



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 06:47 pm BST

PDB ID : 1YAA
Title : ASPARTATE AMINOTRANSFERASE FROM SACCHAROMYCES CEREVISIAE CYTOPLASM
Authors : Jeffery, C.J.
Deposited on : 1998-01-27
Resolution : 2.05 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 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

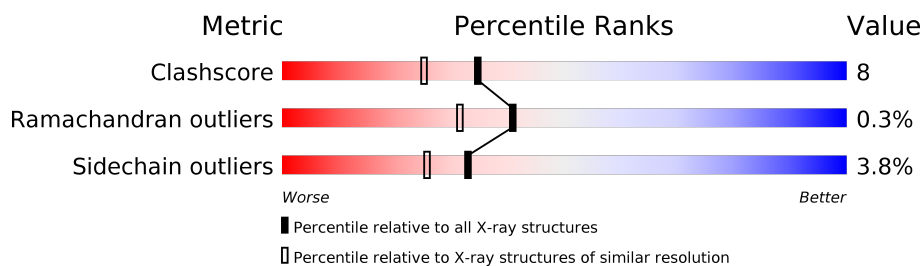
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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	412	
1	B	412	
1	C	412	
1	D	412	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13596 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.

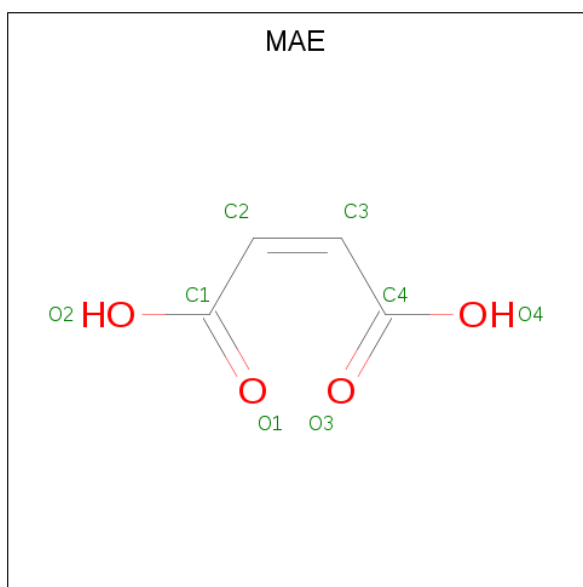
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3197	2039	550	597	11			
1	B	412	Total	C	N	O	S	0	0	0
			3197	2039	550	597	11			
1	C	412	Total	C	N	O	S	0	0	0
			3197	2039	550	597	11			
1	D	412	Total	C	N	O	S	0	0	0
			3197	2039	550	597	11			

There are 4 discrepancies between the modelled and reference sequences:

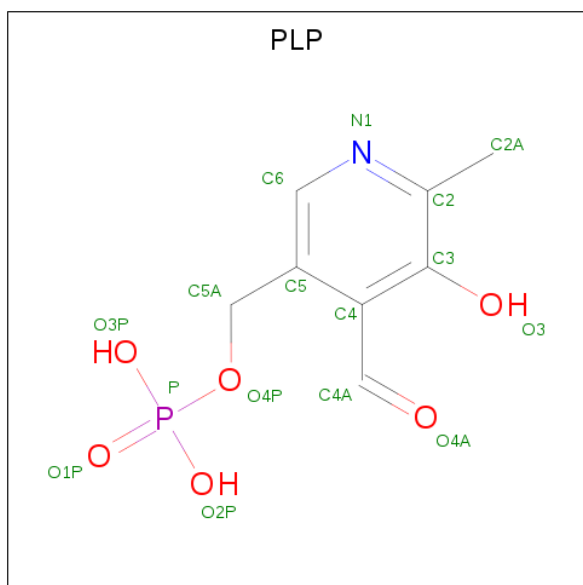
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	LEU	PHE	CONFLICT	UNP P23542
B	95	LEU	PHE	CONFLICT	UNP P23542
C	95	LEU	PHE	CONFLICT	UNP P23542
D	95	LEU	PHE	CONFLICT	UNP P23542

- Molecule 2 is MALEIC ACID (three-letter code: MAE) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	4	4		
2	B	1	Total	C	O	0	0
			8	4	4		
2	C	1	Total	C	O	0	0
			8	4	4		
2	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



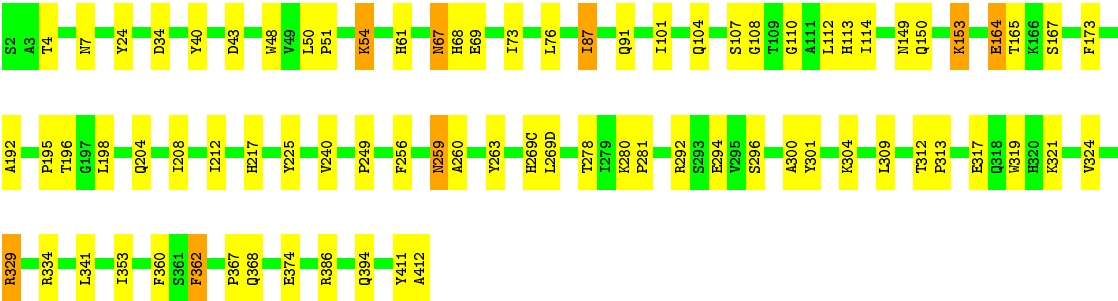
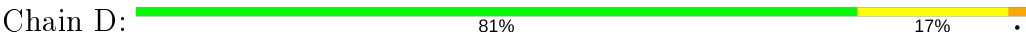
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		
4	B	183	Total	O	0	0
			183	183		
4	C	190	Total	O	0	0
			190	190		
4	D	180	Total	O	0	0
			180	180		



