



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:07 am GMT

PDB ID : 4QF6
Title : Structure of Aldehyde Dehydrogenase from Bacillus cereus, E194S mutant
Authors : Ngo, H.P.T.; Hong, S.H.; Oh, D.K.; Kang, L.W.
Deposited on : 2014-05-19
Resolution : 1.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

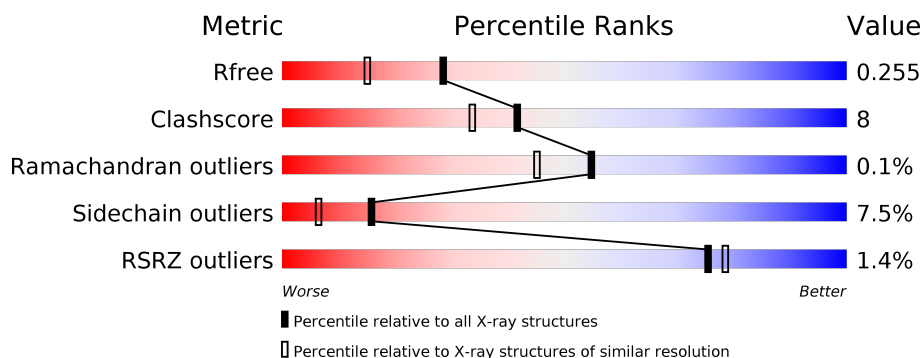
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 $\leq 5\%$. 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	494	<div> <div>81%</div> <div>15%</div> <div>...</div> </div>
1	B	494	<div> <div>%</div> <div>83%</div> <div>13%</div> <div>...</div> </div>
1	C	494	<div> <div>84%</div> <div>13%</div> <div>...</div> </div>
1	D	494	<div> <div>85%</div> <div>12%</div> <div>...</div> </div>
1	E	494	<div> <div>85%</div> <div>12%</div> <div>...</div> </div>
1	F	494	<div> <div>80%</div> <div>17%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	494	
1	H	494	
1	I	494	
1	J	494	
1	K	494	
1	L	494	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	J	501	-	-	-	X
2	NA	K	501	-	-	-	X
2	NA	L	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47191 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	491	Total	C	N	O	S	0	1	0
			3791	2414	630	733	14			
1	B	491	Total	C	N	O	S	0	1	0
			3791	2414	630	733	14			
1	C	491	Total	C	N	O	S	0	1	0
			3793	2415	630	734	14			
1	D	489	Total	C	N	O	S	0	3	0
			3787	2413	628	732	14			
1	E	490	Total	C	N	O	S	0	0	0
			3781	2408	629	730	14			
1	F	491	Total	C	N	O	S	0	2	0
			3794	2416	630	734	14			
1	G	490	Total	C	N	O	S	0	0	0
			3781	2408	629	730	14			
1	H	490	Total	C	N	O	S	0	1	0
			3787	2412	629	732	14			
1	I	491	Total	C	N	O	S	0	0	0
			3788	2412	630	732	14			
1	J	491	Total	C	N	O	S	0	0	0
			3788	2412	630	732	14			
1	K	489	Total	C	N	O	S	0	0	0
			3773	2404	627	728	14			
1	L	488	Total	C	N	O	S	0	0	0
			3764	2398	626	726	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
B	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
C	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
D	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
E	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217

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Chain	Residue	Modelled	Actual	Comment	Reference
F	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
G	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
H	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
I	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
J	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
K	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
L	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Na 2 2	0	0
2	J	2	Total Na 2 2	0	0
2	D	2	Total Na 2 2	0	0
2	K	2	Total Na 2 2	0	0
2	E	2	Total Na 2 2	0	0
2	H	2	Total Na 2 2	0	0
2	B	2	Total Na 2 2	0	0
2	I	2	Total Na 2 2	0	0
2	C	2	Total Na 2 2	0	0
2	A	2	Total Na 2 2	0	0
2	L	2	Total Na 2 2	0	0
2	F	2	Total Na 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	255	Total O 255 255	0	0
3	B	123	Total O 123 123	0	0

