



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 01:25 pm BST

PDB ID : 9S5H / pdb_00009s5h
Title : anammox-specific heterodimeric ketoacyl-ACP synthase (amxFabFhet) from *Brocadia fulgida*
Authors : Granatino, P.; Barends, T.
Deposited on : 2025-07-29
Resolution : 2.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

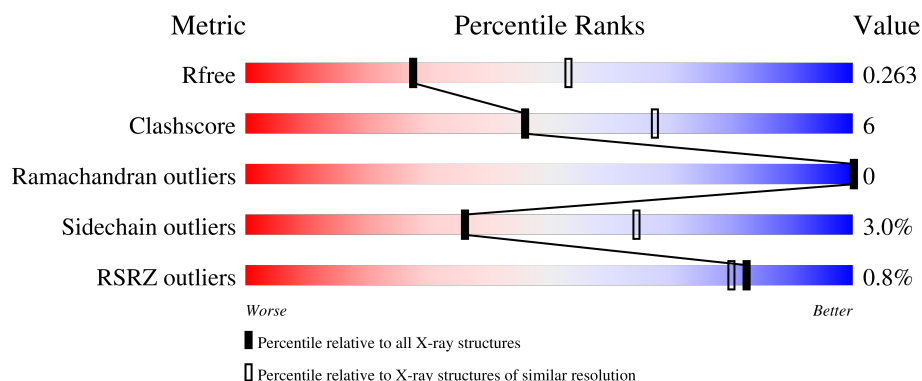
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. 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	413	 86% 14%
1	B	413	 77% 20% 3%
1	E	413	 86% 12% 2%
1	G	413	 82% 17% 1%
1	I	413	 83% 15% 2%

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Mol	Chain	Length	Quality of chain
1	K	413	% 81%16% ..
2	C	412	% 85%14% .
2	D	412	% 87%13%
2	F	412	% 85%14%
2	H	412	% 81%19%
2	J	412	% 84%15% .
2	L	412	% 81%18%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 37500 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	405	Total	C	N	O	S	0	0	0
			3022	1913	516	574	19			
1	A	413	Total	C	N	O	S	0	0	0
			3087	1956	526	585	20			
1	E	408	Total	C	N	O	S	0	0	0
			3039	1923	519	577	20			
1	G	413	Total	C	N	O	S	0	0	0
			3087	1956	526	585	20			
1	I	405	Total	C	N	O	S	0	0	0
			3022	1913	516	574	19			
1	K	404	Total	C	N	O	S	0	0	0
			3014	1909	514	572	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASN	-	expression tag	UNP A0A0M2USV6
B	-3	LEU	-	expression tag	UNP A0A0M2USV6
B	-2	TYR	-	expression tag	UNP A0A0M2USV6
B	-1	PHE	-	expression tag	UNP A0A0M2USV6
B	0	GLN	-	expression tag	UNP A0A0M2USV6
B	1	GLY	-	expression tag	UNP A0A0M2USV6
B	2	ALA	-	expression tag	UNP A0A0M2USV6
A	-4	ASN	-	expression tag	UNP A0A0M2USV6
A	-3	LEU	-	expression tag	UNP A0A0M2USV6
A	-2	TYR	-	expression tag	UNP A0A0M2USV6
A	-1	PHE	-	expression tag	UNP A0A0M2USV6
A	0	GLN	-	expression tag	UNP A0A0M2USV6
A	1	GLY	-	expression tag	UNP A0A0M2USV6
A	2	ALA	-	expression tag	UNP A0A0M2USV6
E	-4	ASN	-	expression tag	UNP A0A0M2USV6
E	-3	LEU	-	expression tag	UNP A0A0M2USV6
E	-2	TYR	-	expression tag	UNP A0A0M2USV6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PHE	-	expression tag	UNP A0A0M2USV6
E	0	GLN	-	expression tag	UNP A0A0M2USV6
E	1	GLY	-	expression tag	UNP A0A0M2USV6
E	2	ALA	-	expression tag	UNP A0A0M2USV6
G	-4	ASN	-	expression tag	UNP A0A0M2USV6
G	-3	LEU	-	expression tag	UNP A0A0M2USV6
G	-2	TYR	-	expression tag	UNP A0A0M2USV6
G	-1	PHE	-	expression tag	UNP A0A0M2USV6
G	0	GLN	-	expression tag	UNP A0A0M2USV6
G	1	GLY	-	expression tag	UNP A0A0M2USV6
G	2	ALA	-	expression tag	UNP A0A0M2USV6
I	-4	ASN	-	expression tag	UNP A0A0M2USV6
I	-3	LEU	-	expression tag	UNP A0A0M2USV6
I	-2	TYR	-	expression tag	UNP A0A0M2USV6
I	-1	PHE	-	expression tag	UNP A0A0M2USV6
I	0	GLN	-	expression tag	UNP A0A0M2USV6
I	1	GLY	-	expression tag	UNP A0A0M2USV6
I	2	ALA	-	expression tag	UNP A0A0M2USV6
K	-4	ASN	-	expression tag	UNP A0A0M2USV6
K	-3	LEU	-	expression tag	UNP A0A0M2USV6
K	-2	TYR	-	expression tag	UNP A0A0M2USV6
K	-1	PHE	-	expression tag	UNP A0A0M2USV6
K	0	GLN	-	expression tag	UNP A0A0M2USV6
K	1	GLY	-	expression tag	UNP A0A0M2USV6
K	2	ALA	-	expression tag	UNP A0A0M2USV6

