wwPDB X-ray Structure Validation Summary Report (i)

Oct 18, 2023 – 04:54 PM EDT

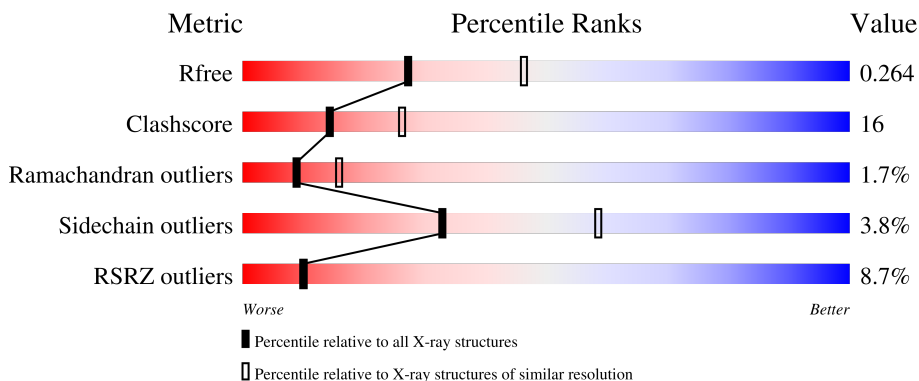|		
PDB ID	:	2E2K
Title	:	Helicobacter pylori formamidase AmiF contains a fine-tuned cysteine-glutamate-lysine catalytic triad
Authors	:	Wang, W.C.; Hung, C.L.
Deposited on	:	2006-11-14
Resolution	:	2.50 Å(reported)

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 2.50 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.
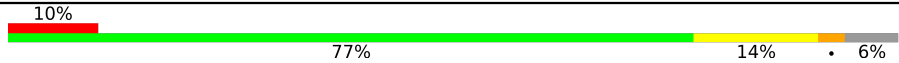

Metric	Percentile Ranks	Value
Rfree		0.264
Clashscore		16
Ramachandran outliers		1.7%
Sidechain outliers		3.8%
RSRZ outliers		8.7%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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	334	8% / 75% 16% · 6%
1	B	334	7% / 74% 18% · 6%
1	C	334	7% / 74% 17% · 6%
1	D	334	7% / 73% 18% · 7%
1	E	334	9% / 74% 17% · 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	334	

10%

77%

14% · 6%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 15744 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 Formamidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2482	1597	416	458	11			
1	B	314	Total	C	N	O	S	0	0	0
			2485	1598	417	459	11			
1	C	314	Total	C	N	O	S	0	0	0
			2489	1600	417	461	11			
1	D	311	Total	C	N	O	S	0	0	0
			2458	1581	412	454	11			
1	E	315	Total	C	N	O	S	0	0	0
			2493	1602	419	461	11			
1	F	314	Total	C	N	O	S	0	0	0
			2487	1601	415	460	11			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	151	Total	O	0	0
			151	151		
2	C	133	Total	O	0	0
			133	133		

Continued on next page...

wwPDB X-ray Structure Validation Summary Report

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	159	Total 159	O 159	0	0
2	E	138	Total 138	O 138	0	0
2	F	121	Total 121	O 121	0	0

3 Residue-property plots ⓘ

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 d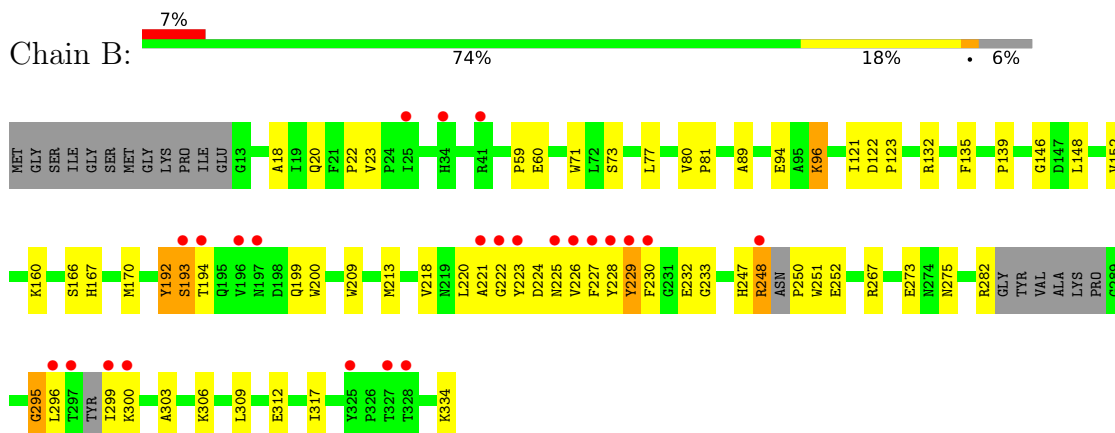isplayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or 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.
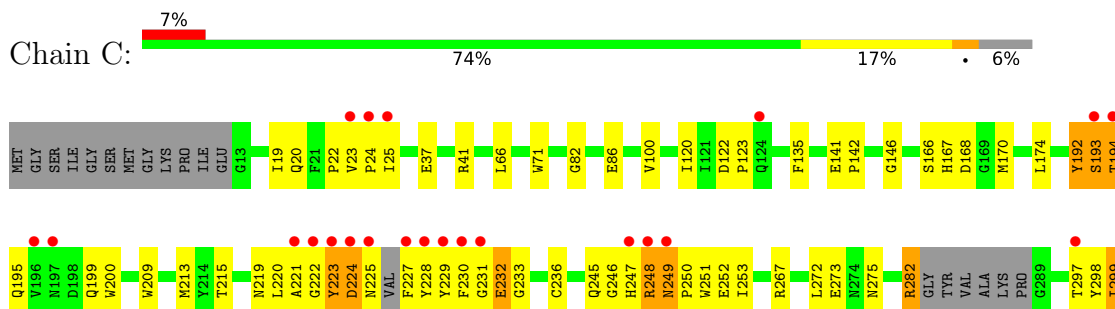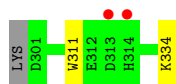
- Molecule 1: Formamidase

