



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 04:46 PM GMT

PDB ID : 2VBG
Title : THE COMPLEX STRUCTURE OF THE BRANCHED-CHAIN KETO ACID
DECARBOXYLASE (KDCA) FROM LACTOCOCCUS LACTIS WITH 2R-
1-HYDROXYETHYL-DEAZATHDP
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Deposited on : 2007-09-12
Resolution : 1.80 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

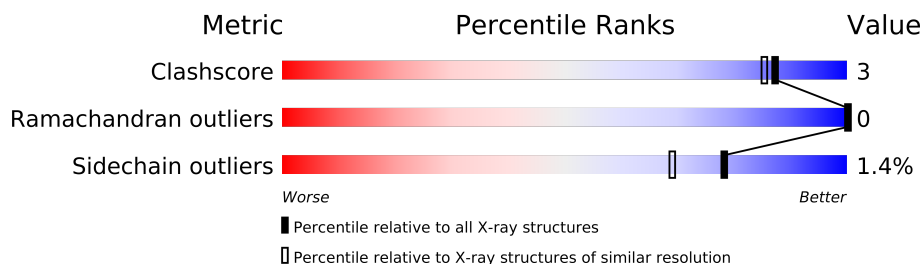
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	570	
1	B	570	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9634 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

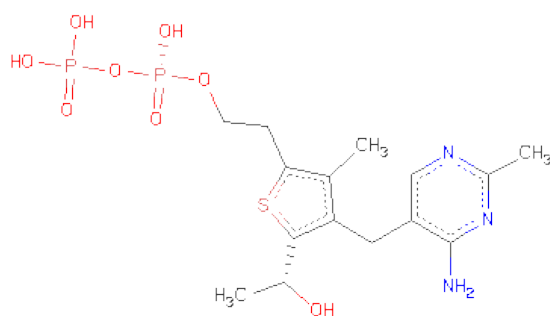
- Molecule 1 is a protein called BRANCHED-CHAIN ALPHA-KETOACID DECARBOXY-LASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	6	12	0
			4330	2770	703	844	13			
1	B	544	Total	C	N	O	S	0	7	0
			4294	2745	700	837	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-5-[(1R)-1-HYDROXYETHYL]-3-METHYL-2-THIENYL}ETHYLTRIHYDROGEN DIPHOSPHATE (three-letter code: R1T) (formula: C₁₅H₂₃N₃O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 29	C 15	N 3	O 8	P 2	S 1	0	0
3	B	1	Total 29	C 15	N 3	O 8	P 2	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	478	Total	O	0	0
			478	478		
4	B	472	Total	O	0	0
			472	472		

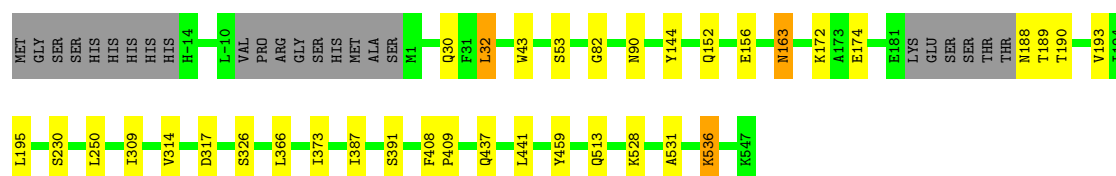
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

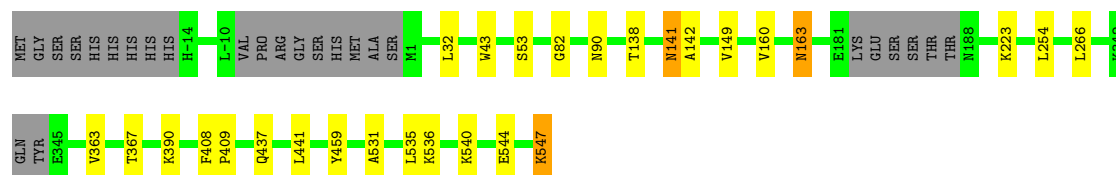
• Molecule 1: BRANCHED-CHAIN ALPHA-KETOACID DECARBOXYLASE

