



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:19 PM UTC

PDB ID : 1AHG / pdb_00001ahg
Title : ASPARTATE AMINOTRANSFERASE HEXAMUTANT
Authors : Malashkevich, V.N.; Jansonius, J.N.
Deposited on : 1995-02-22
Resolution : 2.50 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

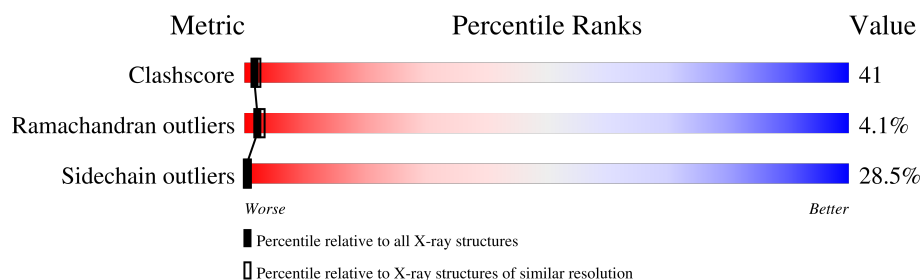
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

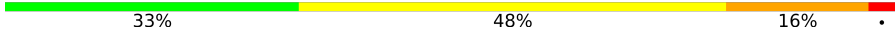
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	 33% 48% 16% .
1	B	396	 31% 49% 17% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6708 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.

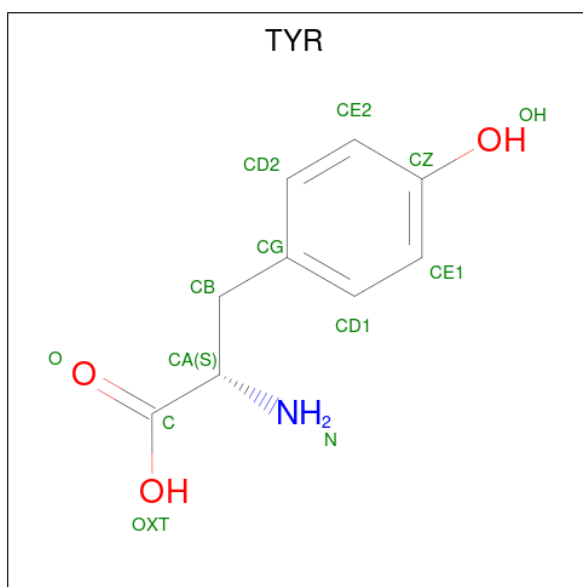
- Molecule 1 is a protein called Aspartate aminotransferase.

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:

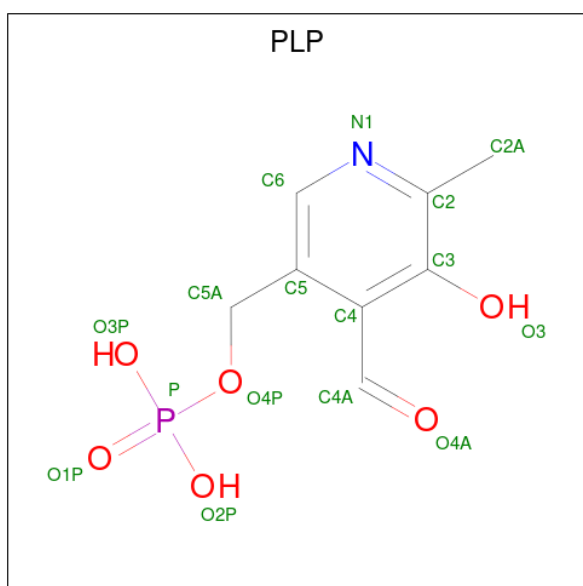
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	VAL	engineered mutation	UNP P00509
A	41	TYR	LYS	engineered mutation	UNP P00509
A	47	ILE	THR	engineered mutation	UNP P00509
A	69	LEU	ASN	engineered mutation	UNP P00509
A	109	SER	THR	engineered mutation	UNP P00509
A	297	SER	ASN	engineered mutation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

- Molecule 2 is TYROSINE (CCD ID: TYR) (formula: C₉H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	1	3		
2	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: 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		

- Molecule 4 is water.

