



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1KKO / pdb_00001kko
Title : CRYSTAL STRUCTURE OF CITROBACTER AMALONATICUS METHYL-
LASPARTATE AMMONIA LYASE
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Deposited on : 2001-12-10
Resolution : 1.33 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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

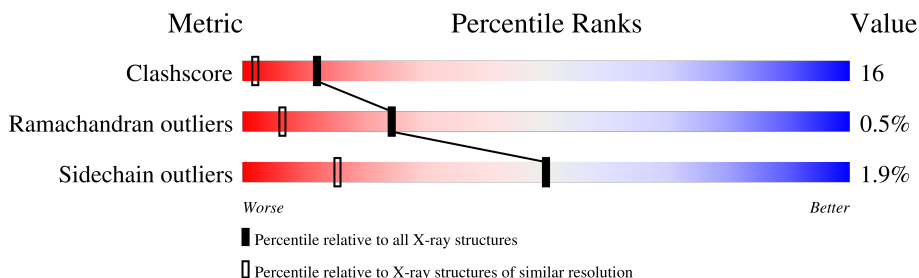
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 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	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	413	 84% 14% .
1	B	413	 80% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8530 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 3-METHYLASPARTATE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	Se	0	0	0
			3164	2010	541	593	10	10			
1	B	411	Total	C	N	O	S	Se	0	0	0
			3158	2006	541	591	10	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O66145
A	184	MSE	MET	modified residue	UNP O66145
A	249	MSE	MET	modified residue	UNP O66145
A	287	MSE	MET	modified residue	UNP O66145
A	327	MSE	MET	modified residue	UNP O66145
A	353	MSE	MET	modified residue	UNP O66145
A	381	MSE	MET	modified residue	UNP O66145
A	383	MSE	MET	modified residue	UNP O66145
A	389	MSE	MET	modified residue	UNP O66145
A	402	MSE	MET	modified residue	UNP O66145
B	1	MSE	MET	modified residue	UNP O66145
B	184	MSE	MET	modified residue	UNP O66145
B	249	MSE	MET	modified residue	UNP O66145
B	287	MSE	MET	modified residue	UNP O66145
B	327	MSE	MET	modified residue	UNP O66145
B	353	MSE	MET	modified residue	UNP O66145
B	381	MSE	MET	modified residue	UNP O66145
B	383	MSE	MET	modified residue	UNP O66145
B	389	MSE	MET	modified residue	UNP O66145
B	402	MSE	MET	modified residue	UNP O66145

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1089	Total	O	0	0
			1089	1089		
3	B	1114	Total	O	0	0
			1114	1114		

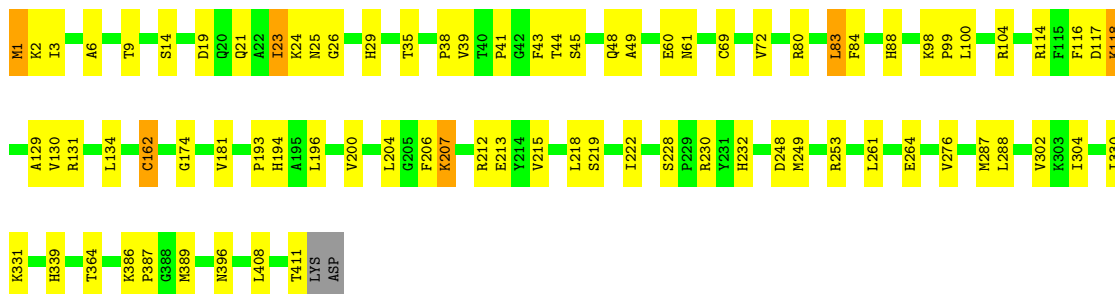
i

Note EDS was not executed.

Chain A: 84% 14%



Chain B: 80% 18%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.34Å 237.36Å 65.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 1.33	Depositor
% Data completeness (in resolution range)	95.7 (119.52-1.33)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.161 , 0.191	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8530	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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

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	0/3220	0.81	0/4354
1	B	0.56	0/3215	0.83	1/4350 (0.0%)
All	All	0.55	0/6435	0.82	1/8704 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MSE	CG-SE-CE	-5.20	87.48	98.92

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	3164	0	3132	87	0
1	B	3158	0	3113	110	0
2	A	5	0	0	0	0
3	A	1089	0	0	63	3
3	B	1114	0	0	67	6
All	All	8530	0	6245	195	7

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 16.

The worst 5 of 195 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:B:207:LYS:HA	1:B:207:LYS:HE3	1.22	1.19
1:B:213:GLU:HB3	3:B:1001:HOH:O	1.43	1.15
1:B:204:LEU:HB3	3:B:1488:HOH:O	1.47	1.14
1:B:200:VAL:HA	3:B:1488:HOH:O	1.52	1.10
1:A:276:VAL:HG21	1:A:287:MSE:HG2	1.34	1.09

The worst 5 of 7 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	Interatomic distance (Å)	Clash overlap (Å)
3:A:4090:HOH:O	3:B:1029:HOH:O[1_556]	0.22	1.98
3:B:680:HOH:O	3:B:1527:HOH:O[6_435]	0.31	1.89
3:B:972:HOH:O	3:B:1527:HOH:O[6_435]	1.29	0.91
3:B:972:HOH:O	3:B:972:HOH:O[6_435]	1.76	0.44
3:B:896:HOH:O	3:B:980:HOH:O[6_435]	1.92	0.28

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	409/413 (99%)	400 (98%)	9 (2%)	0	100	100
1	B	409/413 (99%)	393 (96%)	12 (3%)	4 (1%)	12	1
All	All	818/826 (99%)	793 (97%)	21 (3%)	4 (0%)	24	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	LYS

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Mol	Chain	Res	Type
1	B	26	GLY
1	B	23	ILE
1	B	41	PRO

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	336/331 (102%)	330 (98%)	6 (2%)	51	17
1	B	334/331 (101%)	327 (98%)	7 (2%)	47	13
All	All	670/662 (101%)	657 (98%)	13 (2%)	50	15

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	LEU
1	B	118	LYS
1	B	228	SER
1	B	193	PRO
1	B	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	B	357	GLN
1	A	410	GLN
1	B	396	ASN
1	B	96	HIS

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	SO4	A	3001	-	4,4,4	0.67	0	6,6,6	0.53	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.