



# wwPDB X-ray Structure Validation Summary Report

Nov 17, 2014 – 11:52 AM EST

PDB ID : 4NQZ  
Title : Crystal Structure of the Pseudomonas aeruginosa Enoyl-Acyl Carrier Protein Reductase (FabI) in apo form  
Authors : Chi, Y.M.; Lee, J.H.; Park, A.K.  
Deposited on : 2013-11-26  
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary 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>

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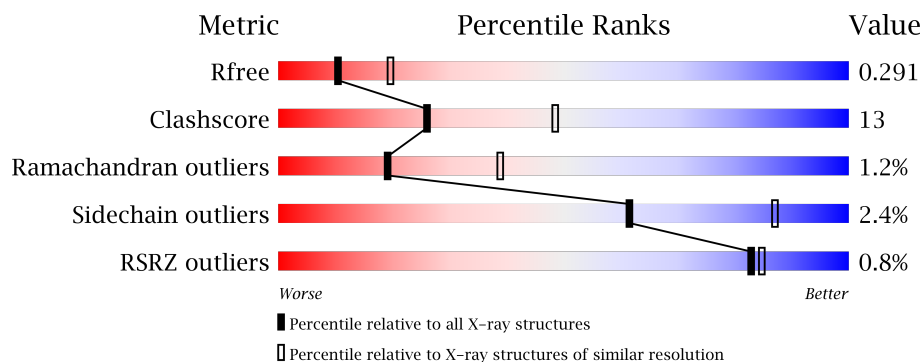
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24195  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24195

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	273	
1	B	273	
1	C	273	
1	D	273	
1	E	273	
1	F	273	
1	G	273	
1	H	273	
1	I	273	
1	J	273	
1	K	273	
1	L	273	
1	M	273	
1	N	273	

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Mol	Chain	Length	Quality of chain
1	O	273	
1	P	273	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29449 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 Enoyl-[acyl-carrier-protein]reductase [NADH] FabI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1840	1151	327	351	11			
1	B	243	Total	C	N	O	S	0	0	0
			1797	1125	318	345	9			
1	C	245	Total	C	N	O	S	0	0	0
			1813	1135	320	347	11			
1	D	246	Total	C	N	O	S	0	0	0
			1822	1141	322	348	11			
1	E	244	Total	C	N	O	S	0	0	0
			1805	1130	319	346	10			
1	F	245	Total	C	N	O	S	0	0	0
			1816	1136	323	347	10			
1	G	244	Total	C	N	O	S	0	0	0
			1805	1130	319	346	10			
1	H	248	Total	C	N	O	S	0	0	0
			1844	1153	330	350	11			
1	I	244	Total	C	N	O	S	0	0	0
			1805	1130	319	346	10			
1	J	245	Total	C	N	O	S	0	0	0
			1813	1135	320	347	11			
1	K	246	Total	C	N	O	S	0	0	0
			1824	1141	324	348	11			
1	L	244	Total	C	N	O	S	0	0	0
			1808	1131	322	346	9			
1	M	245	Total	C	N	O	S	0	0	0
			1816	1136	323	347	10			
1	N	244	Total	C	N	O	S	0	0	0
			1811	1133	322	346	10			
1	O	247	Total	C	N	O	S	0	0	0
			1836	1148	329	349	10			
1	P	248	Total	C	N	O	S	0	0	0
			1837	1149	327	350	11			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
A	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
A	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
A	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
A	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
A	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
A	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
A	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
B	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
B	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
B	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
B	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
B	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
B	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
B	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
B	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
C	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
C	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
C	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
C	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
C	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
C	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
C	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
C	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
D	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
D	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
D	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
D	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
D	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
D	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
D	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
D	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
E	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
E	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
E	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
E	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
E	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
E	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
E	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
E	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
F	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
F	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
F	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
F	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
F	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
F	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
F	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
G	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
G	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
G	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
G	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
G	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
G	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
G	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
G	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
H	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
H	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
H	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
H	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
H	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
H	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
H	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
H	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
I	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
I	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
I	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
I	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
I	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
I	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
I	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
I	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
J	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
J	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
J	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
J	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
J	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
J	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
J	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
J	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
K	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
K	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
K	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
K	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
K	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
K	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
K	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
L	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
L	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
L	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
L	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
L	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
L	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
L	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
L	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
M	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
M	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
M	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
M	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
M	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
M	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
M	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
M	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
N	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
N	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
N	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
N	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
N	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
N	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
N	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
N	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
O	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
O	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
O	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
O	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
O	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
O	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
O	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
O	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
P	266	LEU	-	EXPRESSION TAG	UNP Q9ZFE4
P	267	GLU	-	EXPRESSION TAG	UNP Q9ZFE4
P	268	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
P	269	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
P	270	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
P	271	HIS	-	EXPRESSION TAG	UNP Q9ZFE4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	272	HIS	-	EXPRESSION TAG	UNP Q9ZFE4
P	273	HIS	-	EXPRESSION TAG	UNP Q9ZFE4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	24	Total O 24 24	0	0
2	C	33	Total O 33 33	0	0
2	D	24	Total O 24 24	0	0
2	E	22	Total O 22 22	0	0
2	F	26	Total O 26 26	0	0
2	G	23	Total O 23 23	0	0
2	H	32	Total O 32 32	0	0
2	I	23	Total O 23 23	0	0
2	J	16	Total O 16 16	0	0
2	K	20	Total O 20 20	0	0
2	L	16	Total O 16 16	0	0
2	M	16	Total O 16 16	0	0
2	N	22	Total O 22 22	0	0
2	O	13	Total O 13 13	0	0
2	P	20	Total O 20 20	0	0