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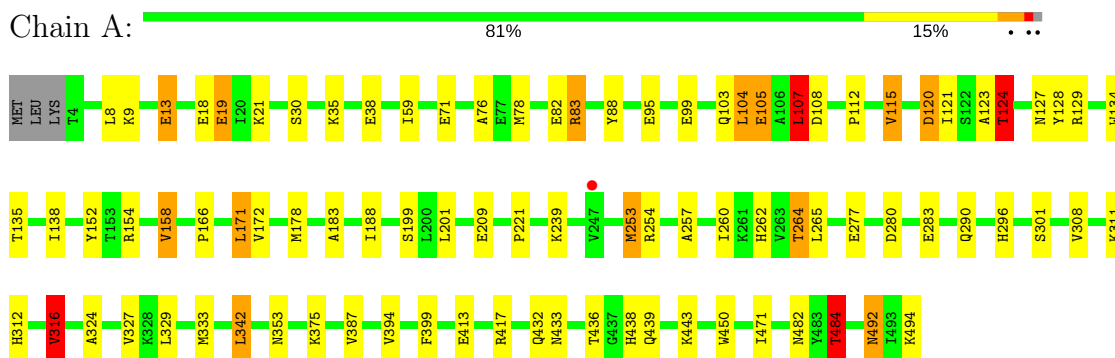
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	197	Total 197	O 197	0	0
3	D	216	Total 216	O 216	0	0
3	E	218	Total 218	O 218	0	0
3	F	124	Total 124	O 124	0	0
3	G	152	Total 152	O 152	0	0
3	H	143	Total 143	O 143	0	0
3	I	109	Total 109	O 109	0	0
3	J	74	Total 74	O 74	0	0
3	K	76	Total 76	O 76	0	0
3	L	62	Total 62	O 62	0	0

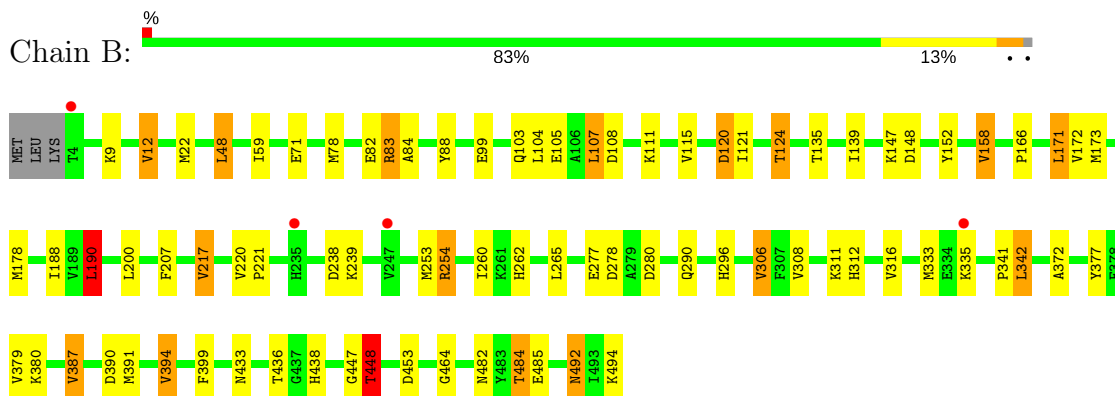
3 Residue-property plots

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.

