



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:58 PM GMT

PDB ID : 4ZWL  
Title : 2.60 Angstrom resolution crystal structure of betaine aldehyde dehydrogenase (betB) H448F/Y450L double mutant from Staphylococcus aureus in complex with NAD<sup>+</sup> and BME-free Cys289  
Authors : Halavaty, A.S.; Minasov, G.; Chen, C.; Joo, J.C.; Yakunin, A.F.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2015-05-19  
Resolution : 2.60 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

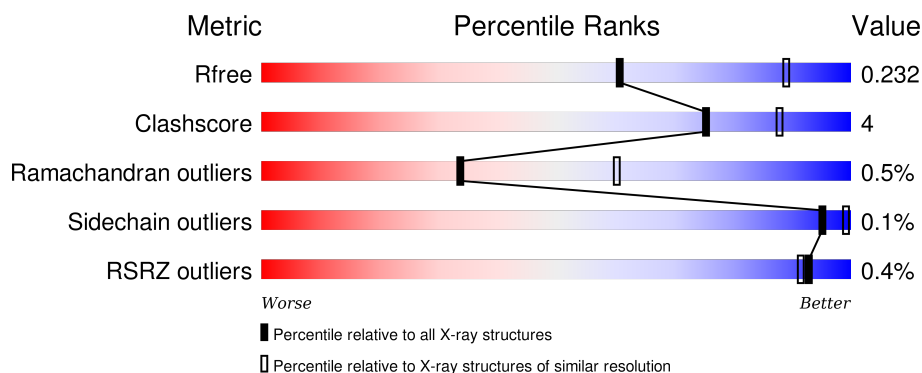
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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  $\geq 3$ , 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	517	<div> <div>87%</div> <div>9% . .</div> </div>
1	B	517	<div> <div>%</div> <div>89%</div> <div>7% .</div> </div>
1	C	517	<div> <div>86%</div> <div>10% .</div> </div>
1	D	517	<div> <div>88%</div> <div>8% .</div> </div>
1	E	517	<div> <div>90%</div> <div>6% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	517	 87% 8% . .
1	G	517	 87% 9% .
1	H	517	 88% 8% .