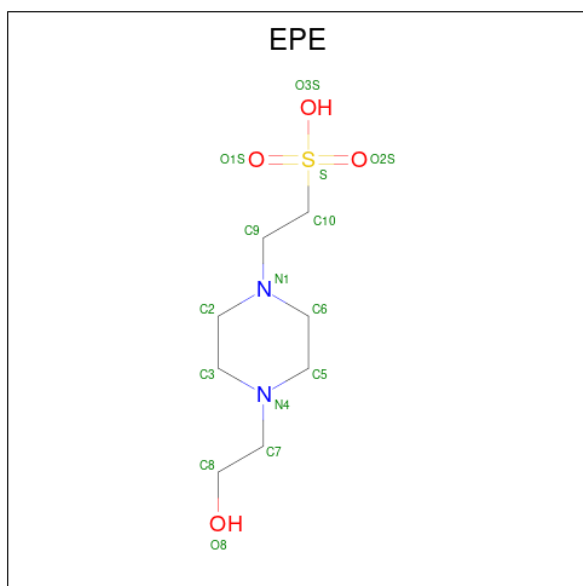
- Molecule 2 is a protein called 3-oxoacyl-(Acyl-carrier-protein) synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	411	Total	C	N	O	S	0	0	0
			3120	1965	535	607	13			
2	D	412	Total	C	N	O	S	0	0	0
			3129	1970	536	610	13			
2	F	412	Total	C	N	O	S	0	0	0
			3129	1970	536	610	13			
2	H	412	Total	C	N	O	S	0	0	0
			3129	1970	536	610	13			
2	J	410	Total	C	N	O	S	0	0	0
			3111	1959	533	606	13			
2	L	411	Total	C	N	O	S	0	0	0
			3120	1965	535	607	13			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).

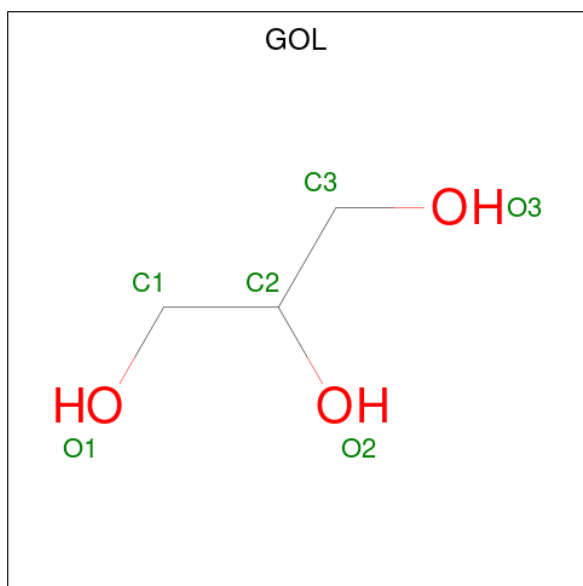


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0
6	F	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0
6	H	1	Total O P 5 4 1	0	0
6	L	1	Total O P 5 4 1	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