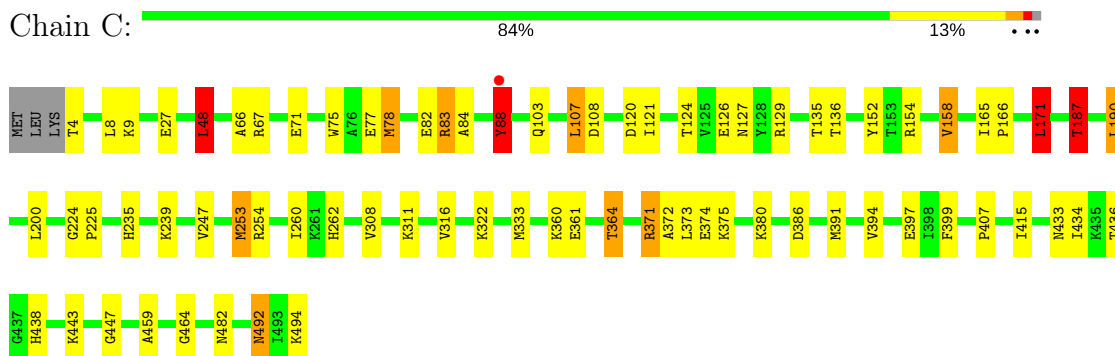
• Molecule 1: Aldehyde dehydrogenase



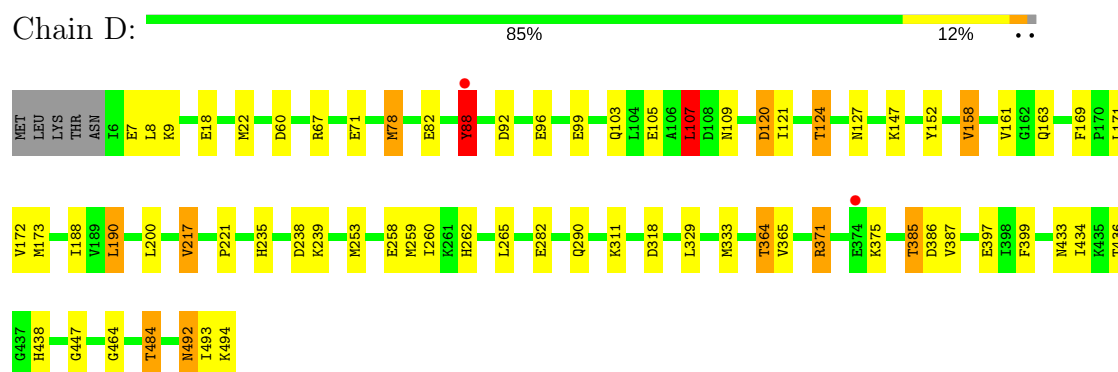
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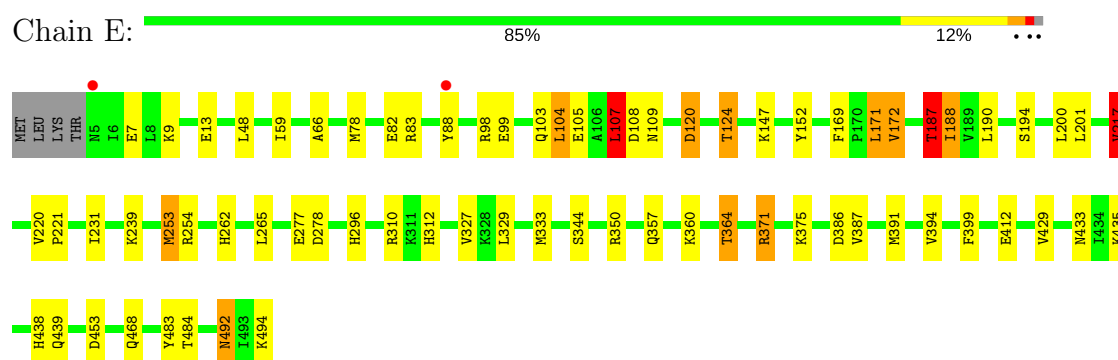
• Molecule 1: Aldehyde dehydrogenase



