



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2022 – 06:05 PM EDT

PDB ID : 8E9S
Title : Crystal structure of E. coli aspartate aminotransferase mutant VFCS bound to maleic acid at 278 K
Authors : Chica, R.A.; St-Jacques, A.D.; Rodriguez, J.M.; Thompson, M.C.
Deposited on : 2022-08-26
Resolution : 2.00 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 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

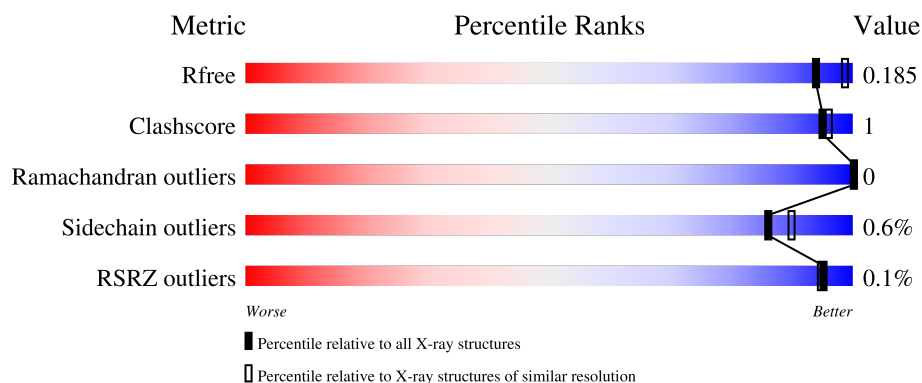
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

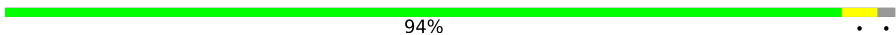
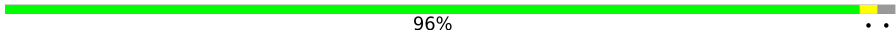
The reported resolution of this entry is 2.00 Å.

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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	406	 94%
1	B	406	 96%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12525 atoms, of which 5961 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
1	A	399	Total	C	H	N	O	S	0	3	0
			6068	1948	2979	537	591	13			
1	B	399	Total	C	H	N	O	S	0	9	0
			6050	1944	2964	536	593	13			

There are 28 discrepancies between the modelled and reference sequences:

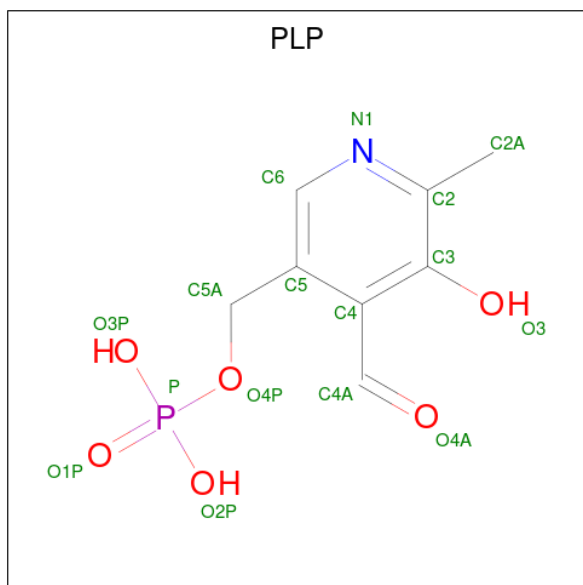
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP P00509
A	-8	ALA	-	expression tag	UNP P00509
A	-7	HIS	-	expression tag	UNP P00509
A	-6	HIS	-	expression tag	UNP P00509
A	-5	HIS	-	expression tag	UNP P00509
A	-4	HIS	-	expression tag	UNP P00509
A	-3	HIS	-	expression tag	UNP P00509
A	-2	HIS	-	expression tag	UNP P00509
A	-1	VAL	-	expression tag	UNP P00509
A	0	GLY	-	expression tag	UNP P00509
A	1	THR	-	expression tag	UNP P00509
A	37	PHE	LYS	engineered mutation	UNP P00509
A	43	CYS	THR	engineered mutation	UNP P00509
A	64	SER	ASN	engineered mutation	UNP P00509
B	-9	MET	-	initiating methionine	UNP P00509
B	-8	ALA	-	expression tag	UNP P00509
B	-7	HIS	-	expression tag	UNP P00509
B	-6	HIS	-	expression tag	UNP P00509
B	-5	HIS	-	expression tag	UNP P00509
B	-4	HIS	-	expression tag	UNP P00509
B	-3	HIS	-	expression tag	UNP P00509
B	-2	HIS	-	expression tag	UNP P00509
B	-1	VAL	-	expression tag	UNP P00509
B	0	GLY	-	expression tag	UNP P00509
B	1	THR	-	expression tag	UNP P00509

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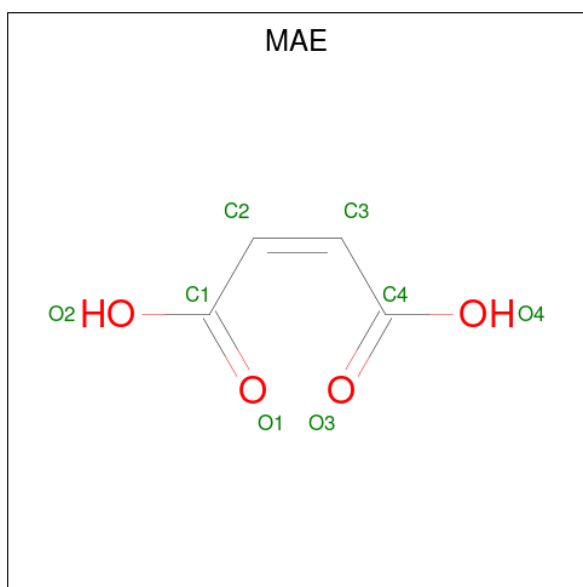
Chain	Residue	Modelled	Actual	Comment	Reference
B	37	PHE	LYS	engineered mutation	UNP P00509
B	43	CYS	THR	engineered mutation	UNP P00509
B	64	SER	ASN	engineered mutation	UNP P00509

