

# Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 - 06:28 pm GMT

PDB ID : 1H4F

Title : E. COLI BETA-KETOACYL [ACYL CARRIER PROTEIN] SYNTHASE I

K328R

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Deposited on : 2003-02-26

Resolution : 2.00 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*A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : FAILED Xtriage (Phenix) : 1.13

EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

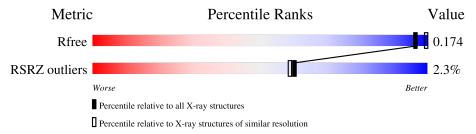
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.00 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 $(\#  ext{Entries})$	Similar resolution $(\#\text{Entries}, \text{resolution range}(\text{Å}))$			
$R_{free}$	130704	8085 (2.00-2.00)			
RSRZ outliers	127900	7900 (2.00-2.00)			

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12848 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 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I.

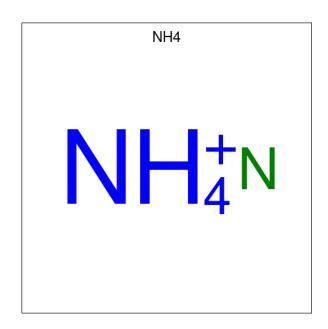
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	406	Total	С	N	О	S	0	0	1
1	A	400	2975	1849	521	582	23	U	U	1
1	В	406	Total	С	N	О	S	0	0	0
1	Б	400	2983	1853	521	586	23	U		U
1	C	406	Total	С	N	О	S	0	0	0
1		400	2983	1853	521	586	23	U		
1	D	406	Total	С	N	О	S	0	0	1
1	ע	400	2975	1849	521	582	23	U	0	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	ARG	LYS	engineered mutation	UNP P14926
В	328	ARG	LYS	engineered mutation	UNP P14926
С	328	ARG	LYS	engineered mutation	UNP P14926
D	328	ARG	LYS	engineered mutation	UNP P14926

• Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Λ	1	Total N	0	0
	A	1	1 1	0	0
2	D	1	Total N		0
	Б	1	1 1	0	U
2	С	1	Total N	0	0
		1	1 1	0	0
2	D	1	Total N	0	0
	ש	1	$\begin{vmatrix} 1 & 1 \end{vmatrix}$		U

#### • Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	223	Total O 223 223	0	0
3	В	265	Total O 265 265	0	0
3	С	250	Total O 250 250	0	0
3	D	190	Total O 190 190	0	0

MolProbity failed to run properly - this section is therefore empty.



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	58.93Å 139.04Å 211.66Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 - 2.00	Depositor
Resolution (A)	29.94 - 1.82	EDS
% Data completeness	90.1 (29.94-2.00)	Depositor
(in resolution range)	87.4 (29.94-1.82)	EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.18 (at 1.82Å)	Xtriage
Refinement program	CNS 1.1	Depositor
$R, R_{free}$	0.178 , $0.227$	Depositor
It, It free	0.175 , $0.174$	DCC
$R_{free}$ test set	6894  reflections  (5.02%)	wwPDB-VP
Wilson B-factor $(\mathring{A}^2)$	17.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38, 51.9	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 4 Model quality (i)

### 4.1 Standard geometry (i)

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### 4.2 Too-close contacts (i)

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### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

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#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are modelled with single atom - leaving 0 for Mogul analysis.

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.

## 4.7 Other polymers (i)

There are no such residues in this entry.

# 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 5 Fit of model and data (i)

### 5.1 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,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	406/406 (100%)	-0.03	16 (3%) 39 38	6, 19, 39, 55	0
1	В	406/406 (100%)	-0.44	1 (0%) 95 94	4, 13, 30, 55	0
1	С	406/406 (100%)	-0.29	8 (1%) 65 63	6, 15, 30, 70	0
1	D	406/406 (100%)	-0.11	12 (2%) 50 49	8, 18, 34, 54	0
All	All	1624/1624 (100%)	-0.22	37 (2%) 60 59	4, 16, 35, 70	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	406	ASP	9.5
1	A	406	ASP	9.4
1	С	404	LEU	8.4
1	С	405	LYS	5.5
1	D	271	ALA	5.5
1	В	406	ASP	5.4
1	D	270	VAL	5.1
1	A	319	ASP	4.8
1	D	1	MET	4.8
1	A	370	GLY	4.4
1	С	1	MET	3.9
1	С	270	VAL	3.7
1	D	213	ASP	3.6
1	С	271	ALA	3.6
1	A	213	ASP	3.2
1	D	62	ARG	3.2
1	A	320	LYS	3.2
1	D	268	ASP	3.0
1	D	366	GLU	2.9
1	A	303	PRO	2.7
1	A	318	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	405	LYS	2.5
1	A	371	LEU	2.4
1	С	286	HIS	2.4
1	С	268	ASP	2.4
1	A	62	ARG	2.3
1	D	273	SER	2.3
1	A	405	LYS	2.2
1	A	214	THR	2.2
1	D	272	PRO	2.2
1	D	57	THR	2.1
1	A	225	HIS	2.1
1	A	372	ASN	2.1
1	A	314	ARG	2.1
1	A	317	PHE	2.0
1	D	90	PRO	2.0
1	A	30	ARG	2.0

#### 5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

### 5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.4 Ligands (i)

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. The B-factors column lists the minimum, median,  $95^{th}$  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	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	NH4	A	1406	1/1	0.95	0.30	17,17,17,17	0
2	NH4	С	1407	1/1	0.97	0.27	10,10,10,10	0
2	NH4	D	1406	1/1	0.98	0.36	12,12,12,12	0
2	NH4	В	1407	1/1	0.99	0.27	9,9,9,9	0



# 5.5 Other polymers (i)

There are no such residues in this entry.

