



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:29 am BST

PDB ID : 1FTE  
Title : CRYSTAL STRUCTURE OF STREPTOCOCCUS PNEUMONIAE ACYL  
CARRIER PROTEIN SYNTHASE (NATIVE 1)  
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Deposited on : 2000-09-12  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

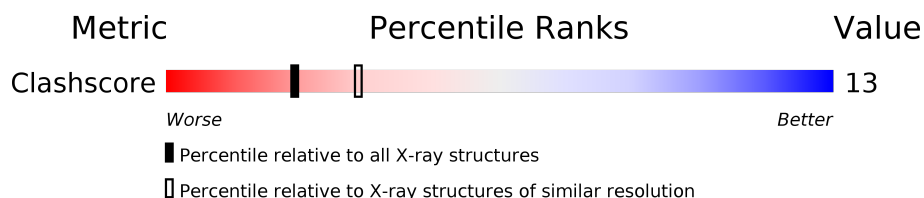
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)

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 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	122	 68% 26% • 5%
1	B	122	 79% 16% 5%
1	C	122	 69% 22% 9%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2793 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 ACYL CARRIER PROTEIN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			909	578	157	171	3			
1	B	116	Total	C	N	O	S	0	0	0
			909	578	157	171	3			
1	C	111	Total	C	N	O	S	0	0	0
			874	555	151	165	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	MET	-	CLONING ARTIFACT	UNP P0A2W6
A	1002	ARG	-	CLONING ARTIFACT	UNP P0A2W6
A	1035	LEU	GLN	CONFLICT	UNP P0A2W6
B	2001	MET	-	CLONING ARTIFACT	UNP P0A2W6
B	2002	ARG	-	CLONING ARTIFACT	UNP P0A2W6
B	2035	LEU	GLN	CONFLICT	UNP P0A2W6
C	3001	MET	-	CLONING ARTIFACT	UNP P0A2W6
C	3002	ARG	-	CLONING ARTIFACT	UNP P0A2W6
C	3035	LEU	GLN	CONFLICT	UNP P0A2W6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	38	Total	O	0	0
			38	38		
3	C	24	Total	O	0	0
			24	24		

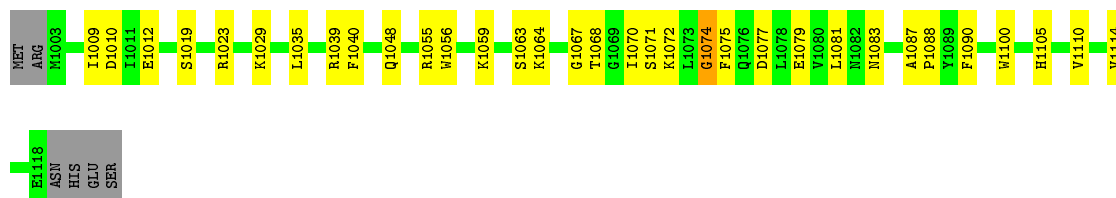
### 3 Residue-property plots [i](#)

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. 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.

Note EDS was not executed.

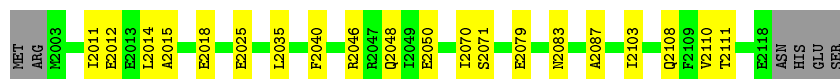
#### • Molecule 1: ACYL CARRIER PROTEIN SYNTHASE

Chain A: 



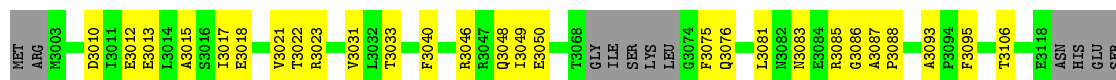
#### • Molecule 1: ACYL CARRIER PROTEIN SYNTHASE

Chain B: 



#### • Molecule 1: ACYL CARRIER PROTEIN SYNTHASE

Chain C: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.82Å 59.56Å 113.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	91.2 (20.00-2.40)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNX	Depositor
R, $R_{free}$	0.229 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.44	0/926	0.72	2/1245 (0.2%)
1	B	0.44	0/926	0.59	0/1245
1	C	0.39	0/890	0.57	0/1196
All	All	0.42	0/2742	0.63	2/3686 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1074	GLY	O-C-N	-12.44	102.79	122.70
1	A	1074	GLY	CA-C-N	8.20	135.23	117.20

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	909	0	904	29	0
1	B	909	0	904	24	0
1	C	874	0	860	22	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	38	0	0	0	0
3	C	24	0	0	0	0
All	All	2793	0	2668	67	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 13.