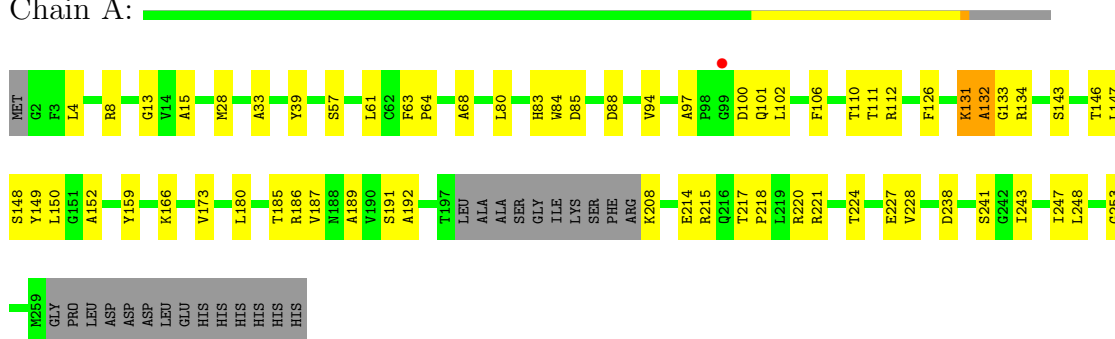


### 3 Residue-property plots

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.

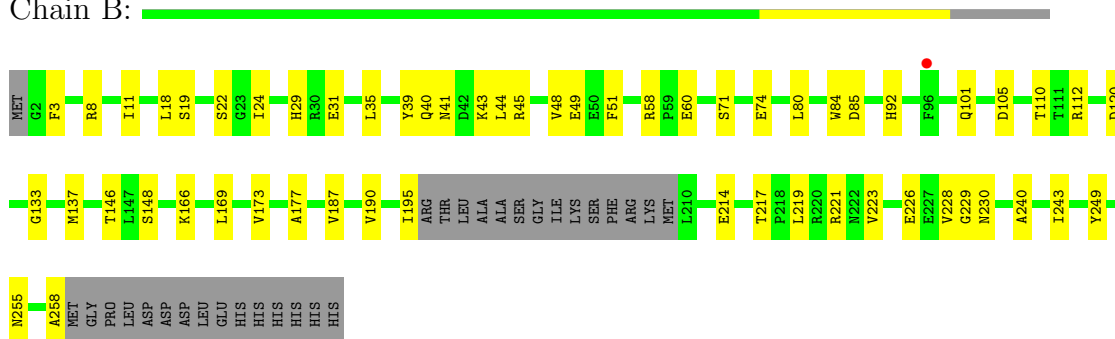
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain A:



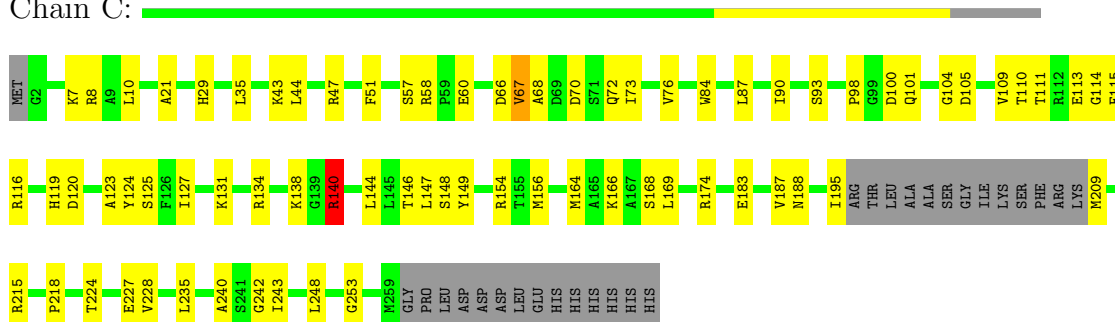
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain B:

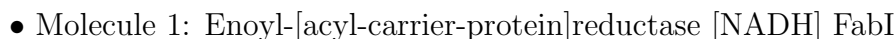
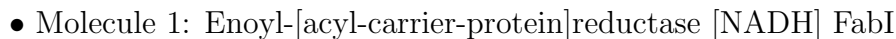


- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

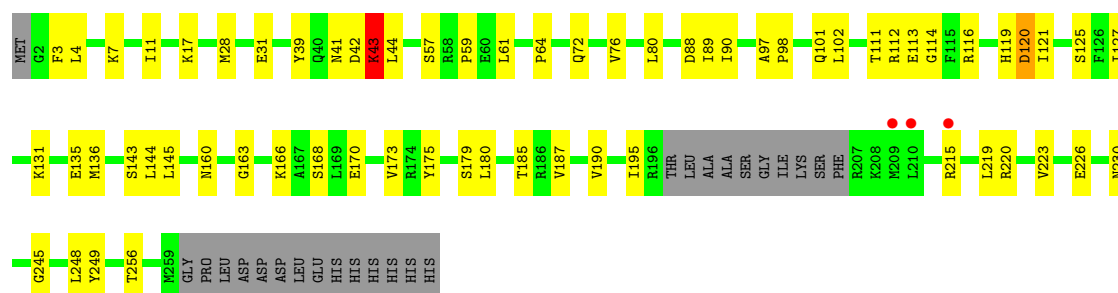
Chain C:



- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

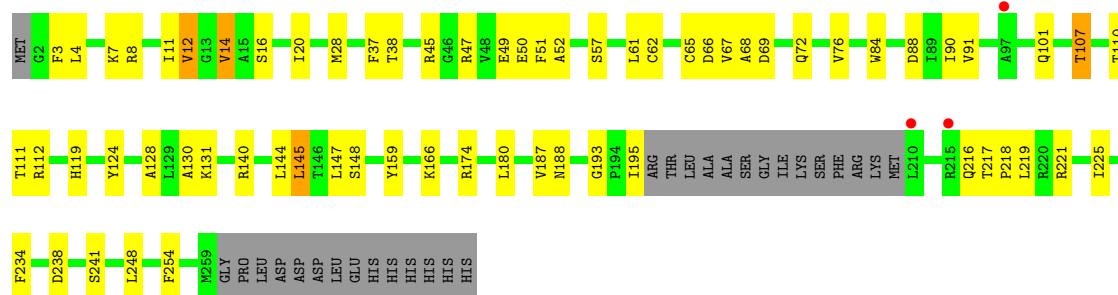


Age Group	Percentage
18-29	90%
30-49	83%
50-64	72%
65+	60%



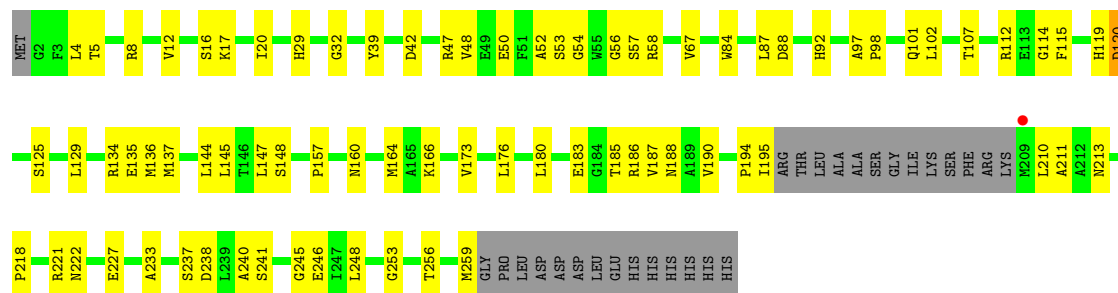
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain I:



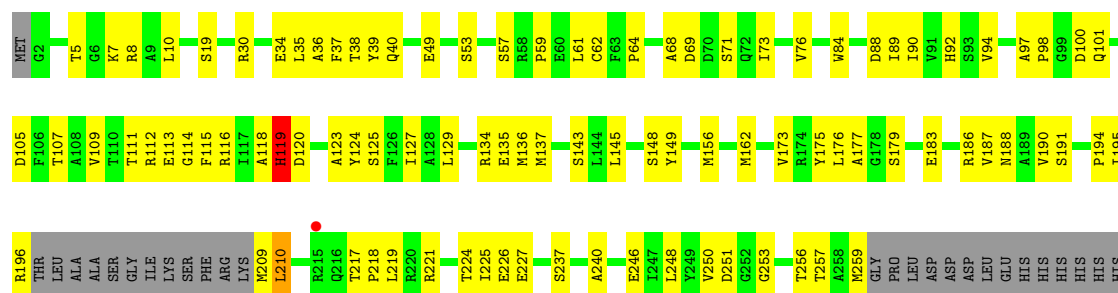
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain J:



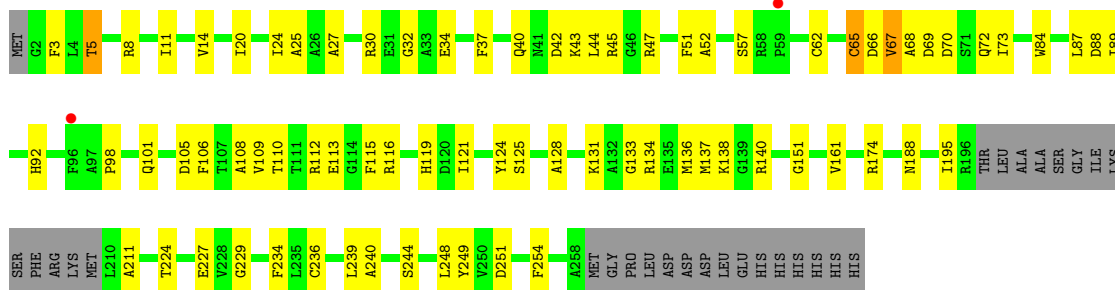
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain K:



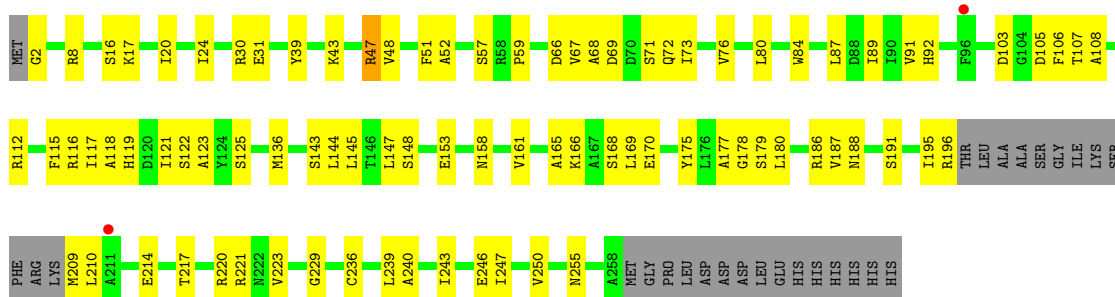
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain L:



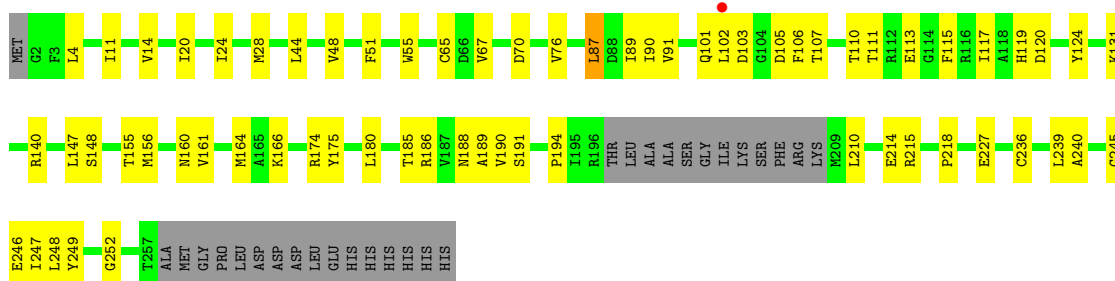
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain M:



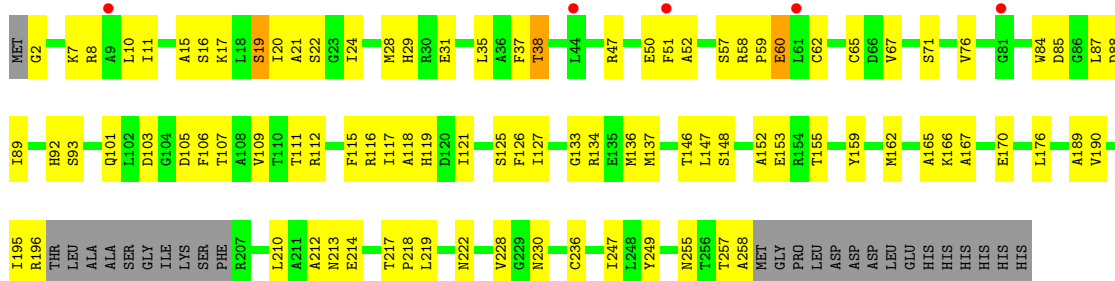
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain N: 



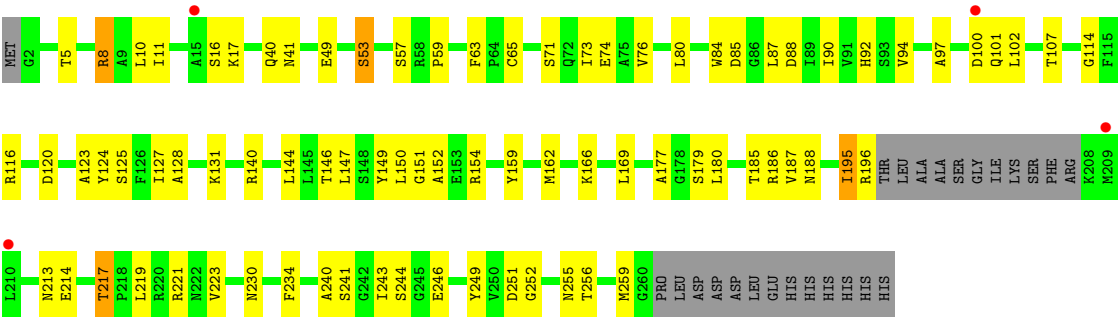
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain 0: 



- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH] FabI

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.32Å 155.84Å 129.45Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	44.39 – 2.60 48.13 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.7 (44.39-2.60) 84.7 (48.13-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.199 , 0.286 0.205 , 0.291	Depositor DCC
$R_{free}$ test set	5659 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 10.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 112300 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	29449	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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	0.50	0/1869	0.65	0/2520
1	B	0.45	0/1826	0.62	0/2465
1	C	0.50	0/1842	0.66	1/2485 (0.0%)
1	D	0.43	0/1851	0.58	0/2496
1	E	0.42	0/1834	0.58	0/2475
1	F	0.46	0/1845	0.66	0/2489
1	G	0.49	0/1834	0.67	0/2475
1	H	0.47	0/1873	0.66	0/2524
1	I	0.45	0/1834	0.63	0/2475
1	J	0.41	0/1842	0.59	0/2485
1	K	0.47	0/1853	0.65	1/2499 (0.0%)
1	L	0.41	0/1837	0.60	0/2479
1	M	0.43	0/1845	0.60	0/2489
1	N	0.45	0/1840	0.63	1/2482 (0.0%)
1	O	0.41	0/1865	0.60	0/2514
1	P	0.42	0/1866	0.61	1/2515 (0.0%)
All	All	0.45	0/29556	0.63	4/39867 (0.0%)

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	O	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	195	ILE	C-N-CA	5.56	135.60	121.70
1	K	210	LEU	CA-CB-CG	5.52	128.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	N	87	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	60	GLU	Peptide

## 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	1840	0	1820	44	0
1	B	1797	0	1769	36	0
1	C	1813	0	1787	55	0
1	D	1822	0	1800	55	0
1	E	1805	0	1778	51	0
1	F	1816	0	1791	48	0
1	G	1805	0	1778	50	1
1	H	1844	0	1826	47	0
1	I	1805	0	1778	48	1
1	J	1813	0	1787	58	0
1	K	1824	0	1800	69	0
1	L	1808	0	1782	59	0
1	M	1816	0	1791	66	0
1	N	1811	0	1786	56	0
1	O	1836	0	1817	67	0
1	P	1837	0	1816	63	0
2	A	27	0	0	6	0
2	B	24	0	0	1	0
2	C	33	0	0	6	0
2	D	24	0	0	3	0
2	E	22	0	0	3	0
2	F	26	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	23	0	0	4	0
2	H	32	0	0	4	0
2	I	23	0	0	2	0
2	J	16	0	0	2	0
2	K	20	0	0	3	0
2	L	16	0	0	7	0
2	M	16	0	0	1	0
2	N	22	0	0	5	0
2	O	13	0	0	2	0
2	P	20	0	0	6	0
All	All	29449	0	28706	772	1

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 13.

The worst 5 of 772 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:101:GLN:HE22	1:F:111:THR:H	1.12	0.96
1:G:153:GLU:OE1	1:G:249:TYR:OH	1.88	0.91
1:N:188:ASN:O	2:N:303:HOH:O	1.91	0.88
1:J:241:SER:HB2	1:L:227:GLU:HG2	1.60	0.84
1:O:107:THR:O	1:P:131:LYS:NZ	2.09	0.83

All (1) 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)
1:G:47:ARG:NH2	1:I:62:CYS:O[2_555]	2.17	0.03

## 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	244/273 (89%)	217 (89%)	24 (10%)	3 (1%)	19	39
1	B	239/273 (88%)	216 (90%)	21 (9%)	2 (1%)	27	53
1	C	241/273 (88%)	215 (89%)	25 (10%)	1 (0%)	43	72
1	D	242/273 (89%)	221 (91%)	20 (8%)	1 (0%)	43	72
1	E	240/273 (88%)	213 (89%)	22 (9%)	5 (2%)	11	19
1	F	241/273 (88%)	212 (88%)	24 (10%)	5 (2%)	11	19
1	G	240/273 (88%)	214 (89%)	23 (10%)	3 (1%)	18	35
1	H	244/273 (89%)	224 (92%)	16 (7%)	4 (2%)	14	28
1	I	240/273 (88%)	217 (90%)	22 (9%)	1 (0%)	43	72
1	J	241/273 (88%)	209 (87%)	27 (11%)	5 (2%)	11	19
1	K	242/273 (89%)	211 (87%)	26 (11%)	5 (2%)	11	19
1	L	240/273 (88%)	217 (90%)	21 (9%)	2 (1%)	27	53
1	M	241/273 (88%)	218 (90%)	21 (9%)	2 (1%)	27	53
1	N	240/273 (88%)	213 (89%)	26 (11%)	1 (0%)	43	72
1	O	243/273 (89%)	211 (87%)	28 (12%)	4 (2%)	14	28
1	P	244/273 (89%)	217 (89%)	26 (11%)	1 (0%)	43	72
All	All	3862/4368 (88%)	3445 (89%)	372 (10%)	45 (1%)	19	39

