



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:05 PM GMT

PDB ID : 1DZN  
Title : ASP170SER MUTANT OF VANILLYL-ALCOHOL OXIDASE  
Authors : Van Den Heuvel, R.H.H.; Fraaije, M.W.; Van Berkel, W.J.H.; Mattevi, A.  
Deposited on : 2000-03-05  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

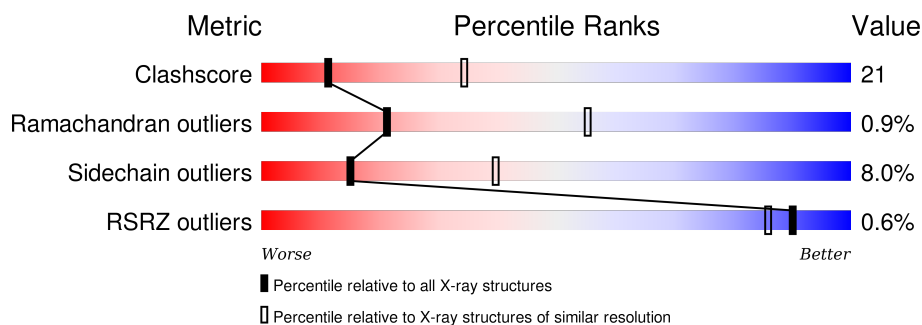
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	560	 57% 34% 6% . .
1	B	560	 54% 35% 7% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	600	-	-	-	X
3	EUG	A	601	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8821 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.

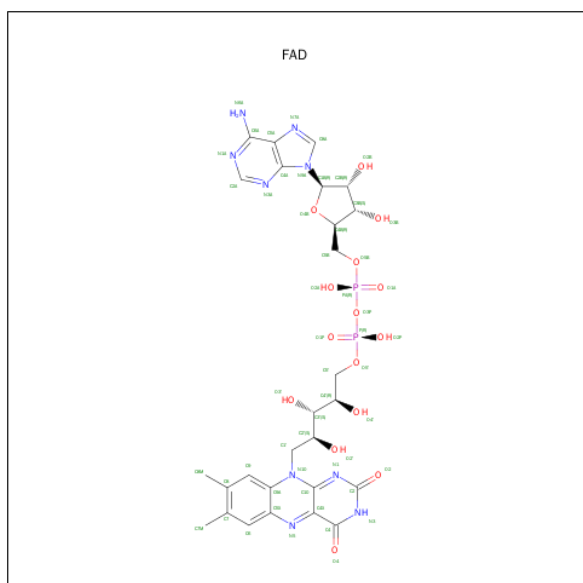
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4315	2774	731	787	23			
1	B	550	Total	C	N	O	S	0	0	0
			4316	2775	731	787	23			

There are 5 discrepancies between the modelled and reference sequences:

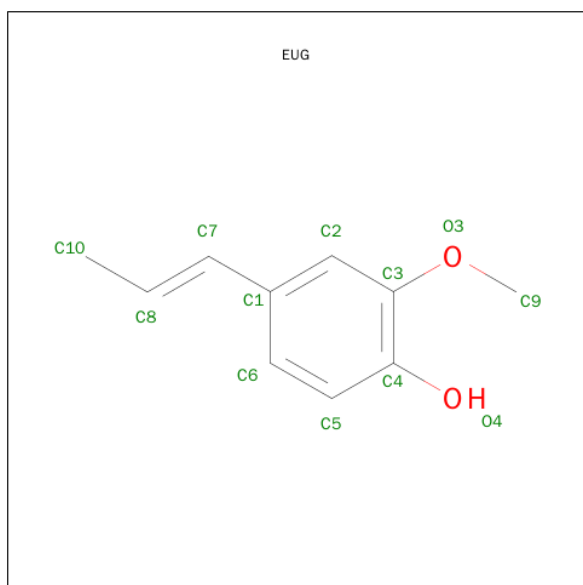
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	GLU	CONFLICT	UNP P56216
B	6	ALA	GLU	CONFLICT	UNP P56216
A	274	GLY	ARG	CONFLICT	UNP P56216
B	274	GLY	ARG	CONFLICT	UNP P56216
B	170	SER	ASP	ENGINEERED	UNP P56216

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-METHOXY-4-VINYL-PHENOL (three-letter code: EUG) (formula:  $C_{10}H_{12}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	32	Total	O	0	0
			32	32		



E529	V530	L531	V535	D536	K545	W549	P550	S551	Q552	Y553	S554	H555	W558	K559	L560	R446	T457	V460	R463	H467	I468	V469	C470	I471	V472	F473	N474	K475	K476	D477	L478	R482	K483	V484	L487	M488	R489	T490	L491	I492	D493	D494	C495	A496	V500	E501	E502	Y503	R504	T505	H506	L507	E508	F509	D510	D511	Q512	I513	H514	E515	T516	N517	N518	H519	L525	R526	I272	P273	S278	Y279	L280	I281	I282	I283	P284	K285	D288	L289	K290	I295	I296	R297	F298	L299	R300	L301	L305	Q306	I307	V308	P309	T310	I311	R312	R313	I314	L315	L316	D317	K324	R325	T331	L334	S335	D336	K341	I342	A343	K344	Q345	L346	N347	I348	K349	R350	N351	I352	F353	Y354	I357	Y358	E361	P362	I363	R364	L367	W368	I371	K372	D373	A374	Y384	F385	P386	S393	V394	L395	R396	V397	R398	D399	K400	T401	Y408	L411	K412	W413	I414	D415	W416	L417	P418	W419	G420	A421	R422	L423	F424	S425	S426	P427	I428	A429	K430	Y431	Q439	T443
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## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.33Å 131.33Å 134.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 31.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.7 (20.00-2.80) 82.9 (31.65-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.227 , 0.291 0.220 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.1	EDS
Estimated twinning fraction	0.025 for l,-k,h 0.038 for -l,-k,-h 0.031 for -h,-l,-k 0.024 for -h,l,k 0.056 for -h,k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 23311 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: EUG, FAD

