

# wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 03:33 am BST

PDB ID : 2IUV

Title : CRYSTAL STRUCTURE OF N-QUINOL FORM OF AROMATIC AMINE

DEHYDROGENASE (AADH) FROM ALCALIGENES FAECALIS, FORM

В

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Deposited on : 2006-06-07

Resolution : 1.55 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 (i) symbol.

The following versions of software and data (see references (1)) 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)

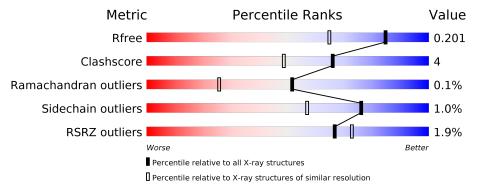
Validation Pipeline (wwPDB-VP) : 2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=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	90%	9% •
1	В	361	90%	8% ••
2	D	135	7% 69% 13%	19%
2	Н	135	83%	7% 10%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8696 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	
1	A	359	Total 2806	C 1770	N 489	O 533	S 14	0	1	0
1	В	358	Total 2791	C 1761	N 486	O 530	S 14	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	110	Total	C	N	0	S	0	0	1
			833	508	149	161	15			
9	П	122	Total	С	N	О	S	0	0	0
	11	122	925	564	163	183	15		U	U

• Molecule 3 is water.

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	509	Total O 509 509	0	0
3	В	560	Total O 560 560	0	0
3	D	115	Total O 115 115	0	0
3	Н	157	Total O 157 157	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 90% • Molecule 1: AROMATIC AMINE DEHYDROGENASE ALPHA SUBUNIT Chain B: • Molecule 2: AROMATIC AMINE DEHYDROGENASE BETA SUBUNIT Chain D: 19% • Molecule 2: AROMATIC AMINE DEHYDROGENASE BETA SUBUNIT Chain H: 83%

# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	89.84Å 96.30Å 118.90Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 - 1.55	Depositor
resolution (A)	29.30 - 1.55	EDS
% Data completeness	89.4 (15.00-1.55)	Depositor
(in resolution range)	89.4 (29.30-1.55)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.56 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
P. P.	0.155 , 0.190	Depositor
$R, R_{free}$	0.168 , 0.201	DCC
$R_{free}$ test set	6708  reflections  (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.6	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34,60.7	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: TQQ

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z >5	
1	A	0.52	0/2874	0.74	5/3894 (0.1%)	
1	В	0.54	0/2859	0.75	$7/3877 \ (0.2\%)$	
2	D	0.50	0/839	0.75	2/1143~(0.2%)	
2	Н	0.52	0/932	0.73	$1/1271 \ (0.1\%)$	
All	All	0.52	0/7504	0.74	$15/10185 \; (0.1\%)$	

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 maintain group or atoms of a sidechain that are expected to be planar.

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	В	218	ASP	CB-CG-OD2	7.88	125.40	118.30
1	В	316	ASP	CB-CG-OD2	6.23	123.91	118.30
1	В	244	ASP	CB-CG-OD2	6.12	123.80	118.30
2	D	121	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	303	ASP	CB-CG-OD2	5.90	123.61	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	SER	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	2806	0	2749	21	0
1	В	2791	0	2722	23	0
2	D	833	0	729	13	0
2	Н	925	0	812	8	0
3	A	509	0	0	3	0
3	В	560	0	0	4	0
3	D	115	0	0	5	0
3	Н	157	0	0	1	0
All	All	8696	0	7012	58	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 4.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap} & ( ext{Å}) \end{aligned}$
1:A:118[A]:MET:SD	3:D:2069:HOH:O	2.40	0.80
1:A:104:ARG:HH11	1:A:106:HIS:HE1	1.36	0.73
1:B:91:TYR:OH	1:B:428:HIS:HD2	1.72	0.72
1:B:104:ARG:HH11	1:B:106:HIS:HE1	1.39	0.71
1:A:124:ASN:HD21	1:A:178:GLY:H	1.40	0.69

