



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 10:19 PM EDT

PDB ID : 3K2W  
Title : CRYSTAL STRUCTURE OF betaine-aldehyde dehydrogenase FROM Pseudoalteromonas atlantica T6c  
Authors : Patskovsky, Y.; Toro, R.; Rutter, M.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-09-30  
Resolution : 1.90 Å(reported)

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<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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

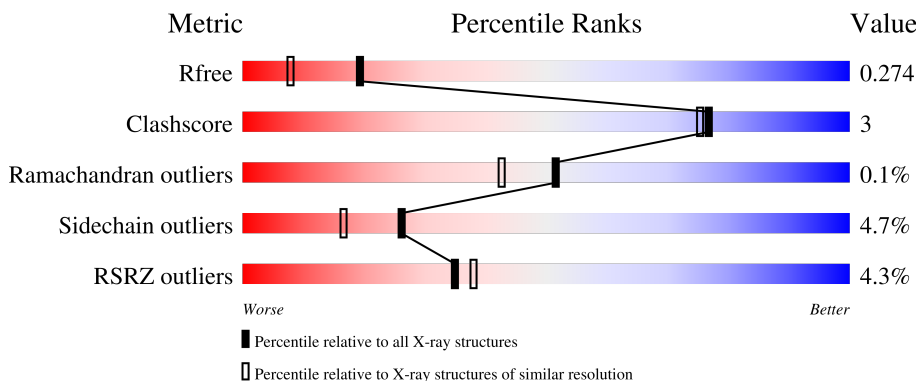
# 1 Overall quality at a glance

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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	497	
1	B	497	
1	C	497	
1	D	497	
1	E	497	

