



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:19 am BST

PDB ID : 1QIT
Title : ASPARTATE AMINOTRANSFERASE FROM ESCHERICHIA COLI,
C191W MUTATION, WITH BOUND MALEATE
Authors : Jeffery, C.J.; Gloss, L.M.; Petsko, G.A.; Ringe, D.
Deposited on : 1999-06-15
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) 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

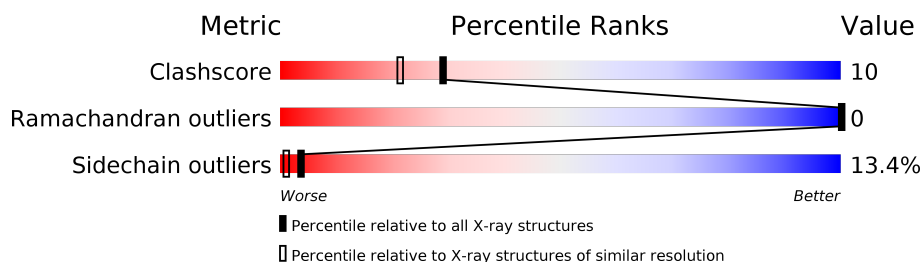
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	 76% 20% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3217 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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3077	1944	537	584	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

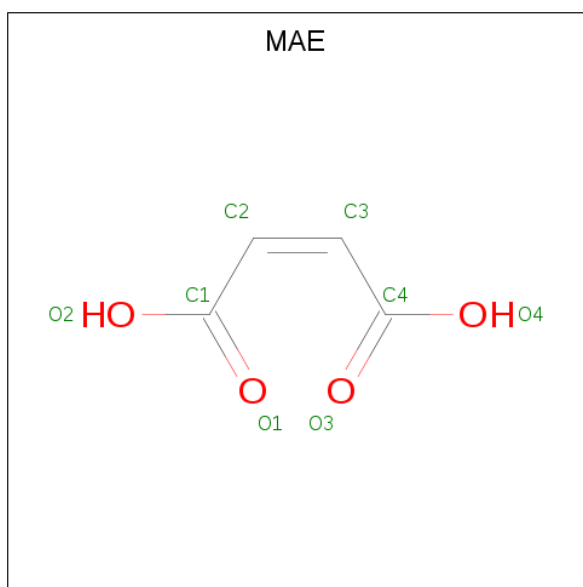
Chain	Residue	Modelled	Actual	Comment	Reference
A	191	TRP	CYS	engineered mutation	UNP P00509

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is water.

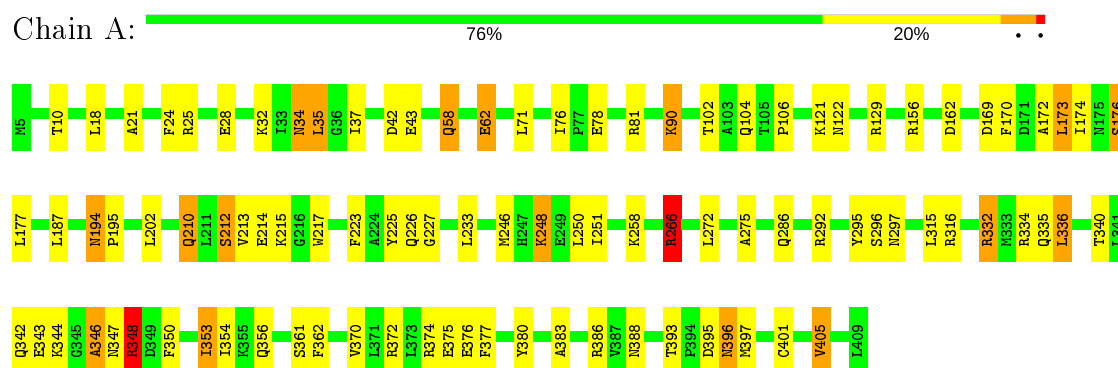
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		

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: ASPARTATE AMINOTRANSFERASE



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 21	Depositor
Cell constants a, b, c, α , β , γ	157.45Å 85.05Å 78.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	80.0 (10.00-1.90)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3217	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: MAE, PLP

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	0.60	0/3140	0.96	7/4255 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	266	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	A	173	LEU	CA-CB-CG	7.47	132.48	115.30
1	A	266	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	348	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	35	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	346	ALA	N-CA-C	-5.65	95.74	111.00
1	A	250	LEU	CA-CB-CG	5.50	127.95	115.30

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	3077	0	3021	59	0
2	A	15	0	7	1	0
3	A	8	0	2	0	0
4	A	117	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3217	0	3030	59	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 10.

