



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 7C0E / pdb\_00007c0e  
Title : Crystal structure of Azospirillum brasilense L-2-keto-3-deoxyarabonate dehydratase (2-oxobutyrate-bound form)  
Authors : Watanabe, Y.; Ono, A.; Watanabe, S.  
Deposited on : 2020-05-01  
Resolution : 2.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

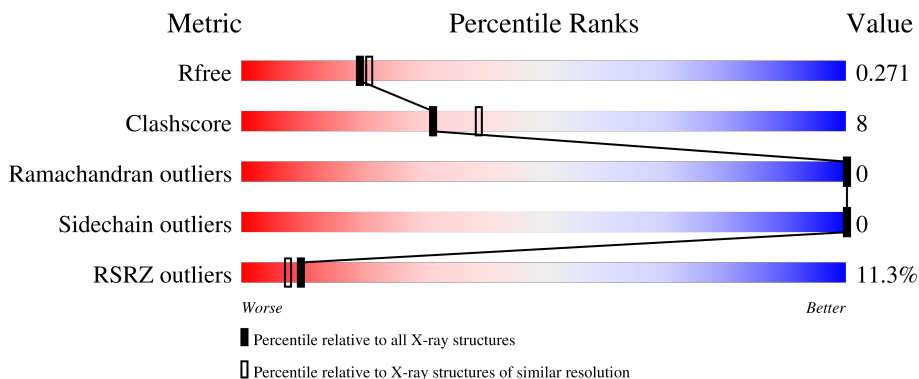
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	320	 86% 9% 5%
1	B	320	 83% 11% 6%
1	C	320	 85% 10% 5%
1	D	320	 86% 8% 5%
1	E	320	 83% 12% 5%

