



Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 05:48 PM GMT

PDB ID : 3CV2
Title : Atomic Resolution Structures of Escherichia coli and Bacillus anthracis Malate Synthase A: Comparison with Isoform G and Implications for Structure Based Drug Design
Authors : Lohman, J.R.; Remington, S.J.
Deposited on : 2008-04-17
Resolution : 1.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

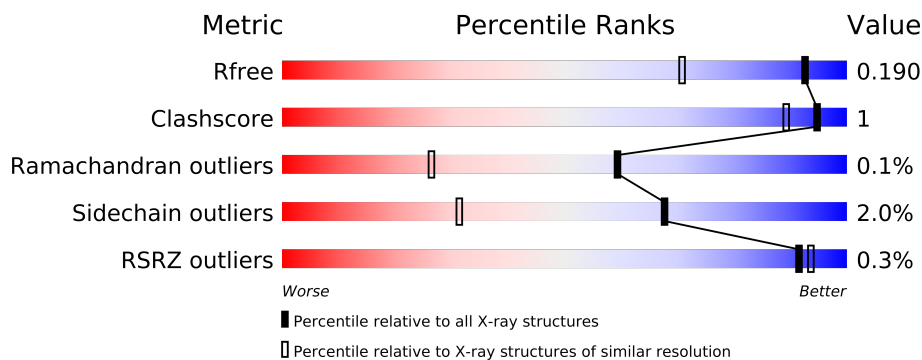
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 1.40 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}	66092	1097 (1.42-1.38)
Clashscore	79885	1246 (1.42-1.38)
Ramachandran outliers	78287	1206 (1.42-1.38)
Sidechain outliers	78261	1205 (1.42-1.38)
RSRZ outliers	66119	1097 (1.42-1.38)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	532	
1	B	532	

2 Entry composition i

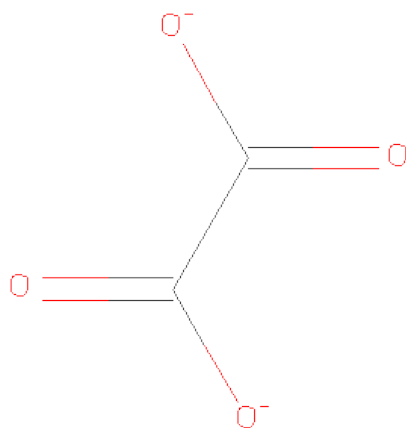
There are 5 unique types of molecules in this entry. The entry contains 9663 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Malate synthase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	3	14	0
			4220	2692	729	779	20			
1	B	525	Total	C	N	O	S	0	10	0
			4210	2683	730	777	20			

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).

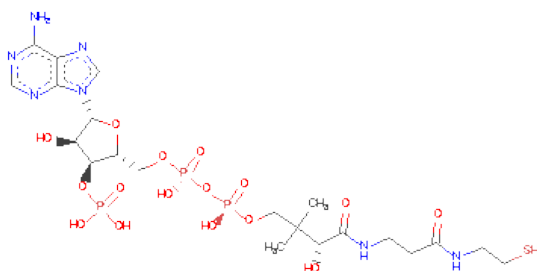


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		
2	B	1	Total	C	O	0	0
			6	2	4		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	2	Total Mg 2 2	0	0

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 31 10 5 13 3	0	0
4	B	1	Total C N O P 31 10 5 13 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	575	Total O 576 576	0	1
5	B	579	Total O 580 580	0	1

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: Malate synthase A

Chain A: 



- Molecule 1: Malate synthase A

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.20Å 71.47Å 103.26Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	25.01 – 1.40 24.42 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (25.01-1.40) 97.2 (24.42-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.200 0.173 , 0.190	Depositor DCC
R_{free} test set	10530 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
Estimated twinning fraction	0.012 for k,h,-l 0.012 for -k,-h,-l 0.469 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 209099 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9663	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: COA, OXL, CSO, MG

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	0.57	3/4346 (0.1%)	0.62	1/5893 (0.0%)
1	B	0.48	1/4321 (0.0%)	0.62	1/5858 (0.0%)
All	All	0.53	4/8667 (0.0%)	0.62	2/11751 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20[A]	GLN	CG-CD	14.52	1.84	1.51
1	A	20[B]	GLN	CG-CD	14.52	1.84	1.51
1	B	319	CYS	CB-SG	-8.03	1.68	1.82
1	A	319	CYS	CB-SG	-5.67	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	TYR	CA-CB-CG	5.35	123.57	113.40
1	B	281	PHE	CB-CG-CD2	-5.28	117.11	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4220	0	0	8	0
1	B	4210	0	0	4	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	0	1	0
4	B	31	0	0	0	0
5	A	576	0	0	4	0
5	B	580	0	0	3	0
All	All	9663	0	0	12	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (12) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:381[B]:ASP:OD1	5:B:1194:HOH:O	1.98	0.81
1:A:381[B]:ASP:OD1	5:A:1186:HOH:O	1.97	0.81
1:A:321[B]:LYS:NZ	5:A:1259:HOH:O	2.16	0.78
1:B:321[B]:LYS:NZ	5:B:1305:HOH:O	2.28	0.66
1:B:357:ALA:CB	1:B:382[B]:ILE:CD1	2.85	0.55
1:B:353:LYS:NZ	5:B:1579:HOH:O	2.39	0.55
1:A:353:LYS:NZ	5:A:1459:HOH:O	2.44	0.50
1:A:382:ILE:CD1	1:A:389:GLN:NE2	2.79	0.45
1:A:112:LYS:NZ	5:A:1385:HOH:O	2.50	0.44
1:A:496:GLU:O	1:A:500:SER:OG	2.39	0.41
1:A:101:LYS:NZ	4:A:1002:COA:O7A	2.55	0.40
1:A:302:THR:OG1	1:A:305:LYS:NZ	2.54	0.40