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	0.66	0/4434	1.87	94/6032 (1.6%)
1	B	0.67	0/4435	1.85	83/6034 (1.4%)
All	All	0.67	0/8869	1.86	177/12066 (1.5%)

There are no bond length outliers.

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	CD-NE-CZ	38.37	177.31	123.60
1	B	398	ARG	CD-NE-CZ	31.00	167.00	123.60
1	B	211	ARG	CD-NE-CZ	19.93	151.50	123.60
1	A	211	ARG	CD-NE-CZ	19.68	151.16	123.60
1	B	446	ARG	NE-CZ-NH1	19.28	129.94	120.30

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	4315	0	4223	175	0
1	B	4316	0	4227	181	0
2	A	53	0	30	9	0
2	B	53	0	30	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	7	0	0
3	B	11	0	7	2	0
4	A	30	0	0	3	0
4	B	32	0	0	2	0
All	All	8821	0	8524	356	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 21.

The worst 5 of 356 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)
2:B:600:FAD:H8A	2:B:600:FAD:C5B	1.74	1.16
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.17	1.15
2:A:600:FAD:H8A	2:A:600:FAD:C5B	1.85	1.06
2:B:600:FAD:H51A	2:B:600:FAD:H8A	1.08	1.05
2:B:600:FAD:H51A	2:B:600:FAD:C8A	1.99	0.93

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	546/560 (98%)	496 (91%)	44 (8%)	6 (1%)	17	50
1	B	546/560 (98%)	491 (90%)	51 (9%)	4 (1%)	26	62
All	All	1092/1120 (98%)	987 (90%)	95 (9%)	10 (1%)	21	55

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	GLY
1	B	420	GLY
1	B	105	ASN
1	A	198	SER
1	A	519	TRP

### 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	463/480 (96%)	430 (93%)	33 (7%)	18	46
1	B	463/480 (96%)	422 (91%)	41 (9%)	12	34
All	All	926/960 (96%)	852 (92%)	74 (8%)	15	40

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	PHE
1	B	114	ARG
1	B	503	TYR
1	B	11	THR
1	B	79	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	GLN
1	B	128	ASN
1	B	552	GLN
1	A	555	HIS
1	B	79	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 carbohydrates 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	FAD	A	600	1	48,58,58	1.76	9 (18%)	54,89,89	2.72	22 (40%)
3	EUG	A	601	-	11,11,12	0.68	0	14,14,15	3.55	6 (42%)
2	FAD	B	600	1	48,58,58	1.75	8 (16%)	54,89,89	2.79	20 (37%)
3	EUG	B	601	-	11,11,12	0.60	0	14,14,15	2.78	7 (50%)

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	FAD	A	600	1	-	0/30/50/50	0/6/6/6
3	EUG	A	601	-	-	0/4/4/5	0/1/1/1
2	FAD	B	600	1	-	0/30/50/50	0/6/6/6
3	EUG	B	601	-	-	0/4/4/5	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C10-N10	-5.38	1.32	1.39
2	B	600	FAD	PA-O2A	-4.86	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C10-N10	-4.49	1.33	1.39
2	A	600	FAD	PA-O2A	-4.31	1.36	1.54
2	A	600	FAD	P-O2P	-3.75	1.38	1.54

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	EUG	O3-C3-C2	-6.90	112.43	124.21
2	A	600	FAD	C4X-C4-N3	-6.30	114.98	123.59
2	B	600	FAD	C4X-C4-N3	-6.19	115.13	123.59
2	B	600	FAD	O4B-C1B-N9A	-5.47	96.65	108.10
2	B	600	FAD	N3A-C2A-N1A	-5.39	124.77	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	9	0
2	B	600	FAD	8	0
3	B	601	EUG	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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	550/560 (98%)	-0.49	1 (0%) 95 94	16, 28, 53, 77	0
1	B	550/560 (98%)	-0.45	6 (1%) 82 74	16, 28, 54, 77	0
All	All	1100/1120 (98%)	-0.47	7 (0%) 90 86	16, 28, 54, 77	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	ASN	4.0
1	B	6	ALA	3.6
1	B	157	ALA	3.0
1	B	161	ARG	2.9
1	B	7	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EUG	A	601	11/12	0.91	0.32	3.25	34,35,37,37	0
2	FAD	A	600	53/53	0.93	0.25	2.82	47,51,52,52	0
2	FAD	B	600	53/53	0.93	0.21	1.95	47,51,52,52	0
3	EUG	B	601	11/12	0.96	0.20	0.96	34,35,37,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.