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Mol	Chain	Length	Quality of chain
1	F	320	 82% 12% 6%
1	G	320	 87% 8% 5%
1	H	320	 83% 12% 5%
1	I	320	 31% 74% 21% 5%
1	J	320	 27% 69% 26% 5%
1	K	320	 30% 67% 28% 5%
1	L	320	 32% 68% 26% 6%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 29111 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 L-2-keto-3-deoxyarabonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2348	1481	424	432	11	0	0	0
1	B	302	2326	1468	420	427	11	0	0	0
1	C	304	2342	1477	424	430	11	0	0	0
1	D	303	2325	1468	418	428	11	0	0	0
1	E	304	2342	1477	424	430	11	0	0	0
1	F	302	2326	1468	420	427	11	0	0	0
1	G	303	2325	1468	418	428	11	0	0	0
1	H	303	2325	1468	418	428	11	0	0	0
1	I	304	2336	1474	421	430	11	0	0	0
1	J	304	2336	1474	421	430	11	0	0	0
1	K	303	2331	1471	421	428	11	0	0	0
1	L	301	2317	1462	419	425	11	0	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q1JUQ0
A	-9	ARG	-	expression tag	UNP Q1JUQ0
A	-8	GLY	-	expression tag	UNP Q1JUQ0
A	-7	SER	-	expression tag	UNP Q1JUQ0
A	-6	HIS	-	expression tag	UNP Q1JUQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q1JUQ0
A	-4	HIS	-	expression tag	UNP Q1JUQ0
A	-3	HIS	-	expression tag	UNP Q1JUQ0
A	-2	HIS	-	expression tag	UNP Q1JUQ0
A	-1	HIS	-	expression tag	UNP Q1JUQ0
A	0	GLY	-	expression tag	UNP Q1JUQ0
A	1	SER	-	expression tag	UNP Q1JUQ0
B	-10	MET	-	expression tag	UNP Q1JUQ0
B	-9	ARG	-	expression tag	UNP Q1JUQ0
B	-8	GLY	-	expression tag	UNP Q1JUQ0
B	-7	SER	-	expression tag	UNP Q1JUQ0
B	-6	HIS	-	expression tag	UNP Q1JUQ0
B	-5	HIS	-	expression tag	UNP Q1JUQ0
B	-4	HIS	-	expression tag	UNP Q1JUQ0
B	-3	HIS	-	expression tag	UNP Q1JUQ0
B	-2	HIS	-	expression tag	UNP Q1JUQ0
B	-1	HIS	-	expression tag	UNP Q1JUQ0
B	0	GLY	-	expression tag	UNP Q1JUQ0
B	1	SER	-	expression tag	UNP Q1JUQ0
C	-10	MET	-	expression tag	UNP Q1JUQ0
C	-9	ARG	-	expression tag	UNP Q1JUQ0
C	-8	GLY	-	expression tag	UNP Q1JUQ0
C	-7	SER	-	expression tag	UNP Q1JUQ0
C	-6	HIS	-	expression tag	UNP Q1JUQ0
C	-5	HIS	-	expression tag	UNP Q1JUQ0
C	-4	HIS	-	expression tag	UNP Q1JUQ0
C	-3	HIS	-	expression tag	UNP Q1JUQ0
C	-2	HIS	-	expression tag	UNP Q1JUQ0
C	-1	HIS	-	expression tag	UNP Q1JUQ0
C	0	GLY	-	expression tag	UNP Q1JUQ0
C	1	SER	-	expression tag	UNP Q1JUQ0
D	-10	MET	-	expression tag	UNP Q1JUQ0
D	-9	ARG	-	expression tag	UNP Q1JUQ0
D	-8	GLY	-	expression tag	UNP Q1JUQ0
D	-7	SER	-	expression tag	UNP Q1JUQ0
D	-6	HIS	-	expression tag	UNP Q1JUQ0
D	-5	HIS	-	expression tag	UNP Q1JUQ0
D	-4	HIS	-	expression tag	UNP Q1JUQ0
D	-3	HIS	-	expression tag	UNP Q1JUQ0
D	-2	HIS	-	expression tag	UNP Q1JUQ0
D	-1	HIS	-	expression tag	UNP Q1JUQ0
D	0	GLY	-	expression tag	UNP Q1JUQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	expression tag	UNP Q1JUQ0
E	-10	MET	-	expression tag	UNP Q1JUQ0
E	-9	ARG	-	expression tag	UNP Q1JUQ0
E	-8	GLY	-	expression tag	UNP Q1JUQ0
E	-7	SER	-	expression tag	UNP Q1JUQ0
E	-6	HIS	-	expression tag	UNP Q1JUQ0
E	-5	HIS	-	expression tag	UNP Q1JUQ0
E	-4	HIS	-	expression tag	UNP Q1JUQ0
E	-3	HIS	-	expression tag	UNP Q1JUQ0
E	-2	HIS	-	expression tag	UNP Q1JUQ0
E	-1	HIS	-	expression tag	UNP Q1JUQ0
E	0	GLY	-	expression tag	UNP Q1JUQ0
E	1	SER	-	expression tag	UNP Q1JUQ0
