



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:41 AM GMT

PDB ID : 3FLM  
Title : Crystal structure of menD from E.coli  
Authors : Priyadarshi, A.; Hwang, K.Y.  
Deposited on : 2008-12-19  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

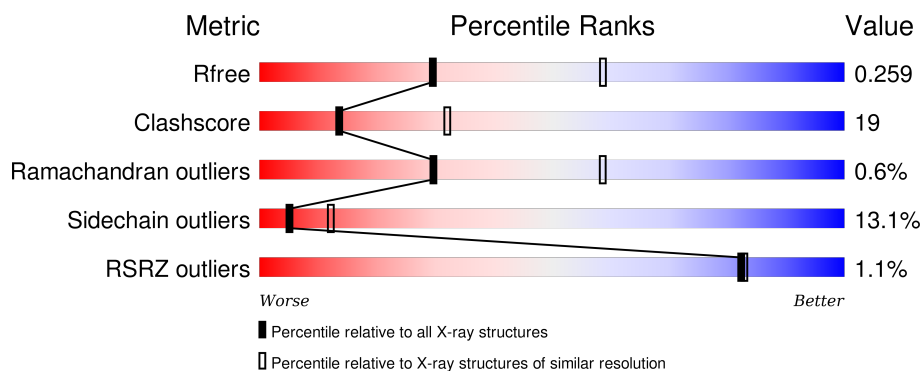
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	556	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>27%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	556	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>32%</div> <div>8%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8317 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4158	2636	752	756	14			
1	B	531	Total	C	N	O	S	0	0	0
			4127	2614	747	752	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	LEU	PRO	ENGINEERED	UNP P17109
B	36	LEU	PRO	ENGINEERED	UNP P17109

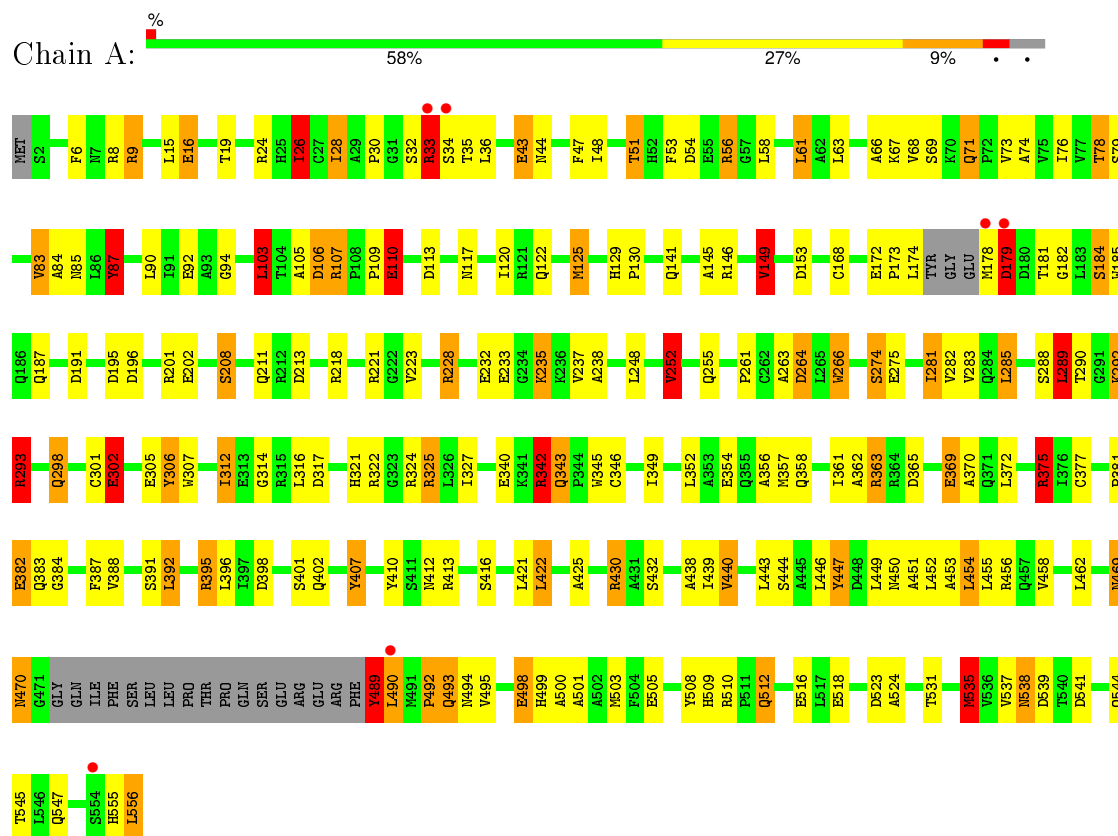
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	18	Total	O	0	0
			18	18		