All (67) 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:1083:ASN:ND2	1:A:1087:ALA:H	1.80	0.79
1:B:2083:ASN:HD21	1:B:2087:ALA:H	1.33	0.76
1:A:1083:ASN:HD21	1:A:1087:ALA:H	1.36	0.74
1:C:3046:ARG:O	1:C:3050:GLU:HG3	1.87	0.74
1:B:2070:ILE:HG13	1:B:2071:SER:N	2.05	0.72
1:A:1074:GLY:HA3	1:A:1077:ASP:OD2	1.90	0.71
1:B:2046:ARG:O	1:B:2050:GLU:HG3	1.90	0.71
1:B:2040:PHE:CE1	1:B:2048:GLN:HG2	2.28	0.69
1:B:2083:ASN:ND2	1:B:2087:ALA:H	1.91	0.68
1:B:2070:ILE:HG13	1:B:2071:SER:H	1.61	0.66
1:A:1040:PHE:CE1	1:A:1048:GLN:HG2	2.33	0.64
1:C:3013:GLU:OE2	1:C:3015:ALA:HB3	1.97	0.64
1:B:2070:ILE:HG23	1:C:3086:GLY:HA3	1.81	0.63
1:A:1105:HIS:HB3	1:A:1110:VAL:HG23	1.84	0.60
1:C:3083:ASN:HD22	1:C:3083:ASN:C	2.07	0.58
1:A:1063:SER:HB3	1:A:1068:THR:HG21	1.85	0.58
1:B:2083:ASN:HD22	1:B:2083:ASN:C	2.06	0.58
1:A:1019:SER:O	1:A:1023:ARG:HG3	2.05	0.57
1:B:2035:LEU:HB2	1:B:2079:GLU:OE2	2.05	0.57
1:C:3046:ARG:O	1:C:3049:ILE:HG22	2.06	0.56
1:A:1083:ASN:C	1:A:1083:ASN:HD22	2.08	0.56
1:A:1064:LYS:NZ	1:B:2103:ILE:O	2.39	0.56
1:C:3040:PHE:CE1	1:C:3048:GLN:HG2	2.42	0.55
1:A:1010:ASP:OD1	1:A:1012:GLU:HG2	2.07	0.54
1:A:1009:ILE:HD12	1:B:2111:THR:HG23	1.89	0.54
1:C:3083:ASN:HD21	1:C:3087:ALA:H	1.57	0.52
1:A:1029:LYS:HD3	1:A:1029:LYS:O	2.10	0.52
1:C:3083:ASN:ND2	1:C:3087:ALA:H	2.08	0.51
1:B:2015:ALA:O	1:B:2018:GLU:HB2	2.11	0.50
1:B:2012:GLU:HB2	1:B:2110:VAL:HG12	1.94	0.50
1:A:1035:LEU:HD12	1:A:1079:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:LEU:O	1:A:1088:PRO:HA	2.12	0.49
1:A:1074:GLY:O	1:A:1075:PHE:C	2.51	0.49
1:C:3081:LEU:O	1:C:3088:PRO:HA	2.13	0.48
1:B:2070:ILE:CG1	1:B:2071:SER:N	2.75	0.48
1:B:2011:ILE:HG23	1:C:3106:THR:HG23	1.95	0.47
1:B:2070:ILE:CG1	1:B:2071:SER:H	2.27	0.47
1:A:1009:ILE:CD1	1:B:2111:THR:HG23	2.45	0.46
1:B:2012:GLU:HB2	1:B:2110:VAL:CG1	2.45	0.46
1:A:1009:ILE:O	1:A:1064:LYS:NZ	2.44	0.46
1:C:3018:GLU:O	1:C:3021:VAL:N	2.49	0.46
1:C:3031:VAL:HG13	1:C:3075:PHE:HD2	1.81	0.46
1:B:2070:ILE:HG12	1:C:3085:ARG:O	2.17	0.44
1:A:1068:THR:HG23	1:A:1071:SER:O	2.16	0.44
1:B:2070:ILE:HG23	1:C:3085:ARG:O	2.16	0.44
1:A:1056:TRP:C	1:A:1056:TRP:CD1	2.91	0.44
1:A:1039:ARG:HG3	1:A:1039:ARG:HH21	1.83	0.44
1:A:1055:ARG:O	1:A:1059:LYS:HG3	2.18	0.44
1:B:2070:ILE:N	1:C:3085:ARG:O	2.46	0.44
1:A:1079:GLU:O	1:A:1090:PHE:HA	2.18	0.43
1:C:3083:ASN:ND2	1:C:3083:ASN:C	2.70	0.43
1:B:2083:ASN:ND2	1:B:2087:ALA:N	2.63	0.43
1:A:1064:LYS:O	1:A:1067:GLY:N	2.44	0.43
1:A:1070:ILE:HG13	1:A:1071:SER:N	2.34	0.43
1:A:1039:ARG:NH2	1:A:1039:ARG:HG3	2.34	0.43
1:A:1100:TRP:O	1:A:1114:VAL:HA	2.19	0.43
1:C:3093:ALA:O	1:C:3095:PHE:N	2.45	0.43
1:C:3010:ASP:OD2	1:C:3012:GLU:HG2	2.18	0.43
1:A:1071:SER:O	1:A:1072:LYS:HG3	2.19	0.42
1:A:1083:ASN:C	1:A:1083:ASN:ND2	2.73	0.42
1:B:2014:LEU:HD23	1:B:2108:GLN:C	2.38	0.42
1:C:3022:THR:O	1:C:3023:ARG:O	2.37	0.42
1:C:3017:ILE:O	1:C:3021:VAL:HG23	2.20	0.42
1:B:2025:GLU:HG3	1:B:2025:GLU:O	2.19	0.41
1:C:3033:THR:HA	1:C:3076:GLN:HE22	1.85	0.41
1:C:3085:ARG:HG3	1:C:3085:ARG:HH11	1.86	0.41
1:A:1012:GLU:HB2	1:A:1110:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

2 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	SO4	C	1200	-	4,4,4	0.65	0	6,6,6	0.19	0
2	SO4	B	2200	-	4,4,4	0.41	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.