



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:06 am BST

PDB ID : 4QYJ
Title : Structure of Phenylacetaldehyde Dehydrogenase from *Pseudomonas putida* S12
Authors : Crabo, A.G.; Gassner, G.T.; Sazinsky, M.H.
Deposited on : 2014-07-24
Resolution : 2.83 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

<https://www.wwpdb.org/validation/2017/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
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

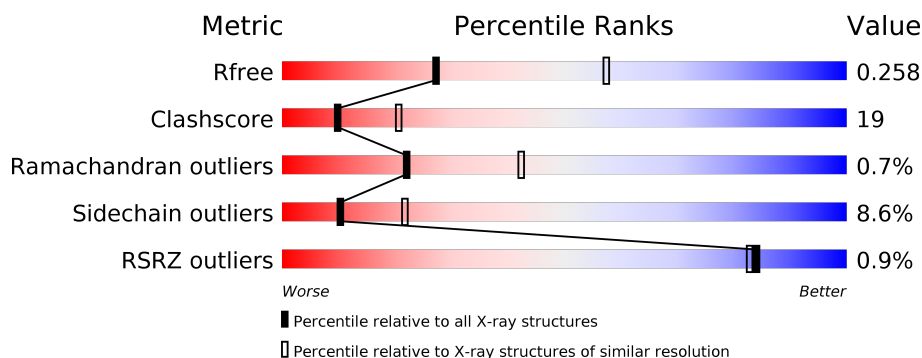
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 $\leq 5\%$. 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	516	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>27%</div> <div>• 7%</div> </div> </div>
1	B	516	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>• 7%</div> </div> </div>
1	C	516	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>• 7%</div> </div> </div>
1	D	516	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>27%</div> <div>6% 7%</div> </div> </div>
1	E	516	<div> <div></div> <div> <div>63%</div> <div>27%</div> <div>• 7%</div> </div> </div>
1	F	516	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	516	<div><div>%</div><div><div></div><div>63%</div><div>26%</div><div>•</div><div>7%</div></div></div>
1	H	516	<div><div>%</div><div><div></div><div>60%</div><div>28%</div><div>6%</div><div>7%</div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27306 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	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3416	2170	580	651	15			
1	B	481	Total	C	N	O	S	0	0	0
			3411	2169	579	648	15			
1	C	481	Total	C	N	O	S	0	0	0
			3409	2167	580	647	15			
1	D	481	Total	C	N	O	S	0	0	0
			3419	2173	584	647	15			
1	E	481	Total	C	N	O	S	0	0	0
			3408	2166	580	647	15			
1	F	481	Total	C	N	O	S	0	0	0
			3411	2169	579	648	15			
1	G	481	Total	C	N	O	S	0	0	0
			3419	2172	584	648	15			
1	H	481	Total	C	N	O	S	0	0	0
			3413	2170	581	647	15			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP V4GH04
A	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
A	-17	SER	-	EXPRESSION TAG	UNP V4GH04
A	-16	SER	-	EXPRESSION TAG	UNP V4GH04
A	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
A	-9	SER	-	EXPRESSION TAG	UNP V4GH04
A	-8	SER	-	EXPRESSION TAG	UNP V4GH04
A	-7	GLY	-	EXPRESSION TAG	UNP V4GH04

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
A	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
A	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
A	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
A	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
A	-1	SER	-	EXPRESSION TAG	UNP V4GH04
A	0	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-19	MET	-	EXPRESSION TAG	UNP V4GH04
B	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
B	-17	SER	-	EXPRESSION TAG	UNP V4GH04
B	-16	SER	-	EXPRESSION TAG	UNP V4GH04
B	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
B	-9	SER	-	EXPRESSION TAG	UNP V4GH04
B	-8	SER	-	EXPRESSION TAG	UNP V4GH04
B	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
B	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
B	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
B	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
B	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
B	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
B	-1	SER	-	EXPRESSION TAG	UNP V4GH04
B	0	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-19	MET	-	EXPRESSION TAG	UNP V4GH04
C	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
C	-17	SER	-	EXPRESSION TAG	UNP V4GH04
C	-16	SER	-	EXPRESSION TAG	UNP V4GH04
C	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
C	-9	SER	-	EXPRESSION TAG	UNP V4GH04
C	-8	SER	-	EXPRESSION TAG	UNP V4GH04
C	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
C	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
C	-5	VAL	-	EXPRESSION TAG	UNP V4GH04

