



# wwPDB X-ray Structure Validation Summary Report

Feb 14, 2017 – 11:49 am GMT

PDB ID : 3NYW  
Title : Crystal Structure of a betaketoacyl-[ACP] reductase (FabG) from *Bacteroides thetaiotaomicron*  
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2010-07-15  
Resolution : 2.16 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](mailto: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.

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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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

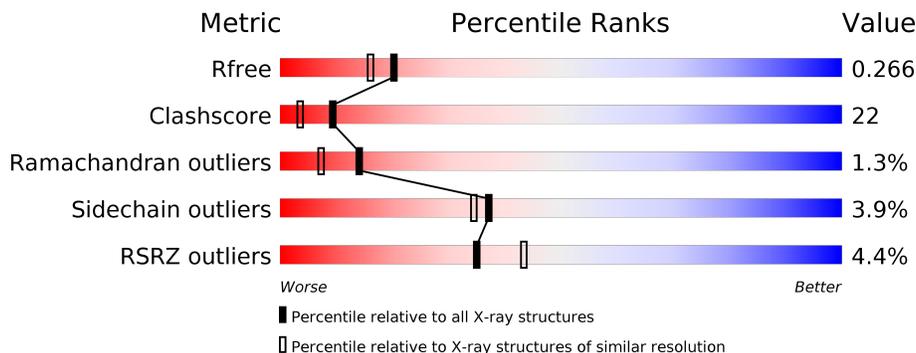
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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))
$R_{free}$	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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. 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	250	
1	B	250	
1	C	250	
1	D	250	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7143 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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	232	Total 1779	C 1131	N 298	O 338	S 4	Se 8	0	0	0
1	B	220	Total 1694	C 1079	N 285	O 318	S 4	Se 8	0	0	0
1	C	228	Total 1755	C 1119	N 293	O 331	S 4	Se 8	0	0	0
1	D	213	Total 1646	C 1048	N 278	O 309	S 4	Se 7	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	EXPRESSION TAG	UNP Q8A562
A	0	SER	-	EXPRESSION TAG	UNP Q8A562
A	1	LEU	-	EXPRESSION TAG	UNP Q8A562
A	241	GLU	-	EXPRESSION TAG	UNP Q8A562
A	242	GLY	-	EXPRESSION TAG	UNP Q8A562
A	243	HIS	-	EXPRESSION TAG	UNP Q8A562
A	244	HIS	-	EXPRESSION TAG	UNP Q8A562
A	245	HIS	-	EXPRESSION TAG	UNP Q8A562
A	246	HIS	-	EXPRESSION TAG	UNP Q8A562
A	247	HIS	-	EXPRESSION TAG	UNP Q8A562
A	248	HIS	-	EXPRESSION TAG	UNP Q8A562
B	-1	MSE	-	EXPRESSION TAG	UNP Q8A562
B	0	SER	-	EXPRESSION TAG	UNP Q8A562
B	1	LEU	-	EXPRESSION TAG	UNP Q8A562
B	241	GLU	-	EXPRESSION TAG	UNP Q8A562
B	242	GLY	-	EXPRESSION TAG	UNP Q8A562
B	243	HIS	-	EXPRESSION TAG	UNP Q8A562
B	244	HIS	-	EXPRESSION TAG	UNP Q8A562
B	245	HIS	-	EXPRESSION TAG	UNP Q8A562
B	246	HIS	-	EXPRESSION TAG	UNP Q8A562
B	247	HIS	-	EXPRESSION TAG	UNP Q8A562

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Chain	Residue	Modelled	Actual	Comment	Reference
B	248	HIS	-	EXPRESSION TAG	UNP Q8A562
C	-1	MSE	-	EXPRESSION TAG	UNP Q8A562
C	0	SER	-	EXPRESSION TAG	UNP Q8A562
C	1	LEU	-	EXPRESSION TAG	UNP Q8A562
C	241	GLU	-	EXPRESSION TAG	UNP Q8A562
C	242	GLY	-	EXPRESSION TAG	UNP Q8A562
C	243	HIS	-	EXPRESSION TAG	UNP Q8A562
C	244	HIS	-	EXPRESSION TAG	UNP Q8A562
C	245	HIS	-	EXPRESSION TAG	UNP Q8A562
C	246	HIS	-	EXPRESSION TAG	UNP Q8A562
C	247	HIS	-	EXPRESSION TAG	UNP Q8A562
C	248	HIS	-	EXPRESSION TAG	UNP Q8A562
D	-1	MSE	-	EXPRESSION TAG	UNP Q8A562
D	0	SER	-	EXPRESSION TAG	UNP Q8A562
D	1	LEU	-	EXPRESSION TAG	UNP Q8A562
D	241	GLU	-	EXPRESSION TAG	UNP Q8A562
D	242	GLY	-	EXPRESSION TAG	UNP Q8A562
D	243	HIS	-	EXPRESSION TAG	UNP Q8A562
D	244	HIS	-	EXPRESSION TAG	UNP Q8A562
D	245	HIS	-	EXPRESSION TAG	UNP Q8A562
D	246	HIS	-	EXPRESSION TAG	UNP Q8A562
D	247	HIS	-	EXPRESSION TAG	UNP Q8A562
D	248	HIS	-	EXPRESSION TAG	UNP Q8A562