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
3	SO4	E	502	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32907 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 Betaine-aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	10	0
			3954	2492	667	780	15			
1	B	499	Total	C	N	O	S	0	6	0
			3916	2469	665	768	14			
1	C	499	Total	C	N	O	S	0	7	0
			3927	2475	665	773	14			
1	D	498	Total	C	N	O	S	0	6	0
			3912	2464	665	769	14			
1	E	496	Total	C	N	O	S	0	10	0
			3929	2474	667	774	14			
1	F	496	Total	C	N	O	S	0	5	0
			3885	2449	658	764	14			
1	G	496	Total	C	N	O	S	0	4	0
			3876	2444	656	762	14			
1	H	496	Total	C	N	O	S	0	4	0
			3877	2445	657	761	14			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q5HCU0
A	-19	GLY	-	expression tag	UNP Q5HCU0
A	-18	SER	-	expression tag	UNP Q5HCU0
A	-17	SER	-	expression tag	UNP Q5HCU0
A	-16	HIS	-	expression tag	UNP Q5HCU0
A	-15	HIS	-	expression tag	UNP Q5HCU0
A	-14	HIS	-	expression tag	UNP Q5HCU0
A	-13	HIS	-	expression tag	UNP Q5HCU0
A	-12	HIS	-	expression tag	UNP Q5HCU0
A	-11	HIS	-	expression tag	UNP Q5HCU0
A	-10	SER	-	expression tag	UNP Q5HCU0
A	-9	SER	-	expression tag	UNP Q5HCU0
A	-8	GLY	-	expression tag	UNP Q5HCU0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ARG	-	expression tag	UNP Q5HCU0
A	-6	GLU	-	expression tag	UNP Q5HCU0
A	-5	ASN	-	expression tag	UNP Q5HCU0
A	-4	LEU	-	expression tag	UNP Q5HCU0
A	-3	TYR	-	expression tag	UNP Q5HCU0
A	-2	PHE	-	expression tag	UNP Q5HCU0
A	-1	GLN	-	expression tag	UNP Q5HCU0
A	0	GLY	-	expression tag	UNP Q5HCU0
A	448	PHE	HIS	engineered mutation	UNP Q5HCU0
A	450	LEU	TYR	engineered mutation	UNP Q5HCU0
B	-20	MET	-	expression tag	UNP Q5HCU0
B	-19	GLY	-	expression tag	UNP Q5HCU0
B	-18	SER	-	expression tag	UNP Q5HCU0
B	-17	SER	-	expression tag	UNP Q5HCU0
B	-16	HIS	-	expression tag	UNP Q5HCU0
B	-15	HIS	-	expression tag	UNP Q5HCU0
B	-14	HIS	-	expression tag	UNP Q5HCU0
B	-13	HIS	-	expression tag	UNP Q5HCU0
B	-12	HIS	-	expression tag	UNP Q5HCU0
B	-11	HIS	-	expression tag	UNP Q5HCU0
B	-10	SER	-	expression tag	UNP Q5HCU0
B	-9	SER	-	expression tag	UNP Q5HCU0
B	-8	GLY	-	expression tag	UNP Q5HCU0
B	-7	ARG	-	expression tag	UNP Q5HCU0
B	-6	GLU	-	expression tag	UNP Q5HCU0
B	-5	ASN	-	expression tag	UNP Q5HCU0
B	-4	LEU	-	expression tag	UNP Q5HCU0
B	-3	TYR	-	expression tag	UNP Q5HCU0
B	-2	PHE	-	expression tag	UNP Q5HCU0
B	-1	GLN	-	expression tag	UNP Q5HCU0
B	0	GLY	-	expression tag	UNP Q5HCU0
B	448	PHE	HIS	engineered mutation	UNP Q5HCU0
B	450	LEU	TYR	engineered mutation	UNP Q5HCU0
C	-20	MET	-	expression tag	UNP Q5HCU0
C	-19	GLY	-	expression tag	UNP Q5HCU0
C	-18	SER	-	expression tag	UNP Q5HCU0
C	-17	SER	-	expression tag	UNP Q5HCU0
C	-16	HIS	-	expression tag	UNP Q5HCU0
C	-15	HIS	-	expression tag	UNP Q5HCU0
C	-14	HIS	-	expression tag	UNP Q5HCU0
C	-13	HIS	-	expression tag	UNP Q5HCU0
C	-12	HIS	-	expression tag	UNP Q5HCU0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	HIS	-	expression tag	UNP Q5HCU0
C	-10	SER	-	expression tag	UNP Q5HCU0
C	-9	SER	-	expression tag	UNP Q5HCU0
C	-8	GLY	-	expression tag	UNP Q5HCU0
C	-7	ARG	-	expression tag	UNP Q5HCU0
C	-6	GLU	-	expression tag	UNP Q5HCU0
C	-5	ASN	-	expression tag	UNP Q5HCU0
C	-4	LEU	-	expression tag	UNP Q5HCU0
C	-3	TYR	-	expression tag	UNP Q5HCU0
C	-2	PHE	-	expression tag	UNP Q5HCU0
C	-1	GLN	-	expression tag	UNP Q5HCU0
C	0	GLY	-	expression tag	UNP Q5HCU0
C	448	PHE	HIS	engineered mutation	UNP Q5HCU0
C	450	LEU	TYR	engineered mutation	UNP Q5HCU0
D	-20	MET	-	expression tag	UNP Q5HCU0
D	-19	GLY	-	expression tag	UNP Q5HCU0
D	-18	SER	-	expression tag	UNP Q5HCU0
D	-17	SER	-	expression tag	UNP Q5HCU0
D	-16	HIS	-	expression tag	UNP Q5HCU0
D	-15	HIS	-	expression tag	UNP Q5HCU0
D	-14	HIS	-	expression tag	UNP Q5HCU0
D	-13	HIS	-	expression tag	UNP Q5HCU0
D	-12	HIS	-	expression tag	UNP Q5HCU0
D	-11	HIS	-	expression tag	UNP Q5HCU0
D	-10	SER	-	expression tag	UNP Q5HCU0
D	-9	SER	-	expression tag	UNP Q5HCU0