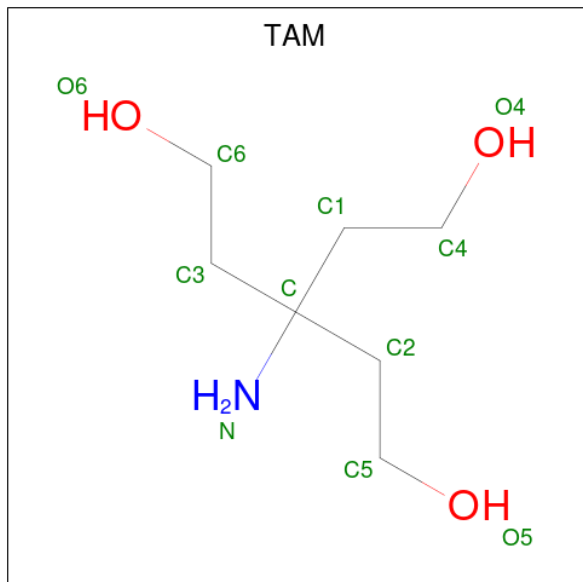
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0
8	J	1	Total C O 6 3 3	0	0

- Molecule 9 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			11	7	1	3		
9	J	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	29	Total	O	0	0
			29	29		
10	C	40	Total	O	0	0
			40	40		
10	A	27	Total	O	0	0
			27	27		
10	D	29	Total	O	0	0
			29	29		
10	E	31	Total	O	0	0
			31	31		
10	F	19	Total	O	0	0
			19	19		
10	G	34	Total	O	0	0
			34	34		
10	H	32	Total	O	0	0
			32	32		

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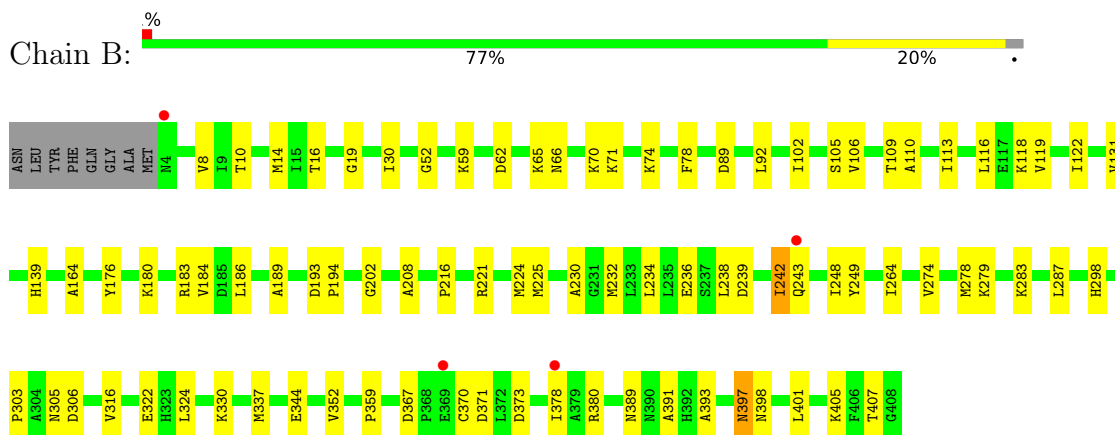
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	I	35	Total 35	O 35	0	0
10	J	27	Total 27	O 27	0	0
10	K	25	Total 25	O 25	0	0
10	L	20	Total 20	O 20	0	0

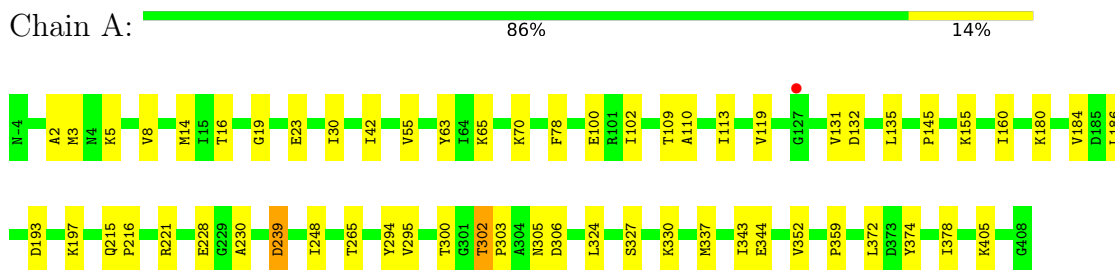
3 Residue-property plots

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.