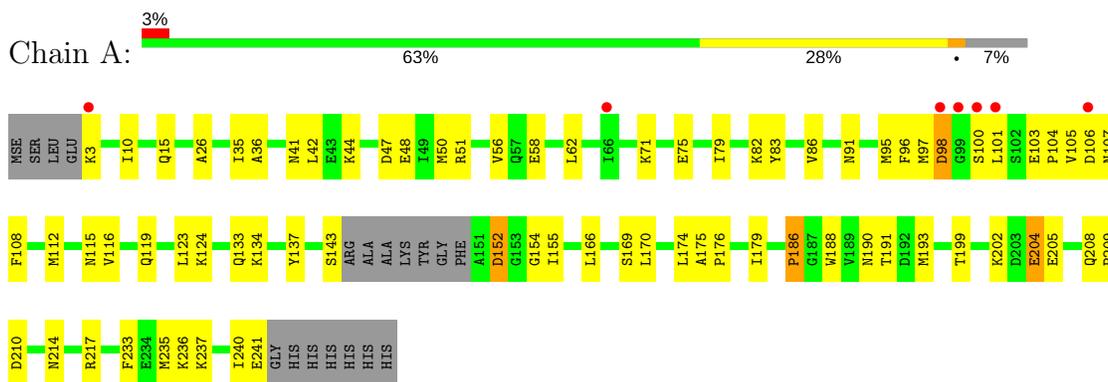
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	104	Total O 104 104	0	0
2	B	48	Total O 48 48	0	0
2	C	88	Total O 88 88	0	0
2	D	29	Total O 29 29	0	0

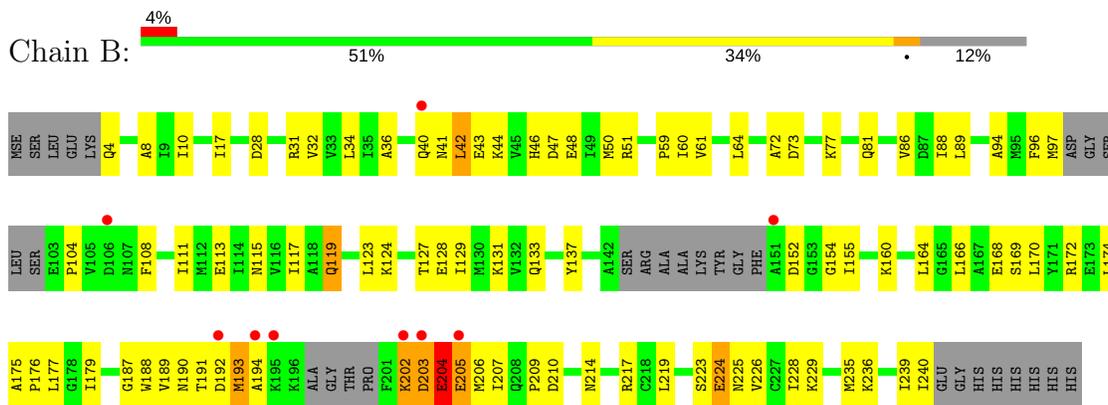
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 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.