D	-8	GLY	-	expression tag	UNP Q5HCU0
D	-7	ARG	-	expression tag	UNP Q5HCU0
D	-6	GLU	-	expression tag	UNP Q5HCU0
D	-5	ASN	-	expression tag	UNP Q5HCU0
D	-4	LEU	-	expression tag	UNP Q5HCU0
D	-3	TYR	-	expression tag	UNP Q5HCU0
D	-2	PHE	-	expression tag	UNP Q5HCU0
D	-1	GLN	-	expression tag	UNP Q5HCU0
D	0	GLY	-	expression tag	UNP Q5HCU0
D	448	PHE	HIS	engineered mutation	UNP Q5HCU0
D	450	LEU	TYR	engineered mutation	UNP Q5HCU0
E	-20	MET	-	expression tag	UNP Q5HCU0
E	-19	GLY	-	expression tag	UNP Q5HCU0
E	-18	SER	-	expression tag	UNP Q5HCU0
E	-17	SER	-	expression tag	UNP Q5HCU0
E	-16	HIS	-	expression tag	UNP Q5HCU0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP Q5HCU0
E	-14	HIS	-	expression tag	UNP Q5HCU0
E	-13	HIS	-	expression tag	UNP Q5HCU0
E	-12	HIS	-	expression tag	UNP Q5HCU0
E	-11	HIS	-	expression tag	UNP Q5HCU0
E	-10	SER	-	expression tag	UNP Q5HCU0
E	-9	SER	-	expression tag	UNP Q5HCU0
E	-8	GLY	-	expression tag	UNP Q5HCU0
E	-7	ARG	-	expression tag	UNP Q5HCU0
E	-6	GLU	-	expression tag	UNP Q5HCU0
E	-5	ASN	-	expression tag	UNP Q5HCU0
E	-4	LEU	-	expression tag	UNP Q5HCU0
E	-3	TYR	-	expression tag	UNP Q5HCU0
E	-2	PHE	-	expression tag	UNP Q5HCU0
E	-1	GLN	-	expression tag	UNP Q5HCU0
E	0	GLY	-	expression tag	UNP Q5HCU0
E	448	PHE	HIS	engineered mutation	UNP Q5HCU0
E	450	LEU	TYR	engineered mutation	UNP Q5HCU0
F	-20	MET	-	expression tag	UNP Q5HCU0
F	-19	GLY	-	expression tag	UNP Q5HCU0
F	-18	SER	-	expression tag	UNP Q5HCU0
F	-17	SER	-	expression tag	UNP Q5HCU0
F	-16	HIS	-	expression tag	UNP Q5HCU0
F	-15	HIS	-	expression tag	UNP Q5HCU0
F	-14	HIS	-	expression tag	UNP Q5HCU0
F	-13	HIS	-	expression tag	UNP Q5HCU0
F	-12	HIS	-	expression tag	UNP Q5HCU0
F	-11	HIS	-	expression tag	UNP Q5HCU0
F	-10	SER	-	expression tag	UNP Q5HCU0
F	-9	SER	-	expression tag	UNP Q5HCU0
F	-8	GLY	-	expression tag	UNP Q5HCU0
F	-7	ARG	-	expression tag	UNP Q5HCU0
F	-6	GLU	-	expression tag	UNP Q5HCU0
F	-5	ASN	-	expression tag	UNP Q5HCU0
F	-4	LEU	-	expression tag	UNP Q5HCU0
F	-3	TYR	-	expression tag	UNP Q5HCU0
F	-2	PHE	-	expression tag	UNP Q5HCU0
F	-1	GLN	-	expression tag	UNP Q5HCU0
F	0	GLY	-	expression tag	UNP Q5HCU0
F	448	PHE	HIS	engineered mutation	UNP Q5HCU0
F	450	LEU	TYR	engineered mutation	UNP Q5HCU0
G	-20	MET	-	expression tag	UNP Q5HCU0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	GLY	-	expression tag	UNP Q5HCU0
G	-18	SER	-	expression tag	UNP Q5HCU0
G	-17	SER	-	expression tag	UNP Q5HCU0
G	-16	HIS	-	expression tag	UNP Q5HCU0
G	-15	HIS	-	expression tag	UNP Q5HCU0
G	-14	HIS	-	expression tag	UNP Q5HCU0
G	-13	HIS	-	expression tag	UNP Q5HCU0
G	-12	HIS	-	expression tag	UNP Q5HCU0
G	-11	HIS	-	expression tag	UNP Q5HCU0
G	-10	SER	-	expression tag	UNP Q5HCU0
G	-9	SER	-	expression tag	UNP Q5HCU0
G	-8	GLY	-	expression tag	UNP Q5HCU0
G	-7	ARG	-	expression tag	UNP Q5HCU0
G	-6	GLU	-	expression tag	UNP Q5HCU0
G	-5	ASN	-	expression tag	UNP Q5HCU0
G	-4	LEU	-	expression tag	UNP Q5HCU0
G	-3	TYR	-	expression tag	UNP Q5HCU0
G	-2	PHE	-	expression tag	UNP Q5HCU0
G	-1	GLN	-	expression tag	UNP Q5HCU0
G	0	GLY	-	expression tag	UNP Q5HCU0
G	448	PHE	HIS	engineered mutation	UNP Q5HCU0
G	450	LEU	TYR	engineered mutation	UNP Q5HCU0
H	-20	MET	-	expression tag	UNP Q5HCU0
H	-19	GLY	-	expression tag	UNP Q5HCU0
H	-18	SER	-	expression tag	UNP Q5HCU0
H	-17	SER	-	expression tag	UNP Q5HCU0
H	-16	HIS	-	expression tag	UNP Q5HCU0
H	-15	HIS	-	expression tag	UNP Q5HCU0
H	-14	HIS	-	expression tag	UNP Q5HCU0
H	-13	HIS	-	expression tag	UNP Q5HCU0
H	-12	HIS	-	expression tag	UNP Q5HCU0
H	-11	HIS	-	expression tag	UNP Q5HCU0
H	-10	SER	-	expression tag	UNP Q5HCU0
H	-9	SER	-	expression tag	UNP Q5HCU0
H	-8	GLY	-	expression tag	UNP Q5HCU0
H	-7	ARG	-	expression tag	UNP Q5HCU0
H	-6	GLU	-	expression tag	UNP Q5HCU0
H	-5	ASN	-	expression tag	UNP Q5HCU0
H	-4	LEU	-	expression tag	UNP Q5HCU0
H	-3	TYR	-	expression tag	UNP Q5HCU0
H	-2	PHE	-	expression tag	UNP Q5HCU0
H	-1	GLN	-	expression tag	UNP Q5HCU0

