

Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 06:52 pm BST

PDB ID : 5MYP

Title : Structure of apo-TbALDH3

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Deposited on : 2017-01-27

Resolution : 1.95 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 (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 : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

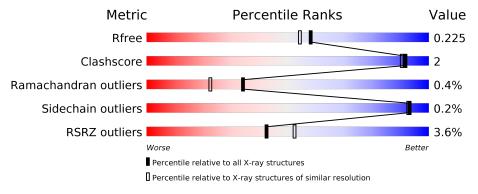
Validation Pipeline (wwPDB-VP) : 2.11

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 1.95 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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 <=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	546	85%	11%
1	В	546	85%	11%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8406 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 Aldehyde dehydrogenase.

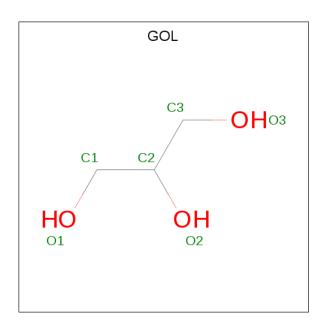
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	485	Total C		N	О	S	0	20	0
1	Α	400	3945	2499	696	731	19	0	20	
1	R	485	Total	С	N	О	S	0	22	0
1	В	400	3959	2508	699	733	19		0 22	

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q583M9
A	2	SER	-	expression tag	UNP Q583M9
A	3	MET	-	expression tag	UNP Q583M9
A	4	ALA	-	expression tag	UNP Q583M9
A	19	VAL	THR	conflict	UNP Q583M9
A	30	ASP	ASN	conflict	UNP Q583M9
A	235	THR	SER	conflict	UNP Q583M9
A	323	GLN	HIS	conflict	UNP Q583M9
A	354	ASN	ASP	conflict	UNP Q583M9
A	465	LEU	PHE	conflict	UNP Q583M9
A	541	SER	GLY	conflict	UNP Q583M9
В	1	GLY	-	expression tag	UNP Q583M9
В	2	SER	-	expression tag	UNP Q583M9
В	3	MET	-	expression tag	UNP Q583M9
В	4	ALA	-	expression tag	UNP Q583M9
В	19	VAL	THR	conflict	UNP Q583M9
В	30	ASP	ASN	conflict	UNP Q583M9
В	235	THR	SER	conflict	UNP Q583M9
В	323	GLN	HIS	conflict	UNP Q583M9
В	354	ASN	ASP	conflict	UNP Q583M9
В	465	LEU	PHE	conflict	UNP Q583M9
В	541	SER	GLY	conflict	UNP Q583M9

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





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

• Molecule 3 is water.

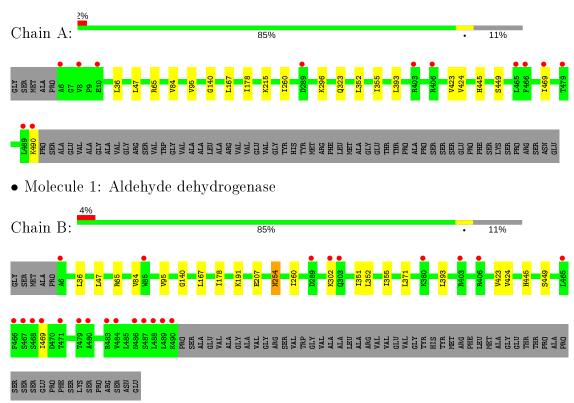
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	252	Total O 252 252	0	0
3	В	238	Total O 238 238	0	0



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 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: Aldehyde dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	87.72Å 63.95Å 91.75Å	Depositor
a, b, c, α , β , γ	90.00° 98.64° 90.00°	Depositor
Resolution (Å)	22.90 - 1.95	Depositor
resolution (A)	22.87 - 1.95	EDS
% Data completeness	99.2 (22.90-1.95)	Depositor
(in resolution range)	99.3 (22.87-1.95)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.70 \; ({\rm at} \; 1.95 {\rm \AA})$	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
D D.	0.200 , 0.223	Depositor
R, R_{free}	0.207 , 0.225	DCC
R_{free} test set	3580 reflections $(4.93%)$	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39 , 43.6	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8406	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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		
MIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.35	0/4014	0.57	0/5429	
1	В	0.35	0/4028	0.56	0/5449	
All	All	0.35	0/8042	0.57	0/10878	