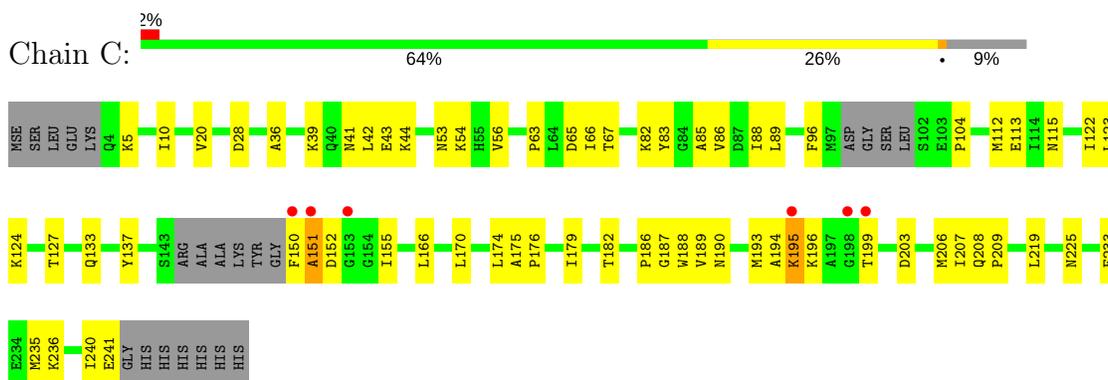
- Molecule 1: Putative oxidoreductase



- Molecule 1: Putative oxidoreductase



- Molecule 1: Putative oxidoreductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.88Å 105.72Å 78.83Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	45.83 – 2.16 45.83 – 2.05	Depositor EDS
% Data completeness (in resolution range)	92.8 (45.83-2.16) 97.8 (45.83-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.05Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.236 , 0.263 0.234 , 0.266	Depositor DCC
$R_{free}$ test set	2023 reflections (3.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.40	0/1793	0.66	0/2406
1	B	0.33	0/1704	0.65	0/2283
1	C	0.38	0/1769	0.66	0/2373
1	D	0.35	0/1657	0.68	1/2223 (0.0%)
All	All	0.37	0/6923	0.66	1/9285 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	MSE	CB-CG-SE	-8.74	86.48	112.70

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	1779	0	1841	66	0
1	B	1694	0	1758	100	0
1	C	1755	0	1813	70	0
1	D	1646	0	1705	100	0
2	A	104	0	0	8	0
2	B	48	0	0	12	0
2	C	88	0	0	8	0
2	D	29	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7143	0	7117	307	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 22.

The worst 5 of 307 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:190:ASN:HD22	1:A:208:GLN:HE22	1.09	0.96
1:A:86:VAL:H	1:A:133:GLN:HE22	1.11	0.93
1:C:124:LYS:HE2	1:D:104:PRO:HG2	1.50	0.92
1:B:96:PHE:H	1:B:115:ASN:HD21	1.17	0.92
1:B:97:MSE:HE3	1:B:111:ILE:HD13	1.52	0.91

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	228/250 (91%)	219 (96%)	8 (4%)	1 (0%)	38	32
1	B	212/250 (85%)	201 (95%)	9 (4%)	2 (1%)	20	12
1	C	222/250 (89%)	213 (96%)	8 (4%)	1 (0%)	32	25
1	D	205/250 (82%)	187 (91%)	11 (5%)	7 (3%)	4	1
All	All	867/1000 (87%)	820 (95%)	36 (4%)	11 (1%)	14	7

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	GLU
1	D	51	ARG

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Mol	Chain	Res	Type
1	A	98	ASP
1	B	193	MSE
1	D	16	GLY

### 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	195/200 (98%)	189 (97%)	6 (3%)	45	44
1	B	185/200 (92%)	175 (95%)	10 (5%)	26	20
1	C	192/200 (96%)	189 (98%)	3 (2%)	68	73
1	D	181/200 (90%)	171 (94%)	10 (6%)	25	19
All	All	753/800 (94%)	724 (96%)	29 (4%)	37	34

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	205	GLU
1	C	137	TYR
1	D	170	LEU
1	B	210	ASP
1	C	166	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	ASN
1	B	221	ASN
1	D	119	GLN
1	B	119	GLN
1	C	91	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

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, 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	224/250 (89%)	0.13	7 (3%) 49 58	20, 34, 59, 78	0
1	B	212/250 (84%)	0.39	9 (4%) 37 45	32, 49, 62, 69	0
1	C	220/250 (88%)	0.21	6 (2%) 55 63	19, 32, 58, 70	0
1	D	206/250 (82%)	0.51	16 (7%) 14 18	32, 50, 67, 73	0
All	All	862/1000 (86%)	0.30	38 (4%) 35 43	19, 42, 64, 78	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	151	ALA	6.6
1	A	99	GLY	5.6
1	D	4	GLN	5.4
1	D	189	VAL	5.2
1	C	198	GLY	4.8

### 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.