



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 1AHF / pdb_00001ahf
Title : ASPARTATE AMINOTRANSFERASE HEXAMUTANT
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Deposited on : 1995-02-22
Resolution : 2.30 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

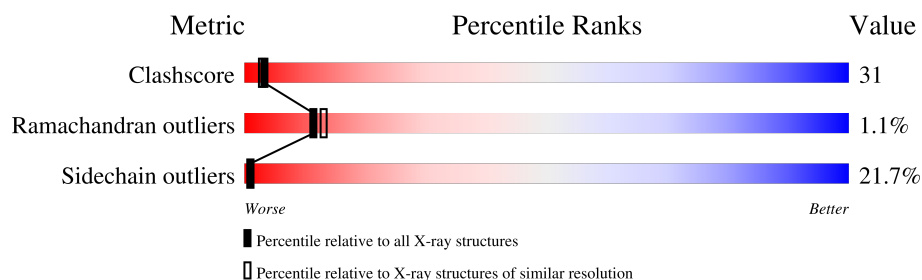
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	47% 36% 16% .
1	B	396	47% 41% 11% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOP	A	411	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6593 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.

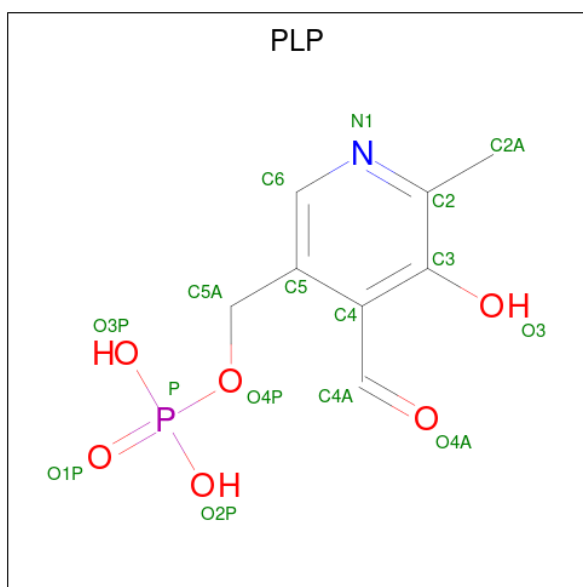
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3071	1942	533	583	13			
1	B	396	Total	C	N	O	S	0	0	0
			3071	1942	533	583	13			

There are 12 discrepancies between the modelled and reference sequences:

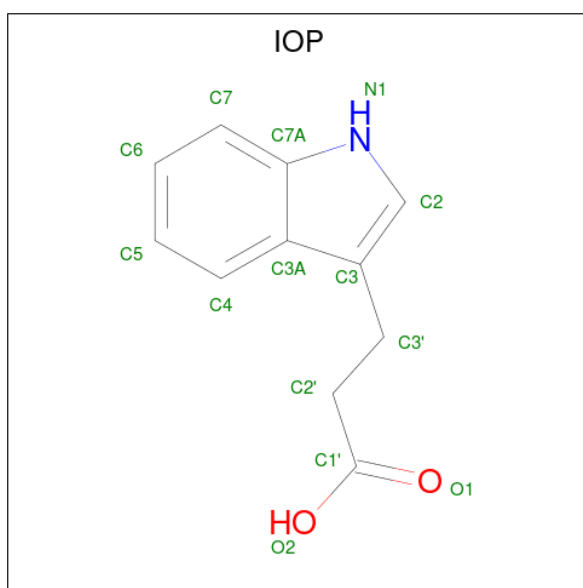
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	VAL	conflict	UNP P00509
A	41	TYR	LYS	conflict	UNP P00509
A	47	ILE	THR	conflict	UNP P00509
A	69	LEU	ASN	conflict	UNP P00509
A	109	SER	THR	conflict	UNP P00509
A	297	SER	ASN	conflict	UNP P00509
B	39	LEU	VAL	conflict	UNP P00509
B	41	TYR	LYS	conflict	UNP P00509
B	47	ILE	THR	conflict	UNP P00509
B	69	LEU	ASN	conflict	UNP P00509
B	109	SER	THR	conflict	UNP P00509
B	297	SER	ASN	conflict	UNP P00509

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 3 is INDOLYLPROPIONIC ACID (CCD ID: IOP) (formula: $C_{11}H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	11	1	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is water.