Chain A: 



• Molecule 1: BRANCHED-CHAIN ALPHA-KETOACID DECARBOXYLASE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.98Å 108.58Å 146.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	97.3 (30.00-1.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.163 , 0.205	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9634	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R1T, MG

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	0.42	1/4443 (0.0%)	0.56	0/6010
1	B	0.42	0/4389	0.55	0/5937
All	All	0.42	1/8832 (0.0%)	0.56	0/11947

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172[A]	LYS	CG-CD	5.30	1.70	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4330	0	4319	21	2
1	B	4294	0	4291	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	20	2	0
3	B	29	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	478	0	0	3	0
4	B	472	0	0	2	0
All	All	9634	0	8650	44	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:LEU:O	4:A:2316:HOH:O	1.82	0.97
1:A:513:GLN:NE2	4:A:2316:HOH:O	1.99	0.88
1:B:141:ASN:HD22	1:B:141:ASN:C	1.87	0.78
1:A:195:LEU:HD21	1:A:326:SER:OG	1.89	0.73
1:B:254:LEU:HB3	1:B:266[B]:LEU:HD13	1.80	0.64
1:A:190:THR:HG21	1:A:317:ASP:OD2	1.98	0.64
1:B:149[B]:VAL:CG1	1:B:160:VAL:HB	2.29	0.63
1:A:152:GLN:NE2	1:A:156:GLU:OE2	2.24	0.63
1:A:373:ILE:CD1	1:A:387[A]:ILE:HD11	2.31	0.61
1:B:363:VAL:O	1:B:367[B]:THR:HG23	2.02	0.60
1:B:163:ASN:C	1:B:163:ASN:HD22	2.05	0.60
1:B:367[A]:THR:HG23	1:B:390:LYS:HD3	1.85	0.58
1:B:141:ASN:C	1:B:141:ASN:ND2	2.56	0.58
1:A:373:ILE:HD12	1:A:387[A]:ILE:HD11	1.86	0.58
1:B:141:ASN:HD22	1:B:142:ALA:N	2.04	0.56
1:A:163:ASN:HD22	1:A:163:ASN:C	2.08	0.55
1:A:309:ILE:HD12	1:A:314:VAL:HG22	1.89	0.55
1:B:138:THR:H	1:B:141:ASN:ND2	2.07	0.52
1:B:223:LYS:NZ	4:B:2228:HOH:O	2.42	0.52
1:B:138:THR:H	1:B:141:ASN:HD21	1.58	0.51
1:A:528:LYS:NZ	4:A:2453:HOH:O	2.44	0.50
1:B:459:TYR:CD1	3:B:1549:R1T:H61	2.49	0.48
1:A:309:ILE:CD1	1:A:314:VAL:HG22	2.45	0.46
1:A:30[A]:GLN:NE2	4:B:2469:HOH:O	2.48	0.46
1:A:53:SER:OG	1:A:82:GLY:HA3	2.15	0.46
1:B:544:GLU:OE1	1:B:547:LYS:NZ	2.49	0.45
1:B:408:PHE:HB3	1:B:409:PRO:HD3	1.98	0.45
1:A:441:LEU:HD23	1:A:441:LEU:C	2.38	0.45
1:A:408:PHE:HB3	1:A:409:PRO:HD3	1.99	0.44
1:B:531:ALA:HB3	1:B:536:LYS:HE2	1.99	0.44
1:A:459:TYR:CD1	3:A:1549:R1T:H61	2.53	0.44
1:A:163:ASN:C	1:A:163:ASN:ND2	2.72	0.43
1:A:189:THR:O	1:A:193:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230[B]:SER:OG	1:A:250:LEU:CD2	2.67	0.43
1:A:32:LEU:HD11	1:A:43:TRP:CD2	2.54	0.42
1:A:531:ALA:HB3	1:A:536:LYS:HE3	2.01	0.42
3:A:1549:R1T:C2	3:A:1549:R1T:H4'2	2.33	0.42
1:B:163:ASN:C	1:B:163:ASN:ND2	2.71	0.42
1:B:254:LEU:CB	1:B:266[B]:LEU:HD13	2.48	0.42
1:B:149[B]:VAL:HG13	1:B:160:VAL:HB	1.99	0.41
1:B:32:LEU:HD21	1:B:43:TRP:CD2	2.56	0.41
1:B:53:SER:OG	1:B:82:GLY:HA3	2.21	0.41
1:B:441:LEU:C	1:B:441:LEU:HD13	2.41	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:144[B]:TYR:CE2	1:A:391[B]:SER:OG[4_555]	1.94	0.26
1:A:144[B]:TYR:CD2	1:A:391[B]:SER:OG[4_555]	1.99	0.21

