



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8R2Q / pdb_00008r2q
Title : Mycobacterium tuberculosis fatty acyl CoA synthetase, FadD5
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Deposited on : 2023-11-07
Resolution : 2.80 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 ⓘ 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

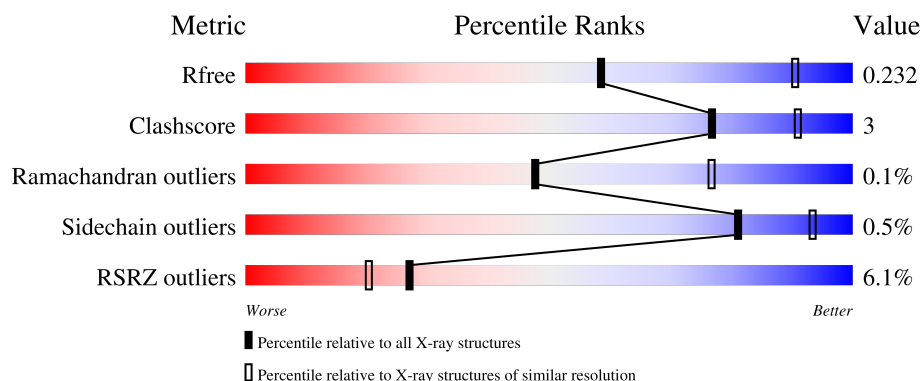
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	570	5% 67% 6% 27%
1	B	570	4% 66% 7% 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6331 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 Probable fatty-acid-CoA ligase FadD5 (Fatty-acid-CoA synthetase) (Fatty-acid-CoA synthase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3116	1981	542	572	21			
1	B	417	Total	C	N	O	S	0	0	0
			3132	1989	545	577	21			

There are 32 discrepancies between the modelled and reference sequences:

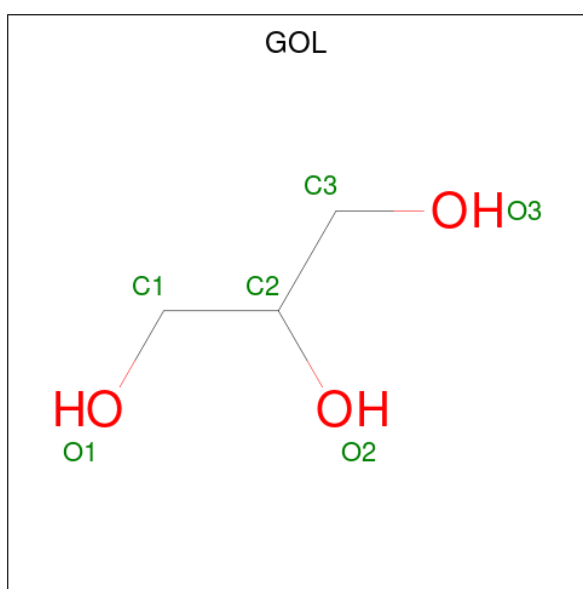
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP O07411
A	-14	GLY	-	expression tag	UNP O07411
A	-13	SER	-	expression tag	UNP O07411
A	-12	SER	-	expression tag	UNP O07411
A	-11	HIS	-	expression tag	UNP O07411
A	-10	HIS	-	expression tag	UNP O07411
A	-9	HIS	-	expression tag	UNP O07411
A	-8	HIS	-	expression tag	UNP O07411
A	-7	HIS	-	expression tag	UNP O07411
A	-6	HIS	-	expression tag	UNP O07411
A	-5	SER	-	expression tag	UNP O07411
A	-4	GLN	-	expression tag	UNP O07411
A	-3	ASP	-	expression tag	UNP O07411
A	-2	PRO	-	expression tag	UNP O07411
A	-1	ASN	-	expression tag	UNP O07411
A	0	SER	-	expression tag	UNP O07411
B	-15	MET	-	initiating methionine	UNP O07411
B	-14	GLY	-	expression tag	UNP O07411
B	-13	SER	-	expression tag	UNP O07411
B	-12	SER	-	expression tag	UNP O07411
B	-11	HIS	-	expression tag	UNP O07411
B	-10	HIS	-	expression tag	UNP O07411
B	-9	HIS	-	expression tag	UNP O07411
B	-8	HIS	-	expression tag	UNP O07411