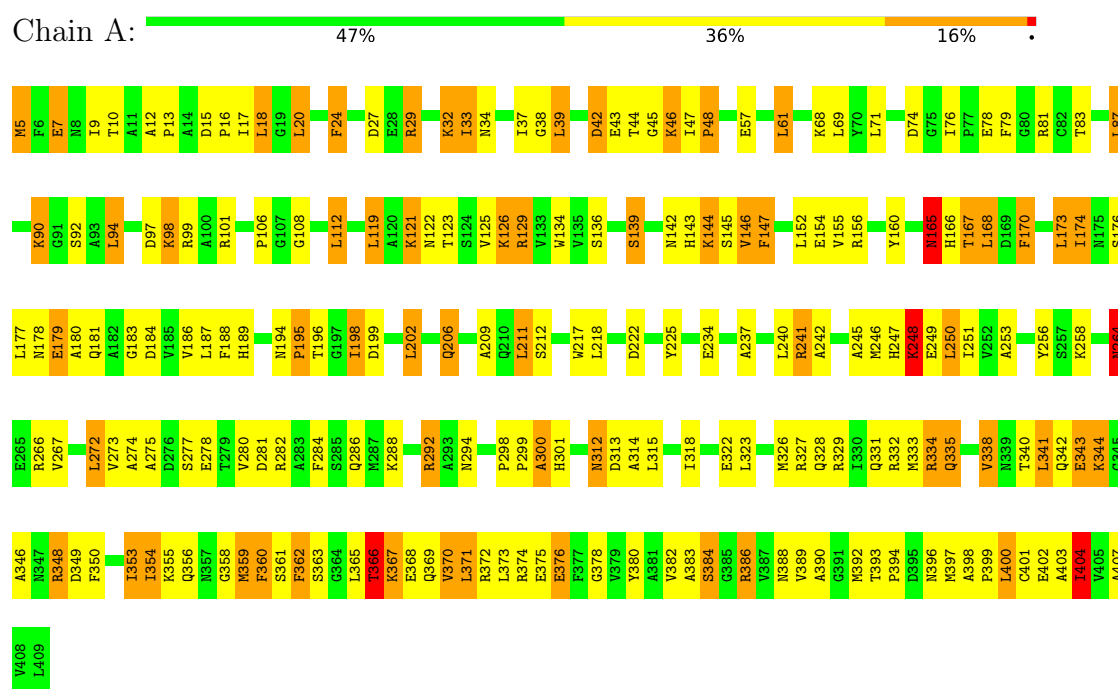
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	187	Total	O	0	0
			187	187		

3 Residue-property plots

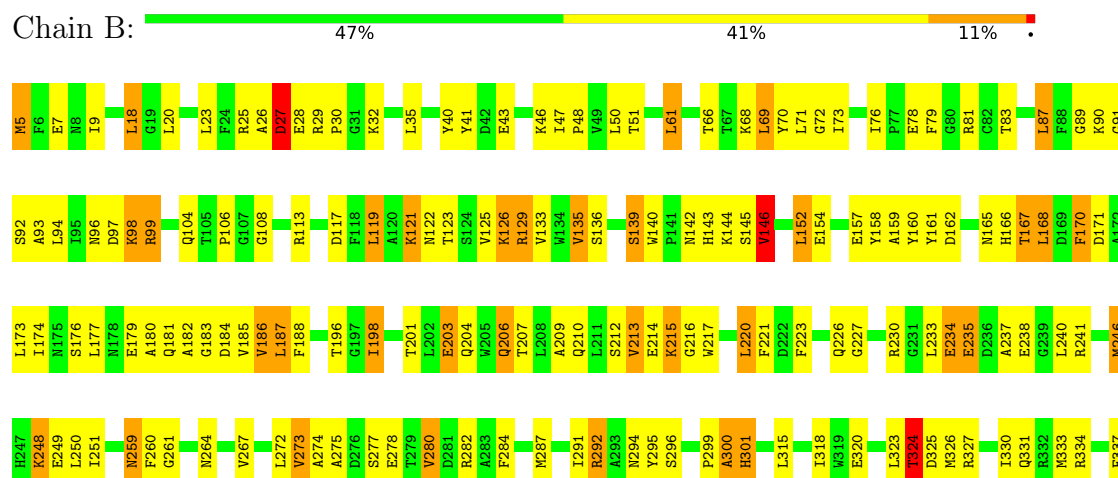
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ASPARTATE AMINOTRANSFERASE



V338		L341		M347		I353		S361		V370		Y380		M397		V408
		Q342		R348		I354		F362		L371		A381		A398		L409
		E343		D349		K355		T366		R372		V382		P399		
		K344		F350		Q356		K367		L373		A383		L400		
						N357				R374		S384		C401		
										E375		G385		E402		
										E376		R386		A403		
										F377		V387		I404		
												N388				
												V389				
												A390				
												G391				
												M392				