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Mol	Chain	Length	Quality of chain
1	F	497	<div><div><div>%</div><div><div></div><div>87%</div><div>9%</div><div></div></div><div></div></div></div>
1	G	497	<div><div><div>2%</div><div><div></div><div>89%</div><div>8%</div><div></div></div><div></div></div></div>
1	H	497	<div><div><div>8%</div><div><div></div><div>89%</div><div>9%</div><div></div></div><div></div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31410 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	475	Total	C	N	O	S	0	7	0
			3659	2311	617	707	24			
1	B	488	Total	C	N	O	S	0	2	0
			3720	2346	622	728	24			
1	C	484	Total	C	N	O	S	0	5	0
			3708	2341	622	721	24			
1	D	483	Total	C	N	O	S	0	8	0
			3712	2346	622	719	25			
1	E	486	Total	C	N	O	S	0	5	0
			3718	2347	620	726	25			
1	F	483	Total	C	N	O	S	0	9	0
			3720	2354	618	723	25			
1	G	484	Total	C	N	O	S	0	6	0
			3708	2343	619	722	24			
1	H	486	Total	C	N	O	S	0	5	0
			3719	2347	624	723	25			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q15SR9
A	0	SER	-	expression tag	UNP Q15SR9
A	1	LEU	-	expression tag	UNP Q15SR9
A	488	GLU	-	expression tag	UNP Q15SR9
A	489	GLY	-	expression tag	UNP Q15SR9
A	490	HIS	-	expression tag	UNP Q15SR9
A	491	HIS	-	expression tag	UNP Q15SR9
A	492	HIS	-	expression tag	UNP Q15SR9
A	493	HIS	-	expression tag	UNP Q15SR9
A	494	HIS	-	expression tag	UNP Q15SR9
A	495	HIS	-	expression tag	UNP Q15SR9
B	-1	MET	-	expression tag	UNP Q15SR9
B	0	SER	-	expression tag	UNP Q15SR9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	expression tag	UNP Q15SR9
B	488	GLU	-	expression tag	UNP Q15SR9
B	489	GLY	-	expression tag	UNP Q15SR9
B	490	HIS	-	expression tag	UNP Q15SR9
B	491	HIS	-	expression tag	UNP Q15SR9
B	492	HIS	-	expression tag	UNP Q15SR9
B	493	HIS	-	expression tag	UNP Q15SR9
B	494	HIS	-	expression tag	UNP Q15SR9
B	495	HIS	-	expression tag	UNP Q15SR9
C	-1	MET	-	expression tag	UNP Q15SR9
C	0	SER	-	expression tag	UNP Q15SR9
C	1	LEU	-	expression tag	UNP Q15SR9
C	488	GLU	-	expression tag	UNP Q15SR9
C	489	GLY	-	expression tag	UNP Q15SR9
C	490	HIS	-	expression tag	UNP Q15SR9
C	491	HIS	-	expression tag	UNP Q15SR9
C	492	HIS	-	expression tag	UNP Q15SR9
C	493	HIS	-	expression tag	UNP Q15SR9
C	494	HIS	-	expression tag	UNP Q15SR9
C	495	HIS	-	expression tag	UNP Q15SR9
D	-1	MET	-	expression tag	UNP Q15SR9
D	0	SER	-	expression tag	UNP Q15SR9
D	1	LEU	-	expression tag	UNP Q15SR9
D	488	GLU	-	expression tag	UNP Q15SR9
D	489	GLY	-	expression tag	UNP Q15SR9
D	490	HIS	-	expression tag	UNP Q15SR9
D	491	HIS	-	expression tag	UNP Q15SR9
D	492	HIS	-	expression tag	UNP Q15SR9
D	493	HIS	-	expression tag	UNP Q15SR9
D	494	HIS	-	expression tag	UNP Q15SR9
D	495	HIS	-	expression tag	UNP Q15SR9
E	-1	MET	-	expression tag	UNP Q15SR9
E	0	SER	-	expression tag	UNP Q15SR9
E	1	LEU	-	expression tag	UNP Q15SR9
E	488	GLU	-	expression tag	UNP Q15SR9
E	489	GLY	-	expression tag	UNP Q15SR9
E	490	HIS	-	expression tag	UNP Q15SR9
E	491	HIS	-	expression tag	UNP Q15SR9
E	492	HIS	-	expression tag	UNP Q15SR9
E	493	HIS	-	expression tag	UNP Q15SR9
E	494	HIS	-	expression tag	UNP Q15SR9
E	495	HIS	-	expression tag	UNP Q15SR9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MET	-	expression tag	UNP Q15SR9
F	0	SER	-	expression tag	UNP Q15SR9
F	1	LEU	-	expression tag	UNP Q15SR9
F	488	GLU	-	expression tag	UNP Q15SR9
F	489	GLY	-	expression tag	UNP Q15SR9
F	490	HIS	-	expression tag	UNP Q15SR9
F	491	HIS	-	expression tag	UNP Q15SR9
F	492	HIS	-	expression tag	UNP Q15SR9
F	493	HIS	-	expression tag	UNP Q15SR9
F	494	HIS	-	expression tag	UNP Q15SR9
F	495	HIS	-	expression tag	UNP Q15SR9
G	-1	MET	-	expression tag	UNP Q15SR9
G	0	SER	-	expression tag	UNP Q15SR9
G	1	LEU	-	expression tag	UNP Q15SR9
G	488	GLU	-	expression tag	UNP Q15SR9
G	489	GLY	-	expression tag	UNP Q15SR9
G	490	HIS	-	expression tag	UNP Q15SR9
G	491	HIS	-	expression tag	UNP Q15SR9
G	492	HIS	-	expression tag	UNP Q15SR9
G	493	HIS	-	expression tag	UNP Q15SR9
G	494	HIS	-	expression tag	UNP Q15SR9
G	495	HIS	-	expression tag	UNP Q15SR9
H	-1	MET	-	expression tag	UNP Q15SR9
H	0	SER	-	expression tag	UNP Q15SR9
H	1	LEU	-	expression tag	UNP Q15SR9
H	488	GLU	-	expression tag	UNP Q15SR9
H	489	GLY	-	expression tag	UNP Q15SR9
H	490	HIS	-	expression tag	UNP Q15SR9
H	491	HIS	-	expression tag	UNP Q15SR9
H	492	HIS	-	expression tag	UNP Q15SR9
H	493	HIS	-	expression tag	UNP Q15SR9
H	494	HIS	-	expression tag	UNP Q15SR9
H	495	HIS	-	expression tag	UNP Q15SR9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

