



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AHZ
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH 4-(1-HEPTENYL)PHENOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 3.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

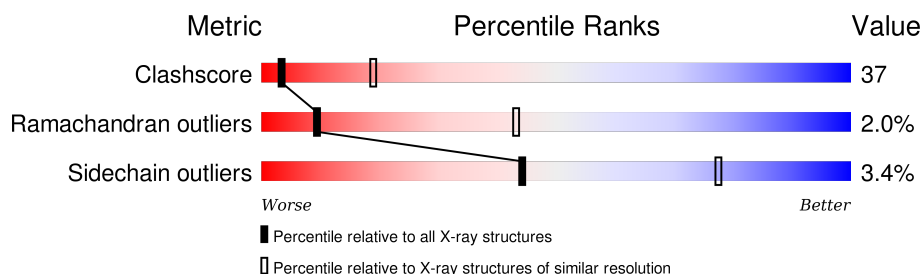
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

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
4	EPT	A	602	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8904 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.

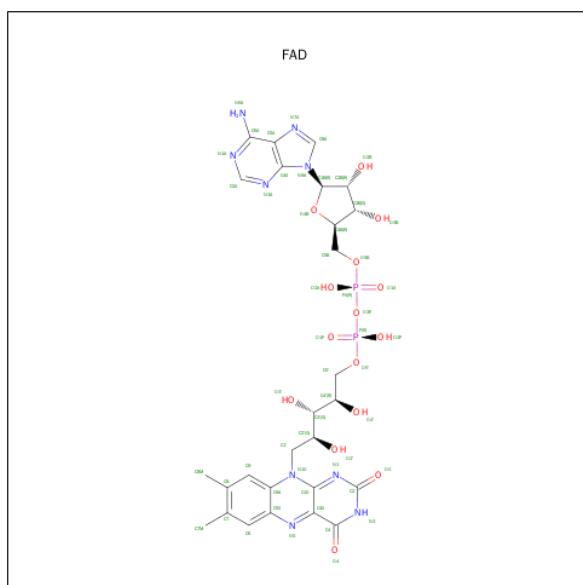
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

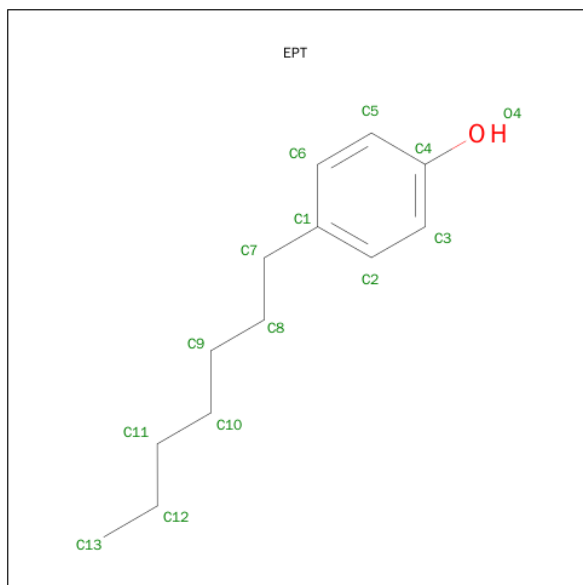
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is HEPTANYL-P-PHENOL (three-letter code: EPT) (formula: $C_{13}H_{20}O$).