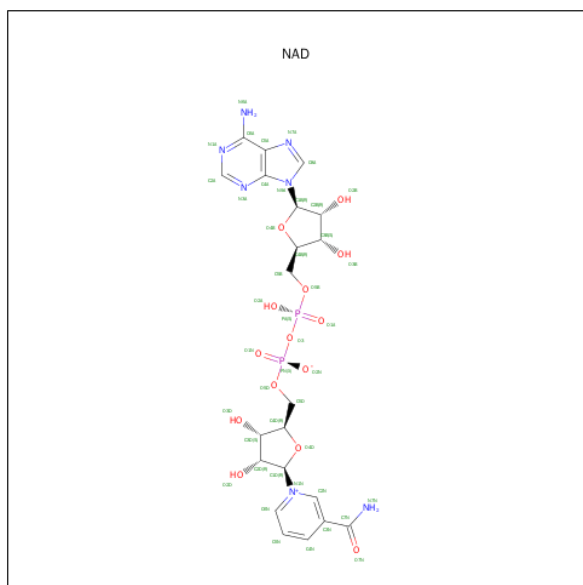
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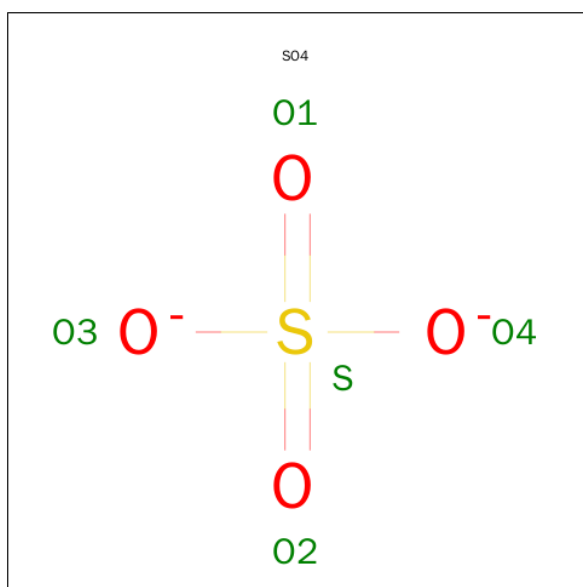
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	GLY	-	expression tag	UNP Q5HCU0
H	448	PHE	HIS	engineered mutation	UNP Q5HCU0
H	450	LEU	TYR	engineered mutation	UNP Q5HCU0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