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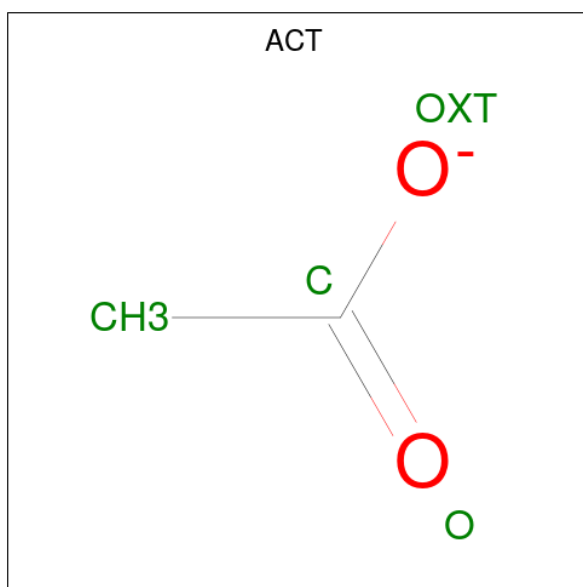
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total	O	0	0
			154	154		
5	B	170	Total	O	0	0
			170	170		
5	C	224	Total	O	0	0
			224	224		
5	D	218	Total	O	0	0
			218	218		
5	E	227	Total	O	0	0
			227	227		
5	F	220	Total	O	0	0
			220	220		

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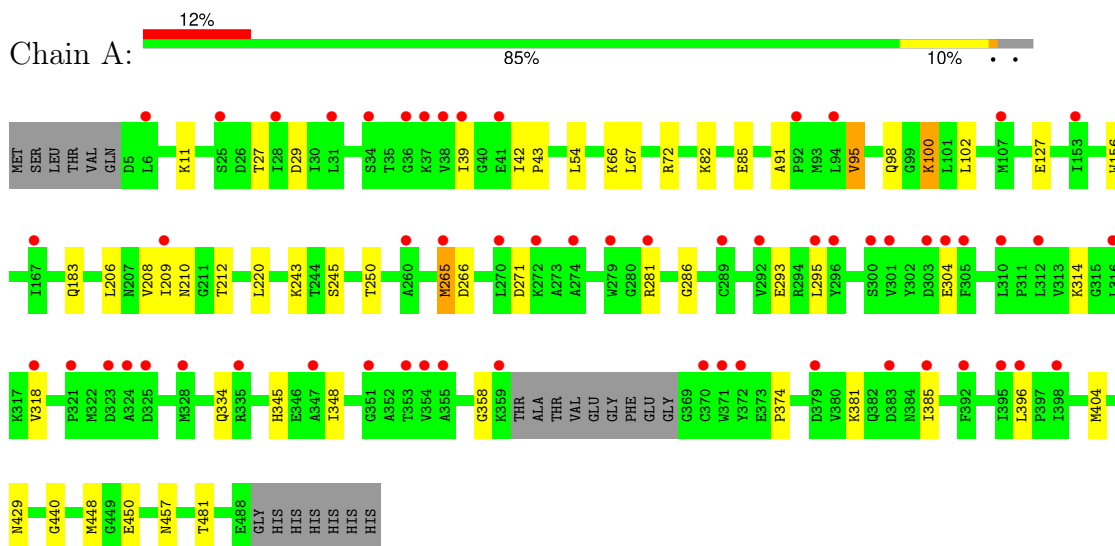
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	220	Total 220	O 220	0	0
5	H	179	Total 179	O 179	0	0