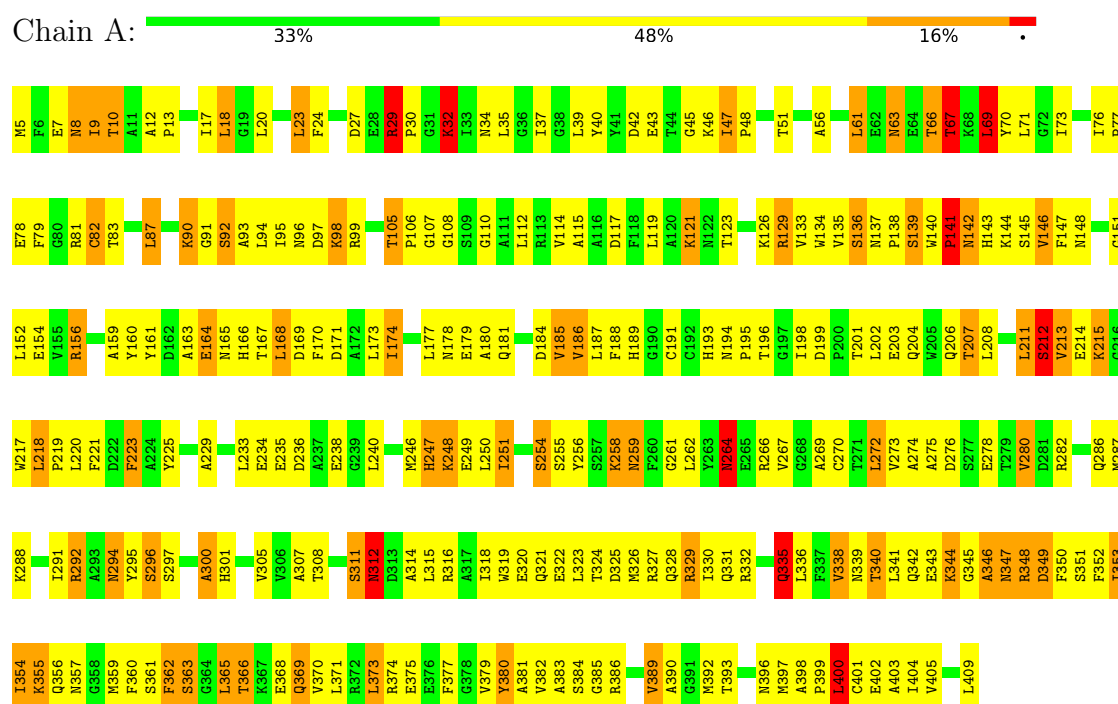
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total 249	O 249	0	0
4	B	261	Total 261	O 261	0	0

3 Residue-property plots

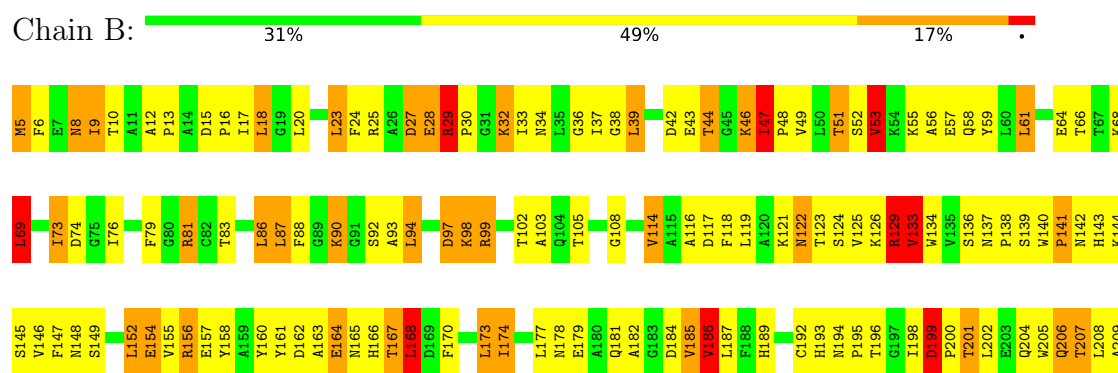
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



R348	D349	F350	S351	F352	I353	I354	K355	Q356	N357	G358	M359	F360	S361	F362	S363				K367	E368				L371	R372	L373	R374	E375	E376	F377	G378	V379	Y380	A381	V382	A383	S384	G385	R386				V389	A390	G391	M392	T393	P394	D395	N396	M397	A398	P399	C401	L400	E402	A403	I404	V405	A407	V408	L409								
V280	D281	R282				S285	Q286	M287	K288				I291	R292	A293	N294	Y295	S296	S297				H301				S304	V305	V306	A307	T308	I309				N312	D313	A314	L315	R316	A317	I318	W319	E320	Q321	E322	L323	T324	D325	M326	R327	Q328	R329	I330	Q331	R332	M333	R334				V338	N339	T340	L341	Q342	E343	K344	G345	N347
Q210	L211	S212	E213	K215	G216	W217	L218	P219	L220	F221	D222	F223				Q226				A229	R230	G231	L233	E234	E235	D236	A237				L240	R241	A242	F243	A244	L245	M246	H247	K248	E249	L250	L251	V252	A253	S254	S255	Y256	S257	K258	N259				M264	E265	R266	V267				L272	V273	A274	L275	D276	S277	E278	T279		