F	-10	MET	-	expression tag	UNP Q1JUQ0
F	-9	ARG	-	expression tag	UNP Q1JUQ0
F	-8	GLY	-	expression tag	UNP Q1JUQ0
F	-7	SER	-	expression tag	UNP Q1JUQ0
F	-6	HIS	-	expression tag	UNP Q1JUQ0
F	-5	HIS	-	expression tag	UNP Q1JUQ0
F	-4	HIS	-	expression tag	UNP Q1JUQ0
F	-3	HIS	-	expression tag	UNP Q1JUQ0
F	-2	HIS	-	expression tag	UNP Q1JUQ0
F	-1	HIS	-	expression tag	UNP Q1JUQ0
F	0	GLY	-	expression tag	UNP Q1JUQ0
F	1	SER	-	expression tag	UNP Q1JUQ0
G	-10	MET	-	expression tag	UNP Q1JUQ0
G	-9	ARG	-	expression tag	UNP Q1JUQ0
G	-8	GLY	-	expression tag	UNP Q1JUQ0
G	-7	SER	-	expression tag	UNP Q1JUQ0
G	-6	HIS	-	expression tag	UNP Q1JUQ0
G	-5	HIS	-	expression tag	UNP Q1JUQ0
G	-4	HIS	-	expression tag	UNP Q1JUQ0
G	-3	HIS	-	expression tag	UNP Q1JUQ0
G	-2	HIS	-	expression tag	UNP Q1JUQ0
G	-1	HIS	-	expression tag	UNP Q1JUQ0
G	0	GLY	-	expression tag	UNP Q1JUQ0
G	1	SER	-	expression tag	UNP Q1JUQ0
H	-10	MET	-	expression tag	UNP Q1JUQ0
H	-9	ARG	-	expression tag	UNP Q1JUQ0
H	-8	GLY	-	expression tag	UNP Q1JUQ0
H	-7	SER	-	expression tag	UNP Q1JUQ0
H	-6	HIS	-	expression tag	UNP Q1JUQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP Q1JUQ0
H	-4	HIS	-	expression tag	UNP Q1JUQ0
H	-3	HIS	-	expression tag	UNP Q1JUQ0
H	-2	HIS	-	expression tag	UNP Q1JUQ0
H	-1	HIS	-	expression tag	UNP Q1JUQ0
H	0	GLY	-	expression tag	UNP Q1JUQ0
H	1	SER	-	expression tag	UNP Q1JUQ0
I	-10	MET	-	expression tag	UNP Q1JUQ0
I	-9	ARG	-	expression tag	UNP Q1JUQ0
I	-8	GLY	-	expression tag	UNP Q1JUQ0
I	-7	SER	-	expression tag	UNP Q1JUQ0
I	-6	HIS	-	expression tag	UNP Q1JUQ0
I	-5	HIS	-	expression tag	UNP Q1JUQ0
I	-4	HIS	-	expression tag	UNP Q1JUQ0
I	-3	HIS	-	expression tag	UNP Q1JUQ0
I	-2	HIS	-	expression tag	UNP Q1JUQ0
I	-1	HIS	-	expression tag	UNP Q1JUQ0
I	0	GLY	-	expression tag	UNP Q1JUQ0
I	1	SER	-	expression tag	UNP Q1JUQ0
J	-10	MET	-	expression tag	UNP Q1JUQ0
J	-9	ARG	-	expression tag	UNP Q1JUQ0
J	-8	GLY	-	expression tag	UNP Q1JUQ0
J	-7	SER	-	expression tag	UNP Q1JUQ0
J	-6	HIS	-	expression tag	UNP Q1JUQ0
J	-5	HIS	-	expression tag	UNP Q1JUQ0
J	-4	HIS	-	expression tag	UNP Q1JUQ0
J	-3	HIS	-	expression tag	UNP Q1JUQ0
J	-2	HIS	-	expression tag	UNP Q1JUQ0
J	-1	HIS	-	expression tag	UNP Q1JUQ0
J	0	GLY	-	expression tag	UNP Q1JUQ0
J	1	SER	-	expression tag	UNP Q1JUQ0
K	-10	MET	-	expression tag	UNP Q1JUQ0
K	-9	ARG	-	expression tag	UNP Q1JUQ0
K	-8	GLY	-	expression tag	UNP Q1JUQ0
K	-7	SER	-	expression tag	UNP Q1JUQ0
K	-6	HIS	-	expression tag	UNP Q1JUQ0
K	-5	HIS	-	expression tag	UNP Q1JUQ0
K	-4	HIS	-	expression tag	UNP Q1JUQ0
K	-3	HIS	-	expression tag	UNP Q1JUQ0
K	-2	HIS	-	expression tag	UNP Q1JUQ0
K	-1	HIS	-	expression tag	UNP Q1JUQ0
K	0	GLY	-	expression tag	UNP Q1JUQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	SER	-	expression tag	UNP Q1JUQ0
L	-10	MET	-	expression tag	UNP Q1JUQ0
L	-9	ARG	-	expression tag	UNP Q1JUQ0
L	-8	GLY	-	expression tag	UNP Q1JUQ0
L	-7	SER	-	expression tag	UNP Q1JUQ0
L	-6	HIS	-	expression tag	UNP Q1JUQ0
L	-5	HIS	-	expression tag	UNP Q1JUQ0
L	-4	HIS	-	expression tag	UNP Q1JUQ0
L	-3	HIS	-	expression tag	UNP Q1JUQ0
L	-2	HIS	-	expression tag	UNP Q1JUQ0
L	-1	HIS	-	expression tag	UNP Q1JUQ0
L	0	GLY	-	expression tag	UNP Q1JUQ0
L	1	SER	-	expression tag	UNP Q1JUQ0

