



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:12 PM UTC

PDB ID : 1Q2X / pdb_00001q2x
Title : Crystal Structure of the E243D Mutant of Aspartate Semialdehyde Dehydrogenase from Haemophilus influenzae bound with substrate aspartate semialdehyde
Authors : Blanco, J.; Moore, R.A.; Faehnle, C.R.; Coe, D.M.; Viola, R.E.
Deposited on : 2003-07-26
Resolution : 2.05 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 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

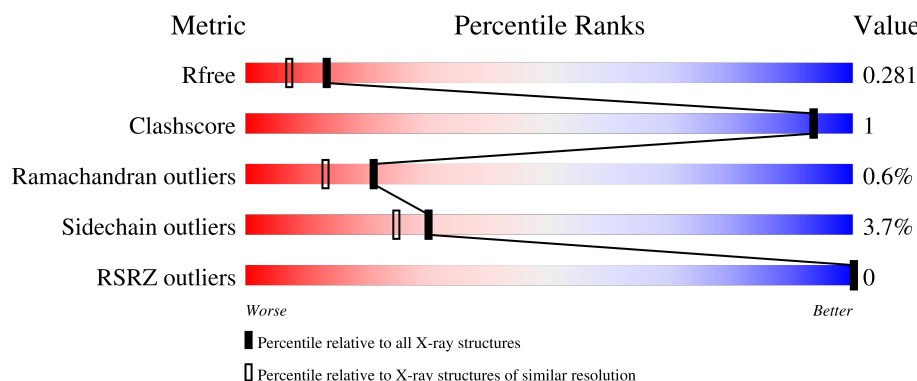
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	371	 83% 13% . .
1	B	371	 85% 11% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5734 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-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2761	1761	464	521	15			
1	B	357	Total	C	N	O	S	0	0	0
			2761	1761	464	521	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	HTI	CYS	modified residue	UNP P44801
A	243	ASP	GLU	engineered mutation	UNP P44801
B	136	HTI	CYS	modified residue	UNP P44801
B	243	ASP	GLU	engineered mutation	UNP P44801

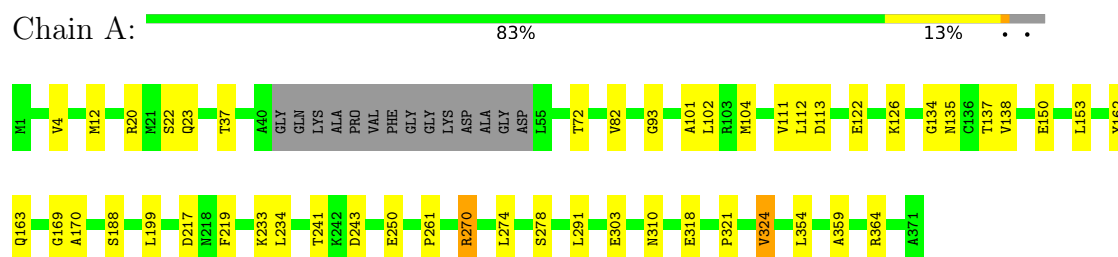
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total	O	0	0
			108	108		
2	B	104	Total	O	0	0
			104	104		

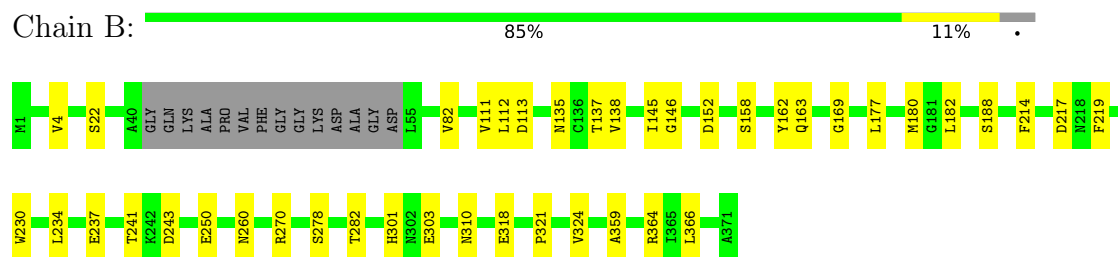
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Aspartate-semialdehyde dehydrogenase



