



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 12:17 AM EDT

PDB ID : 7KQV
Title : Crystal Structure of aldehyde dehydrogenase (ChALDH) from *Cladosporium herbarum*
Authors : Lee, S.G.; Jez, J.M.
Deposited on : 2020-11-17
Resolution : 3.18 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 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

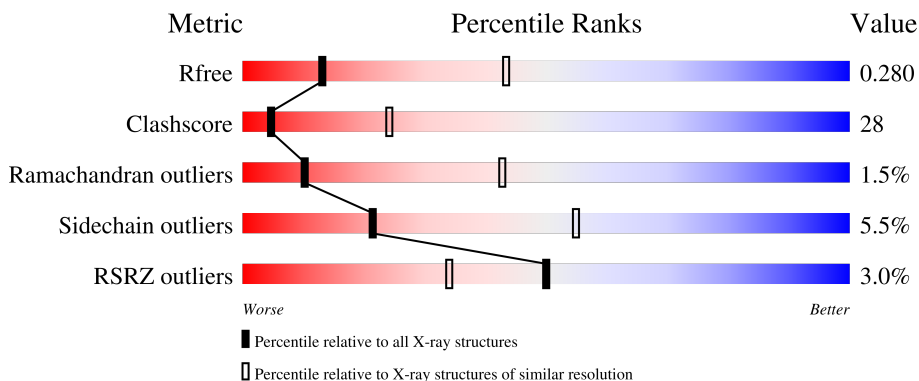
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 ≥ 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	496	 2% 45% 42% 9%
1	B	496	 3% 50% 40% 7%
1	C	496	 3% 42% 34% 20%
1	D	496	 3% 49% 43% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13484 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.

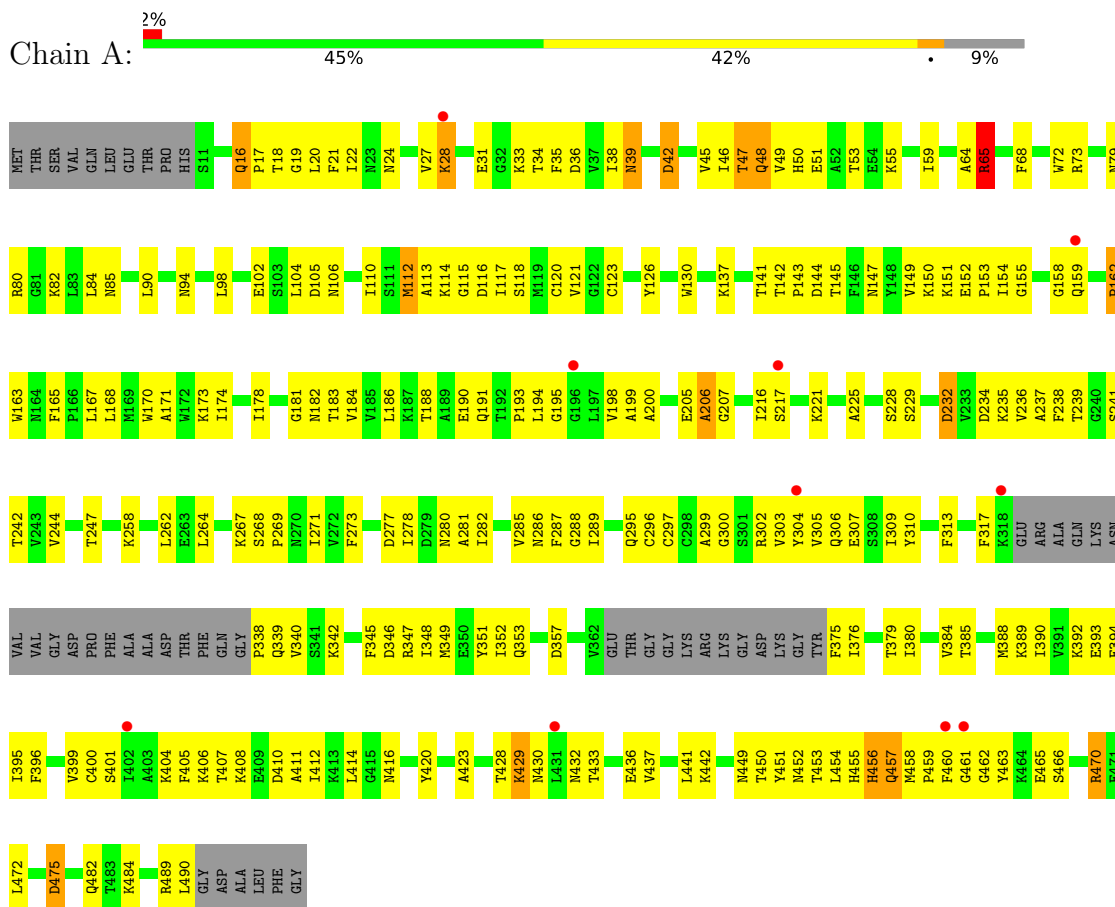
- Molecule 1 is a protein called Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	449	Total 3418	C 2181	N 572	O 650	S 15	0	0	0
1	B	460	Total 3485	C 2219	N 582	O 669	S 15	0	0	0
1	C	399	Total 3016	C 1923	N 507	O 573	S 13	0	0	0
1	D	469	Total 3565	C 2269	N 601	O 680	S 15	0	0	0