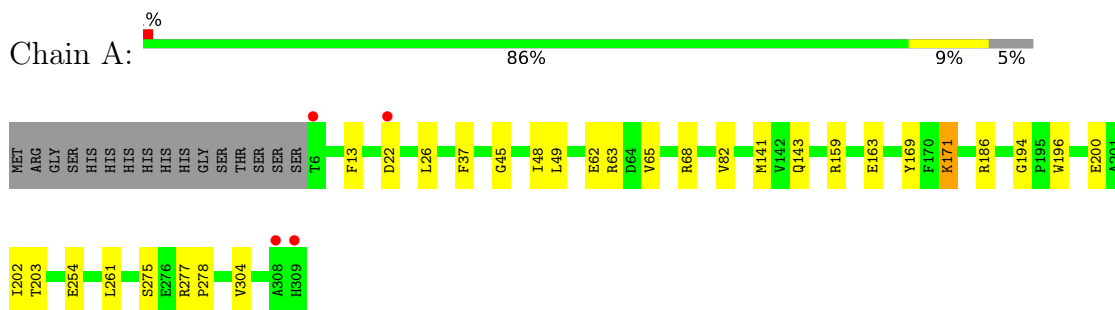
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	105	Total O 105 105	0	0
2	B	92	Total O 92 92	0	0
2	C	107	Total O 107 107	0	0
2	D	111	Total O 111 111	0	0
2	E	112	Total O 112 112	0	0
2	F	105	Total O 105 105	0	0
2	G	116	Total O 116 116	0	0
2	H	97	Total O 97 97	0	0
2	I	65	Total O 65 65	0	0
2	J	71	Total O 71 71	0	0
2	K	89	Total O 89 89	0	0
2	L	62	Total O 62 62	0	0