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	86.00Å 79.10Å 89.60Å 90.00° 118.67° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.5 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.250 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6708	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: 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	1.14	0/3133	1.66	31/4244 (0.7%)
1	B	1.12	6/3133 (0.2%)	1.65	38/4244 (0.9%)
All	All	1.13	6/6266 (0.1%)	1.66	69/8488 (0.8%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	THR	N-CA	6.91	1.54	1.46
1	B	168	LEU	N-CA	-6.73	1.38	1.46
1	B	167	THR	CA-C	-6.22	1.45	1.52
1	B	166	HIS	CA-C	5.82	1.59	1.53
1	B	166	HIS	N-CA	5.77	1.54	1.46

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ALA	N-CA-C	10.62	124.36	111.40
1	A	373	LEU	N-CA-C	-9.39	100.74	110.97
1	B	167	THR	O-C-N	9.23	132.87	122.99
1	B	117	ASP	N-CA-C	-8.99	102.44	113.50
1	B	199	ASP	CA-CB-CG	8.90	121.50	112.60

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	3071	0	3022	244	0
1	B	3071	0	3022	286	0
2	A	13	0	8	2	0
2	B	13	0	8	1	0
3	A	15	0	6	1	0
3	B	15	0	6	2	0
4	A	249	0	0	22	0
4	B	261	0	0	19	0
All	All	6708	0	6072	508	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 41.

The worst 5 of 508 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:129:ARG:HB2	1:A:154:GLU:HB3	1.32	1.10
1:A:312:ASN:ND2	1:A:315:LEU:H	1.50	1.09
1:A:397:MET:HE3	1:A:397:MET:HA	1.37	1.07
1:B:46:LYS:HD2	1:B:47:ILE:HG13	1.38	1.04
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.22	1.03

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%)	331 (84%)	48 (12%)	15 (4%)	2 3
1	B	394/396 (100%)	328 (83%)	49 (12%)	17 (4%)	2 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	788/792 (100%)	659 (84%)	97 (12%)	32 (4%)	2 3

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	301	HIS
1	A	346	ALA
1	B	233	LEU
1	B	234	GLU

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%)	227 (71%)	93 (29%)	0 0
1	B	320/320 (100%)	231 (72%)	89 (28%)	0 1
All	All	640/640 (100%)	458 (72%)	182 (28%)	0 0

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90	LYS
1	B	207	THR
1	B	105	THR
1	B	145	SER
1	B	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
1	B	148	ASN
1	B	339	ASN

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Mol	Chain	Res	Type
1	B	104	GLN
1	B	165	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 oligosaccharides 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	TYR	A	501	3	12,13,13	0.77	0	13,17,17	0.31	0
3	PLP	A	500	2	15,15,16	1.70	3 (20%)	21,22,23	1.99	8 (38%)
2	TYR	B	501	3	12,13,13	0.79	0	13,17,17	0.59	0
3	PLP	B	500	2	15,15,16	1.70	2 (13%)	21,22,23	2.27	7 (33%)

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	TYR	A	501	3	-	0/8/8/8	0/1/1/1
3	PLP	A	500	2	-	2/6/6/8	0/1/1/1
2	TYR	B	501	3	-	4/8/8/8	0/1/1/1
3	PLP	B	500	2	-	3/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	PLP	C4A-C4	-4.73	1.42	1.51
3	A	500	PLP	C4A-C4	-3.97	1.43	1.51
3	A	500	PLP	C5-C4	2.60	1.43	1.40
3	A	500	PLP	P-O3P	-2.60	1.45	1.54
3	B	500	PLP	P-O3P	-2.36	1.46	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	PLP	C6-C5-C4	5.32	122.46	118.10
3	A	500	PLP	C4A-C4-C5	3.87	124.93	120.94
3	A	500	PLP	C6-C5-C4	3.86	121.26	118.10
3	B	500	PLP	C5A-C5-C4	-3.60	115.53	122.64
3	B	500	PLP	C5-C6-N1	-3.50	118.14	123.83

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	PLP	C4-C5-C5A-O4P
3	A	500	PLP	C6-C5-C5A-O4P
3	B	500	PLP	C4-C5-C5A-O4P
3	B	500	PLP	C6-C5-C5A-O4P
2	B	501	TYR	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TYR	2	0
3	A	500	PLP	1	0
2	B	501	TYR	1	0
3	B	500	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 [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.