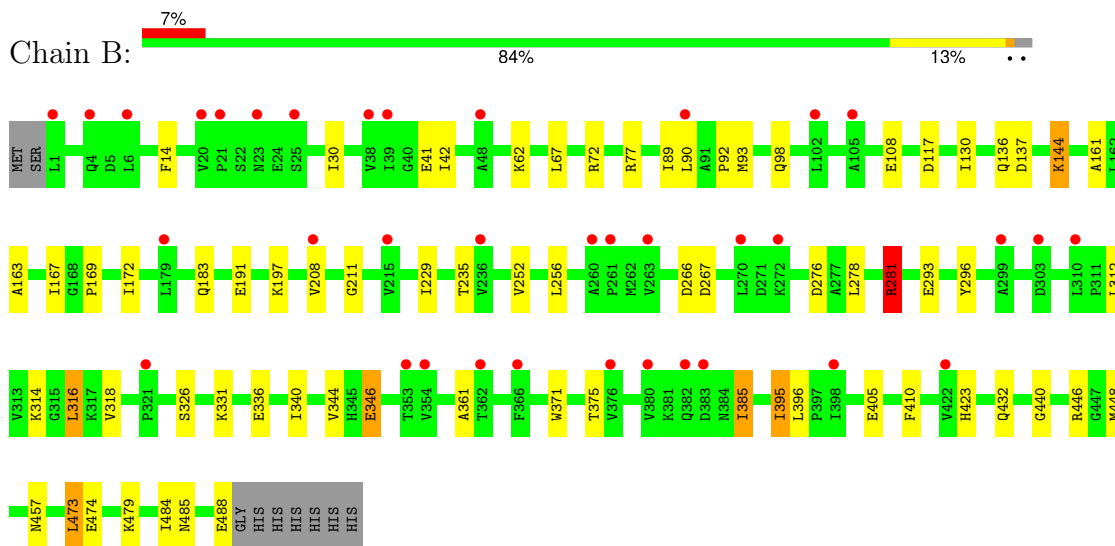
### 3 Residue-property plots [i](#)

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.

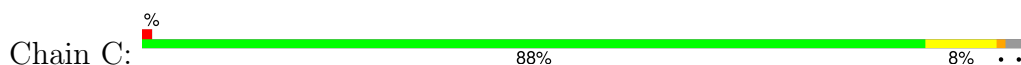
- Molecule 1: Betaine-aldehyde dehydrogenase

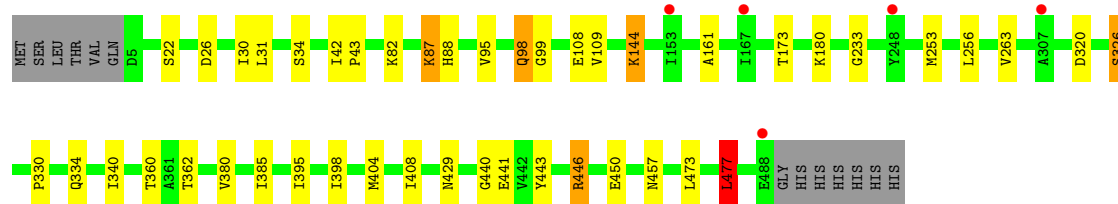


- Molecule 1: Betaine-aldehyde dehydrogenase

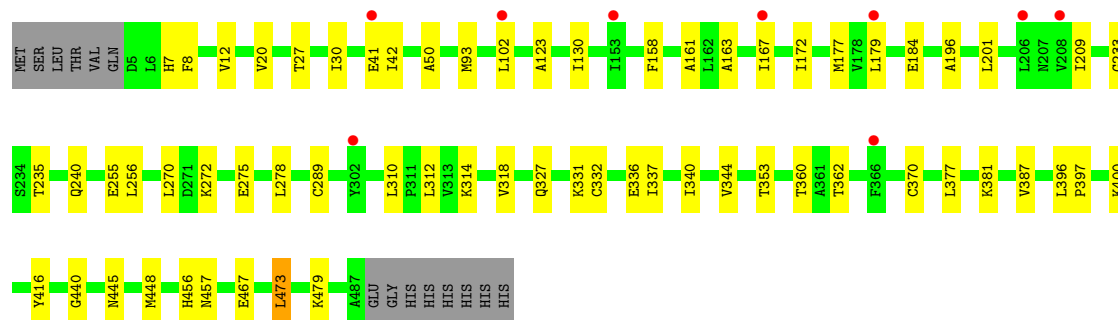
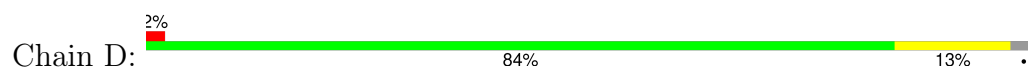


