Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 06:57 AM EDT

PDB ID	:	1G4X
Title	:	ASPARTATE AMINOTRANSFERASE ACTIVE SITE MUTANT N194A/R292L
Authors	:	Mizuguchi, H.
Deposited on	:	2000-10-29
Resolution	:	2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

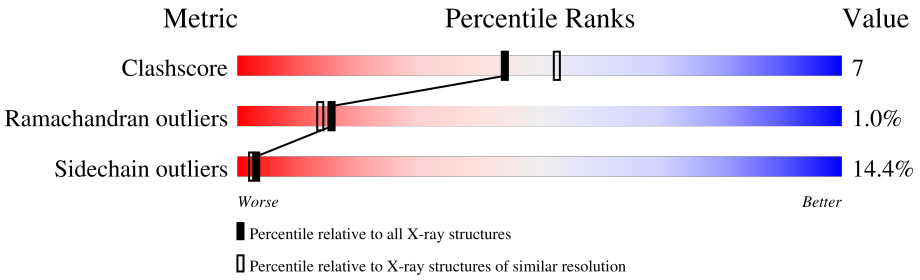
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	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	396	76% 19% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3228 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.

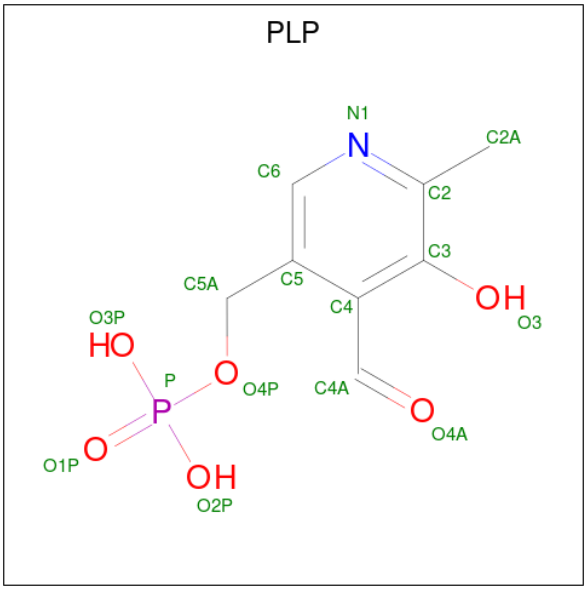
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3063	1935	532	583	13	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	ALA	ASN	engineered mutation	UNP P00509
A	292	LEU	ARG	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
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		

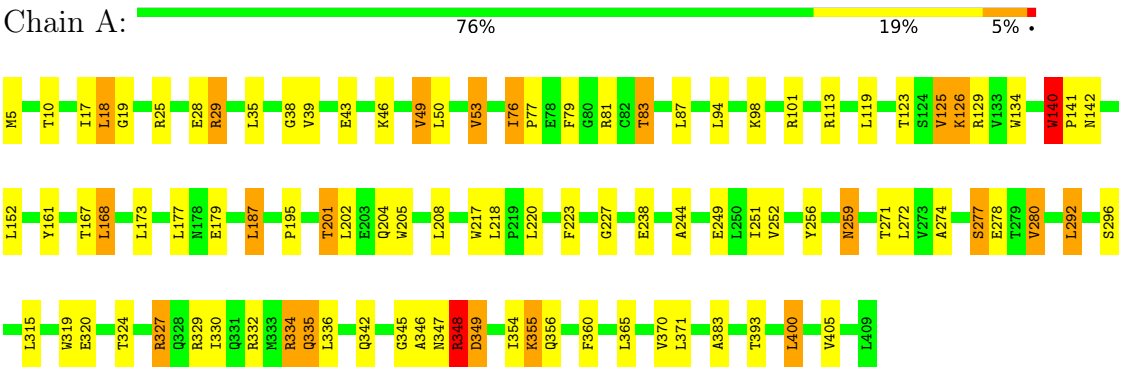
3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	155.04Å 88.75Å 80.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.229 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3228	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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: 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	0.69	0/3124	1.35	27/4233 (0.6%)

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	A	0	2

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	334	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	A	334	ARG	NE-CZ-NH1	-9.44	115.58	120.30
1	A	347	ASN	CA-C-N	-9.16	97.04	117.20
1	A	18	LEU	CA-CB-CG	8.73	135.37	115.30
1	A	319	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	A	134	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	319	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	A	134	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	A	140	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	A	205	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	A	217	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	A	140	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	217	TRP	CB-CG-CD1	-6.95	117.97	127.00
1	A	205	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	A	217	TRP	CE2-CD2-CG	-6.46	102.14	107.30
1	A	327	ARG	NE-CZ-NH2	6.30	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	187	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	280	VAL	CA-CB-CG2	-5.77	102.24	110.90
1	A	349	ASP	CA-C-N	-5.58	104.92	117.20
1	A	18	LEU	CA-C-N	-5.52	105.16	116.20
1	A	217	TRP	CA-CB-CG	5.46	124.07	113.70
1	A	161	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	348	ARG	CA-CB-CG	5.26	124.96	113.40
1	A	140	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	A	319	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	A	329	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	A	205	TRP	CG-CD2-CE3	5.05	138.45	133.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	TRP	Peptide
1	A	348	ARG	Peptide