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	535/532 (101%)	523 (98%)	12 (2%)	0	100	100
1	B	532/532 (100%)	522 (98%)	9 (2%)	1 (0%)	56	24
All	All	1067/1064 (100%)	1045 (98%)	21 (2%)	1 (0%)	59	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	VAL

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	445/447 (100%)	435 (98%)	10 (2%)	64	27
1	B	440/447 (98%)	431 (98%)	9 (2%)	68	31
All	All	885/894 (99%)	866 (98%)	19 (2%)	68	29

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43[A]	GLN
1	A	43[B]	GLN
1	A	102	MET
1	A	212	TYR
1	A	259	ASP
1	A	291	PRO
1	A	382	ILE
1	A	396	GLN
1	A	408	PRO
1	A	494	LEU
1	B	15	ARG
1	B	44	ARG
1	B	212	TYR
1	B	259	ASP
1	B	265	LEU
1	B	311	TYR

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Mol	Chain	Res	Type
1	B	330[A]	MET
1	B	330[B]	MET
1	B	409	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	CSO	A	438	1	6,6,7	7.54	3 (50%)	3,6,8	3.04	1 (33%)
1	CSO	B	438	1	6,6,7	7.31	3 (50%)	3,6,8	2.70	1 (33%)

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
1	CSO	A	438	1	-	0/2/5/7	0/0/0/0
1	CSO	B	438	1	-	0/2/5/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	CSO	O-C	17.45	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	438	CSO	O-C	16.96	1.23	1.11
1	A	438	CSO	CB-SG	-5.27	1.76	1.82
1	B	438	CSO	CB-SG	-5.02	1.76	1.82
1	A	438	CSO	OD-SG	2.87	1.74	1.62
1	B	438	CSO	OD-SG	2.62	1.73	1.62

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	CSO	C-CA-N	-4.94	108.89	113.83
1	B	438	CSO	C-CA-N	-4.55	109.28	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
2	OXL	A	1000	3	0,5,5	0.00	-	0,6,6	0.00	-
4	COA	A	1002	-	33,33,50	1.13	3 (9%)	52,52,75	1.66	6 (11%)
2	OXL	B	1000	3	0,5,5	0.00	-	0,6,6	0.00	-
4	COA	B	1001	-	33,33,50	1.11	3 (9%)	52,52,75	1.76	7 (13%)

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	OXL	A	1000	3	-	0/0/4/4	0/0/0/0
4	COA	A	1002	-	-	0/21/37/64	0/1/3/3
2	OXL	B	1000	3	-	0/0/4/4	0/0/0/0
4	COA	B	1001	-	-	0/21/37/64	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	COA	P2A-O4A	3.61	1.62	1.50
4	B	1001	COA	P2A-O4A	3.47	1.61	1.50
4	B	1001	COA	C2A-N3A	3.00	1.38	1.32
4	A	1002	COA	C2A-N3A	2.80	1.37	1.32
4	B	1001	COA	C2A-N1A	2.32	1.38	1.33
4	A	1002	COA	C2A-N1A	2.21	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	COA	N3A-C2A-N1A	-9.42	120.83	128.71
4	A	1002	COA	N3A-C2A-N1A	-8.77	121.38	128.71
4	A	1002	COA	N3A-C4A-N9A	3.49	131.74	125.43
4	B	1001	COA	N3A-C4A-N9A	3.46	131.69	125.43
4	B	1001	COA	O4B-C1B-N9A	3.25	111.46	108.44
4	A	1002	COA	O4B-C1B-N9A	3.04	111.27	108.44
4	B	1001	COA	P2A-O3A-P1A	-2.37	122.79	132.95
4	A	1002	COA	C5A-C4A-N3A	-2.11	121.11	125.70
4	B	1001	COA	C5A-C4A-N3A	-2.08	121.16	125.70
4	B	1001	COA	O5A-P2A-O3A	2.08	110.92	104.29
4	A	1002	COA	N7A-C8A-N9A	-2.06	108.54	114.36
4	B	1001	COA	C4A-C5A-N7A	-2.04	107.78	109.52
4	A	1002	COA	P2A-O3A-P1A	-2.02	124.27	132.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	524/532 (98%)	-0.47	1 (0%) 93 94	11, 18, 31, 35	12 (2%)
1	B	525/532 (98%)	-0.47	2 (0%) 90 92	11, 18, 30, 39	13 (2%)
All	All	1049/1064 (98%)	-0.47	3 (0%) 91 93	11, 18, 31, 39	25 (2%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	CYS	6.3
1	B	409	CYS	4.4
1	B	408	PRO	3.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSO	B	438	7/8	0.08	0.50	16,19,19,20	1
1	CSO	A	438	7/8	0.07	0.29	15,19,20,21	1

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	1001	1/1	0.15	1.94	33,33,33,33	0
4	COA	A	1002	31/48	0.09	1.35	13,23,44,45	31
3	MG	A	1	1/1	0.06	0.93	12,12,12,12	0
4	COA	B	1001	31/48	0.09	0.89	15,23,43,44	31
2	OXL	B	1000	6/6	0.05	-0.48	12,12,16,20	0
3	MG	B	1	1/1	0.05	-0.62	11,11,11,11	0
2	OXL	A	1000	6/6	0.04	-0.88	11,13,15,19	0

6.5 Other polymers

There are no such residues in this entry.