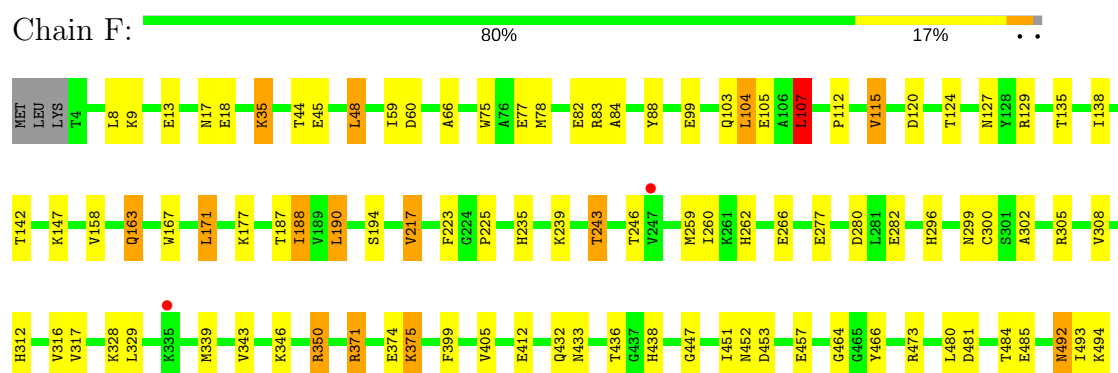
- Molecule 1: Aldehyde dehydrogenase



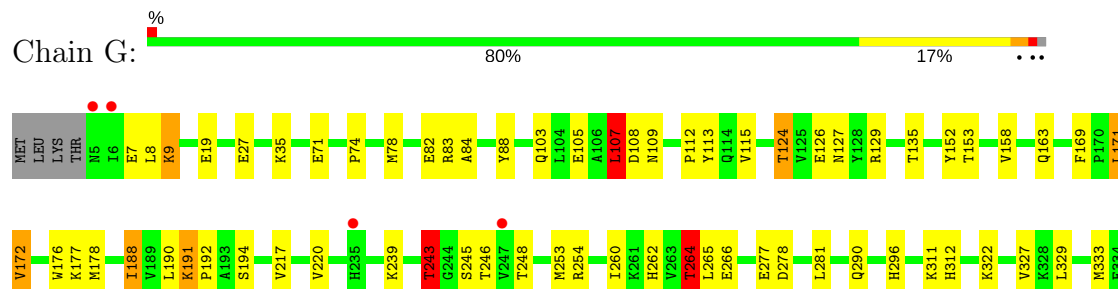
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase

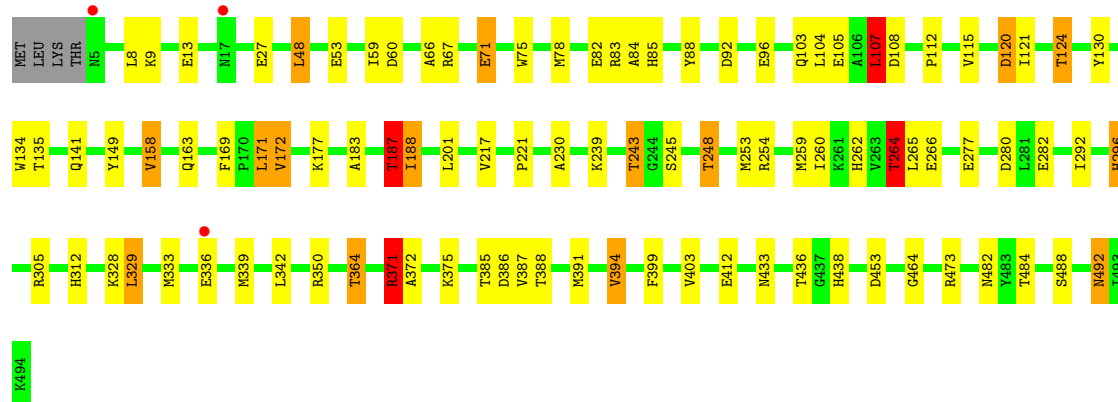
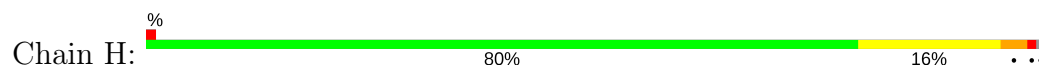