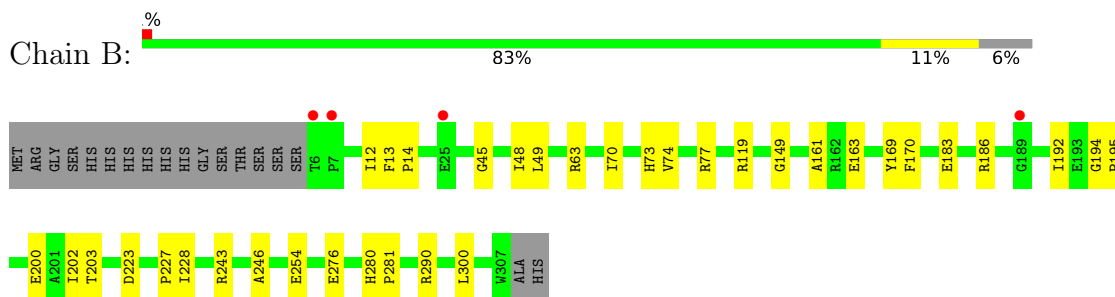
### 3 Residue-property plots [i](#)

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.

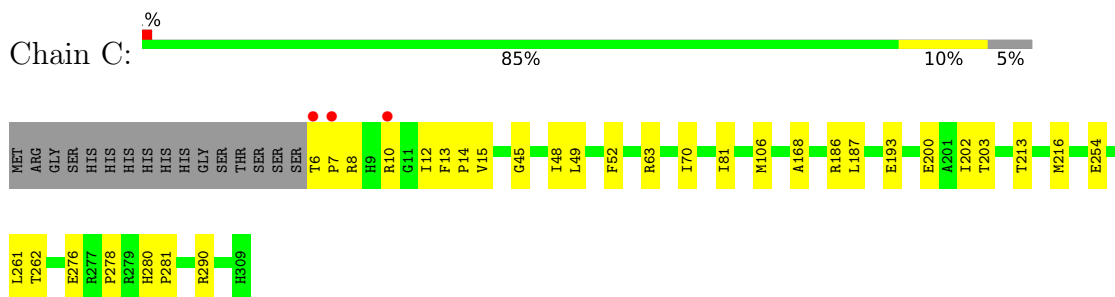
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



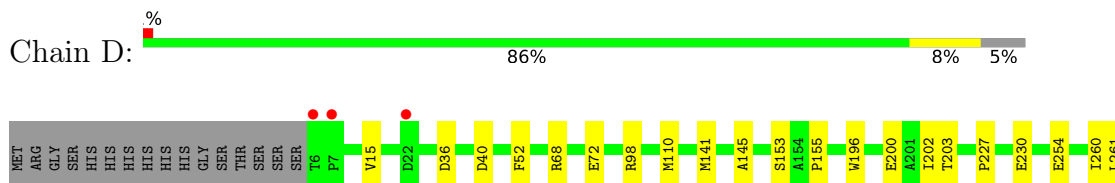
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

