wwPDB X-ray Structure Validation Summary Report (i)

May 28, 2020 – 07:55 pm BST

PDB ID	:	1KKO
Title	:	CRYSTAL STRUCTURE OF CITROBACTER AMALONATICUS METHYLASPARTATE AMMONIA LYASE
Authors	:	Levy, C.W.; Buckley, P.A.; Sedelnikova, S.; Kato, Y.; Asano, Y.; Rice, D.W.; Baker, P.J.
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 (i) symbol.

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

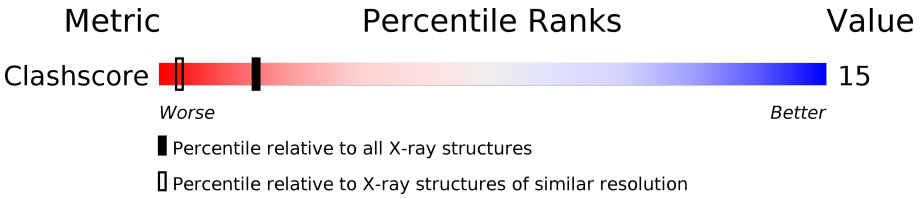
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	1417 (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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	413	84% 16%
1	B	413	81% 18%

2 Entry composition (i)

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.

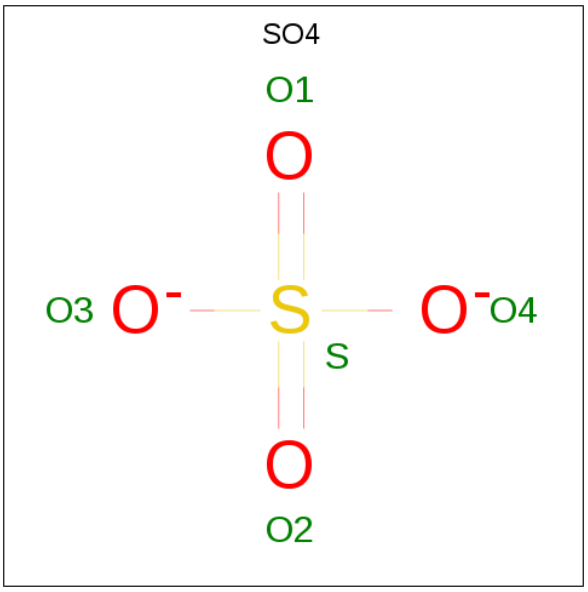
- Molecule 1 is a protein called 3-METHYLASPARTATE AMMONIA-LYASE.

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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

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

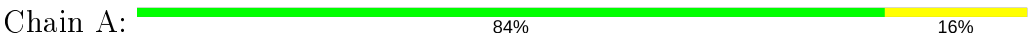
3 Residue-property plots (i)

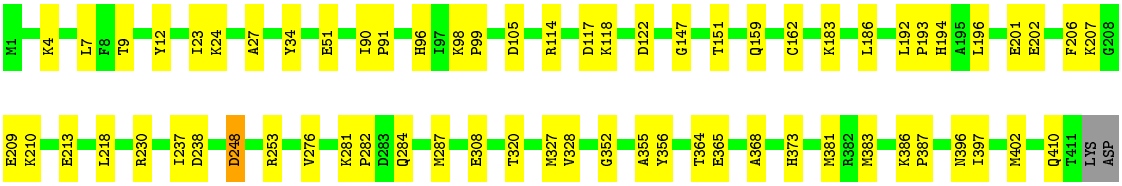
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: 3-METHYLASPARTATE AMMONIA-LYASE

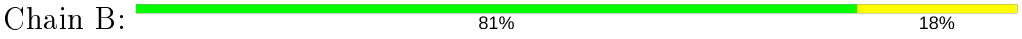
Chain A:

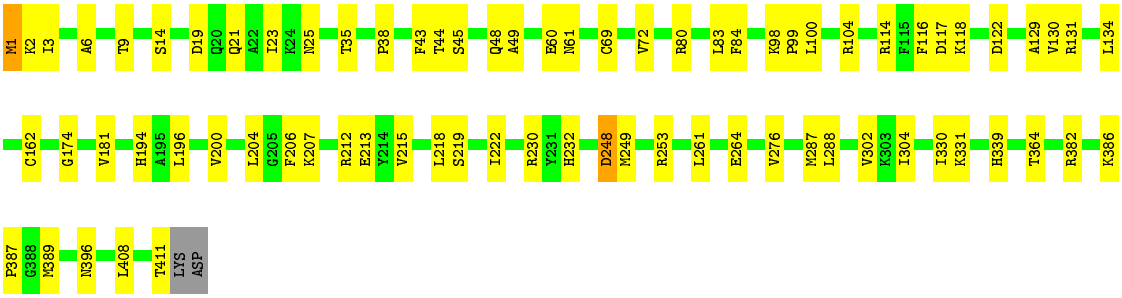




- Molecule 1: 3-METHYLASPARTATE AMMONIA-LYASE

Chain B:





4 Data and refinement statistics (i)

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

5.1 Standard geometry

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	0.41	0/3220	0.74	3/4354 (0.1%)
1	B	0.42	0/3215	0.76	4/4350 (0.1%)
All	All	0.41	0/6435	0.75	7/8704 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	248	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	122	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	248	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	382	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	105	ASP	CB-CG-OD2	5.21	122.99	118.30

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	3164	0	3132	86	0
1	B	3158	0	3113	109	0
2	A	5	0	0	0	0
3	A	1089	0	0	62	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1114	0	0	66	6
All	All	8530	0	6245	193	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 15.

The worst 5 of 193 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

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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

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 carbohydrates 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	0.59	0	6,6,6	0.54	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.