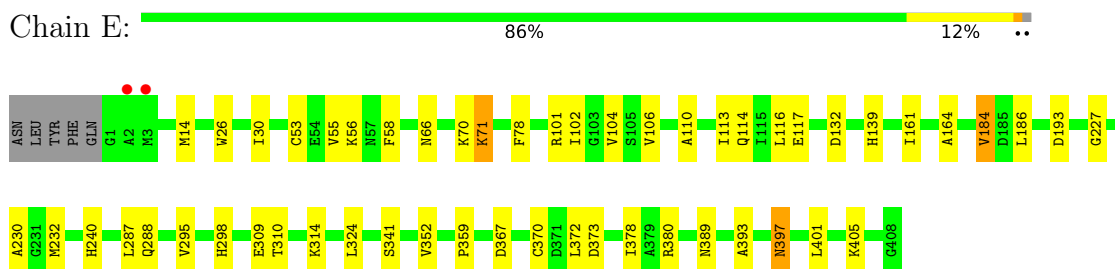
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) synthase



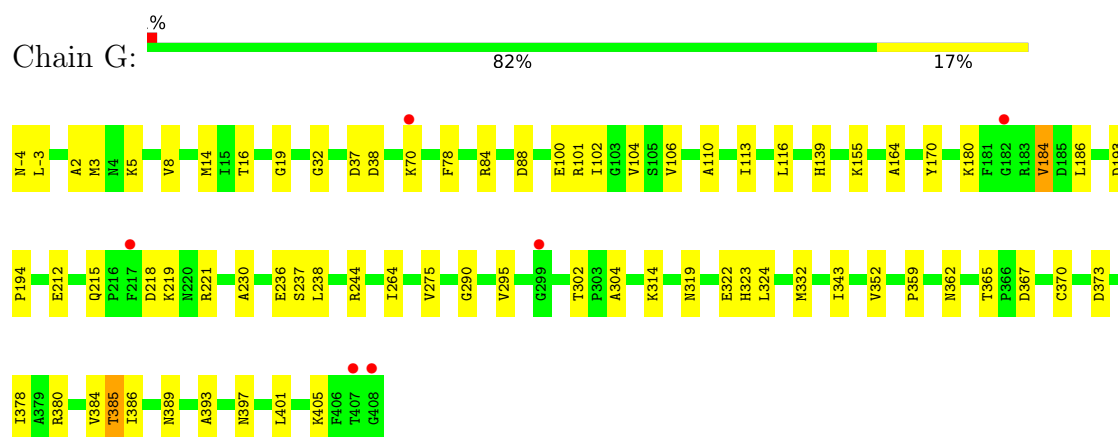
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) synthase



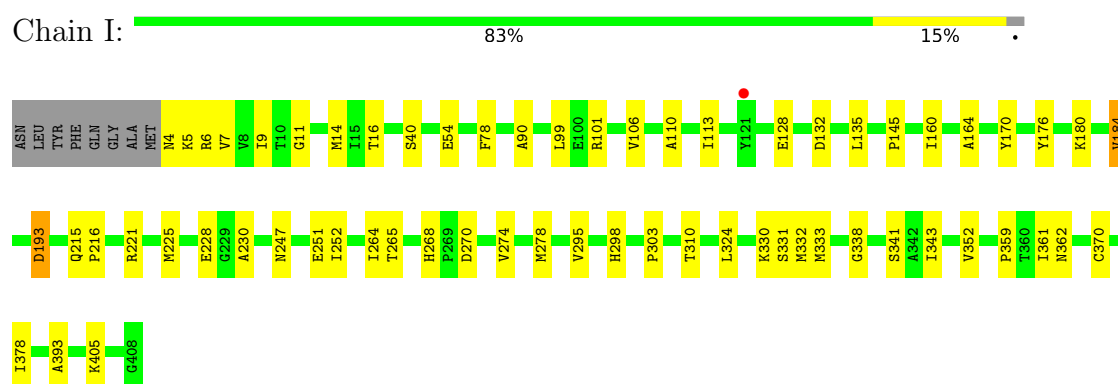
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) synthase



