



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2025 – 04:18 PM EDT

PDB ID : 9MQF / pdb\_00009mqf  
Title : Chloroplast acyl-ACP thioesterase from Chlamydomonas reinhardtii  
Authors : Chen, J.A.; Suo, Y.; Mayfield, S.P.; Burkart, M.D.  
Deposited on : 2025-01-02  
Resolution : 2.50 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

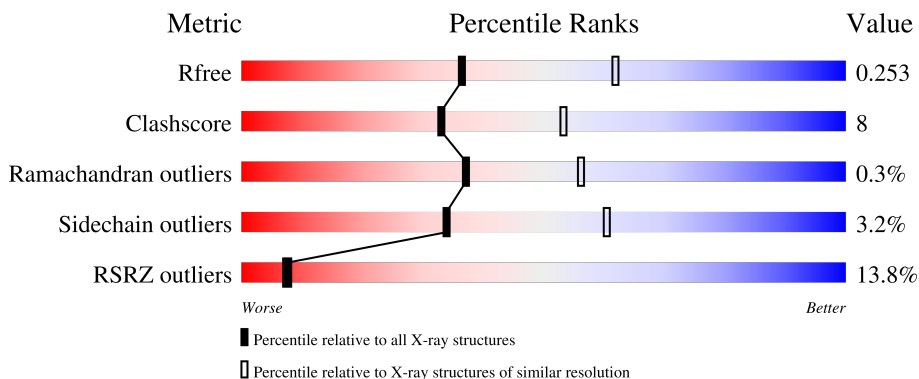
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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  $\geq 3$ , 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	351	<div> <div>11%</div> <div>67%</div> <div>14%</div> <div>••</div> <div>17%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2299 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 Acyl-[acyl-carrier-protein] hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2291	1440	407	429	15			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	MET	-	initiating methionine	UNP A8HY17
A	84	VAL	-	expression tag	UNP A8HY17
A	85	PRO	-	expression tag	UNP A8HY17
A	396	GLY	-	expression tag	UNP A8HY17
A	397	THR	-	expression tag	UNP A8HY17
A	398	GLY	-	expression tag	UNP A8HY17
A	399	GLU	-	expression tag	UNP A8HY17
A	400	ASN	-	expression tag	UNP A8HY17
A	401	LEU	-	expression tag	UNP A8HY17
A	402	TYR	-	expression tag	UNP A8HY17
A	403	PHE	-	expression tag	UNP A8HY17
A	404	GLN	-	expression tag	UNP A8HY17
A	405	GLY	-	expression tag	UNP A8HY17
A	406	SER	-	expression tag	UNP A8HY17
A	407	GLY	-	expression tag	UNP A8HY17
A	408	GLY	-	expression tag	UNP A8HY17
A	409	GLY	-	expression tag	UNP A8HY17
A	410	GLY	-	expression tag	UNP A8HY17
A	411	SER	-	expression tag	UNP A8HY17
A	412	ASP	-	expression tag	UNP A8HY17
A	413	TYR	-	expression tag	UNP A8HY17
A	414	LYS	-	expression tag	UNP A8HY17
A	415	ASP	-	expression tag	UNP A8HY17
A	416	ASP	-	expression tag	UNP A8HY17
A	417	ASP	-	expression tag	UNP A8HY17
A	418	ASP	-	expression tag	UNP A8HY17
A	419	LYS	-	expression tag	UNP A8HY17

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Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLY	-	expression tag	UNP A8HY17
A	421	THR	-	expression tag	UNP A8HY17
A	422	GLY	-	expression tag	UNP A8HY17
A	423	ARG	-	expression tag	UNP A8HY17
A	424	SER	-	expression tag	UNP A8HY17
A	425	ARG	-	expression tag	UNP A8HY17
A	426	LEU	-	expression tag	UNP A8HY17
A	427	GLU	-	expression tag	UNP A8HY17
A	428	HIS	-	expression tag	UNP A8HY17
A	429	HIS	-	expression tag	UNP A8HY17
A	430	HIS	-	expression tag	UNP A8HY17
A	431	HIS	-	expression tag	UNP A8HY17
A	432	HIS	-	expression tag	UNP A8HY17
A	433	HIS	-	expression tag	UNP A8HY17

