



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:12 am BST

PDB ID : 2IUP
Title : CRYSTAL STRUCTURE OF DITHIONITE-REDUCED AROMATIC AMINE DEHYDROGENASE (AADH) FROM ALCALIGENES FAECALIS
Authors : Roujeinikova, A.; Scrutton, N.; Leys, D.
Deposited on : 2006-06-07
Resolution : 1.80 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) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

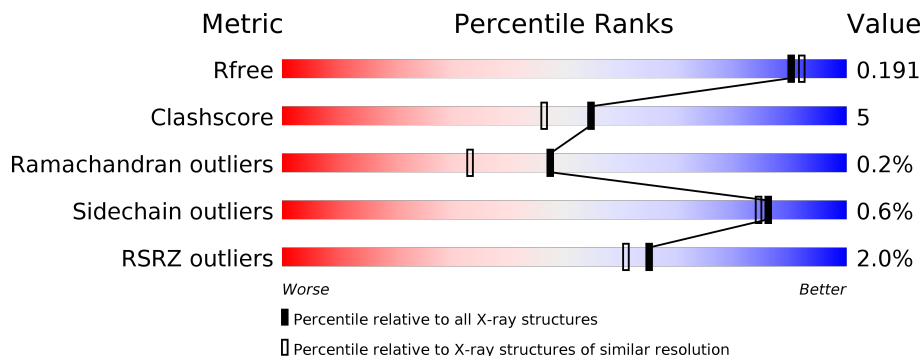
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 $\leq 5\%$. 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	361	
1	B	361	
2	D	135	
2	H	135	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8534 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 AROMATIC AMINE DEHYDROGENASE ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2819	1778	491	536	14	0	4	0
1	B	361	2799	1764	488	533	14	0	2	0

- Molecule 2 is a protein called AROMATIC AMINE DEHYDROGENASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	109	840	513	147	165	15	0	1	0
2	H	119	903	551	159	178	15	0	0	0

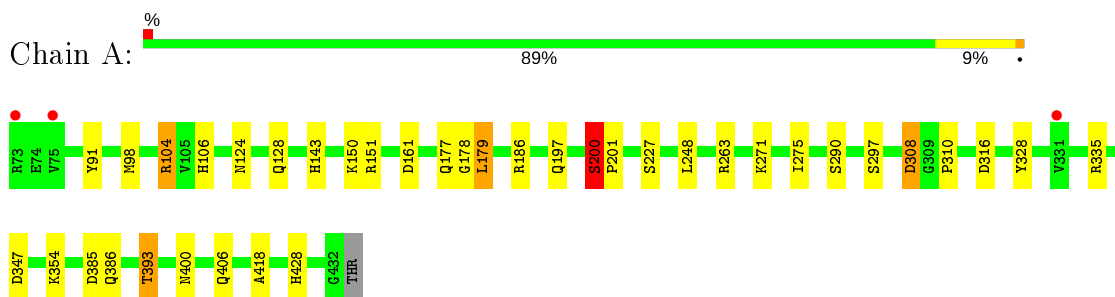
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	501	Total 501	O 501	0	0
3	B	421	Total 421	O 421	0	0
3	D	132	Total 132	O 132	0	0
3	H	119	Total 119	O 119	0	0

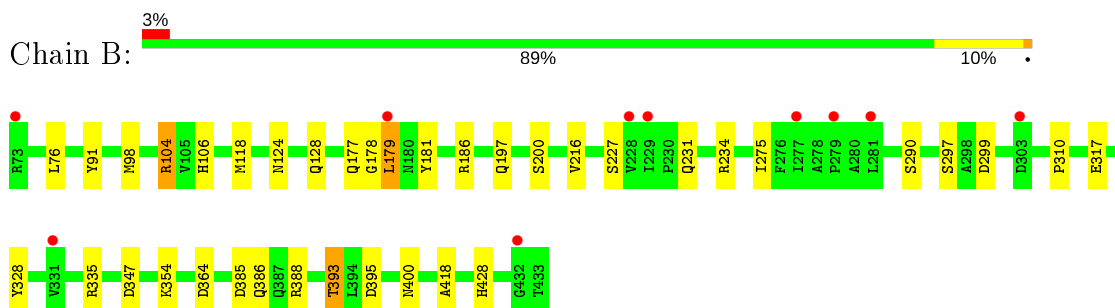
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

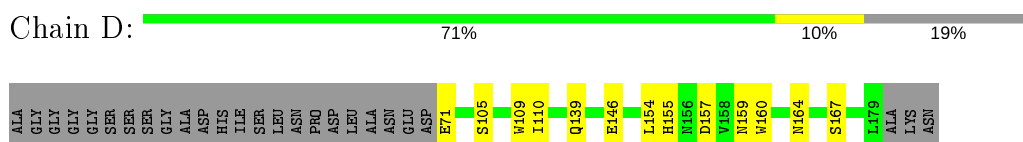
- Molecule 1: AROMATIC AMINE DEHYDROGENASE ALPHA SUBUNIT



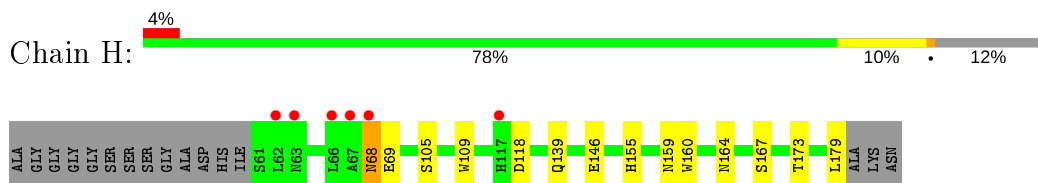
- Molecule 1: AROMATIC AMINE DEHYDROGENASE ALPHA SUBUNIT