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
C	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
C	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
C	-1	SER	-	EXPRESSION TAG	UNP V4GH04
C	0	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-19	MET	-	EXPRESSION TAG	UNP V4GH04
D	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
D	-17	SER	-	EXPRESSION TAG	UNP V4GH04
D	-16	SER	-	EXPRESSION TAG	UNP V4GH04
D	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
D	-9	SER	-	EXPRESSION TAG	UNP V4GH04
D	-8	SER	-	EXPRESSION TAG	UNP V4GH04
D	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
D	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
D	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
D	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
D	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
D	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
D	-1	SER	-	EXPRESSION TAG	UNP V4GH04
D	0	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-19	MET	-	EXPRESSION TAG	UNP V4GH04
E	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
E	-17	SER	-	EXPRESSION TAG	UNP V4GH04
E	-16	SER	-	EXPRESSION TAG	UNP V4GH04
E	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
E	-9	SER	-	EXPRESSION TAG	UNP V4GH04
E	-8	SER	-	EXPRESSION TAG	UNP V4GH04
E	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
E	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
E	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
E	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
E	-3	ARG	-	EXPRESSION TAG	UNP V4GH04

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
E	-1	SER	-	EXPRESSION TAG	UNP V4GH04
E	0	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-19	MET	-	EXPRESSION TAG	UNP V4GH04
F	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
F	-17	SER	-	EXPRESSION TAG	UNP V4GH04
F	-16	SER	-	EXPRESSION TAG	UNP V4GH04
F	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
F	-9	SER	-	EXPRESSION TAG	UNP V4GH04
F	-8	SER	-	EXPRESSION TAG	UNP V4GH04
F	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
F	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
F	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
F	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
F	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
F	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
F	-1	SER	-	EXPRESSION TAG	UNP V4GH04
F	0	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-19	MET	-	EXPRESSION TAG	UNP V4GH04
G	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
G	-17	SER	-	EXPRESSION TAG	UNP V4GH04
G	-16	SER	-	EXPRESSION TAG	UNP V4GH04
G	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
G	-9	SER	-	EXPRESSION TAG	UNP V4GH04
G	-8	SER	-	EXPRESSION TAG	UNP V4GH04
G	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
G	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
G	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
G	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
G	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
G	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
G	-1	SER	-	EXPRESSION TAG	UNP V4GH04

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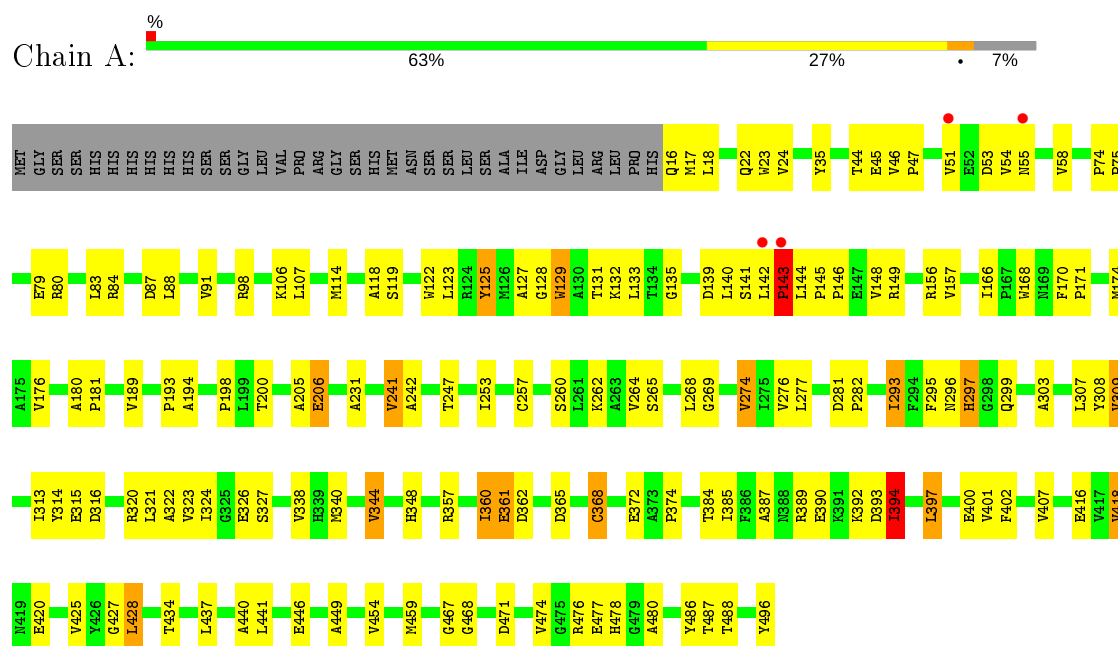
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-19	MET	-	EXPRESSION TAG	UNP V4GH04
H	-18	GLY	-	EXPRESSION TAG	UNP V4GH04
H	-17	SER	-	EXPRESSION TAG	UNP V4GH04
H	-16	SER	-	EXPRESSION TAG	UNP V4GH04
H	-15	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-14	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-13	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-12	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-11	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-10	HIS	-	EXPRESSION TAG	UNP V4GH04
H	-9	SER	-	EXPRESSION TAG	UNP V4GH04
H	-8	SER	-	EXPRESSION TAG	UNP V4GH04
H	-7	GLY	-	EXPRESSION TAG	UNP V4GH04
H	-6	LEU	-	EXPRESSION TAG	UNP V4GH04
H	-5	VAL	-	EXPRESSION TAG	UNP V4GH04
H	-4	PRO	-	EXPRESSION TAG	UNP V4GH04
H	-3	ARG	-	EXPRESSION TAG	UNP V4GH04
H	-2	GLY	-	EXPRESSION TAG	UNP V4GH04
H	-1	SER	-	EXPRESSION TAG	UNP V4GH04
H	0	HIS	-	EXPRESSION TAG	UNP V4GH04

