

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 10:25 AM EDT

PDB ID : 2QO0

> Title Crystal structure of the complex between the A246F mutant of mycobacterium

> > beta-ketoacyl-acyl carrier protein synthase III (FABH) and 11-(decyldithioca

rbonyloxy)-undecanoic acid

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2007-07-19 Deposited on

Resolution 1.85 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 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.35

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)

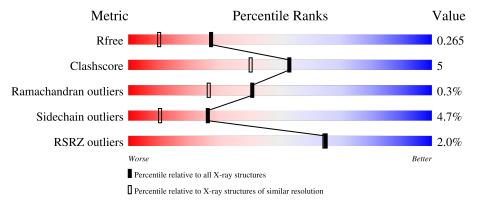
Validation Pipeline (wwPDB-VP) 2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	335	86%	11%	
1	В	335	84%	13%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5153 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.

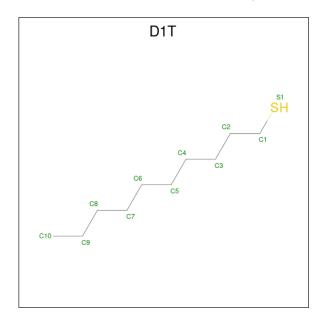
• Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] synthase 3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	328	Total	С	N	О	S	0	2	0
1	11	320	2380	1486	424	457	13		2	
1	D	331	Total	С	N	О	S	0	4	0
1	Б	991	2431	1520	428	470	13	0	4	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	PHE	ALA	engineered mutation	UNP P0A574
В	246	PHE	ALA	engineered mutation	UNP P0A574

• Molecule 2 is DECANE-1-THIOL (three-letter code: D1T) (formula: C₁₀H₂₂S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total 11	C 10	S 1	0	0



 $Continued\ from\ previous\ page...$

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	В	1	Total	С	S	0	0
	Ъ	1	11	10	1	0	U

• Molecule 3 is water.

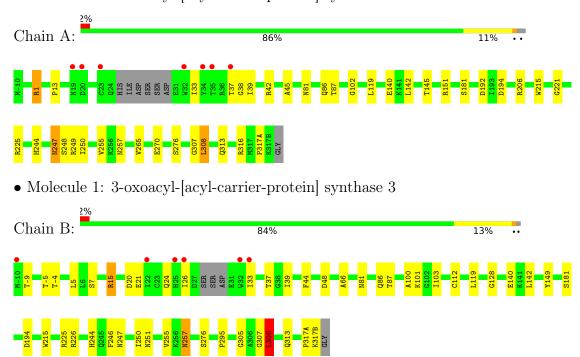
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	142	Total O 142 142	0	0
3	В	177	Total O 178 178	0	1



3 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 3





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	55.30Å 93.05Å 104.72Å	Donogitor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	25.00 - 1.85	Depositor	
rtesolution (A)	24.93 - 1.85	EDS	
% Data completeness	99.8 (25.00-1.85)	Depositor	
(in resolution range)	99.8 (24.93-1.85)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	0.10	Depositor	
$< I/\sigma(I) > 1$	5.90 (at 1.85Å)	Xtriage	
Refinement program	REFMAC 5.2.0019, CNS	Depositor	
P. P.	0.194 , 0.264	Depositor	
R, R_{free}	0.194 , 0.265	DCC	
R_{free} test set	4710 reflections (10.07%)	wwPDB-VP	
Wilson B-factor (\mathring{A}^2)	17.8	Xtriage	
Anisotropy	0.355	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 50.1	EDS	
L-test for twinning ²	$ < L > = 0.37, < L^2> = 0.20$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	5153	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	22.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.09% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: D1T

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.42	0/2421	0.59	0/3294	
1	В	0.44	0/2475	0.62	0/3369	
All	All	0.43	0/4896	0.60	0/6663	

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	A	0	1
1	В	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	307	GLY	Peptide
1	В	307	GLY	Peptide