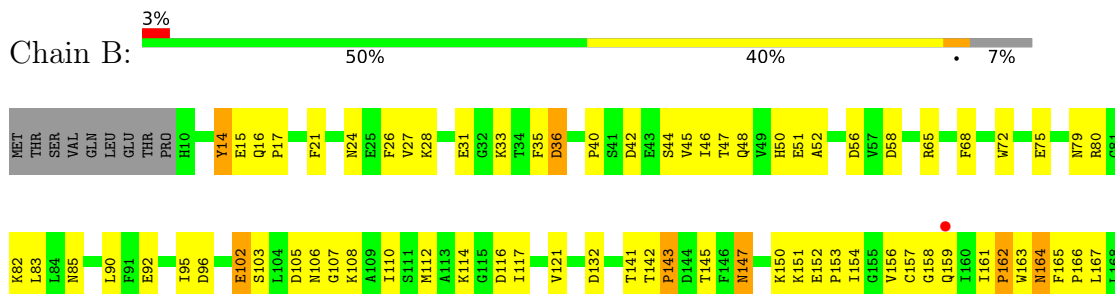
3 Residue-property plots

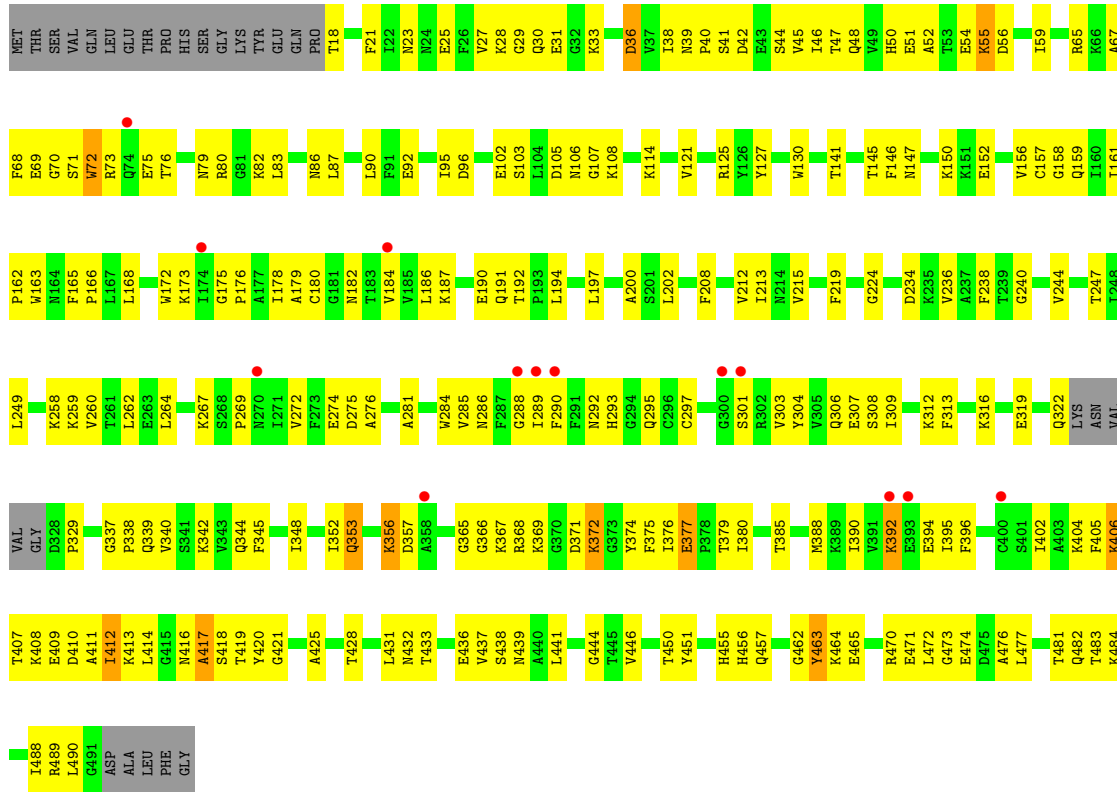
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	157.18Å 157.18Å 164.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 3.18 49.70 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.70-3.18) 99.5 (49.70-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.233 , 0.281 0.233 , 0.280	Depositor DCC
R_{free} test set	1692 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h 0.014 for -l,-k,-h 0.008 for -h,-l,-k 0.005 for -h,l,k 0.458 for -h,k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13484	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 [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	0.52	1/3484 (0.0%)	0.78	4/4716 (0.1%)
1	B	0.55	0/3554	0.74	0/4817
1	C	0.55	2/3076 (0.1%)	0.75	0/4170
1	D	0.55	1/3634 (0.0%)	0.73	2/4917 (0.0%)
All	All	0.54	4/13748 (0.0%)	0.75	6/18620 (0.0%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	ARG	CZ-NH1	6.17	1.41	1.33
1	C	172	TRP	CB-CG	-5.99	1.39	1.50
1	C	485	THR	CB-CG2	5.23	1.69	1.52
1	D	377	GLU	CD-OE1	-5.09	1.20	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH1	11.13	125.87	120.30
1	A	28	LYS	CD-CE-NZ	9.54	133.64	111.70
1	A	232	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	429	LYS	CD-CE-NZ	-5.49	99.07	111.70
1	D	431	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	276	ALA	Peptide
1	B	277	ASP	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	3418	0	3422	216	1
1	B	3485	0	3457	194	1
1	C	3016	0	3011	175	0
1	D	3565	0	3557	198	0
All	All	13484	0	13447	754	1