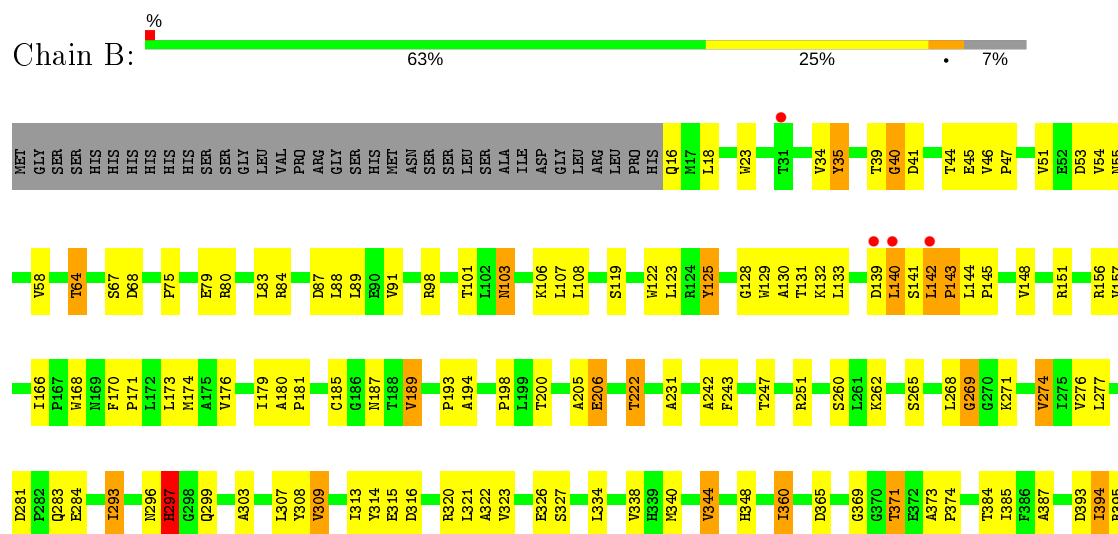
3 Residue-property plots [i](#)

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

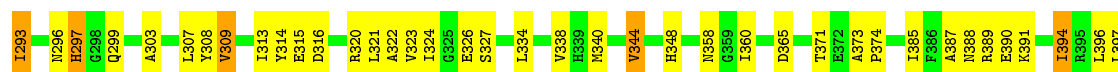
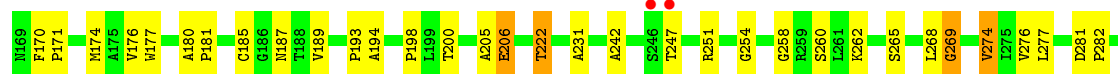
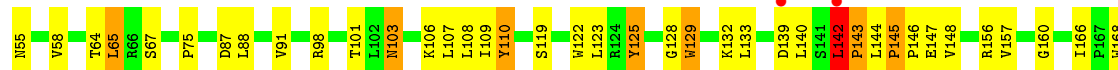
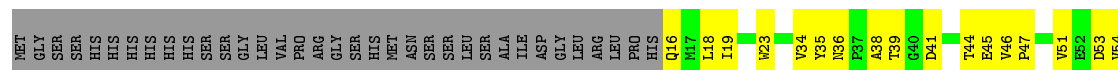