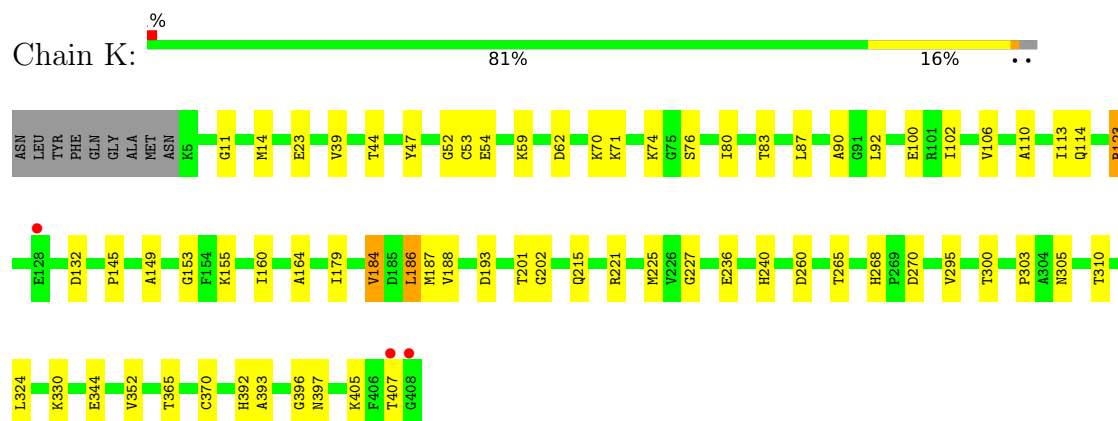
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) synthase



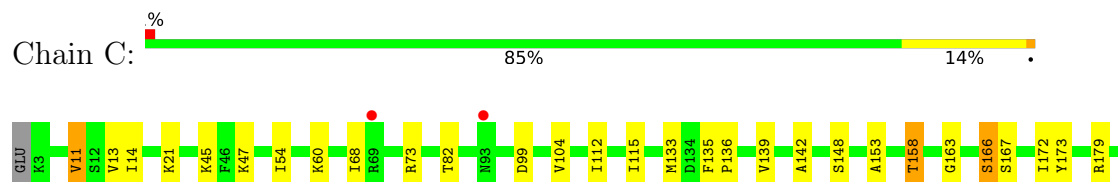
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) synthase

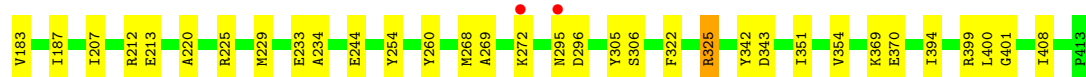


- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) synthase

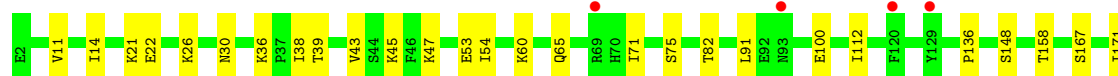
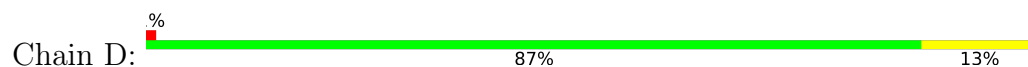


- Molecule 2: 3-oxoacyl-(Acyl-carrier-protein) synthase

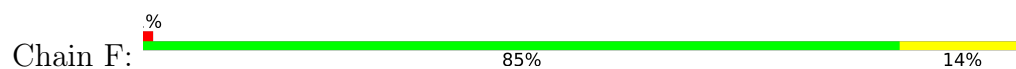




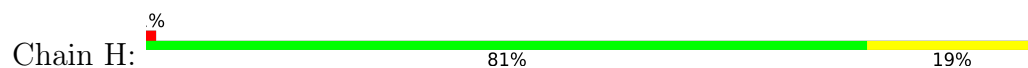
- Molecule 2: 3-oxoacyl-(Acyl-carrier-protein) synthase