- Molecule 1: Betaine-aldehyde dehydrogenase

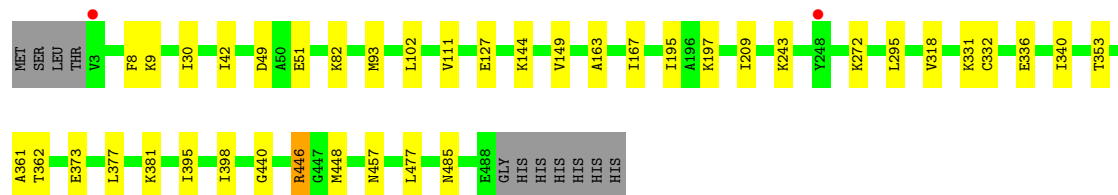




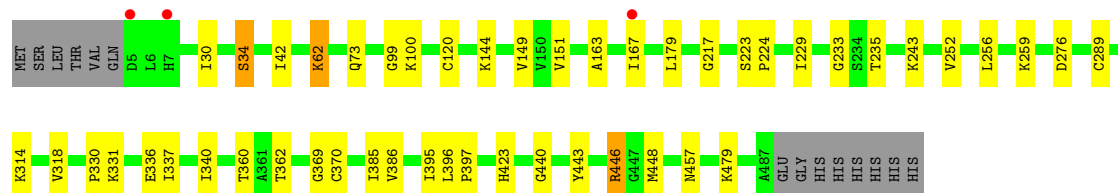
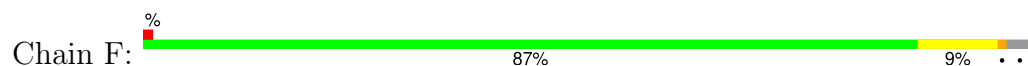
• Molecule 1: Betaine-aldehyde dehydrogenase



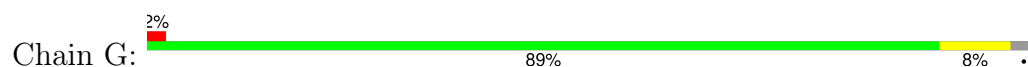
• Molecule 1: Betaine-aldehyde dehydrogenase

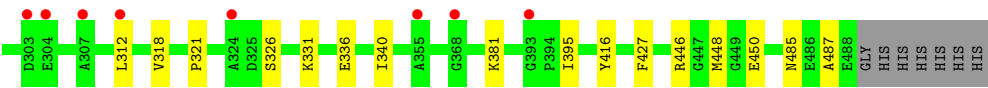


• Molecule 1: Betaine-aldehyde dehydrogenase

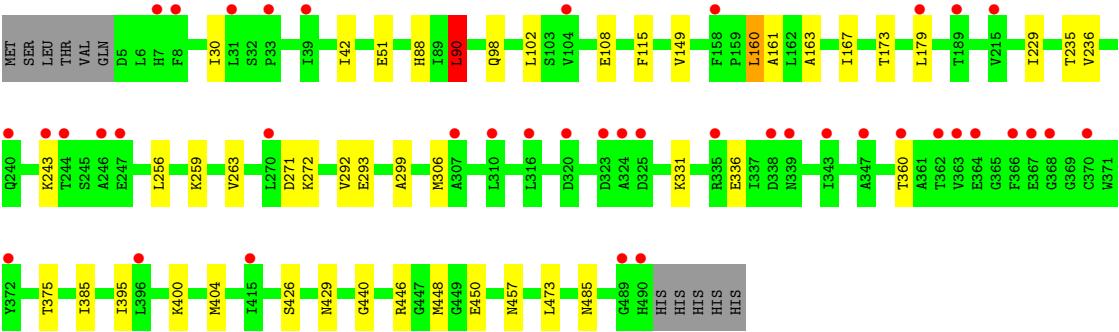
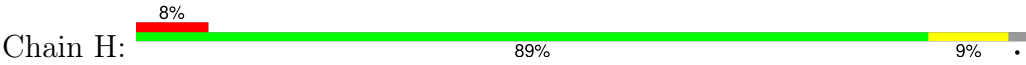