- Molecule 1: Aldehyde dehydrogenase

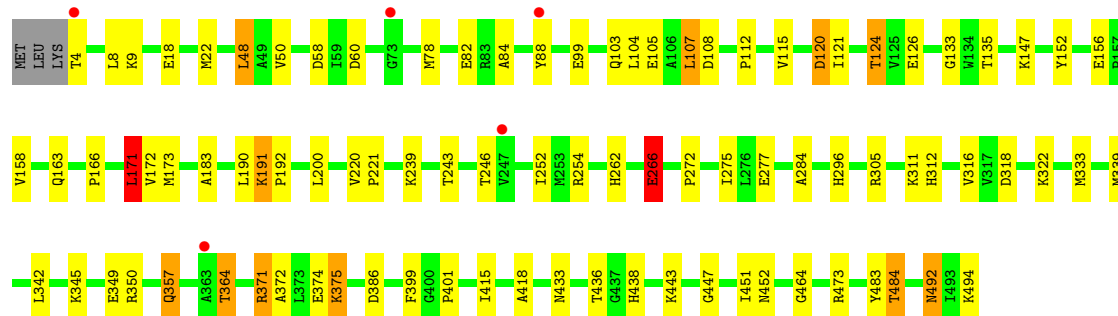
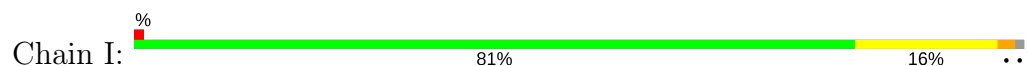




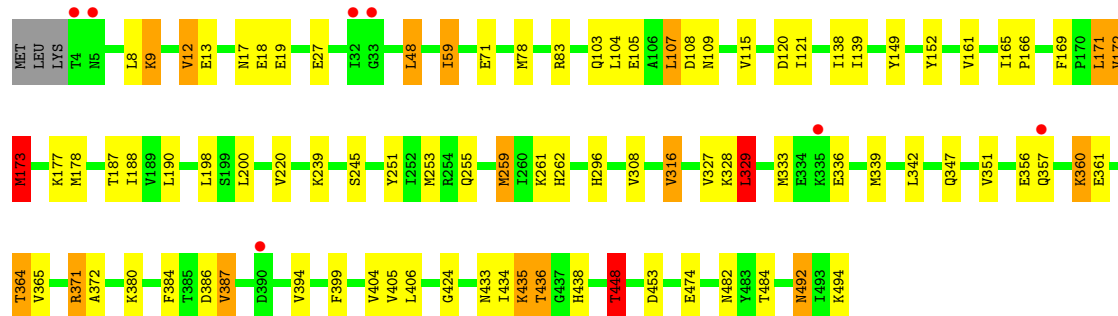
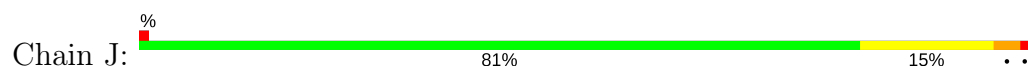
• Molecule 1: Aldehyde dehydrogenase