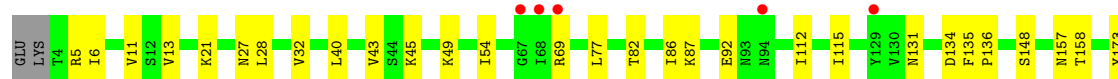
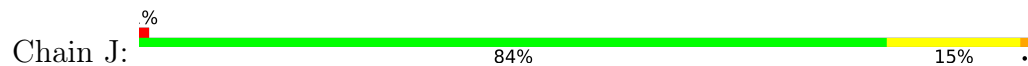
- Molecule 2: 3-oxoacyl-(Acyl-carrier-protein) synthase

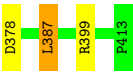


- Molecule 2: 3-oxoacyl-(Acyl-carrier-protein) synthase

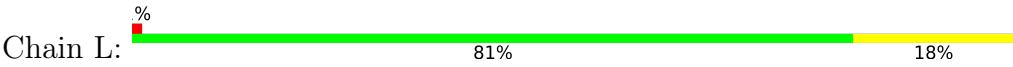


- Molecule 2: 3-oxoacyl-(Acyl-carrier-protein) synthase





● Molecule 2: 3-oxoacyl-(Acyl-carrier-protein) synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.92Å 119.96Å 374.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.60 48.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.86-2.60) 99.6 (48.86-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.267 0.213 , 0.263	Depositor DCC
R_{free} test set	7884 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	37500	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, TAM, 1PE, GOL, MG, PO4, 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	0.10	0/3147	0.29	0/4259
1	B	0.10	0/3080	0.30	0/4169
1	E	0.10	0/3097	0.29	0/4191
1	G	0.09	0/3147	0.28	0/4259
1	I	0.10	0/3080	0.28	0/4169
1	K	0.09	0/3072	0.28	0/4158
2	C	0.09	0/3172	0.26	0/4297
2	D	0.10	0/3181	0.27	0/4309
2	F	0.09	0/3181	0.26	0/4309
2	H	0.09	0/3181	0.26	0/4309
2	J	0.10	0/3163	0.28	0/4286
2	L	0.11	0/3172	0.28	0/4297
All	All	0.10	0/37673	0.28	0/51012

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	243	GLN	Peptide

5.2 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	3087	0	3098	33	0
1	B	3022	0	3035	47	0
1	E	3039	0	3055	28	0
1	G	3087	0	3098	41	0
1	I	3022	0	3035	33	0
1	K	3014	0	3029	41	0
2	C	3120	0	3136	40	0
2	D	3129	0	3142	25	0
2	F	3129	0	3142	33	0
2	H	3129	0	3142	46	0
2	J	3111	0	3123	39	0
2	L	3120	0	3136	42	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	B	15	0	17	4	0
5	C	16	0	22	3	0
5	D	12	0	15	0	0
5	F	16	0	22	2	0
5	H	8	0	9	1	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	G	5	0	0	0	0
6	H	5	0	0	0	0
6	L	5	0	0	0	0
7	A	1	0	0	1	0
8	D	6	0	8	1	0
8	F	6	0	8	0	0
8	J	6	0	8	1	0
9	H	11	0	17	5	0
9	J	11	0	17	3	0
10	A	27	0	0	1	0
10	B	29	0	0	1	0
10	C	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	29	0	0	1	0
10	E	31	0	0	1	0
10	F	19	0	0	2	0
10	G	34	0	0	0	0
10	H	32	0	0	3	0
10	I	35	0	0	0	0
10	J	27	0	0	1	0
10	K	25	0	0	0	0
10	L	20	0	0	1	0
All	All	37500	0	37314	432	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 6.

The worst 5 of 432 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:5:LYS:NZ	1:A:239:ASP:OD2	2.09	0.85
2:J:241:GLU:OE2	2:J:249:ARG:NH2	2.13	0.81
1:A:2:ALA:O	1:A:180:LYS:NZ	2.14	0.80
2:H:229:MET:HE1	9:H:502:TAM:H22	1.69	0.74
2:F:46:PHE:O	2:F:49:LYS:NZ	2.22	0.73

There are no symmetry-related clashes.