• Molecule 1: Betaine-aldehyde dehydrogenase





• Molecule 1: Betaine-aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.78Å 163.72Å 142.07Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 29.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.90) 97.6 (29.97-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, $R_{free}$	0.210 , 0.274 0.211 , 0.274	Depositor DCC
$R_{free}$ test set	9237 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	31410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, ACT

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	0.55	2/3745 (0.1%)	0.65	0/5073
1	B	0.56	0/3793	0.67	1/5143 (0.0%)
1	C	0.55	0/3791	0.68	1/5139 (0.0%)
1	D	0.54	0/3804	0.68	1/5154 (0.0%)
1	E	0.56	0/3800	0.67	1/5151 (0.0%)
1	F	0.57	0/3814	0.66	0/5168
1	G	0.54	0/3793	0.66	0/5140
1	H	0.53	0/3802	0.65	1/5151 (0.0%)
All	All	0.55	2/30342 (0.0%)	0.67	5/41119 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLU	CD-OE2	-5.36	1.19	1.25
1	A	127	GLU	CD-OE1	-5.15	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	446	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	477	LEU	CA-CB-CG	5.58	128.13	115.30
1	D	473	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	281	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	H	90	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3659	0	3659	21	0
1	B	3720	0	3693	33	0
1	C	3708	0	3689	26	0
1	D	3712	0	3708	25	0
1	E	3718	0	3697	16	0
1	F	3720	0	3720	23	0
1	G	3708	0	3700	17	0
1	H	3719	0	3700	16	0
2	A	6	0	8	0	0
2	B	18	0	24	3	0
2	C	6	0	8	2	0
2	D	18	0	24	1	0
2	E	12	0	16	0	0
2	F	18	0	24	1	0
2	G	18	0	24	2	0
2	H	6	0	8	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	1	0
4	E	4	0	3	0	0
4	F	4	0	3	0	0
5	A	154	0	0	0	0
5	B	170	0	0	1	0
5	C	224	0	0	2	0
5	D	218	0	0	1	0
5	E	227	0	0	3	0
5	F	220	0	0	1	0
5	G	220	0	0	2	0
5	H	179	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31410	0	29720	176	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 3.

The worst 5 of 176 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:E:332:CYS:HB3	5:E:1434:HOH:O	1.73	0.87
1:B:163:ALA:O	1:B:167:ILE:HG12	1.77	0.84
1:G:340:ILE:HB	1:G:395:ILE:HD11	1.62	0.80
1:C:95:VAL:O	1:C:99:GLY:HA2	1.84	0.76
1:A:404:MET:HG2	1:A:429[A]:ASN:HB2	1.68	0.76

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	478/497 (96%)	456 (95%)	20 (4%)	2 (0%)	34	24
1	B	488/497 (98%)	468 (96%)	20 (4%)	0	100	100
1	C	487/497 (98%)	474 (97%)	13 (3%)	0	100	100
1	D	489/497 (98%)	472 (96%)	17 (4%)	0	100	100
1	E	489/497 (98%)	475 (97%)	14 (3%)	0	100	100
1	F	490/497 (99%)	481 (98%)	9 (2%)	0	100	100
1	G	488/497 (98%)	474 (97%)	14 (3%)	0	100	100
1	H	489/497 (98%)	474 (97%)	14 (3%)	1 (0%)	47	38
All	All	3898/3976 (98%)	3774 (97%)	121 (3%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO
1	H	292	VAL
1	A	358	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	396/407 (97%)	375 (95%)	21 (5%)	22	13
1	B	401/407 (98%)	377 (94%)	24 (6%)	19	9
1	C	400/407 (98%)	382 (96%)	18 (4%)	27	18
1	D	402/407 (99%)	379 (94%)	23 (6%)	20	11
1	E	402/407 (99%)	388 (96%)	14 (4%)	36	27
1	F	403/407 (99%)	390 (97%)	13 (3%)	39	30
1	G	401/407 (98%)	387 (96%)	14 (4%)	36	27
1	H	401/407 (98%)	379 (94%)	22 (6%)	21	12
All	All	3206/3256 (98%)	3057 (95%)	149 (5%)	26	17