All (59) 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:233:LEU:HA	4:A:2077:HOH:O	1.71	0.89
1:A:346:ALA:HB2	1:A:405:VAL:HG12	1.58	0.85
1:A:348:ARG:HG3	1:A:348:ARG:HH11	1.42	0.83
1:A:233:LEU:HD23	4:A:2077:HOH:O	1.80	0.82
1:A:78:GLU:HG3	1:A:81:ARG:HH12	1.47	0.78
1:A:121:LYS:HG3	1:A:122:ASN:ND2	2.08	0.69
1:A:34:ASN:O	1:A:380:TYR:O	2.11	0.68
1:A:356:GLN:NE2	1:A:361:SER:HA	2.10	0.66
1:A:194:ASN:HD21	1:A:386:ARG:HH11	1.43	0.66
1:A:78:GLU:HG3	1:A:81:ARG:NH1	2.10	0.66
1:A:266:ARG:HH22	2:A:410:PLP:P	2.20	0.65
1:A:226:GLN:HG2	4:A:2077:HOH:O	1.97	0.64
1:A:401:CYS:O	1:A:405:VAL:HG13	2.00	0.62
1:A:350:PHE:O	1:A:353:ILE:HG23	1.99	0.62
1:A:18:LEU:HD23	1:A:37:ILE:HD12	1.82	0.62
1:A:210:GLN:O	1:A:213:VAL:HG12	2.01	0.61
1:A:376:GLU:HG2	1:A:377:PHE:CE1	2.37	0.60
1:A:90:LYS:H	1:A:90:LYS:CD	2.14	0.60
1:A:374:ARG:HD2	1:A:380:TYR:CE2	2.38	0.58
1:A:121:LYS:NZ	1:A:122:ASN:HD21	2.02	0.57
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.88	0.55
1:A:212:SER:HA	1:A:217:TRP:CE3	2.44	0.53
1:A:396:ASN:HD22	1:A:396:ASN:C	2.12	0.52
1:A:393:THR:H	1:A:396:ASN:ND2	2.08	0.51
1:A:121:LYS:CG	1:A:122:ASN:ND2	2.74	0.51
1:A:76:ILE:H	1:A:104:GLN:NE2	2.08	0.50
1:A:227:GLY:N	4:A:2077:HOH:O	2.45	0.49
1:A:35:LEU:HA	1:A:388:ASN:HB3	1.94	0.49
1:A:58:GLN:O	1:A:62:GLU:HG2	2.12	0.49
1:A:374:ARG:HD3	4:A:2113:HOH:O	2.12	0.49
1:A:348:ARG:CG	1:A:348:ARG:HH11	2.17	0.49
1:A:43:GLU:CD	1:A:43:GLU:H	2.15	0.48
1:A:225:TYR:CE1	1:A:258:LYS:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HG2	1:A:275:ALA:CB	2.44	0.48
1:A:348:ARG:NH1	1:A:348:ARG:HG3	2.18	0.48
1:A:121:LYS:HZ3	1:A:122:ASN:HD21	1.63	0.47
1:A:248:LYS:HG2	1:A:275:ALA:HB2	1.96	0.47
1:A:336:LEU:CD2	1:A:397:MET:HG2	2.46	0.46
1:A:225:TYR:CZ	1:A:258:LYS:HD3	2.51	0.46
1:A:393:THR:H	1:A:396:ASN:HD21	1.64	0.46
1:A:194:ASN:HD21	1:A:386:ARG:NH1	2.11	0.46
1:A:42:ASP:HB2	1:A:43:GLU:OE2	2.16	0.45
1:A:172:ALA:O	1:A:176:SER:HB2	2.15	0.45
1:A:24:PHE:HD1	1:A:380:TYR:CD1	2.34	0.45
1:A:335:GLN:HA	1:A:354:ILE:HD11	1.98	0.45
1:A:106:PRO:HD3	1:A:295:TYR:CZ	2.52	0.45
1:A:90:LYS:H	1:A:90:LYS:HE2	1.81	0.45
1:A:340:THR:O	1:A:344:LYS:HG2	2.17	0.44
1:A:356:GLN:HE21	1:A:361:SER:HA	1.83	0.44
1:A:121:LYS:NZ	1:A:286:GLN:HE21	2.15	0.44
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.77	0.43
1:A:162:ASP:HB2	1:A:169:ASP:HB2	2.00	0.43
1:A:90:LYS:CE	1:A:90:LYS:H	2.32	0.42
1:A:21:ALA:O	1:A:25:ARG:HG2	2.19	0.42
1:A:336:LEU:HD23	1:A:397:MET:HG2	2.01	0.42
1:A:210:GLN:O	1:A:214:GLU:HB2	2.20	0.41
1:A:332:ARG:HD3	4:A:2044:HOH:O	2.21	0.40
1:A:170:PHE:O	1:A:174:ILE:HG12	2.22	0.40
1:A:292:ARG:HA	1:A:296:SER:HA	2.03	0.40