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	550/570 (96%)	540 (98%)	10 (2%)	0	100	100
1	B	543/570 (95%)	535 (98%)	8 (2%)	0	100	100
All	All	1093/1140 (96%)	1075 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	481/492 (98%)	474 (98%)	7 (2%)	76	66
1	B	476/492 (97%)	470 (99%)	6 (1%)	80	71
All	All	957/984 (97%)	944 (99%)	13 (1%)	78	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	90	ASN
1	A	163	ASN
1	A	174	GLU
1	A	188	ASN
1	A	437	GLN
1	A	536	LYS
1	B	90	ASN
1	B	141	ASN
1	B	163	ASN
1	B	437	GLN
1	B	540	LYS
1	B	547	LYS

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

Mol	Chain	Res	Type
1	A	163	ASN
1	B	141	ASN
1	B	163	ASN
1	B	377	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	R1T	A	1549	2	30,30,30	1.91	6 (20%)	44,45,45	2.07	9 (20%)
3	R1T	B	1549	2	30,30,30	1.96	5 (16%)	44,45,45	1.85	9 (20%)

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
3	R1T	A	1549	2	-	0/17/21/21	0/2/2/2
3	R1T	B	1549	2	-	0/17/21/21	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1549	R1T	C3-C4	5.58	1.54	1.37
3	A	1549	R1T	C3-C4	5.36	1.53	1.37
3	B	1549	R1T	C2-S1	5.07	1.83	1.73
3	A	1549	R1T	C2-S1	4.30	1.82	1.73
3	B	1549	R1T	C2-C3	4.30	1.43	1.36
3	A	1549	R1T	C2-C3	3.80	1.42	1.36
3	A	1549	R1T	C5-C4	3.62	1.42	1.36
3	B	1549	R1T	C5-C4	3.60	1.42	1.36
3	A	1549	R1T	C5-S1	3.21	1.79	1.73
3	A	1549	R1T	PB-O3A	2.47	1.64	1.60
3	B	1549	R1T	PB-O3A	2.32	1.64	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1549	R1T	OP1-CP1-C2	-8.45	98.78	112.64
3	B	1549	R1T	OP1-CP1-C2	-7.23	100.78	112.64
3	A	1549	R1T	CP2-CP1-C2	4.51	119.07	112.23
3	B	1549	R1T	N1'-C2'-N3'	-3.39	119.53	125.65
3	A	1549	R1T	C6'-N1'-C2'	3.26	121.40	115.68
3	A	1549	R1T	C7'-C5'-C4'	3.21	126.13	122.17
3	A	1549	R1T	N1'-C2'-N3'	-3.15	119.96	125.65
3	B	1549	R1T	CP2-CP1-C2	3.15	117.01	112.23
3	B	1549	R1T	C6'-N1'-C2'	3.08	121.10	115.68
3	A	1549	R1T	C7'-C5'-C6'	-3.00	117.89	121.82
3	B	1549	R1T	CM2-C2'-N1'	2.99	120.58	117.02
3	B	1549	R1T	C7'-C5'-C4'	2.94	125.80	122.17
3	B	1549	R1T	C7'-C5'-C6'	-2.83	118.12	121.82
3	A	1549	R1T	C3-C2-S1	-2.59	105.89	111.18
3	B	1549	R1T	C3-C2-S1	-2.46	106.17	111.18
3	A	1549	R1T	CM2-C2'-N1'	2.43	119.92	117.02
3	A	1549	R1T	C7'-C3-C4	-2.40	121.77	126.85
3	B	1549	R1T	C7'-C3-C4	-2.02	122.57	126.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.