wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 06:45 am GMT

PDB ID	:	2VB8
Title	:	beta-ketoacyl-ACP synthase I (KAS) from E. coli with bound inhibitor thiolactomycin
Authors	:	Pappenberger, G.; Schulz-Gasch, T.; Bailly, J.; Hennig, M.
Deposited on	:	2007-09-06
Resolution	:	1.52 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*
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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
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

PERCENTILES INFOmissingINFO

1 Entry composition

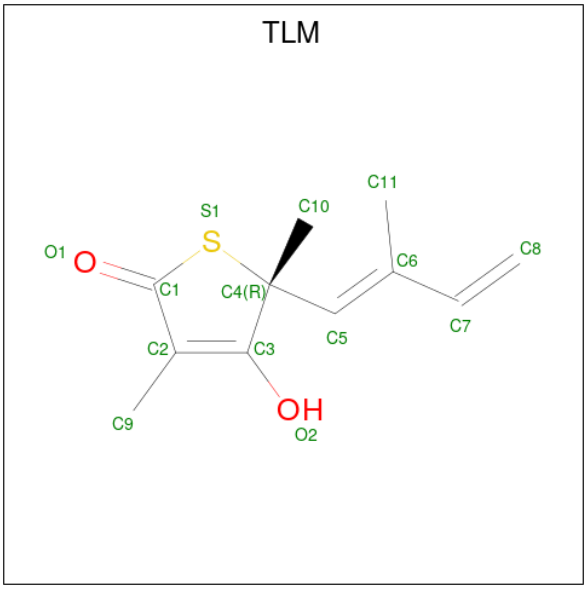
There are 4 unique types of molecules in this entry. The entry contains 14694 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	23	1
			2983	1859	515	581	28			
1	B	404	Total	C	N	O	S	0	27	1
			3002	1867	522	588	25			
1	C	406	Total	C	N	O	S	0	21	1
			2997	1869	517	584	27			
1	D	404	Total	C	N	O	S	0	28	1
			3009	1868	522	592	27			

- Molecule 2 is THIOLACTOMYCIN (three-letter code: TLM) (formula: $C_{11}H_{14}O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			14	11	2	1		
2	B	1	Total	C	O	S	0	0
			14	11	2	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O S 14 11 2 1	0	0
2	D	1	Total C O S 14 11 2 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is water.

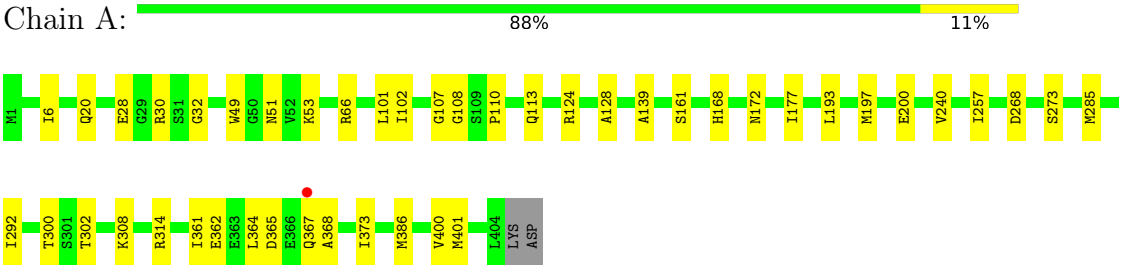
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	679	Total O 679 679	0	0
4	B	667	Total O 667 667	0	0
4	C	679	Total O 679 679	0	0
4	D	620	Total O 620 620	0	0

2 Residue-property plots (i)

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 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.

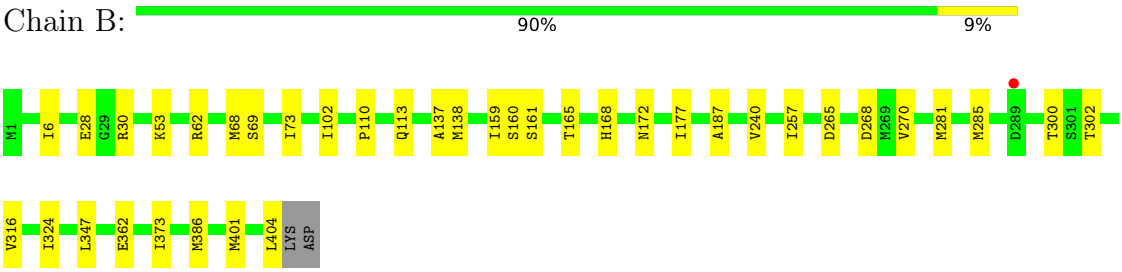
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

Chain A:



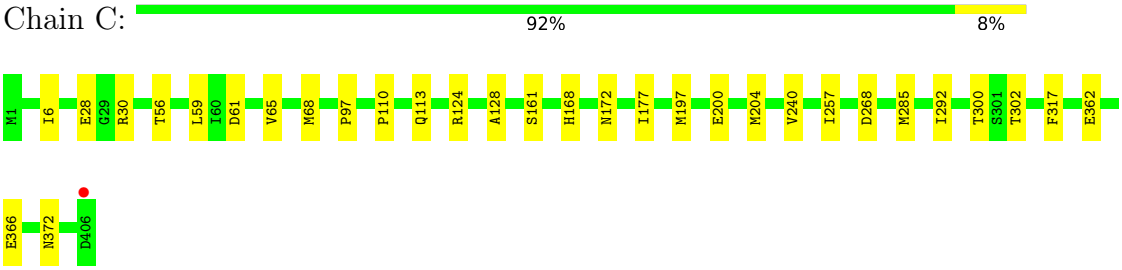
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