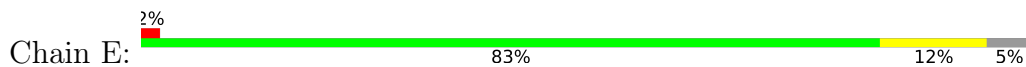


- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

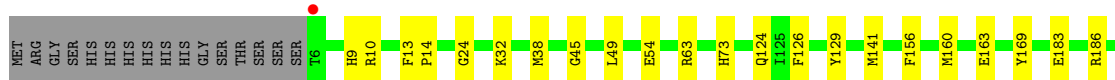
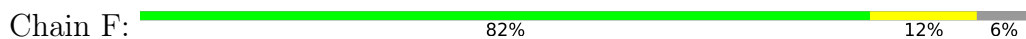




- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



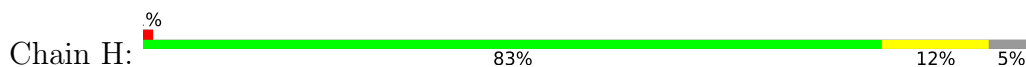
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

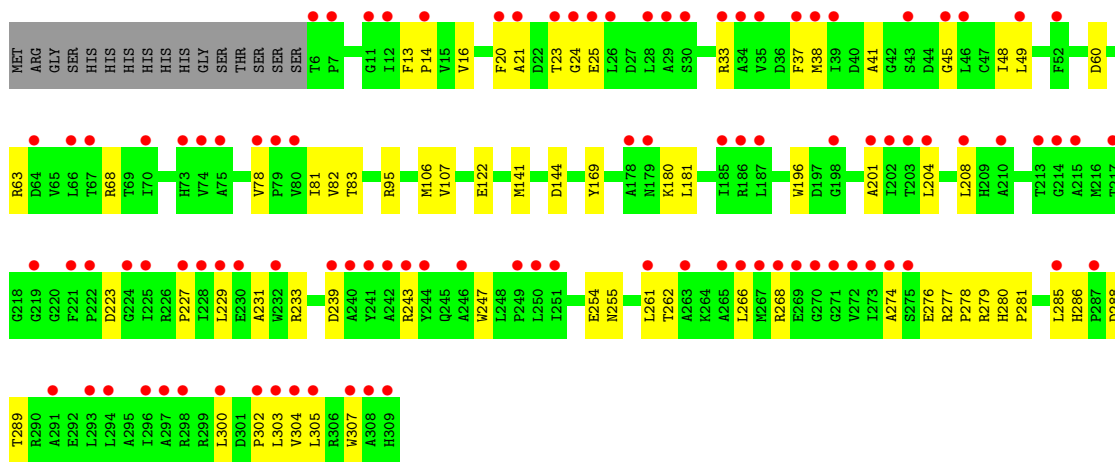


- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

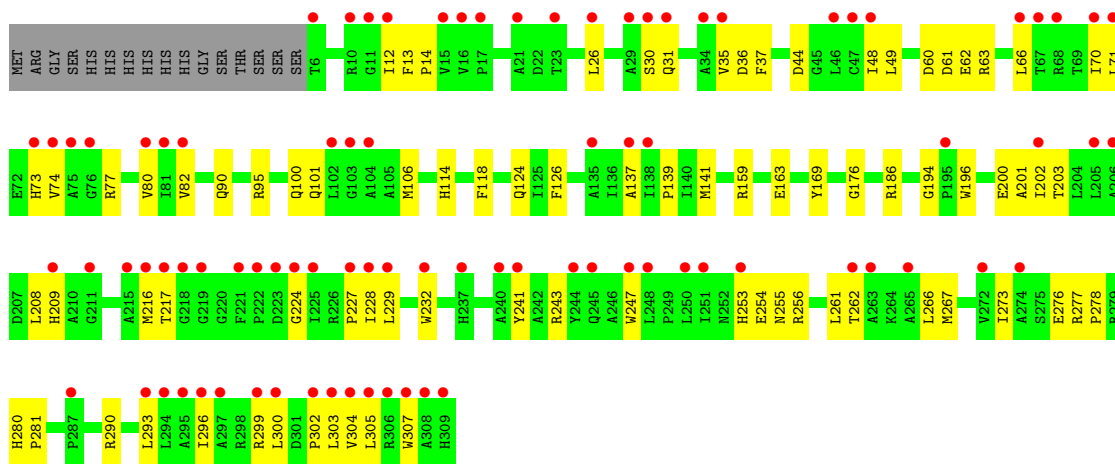


- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

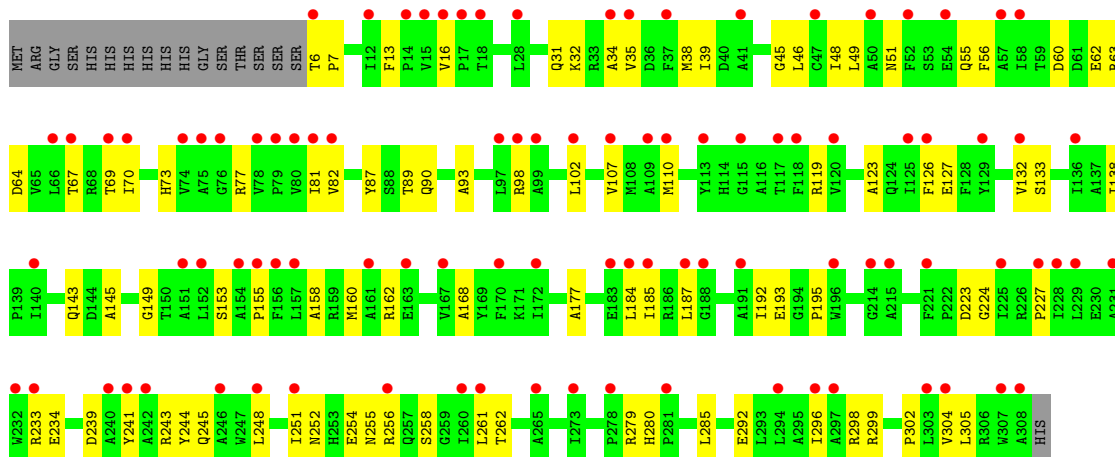




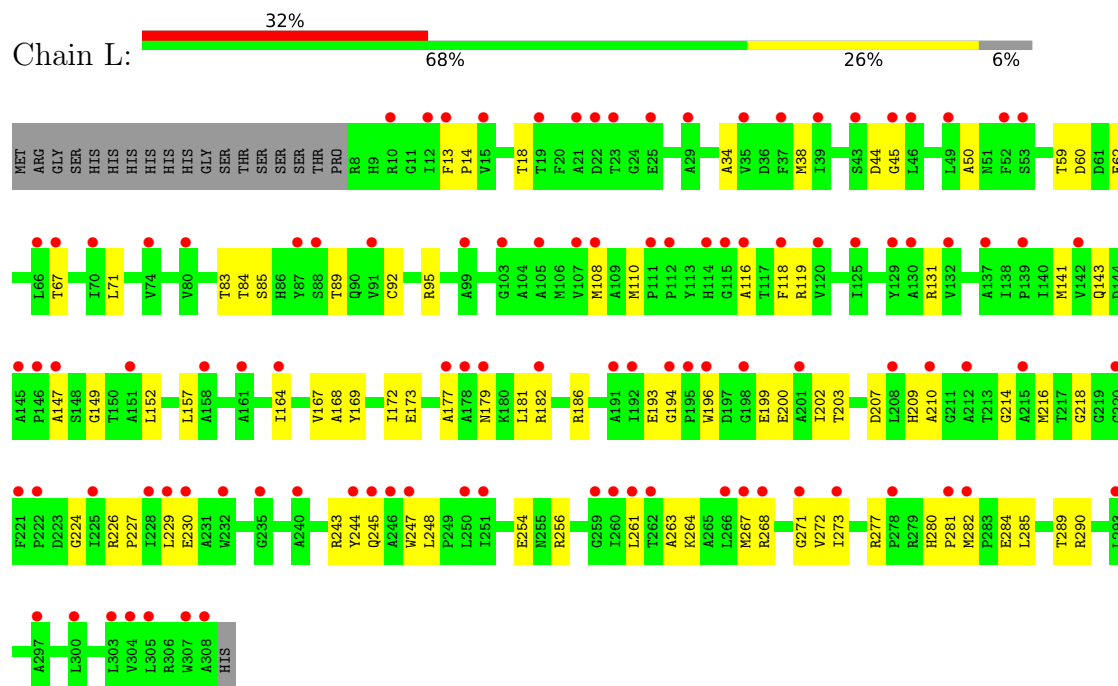
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.52Å 81.20Å 142.84Å 85.71° 88.43° 75.39°	Depositor
Resolution (Å)	47.95 – 2.20 47.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.95-2.20) 98.3 (47.95-2.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.221 , 0.269 0.227 , 0.271	Depositor DCC
$R_{free}$ test set	8087 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	29111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FF9