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP O07411
B	-6	HIS	-	expression tag	UNP O07411
B	-5	SER	-	expression tag	UNP O07411
B	-4	GLN	-	expression tag	UNP O07411
B	-3	ASP	-	expression tag	UNP O07411
B	-2	PRO	-	expression tag	UNP O07411
B	-1	ASN	-	expression tag	UNP O07411
B	0	SER	-	expression tag	UNP O07411

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total 27	O 27	0	0
3	B	26	Total 26	O 26	0	0

SER
ALA
GLY
PHE
THR
GLU
ARG
ARG
GLU
ASN
ARG
GLN
LYS
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.91Å 120.91Å 247.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.56 – 2.80 86.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (86.56-2.80) 99.4 (86.56-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.205 , 0.238 0.205 , 0.232	Depositor DCC
R_{free} test set	2345 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6331	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.09	0/3181	0.27	0/4344
1	B	0.10	0/3197	0.27	0/4364
All	All	0.09	0/6378	0.27	0/8708

There are no bond length outliers.

There are no bond angle outliers.

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	3116	0	3123	20	0
1	B	3132	0	3145	22	0
2	A	18	0	24	1	0
2	B	12	0	16	1	0
3	A	27	0	0	0	0
3	B	26	0	0	0	0
All	All	6331	0	6308	37	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 3.

All (37) 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:B:80:MET:HE3	1:B:106:LEU:HD11	1.70	0.73
1:A:191:THR:HG22	1:A:193:GLY:H	1.57	0.69
1:A:98:MET:HG2	1:A:174:VAL:HG21	1.75	0.68
1:A:208:LEU:HB2	2:A:602:GOL:H11	1.80	0.63
1:A:34:ARG:NH2	1:B:361:PRO:HA	2.18	0.58
1:B:218:THR:HG21	1:B:343:MET:HE3	1.90	0.54
1:A:329:LEU:HB3	1:A:343:MET:HE1	1.88	0.54
1:A:37:MET:HE1	1:B:364:ALA:HB1	1.89	0.54
1:A:352:LYS:NZ	1:A:419:ASP:OD2	2.40	0.54
1:B:282:PRO:HD2	1:B:309:ALA:HB3	1.91	0.53
1:B:226:ASP:OD2	1:B:302:ARG:NH2	2.43	0.51
1:A:280:LEU:HB2	1:A:285:TRP:CE2	2.48	0.49
1:B:107:ASN:HB3	1:B:110:LEU:HG	1.95	0.49
1:B:46:ARG:HD3	1:B:273:GLU:OE1	2.13	0.48
1:A:89:PHE:HE1	1:A:240:ILE:HD13	1.79	0.48
1:A:361:PRO:HA	1:B:34:ARG:NH2	2.28	0.48
1:A:32:LEU:HD22	1:A:94:LEU:HD13	1.97	0.47
1:A:107:ASN:HB3	1:A:110:LEU:HG	1.96	0.46
1:B:190:TYR:HA	1:B:200:GLY:HA2	1.99	0.45
1:A:348:ASP:OD2	1:B:224:ASN:ND2	2.50	0.45
1:A:218:THR:HG21	1:A:343:MET:HG3	1.99	0.44
1:B:82:LEU:HG	1:B:133:LEU:HD13	1.99	0.44
1:B:190:TYR:O	2:B:601:GOL:H2	2.18	0.43
1:A:306:TRP:CE2	1:A:330:ALA:HB2	2.54	0.42
1:B:212:ALA:HB2	1:B:244:LEU:HB3	2.00	0.42
1:A:226:ASP:HB2	1:A:251:LEU:HD13	2.02	0.42
1:A:199:LYS:HB3	1:A:394:TYR:CD1	2.54	0.42
1:B:28:TRP:HA	1:B:31:GLN:CD	2.45	0.42
1:A:245:THR:HG23	1:A:249:LEU:HD12	2.01	0.41
1:B:197:ARG:NH2	1:B:396:ASN:O	2.53	0.41
1:A:68:LEU:O	1:A:73:VAL:HG12	2.20	0.41
1:B:372:MET:HE2	1:B:407:GLY:HA3	2.03	0.41
1:A:216:LEU:HD22	1:B:217:TYR:HB3	2.03	0.41
1:B:433:MET:SD	1:B:433:MET:N	2.94	0.41
1:B:80:MET:HE2	1:B:119:VAL:HG22	2.03	0.40
1:B:285:TRP:CH2	1:B:304:LEU:HD22	2.57	0.40
1:B:383:ILE:HB	1:B:416:VAL:HG21	2.04	0.40