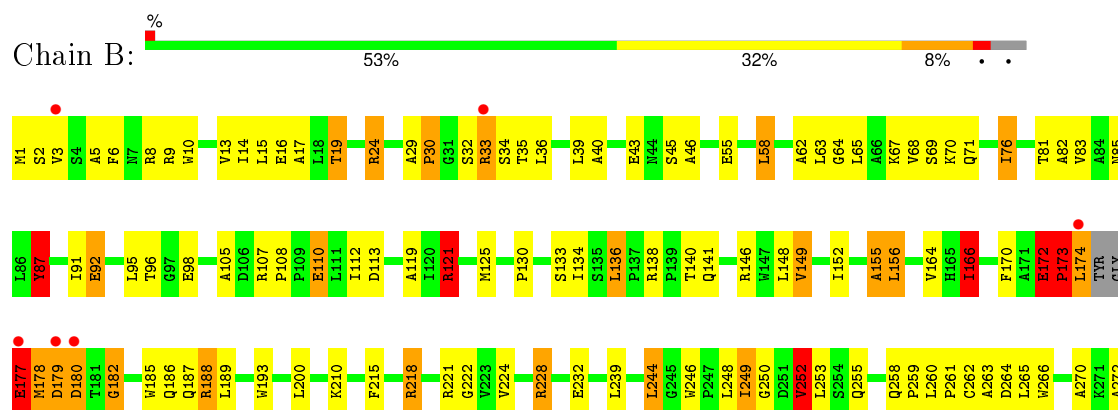
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



T273	Q358	V440	R526
S274	A359	G441	T527
E275	V360	D442	P528
L276	I361	L443	T529
Q277	A362	S444	T530
Q280	R363	Y447	M535
I281	R364	L452	V536
V282	D365	A453	M538
V283	A366	L454	D539
Q284	A370	L455	T540
L285	Q371	R456	Q544
L289	I372	Q457	Q547
T290	R375	L462	L550
R293	I376	I465	A551
L294	D377	V466	Q552
W297	Y379	V467	L556
E302	L380	N470	
P303	P381	GLY	
E304	E382	GLY	
F305	Q383	GLN	
Y306	G384	TLE	
	Q385	PHE	
	L386	SER	
	F387	LEU	
I312	V388	LEU	
R315	G389	PRO	
	S391	THR	
R322	L392	PRO	
G323	V393	GLN	
R324	V394	SER	
R325	R395	GLU	
L326	L396	ARG	
I327	I397	GLU	
	D398	ARG	
T330	S401	PHE	
L334	Q402	TYR	
	LEU	LEU	
A339	Y407	NET	
E340	P408	PRO	
F341	V409	GLN	
R342	Y410	N494	
Q343	S411	V495	
	N412	H496	
	R413	F497	
C346		F498	
V347		H499	
E348	A426		
I349	G427	K507	
P350	R430	Q512	
L352	R351	L517	
A353	A431	A524	
E354	T436	M525	
Q355	L437		
A356	A438		
M357	I439		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.07Å 118.07Å 176.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 41.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.70) 98.3 (41.74-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.182 , 0.270 0.178 , 0.259	Depositor DCC
$R_{free}$ test set	1725 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 34334 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.57	41/4258 (1.0%)	1.42	64/5806 (1.1%)
1	B	1.51	33/4225 (0.8%)	1.39	44/5760 (0.8%)
All	All	1.54	74/8483 (0.9%)	1.41	108/11566 (0.9%)

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	3	5
1	B	0	6
All	All	3	11

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	GLU	CG-CD	10.85	1.68	1.51
1	A	110	GLU	CB-CG	-10.21	1.32	1.52
1	B	105	ALA	CA-CB	-9.62	1.32	1.52
1	A	518	GLU	CG-CD	8.62	1.64	1.51
1	A	105	ALA	CA-CB	-8.26	1.35	1.52

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	107	ARG	NE-CZ-NH1	-11.03	114.79	120.30
1	B	218	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	B	228	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	61	LEU	CB-CG-CD1	-9.77	94.39	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	35	THR	CB
1	A	302	GLU	CA
1	A	493	GLN	CA

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	ASP	Peptide
1	A	302	GLU	Peptide
1	A	469	ASN	Peptide
1	A	489	TYR	Peptide
1	A	492	PRO	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	4158	0	4131	152	0
1	B	4127	0	4102	160	0
2	A	14	0	0	0	0
2	B	18	0	0	0	0
All	All	8317	0	8233	304	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 19.

The worst 5 of 304 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:33:ARG:NH2	1:B:174:LEU:HD21	1.51	1.25
1:A:493:GLN:HG2	1:A:494:ASN:N	1.60	1.16
1:B:33:ARG:HH22	1:B:174:LEU:HD21	1.00	1.14
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.03	1.13
1:B:363:ARG:HB3	1:B:363:ARG:HH11	1.16	1.10

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	529/556 (95%)	489 (92%)	37 (7%)	3 (1%)	30	59
1	B	525/556 (94%)	487 (93%)	35 (7%)	3 (1%)	30	59
All	All	1054/1112 (95%)	976 (93%)	72 (7%)	6 (1%)	30	59

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	PRO
1	A	492	PRO
1	A	30	PRO
1	B	64	GLY
1	A	302	GLU

### 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	433/452 (96%)	378 (87%)	55 (13%)	5	13
1	B	430/452 (95%)	372 (86%)	58 (14%)	5	11
All	All	863/904 (96%)	750 (87%)	113 (13%)	5	12

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	535	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	166	ILE
1	B	495	VAL
1	A	539	ASP
1	B	32	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	141	GLN
1	B	355	GLN
1	B	71	GLN
1	B	277	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<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	535/556 (96%)	-0.48	6 (1%) 82 83	13, 25, 49, 80	10 (1%)
1	B	531/556 (95%)	-0.39	6 (1%) 82 83	13, 28, 52, 87	11 (2%)
All	All	1066/1112 (95%)	-0.44	12 (1%) 82 83	13, 26, 50, 87	21 (1%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	SER	4.1
1	B	177	GLU	3.5
1	B	33	ARG	3.2
1	A	33	ARG	3.0
1	A	178	MET	2.5

### 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 carbohydrates 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.