



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2024 – 06:13 PM EST

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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.36  
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) : 2.36

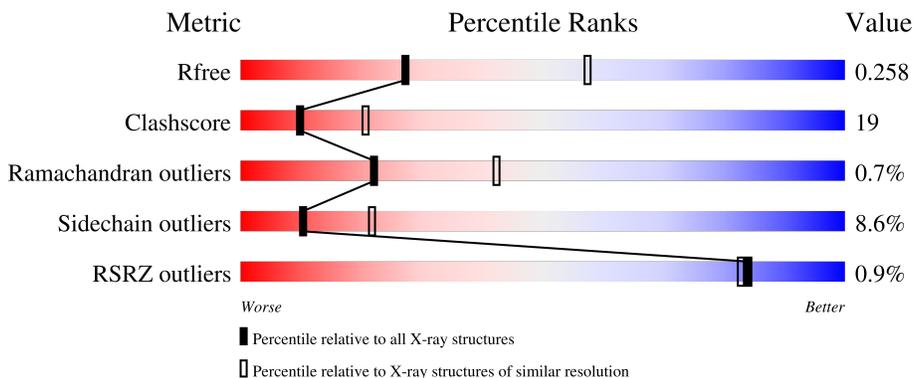
# 1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 63% 27% 7%
1	B	516	 63% 25% 7%
1	C	516	 62% 28% 7%
1	D	516	 60% 27% 6% 7%
1	E	516	 63% 27% 7%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	516	
1	G	516	
1	H	516	

## 2 Entry composition i

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
			Total	C	N	O	S			
1	A	481	Total 3416	C 2170	N 580	O 651	S 15	0	0	0
1	B	481	Total 3411	C 2169	N 579	O 648	S 15	0	0	0
1	C	481	Total 3409	C 2167	N 580	O 647	S 15	0	0	0
1	D	481	Total 3419	C 2173	N 584	O 647	S 15	0	0	0
1	E	481	Total 3408	C 2166	N 580	O 647	S 15	0	0	0
1	F	481	Total 3411	C 2169	N 579	O 648	S 15	0	0	0
1	G	481	Total 3419	C 2172	N 584	O 648	S 15	0	0	0
1	H	481	Total 3413	C 2170	N 581	O 647	S 15	0	0	0