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	411/413 (100%)	402 (98%)	9 (2%)	0	100	100
1	B	403/413 (98%)	392 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	406/413 (98%)	394 (97%)	12 (3%)	0	100	100
1	G	411/413 (100%)	401 (98%)	10 (2%)	0	100	100
1	I	403/413 (98%)	390 (97%)	13 (3%)	0	100	100
1	K	402/413 (97%)	396 (98%)	6 (2%)	0	100	100
2	C	409/412 (99%)	399 (98%)	10 (2%)	0	100	100
2	D	410/412 (100%)	401 (98%)	9 (2%)	0	100	100
2	F	410/412 (100%)	400 (98%)	10 (2%)	0	100	100
2	H	410/412 (100%)	402 (98%)	8 (2%)	0	100	100
2	J	408/412 (99%)	399 (98%)	9 (2%)	0	100	100
2	L	409/412 (99%)	399 (98%)	10 (2%)	0	100	100
All	All	4892/4950 (99%)	4775 (98%)	117 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	326/326 (100%)	318 (98%)	8 (2%)	42	69
1	B	320/326 (98%)	310 (97%)	10 (3%)	35	63
1	E	321/326 (98%)	313 (98%)	8 (2%)	42	69
1	G	326/326 (100%)	318 (98%)	8 (2%)	42	69
1	I	320/326 (98%)	312 (98%)	8 (2%)	42	69
1	K	319/326 (98%)	311 (98%)	8 (2%)	42	69
2	C	341/342 (100%)	330 (97%)	11 (3%)	34	62
2	D	342/342 (100%)	332 (97%)	10 (3%)	37	65
2	F	342/342 (100%)	332 (97%)	10 (3%)	37	65
2	H	342/342 (100%)	329 (96%)	13 (4%)	29	56
2	J	340/342 (99%)	330 (97%)	10 (3%)	37	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	341/342 (100%)	326 (96%)	15 (4%)	25	50
All	All	3980/4008 (99%)	3861 (97%)	119 (3%)	36	64

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3	MET
2	L	148	SER
2	H	224	LYS
2	L	94	ASN
2	L	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	279	ASN
1	G	354	ASN
2	L	30	ASN
2	F	288	GLN
1	G	305	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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
6	PO4	D	501	-	4,4,4	0.93	0	6,6,6	0.44	0
8	GOL	J	502	-	5,5,5	0.90	0	5,5,5	1.01	0
9	TAM	H	502	-	7,10,10	0.43	0	9,12,12	0.93	0
5	1PE	D	502	-	11,11,15	0.15	0	10,10,14	0.13	0
6	PO4	G	502	-	4,4,4	0.92	0	6,6,6	0.38	0
6	PO4	F	501	-	4,4,4	0.94	0	6,6,6	0.47	0
9	TAM	J	501	-	7,10,10	0.32	0	9,12,12	0.99	1 (11%)
5	1PE	F	502	-	15,15,15	0.12	0	14,14,14	0.10	0
5	1PE	C	501	-	15,15,15	0.13	0	14,14,14	0.07	0
6	PO4	L	501	-	4,4,4	0.91	0	6,6,6	0.46	0
4	EPE	B	502	-	15,15,15	0.79	1 (6%)	18,20,20	1.65	4 (22%)
8	GOL	F	503	-	5,5,5	0.95	0	5,5,5	0.98	0
6	PO4	H	501	-	4,4,4	0.92	0	6,6,6	0.38	0
6	PO4	C	502	-	4,4,4	0.93	0	6,6,6	0.46	0
5	1PE	H	503	-	7,7,15	0.17	0	6,6,14	0.08	0
8	GOL	D	503	-	5,5,5	1.00	0	5,5,5	0.94	0

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
8	GOL	J	502	-	-	2/4/4/4	-
9	TAM	H	502	-	-	4/12/12/12	-
5	1PE	D	502	-	-	6/9/9/13	-
9	TAM	J	501	-	-	6/12/12/12	-
5	1PE	F	502	-	-	6/13/13/13	-
5	1PE	C	501	-	-	9/13/13/13	-
4	EPE	B	502	-	-	4/9/19/19	0/1/1/1
8	GOL	F	503	-	-	2/4/4/4	-
5	1PE	H	503	-	-	2/5/5/13	-
8	GOL	D	503	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	EPE	C10-S	2.55	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	EPE	C5-N4-C3	3.71	117.18	108.83
4	B	502	EPE	C7-N4-C3	2.97	118.82	111.23
4	B	502	EPE	C7-N4-C5	2.59	117.86	111.23
4	B	502	EPE	O1S-S-C10	2.43	109.84	106.92
9	J	501	TAM	C2-C-C1	-2.10	106.80	110.50