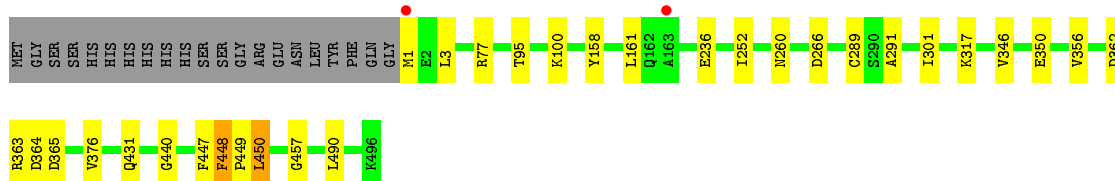
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	177	Total	O		0	5
			180	180			
4	B	182	Total	O		0	2
			183	183			
4	C	166	Total	O		0	3
			168	168			
4	D	174	Total	O		0	3
			176	176			
4	E	125	Total	O		0	2
			125	125			
4	F	151	Total	O		0	2
			151	151			
4	G	122	Total	O		0	1
			123	123			
4	H	98	Total	O		0	1
			98	98			





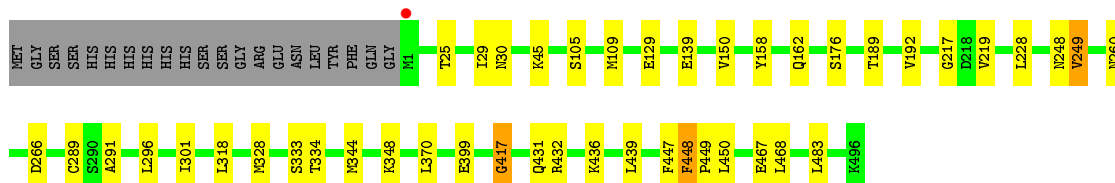
• Molecule 1: Betaine-aldehyde dehydrogenase

Chain E: 90% 6% .



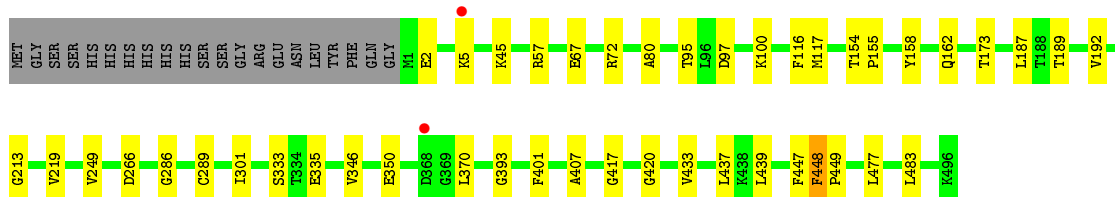
• Molecule 1: Betaine-aldehyde dehydrogenase

Chain F: 87% 8% . .



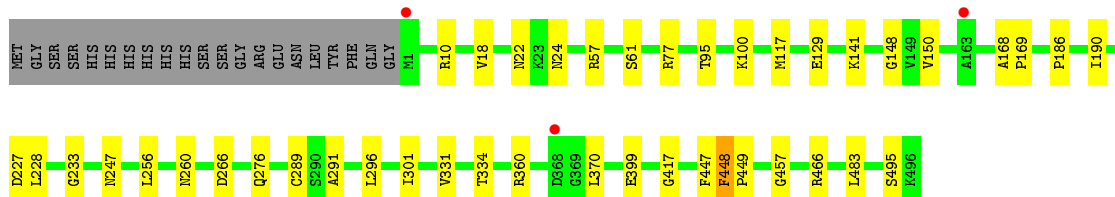
• Molecule 1: Betaine-aldehyde dehydrogenase

Chain G: 87% 9% .