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	0.15	0/2386	0.36	0/3244
1	B	0.14	0/2369	0.35	0/3222
1	C	0.14	0/2386	0.34	0/3244
1	D	0.14	0/2368	0.35	0/3222
1	E	0.14	0/2386	0.36	0/3244
1	F	0.14	0/2369	0.36	0/3222
1	G	0.14	0/2368	0.35	0/3222
1	H	0.14	0/2368	0.35	0/3222
1	I	0.17	0/2380	0.39	0/3237
1	J	0.18	0/2380	0.39	0/3237
1	K	0.17	0/2374	0.44	0/3229
1	L	0.18	0/2359	0.38	0/3207
All	All	0.15	0/28493	0.37	0/38752

There are no bond length outliers.

There are no bond angle outliers.

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	2348	0	2308	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2326	0	2296	24	0
1	C	2342	0	2308	19	0
1	D	2325	0	2290	16	0
1	E	2342	0	2308	27	0
1	F	2326	0	2296	32	0
1	G	2325	0	2290	15	0
1	H	2325	0	2290	25	0
1	I	2336	0	2297	56	0
1	J	2336	0	2297	82	0
1	K	2331	0	2301	96	0
1	L	2317	0	2287	64	0
2	A	105	0	0	0	0
2	B	92	0	0	0	0
2	C	107	0	0	1	0
2	D	111	0	0	3	0
2	E	112	0	0	0	0
2	F	105	0	0	3	0
2	G	116	0	0	2	0
2	H	97	0	0	4	0
2	I	65	0	0	6	0
2	J	71	0	0	5	0
2	K	89	0	0	36	0
2	L	62	0	0	9	0
All	All	29111	0	27568	448	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 448 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:J:203:THR:CG2	1:K:256:ARG:HD2	1.87	1.05
1:J:203:THR:HG21	1:K:256:ARG:CD	1.87	1.04
1:J:203:THR:HG21	1:K:256:ARG:HD2	0.98	0.97
1:J:100:GLN:HE22	1:J:137:ALA:H	1.11	0.96
1:K:63:ARG:NH1	2:K:403:HOH:O	2.04	0.90

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	301/320 (94%)	291 (97%)	10 (3%)	0	100	100
1	B	299/320 (93%)	292 (98%)	7 (2%)	0	100	100
1	C	301/320 (94%)	293 (97%)	8 (3%)	0	100	100
1	D	300/320 (94%)	295 (98%)	5 (2%)	0	100	100
1	E	301/320 (94%)	292 (97%)	9 (3%)	0	100	100
1	F	299/320 (93%)	292 (98%)	7 (2%)	0	100	100
1	G	300/320 (94%)	294 (98%)	6 (2%)	0	100	100
1	H	300/320 (94%)	292 (97%)	8 (3%)	0	100	100
1	I	301/320 (94%)	293 (97%)	8 (3%)	0	100	100
1	J	301/320 (94%)	294 (98%)	7 (2%)	0	100	100
1	K	300/320 (94%)	293 (98%)	7 (2%)	0	100	100
1	L	298/320 (93%)	291 (98%)	7 (2%)	0	100	100
All	All	3601/3840 (94%)	3512 (98%)	89 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	192/250 (77%)	192 (100%)	0	100	100
1	B	235/250 (94%)	235 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	236/250 (94%)	236 (100%)	0	100	100
1	D	234/250 (94%)	234 (100%)	0	100	100
1	E	236/250 (94%)	236 (100%)	0	100	100
1	F	235/250 (94%)	235 (100%)	0	100	100
1	G	234/250 (94%)	234 (100%)	0	100	100
1	H	234/250 (94%)	234 (100%)	0	100	100
1	I	235/250 (94%)	235 (100%)	0	100	100
1	J	235/250 (94%)	235 (100%)	0	100	100
1	K	235/250 (94%)	235 (100%)	0	100	100
1	L	233/250 (93%)	233 (100%)	0	100	100
All	All	2774/3000 (92%)	2774 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	124	GLN
1	H	124	GLN
1	G	252	ASN
1	H	252	ASN
1	D	252	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](#)