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	2380	0	2335	24	0
1	В	2431	0	2366	33	0
2	A	11	0	21	1	0
2	В	11	0	21	1	0
3	A	142	0	0	0	0
3	В	178	0	0	2	0
All	All	5153	0	4743	52	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 5.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance} (\text{\AA})$	overlap(Å)
1:A:225:ARG:HH22	1:A:257:ASN:HD21	1.13	0.93
1:B:225:ARG:HH22	1:B:257:ASN:HD21	1.23	0.83
1:B:33:ILE:O	1:B:37:THR:HG22	1.80	0.80
1:B:37:THR:HG23	1:B:39:ILE:H	1.45	0.79
1:B:295:PRO:HG3	1:B:317(B):LYS:HB3	1.65	0.78
1:A:33:ILE:O	1:A:37:THR:HG22	1.89	0.72
1:A:225:ARG:HH22	1:A:257:ASN:ND2	1.89	0.69
1:B:251:ASN:O	1:B:255:VAL:HG23	1.94	0.66
1:B:140:GLU:HG2	1:B:276[B]:SER:HB2	1.78	0.65
1:B:15[B]:ARG:NH2	1:B:21:GLU:OE2	2.31	0.63
1:B:317(A):PRO:O	1:B:317(B):LYS:HB2	2.00	0.60
1:A:140:GLU:HG3	1:A:142:LEU:HG	1.84	0.58
1:B:15[A]:ARG:HG2	1:B:44:PHE:HB2	1.84	0.57
1:B:112:CYS:HB2	1:B:305:GLY:HA3	1.87	0.56
1:B:308:LEU:H	1:B:308:LEU:HD23	1.69	0.56
1:A:1:ARG:CZ	1:B:-5:THR:HG21	2.37	0.54
1:A:247:ASN:ND2	1:A:249:ARG:H	2.08	0.52
1:B:247:ASN:HB3	1:B:250:ILE:HD12	1.92	0.52
1:B:244:HIS:HE1	1:B:276[A]:SER:O	1.93	0.51
1:A:244:HIS:HE1	1:A:276[A]:SER:O	1.93	0.51
1:A:316:ARG:NH2	1:B:-9:THR:O	2.44	0.51
1:B:112:CYS:HB3	1:B:244:HIS:CE1	2.46	0.51
1:A:244:HIS:HE1	1:A:276[B]:SER:O	1.94	0.50
1:B:140:GLU:HG2	1:B:276[A]:SER:HB3	1.93	0.50
1:A:37:THR:HG23	1:A:39:ILE:H	1.77	0.49
1:A:247:ASN:HB3	1:A:250:ILE:HD12	1.94	0.49
1:B:244:HIS:HE1	1:B:276[B]:SER:O	1.96	0.49
1:B:5:LEU:HB3	1:B:317(A):PRO:HB3	1.95	0.48



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A	A. 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} (\mathring{\rm A})$	overlap (Å)
1:A:140:GLU:HG2	1:A:276[B]:SER:HB2	1.95	0.48
1:B:308:LEU:HD23	1:B:308:LEU:N	2.29	0.48
1:A:38:GLY:O	1:A:270:GLU:HA	2.14	0.46
1:A:255:VAL:HG21	1:A:265:VAL:HG21	1.96	0.46
1:B:-4:THR:HG23	1:B:128:GLY:O	2.14	0.46
1:B:101:LYS:HB3	3:B:513:HOH:O	2.16	0.46
1:B:140:GLU:HG3	1:B:142:LEU:HG	1.96	0.46
1:B:226:ARG:NH1	3:B:450:HOH:O	2.49	0.46
1:A:221:GLY:HA3	1:A:257:ASN:ND2	2.30	0.46
1:B:100:ALA:O	1:B:103:ILE:HG12	2.16	0.45
1:B:215:TRP:CD2	1:B:308:LEU:HD13	2.52	0.45
1:B:7:SER:HB3	1:B:66:ALA:HB2	1.98	0.44
1:A:215:TRP:CD2	1:A:308:LEU:HD13	2.53	0.44
1:A:86:GLN:HB3	1:B:81:ASN:O	2.17	0.43
1:A:145:THR:HB	2:A:761:D1T:H82	2.01	0.43
1:A:13:PRO:HB3	1:A:45:ALA:HA	2.01	0.42
1:A:86:GLN:HB2	2:B:761:D1T:H71	2.00	0.42
1:A:192:ASP:HB3	1:A:206:ARG:HG3	1.99	0.42
1:B:317(A):PRO:O	1:B:317(B):LYS:CB	2.66	0.42
1:A:102:GLY:HA2	1:B:181[B]:SER:O	2.20	0.42
1:A:81:ASN:O	1:B:86:GLN:HB3	2.20	0.42
1:B:37:THR:HG23	1:B:39:ILE:HG13	2.02	0.42
1:A:140:GLU:HG2	1:A:276[A]:SER:HB3	2.02	0.41
1:B:24:GLN:HG2	1:B:149:TYR:HD2	1.86	0.41

