wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:24 AM GMT

PDB ID	:	2AAL
Title	:	Crystal Structures of the Wild-type, Mutant-P1A and Inactivated Malonate Semialdehyde Decarboxylase: A Structural Basis for the Decarboxylase and Hydratase Activities
Authors	:	Almrud, J.J.; Poelarends, G.J.; Johnson Jr., W.H.; Serrano, H.; Hackert, M.L.; Whitman, C.P.
Deposited on	:	2005-07-13
Resolution	:	1.65 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

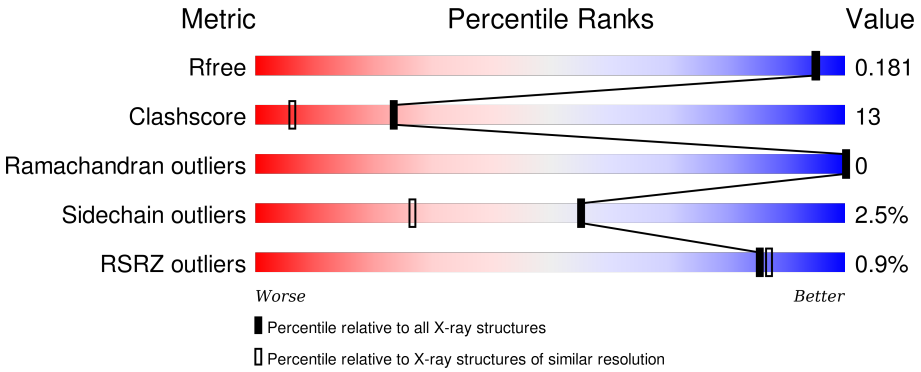
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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.



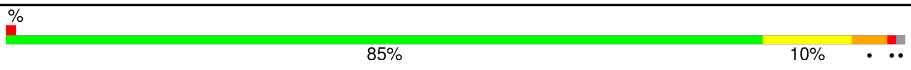
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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. 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	131	72% 24%
1	B	131	74% 21%
1	C	131	77% 15% 6%
1	D	131	78% 17%
1	E	131	73% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	131	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7105 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 Malonate Semialdehyde Decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	5	0
			1040	651	182	203	4			
1	B	131	Total	C	N	O	S	0	1	0
			1009	634	173	198	4			
1	C	130	Total	C	N	O	S	0	5	0
			1035	650	177	204	4			
1	D	130	Total	C	N	O	S	0	6	0
			1041	654	177	205	5			
1	E	130	Total	C	N	O	S	0	3	0
			1020	643	174	199	4			
1	F	130	Total	C	N	O	S	0	1	0
			1004	631	172	196	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MLI	-	PROPIONATION	GB 10637971
A	7	LEU	ILE	CONFLICT	GB 10637971
A	130	GLY	-	CLONING ARTIFACT	GB 10637971
B	0	MLI	-	PROPIONATION	GB 10637971
B	7	LEU	ILE	CONFLICT	GB 10637971
B	130	GLY	-	CLONING ARTIFACT	GB 10637971
C	0	MLI	-	PROPIONATION	GB 10637971
C	7	LEU	ILE	CONFLICT	GB 10637971
C	130	GLY	-	CLONING ARTIFACT	GB 10637971
D	0	MLI	-	PROPIONATION	GB 10637971
D	7	LEU	ILE	CONFLICT	GB 10637971
D	130	GLY	-	CLONING ARTIFACT	GB 10637971
E	0	MLI	-	PROPIONATION	GB 10637971
E	7	LEU	ILE	CONFLICT	GB 10637971
E	130	GLY	-	CLONING ARTIFACT	GB 10637971
F	0	MLI	-	PROPIONATION	GB 10637971
F	7	LEU	ILE	CONFLICT	GB 10637971

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	130	GLY	-	CLONING ARTIFACT	GB 10637971

- Molecule 2 is water.

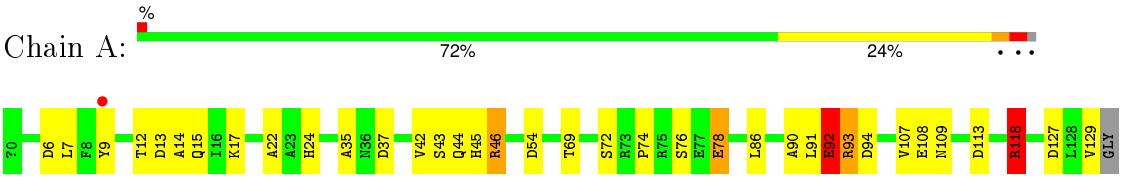
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	148	Total O 148 148	0	0
2	B	135	Total O 135 135	0	0
2	C	158	Total O 158 158	0	0
2	D	168	Total O 168 168	0	0
2	E	171	Total O 171 171	0	0
2	F	176	Total O 176 176	0	0

3 Residue-property plots (i)

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.

