



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3CB3 / pdb_00003cb3
Title : Crystal structure of L-Talarate dehydratase from Polaromonas sp. JS666 complexed with Mg and L-glucarate
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Deposited on : 2008-02-21
Resolution : 2.00 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>.

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

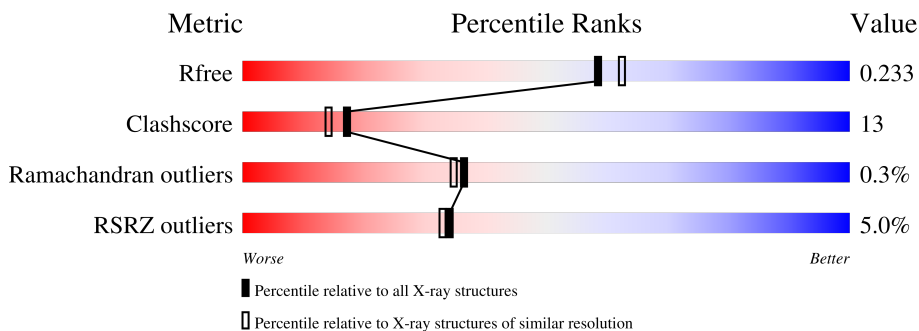
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 ≥ 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	393	 2% 78% 16% • 5%
1	B	393	 8% 63% 27% • 8%
1	C	393	 8% 65% 26% • 9%
1	D	393	 2% 72% 19% 9%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11715 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	373	2867	1821	513	520	13	0	0	0
1	B	361	2777	1766	495	503	13	0	0	0
1	C	357	2750	1748	491	498	13	0	0	0
1	D	358	2757	1753	492	499	13	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q12GE3
A	0	SER	-	expression tag	UNP Q12GE3
A	1	LEU	-	expression tag	UNP Q12GE3
A	384	GLU	-	expression tag	UNP Q12GE3
A	385	GLY	-	expression tag	UNP Q12GE3
A	386	HIS	-	expression tag	UNP Q12GE3
A	387	HIS	-	expression tag	UNP Q12GE3
A	388	HIS	-	expression tag	UNP Q12GE3
A	389	HIS	-	expression tag	UNP Q12GE3
A	390	HIS	-	expression tag	UNP Q12GE3
A	391	HIS	-	expression tag	UNP Q12GE3
B	-1	MET	-	expression tag	UNP Q12GE3
B	0	SER	-	expression tag	UNP Q12GE3
B	1	LEU	-	expression tag	UNP Q12GE3
B	384	GLU	-	expression tag	UNP Q12GE3
B	385	GLY	-	expression tag	UNP Q12GE3
B	386	HIS	-	expression tag	UNP Q12GE3
B	387	HIS	-	expression tag	UNP Q12GE3
B	388	HIS	-	expression tag	UNP Q12GE3
B	389	HIS	-	expression tag	UNP Q12GE3
B	390	HIS	-	expression tag	UNP Q12GE3

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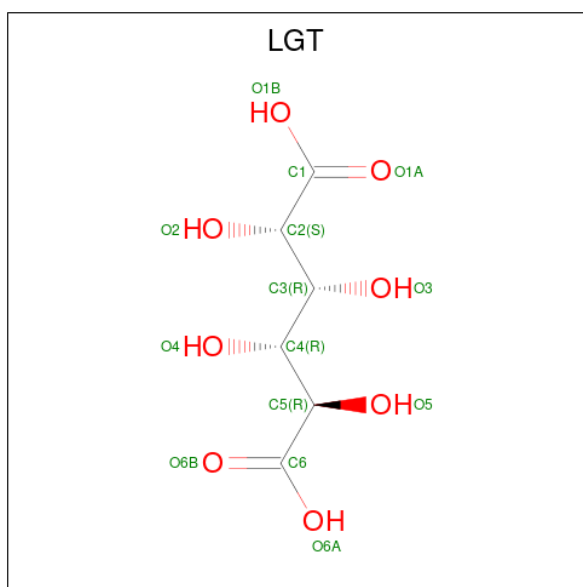
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Chain	Residue	Modelled	Actual	Comment	Reference
B	391	HIS	-	expression tag	UNP Q12GE3
C	-1	MET	-	expression tag	UNP Q12GE3
C	0	SER	-	expression tag	UNP Q12GE3
C	1	LEU	-	expression tag	UNP Q12GE3
C	384	GLU	-	expression tag	UNP Q12GE3
C	385	GLY	-	expression tag	UNP Q12GE3
C	386	HIS	-	expression tag	UNP Q12GE3
C	387	HIS	-	expression tag	UNP Q12GE3
C	388	HIS	-	expression tag	UNP Q12GE3
C	389	HIS	-	expression tag	UNP Q12GE3
C	390	HIS	-	expression tag	UNP Q12GE3
C	391	HIS	-	expression tag	UNP Q12GE3
D	-1	MET	-	expression tag	UNP Q12GE3
D	0	SER	-	expression tag	UNP Q12GE3
D	1	LEU	-	expression tag	UNP Q12GE3
D	384	GLU	-	expression tag	UNP Q12GE3
D	385	GLY	-	expression tag	UNP Q12GE3
D	386	HIS	-	expression tag	UNP Q12GE3
D	387	HIS	-	expression tag	UNP Q12GE3
D	388	HIS	-	expression tag	UNP Q12GE3
D	389	HIS	-	expression tag	UNP Q12GE3
D	390	HIS	-	expression tag	UNP Q12GE3
D	391	HIS	-	expression tag	UNP Q12GE3