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	3945	0	4034	12	0
1	В	3959	0	4049	17	0
2	A	12	0	16	0	0
3	A	252	0	0	0	0
3	В	238	0	0	0	0
All	All	8406	0	8099	26	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 2.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance} \left(\operatorname{\AA} \right)$	overlap (Å)
1:B:36:LEU:HD21	1:B:95:VAL:HG21	1.81	0.62
1:B:191[B]:LYS:NZ	1:B:191[B]:LYS:HB3	2.17	0.60
1:A:47:LEU:HB2	1:A:84:VAL:HG11	1.83	0.60
1:B:47:LEU:HB2	1:B:84:VAL:HG11	1.84	0.59
1:A:36:LEU:HD21	1:A:95:VAL:HG21	1.84	0.58
1:A:167:LEU:HD23	1:A:178:ILE:HD11	1.88	0.56
1:B:191[B]:LYS:HZ3	1:B:191[B]:LYS:HB3	1.71	0.56
1:B:167:LEU:HD23	1:B:178:ILE:HD11	1.88	0.54
1:B:191[B]:LYS:NZ	1:B:191[B]:LYS:CB	2.74	0.49
1:B:351:ILE:HD12	1:B:371:LEU:HD23	1.95	0.48
1:A:424:VAL:HG11	1:B:469:ILE:HD12	1.95	0.48
1:A:323[B]:GLN:HA	1:A:323[B]:GLN:OE1	2.12	0.47
1:B:65[A]:ARG:HA	1:B:65[A]:ARG:CZ	2.46	0.45
1:B:302[A]:LYS:HD3	1:B:302[A]:LYS:HA	1.91	0.43
1:A:260:ILE:HG23	1:A:393:LEU:HD23	2.01	0.43
1:B:260:ILE:HG23	1:B:393:LEU:HD23	2.00	0.43
1:B:352:LEU:CB	1:B:355:ILE:HD11	2.49	0.42
1:A:469:ILE:HD12	1:B:424:VAL:HG11	2.02	0.42
1:A:215[A]:LYS:HD2	1:B:207[A]:GLU:OE1	2.20	0.42
1:A:352:LEU:CB	1:A:355:ILE:HD11	2.50	0.42
1:A:140:GLY:HA3	1:A:449:SER:HB3	2.00	0.42
1:A:65[A]:ARG:HA	1:A:65[A]:ARG:CZ	2.49	0.42
1:A:296[A]:LYS:HD2	1:A:296[A]:LYS:HA	1.84	0.41
1:B:351:ILE:CD1	1:B:371:LEU:HD23	2.51	0.41
1:B:140:GLY:HA3	1:B:449:SER:HB3	2.02	0.41
1:B:65[A]:ARG:HD3	1:B:254:ASN:HD21	1.86	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	503/546~(92%)	494 (98%)	7 (1%)	2 (0%)	34 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	505/546~(92%)	496 (98%)	7 (1%)	2 (0%)	34	22
All	All	1008/1092 (92%)	990 (98%)	14 (1%)	4 (0%)	34	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	HIS
1	В	445	HIS
1	A	423	VAL
1	В	423	VAL

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	1 Analysed Rotameric Outliers		Percentiles	
1	A	433/459 (94%)	432 (100%)	1 (0%)	93 93
1	В	$435/459 \ (95\%)$	434 (100%)	1 (0%)	93 93
All	All	868/918 (95%)	866 (100%)	2 (0%)	93 93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	LYS
1	В	254	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	48	ASN
1	A	62	HIS
1	A	239	ASN
1	A	400	ASN

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Mol	Chain	Res	Type
1	A	455	HIS
1	В	16	ASN
1	В	62	HIS
1	В	136	GLN
1	В	180	ASN
1	В	196	HIS
1	В	239	ASN
1	В	254	ASN
1	В	359	HIS
1	В	400	ASN

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)

2 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	Tuno	Chain	Res	Link	В	ond leng	${ m gths}$	В	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	602	-	5,5,5	0.40	0	5,5,5	0.42	0
2	GOL	A	601	_	5,5,5	0.30	0	5,5,5	0.25	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	602	_	-	4/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	C1-C2-C3-O3
2	A	602	GOL	O2-C2-C3-O3
2	A	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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^{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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	485/546 (88%)	0.19	12 (2%) 57 66	10, 18, 30, 53	0
1	В	485/546 (88%)	0.30	23 (4%) 31 41	9, 17, 33, 58	0
All	All	970/1092 (88%)	0.25	35 (3%) 42 52	9, 17, 31, 58	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	7.4
1	В	6	ALA	6.4
1	В	469	ILE	5.7
1	В	466	PHE	5.0
1	В	468	SER	4.7
1	A	490	LYS	4.6
1	В	479	THR	4.2
1	В	465	LEU	3.7
1	В	403	ARG	3.6
1	В	471	THR	3.5
1	A	466	PHE	3.5
1	В	483[A]	ARG	3.4
1	В	488	LEU	3.4
1	В	289	ASP	3.3
1	В	487	SER	3.3
1	В	484	VAL	3.3
1	В	489	LEU	3.2
1	В	490	LYS	3.2
1	A	469	ILE	3.0
1	В	302[A]	LYS	3.0
1	A	465	LEU	2.8
1	В	303	GLN	2.7
1	A	403[A]	ARG	2.7
1	A	406	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	В	486	ASN	2.6
1	A	289	ASP	2.5
1	В	467	SER	2.5
1	В	85	TRP	2.4
1	A	489	LEU	2.4
1	В	406	ARG	2.3
1	A	8	VAL	2.3
1	В	480	ALA	2.2
1	В	380	LYS	2.2
1	A	479	THR	2.0
1	A	10	GLU	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 carbohydrates 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	GOL	A	602	6/6	0.60	0.21	43,43,44,44	0
2	GOL	A	601	6/6	0.85	0.17	24,25,26,27	0

6.5 Other polymers (i)

There are no such residues in this entry.