- Molecule 1: Aspartate-semialdehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.61Å 113.86Å 57.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.38 – 2.05 40.38 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.5 (40.38-2.05) 93.5 (40.38-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 2.05Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.238 , 0.279 0.243 , 0.281	Depositor DCC
R_{free} test set	4124 reflections (9.60%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,k,-h 0.487 for h,-k,-l 0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5734	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HTI

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	0.76	0/2795	1.20	25/3779 (0.7%)
1	B	0.75	0/2795	1.19	19/3779 (0.5%)
All	All	0.75	0/5590	1.19	44/7558 (0.6%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	VAL	N-CA-C	8.45	119.02	110.82
1	A	82	VAL	N-CA-C	7.47	118.07	110.82
1	A	111	VAL	N-CA-C	6.99	119.50	108.87
1	A	113	ASP	N-CA-C	6.88	123.06	113.57
1	B	359	ALA	N-CA-C	6.74	120.72	112.23
1	A	169	GLY	N-CA-C	6.71	118.97	111.85
1	B	169	GLY	N-CA-C	6.71	118.96	111.85
1	A	217	ASP	N-CA-C	6.67	118.20	111.07
1	B	111	VAL	N-CA-C	6.61	118.92	108.87
1	A	188	SER	N-CA-C	6.47	117.99	111.07
1	A	318	GLU	N-CA-C	6.43	121.66	113.55
1	B	217	ASP	N-CA-C	6.38	118.23	111.28
1	B	237	GLU	N-CA-C	6.29	118.22	111.36
1	B	364	ARG	N-CA-C	6.25	119.07	111.82
1	A	359	ALA	N-CA-C	6.22	120.06	112.23
1	B	250	GLU	N-CA-C	6.18	120.02	112.23
1	A	324	VAL	N-CA-C	6.10	121.37	113.07
1	A	93	GLY	N-CA-C	6.09	122.53	112.30
1	A	364	ARG	N-CA-C	6.06	118.86	111.82
1	B	113	ASP	N-CA-C	6.00	123.07	109.81
1	B	301	HIS	N-CA-C	5.91	117.39	111.07
1	B	318	GLU	N-CA-C	5.88	120.96	113.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	GLN	N-CA-C	5.83	119.76	109.96
1	A	261	PRO	N-CA-C	5.77	120.29	110.95
1	A	250	GLU	N-CA-C	5.71	119.43	112.23
1	A	241	THR	N-CA-C	-5.62	101.70	110.42
1	A	134	GLY	N-CA-C	5.54	121.08	112.60
1	B	324	VAL	N-CA-C	5.53	120.19	112.50
1	B	4	VAL	N-CA-C	5.52	115.89	108.17
1	B	146	GLY	N-CA-C	5.52	120.47	113.24
1	A	37	THR	N-CA-C	-5.51	106.61	113.38
1	A	4	VAL	N-CA-C	5.49	115.86	108.17
1	B	241	THR	N-CA-C	-5.43	102.42	110.46
1	A	274	LEU	N-CA-C	5.38	118.17	111.24
1	A	104	MET	N-CA-C	5.25	119.32	113.02
1	B	163	GLN	N-CA-C	5.24	118.76	109.96
1	A	72	THR	N-CA-C	5.22	117.59	108.76
1	B	214	PHE	CA-C-N	5.21	126.35	119.84
1	B	214	PHE	C-N-CA	5.21	126.35	119.84
1	A	233	LYS	N-CA-C	5.20	117.42	110.35
1	A	102	LEU	N-CA-C	5.13	119.69	113.38
1	A	170	ALA	N-CA-C	5.12	116.55	111.07
1	A	101	ALA	N-CA-C	5.11	119.81	111.37
1	B	188	SER	N-CA-C	5.02	116.75	111.28

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	2761	0	2817	8	0
1	B	2761	0	2817	8	0
2	A	108	0	0	0	0
2	B	104	0	0	0	0
All	All	5734	0	5634	16	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 1.