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.92Å 79.39Å 88.80Å 90.00° 118.99° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.0 (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.232 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: IOP, SO4, 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	1.17	1/3133 (0.0%)	1.61	32/4244 (0.8%)
1	B	1.24	3/3133 (0.1%)	1.64	31/4244 (0.7%)
All	All	1.20	4/6266 (0.1%)	1.63	63/8488 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	GLY	C-N	-14.95	1.12	1.33
1	B	92	SER	N-CA	-8.32	1.35	1.46
1	B	89	GLY	N-CA	7.26	1.54	1.45
1	A	366	THR	CB-OG1	5.40	1.52	1.43

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	THR	N-CA-C	8.41	120.52	111.36
1	A	300	ALA	N-CA-C	8.12	119.91	111.14
1	A	248	LYS	N-CA-C	-8.06	103.39	113.55
1	B	91	GLY	O-C-N	-7.93	112.39	122.70
1	B	196	THR	N-CA-C	7.86	121.36	111.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	409	LEU	CA

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	3071	0	3020	194	0
1	B	3071	0	3020	198	0
2	A	15	0	6	1	0
2	B	15	0	6	0	0
3	A	14	0	10	8	0
4	B	5	0	0	1	0
5	A	215	0	0	11	0
5	B	187	0	0	12	0
All	All	6593	0	6062	374	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 31.

The worst 5 of 374 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:117:ASP:O	1:B:121:LYS:HD2	1.57	1.03
1:B:272:LEU:HD22	1:B:287:MET:HE2	1.42	1.02
1:A:17:ILE:HG21	3:A:411:IOP:H2	1.43	1.00
1:A:37:ILE:HG13	3:A:411:IOP:H3'2	1.44	0.96
1:B:129:ARG:HG3	5:B:426:HOH:O	1.69	0.89

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%)	358 (91%)	31 (8%)	5 (1%)	9	10
1	B	394/396 (100%)	370 (94%)	20 (5%)	4 (1%)	12	15
All	All	788/792 (100%)	728 (92%)	51 (6%)	9 (1%)	11	13

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ALA
1	A	343	GLU
1	A	374	ARG
1	B	30	PRO
1	B	301	HIS

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	320/320 (100%)	246 (77%)	74 (23%)	1	1
1	B	320/320 (100%)	255 (80%)	65 (20%)	1	1
All	All	640/640 (100%)	501 (78%)	139 (22%)	1	1

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	267	VAL

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Mol	Chain	Res	Type
1	B	318	ILE
1	B	357	ASN
1	A	292	ARG
1	A	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	294	ASN
1	B	328	GLN
1	A	328	GLN
1	A	312	ASN
1	B	339	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	412	1	15,15,16	1.34	3 (20%)	21,22,23	2.03	8 (38%)
4	SO4	B	411	-	4,4,4	0.29	0	6,6,6	0.46	0
2	PLP	A	410	1	15,15,16	1.12	1 (6%)	21,22,23	2.05	10 (47%)
3	IOP	A	411	-	15,15,15	0.65	0	20,20,20	1.45	4 (20%)

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	B	412	1	-	2/6/6/8	0/1/1/1
2	PLP	A	410	1	-	2/6/6/8	0/1/1/1
3	IOP	A	411	-	-	2/5/5/5	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	412	PLP	C5-C4	2.82	1.43	1.40
2	A	410	PLP	C5-C4	2.60	1.43	1.40
2	B	412	PLP	C4A-C4	-2.43	1.46	1.51
2	B	412	PLP	P-O3P	-2.08	1.47	1.54

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	412	PLP	C4A-C4-C5	5.24	126.35	120.94
2	A	410	PLP	C4A-C4-C5	4.22	125.29	120.94
2	A	410	PLP	C6-C5-C4	3.59	121.04	118.10
3	A	411	IOP	C3'-C2'-C1'	-3.23	105.09	113.67
3	A	411	IOP	O1-C1'-C2'	-3.01	113.54	123.09

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	410	PLP	C4-C5-C5A-O4P
2	A	410	PLP	C6-C5-C5A-O4P
2	B	412	PLP	C4-C5-C5A-O4P
2	B	412	PLP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
3	A	411	IOP	O1-C1'-C2'-C3'

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	411	SO4	1	0
2	A	410	PLP	1	0
3	A	411	IOP	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	91:GLY	C	92:SER	N	1.12

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.