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			22	8	7	1	5	1		
2	B	1	Total	C	H	N	O	P	0	0
			22	8	7	1	5	1		

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	4	2	4		
3	B	1	Total	C	H	O	0	0
			10	4	2	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	183	Total	O	0	0
			183	183		
4	B	160	Total	O	0	0
			160	160		

- Molecule 1: Aspartate aminotransferase



- Chain B:  96%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	143.83Å 143.83Å 81.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	124.49 – 2.00 124.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (124.49-2.00) 99.3 (124.56-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.148 , 0.185 0.148 , 0.185	Depositor DCC
R_{free} test set	6537 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.040 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12525	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

5.1 Standard geometry

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	0.33	0/3158	0.56	0/4285
1	B	0.32	0/3194	0.54	0/4339
All	All	0.32	0/6352	0.55	0/8624

There are no bond length outliers.

There are no bond angle outliers.

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	3089	2979	2996	10	0
1	B	3086	2964	2930	5	0
2	A	15	7	7	1	0
2	B	15	7	7	0	0
3	A	8	2	2	0	0
3	B	8	2	2	0	0
4	A	183	0	0	0	0
4	B	160	0	0	2	0
All	All	6564	5961	5944	15	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 1.

All (15) 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:39:GLU:OE2	4:B:501:HOH:O	2.10	0.68
1:B:18:ASP:OD1	1:B:21:ARG:NH2	2.38	0.57
1:A:-1:VAL:HG13	1:A:0:GLY:H	1.74	0.52
1:A:-1:VAL:HG13	1:A:0:GLY:N	2.25	0.52
1:A:76:ARG:NH2	1:A:80:GLU:OE2	2.44	0.51
1:B:159:PHE:CE2	1:B:163:ILE:HD11	2.46	0.50
1:A:199:GLN:HA	1:A:234:MET:HE1	1.95	0.48
1:A:149:TYR:O	1:A:157:LEU:HD12	2.16	0.46
1:A:280:ARG:HA	1:A:284:SER:HA	2.01	0.42
1:A:362:ARG:HG3	1:A:368:TYR:CE2	2.54	0.42
1:B:388:LEU:HD23	1:B:388:LEU:C	2.41	0.41
1:A:386:ALA:HB3	1:A:387:PRO:HD3	2.02	0.41
1:B:39:GLU:HG3	4:B:629:HOH:O	2.20	0.41
1:A:89:LEU:HD11	1:A:232:ALA:HB1	2.03	0.40
1:A:211:ASP:OD2	2:A:401:PLP:N1	2.54	0.40

There are no symmetry-related clashes.

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	400/406 (98%)	392 (98%)	8 (2%)	0	100	100
1	B	406/406 (100%)	398 (98%)	8 (2%)	0	100	100
All	All	806/812 (99%)	790 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	321/328 (98%)	320 (100%)	1 (0%)	92	95
1	B	322/328 (98%)	319 (99%)	3 (1%)	78	83
All	All	643/656 (98%)	639 (99%)	4 (1%)	86	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	PHE
1	B	209	LEU
1	B	212	PHE
1	B	350	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	401	1	15,15,16	0.87	0	20,22,23	1.15	2 (10%)
3	MAE	A	402	-	7,7,7	1.62	1 (14%)	8,8,8	0.73	0
2	PLP	B	401	1	15,15,16	0.94	1 (6%)	20,22,23	1.17	1 (5%)
3	MAE	B	402	-	7,7,7	1.48	1 (14%)	8,8,8	0.86	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	401	1	-	2/6/6/8	0/1/1/1
3	MAE	A	402	-	-	2/5/5/5	-
2	PLP	B	401	1	-	1/6/6/8	0/1/1/1
3	MAE	B	402	-	-	2/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	MAE	C3-C4	2.38	1.53	1.48
2	B	401	PLP	C2-N1	2.20	1.38	1.33
3	B	402	MAE	C3-C4	2.11	1.53	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PLP	O4P-C5A-C5	3.08	115.22	109.35
2	A	401	PLP	C5A-C5-C6	-2.35	115.51	119.37
2	A	401	PLP	O4P-C5A-C5	2.28	113.69	109.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PLP	C5A-O4P-P-O2P
2	A	401	PLP	C5A-O4P-P-O3P
3	A	402	MAE	O2-C1-C2-C3
3	B	402	MAE	O1-C1-C2-C3
3	A	402	MAE	O1-C1-C2-C3
3	B	402	MAE	O2-C1-C2-C3
2	B	401	PLP	C5A-O4P-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	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 [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	399/406 (98%)	-0.51	0	100 100	18, 28, 57, 88	0
1	B	399/406 (98%)	-0.49	1 (0%)	94 93	16, 33, 63, 98	0
All	All	798/812 (98%)	-0.50	1 (0%)	95 95	16, 30, 59, 98	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	VAL	2.9

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 monosaccharides 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(Å ²)	Q<0.9
2	PLP	B	401	15/16	0.98	0.10	15,22,27,30	0
3	MAE	A	402	8/8	0.98	0.11	19,22,29,30	0
3	MAE	B	402	8/8	0.98	0.10	19,21,26,27	0
2	PLP	A	401	15/16	0.99	0.11	12,20,25,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.