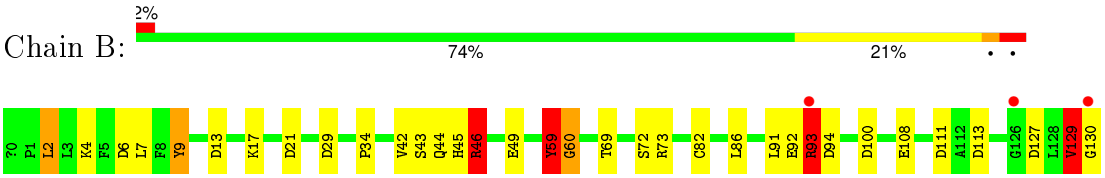
- Molecule 1: Malonate Semialdehyde Decarboxylase

Chain A:



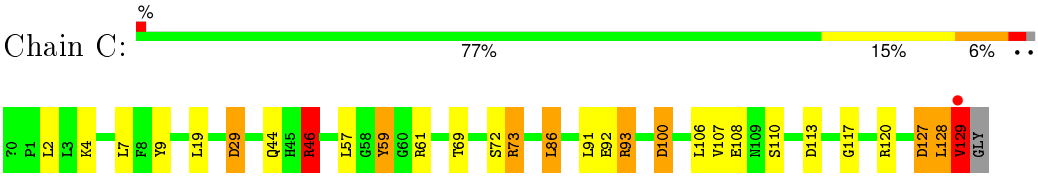
- Molecule 1: Malonate Semialdehyde Decarboxylase

Chain B:



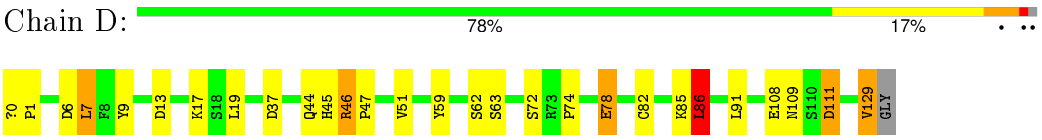
- Molecule 1: Malonate Semialdehyde Decarboxylase

Chain C:



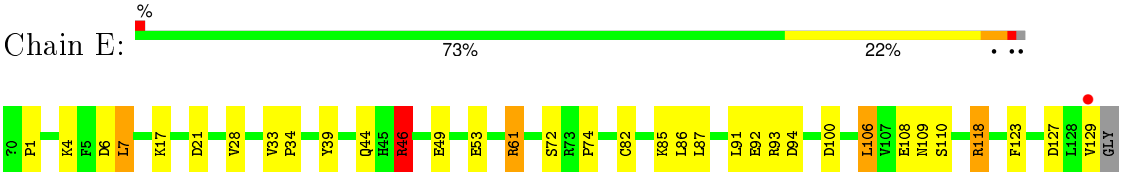
- Molecule 1: Malonate Semialdehyde Decarboxylase

Chain D:



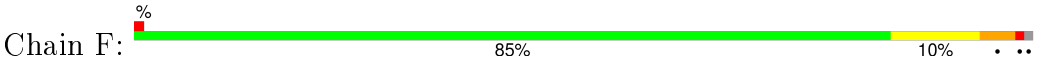
- Molecule 1: Malonate Semialdehyde Decarboxylase

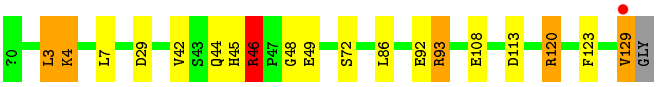
Chain E:



- Molecule 1: Malonate Semialdehyde Decarboxylase

Chain F:




?0
L3
K4
L7
D29
V42
S43
Q44
H45
R46
P47
G48
E49
S72
L86
E92
R93
E108
D113
R120
F123
V129
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	51.89Å 51.89Å 219.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.55 – 1.65 73.03 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (72.55-1.65) 98.8 (73.03-1.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.184 , 0.239 0.188 , 0.181	Depositor DCC
R_{free} test set	3962 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	9.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 17.5	EDS
Estimated twinning fraction	0.069 for -h,-k,l 0.237 for h,-h-k,-l 0.074 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 86018 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7105	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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

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	1.32	6/1052 (0.6%)	1.47	16/1423 (1.1%)
1	B	1.42	13/1021 (1.3%)	1.58	19/1382 (1.4%)
1	C	1.52	10/1047 (1.0%)	1.57	18/1417 (1.3%)
1	D	1.56	13/1054 (1.2%)	1.34	19/1426 (1.3%)
1	E	1.64	14/1032 (1.4%)	1.72	23/1397 (1.6%)
1	F	1.33	8/1016 (0.8%)	1.58	11/1375 (0.8%)
All	All	1.47	64/6222 (1.0%)	1.55	106/8420 (1.3%)