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 28.

The worst 5 of 754 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:D:356:LYS:NZ	1:D:357:ASP:OD1	1.74	1.20
1:D:353:GLN:HG3	1:D:356:LYS:CE	1.77	1.15
1:B:343:VAL:O	1:B:347:ARG:HD3	1.50	1.09
1:D:353:GLN:HG3	1:D:356:LYS:HE3	1.28	1.08
1:D:353:GLN:CG	1:D:356:LYS:HE3	1.84	1.08

All (1) 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)
1:A:429:LYS:NZ	1:B:432:ASN:OD1[6_455]	2.05	0.15

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	443/496 (89%)	401 (90%)	36 (8%)	6 (1%)	11	44
1	B	454/496 (92%)	411 (90%)	38 (8%)	5 (1%)	14	50
1	C	393/496 (79%)	351 (89%)	34 (9%)	8 (2%)	7	35
1	D	465/496 (94%)	428 (92%)	30 (6%)	7 (2%)	10	43
All	All	1755/1984 (88%)	1591 (91%)	138 (8%)	26 (2%)	10	43

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	B	276	ALA
1	B	326	VAL
1	D	70	GLY
1	A	115	GLY

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	365/400 (91%)	346 (95%)	19 (5%)	23	56
1	B	370/400 (92%)	349 (94%)	21 (6%)	20	54
1	C	320/400 (80%)	298 (93%)	22 (7%)	15	46
1	D	377/400 (94%)	360 (96%)	17 (4%)	27	61
All	All	1432/1600 (90%)	1353 (94%)	79 (6%)	21	55

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	400	CYS
1	D	322	GLN
1	C	427	HIS
1	D	72	TRP
1	D	372	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	50	HIS
1	D	456	HIS
1	D	293	HIS
1	A	482	GLN
1	C	427	HIS

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 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

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, 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	449/496 (90%)	0.12	10 (2%) 62 48	54, 85, 137, 251	0
1	B	460/496 (92%)	0.06	13 (2%) 53 37	48, 74, 118, 222	0
1	C	399/496 (80%)	0.17	17 (4%) 35 21	54, 79, 130, 177	0
1	D	469/496 (94%)	0.09	13 (2%) 53 37	47, 74, 119, 195	0
All	All	1777/1984 (89%)	0.11	53 (2%) 50 34	47, 78, 129, 251	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	385	THR	5.1
1	A	460	PHE	4.7
1	B	392	LYS	4.5
1	C	271	ILE	4.1
1	C	300	GLY	4.1

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.