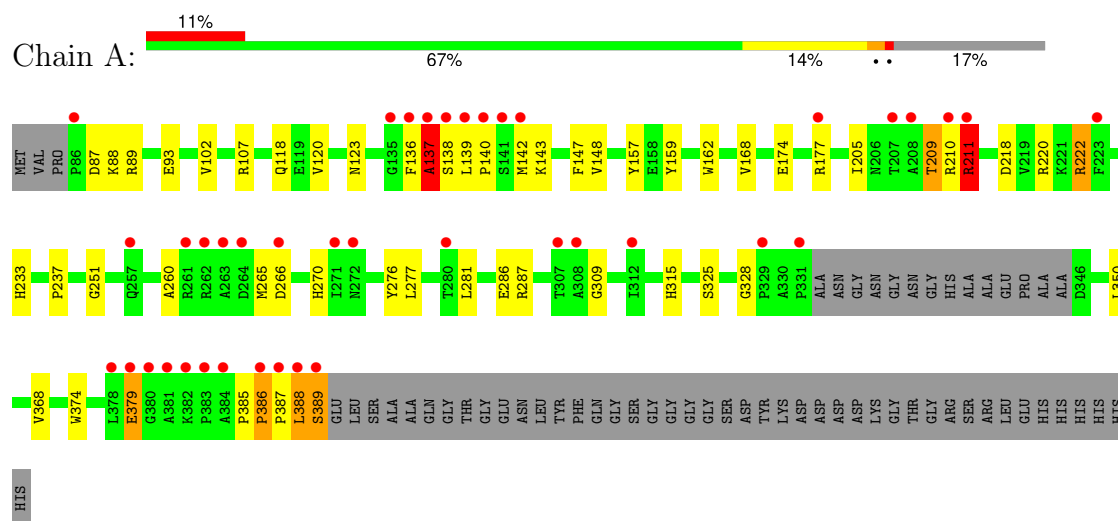
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0

### 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: Acyl-[acyl-carrier-protein] hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.26Å 67.26Å 207.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 2.50 48.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.20-2.50) 99.9 (48.20-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487-000, REFMAC 5	Depositor
R, $R_{free}$	0.237 , 0.253 0.238 , 0.253	Depositor DCC
$R_{free}$ test set	851 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.27	0/2343	0.71	10/3174 (0.3%)

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	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	389	SER	N-CA-CB	13.66	133.73	110.50
1	A	388	LEU	N-CA-C	-11.02	91.00	108.63
1	A	389	SER	N-CA-C	-9.55	84.25	111.00
1	A	138	SER	N-CA-CB	-7.35	99.54	111.01
1	A	388	LEU	CB-CA-C	-7.07	99.56	110.88
1	A	386	PRO	CB-CA-C	-6.52	102.96	110.92
1	A	87	ASP	N-CA-C	-5.64	106.21	114.39
1	A	137	ALA	N-CA-C	-5.64	98.79	110.80
1	A	386	PRO	O-C-N	-5.26	115.25	121.46
1	A	88	LYS	N-CA-C	-5.11	106.89	112.72

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	210	ARG	Sidechain
1	A	211	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	386	PRO	Mainchain

## 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	2291	0	2264	35	0
2	A	8	0	0	0	0
All	All	2299	0	2264	35	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 8.

