WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 08:35 AM EST

PDB ID	:	1AW8
Title	:	PYRUVOYL DEPENDENT ASPARTATE DECARBOXYLASE
Authors	:	Albert, A.; Dhanaraj, V.; Genschel, U.; Khan, G.; Ramjee, M.K.; Pulido, R.; Sybanda, B.L.; von Delf, F.; Witty, M.; Blundell, T.L.; Smith, A.G.; Abell, C.
Deposited on	:	1997-10-12
Resolution	:	2.20 Å(reported)

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

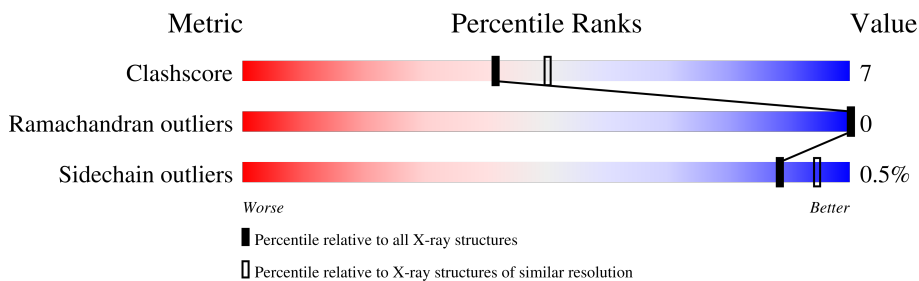|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0.5%

Worse ⟷ *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	24	67% 21% 12%
1	D	24	92% 8%
2	B	92	85% 15%
2	E	92	88% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1917 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 L-ASPARTATE-ALPHA-DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	24	Total	C	N	O	S	0	4	0
			232	146	45	39	2			
1	D	24	Total	C	N	O	S	0	0	0
			197	124	39	32	2			

- Molecule 2 is a protein called L-ASPARTATE-ALPHA-DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	S	0	1	0
			698	435	119	140	4			
2	E	91	Total	C	N	O	S	0	0	0
			692	432	118	138	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	PYR	SER	microheterogeneity	UNP P0A790
E	25	PYR	SER	conflict	UNP P0A790

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	34	Total	O	0	0
			34	34		
3	D	9	Total	O	0	0
			9	9		
3	E	45	Total	O	0	0
			45	45		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: L-ASPARTATE-ALPHA-DECARBOXYLASE

Chain A:

67%　　　　　　21%　　12%

M1 I2 Q7 H11 L20 H21 Y22 E23 G24

• Molecule 1: L-ASPARTATE-ALPHA-DECARBOXYLASE

Chain D:

92%　　　　　　8%

M1 H17 E23 G24

• Molecule 2: L-ASPARTATE-ALPHA-DECARBOXYLASE

Chain B:

85%　　　　　　15%

PYR25 S25 C26 E40 N41 Y58 A59 I60 E63 S66 S70 V71 N72 A76 H77 T92 E97 N104 K115

• Molecule 2: L-ASPARTATE-ALPHA-DECARBOXYLASE

Chain E:

88%　　　　　　12%

PYR25 S25 C26 Q30 D31 F32 E40 N41 R64 S70 T92 D95 E96 R99 K115
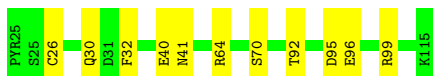
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	72.17Å 72.17Å 216.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	97.0 (8.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.200 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1917	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: PYR

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	1.81	2/236 (0.8%)	1.50	8/313 (2.6%)
1	D	0.35	0/200	0.66	0/266
2	B	0.38	0/705	0.65	0/957
2	E	0.33	0/699	0.61	0/949
All	All	0.73	2/1840 (0.1%)	0.80	8/2485 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23[A]	GLU	C-N	-17.70	1.01	1.33
1	A	23[B]	GLU	C-N	-17.70	1.01	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24[A]	GLY	N-CA-C	8.79	135.07	113.10
1	A	24[B]	GLY	N-CA-C	8.79	135.07	113.10
1	A	23[A]	GLU	C-N-CA	6.99	136.99	122.30
1	A	23[B]	GLU	C-N-CA	6.99	136.99	122.30
1	A	21[A]	HIS	N-CA-C	6.16	127.63	111.00
1	A	21[B]	HIS	N-CA-C	6.16	127.63	111.00
1	A	24[A]	GLY	CA-C-O	6.14	131.66	120.60
1	A	24[B]	GLY	CA-C-O	6.14	131.66	120.60

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	232	0	231	11	0
1	D	197	0	207	2	0
2	B	698	0	657	12	0
2	E	692	0	655	8	0
3	A	10	0	0	0	0
3	B	34	0	0	1	0
3	D	9	0	0	0	0
3	E	45	0	0	1	0
All	All	1917	0	1750	23	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 7.

All (23) 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:22[A]:TYR:CG	1:A:23[A]:GLU:N	2.67	0.63
1:A:11:HIS:NE2	1:D:23:GLU:HA	2.14	0.62
1:A:20:LEU:HD22	2:B:76:ALA:HB3	1.80	0.62
2:B:26:CYS:HA	2:B:70:SER:O	2.01	0.59
1:A:20:LEU:HD22	2:B:76:ALA:CB	2.33	0.59
1:A:22[B]:TYR:CB	2:B:72:ASN:HB3	2.39	0.53
2:E:96:GLU:HG3	3:E:1007:HOH:O	2.09	0.53
1:A:2:ILE:HB	2:E:92:THR:OG1	2.12	0.49
2:E:95:ASP:O	2:E:99:ARG:HG2	2.15	0.47
2:E:30:GLN:HB3	2:E:64:ARG:HG2	1.97	0.46
1:A:20:LEU:HD11	2:B:77:HIS:NE2	2.30	0.45
1:A:2:ILE:CG2	2:B:92:THR:HB	2.47	0.45
2:B:97:GLU:HB2	3:B:1044:HOH:O	2.17	0.44
2:E:26:CYS:HA	2:E:70:SER:O	2.17	0.43
1:D:17:HIS:O	2:E:70:SER:HA	2.19	0.43
1:A:7:GLN:NE2	2:B:104:ASN:HD22	2.15	0.43
1:A:21[A]:HIS:O	1:A:22[A]:TYR:CB	2.67	0.43
1:A:23[A]:GLU:HB3	2:B:72:ASN:ND2	2.35	0.41
2:B:40:GLU:O	2:B:41:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:GLU:HG3	2:B:66:SER:HB3	2.02	0.41
2:B:58:TYR:HE2	2:B:60:ILE:HD11	1.85	0.41
2:E:32:PHE:N	2:E:32:PHE:CD1	2.89	0.41
2:E:40:GLU:O	2:E:41:ASN:HB2	2.20	0.41

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	25/24 (104%)	25 (100%)	0	0	100	100
1	D	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
2	B	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
2	E	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
All	All	225/232 (97%)	219 (97%)	6 (3%)	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	24/21 (114%)	23 (96%)	1 (4%)	30	38
1	D	21/21 (100%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	71/71 (100%)	71 (100%)	0	100	100
2	E	70/71 (99%)	70 (100%)	0	100	100
All	All	186/184 (101%)	185 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	D	7	GLN
1	D	17	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	23[A]:GLU	C	24[A]:GLY	N	1.01

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.