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is L-GLUCARIC ACID (CCD ID: LGT) (formula: C₆H₁₀O₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 14 6 8	0	0
3	B	1	Total C O 14 6 8	0	0
3	C	1	Total C O 14 6 8	0	0
3	D	1	Total C O 14 6 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	141	Total O 141 141	0	0
4	B	123	Total O 123 123	0	0
4	C	107	Total O 107 107	0	0
4	D	129	Total O 129 129	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.47Å 84.74Å 118.25Å 90.00° 126.04° 90.00°	Depositor
Resolution (Å)	24.91 – 2.00 24.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (24.91-2.00) 94.7 (24.91-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.239 0.207 , 0.233	Depositor DCC
R_{free} test set	5205 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.022 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11715	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, LGT

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	0.40	0/2938	0.88	8/3991 (0.2%)
1	B	0.39	0/2846	0.87	7/3866 (0.2%)
1	C	0.39	0/2818	0.87	5/3826 (0.1%)
1	D	0.40	0/2826	0.87	8/3837 (0.2%)
All	All	0.40	0/11428	0.87	28/15520 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	ILE	N-CA-C	7.56	117.68	110.42
1	A	93	ILE	N-CA-C	7.18	117.31	110.42
1	D	93	ILE	N-CA-C	6.30	116.47	110.42
1	B	217	ASP	N-CA-C	-6.29	101.46	110.59
1	B	93	ILE	N-CA-C	6.19	116.36	110.42

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	2867	0	2851	56	0
1	B	2777	0	2752	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2750	0	2722	82	0
1	D	2757	0	2730	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	14	0	7	0	0
3	B	14	0	7	0	0
3	C	14	0	7	2	0
3	D	14	0	7	0	0
4	A	141	0	0	4	0
4	B	123	0	0	8	0
4	C	107	0	0	5	0
4	D	129	0	0	6	0
All	All	11715	0	11083	280	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 13.

The worst 5 of 280 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:A:358:ARG:HH11	1:A:358:ARG:HB2	1.24	1.03
1:C:214:GLN:HE21	1:C:242:ALA:H	1.10	0.98
1:B:214:GLN:HE21	1:B:242:ALA:H	1.21	0.89
1:A:346:ILE:HG21	1:A:353:MET:HE3	1.60	0.83
1:B:192:ILE:HD13	1:B:227:ILE:HG21	1.60	0.83

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	371/393 (94%)	364 (98%)	6 (2%)	1 (0%)	36	35
1	B	357/393 (91%)	346 (97%)	9 (2%)	2 (1%)	21	17
1	C	353/393 (90%)	341 (97%)	11 (3%)	1 (0%)	36	35
1	D	354/393 (90%)	347 (98%)	7 (2%)	0	100	100
All	All	1435/1572 (91%)	1398 (97%)	33 (2%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	315	ALA
1	C	315	ALA
1	A	315	ALA
1	B	161	ILE

5.3.2 Protein sidechains [i](#)

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

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	LGT	C	601	2	13,13,13	1.43	3 (23%)	16,18,18	0.71	0
3	LGT	B	601	2	13,13,13	1.47	3 (23%)	16,18,18	0.69	0
3	LGT	A	601	2	13,13,13	1.41	2 (15%)	16,18,18	0.79	0
3	LGT	D	601	2	13,13,13	1.32	1 (7%)	16,18,18	0.76	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
3	LGT	C	601	2	-	9/20/20/20	-
3	LGT	B	601	2	-	4/20/20/20	-
3	LGT	A	601	2	-	7/20/20/20	-
3	LGT	D	601	2	-	6/20/20/20	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	LGT	C2-C1	2.74	1.56	1.52
3	C	601	LGT	C5-C6	2.52	1.56	1.52
3	B	601	LGT	C5-C6	2.39	1.56	1.52
3	B	601	LGT	C2-C1	2.34	1.56	1.52
3	C	601	LGT	C2-C1	2.20	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	LGT	C2-C3-C4-O4
3	A	601	LGT	C2-C3-C4-C5
3	A	601	LGT	O3-C3-C4-O4
3	A	601	LGT	O3-C3-C4-C5
3	B	601	LGT	C2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	LGT	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	373/393 (94%)	0.04	2 (0%) 87 87	15, 25, 40, 51	0
1	B	361/393 (91%)	0.32	30 (8%) 17 16	14, 26, 51, 62	0
1	C	357/393 (90%)	0.38	31 (8%) 16 15	15, 27, 52, 61	0
1	D	358/393 (91%)	0.05	9 (2%) 58 58	15, 25, 41, 56	0
All	All	1449/1572 (92%)	0.19	72 (4%) 34 33	14, 26, 46, 62	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	TRP	5.1
1	B	102	TRP	4.5
1	B	156	PHE	4.1
1	C	102	TRP	4.0
1	C	164	LEU	4.0

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LGT	B	601	14/14	0.65	0.15	37,43,47,48	0
3	LGT	C	601	14/14	0.74	0.14	34,41,49,51	0
3	LGT	D	601	14/14	0.82	0.12	29,38,47,48	0
3	LGT	A	601	14/14	0.85	0.11	32,39,45,46	0
2	MG	B	502	1/1	0.91	0.05	31,31,31,31	0
2	MG	B	503	1/1	0.94	0.10	28,28,28,28	0
2	MG	D	502	1/1	0.97	0.03	29,29,29,29	0
2	MG	D	503	1/1	0.97	0.03	21,21,21,21	0
2	MG	A	502	1/1	0.98	0.03	21,21,21,21	0
2	MG	C	501	1/1	0.98	0.04	36,36,36,36	0
2	MG	C	502	1/1	0.98	0.08	32,32,32,32	0
2	MG	A	501	1/1	0.99	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.