• Molecule 1: Betaine-aldehyde dehydrogenase

Chain H: 88% 8% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.14Å 170.97Å 137.58Å 90.00° 102.77° 90.00°	Depositor
Resolution (Å)	29.95 – 2.60 29.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.95-2.60) 100.0 (29.95-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.158 , 0.232 0.163 , 0.232	Depositor DCC
$R_{free}$ test set	6075 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 123078 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: SO4, NAD

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	0.56	0/4025	0.86	1/5438 (0.0%)
1	B	0.56	0/3991	0.84	0/5393
1	C	0.53	0/3998	0.82	0/5403
1	D	0.53	0/3982	0.80	1/5381 (0.0%)
1	E	0.52	0/4001	0.81	0/5406
1	F	0.53	0/3955	0.82	0/5346
1	G	0.50	0/3946	0.81	0/5334
1	H	0.49	0/3947	0.79	1/5335 (0.0%)
All	All	0.53	0/31845	0.82	3/43036 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	LYS	N-CA-C	-5.53	96.06	111.00
1	A	354	ILE	N-CA-C	-5.49	96.17	111.00
1	H	57	ARG	NE-CZ-NH1	5.17	122.88	120.30

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	3954	0	3889	39	0
1	B	3916	0	3865	30	0
1	C	3927	0	3867	39	0
1	D	3912	0	3858	27	0
1	E	3929	0	3871	27	0
1	F	3885	0	3834	35	0
1	G	3876	0	3828	29	0
1	H	3877	0	3832	33	0
2	A	44	0	26	7	0
2	B	44	0	26	5	0
2	C	44	0	26	4	0
2	D	44	0	26	2	0
2	E	44	0	26	5	0
2	F	44	0	26	5	0
2	G	44	0	26	2	0
2	H	44	0	26	5	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
3	G	15	0	0	0	0
4	A	180	0	0	4	0
4	B	183	0	0	5	0
4	C	168	0	0	4	0
4	D	176	0	0	3	0
4	E	125	0	0	3	0
4	F	151	0	0	3	0
4	G	123	0	0	3	0
4	H	98	0	0	6	0
All	All	32907	0	31052	246	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 4.

The worst 5 of 246 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:431[A]:GLN:HG2	4:D:704[A]:HOH:O	1.26	1.25
1:E:289:CYS:SG	2:E:501:NAD:C4N	2.29	1.20
1:B:289:CYS:SG	2:B:501:NAD:C4N	2.38	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:CYS:SG	2:A:501:NAD:C4N	2.42	1.07
1:F:289:CYS:SG	2:F:501:NAD:C4N	2.49	0.99

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	507/517 (98%)	490 (97%)	14 (3%)	3 (1%)	30	56
1	B	503/517 (97%)	488 (97%)	13 (3%)	2 (0%)	39	65
1	C	504/517 (98%)	483 (96%)	18 (4%)	3 (1%)	30	56
1	D	502/517 (97%)	487 (97%)	12 (2%)	3 (1%)	30	56
1	E	504/517 (98%)	488 (97%)	15 (3%)	1 (0%)	52	77
1	F	499/517 (96%)	485 (97%)	11 (2%)	3 (1%)	30	56
1	G	498/517 (96%)	475 (95%)	21 (4%)	2 (0%)	39	65
1	H	498/517 (96%)	475 (95%)	20 (4%)	3 (1%)	30	56
All	All	4015/4136 (97%)	3871 (96%)	124 (3%)	20 (0%)	34	60

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	PHE
1	B	448	PHE
1	C	363	ARG
1	C	448	PHE
1	D	448	PHE