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	59	PRO
1	E	215	ARG
1	F	103	ASP
1	F	131	LYS
1	G	214	GLU

### 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	184/205 (90%)	181 (98%)	3 (2%)	75	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	179/205 (87%)	176 (98%)	3 (2%)	73	92
1	C	181/205 (88%)	180 (99%)	1 (1%)	92	98
1	D	182/205 (89%)	177 (97%)	5 (3%)	57	85
1	E	180/205 (88%)	179 (99%)	1 (1%)	92	98
1	F	181/205 (88%)	173 (96%)	8 (4%)	39	68
1	G	180/205 (88%)	175 (97%)	5 (3%)	56	84
1	H	184/205 (90%)	182 (99%)	2 (1%)	84	96
1	I	180/205 (88%)	172 (96%)	8 (4%)	39	68
1	J	181/205 (88%)	180 (99%)	1 (1%)	92	98
1	K	182/205 (89%)	176 (97%)	6 (3%)	50	79
1	L	180/205 (88%)	174 (97%)	6 (3%)	50	79
1	M	181/205 (88%)	179 (99%)	2 (1%)	84	96
1	N	181/205 (88%)	177 (98%)	4 (2%)	64	89
1	O	183/205 (89%)	176 (96%)	7 (4%)	44	74
1	P	183/205 (89%)	176 (96%)	7 (4%)	44	74
All	All	2902/3280 (88%)	2833 (98%)	69 (2%)	61	87

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	50	GLU
1	K	19	SER
1	P	8	ARG
1	I	107	THR
1	I	234	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	216	GLN
1	P	213	ASN
1	O	101	GLN
1	E	101	GLN
1	N	101	GLN

### 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	248/273 (90%)	-0.45	1 (0%) 90 91	19, 29, 53, 77	0
1	B	243/273 (89%)	-0.41	1 (0%) 90 91	27, 37, 55, 66	0
1	C	245/273 (89%)	-0.54	0 100 100	17, 28, 45, 62	0
1	D	246/273 (90%)	-0.37	1 (0%) 90 91	26, 41, 58, 88	0
1	E	244/273 (89%)	-0.12	4 (1%) 68 69	28, 46, 68, 75	0
1	F	245/273 (89%)	-0.45	0 100 100	22, 35, 54, 64	0
1	G	244/273 (89%)	-0.51	1 (0%) 90 91	22, 33, 49, 75	0
1	H	248/273 (90%)	-0.54	3 (1%) 75 77	21, 30, 54, 85	0
1	I	244/273 (89%)	-0.46	3 (1%) 75 77	18, 32, 57, 76	0
1	J	245/273 (89%)	-0.25	1 (0%) 90 91	26, 45, 63, 76	0
1	K	246/273 (90%)	-0.46	1 (0%) 90 91	23, 36, 59, 82	0
1	L	244/273 (89%)	-0.30	2 (0%) 83 85	27, 45, 61, 72	0
1	M	245/273 (89%)	-0.33	2 (0%) 83 85	31, 43, 58, 67	0
1	N	244/273 (89%)	-0.30	1 (0%) 90 91	26, 37, 64, 76	0
1	O	247/273 (90%)	0.05	5 (2%) 62 60	34, 51, 71, 80	0
1	P	248/273 (90%)	-0.26	4 (1%) 68 69	27, 40, 66, 80	0
All	All	3926/4368 (89%)	-0.36	30 (0%) 83 85	17, 38, 62, 88	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	209	MET	4.3
1	I	215	ARG	3.8
1	A	99	GLY	3.7
1	K	215	ARG	3.6
1	N	102	LEU	3.2

## 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.