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	EPE	C8-C7-N4-C5
4	B	502	EPE	S-C10-C9-N1
4	B	502	EPE	C9-C10-S-O2S
9	H	502	TAM	C1-C-C2-C5
9	H	502	TAM	C3-C-C2-C5

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	502	GOL	1	0
9	H	502	TAM	5	0
9	J	501	TAM	3	0
5	F	502	1PE	2	0
5	C	501	1PE	3	0
4	B	502	EPE	4	0
5	H	503	1PE	1	0
8	D	503	GOL	1	0

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 [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, 95th 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	413/413 (100%)	-0.07	1 (0%) 91 90	37, 46, 62, 74	0
1	B	405/413 (98%)	0.01	4 (0%) 79 76	35, 46, 61, 83	0
1	E	408/413 (98%)	0.13	2 (0%) 87 85	37, 51, 68, 93	0
1	G	413/413 (100%)	0.15	6 (1%) 72 68	36, 52, 70, 85	0
1	I	405/413 (98%)	0.13	1 (0%) 91 90	38, 52, 69, 94	0
1	K	404/413 (97%)	0.06	3 (0%) 84 82	39, 50, 72, 94	0
2	C	411/412 (99%)	0.06	4 (0%) 79 76	35, 46, 64, 87	0
2	D	412/412 (100%)	0.03	4 (0%) 79 76	37, 47, 66, 87	0
2	F	412/412 (100%)	0.17	3 (0%) 84 82	38, 52, 70, 87	0
2	H	412/412 (100%)	0.05	3 (0%) 84 82	37, 48, 68, 91	0
2	J	410/412 (99%)	0.10	5 (1%) 76 73	37, 50, 72, 91	0
2	L	411/412 (99%)	0.21	5 (1%) 76 73	39, 52, 77, 96	0
All	All	4916/4950 (99%)	0.09	41 (0%) 82 80	35, 49, 70, 96	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	ALA	5.0
1	G	408	GLY	3.1
2	J	94	ASN	3.0
1	B	369	GLU	3.0
1	A	127	GLY	3.0

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 oligosaccharides in this entry.

6.4 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, 95th 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($\text{\AA}^2$)	Q<0.9
4	EPE	B	502	15/15	0.67	0.21	60,69,92,104	0
8	GOL	D	503	6/6	0.72	0.22	47,55,57,60	0
8	GOL	F	503	6/6	0.74	0.19	50,66,68,70	0
5	1PE	F	502	16/16	0.80	0.17	51,60,68,71	0
8	GOL	J	502	6/6	0.82	0.22	43,50,62,66	0
9	TAM	J	501	11/11	0.83	0.15	53,55,63,64	0
9	TAM	H	502	11/11	0.85	0.13	44,49,55,56	0
5	1PE	H	503	8/16	0.89	0.14	50,56,59,61	0
5	1PE	D	502	12/16	0.90	0.11	48,52,57,58	0
5	1PE	C	501	16/16	0.90	0.11	40,46,57,58	0
7	CL	A	501	1/1	0.91	0.14	63,63,63,63	0
6	PO4	L	501	5/5	0.91	0.10	62,63,77,79	0
6	PO4	G	502	5/5	0.92	0.15	62,66,80,90	0
3	MG	B	501	1/1	0.93	0.06	36,36,36,36	0
6	PO4	F	501	5/5	0.93	0.09	58,61,65,75	0
6	PO4	H	501	5/5	0.95	0.08	43,56,65,68	0
6	PO4	D	501	5/5	0.95	0.07	49,50,53,54	0
3	MG	E	501	1/1	0.96	0.05	41,41,41,41	0
6	PO4	C	502	5/5	0.97	0.05	43,48,50,56	0
3	MG	I	501	1/1	0.97	0.09	38,38,38,38	0
3	MG	G	501	1/1	0.98	0.04	44,44,44,44	0
3	MG	K	501	1/1	0.99	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.