- Molecule 1: Aldehyde dehydrogenase

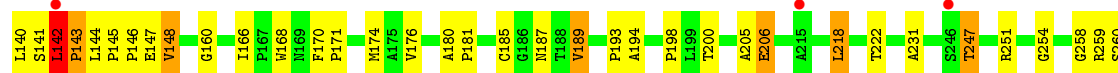
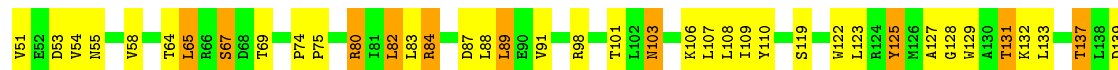
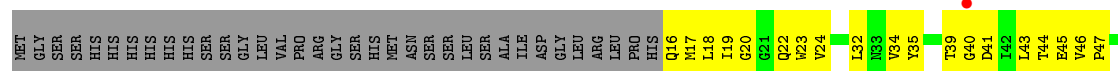




• Molecule 1: Aldehyde dehydrogenase

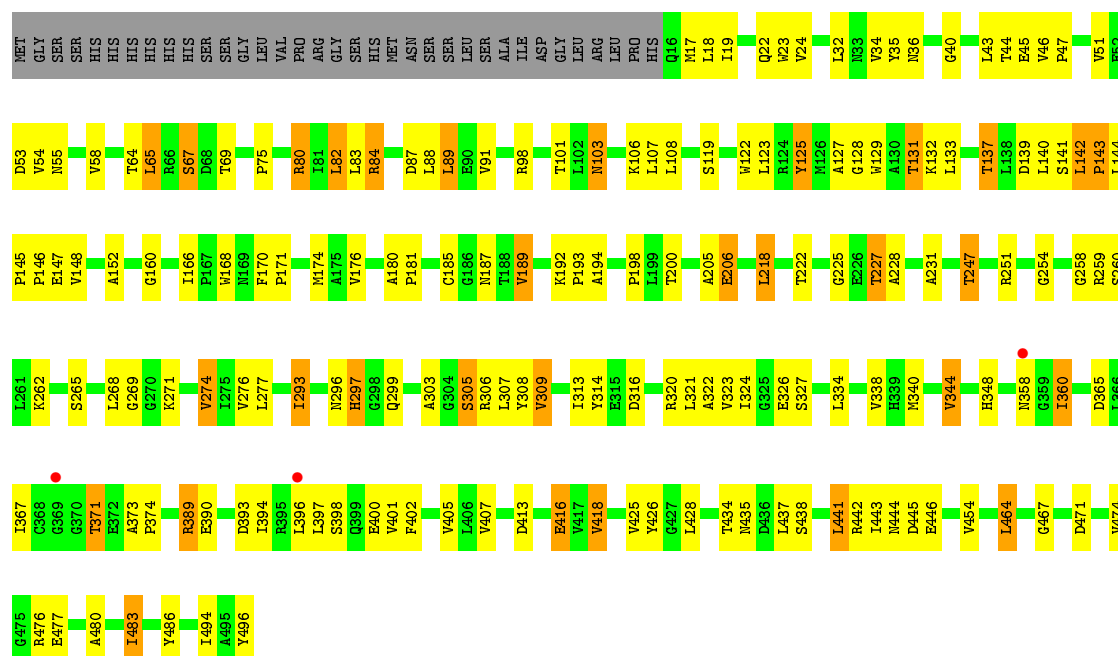


• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.09Å 118.69Å 304.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.83 49.99 – 2.83	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.99-2.83) 81.4 (49.99-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.254 , 0.258 0.254 , 0.258	Depositor DCC
R_{free} test set	4677 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , -2.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	27306	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.70	20/3485 (0.6%)	1.09	16/4781 (0.3%)
1	B	1.70	18/3480 (0.5%)	1.11	23/4774 (0.5%)
1	C	1.70	23/3478 (0.7%)	1.08	16/4772 (0.3%)
1	D	1.69	21/3488 (0.6%)	1.10	15/4783 (0.3%)
1	E	1.68	23/3477 (0.7%)	1.08	16/4771 (0.3%)
1	F	1.70	17/3480 (0.5%)	1.09	15/4774 (0.3%)
1	G	1.73	23/3488 (0.7%)	1.11	16/4784 (0.3%)
1	H	1.71	19/3482 (0.5%)	1.11	15/4776 (0.3%)
All	All	1.70	164/27858 (0.6%)	1.10	132/38215 (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	G	0	1