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	B	0	2
1	C	0	3
1	F	0	1
All	All	0	6

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	39	TYR	CE1-CZ	-16.42	1.17	1.38
1	D	59	TYR	CE1-CZ	-15.58	1.18	1.38
1	C	129	VAL	CA-CB	-14.02	1.25	1.54
1	C	129	VAL	CB-CG1	-13.67	1.24	1.52
1	D	59	TYR	CG-CD2	-12.92	1.22	1.39

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	61	ARG	NE-CZ-NH1	33.53	137.07	120.30
1	F	3	LEU	O-C-N	-31.10	72.95	122.70
1	C	129	VAL	CB-CA-C	-24.75	64.37	111.40
1	B	93	ARG	NE-CZ-NH2	-21.31	109.65	120.30
1	B	46	ARG	NE-CZ-NH1	-19.91	110.35	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	TYR	Peptide
1	B	93	ARG	Sidechain
1	C	128	LEU	Mainchain,Peptide
1	C	59	TYR	Peptide
1	F	3	LEU	Mainchain

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	1040	0	1017	42	2
1	B	1009	0	986	43	3
1	C	1035	0	1010	23	2
1	D	1041	0	1015	28	0
1	E	1020	0	1002	17	0
1	F	1004	0	981	18	0
2	A	148	0	0	16	4
2	B	135	0	0	15	1
2	C	158	0	0	7	6
2	D	168	0	0	10	3
2	E	171	0	0	8	4
2	F	176	0	0	7	3
All	All	7105	0	6011	162	14

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 13.

The worst 5 of 162 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:46:ARG:CG	1:B:46:ARG:HH11	1.16	1.35
1:E:4:LYS:HE2	2:E:264:HOH:O	1.25	1.31
1:A:46:ARG:NH2	1:B:9:TYR:OH	1.73	1.21
1:D:78:GLU:HG2	2:D:179:HOH:O	1.33	1.19
1:F:93:ARG:HD2	2:F:173:HOH:O	1.49	1.11

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:HOH:O	2:D:279:HOH:O[1_444]	1.18	1.02
1:B:93:ARG:NH2	1:C:93:ARG:CB[1_455]	1.67	0.53
1:A:93:ARG:O	1:B:93:ARG:NH1[1_665]	1.86	0.34
2:A:269:HOH:O	2:C:172:HOH:O[1_455]	1.89	0.31
1:C:46:ARG:NH2	2:D:216:HOH:O[1_544]	1.95	0.25

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	132/131 (101%)	128 (97%)	4 (3%)	0	100	100
1	B	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	C	132/131 (101%)	128 (97%)	4 (3%)	0	100	100
1	D	133/131 (102%)	130 (98%)	3 (2%)	0	100	100
1	E	130/131 (99%)	125 (96%)	5 (4%)	0	100	100
1	F	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
All	All	784/786 (100%)	762 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	111/106 (105%)	108 (97%)	3 (3%)	52 23
1	B	107/106 (101%)	105 (98%)	2 (2%)	65 40
1	C	111/106 (105%)	109 (98%)	2 (2%)	66 43
1	D	112/106 (106%)	109 (97%)	3 (3%)	52 23
1	E	109/106 (103%)	104 (95%)	5 (5%)	33 8
1	F	107/106 (101%)	105 (98%)	2 (2%)	65 40
All	All	657/636 (103%)	640 (97%)	17 (3%)	55 25

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1	PRO
1	D	7	LEU
1	E	61	ARG
1	C	129	VAL
1	E	106	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	45	HIS
1	D	24	HIS
1	D	45	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates 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^{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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	129/131 (98%)	-0.47	1 (0%)	87	88	6, 9, 15, 19	0
1	B	130/131 (99%)	-0.40	3 (2%)	64	65	6, 9, 15, 25	0
1	C	129/131 (98%)	-0.43	1 (0%)	87	88	6, 9, 15, 19	0
1	D	129/131 (98%)	-0.49	0	100	100	6, 9, 15, 19	0
1	E	129/131 (98%)	-0.48	1 (0%)	87	88	6, 9, 15, 19	0
1	F	129/131 (98%)	-0.50	1 (0%)	87	88	6, 9, 15, 19	0
All	All	775/786 (98%)	-0.46	7 (0%)	85	87	6, 9, 15, 25	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	VAL	5.2
1	B	130	GLY	3.9
1	F	129	VAL	2.7
1	B	126	GLY	2.5
1	B	93	ARG	2.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.