0.50	0/3498
1	B	0.33	0/2574	0.48	0/3498
1	C	0.33	0/2574	0.50	0/3498
1	D	0.33	0/2574	0.49	0/3498
1	E	0.33	0/2562	0.48	0/3481
1	F	0.33	0/2574	0.48	0/3498
All	All	0.33	0/15432	0.49	0/20971

There are no bond length outliers.

There are no bond angle outliers.

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	2503	0	2442	43	0
1	B	2503	0	2442	47	0
1	C	2503	0	2442	48	0
1	D	2503	0	2442	41	0
1	E	2492	0	2428	24	0
1	F	2503	0	2442	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	3	2	0
2	C	3	0	3	1	0
2	F	3	0	3	0	0
3	A	133	0	0	3	0
3	B	131	0	0	1	0
3	C	143	0	0	1	0
3	D	102	0	0	2	0
3	E	114	0	0	1	0
3	F	112	0	0	0	0
All	All	15751	0	14647	185	0

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 6.

The worst 5 of 185 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:170:MET:CE	1:D:209:TRP:HE1	1.66	1.08
1:C:170:MET:HE2	1:D:209:TRP:HE1	1.24	1.00
1:A:192:TYR:HD2	2:A:1335:ARF:HN2	1.27	0.81
1:C:170:MET:HE2	1:D:209:TRP:NE1	1.96	0.80
1:C:170:MET:CE	1:D:209:TRP:NE1	2.47	0.77

There are no symmetry-related clashes.

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	313/334 (94%)	300 (96%)	12 (4%)	1 (0%)	50	60
1	B	313/334 (94%)	298 (95%)	11 (4%)	4 (1%)	18	17
1	C	313/334 (94%)	298 (95%)	13 (4%)	2 (1%)	33	39
1	D	313/334 (94%)	302 (96%)	10 (3%)	1 (0%)	50	60
1	E	310/334 (93%)	299 (96%)	9 (3%)	2 (1%)	33	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	313/334 (94%)	299 (96%)	13 (4%)	1 (0%)	50 60
All	All	1875/2004 (94%)	1796 (96%)	68 (4%)	11 (1%)	33 39

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	B	193	SER
1	C	231	GLY
1	E	166	SER
1	F	166	SER

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	263/277 (95%)	257 (98%)	6 (2%)	63 80
1	B	263/277 (95%)	258 (98%)	5 (2%)	69 85
1	C	263/277 (95%)	257 (98%)	6 (2%)	63 80
1	D	263/277 (95%)	257 (98%)	6 (2%)	63 80
1	E	262/277 (95%)	256 (98%)	6 (2%)	63 80
1	F	263/277 (95%)	256 (97%)	7 (3%)	57 74
All	All	1577/1662 (95%)	1541 (98%)	36 (2%)	63 80

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	334	LYS
1	D	228	TYR
1	F	220	LEU
1	D	192	TYR
1	D	298	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	249	ASN
1	D	167	HIS
1	F	167	HIS
1	C	275	ASN
1	C	278	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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ARF	A	1335	-	2,2,2	1.96	1 (50%)	1,1,1	0.78	0
2	ARF	C	2335	-	2,2,2	1.96	1 (50%)	1,1,1	0.79	0
2	ARF	F	3335	-	2,2,2	2.02	1 (50%)	1,1,1	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARF	A	1335	-	-	0/0/0/0	0/0/0/0
2	ARF	C	2335	-	-	0/0/0/0	0/0/0/0
2	ARF	F	3335	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3335	ARF	O-C	2.74	1.33	1.23
2	C	2335	ARF	O-C	2.66	1.33	1.23
2	A	1335	ARF	O-C	2.65	1.33	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	317/334 (94%)	0.52	24 (7%)	14 20	24, 34, 42, 49	0
1	B	317/334 (94%)	0.58	35 (11%)	6 10	24, 35, 49, 52	0
1	C	317/334 (94%)	0.48	25 (7%)	13 19	25, 34, 44, 47	0
1	D	317/334 (94%)	0.55	26 (8%)	12 18	27, 36, 51, 56	0
1	E	316/334 (94%)	0.68	34 (10%)	6 10	28, 39, 55, 59	0
1	F	317/334 (94%)	0.76	40 (12%)	4 7	28, 39, 48, 51	0
All	All	1901/2004 (94%)	0.60	184 (9%)	8 13	24, 36, 48, 59	0

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	193	SER	12.3
1	A	229	TYR	11.7
1	F	228	TYR	11.2
1	B	192	TYR	10.8
1	A	228	TYR	10.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ARF	A	1335	3/3	0.27	0.40	36,36,40,40	0
2	ARF	C	2335	3/3	0.25	-0.05	41,41,44,44	0
2	ARF	F	3335	3/3	0.25	-0.40	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.