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	102	LEU
1	H	385	ILE
1	G	243	LYS
1	H	98	GLN
1	C	82	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	485	ASN
1	H	485	ASN

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Mol	Chain	Res	Type
1	C	23	ASN
1	C	74	ASN
1	C	135	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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	$\# Z  > 2$
4	ACT	B	498	-	3,3,3	0.80	0	3,3,3	1.24	0
2	GOL	F	496	-	5,5,5	0.49	0	5,5,5	0.93	0
2	GOL	E	496	-	5,5,5	0.53	0	5,5,5	0.51	0
2	GOL	H	496	-	5,5,5	0.43	0	5,5,5	0.56	0
2	GOL	B	496	-	5,5,5	0.38	0	5,5,5	1.07	0
2	GOL	G	496	-	5,5,5	0.47	0	5,5,5	0.41	0
4	ACT	D	500	-	3,3,3	0.82	0	3,3,3	1.32	0
4	ACT	C	499	-	3,3,3	0.78	0	3,3,3	1.44	0
4	ACT	C	498	-	3,3,3	0.83	0	3,3,3	1.12	0
2	GOL	E	497	-	5,5,5	0.60	0	5,5,5	0.72	0
2	GOL	D	498	-	5,5,5	0.36	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	497	-	5,5,5	0.52	0	5,5,5	0.75	0
2	GOL	C	497	-	5,5,5	0.40	0	5,5,5	0.43	0
4	ACT	F	500	-	3,3,3	0.78	0	3,3,3	1.10	0
2	GOL	G	498	-	5,5,5	0.30	0	5,5,5	0.49	0
2	GOL	F	498	-	5,5,5	0.36	0	5,5,5	0.39	0
2	GOL	A	496	-	5,5,5	0.48	0	5,5,5	0.11	0
2	GOL	D	497	-	5,5,5	0.38	0	5,5,5	0.71	0
2	GOL	B	499	-	5,5,5	0.42	0	5,5,5	0.81	0
2	GOL	F	497	-	5,5,5	0.35	0	5,5,5	0.38	0
4	ACT	E	499	-	3,3,3	0.76	0	3,3,3	0.98	0
2	GOL	D	496	-	5,5,5	0.44	0	5,5,5	0.54	0
2	GOL	G	497	-	5,5,5	0.41	0	5,5,5	0.78	0