Chain B:



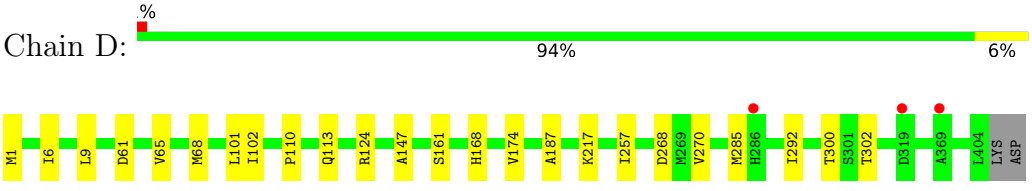
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

Chain C:



• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

Chain D:



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.14Å 138.34Å 211.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 1.52 19.91 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.3 (119.52-1.52) 99.4 (19.91-1.52)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.151 , 0.185 0.150 , 0.183	Depositor DCC
R_{free} test set	13446 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	12.8	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 69.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14694	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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.

4 Model quality

4.1 Standard geometry

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

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	0.69	0/3157	0.72	0/4262
1	B	0.71	0/3206	0.76	1/4328 (0.0%)
1	C	0.71	0/3161	0.76	0/4265
1	D	0.69	0/3211	0.72	0/4333
All	All	0.70	0/12735	0.74	1/17188 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	265	ASP	CB-CG-OD2	-5.29	113.54	118.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2983	0	2921	68	0
1	B	3002	0	2941	49	0
1	C	2997	0	2946	33	0
1	D	3009	0	2936	30	0
2	A	14	0	13	1	0
2	B	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	14	0	13	0	0
2	D	14	0	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	679	0	0	17	3
4	B	667	0	0	10	3
4	C	679	0	0	12	4
4	D	620	0	0	13	4
All	All	14694	0	11796	171	7

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 7.

The worst 5 of 171 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:D:268:ASP:HB2	4:D:2487:HOH:O	1.46	1.12
1:D:285[A]:MET:CE	4:D:2514:HOH:O	2.04	1.06
1:C:268[A]:ASP:OD1	4:C:2514:HOH:O	1.73	1.05
1:B:268[A]:ASP:OD1	4:B:2495:HOH:O	1.76	1.04
1:A:314[B]:ARG:NH2	1:A:367:GLN:O	1.91	1.04

The worst 5 of 7 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	Interatomic distance (Å)	Clash overlap (Å)
4:A:2590:HOH:O	4:B:2636:HOH:O[3_655]	1.79	0.41
4:C:2213:HOH:O	4:D:2065:HOH:O[1_455]	1.95	0.25
4:C:2276:HOH:O	4:D:2060:HOH:O[1_455]	1.99	0.21
4:A:2491:HOH:O	4:B:2092:HOH:O[1_455]	2.09	0.11
4:A:2639:HOH:O	4:B:2645:HOH:O[3_655]	2.14	0.06

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains

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

4.3.3 RNA

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	TLM	D	1405	-	7,14,14	0.90	0	10,21,21	1.50	2 (20%)
2	TLM	C	1405	-	7,14,14	1.16	1 (14%)	10,21,21	1.59	2 (20%)
2	TLM	A	1405	-	7,14,14	0.81	0	10,21,21	1.51	3 (30%)
2	TLM	B	1405	-	7,14,14	0.72	0	10,21,21	1.69	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLM	D	1405	-	-	0/4/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLM	C	1405	-	-	0/4/26/26	0/1/1/1
2	TLM	A	1405	-	-	0/4/26/26	0/1/1/1
2	TLM	B	1405	-	-	0/4/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1405	TLM	C7-C6	2.30	1.50	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1405	TLM	C9-C2-C3	-3.61	121.94	131.27
2	B	1405	TLM	C9-C2-C3	-3.46	122.33	131.27
2	D	1405	TLM	O1-C1-C2	-3.19	122.60	128.35
2	A	1405	TLM	C9-C2-C3	-2.80	124.04	131.27
2	C	1405	TLM	C1-C2-C3	2.66	113.99	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1405	TLM	2	0
2	A	1405	TLM	1	0
2	B	1405	TLM	1	0

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

5.1 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^{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>2			OWAB(Å^2)	Q<0.9
1	A	404/406 (99%)	-0.45	1 (0%)	95	95	8, 13, 22, 39	0
1	B	404/406 (99%)	-0.55	1 (0%)	95	95	6, 11, 19, 34	0
1	C	406/406 (100%)	-0.53	1 (0%)	95	95	7, 11, 20, 35	0
1	D	404/406 (99%)	-0.37	3 (0%)	87	90	7, 13, 25, 45	0
All	All	1618/1624 (99%)	-0.47	6 (0%)	92	94	6, 12, 22, 45	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	319[A]	ASP	5.3
1	C	406	ASP	2.8
1	D	369	ALA	2.7
1	A	367	GLN	2.3
1	D	286	HIS	2.3

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

There are no monosaccharides in this entry.

5.4 Ligands

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	B-factors(Å^2)	Q<0.9
3	CL	A	1406	1/1	0.91	0.07	45,45,45,45	0
3	CL	B	1406	1/1	0.94	0.04	39,39,39,39	0
2	TLM	A	1405	14/14	0.95	0.09	13,15,19,20	0
2	TLM	D	1405	14/14	0.95	0.10	12,17,20,21	0
2	TLM	C	1405	14/14	0.96	0.08	11,15,17,19	0
2	TLM	B	1405	14/14	0.96	0.08	11,16,18,19	0

5.5 Other polymers (i)

There are no such residues in this entry.