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	326/335 (97%)	312 (96%)	13 (4%)	1 (0%)	41 26	



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	В	331/335 (99%)	319 (96%)	11 (3%)	1 (0%)	41 26
All	All	657/670 (98%)	631 (96%)	24 (4%)	2 (0%)	41 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
1	В	308	LEU	
1	A	317(A)	PRO	

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	Rotameric Outliers	
1	A	$234/247 \ (95\%)$	223~(95%)	11 (5%)	26 10
1	В	241/247 (98%)	229 (95%)	12 (5%)	24 9
All	All	475/494 (96%)	452 (95%)	23 (5%)	26 10

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	42	ARG
1	A	87	THR
1	A	119	LEU
1	A	151	ARG
1	A	181	SER
1	A	194	ASP
1	A	247	ASN
1	A	248	SER
1	A	308	LEU
1	A	313	GLN
1	В	15[A]	ARG
1	В	15[B]	ARG
1	В	20	ASP



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Mol	Chain	Res	Type
1	В	26	ILE
1	В	48	ASP
1	В	87	THR
1	В	119	LEU
1	В	194	ASP
1	В	246	PHE
1	В	257	ASN
1	В	308	LEU
1	В	313	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	A	247	ASN
1	A	251	ASN
1	A	257	ASN
1	В	251	ASN
1	В	257	ASN
1	В	271	HIS

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 monosaccharides 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				
IVIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	D1T	A	761	1	10,10,10	0.50	0	9,9,9	1.03	1 (11%)
2	D1T	В	761	1	10,10,10	0.56	0	9,9,9	0.69	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
2	D1T	A	761	1	-	3/8/8/8	_
2	D1T	В	761	1	-	1/8/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^o)$
2	A	761	D1T	C3-C2-C1	-2.75	108.19	113.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	761	D1T	C4-C5-C6-C7
2	A	761	D1T	C6-C7-C8-C9
2	В	761	D1T	C4-C5-C6-C7
2	A	761	D1T	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	761	D1T	1	0
2	В	761	D1T	1	0



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^{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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	328/335~(97%)	-0.10	7 (2%) 63 63	13, 21, 37, 56	0
1	В	331/335 (98%)	-0.25	6 (1%) 68 68	13, 20, 36, 62	0
All	All	659/670 (98%)	-0.17	13 (1%) 65 64	13, 20, 36, 62	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	32	TRP	6.4
1	A	32	TRP	4.8
1	A	23	CYS	3.9
1	В	-10	MET	3.4
1	A	20	ASP	3.3
1	A	35	THR	3.2
1	A	34	TYR	3.2
1	A	37	THR	2.8
1	В	26	ILE	2.7
1	В	22	ILE	2.7
1	В	33	ILE	2.5
1	В	25	HIS	2.4
1	A	19	ASN	2.1

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 monosaccharides 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, 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	D1T	A	761	11/11	0.95	0.09	6,16,23,27	0
2	D1T	В	761	11/11	0.96	0.14	10,16,26,34	0

6.5 Other polymers (i)

There are no such residues in this entry.