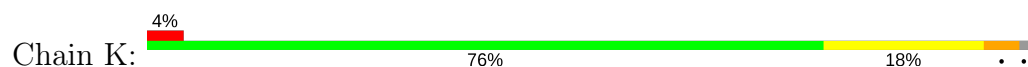
• Molecule 1: Aldehyde dehydrogenase

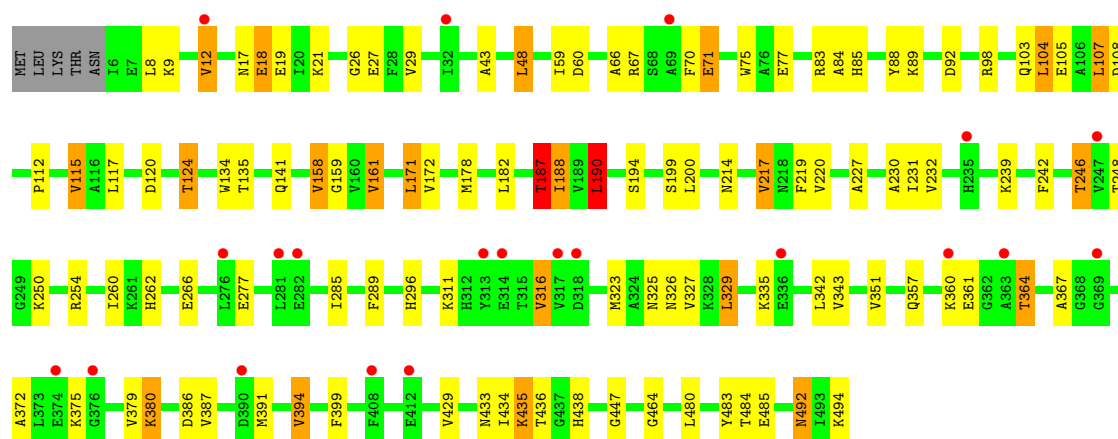


• Molecule 1: Aldehyde dehydrogenase

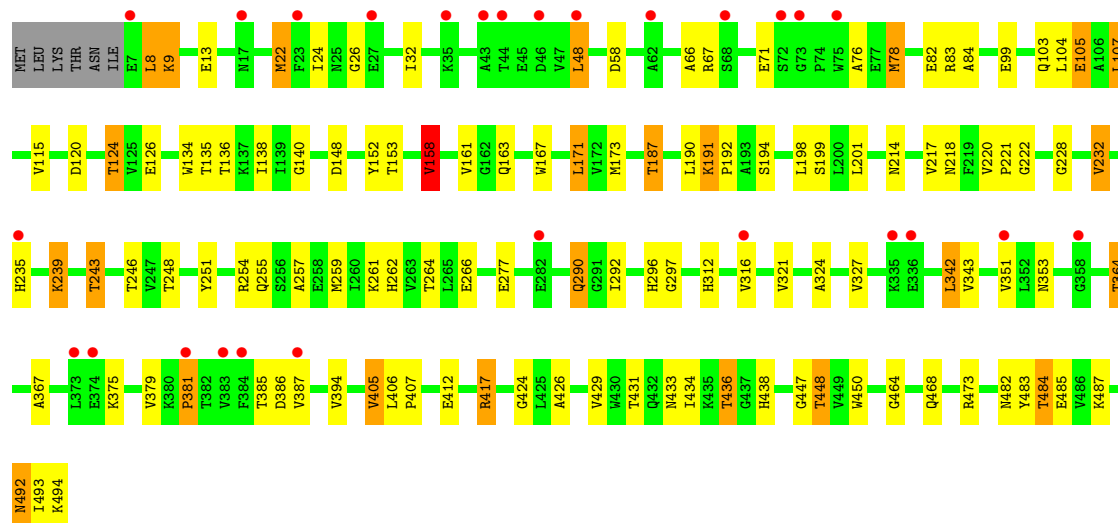
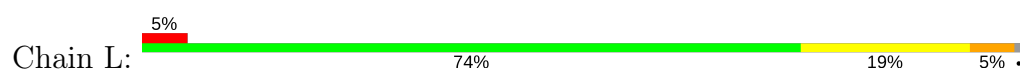


• Molecule 1: Aldehyde dehydrogenase





• Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.56Å 93.66Å 247.85Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	43.56 – 1.90 43.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.9 (43.56-1.90) 84.9 (43.56-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.47 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.204 , 0.252 0.211 , 0.255	Depositor DCC
R_{free} test set	22144 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	47191	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.04 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3627e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.18	11/3873 (0.3%)	1.11	22/5254 (0.4%)
1	B	1.03	1/3873 (0.0%)	1.07	11/5254 (0.2%)
1	C	1.08	3/3875 (0.1%)	1.08	14/5257 (0.3%)
1	D	1.07	5/3875 (0.1%)	1.07	19/5256 (0.4%)
1	E	1.13	6/3860 (0.2%)	1.08	17/5236 (0.3%)
1	F	1.06	2/3879 (0.1%)	1.07	14/5262 (0.3%)
1	G	1.05	4/3860 (0.1%)	1.01	7/5236 (0.1%)
1	H	1.02	4/3869 (0.1%)	1.04	12/5248 (0.2%)
1	I	0.98	2/3867 (0.1%)	0.98	8/5246 (0.2%)
1	J	0.94	1/3867 (0.0%)	0.98	4/5246 (0.1%)
1	K	1.02	1/3852 (0.0%)	1.00	7/5225 (0.1%)
1	L	1.01	1/3843 (0.0%)	1.00	3/5214 (0.1%)
All	All	1.05	41/46393 (0.1%)	1.04	138/62934 (0.2%)