All (16) 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:135:ASN:HD22	1:B:138:VAL:H	1.45	0.64
1:A:20:ARG:HH11	1:A:23:GLN:NE2	2.05	0.54
1:A:219:PHE:HE2	1:A:270:ARG:HD3	1.73	0.54
1:B:219:PHE:HE2	1:B:270:ARG:HD3	1.73	0.52
1:A:20:ARG:HH11	1:A:23:GLN:HE21	1.56	0.52
1:A:135:ASN:HD22	1:A:138:VAL:HG23	1.78	0.47
1:A:12:MET:HE3	1:A:354:LEU:HD21	1.96	0.47
1:B:162:TYR:HB2	1:B:278:SER:HB2	1.98	0.46
1:B:135:ASN:ND2	1:B:138:VAL:H	2.14	0.45
1:B:219:PHE:CE2	1:B:270:ARG:HD3	2.52	0.43
1:A:122:GLU:O	1:A:126:LYS:HB2	2.17	0.43
1:B:177:LEU:HD23	1:B:180:MET:HE3	2.02	0.42
1:A:162:TYR:HB2	1:A:278:SER:HB2	2.02	0.42
1:B:158:SER:HB3	1:B:282:THR:HB	2.01	0.41
1:B:230:TRP:HZ2	1:B:234:LEU:HB2	1.86	0.41
1:A:135:ASN:HD22	1:A:138:VAL:H	1.67	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	352/371 (95%)	338 (96%)	12 (3%)	2 (1%)	21	13
1	B	352/371 (95%)	338 (96%)	12 (3%)	2 (1%)	21	13
All	All	704/742 (95%)	676 (96%)	24 (3%)	4 (1%)	21	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	B	112	LEU
1	B	310	ASN
1	A	310	ASN

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	296/304 (97%)	284 (96%)	12 (4%)	27	21
1	B	296/304 (97%)	286 (97%)	10 (3%)	32	27
All	All	592/608 (97%)	570 (96%)	22 (4%)	30	25

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	137	THR
1	A	150	GLU
1	A	153	LEU
1	A	199	LEU
1	A	234	LEU
1	A	243	ASP
1	A	270	ARG
1	A	291	LEU
1	A	303	GLU
1	A	321	PRO
1	A	324	VAL
1	B	22	SER
1	B	137	THR
1	B	145	ILE
1	B	152	ASP
1	B	182	LEU
1	B	243	ASP
1	B	260	ASN
1	B	303	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	321	PRO
1	B	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	39	GLN
1	A	135	ASN
1	A	163	GLN
1	A	185	GLN
1	A	296	GLN
1	B	3	ASN
1	B	31	ASN
1	B	135	ASN
1	B	163	GLN
1	B	172	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	HTI	A	136	1	7,13,14	0.98	0	5,16,18	0.66	0
1	HTI	B	136	1	7,13,14	0.95	0	5,16,18	0.68	0

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
1	HTI	A	136	1	-	2/11/15/17	-
1	HTI	B	136	1	-	2/11/15/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	136	HTI	CAH-CAJ-CAK-NAL
1	B	136	HTI	CAH-CAJ-CAK-NAL
1	A	136	HTI	CAH-CAJ-CAK-CAM
1	B	136	HTI	CAH-CAJ-CAK-CAM

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	356/371 (95%)	-1.21	0 100 100	11, 30, 57, 67	0
1	B	356/371 (95%)	-1.21	0 100 100	11, 30, 57, 68	0
All	All	712/742 (95%)	-1.21	0 100 100	11, 30, 57, 68	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	HTI	A	136	14/15	0.99	0.05	23,31,34,35	0
1	HTI	B	136	14/15	0.99	0.04	23,31,33,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.