12 non-standard protein/DNA/RNA residues 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
1	FF9	E	171	1	7,8,15	0.53	0	3,8,18	0.40	0
1	FF9	D	171	1	7,8,15	0.47	0	3,8,18	0.47	0
1	FF9	F	171	1	7,8,15	0.50	0	3,8,18	0.23	0
1	FF9	G	171	1	7,8,15	0.51	0	3,8,18	0.24	0
1	FF9	H	171	1	7,8,15	0.52	0	3,8,18	0.66	0
1	FF9	C	171	1	7,8,15	0.52	0	3,8,18	0.58	0
1	FF9	K	171	1	7,8,15	0.54	0	3,8,18	0.42	0
1	FF9	J	171	1	7,8,15	0.50	0	3,8,18	0.36	0
1	FF9	I	171	1	7,8,15	0.51	0	3,8,18	0.53	0
1	FF9	A	171	1	12,14,15	0.84	1 (8%)	6,16,18	1.59	1 (16%)
1	FF9	B	171	1	7,8,15	0.51	0	3,8,18	0.37	0
1	FF9	L	171	1	7,8,15	0.53	0	3,8,18	0.48	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
1	FF9	E	171	1	-	0/6/7/18	-
1	FF9	D	171	1	-	1/6/7/18	-
1	FF9	F	171	1	-	2/6/7/18	-
1	FF9	G	171	1	-	0/6/7/18	-
1	FF9	H	171	1	-	1/6/7/18	-
1	FF9	C	171	1	-	0/6/7/18	-
1	FF9	K	171	1	-	2/6/7/18	-
1	FF9	J	171	1	-	3/6/7/18	-
1	FF9	I	171	1	-	1/6/7/18	-
1	FF9	A	171	1	-	5/14/16/18	-
1	FF9	B	171	1	-	2/6/7/18	-
1	FF9	L	171	1	-	1/6/7/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	FF9	O1-CX2	-2.05	1.25	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	FF9	CD-CE-NZ	-3.15	105.09	110.67

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	171	FF9	O-C-CA-CB
1	A	171	FF9	C1-CX1-CX2-O1
1	A	171	FF9	C1-CX1-CX2-O2
1	A	171	FF9	NZ-CX1-CX2-O1
1	A	171	FF9	NZ-CX1-CX2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	171	FF9	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	303/320 (94%)	0.04	4 (1%) 75 73	19, 28, 42, 65	0
1	B	301/320 (94%)	0.27	4 (1%) 75 73	23, 32, 45, 67	0
1	C	303/320 (94%)	-0.04	3 (0%) 79 77	21, 27, 38, 62	0
1	D	302/320 (94%)	0.12	4 (1%) 75 73	22, 30, 43, 77	0
1	E	303/320 (94%)	0.06	5 (1%) 69 66	21, 30, 42, 82	0
1	F	301/320 (94%)	0.08	1 (0%) 90 88	20, 30, 40, 57	0
1	G	302/320 (94%)	-0.00	1 (0%) 90 88	23, 28, 40, 71	0
1	H	302/320 (94%)	0.11	2 (0%) 84 82	22, 30, 42, 57	0
1	I	303/320 (94%)	1.47	100 (33%) 1 0	23, 47, 59, 74	0
1	J	303/320 (94%)	1.35	87 (28%) 1 1	20, 44, 58, 73	0
1	K	302/320 (94%)	1.75	96 (31%) 1 1	35, 43, 53, 75	0
1	L	300/320 (93%)	1.73	104 (34%) 1 0	34, 46, 55, 70	0
All	All	3625/3840 (94%)	0.58	411 (11%) 10 8	19, 32, 52, 82	0

The worst 5 of 411 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	240	ALA	6.1
1	A	308	ALA	5.5
1	E	6	THR	5.2
1	I	21	ALA	4.8
1	I	228	ILE	4.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	FF9	K	171	9/16	0.72	0.18	36,46,49,51	0
1	FF9	L	171	9/16	0.74	0.17	36,48,50,50	0
1	FF9	A	171	15/16	0.77	0.15	21,26,33,34	6
1	FF9	I	171	9/16	0.84	0.14	38,42,49,52	0
1	FF9	J	171	9/16	0.89	0.11	31,37,43,44	0
1	FF9	D	171	9/16	0.91	0.08	24,30,33,36	0
1	FF9	E	171	9/16	0.91	0.12	23,26,39,40	0
1	FF9	G	171	9/16	0.92	0.09	24,25,28,35	0
1	FF9	F	171	9/16	0.93	0.08	24,26,31,32	0
1	FF9	H	171	9/16	0.93	0.09	24,28,35,37	0
1	FF9	C	171	9/16	0.94	0.08	21,23,31,36	0
1	FF9	B	171	9/16	0.95	0.09	27,28,34,36	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.