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	Perce	ntiles
1	A	358/361~(99%)	344 (96%)	14 (4%)	0	100	100
1	В	357/361 (99%)	344 (96%)	12 (3%)	1 (0%)	41	19
2	D	107/135~(79%)	105 (98%)	2 (2%)	0	100	100
2	Н	119/135~(88%)	115 (97%)	4 (3%)	0	100	100
All	All	941/992 (95%)	908 (96%)	32 (3%)	1 (0%)	51	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
1	В	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	$305/305 \; (100\%)$	301 (99%)	4 (1%)	69	44	
1	В	302/305 (99%)	299 (99%)	3 (1%)	76	57	
2	D	94/112 (84%)	94 (100%)	0	100	100	
2	Н	104/112 (93%)	103 (99%)	1 (1%)	76	57	
All	All	805/834 (96%)	797 (99%)	8 (1%)	76	57	

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	${ m Res}$	$\mathbf{Type}$
1	A	263	ARG
2	Н	123	LEU
1	В	218	ASP
1	A	261	GLN
1	В	104	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:



Mol	Chain	Res	Type
1	В	106	HIS
1	В	177	GLN
2	Н	143	GLN
1	В	128	GLN
1	В	180	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)

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		
IVIOI					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TQQ	D	109	2	12,17,18	4.33	5 (41%)	11,24,26	2.67	4 (36%)
2	TQQ	Н	109	2	12,17,18	4.44	6 (50%)	11,24,26	2.32	3 (27%)

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.

$\mathbf{Mol}$	Type	Chain	${ m Res}$	Link	Chirals	Torsions	$\mathbf{Rings}$
2	TQQ	D	109	2	-	0/4/19/21	0/2/2/2
2	TQQ	Н	109	2	-	0/4/19/21	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
2	Н	109	TQQ	O2-CZ2	10.01	1.44	1.23
2	D	109	TQQ	O2-CZ2	9.47	1.43	1.23
2	Н	109	TQQ	CE2-CZ2	-8.61	1.38	1.50

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
2	D	109	TQQ	CE2-CZ2	-8.34	1.39	1.50
2	Н	109	TQQ	CH2-CZ2	-5.14	1.35	1.49

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	Н	109	TQQ	CZ2-CE2-NE1	6.18	129.81	119.94
2	D	109	TQQ	CZ2-CE2-NE1	5.98	129.50	119.94
2	D	109	TQQ	O2-CZ2-CE2	-4.46	117.12	121.84
2	D	109	TQQ	CG-CB-CA	2.58	118.52	114.53
2	D	109	TQQ	CD2-CE3-CZ3	-2.42	118.17	121.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	109	TQQ	2	0
2	Н	109	TQQ	2	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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	359/361 (99%)	-0.04	3 (0%) 86 89	7, 13, 27, 50	0
1	В	358/361 (99%)	-0.30	2 (0%) 89 92	6, 11, 22, 34	0
2	D	109/135 (80%)	0.30	10 (9%) 9 10	9, 16, 40, 54	0
2	Н	121/135 (89%)	-0.13	3 (2%) 57 64	7, 11, 26, 33	0
All	All	947/992 (95%)	-0.11	18 (1%) 66 73	6, 13, 27, 54	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	GLY	5.9
2	D	117	HIS	5.2
2	D	179	LEU	4.6
2	D	116	PRO	4.5
2	D	120	LYS	3.8

#### 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,  $95^{th}$  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	${f Res}$	Atoms	RSCC	RSR	${f B-factors({ m \AA}^2)}$	Q<0.9
2	TQQ	D	109	16/17	0.94	0.08	9,13,19,25	0
2	TQQ	Н	109	16/17	0.96	0.08	7,10,14,15	0

#### 6.3 Carbohydrates (i)

There are no carbohydrates 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.