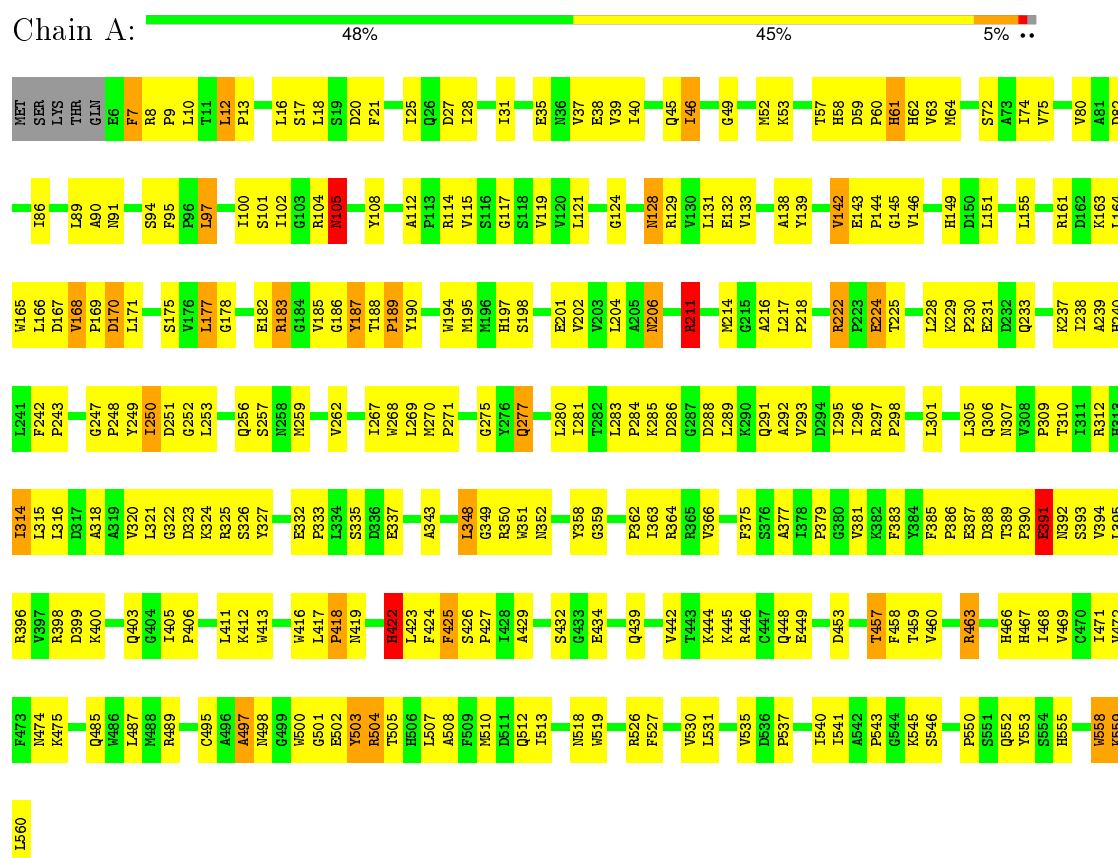
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	13	1		

3 Residue-property plots

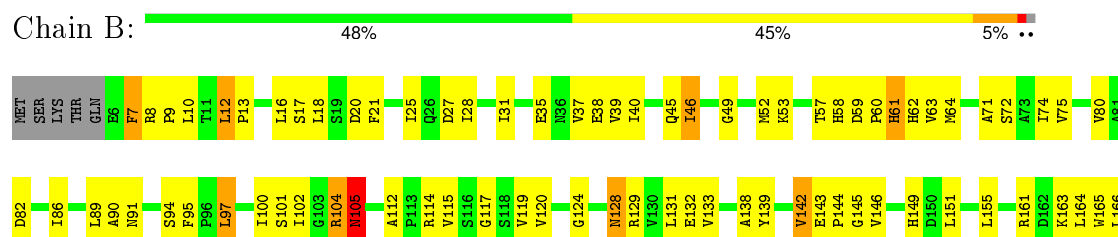
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