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	3063	0	3013	40	0
2	A	15	0	7	0	0
3	A	150	0	0	6	0
All	All	3228	0	3020	40	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 (40) 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:334:ARG:NH1	1:A:356:GLN:HB2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HG21	3:A:447:HOH:O	1.93	0.67
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.84	0.59
1:A:168:LEU:HD21	1:A:173:LEU:HD12	1.87	0.57
1:A:252:VAL:HG13	1:A:271:THR:HB	1.87	0.57
1:A:249:GLU:HG2	1:A:274:ALA:HA	1.87	0.56
1:A:50:LEU:HB2	1:A:53:VAL:HG13	1.88	0.56
1:A:202:LEU:HD13	1:A:238:GLU:HG2	1.88	0.55
1:A:320:GLU:O	1:A:324:THR:HG23	2.09	0.53
1:A:123:THR:OG1	1:A:125:VAL:HG13	2.09	0.53
1:A:355:LYS:HB3	1:A:355:LYS:NZ	2.25	0.52
1:A:101:ARG:HG2	1:A:280:VAL:CG2	2.40	0.52
1:A:348:ARG:HH22	1:A:405:VAL:HG22	1.75	0.51
1:A:201:THR:HG22	1:A:204:GLN:H	1.75	0.51
1:A:43:GLU:HB2	3:A:540:HOH:O	2.10	0.51
1:A:274:ALA:N	3:A:477:HOH:O	2.44	0.51
1:A:292:LEU:HA	1:A:296:SER:HA	1.92	0.50
1:A:38:GLY:HA2	1:A:360:PHE:HZ	1.77	0.49
1:A:28:GLU:HB3	1:A:29:ARG:NH1	2.28	0.49
1:A:346:ALA:HB2	1:A:405:VAL:HG13	1.95	0.48
1:A:278:GLU:HB2	3:A:463:HOH:O	2.15	0.47
1:A:49:VAL:HG23	1:A:53:VAL:CG2	2.45	0.46
1:A:126:LYS:HE3	1:A:126:LYS:HA	1.97	0.46
1:A:274:ALA:HB3	3:A:477:HOH:O	2.16	0.46
1:A:227:GLY:O	1:A:327:ARG:HD3	2.16	0.45
1:A:335:GLN:HA	1:A:354:ILE:CD1	2.46	0.45
1:A:393:THR:HB	3:A:532:HOH:O	2.17	0.44
1:A:251:ILE:HG12	1:A:272:LEU:HD23	2.00	0.44
1:A:330:ILE:O	1:A:334:ARG:HG3	2.18	0.43
1:A:76:ILE:O	1:A:76:ILE:HG13	2.17	0.43
1:A:101:ARG:HG2	1:A:280:VAL:HG22	2.01	0.43
1:A:346:ALA:HB3	1:A:348:ARG:CZ	2.50	0.42
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.87	0.42
1:A:277:SER:O	1:A:280:VAL:HG12	2.20	0.42
1:A:256:TYR:HA	1:A:259:ASN:ND2	2.35	0.42
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.86	0.41
1:A:94:LEU:HD11	1:A:244:ALA:HB1	2.03	0.41
1:A:35:LEU:HD11	1:A:400:LEU:HD21	2.03	0.40
1:A:79:PHE:O	1:A:83:THR:HG23	2.21	0.40
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.86	0.40

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%)	372 (94%)	18 (5%)	4 (1%)	15 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLY
1	A	141	PRO
1	A	345	GLY
1	A	142	ASN

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	319/319 (100%)	273 (86%)	46 (14%)	3 2

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	10	THR
1	A	17	ILE
1	A	18	LEU
1	A	25	ARG
1	A	29	ARG
1	A	39	VAL

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Mol	Chain	Res	Type
1	A	46	LYS
1	A	49	VAL
1	A	53	VAL
1	A	76	ILE
1	A	81	ARG
1	A	83	THR
1	A	87	LEU
1	A	98	LYS
1	A	113	ARG
1	A	119	LEU
1	A	125	VAL
1	A	126	LYS
1	A	129	ARG
1	A	140	TRP
1	A	152	LEU
1	A	167	THR
1	A	168	LEU
1	A	179	GLU
1	A	187	LEU
1	A	195	PRO
1	A	201	THR
1	A	208	LEU
1	A	218	LEU
1	A	220	LEU
1	A	223	PHE
1	A	259	ASN
1	A	277	SER
1	A	292	LEU
1	A	315	LEU
1	A	332	ARG
1	A	335	GLN
1	A	336	LEU
1	A	342	GLN
1	A	348	ARG
1	A	349	ASP
1	A	355	LYS
1	A	365	LEU
1	A	371	LEU
1	A	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	178	ASN
1	A	193	HIS
1	A	259	ASN
1	A	335	GLN
1	A	347	ASN
1	A	356	GLN

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 (i)

1 ligand is 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	413	1	15,15,16	1.20	1 (6%)	20,22,23	1.43	3 (15%)

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	413	1	-	1/6/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PLP	C3-C2	-2.64	1.38	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	413	PLP	O4P-C5A-C5	4.60	118.12	109.35
2	A	413	PLP	C6-C5-C4	2.48	120.11	118.16
2	A	413	PLP	C5-C6-N1	-2.25	120.07	123.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	413	PLP	C5A-O4P-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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.