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	414/570 (73%)	396 (96%)	18 (4%)	0	100	100
1	B	415/570 (73%)	395 (95%)	19 (5%)	1 (0%)	43	72
All	All	829/1140 (73%)	791 (95%)	37 (4%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	GLU

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	Outliers	Percentiles	
1	A	325/456 (71%)	324 (100%)	1 (0%)	86	95
1	B	329/456 (72%)	327 (99%)	2 (1%)	78	92
All	All	654/912 (72%)	651 (100%)	3 (0%)	81	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	THR
1	B	230	VAL
1	B	303	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	211	GLN
1	A	334	GLN
1	B	211	GLN
1	B	334	GLN

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](#)

5 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	GOL	B	601	-	5,5,5	0.90	0	5,5,5	1.11	0
2	GOL	B	602	-	5,5,5	0.95	0	5,5,5	1.06	0
2	GOL	A	602	-	5,5,5	0.97	0	5,5,5	1.04	0
2	GOL	A	603	-	5,5,5	0.92	0	5,5,5	1.08	0
2	GOL	A	601	-	5,5,5	0.93	0	5,5,5	1.08	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	GOL	B	601	-	-	0/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	A	603	-	-	2/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-C3
2	A	602	GOL	O1-C1-C2-O2
2	A	603	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-C3
2	A	603	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GOL	1	0
2	A	602	GOL	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

6.1 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, 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	416/570 (72%)	0.06	28 (6%) 24 17	51, 71, 137, 186	0
1	B	417/570 (73%)	-0.06	23 (5%) 30 23	50, 67, 121, 179	0
All	All	833/1140 (73%)	-0.00	51 (6%) 27 20	50, 70, 129, 186	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	LEU	9.3
1	B	22	LEU	9.3
1	A	23	ALA	8.1
1	B	174	VAL	6.9
1	A	173	ASP	6.4
1	A	20	PRO	6.4
1	B	23	ALA	6.3
1	A	159	ASP	5.9
1	B	428	ASP	5.5
1	B	430	LYS	5.5
1	B	171	ALA	5.3
1	B	20	PRO	5.2
1	A	174	VAL	4.6
1	B	21	TYR	4.4
1	A	21	TYR	4.2
1	A	428	ASP	4.0
1	A	430	LYS	3.8
1	A	435	ILE	3.8
1	B	172	GLY	3.7
1	A	195	THR	3.7
1	B	175	HIS	3.6
1	B	176	GLU	3.5
1	B	195	THR	3.5
1	A	162	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	435	ILE	3.4
1	A	177	PRO	3.2
1	A	433	MET	3.2
1	B	173	ASP	3.0
1	A	158	GLN	2.9
1	B	436	SER	2.9
1	A	192	SER	2.6
1	B	433	MET	2.6
1	A	172	GLY	2.6
1	B	194	THR	2.6
1	A	175	HIS	2.5
1	A	193	GLY	2.4
1	B	193	GLY	2.3
1	A	176	GLU	2.3
1	B	325	GLU	2.3
1	B	350	ILE	2.3
1	A	194	THR	2.2
1	A	170	GLU	2.2
1	B	353	ARG	2.1
1	A	164	TYR	2.1
1	B	192	SER	2.1
1	B	177	PRO	2.1
1	A	153	ALA	2.1
1	A	198	PRO	2.1
1	A	24	ARG	2.0
1	A	146	LEU	2.0
1	A	171	ALA	2.0

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(Å ²)	Q<0.9
2	GOL	B	602	6/6	0.85	0.20	76,81,84,84	0
2	GOL	A	601	6/6	0.89	0.17	71,77,81,91	0
2	GOL	B	601	6/6	0.90	0.17	63,68,85,93	0
2	GOL	A	603	6/6	0.91	0.19	76,84,91,97	0
2	GOL	A	602	6/6	0.93	0.23	68,72,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.