● 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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.31Å 134.63Å 98.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05	Depositor
% Data completeness (in resolution range)	93.0 (10.00-2.05)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.231 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13596	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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	0.37	1/3271 (0.0%)	0.59	0/4439
1	B	0.32	0/3271	0.72	7/4439 (0.2%)
1	C	0.33	0/3271	0.62	3/4439 (0.1%)
1	D	0.32	0/3271	0.61	0/4439
All	All	0.34	1/13084 (0.0%)	0.64	10/17756 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	LYS	CD-CE	10.23	1.76	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	LYS	C-N-CD	-20.74	74.98	120.60
1	B	137	LYS	C-N-CA	9.14	160.38	122.00
1	B	137	LYS	N-CA-C	-9.04	86.61	111.00
1	B	194	ASN	N-CA-C	-7.57	90.55	111.00
1	C	194	ASN	C-N-CD	-7.31	104.51	120.60

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	3197	0	3182	60	0
1	B	3197	0	3182	60	0
1	C	3197	0	3182	54	0
1	D	3197	0	3181	48	0
2	A	8	0	2	0	0
2	B	8	0	2	0	0
2	C	8	0	2	0	0
2	D	8	0	2	0	0
3	A	15	0	6	2	0
3	B	15	0	6	3	0
3	C	15	0	6	3	0
3	D	15	0	6	1	0
4	A	163	0	0	1	0
4	B	183	0	0	3	0
4	C	190	0	0	2	0
4	D	180	0	0	4	0
All	All	13596	0	12759	213	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 8.

The worst 5 of 213 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:258:LYS:CE	1:A:258:LYS:CD	1.76	1.61
1:A:280:LYS:HB3	1:A:281:PRO:HD3	1.69	0.74
1:B:20:ILE:HG22	1:B:23:ARG:HH22	1.51	0.73
1:B:393:ASN:O	1:B:397:VAL:HG23	1.89	0.72
1:A:244:LEU:HA	1:A:247:VAL:HG13	1.71	0.72

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	410/412 (100%)	393 (96%)	16 (4%)	1 (0%)	47	39
1	B	410/412 (100%)	393 (96%)	15 (4%)	2 (0%)	29	18
1	C	410/412 (100%)	393 (96%)	16 (4%)	1 (0%)	47	39
1	D	410/412 (100%)	403 (98%)	6 (2%)	1 (0%)	47	39
All	All	1640/1648 (100%)	1582 (96%)	53 (3%)	5 (0%)	41	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	138	PRO
1	C	263	TYR
1	D	263	TYR
1	B	263	TYR

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	342/342 (100%)	328 (96%)	14 (4%)	30	23
1	B	342/342 (100%)	333 (97%)	9 (3%)	46	39
1	C	342/342 (100%)	327 (96%)	15 (4%)	28	21
1	D	342/342 (100%)	328 (96%)	14 (4%)	30	23
All	All	1368/1368 (100%)	1316 (96%)	52 (4%)	33	26

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	17	LEU
1	C	153	LYS
1	D	329	ARG
1	C	32	LYS
1	C	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	368	GLN
1	C	113	HIS
1	D	349	ASN
1	C	22	GLN
1	C	142	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	MAE	B	902	-	1,7,7	0.47	0	2,8,8	3.00	2 (100%)
2	MAE	A	901	-	1,7,7	0.23	0	2,8,8	2.52	2 (100%)
3	PLP	C	907	1	15,15,16	2.11	2 (13%)	20,22,23	1.70	4 (20%)
3	PLP	D	908	1	15,15,16	1.82	4 (26%)	20,22,23	1.92	5 (25%)
2	MAE	D	904	-	1,7,7	0.49	0	2,8,8	2.74	2 (100%)
3	PLP	B	906	1	15,15,16	2.21	2 (13%)	20,22,23	2.15	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAE	C	903	-	1,7,7	0.25	0	2,8,8	2.35	2 (100%)
3	PLP	A	905	1	15,15,16	2.48	3 (20%)	20,22,23	2.00	6 (30%)

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	MAE	B	902	-	-	0/0/5/5	-
2	MAE	A	901	-	-	0/0/5/5	-
3	PLP	C	907	1	-	2/6/6/8	0/1/1/1
3	PLP	D	908	1	-	2/6/6/8	0/1/1/1
2	MAE	D	904	-	-	0/0/5/5	-
3	PLP	B	906	1	-	2/6/6/8	0/1/1/1
2	MAE	C	903	-	-	0/0/5/5	-
3	PLP	A	905	1	-	2/6/6/8	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	905	PLP	C4A-C4	-8.23	1.34	1.51
3	B	906	PLP	C3-C2	-7.03	1.33	1.40
3	C	907	PLP	C3-C2	-6.33	1.34	1.40
3	D	908	PLP	C3-C2	-3.83	1.37	1.40
3	D	908	PLP	C4A-C4	2.82	1.57	1.51

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	906	PLP	O4P-C5A-C5	6.10	120.97	109.35
3	D	908	PLP	O4P-C5A-C5	5.94	120.68	109.35
3	A	905	PLP	C6-C5-C4	4.89	122.01	118.16
3	A	905	PLP	O4P-C5A-C5	4.89	118.66	109.35
3	C	907	PLP	O4P-C5A-C5	4.57	118.07	109.35

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	907	PLP	C4-C5-C5A-O4P
3	C	907	PLP	C6-C5-C5A-O4P
3	D	908	PLP	C4-C5-C5A-O4P
3	D	908	PLP	C6-C5-C5A-O4P
3	B	906	PLP	C4-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	907	PLP	3	0
3	D	908	PLP	1	0
3	B	906	PLP	3	0
3	A	905	PLP	2	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.