### 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	423/429 (99%)	423 (100%)	0	100	100
1	B	419/429 (98%)	419 (100%)	0	100	100
1	C	420/429 (98%)	420 (100%)	0	100	100
1	D	418/429 (97%)	417 (100%)	1 (0%)	95	99
1	E	421/429 (98%)	419 (100%)	2 (0%)	92	98
1	F	416/429 (97%)	415 (100%)	1 (0%)	95	99
1	G	415/429 (97%)	415 (100%)	0	100	100
1	H	415/429 (97%)	415 (100%)	0	100	100
All	All	3347/3432 (98%)	3343 (100%)	4 (0%)	95	99

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	146	PRO
1	E	364	ASP
1	E	450	LEU
1	F	450	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	431	GLN
1	C	251	ASN
1	C	409	GLN
1	F	435	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](#)

23 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAD	A	501	-	38,48,48	0.90	1 (2%)	47,73,73	2.04	8 (17%)
3	SO4	A	502	-	4,4,4	0.51	0	6,6,6	0.11	0
3	SO4	A	503	-	4,4,4	0.44	0	6,6,6	0.22	0
2	NAD	B	501	-	38,48,48	0.86	1 (2%)	47,73,73	2.54	8 (17%)
3	SO4	B	502	-	4,4,4	0.25	0	6,6,6	0.50	0
3	SO4	B	503	-	4,4,4	0.54	0	6,6,6	0.21	0
2	NAD	C	501	-	38,48,48	0.90	1 (2%)	47,73,73	1.83	6 (12%)
3	SO4	C	502	-	4,4,4	0.46	0	6,6,6	0.36	0
3	SO4	C	503	-	4,4,4	0.63	0	6,6,6	0.43	0
2	NAD	D	501	-	38,48,48	0.95	1 (2%)	47,73,73	1.95	5 (10%)
3	SO4	D	502	-	4,4,4	0.48	0	6,6,6	0.28	0
2	NAD	E	501	-	38,48,48	0.91	1 (2%)	47,73,73	2.14	5 (10%)
3	SO4	E	502	-	4,4,4	0.50	0	6,6,6	0.21	0
3	SO4	E	503	-	4,4,4	0.49	0	6,6,6	0.57	0
2	NAD	F	501	-	38,48,48	1.01	1 (2%)	47,73,73	1.91	5 (10%)
3	SO4	F	502	-	4,4,4	0.50	0	6,6,6	0.24	0
3	SO4	F	503	-	4,4,4	0.47	0	6,6,6	0.94	1 (16%)
3	SO4	F	504	-	4,4,4	0.48	0	6,6,6	0.36	0
2	NAD	G	501	-	38,48,48	1.02	1 (2%)	47,73,73	2.11	8 (17%)
3	SO4	G	502	-	4,4,4	0.46	0	6,6,6	0.26	0
3	SO4	G	503	-	4,4,4	0.50	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	G	504	-	4,4,4	0.51	0	6,6,6	0.30	0
2	NAD	H	501	-	38,48,48	1.00	1 (2%)	47,73,73	1.79	5 (10%)

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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
3	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
3	SO4	B	502	-	-	0/0/0/0	0/0/0/0
3	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	NAD	C	501	-	-	0/22/62/62	0/5/5/5
3	SO4	C	502	-	-	0/0/0/0	0/0/0/0
3	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	NAD	D	501	-	-	0/22/62/62	0/5/5/5
3	SO4	D	502	-	-	0/0/0/0	0/0/0/0
2	NAD	E	501	-	-	0/22/62/62	0/5/5/5
3	SO4	E	502	-	-	0/0/0/0	0/0/0/0
3	SO4	E	503	-	-	0/0/0/0	0/0/0/0
2	NAD	F	501	-	-	0/22/62/62	0/5/5/5
3	SO4	F	502	-	-	0/0/0/0	0/0/0/0
3	SO4	F	503	-	-	0/0/0/0	0/0/0/0
3	SO4	F	504	-	-	0/0/0/0	0/0/0/0
2	NAD	G	501	-	-	0/22/62/62	0/5/5/5
3	SO4	G	502	-	-	0/0/0/0	0/0/0/0
3	SO4	G	503	-	-	0/0/0/0	0/0/0/0
3	SO4	G	504	-	-	0/0/0/0	0/0/0/0
2	NAD	H	501	-	-	0/22/62/62	0/5/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O7N-C7N	3.32	1.31	1.24
2	A	501	NAD	O7N-C7N	3.36	1.31	1.24
2	C	501	NAD	O7N-C7N	3.48	1.31	1.24
2	E	501	NAD	O7N-C7N	4.05	1.32	1.24
2	F	501	NAD	O7N-C7N	4.16	1.33	1.24