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	394/396 (100%)	379 (96%)	15 (4%)	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	320/320 (100%)	277 (87%)	43 (13%)	4	1

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	28	GLU
1	A	32	LYS
1	A	34	ASN
1	A	58	GLN
1	A	62	GLU
1	A	71	LEU
1	A	90	LYS
1	A	102	THR
1	A	129	ARG
1	A	156	ARG
1	A	173	LEU
1	A	176	SER
1	A	187	LEU
1	A	194	ASN
1	A	195	PRO
1	A	202	LEU
1	A	210	GLN
1	A	212	SER
1	A	215	LYS
1	A	223	PHE
1	A	246	MET
1	A	248	LYS

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Mol	Chain	Res	Type
1	A	251	ILE
1	A	266	ARG
1	A	272	LEU
1	A	297	ASN
1	A	315	LEU
1	A	316	ARG
1	A	332	ARG
1	A	334	ARG
1	A	336	LEU
1	A	342	GLN
1	A	343	GLU
1	A	347	ASN
1	A	348	ARG
1	A	353	ILE
1	A	362	PHE
1	A	372	ARG
1	A	375	GLU
1	A	395	ASP
1	A	396	ASN
1	A	405	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	34	ASN
1	A	58	GLN
1	A	63	ASN
1	A	96	ASN
1	A	104	GLN
1	A	122	ASN
1	A	175	ASN
1	A	178	ASN
1	A	194	ASN
1	A	210	GLN
1	A	226	GLN
1	A	286	GLN
1	A	297	ASN
1	A	328	GLN
1	A	339	ASN
1	A	356	GLN
1	A	396	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](#)

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](#)

2 ligands 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	$\# Z > 2$
2	PLP	A	410	1	15,15,16	1.97	3 (20%)	20,22,23	2.19	4 (20%)
3	MAE	A	411	-	1,7,7	0.80	0	2,8,8	1.06	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
2	PLP	A	410	1	-	0/6/6/8	0/1/1/1
3	MAE	A	411	-	-	0/0/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	PLP	C3-C2	-5.80	1.35	1.40
2	A	410	PLP	C5-C4	-2.46	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	PLP	C2A-C2	2.33	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	410	PLP	O4P-C5A-C5	6.59	121.91	109.35
2	A	410	PLP	C5-C6-N1	-3.36	118.23	123.82
2	A	410	PLP	C6-C5-C4	3.30	120.76	118.16
2	A	410	PLP	O2P-P-O4P	-3.28	97.99	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	410	PLP	1	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 ⓘ

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.