	D899	Q485		Q403	Q404	I405	P406		L411	K412	W413		W416	L417	P418	N419		R422	L423	F424		F425	S426	P427		I428	A429		S432	G433	E434		Q439		V442	T443	K444	K445	R446	G447	Q448	E449		D453		T457	F458	T459	V460		R463		H466	H467	I468	V469	Q470	I471	V472	F473	N474	K475																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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	P168	P243		A319	V320	L321	G322	D323	K324	R325	S326	Y327		E332	P333	L334	S335	D336	E337		A343		L348	G349	R350	H351	R352		Y358	G359		P362	L363	R364	R365	V366		F375	S376	A377	I378	P379	G380	V381	R382	F383	V384	F385	P386	E387	D388	T389	P390	E391	R392	S393	V394	L395	R396																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	140.97Å 140.97Å 133.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30	Depositor
% Data completeness (in resolution range)	90.7 (30.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.224 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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: EPT, FAD, CL

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	0.50	0/4511	1.23	26/6131 (0.4%)
1	B	0.50	0/4511	1.23	26/6131 (0.4%)
All	All	0.50	0/9022	1.23	52/12262 (0.4%)

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	183	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	375	PHE	CB-CG-CD1	7.62	126.13	120.80
1	B	375	PHE	CB-CG-CD1	7.61	126.12	120.80
1	A	97	LEU	CA-CB-CG	-7.36	98.36	115.30

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	4391	0	4330	337	0
1	B	4391	0	4330	333	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	29	9	0
3	B	53	0	29	8	0
4	A	14	0	20	14	0
All	All	8904	0	8738	642	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 37.

The worst 5 of 642 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)
3:A:600:FAD:H8A	3:A:600:FAD:H51A	1.31	1.10
1:A:314:ILE:HD11	1:A:350:ARG:HG3	1.37	1.06
3:B:600:FAD:H51A	3:B:600:FAD:H8A	1.31	1.06
1:B:314:ILE:HD11	1:B:350:ARG:HG3	1.37	1.03
1:A:280:LEU:HD12	1:A:281:ILE:H	1.28	0.99

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	553/560 (99%)	503 (91%)	39 (7%)	11 (2%)	9	43
1	B	553/560 (99%)	504 (91%)	38 (7%)	11 (2%)	9	43
All	All	1106/1120 (99%)	1007 (91%)	77 (7%)	22 (2%)	9	43

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE

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Mol	Chain	Res	Type
1	A	388	ASP
1	A	418	PRO
1	A	475	LYS
1	B	46	ILE

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	475/482 (98%)	459 (97%)	16 (3%)	44	77
1	B	475/482 (98%)	459 (97%)	16 (3%)	44	77
All	All	950/964 (98%)	918 (97%)	32 (3%)	44	77

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	HIS
1	B	105	ASN
1	B	391	GLU
1	B	61	HIS
1	B	114	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	498	ASN
1	B	91	ASN
1	B	498	ASN
1	A	520	ASN
1	B	61	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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$
3	FAD	A	600	1	48,58,58	0.84	1 (2%)	54,89,89	1.42	2 (3%)
4	EPT	A	602	-	14,14,14	1.18	1 (7%)	16,16,16	1.67	5 (31%)
3	FAD	B	600	1	48,58,58	0.85	1 (2%)	54,89,89	1.43	3 (5%)

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
3	FAD	A	600	1	-	0/30/50/50	0/6/6/6
4	EPT	A	602	-	-	0/7/7/7	0/1/1/1
3	FAD	B	600	1	-	0/30/50/50	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	EPT	C5-C4	-2.88	1.33	1.38
3	A	600	FAD	C4-N3	3.22	1.39	1.33
3	B	600	FAD	C4-N3	3.24	1.39	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	600	FAD	C4X-C4-N3	-5.22	116.45	123.59
3	A	600	FAD	C4X-C4-N3	-5.19	116.49	123.59
4	A	602	EPT	C9-C8-C7	-3.02	101.14	113.90
4	A	602	EPT	C5-C6-C1	-2.75	117.27	121.04
4	A	602	EPT	C2-C3-C4	-2.60	116.86	119.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	9	0
4	A	602	EPT	14	0
3	B	600	FAD	8	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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.