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	D	0	1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	GLU	CD-OE1	8.67	1.35	1.25
1	G	264	THR	CB-CG2	8.24	1.79	1.52
1	D	88	TYR	CE1-CZ	7.98	1.49	1.38
1	C	88	TYR	CE1-CZ	7.86	1.48	1.38
1	H	264	THR	CB-CG2	7.09	1.75	1.52

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	278	ASP	CB-CG-OD1	11.71	128.84	118.30
1	G	108	ASP	CB-CG-OD2	-10.16	109.16	118.30
1	I	108	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	C	254	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	D	158	VAL	CB-CA-C	-9.20	93.92	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	493	ILE	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	3791	0	3743	61	0
1	B	3791	0	3743	57	0
1	C	3793	0	3742	53	0
1	D	3787	0	3742	54	0
1	E	3781	0	3731	53	0
1	F	3794	0	3748	75	0
1	G	3781	0	3731	73	0
1	H	3787	0	3737	74	0
1	I	3788	0	3738	66	0
1	J	3788	0	3738	65	0
1	K	3773	0	3725	83	0
1	L	3764	0	3714	89	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	255	0	0	11	0
3	B	123	0	0	3	0
3	C	197	0	0	3	0
3	D	216	0	0	5	0
3	E	218	0	0	1	0
3	F	124	0	0	2	0
3	G	152	0	0	4	0
3	H	143	0	0	3	0
3	I	109	0	0	1	0
3	J	74	0	0	4	0
3	K	76	0	0	3	0
3	L	62	0	0	4	0
All	All	47191	0	44832	720	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 8.

The worst 5 of 720 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:H:264:THR:CG2	1:H:264:THR:CB	1.75	1.63
1:G:264:THR:CB	1:G:264:THR:CG2	1.79	1.58
1:L:448:THR:HG23	3:L:627:HOH:O	1.60	1.02
1:D:88:TYR:CE2	3:D:689:HOH:O	2.12	1.01
1:I:173:MET:HE1	1:I:243:THR:HG21	1.48	0.92

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	490/494 (99%)	478 (98%)	12 (2%)	0	100	100
1	B	490/494 (99%)	471 (96%)	19 (4%)	0	100	100
1	C	490/494 (99%)	476 (97%)	13 (3%)	1 (0%)	51	41
1	D	490/494 (99%)	476 (97%)	14 (3%)	0	100	100
1	E	488/494 (99%)	474 (97%)	14 (3%)	0	100	100
1	F	491/494 (99%)	475 (97%)	16 (3%)	0	100	100
1	G	488/494 (99%)	473 (97%)	15 (3%)	0	100	100
1	H	489/494 (99%)	473 (97%)	16 (3%)	0	100	100
1	I	489/494 (99%)	471 (96%)	18 (4%)	0	100	100
1	J	489/494 (99%)	471 (96%)	17 (4%)	1 (0%)	51	41
1	K	487/494 (99%)	470 (96%)	17 (4%)	0	100	100
1	L	486/494 (98%)	466 (96%)	18 (4%)	2 (0%)	38	26
All	All	5867/5928 (99%)	5674 (97%)	189 (3%)	4 (0%)	55	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	78	MET
1	C	373	LEU
1	L	424	GLY
1	J	424	GLY

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	399/401 (100%)	375 (94%)	24 (6%)	22	11
1	B	399/401 (100%)	369 (92%)	30 (8%)	16	6
1	C	399/401 (100%)	376 (94%)	23 (6%)	23	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	399/401 (100%)	374 (94%)	25 (6%)	21	10
1	E	397/401 (99%)	373 (94%)	24 (6%)	22	11
1	F	400/401 (100%)	372 (93%)	28 (7%)	18	8
1	G	397/401 (99%)	367 (92%)	30 (8%)	15	6
1	H	398/401 (99%)	364 (92%)	34 (8%)	12	5
1	I	398/401 (99%)	370 (93%)	28 (7%)	18	8
1	J	398/401 (99%)	360 (90%)	38 (10%)	10	3
1	K	396/401 (99%)	361 (91%)	35 (9%)	12	4
1	L	395/401 (98%)	355 (90%)	40 (10%)	9	3
All	All	4775/4812 (99%)	4416 (92%)	359 (8%)	16	6