Chain A:

- Molecule 1: Formamidase

Chain B:

- Molecule 1: Formamidase

Chain C:

LYS D301 W311 E312 D313 H314 K334

• Molecule 1: Formamidase

Chain D:

7%

73%   18%   •   7%

MET GLY SER ILE GLY SER MET GLY LYS PRO ILE GLU G13 A18 I19 Q20 F21 P22 V23 P24 I25 E37 R41 Y61 W71 L72 S73 K83 L87 S110 I120 I121 D122 P123 L129 K133 P136 W137 N138 P139 I140 E141 P142 G146 I165 S166

H167 D168 G169 M170 L174 Y186 Y192 S193 THR Q195 V196 N197 D198 Q199 W209 M213 Y214 T215 V218 N219 L220 A221 G222 Y223 D224 N225 V226 F227 Y228 Y229 F230 G231 GLU G233 G246 H247 ARG N249 P250 W251 R267 L268 S269 W270 E273 N274 N275 R282 GLY TYR

VAL ALA LYS PRO G289 G295 LEU T297 TYR I299 K300 L309 E312 K316 I317 R331 K334

• Molecule 1: Formamidase

Chain E:

9%

74%   17%   •   6%

MET GLY SER ILE GLY SER MET GLY LYS PRO ILE GLU G13 Q20 F21 P22 V23 P24 I25 H34 R41 S62 W71 V80 P81 G82 K83 K90 E94 V100 P108 I120 I121 D122 P123 L129 P139 I140 E141 P142 G146 M150 S166 H167

D168 G169 M170 L174 Y180 K181 Y186 Y192 S193 T194 Q195 V196 N197 D198 Q199 W200 T203 W209 T215 N219 L220 A221 G222 Y223 D224 N225 V226 F227 Y228 Y229 F230 G231 E232 H247 R248 N249 P250 W251 W270 G271 L272 E273 N274 N275 N278 R282 GLY TYR
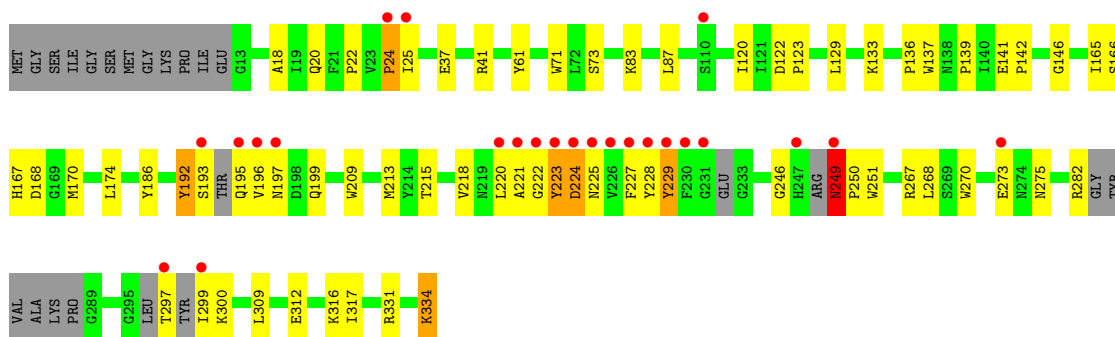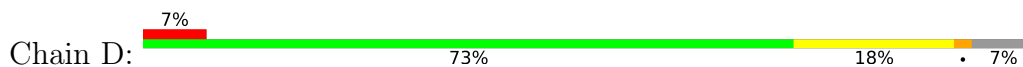
VAL ALA LYS PRO G289 G295 L296 T297 TYR I299 K300 D301 D313 I317 S321 K334

• Molecule 1: Formamidase

Chain F:

10%

77%   14%   •   6%

MET GLY SER ILE GLY SER MET GLY LYS PRO ILE GLU G13 A18 I19 Q20 F21 P22 V23 P24 I25 K30 H34 E60 W71 K93 P108 D109 S110 N111 D122 P123 P139 I140 E141 P142 G146 S166 H167 D168 L174 Y186 Y192 S193 THR Q195

V196 N197 D198 Q199 W209 T215 V218 N219 L220 A221 G222 Y223 D224 N225 V226 F227 Y228 Y229 F230 G231 E232 C236 G246 H247 ARG N249 P250 W251 E252 M262 N275 R282 GLY TYR VAL ALA LYS PRO G289 D293 A294 G295 L296 T297 Y298 I299 K300 L309 E312

D313 H314 I317 G324 T327 K334

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.72Å 130.53Å 144.59Å 90.00° 99.44° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 26.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.50) 99.8 (26.90-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	13.24 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.256 , 0.294 0.256 , 0.264	Depositor DCC
R_{free} test set	3760 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	15744	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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	0.26	0/2550	0.46	0/3459
1	B	0.27	0/2553	0.47	0/3465
1	C	0.26	0/2558	0.47	0/3474
1	D	0.27	0/2523	0.46	0/3421
1	E	0.27	0/2562	0.46	0/3480
1	F	0.26	0/2556	0.47	0/3471
All	All	0.27	0/15302	0.46	0/20770

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	249	ASN	Peptide

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2482	0	2407	111	0
1	B	2485	0	2417	84	0
1	C	2489	0	2409	101	0
1	D	2458	0	2382	83	0
1	E	2493	0	2423	92	0
1	F	2487	0	2411	75	0
2	A	148	0	0	6	0
2	B	151	0	0	1	0
2	C	133	0	0	6	0
2	D	159	0	0	4	0
2	E	138	0	0	3	0
2	F	121	0	0	0	0
All	All	15744	0	14449	455	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 455 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:F:192:TYR:HB3	1:F:193:SER:CA	1.69	1.23
1:E:248:ARG:H	1:E:248:ARG:HD3	1.06	1.20
1:A:192:TYR:CB	1:A:193:SER:HA	1.73	1.18
1:D:192:TYR:HB3	1:D:193:SER:CA	1.76	1.14
1:C:192:TYR:HB3	1:C:193:SER:CA	1.78	1.13

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	303/334 (91%)	282 (93%)	19 (6%)	2 (1%)	22	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	306/334 (92%)	282 (92%)	18 (6%)	6 (2%)	7	12
1	C	306/334 (92%)	287 (94%)	12 (4%)	7 (2%)	6	10
1	D	298/334 (89%)	278 (93%)	16 (5%)	4 (1%)	12	21
1	E	309/334 (92%)	281 (91%)	22 (7%)	6 (2%)	8	13
1	F	306/334 (92%)	278 (91%)	22 (7%)	6 (2%)	7	12
All	All	1828/2004 (91%)	1688 (92%)	109 (6%)	31 (2%)	9	16

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	194	THR
1	C	194	THR
1	E	194	THR
1	E	226	VAL
1	F	250	PRO

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	261/277 (94%)	247 (95%)	14 (5%)	22	42
1	B	262/277 (95%)	252 (96%)	10 (4%)	33	58
1	C	262/277 (95%)	254 (97%)	8 (3%)	40	67
1	D	259/277 (94%)	252 (97%)	7 (3%)	44	71
1	E	263/277 (95%)	254 (97%)	9 (3%)	37	63
1	F	262/277 (95%)	251 (96%)	11 (4%)	30	54
All	All	1569/1662 (94%)	1510 (96%)	59 (4%)	33	58

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	282	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	247	HIS
1	D	229	TYR
1	F	232	GLU
1	F	71	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	281	HIS
1	E	275	ASN
1	E	20	GLN
1	E	210	HIS
1	F	20	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 ⓘ

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(Å²)	Q<0.9
1	A	313/334 (93%)	0.47	27 (8%)	10	10	2, 8, 20, 28	0
1	B	314/334 (94%)	0.41	24 (7%)	13	14	3, 8, 18, 25	0
1	C	314/334 (94%)	0.35	24 (7%)	13	14	2, 7, 15, 24	0
1	D	311/334 (93%)	0.40	24 (7%)	13	13	2, 7, 17, 28	0
1	E	315/334 (94%)	0.59	29 (9%)	9	9	3, 10, 21, 29	0
1	F	314/334 (94%)	0.59	35 (11%)	5	5	4, 10, 21, 26	0
All	All	1881/2004 (93%)	0.47	163 (8%)	10	10	2, 8, 20, 29	0

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	222	GLY	13.2
1	A	222	GLY	12.3
1	B	222	GLY	11.7
1	E	228	TYR	10.8
1	F	228	TYR	10.5

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 monosaccharides 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.