- Molecule 2: AROMATIC AMINE DEHYDROGENASE BETA SUBUNIT



- Molecule 2: AROMATIC AMINE DEHYDROGENASE BETA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.96Å 89.06Å 80.80Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 29.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-1.80) 97.9 (29.92-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.147 , 0.180 0.158 , 0.191	Depositor DCC
R_{free} test set	4552 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8534	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 i

5.1 Standard geometry i

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

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	0.65	1/2897 (0.0%)	0.72	7/3926 (0.2%)
1	B	0.61	1/2872 (0.0%)	0.70	6/3895 (0.2%)
2	D	0.58	0/849	0.68	0/1156
2	H	0.58	0/910	0.67	1/1241 (0.1%)
All	All	0.62	2/7528 (0.0%)	0.70	14/10218 (0.1%)

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	1	2
1	B	1	2
All	All	2	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	THR	CB-OG1	7.25	1.57	1.43
1	B	393	THR	CB-OG1	5.24	1.53	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	179	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	364	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	179	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	308[A]	ASP	CB-CG-OD2	5.43	123.18	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	393	THR	CB
1	B	393	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	SER	Peptide
1	A	310	PRO	Peptide
1	B	200	SER	Peptide
1	B	310	PRO	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	2819	0	2761	33	0
1	B	2799	0	2713	28	0
2	D	840	0	739	11	0
2	H	903	0	788	11	0
3	A	501	0	0	8	0
3	B	421	0	0	3	0
3	D	132	0	0	5	0
3	H	119	0	0	6	0
All	All	8534	0	7001	75	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 5.

The worst 5 of 75 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:179:LEU:HB3	3:B:2158:HOH:O	1.67	0.95
1:A:393:THR:HG21	3:A:2428:HOH:O	1.70	0.91
1:A:179:LEU:HB3	3:A:2039:HOH:O	1.73	0.88
1:B:393:THR:HG21	3:B:2358:HOH:O	1.74	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:SER:HA	2:H:164:ASN:HD21	1.50	0.76

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	362/361 (100%)	350 (97%)	11 (3%)	1 (0%)	41	27
1	B	360/361 (100%)	347 (96%)	12 (3%)	1 (0%)	41	27
2	D	107/135 (79%)	105 (98%)	2 (2%)	0	100	100
2	H	116/135 (86%)	114 (98%)	2 (2%)	0	100	100
All	All	945/992 (95%)	916 (97%)	27 (3%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	VAL
1	A	200	SER

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	307/305 (101%)	306 (100%)	1 (0%)	92	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	302/305 (99%)	299 (99%)	3 (1%)	76	71
2	D	96/112 (86%)	96 (100%)	0	100	100
2	H	101/112 (90%)	100 (99%)	1 (1%)	76	71
All	All	806/834 (97%)	801 (99%)	5 (1%)	86	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	B	104	ARG
1	B	297	SER
1	B	388	ARG
2	H	68	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	106	HIS
1	B	177	GLN
2	H	143	GLN
1	B	124	ASN
1	B	128	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](#)

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
2	TRQ	D	109	2	13,17,18	5.97	6 (46%)	14,24,26	1.99	2 (14%)
2	TRQ	H	109	2	13,17,18	6.26	6 (46%)	14,24,26	3.33	4 (28%)

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	TRQ	D	109	2	-	0/4/19/21	0/2/2/2
2	TRQ	H	109	2	-	0/4/19/21	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	109	TRQ	CH2-CZ2	-16.30	1.35	1.54
2	D	109	TRQ	CH2-CZ2	-15.23	1.36	1.54
2	H	109	TRQ	O7-CZ2	9.45	1.43	1.23
2	H	109	TRQ	CE2-CZ2	-8.92	1.38	1.50
2	D	109	TRQ	O7-CZ2	8.82	1.41	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	109	TRQ	O7-CZ2-CH2	7.15	127.42	119.00
2	H	109	TRQ	O7-CZ2-CE2	-6.83	114.61	121.84
2	H	109	TRQ	CZ2-CE2-NE1	6.17	129.79	119.94
2	D	109	TRQ	CZ2-CE2-NE1	6.05	129.59	119.94
2	D	109	TRQ	CD2-CE3-CZ3	-2.30	118.31	121.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	109	TRQ	1	0
2	H	109	TRQ	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	360/361 (99%)	-0.45	3 (0%) 86 84	10, 15, 26, 56	0
1	B	361/361 (100%)	-0.24	10 (2%) 53 47	11, 21, 34, 53	0
2	D	108/135 (80%)	-0.40	0 100 100	12, 20, 30, 36	0
2	H	118/135 (87%)	-0.11	6 (5%) 28 22	13, 20, 47, 55	0
All	All	947/992 (95%)	-0.32	19 (2%) 65 61	10, 18, 34, 56	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	62	LEU	4.1
2	H	66	LEU	3.6
1	B	228	VAL	3.4
2	H	67	ALA	3.0
2	H	117	HIS	2.9

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
2	TRQ	D	109	16/17	0.94	0.08	16,20,22,32	0
2	TRQ	H	109	16/17	0.96	0.08	15,17,23,39	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.