All (35) 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:388:LEU:HD12	1:A:388:LEU:O	1.52	1.07
1:A:388:LEU:O	1:A:388:LEU:CD1	2.08	1.01
1:A:388:LEU:O	1:A:388:LEU:CG	2.11	0.94
1:A:136:PHE:O	1:A:137:ALA:O	1.87	0.92
1:A:136:PHE:O	1:A:137:ALA:C	2.13	0.91
1:A:388:LEU:O	1:A:388:LEU:HG	1.73	0.88
1:A:136:PHE:C	1:A:137:ALA:O	2.31	0.72
1:A:385:PRO:HB2	1:A:387:PRO:HD2	1.76	0.68
1:A:388:LEU:HD12	1:A:388:LEU:C	2.19	0.66
1:A:350:LEU:HB2	1:A:374:TRP:HB2	1.78	0.64
1:A:120:VAL:HG21	1:A:168:VAL:HB	1.80	0.63
1:A:148:VAL:HG21	1:A:205:ILE:HD13	1.82	0.60
1:A:139:LEU:HB3	1:A:143:LYS:HA	1.86	0.58
1:A:139:LEU:N	1:A:140:PRO:HD3	2.22	0.54
1:A:139:LEU:HA	1:A:142:MET:HB2	1.90	0.53
1:A:287:ARG:NH2	1:A:325:SER:O	2.41	0.53
1:A:218:ASP:OD1	1:A:222:ARG:NH1	2.42	0.53
1:A:157:TYR:HB3	1:A:379:GLU:O	2.10	0.52
1:A:93:GLU:OE2	1:A:123:ASN:ND2	2.44	0.51
1:A:140:PRO:HD2	1:A:142:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:CD2	1:A:237:PRO:HG3	2.47	0.49
1:A:387:PRO:O	1:A:389:SER:N	2.46	0.49
1:A:136:PHE:HE1	1:A:147:PHE:HB2	1.78	0.48
1:A:388:LEU:CD1	1:A:388:LEU:C	2.82	0.48
1:A:260:ALA:O	1:A:309:GLY:HA2	2.14	0.47
1:A:209:THR:C	1:A:211:ARG:N	2.74	0.45
1:A:251:GLY:HA3	1:A:315:HIS:HB3	1.98	0.45
1:A:276:TYR:HB3	1:A:368:VAL:HG21	1.99	0.44
1:A:174:GLU:HG3	1:A:220:ARG:HH21	1.84	0.43
1:A:287:ARG:NE	1:A:328:GLY:O	2.32	0.42
1:A:102:VAL:HG11	1:A:162:TRP:HB2	2.02	0.42
1:A:266:ASP:OD1	1:A:270:HIS:O	2.37	0.42
1:A:277:LEU:O	1:A:281:LEU:HG	2.19	0.42
1:A:209:THR:C	1:A:211:ARG:H	2.28	0.41
1:A:107:ARG:NH2	1:A:159:TYR:H	2.19	0.41

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	286/351 (82%)	269 (94%)	16 (6%)	1 (0%)	37 56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ALA

### 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	247/289 (86%)	239 (97%)	8 (3%)	34 60

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ARG
1	A	118	GLN
1	A	209	THR
1	A	211	ARG
1	A	222	ARG
1	A	265	MET
1	A	286	GLU
1	A	379	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	252	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

There are no ligands in this entry.

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	290/351 (82%)	0.92	40 (13%) 8 7	44, 76, 144, 216	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	PRO	6.9
1	A	208	ALA	6.8
1	A	137	ALA	6.7
1	A	388	LEU	5.5
1	A	384	ALA	5.5
1	A	389	SER	5.5
1	A	86	PRO	5.4
1	A	136	PHE	5.2
1	A	142	MET	4.9
1	A	177	ARG	4.6
1	A	382	LYS	4.2
1	A	331	PRO	4.2
1	A	139	LEU	4.1
1	A	263	ALA	3.9
1	A	383	PRO	3.7
1	A	135	GLY	3.6
1	A	379	GLU	3.6
1	A	141	SER	3.6
1	A	262	ARG	3.5
1	A	307	THR	3.5
1	A	308	ALA	3.2
1	A	211	ARG	3.2
1	A	261	ARG	3.1
1	A	387	PRO	3.1
1	A	381	ALA	2.9
1	A	264	ASP	2.9
1	A	210	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	329	PRO	2.8
1	A	223	PHE	2.6
1	A	386	PRO	2.6
1	A	312	ILE	2.6
1	A	271	ILE	2.5
1	A	207	THR	2.5
1	A	257	GLN	2.5
1	A	380	GLY	2.5
1	A	266	ASP	2.4
1	A	378	LEU	2.4
1	A	272	ASN	2.2
1	A	138	SER	2.2
1	A	280	THR	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.