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	GOL	B	497	-	-	2/4/4/4	-
2	GOL	A	496	-	-	1/4/4/4	-
2	GOL	C	497	-	-	0/4/4/4	-
2	GOL	B	499	-	-	2/4/4/4	-
2	GOL	F	496	-	-	0/4/4/4	-
2	GOL	G	498	-	-	2/4/4/4	-
2	GOL	F	497	-	-	2/4/4/4	-
2	GOL	E	496	-	-	0/4/4/4	-
2	GOL	H	496	-	-	4/4/4/4	-
2	GOL	F	498	-	-	2/4/4/4	-
2	GOL	B	496	-	-	3/4/4/4	-
2	GOL	G	496	-	-	4/4/4/4	-
2	GOL	D	496	-	-	0/4/4/4	-
2	GOL	G	497	-	-	4/4/4/4	-
2	GOL	D	497	-	-	2/4/4/4	-
2	GOL	E	497	-	-	4/4/4/4	-
2	GOL	D	498	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	496	GOL	C1-C2-C3-O3
2	B	497	GOL	C1-C2-C3-O3
2	B	499	GOL	C1-C2-C3-O3
2	D	498	GOL	O1-C1-C2-C3
2	E	497	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	496	GOL	1	0
2	G	496	GOL	1	0
4	D	500	ACT	1	0
2	B	497	GOL	1	0
2	C	497	GOL	2	0
2	F	498	GOL	1	0
2	D	497	GOL	1	0
2	B	499	GOL	2	0
2	G	497	GOL	1	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 [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	475/497 (95%)	0.69	58 (12%) 4 4	21, 48, 75, 92	0
1	B	488/497 (98%)	0.55	36 (7%) 14 16	20, 42, 62, 72	0
1	C	484/497 (97%)	0.02	5 (1%) 82 84	20, 34, 50, 93	0
1	D	483/497 (97%)	0.14	9 (1%) 66 69	21, 36, 54, 76	0
1	E	486/497 (97%)	-0.04	2 (0%) 92 93	21, 35, 52, 78	0
1	F	483/497 (97%)	-0.01	3 (0%) 89 90	22, 34, 49, 81	0
1	G	484/497 (97%)	0.17	12 (2%) 57 60	20, 39, 60, 79	0
1	H	486/497 (97%)	0.58	41 (8%) 11 12	20, 45, 70, 93	0
All	All	3869/3976 (97%)	0.26	166 (4%) 35 38	20, 38, 63, 93	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	363	VAL	5.4
1	H	490	HIS	5.3
1	A	396	LEU	4.7
1	B	20	VAL	4.7
1	A	39	ILE	4.5

### 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](#)

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	ACT	B	498	4/4	0.71	0.18	44,48,52,56	0
2	GOL	F	497	6/6	0.84	0.20	35,59,67,72	0
3	CL	B	500	1/1	0.87	0.11	47,47,47,47	0
4	ACT	C	499	4/4	0.87	0.15	40,47,47,57	0
2	GOL	B	499	6/6	0.88	0.17	31,43,50,58	0
2	GOL	C	497	6/6	0.88	0.17	39,43,58,59	0
2	GOL	F	498	6/6	0.91	0.12	46,57,58,70	0
2	GOL	G	496	6/6	0.92	0.22	39,44,55,59	0
3	CL	A	497	1/1	0.93	0.07	51,51,51,51	0
2	GOL	A	496	6/6	0.93	0.13	25,45,47,49	0
4	ACT	E	499	4/4	0.93	0.12	32,34,42,47	0
2	GOL	E	497	6/6	0.94	0.18	26,30,50,65	0
2	GOL	B	496	6/6	0.94	0.11	21,29,39,50	0
2	GOL	D	498	6/6	0.94	0.12	27,45,50,56	0
4	ACT	F	500	4/4	0.94	0.17	38,41,46,51	0
2	GOL	H	496	6/6	0.95	0.11	40,41,46,54	0
2	GOL	G	497	6/6	0.96	0.08	23,33,34,40	0
4	ACT	D	500	4/4	0.96	0.23	34,38,44,54	0
2	GOL	G	498	6/6	0.96	0.13	19,27,32,35	0
2	GOL	E	496	6/6	0.96	0.10	21,34,37,42	0
3	CL	G	499	1/1	0.97	0.06	49,49,49,49	0
2	GOL	D	496	6/6	0.97	0.13	28,33,39,41	0
2	GOL	B	497	6/6	0.97	0.10	19,28,44,51	0
2	GOL	F	496	6/6	0.98	0.08	22,28,32,35	0
4	ACT	C	498	4/4	0.98	0.08	47,53,54,56	0
3	CL	C	496	1/1	0.98	0.06	38,38,38,38	0
3	CL	F	499	1/1	0.98	0.04	31,31,31,31	0
2	GOL	D	497	6/6	0.98	0.10	24,38,41,45	0
3	CL	H	497	1/1	0.98	0.05	42,42,42,42	0
3	CL	E	498	1/1	0.99	0.05	34,34,34,34	0
3	CL	D	499	1/1	0.99	0.04	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.