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	N3A-C2A-N1A	-12.52	119.31	128.89
2	E	501	NAD	N3A-C2A-N1A	-10.97	120.49	128.89
2	D	501	NAD	N3A-C2A-N1A	-10.54	120.83	128.89
2	A	501	NAD	N3A-C2A-N1A	-9.95	121.27	128.89
2	G	501	NAD	N3A-C2A-N1A	-9.20	121.85	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	7	0
2	B	501	NAD	5	0
2	C	501	NAD	4	0
2	D	501	NAD	2	0
2	E	501	NAD	5	0
2	F	501	NAD	5	0
2	G	501	NAD	2	0
2	H	501	NAD	5	0

## 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, 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	499/517 (96%)	-0.80	2 (0%) 93 91	20, 30, 47, 122	0
1	B	499/517 (96%)	-0.80	4 (0%) 87 85	20, 31, 48, 87	0
1	C	499/517 (96%)	-0.78	0 100 100	22, 34, 55, 80	0
1	D	498/517 (96%)	-0.72	0 100 100	22, 35, 54, 102	0
1	E	496/517 (95%)	-0.64	2 (0%) 93 91	20, 35, 57, 98	0
1	F	496/517 (95%)	-0.73	1 (0%) 95 95	20, 34, 54, 93	0
1	G	496/517 (95%)	-0.57	2 (0%) 93 91	26, 41, 63, 104	0
1	H	496/517 (95%)	-0.53	3 (0%) 90 88	24, 44, 70, 111	0
All	All	3979/4136 (96%)	-0.70	14 (0%) 93 91	20, 35, 60, 122	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	GLN	3.8
1	B	496	LYS	3.3
1	E	163	ALA	3.0
1	B	-2	PHE	2.7
1	H	368	ASP	2.6

### 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	E	502	5/5	0.89	0.23	9.44	75,76,91,106	0
3	SO4	F	503	5/5	0.96	0.15	1.34	37,42,52,53	0
3	SO4	B	502	5/5	0.98	0.14	1.19	39,42,48,56	0
3	SO4	B	503	5/5	0.92	0.20	0.75	46,69,76,83	0
2	NAD	G	501	44/44	0.96	0.12	-0.08	23,37,48,60	0
3	SO4	A	503	5/5	0.97	0.10	-0.11	36,43,48,51	0
2	NAD	E	501	44/44	0.97	0.11	-0.27	22,38,45,49	0
2	NAD	A	501	44/44	0.97	0.10	-0.36	21,30,38,41	0
2	NAD	D	501	44/44	0.96	0.12	-0.36	26,36,41,45	0
2	NAD	H	501	44/44	0.96	0.12	-0.39	29,41,51,57	0
2	NAD	B	501	44/44	0.98	0.09	-0.69	17,29,35,40	0
2	NAD	F	501	44/44	0.97	0.09	-0.71	18,30,35,38	0
2	NAD	C	501	44/44	0.97	0.10	-0.85	25,33,44,50	0
3	SO4	G	504	5/5	0.96	0.25	-	48,51,57,62	5
3	SO4	F	504	5/5	0.80	0.46	-	70,72,75,86	5
3	SO4	C	502	5/5	0.78	0.38	-	75,89,99,124	0
3	SO4	A	502	5/5	0.85	0.37	-	61,62,78,80	5
3	SO4	E	503	5/5	0.90	0.27	-	60,67,78,85	0
3	SO4	F	502	5/5	0.84	0.28	-	58,93,97,107	0
3	SO4	C	503	5/5	0.94	0.18	-	49,58,67,80	0
3	SO4	G	502	5/5	0.95	0.19	-	42,49,64,66	5
3	SO4	G	503	5/5	0.91	0.28	-	62,65,71,73	5
3	SO4	D	502	5/5	0.96	0.24	-	46,47,57,60	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.