5 of 359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	124	THR
1	H	217	VAL
1	L	158	VAL
1	G	194	SER
1	G	453	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	353	ASN
1	G	438	HIS
1	L	114	GLN
1	F	433	ASN
1	G	214	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	491/494 (99%)	-0.14	1 (0%) 94 95	5, 10, 21, 35	0
1	B	491/494 (99%)	0.02	4 (0%) 86 87	10, 17, 30, 45	0
1	C	491/494 (99%)	-0.12	1 (0%) 94 95	5, 12, 25, 43	0
1	D	489/494 (98%)	-0.07	2 (0%) 92 93	5, 12, 25, 37	0
1	E	490/494 (99%)	-0.12	2 (0%) 92 93	5, 11, 23, 43	0
1	F	491/494 (99%)	0.07	2 (0%) 92 93	9, 17, 31, 43	0
1	G	490/494 (99%)	0.02	5 (1%) 82 84	10, 16, 29, 52	0
1	H	490/494 (99%)	0.03	3 (0%) 89 90	10, 16, 29, 58	0
1	I	491/494 (99%)	0.02	5 (1%) 82 84	11, 18, 30, 46	0
1	J	491/494 (99%)	0.15	7 (1%) 75 78	10, 21, 34, 53	0
1	K	489/494 (98%)	0.46	21 (4%) 36 39	13, 21, 34, 50	0
1	L	488/494 (98%)	0.56	27 (5%) 26 29	13, 22, 35, 57	0
All	All	5882/5928 (99%)	0.08	80 (1%) 75 78	5, 17, 30, 58	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	43	ALA	5.5
1	H	5	ASN	4.6
1	J	33	GLY	4.3
1	E	5	ASN	3.8
1	K	390	ASP	3.4

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	NA	J	501	1/1	0.97	0.26	12.76	20,20,20,20	0
2	NA	L	501	1/1	0.94	0.21	3.78	21,21,21,21	0
2	NA	K	501	1/1	0.95	0.18	2.15	20,20,20,20	0
2	NA	A	501	1/1	0.99	0.10	1.69	10,10,10,10	0
2	NA	E	501	1/1	0.99	0.13	1.48	10,10,10,10	0
2	NA	K	502	1/1	0.94	0.14	0.38	23,23,23,23	0
2	NA	D	501	1/1	0.99	0.11	0.37	11,11,11,11	0
2	NA	I	501	1/1	0.98	0.10	-0.15	19,19,19,19	0
2	NA	C	501	1/1	0.98	0.09	-0.35	12,12,12,12	0
2	NA	F	501	1/1	0.93	0.10	-0.48	16,16,16,16	0
2	NA	J	502	1/1	0.94	0.10	-0.60	21,21,21,21	0
2	NA	I	502	1/1	0.98	0.09	-1.07	15,15,15,15	0
2	NA	G	501	1/1	0.99	0.09	-1.58	14,14,14,14	0
2	NA	C	502	1/1	0.99	0.08	-1.90	9,9,9,9	0
2	NA	L	502	1/1	0.98	0.07	-2.22	23,23,23,23	0
2	NA	H	502	1/1	0.98	0.06	-2.28	16,16,16,16	0
2	NA	H	501	1/1	0.97	0.07	-2.36	15,15,15,15	0
2	NA	E	502	1/1	1.00	0.06	-2.37	12,12,12,12	0
2	NA	B	502	1/1	0.96	0.07	-2.47	14,14,14,14	0
2	NA	D	502	1/1	0.98	0.07	-2.55	12,12,12,12	0
2	NA	A	502	1/1	0.99	0.06	-2.96	10,10,10,10	0
2	NA	B	501	1/1	0.94	0.09	-3.96	17,17,17,17	0
2	NA	F	502	1/1	0.98	0.06	-4.14	13,13,13,13	0
2	NA	G	502	1/1	0.99	0.05	-7.72	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.