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

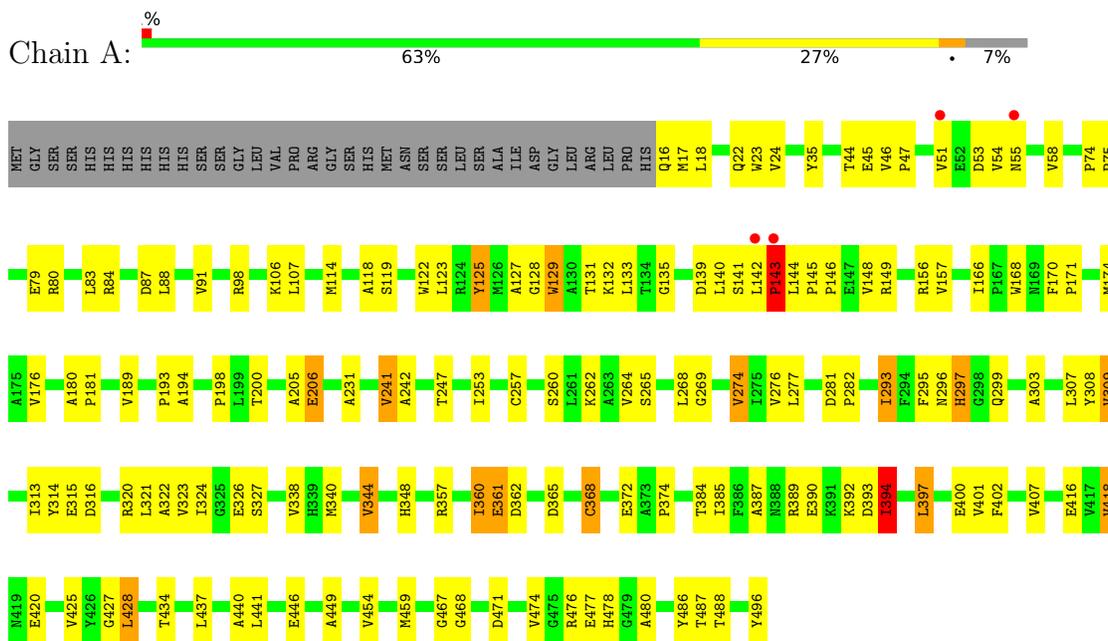
*Continued from previous page...*

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

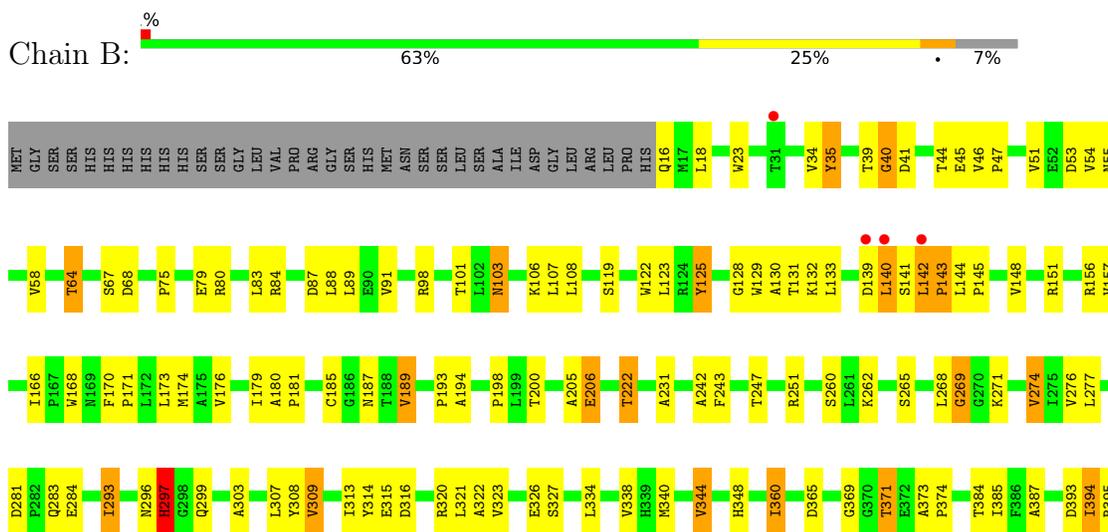
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