The worst 5 of 164 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	496	TYR	CD2-CE2	-5.97	1.30	1.39
1	C	496	TYR	CD2-CE2	-5.94	1.30	1.39
1	H	398	SER	CB-OG	-5.88	1.34	1.42
1	E	143	PRO	N-CD	5.80	1.55	1.47
1	G	146	PRO	N-CD	-5.80	1.39	1.47

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	LEU	C-N-CD	-8.38	102.15	120.60
1	G	142	LEU	N-CA-C	6.28	127.95	111.00
1	E	428	LEU	N-CA-C	5.96	127.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	360	ILE	CG1-CB-CG2	-5.95	98.32	111.40
1	C	360	ILE	CG1-CB-CG2	-5.94	98.33	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	141	SER	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	3416	0	3298	161	0
1	B	3411	0	3298	134	0
1	C	3409	0	3292	138	0
1	D	3419	0	3314	132	0
1	E	3408	0	3290	146	0
1	F	3411	0	3298	121	0
1	G	3419	0	3309	120	0
1	H	3413	0	3303	140	0
All	All	27306	0	26402	1033	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 1033 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:C:156:ARG:CG	1:C:487:THR:HG21	1.58	1.34
1:B:397:LEU:CD1	1:B:407:VAL:HG11	1.57	1.34
1:E:156:ARG:CG	1:E:487:THR:HG21	1.58	1.33
1:B:156:ARG:CG	1:B:487:THR:HG21	1.58	1.33
1:G:156:ARG:CG	1:G:487:THR:HG21	1.58	1.32

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	479/516 (93%)	440 (92%)	36 (8%)	3 (1%)	25	46
1	B	479/516 (93%)	429 (90%)	46 (10%)	4 (1%)	19	38
1	C	479/516 (93%)	439 (92%)	36 (8%)	4 (1%)	19	38
1	D	479/516 (93%)	434 (91%)	42 (9%)	3 (1%)	25	46
1	E	479/516 (93%)	439 (92%)	38 (8%)	2 (0%)	34	56
1	F	479/516 (93%)	433 (90%)	43 (9%)	3 (1%)	25	46
1	G	479/516 (93%)	439 (92%)	38 (8%)	2 (0%)	34	56
1	H	479/516 (93%)	436 (91%)	39 (8%)	4 (1%)	19	38
All	All	3832/4128 (93%)	3489 (91%)	318 (8%)	25 (1%)	22	42

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	C	143	PRO
1	D	143	PRO
1	F	143	PRO
1	A	394	ILE

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	338/408 (83%)	320 (95%)	18 (5%)	22	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	337/408 (83%)	315 (94%)	22 (6%)	17	33
1	C	336/408 (82%)	316 (94%)	20 (6%)	19	37
1	D	338/408 (83%)	281 (83%)	57 (17%)	2	3
1	E	336/408 (82%)	319 (95%)	17 (5%)	24	45
1	F	337/408 (83%)	315 (94%)	22 (6%)	17	33
1	G	338/408 (83%)	314 (93%)	24 (7%)	14	30
1	H	337/408 (83%)	286 (85%)	51 (15%)	3	5
All	All	2697/3264 (83%)	2466 (91%)	231 (9%)	10	22

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	389	ARG
1	E	340	MET
1	H	305	SER
1	D	413	ASP
1	E	91	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	296	ASN
1	E	121	GLN
1	H	103	ASN
1	D	319	GLN
1	E	319	GLN

5.3.3 RNA ⓘ

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 [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 ⓘ

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	481/516 (93%)	-0.05	4 (0%) 86 85	16, 27, 35, 41	0
1	B	481/516 (93%)	-0.04	4 (0%) 86 85	16, 25, 33, 45	0
1	C	481/516 (93%)	0.04	4 (0%) 86 85	17, 27, 37, 44	0
1	D	481/516 (93%)	0.04	7 (1%) 73 70	16, 28, 38, 44	0
1	E	481/516 (93%)	0.00	1 (0%) 95 94	17, 26, 35, 43	0
1	F	481/516 (93%)	0.05	8 (1%) 70 66	17, 25, 33, 43	0
1	G	481/516 (93%)	0.01	3 (0%) 89 88	18, 28, 35, 46	0
1	H	481/516 (93%)	0.22	3 (0%) 89 88	18, 29, 37, 45	0
All	All	3848/4128 (93%)	0.03	34 (0%) 84 83	16, 27, 36, 46	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	396	LEU	4.8
1	E	142	LEU	3.6
1	B	140	LEU	3.2
1	D	246	SER	3.0
1	C	246	SER	2.9

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

There are no such residues in this entry.