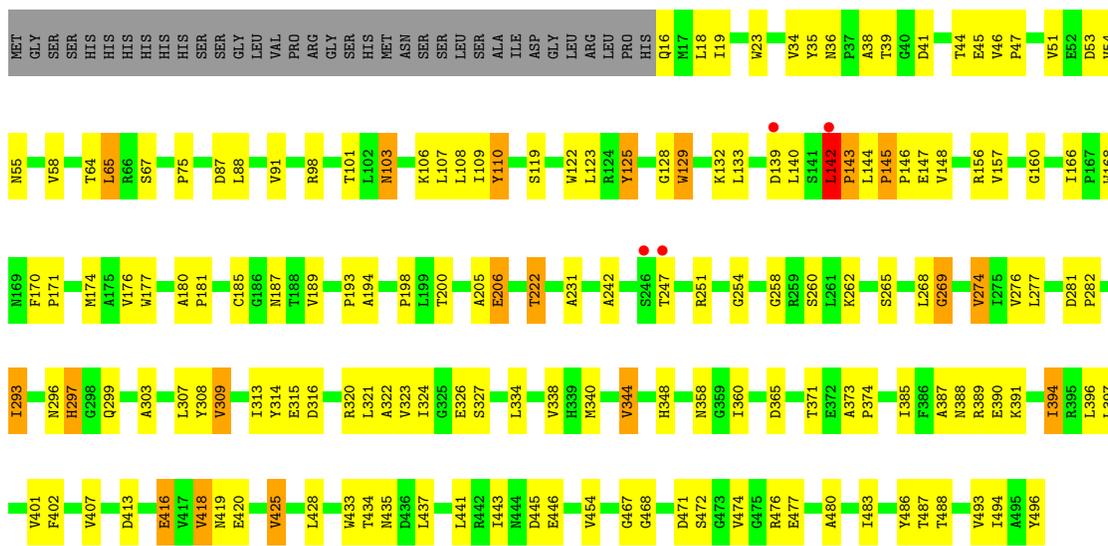


- Molecule 1: Aldehyde dehydrogenase

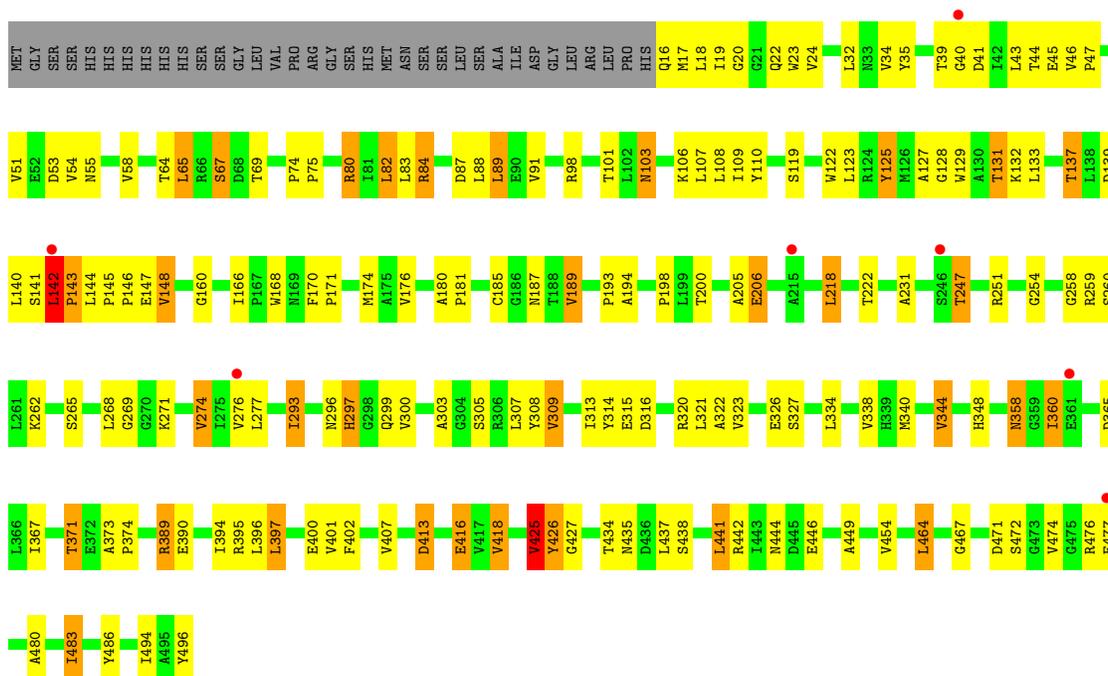




● Molecule 1: Aldehyde dehydrogenase

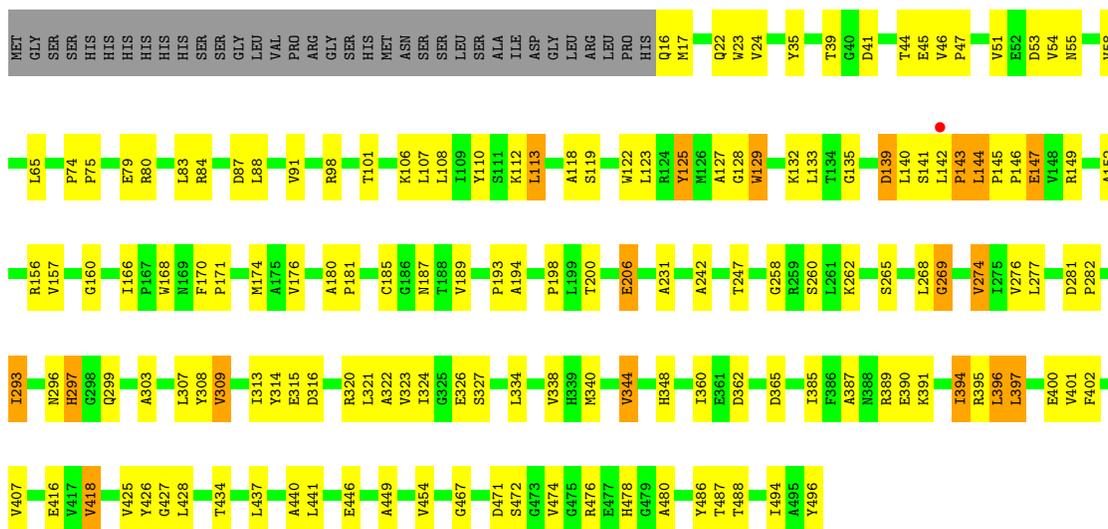


● Molecule 1: Aldehyde dehydrogenase



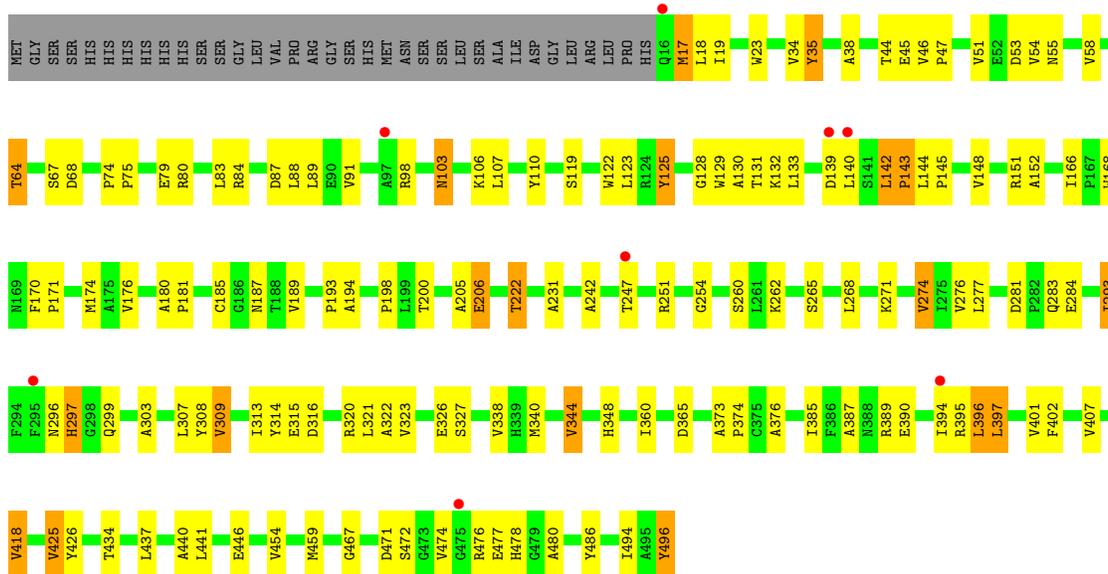
● Molecule 1: Aldehyde dehydrogenase

Chain E: 63% 27% 7%



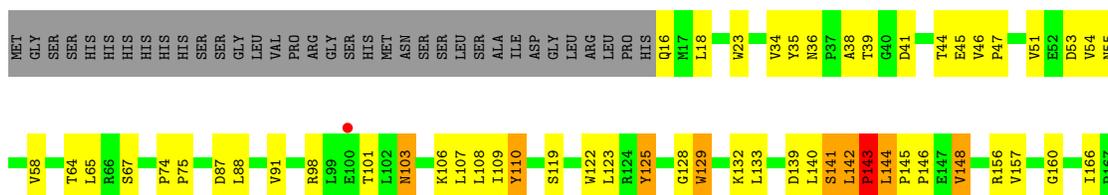
• Molecule 1: Aldehyde dehydrogenase

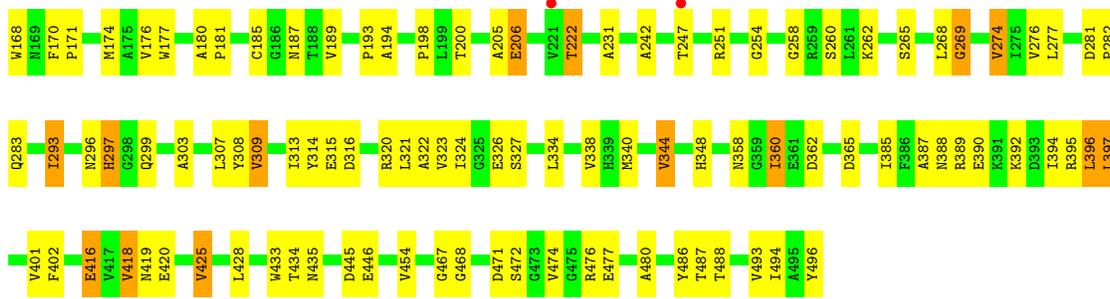
Chain F: 2% 65% 25% 7%



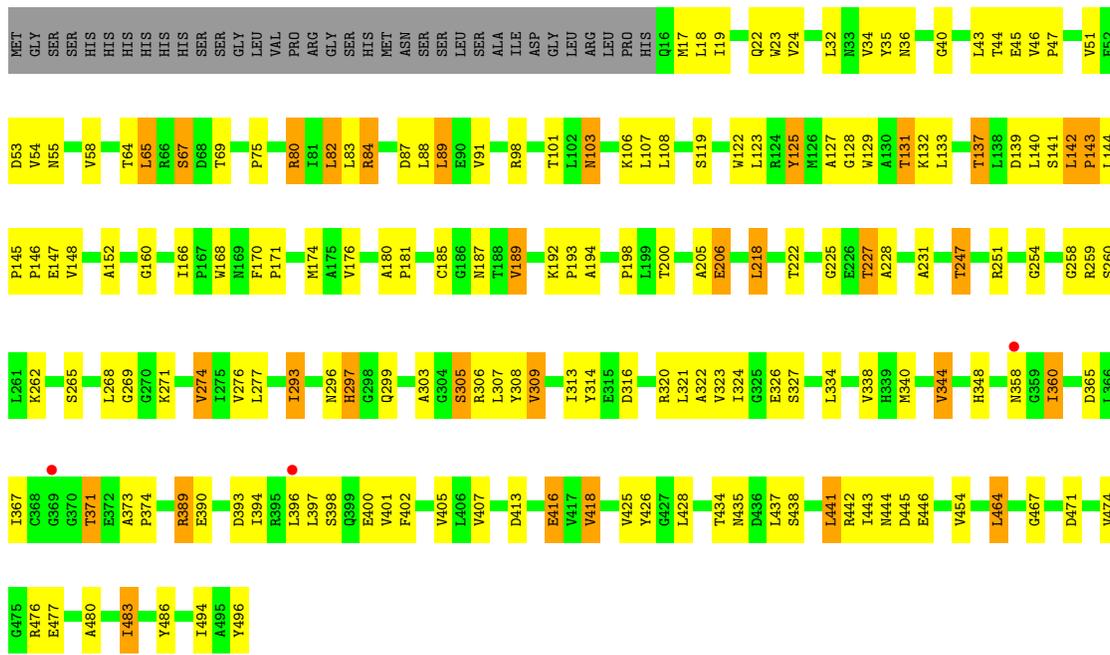
• Molecule 1: Aldehyde dehydrogenase

Chain G: 63% 26% 7%





● Molecule 1: Aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.81Å)	Xtrriage
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 <sup>2</sup> )	38.3	Xtrriage
Anisotropy	0.077	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , -2.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	27306	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage'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.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

*Continued on next page...*

Continued from previous page...

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

*Continued on next page...*

Continued from previous page...

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	464	LEU
1	H	371	THR
1	F	200	THR
1	H	365	ASP
1	H	131	THR

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

Mol	Chain	Res	Type
1	E	319	GLN
1	F	319	GLN
1	H	319	GLN
1	F	121	GLN
1	F	358	ASN

### 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 monosaccharides 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	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, 34, 43	0
1	F	481/516 (93%)	0.05	8 (1%) 70 66	16, 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 [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.