



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:51 PM GMT

PDB ID : 1VAO
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

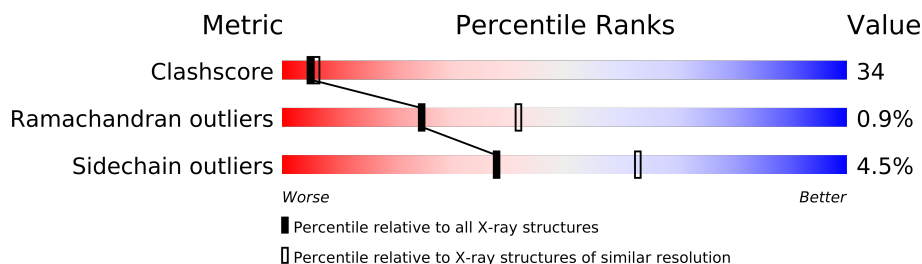
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9134 atoms, of which 0 are hydrogen and 0 are deuterium.

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	36	0	0
			4351	2793	744	790	24			
1	B	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

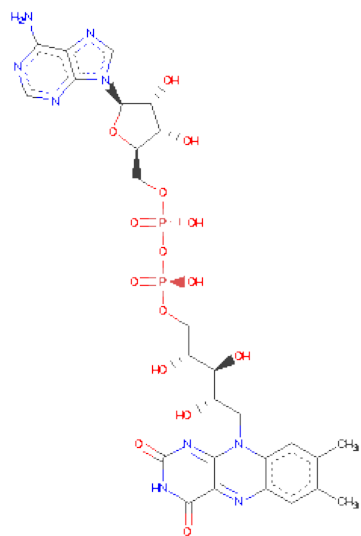


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is water.

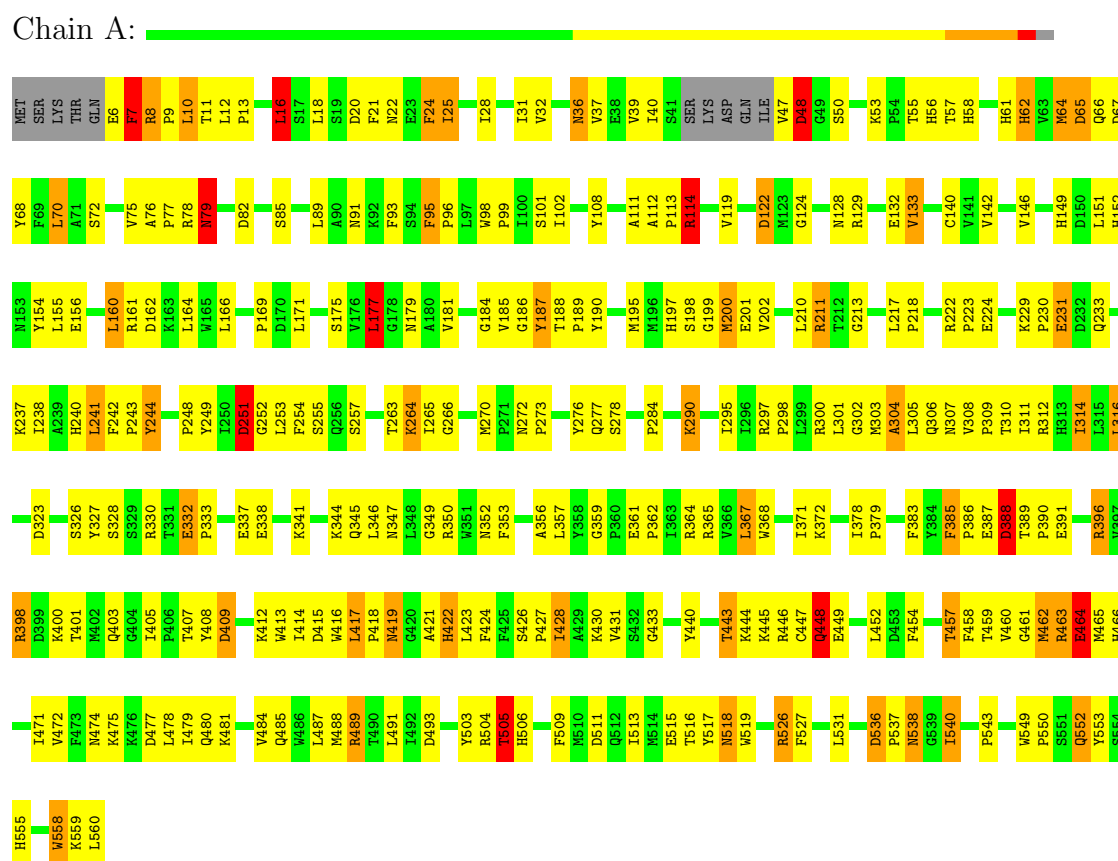
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0
5	B	150	Total O 150 150	0	0

3 Residue-property plots

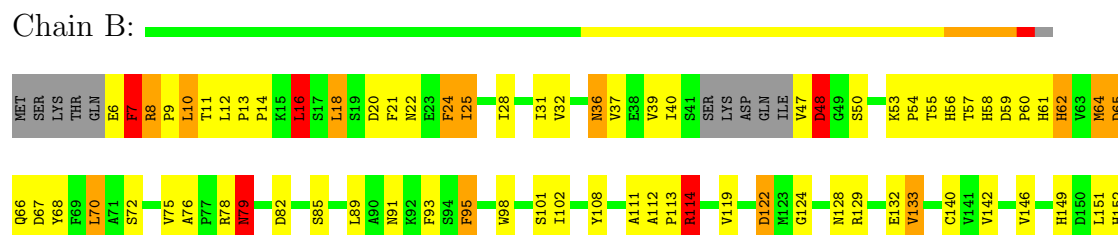
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



Q480	Q481	K482	K483	Y484	Q485	Q486	L487	M488	R489	T490	L491	T492	D493	M500	Y503	R504	T505	H506	F509	N510	D511	Q512	L513	N514	E515	T516	N517	N518	N519	R526	F527	L531	D536	P537	N538	Q539	T540	P543	N549	P550	P550	S551	Q552	Y553	H555	N558	K559	L560				
G404	I405	P406	T407	Y408	D409	K412	W413	I414	D415	W416	L417	P418	M419	G420	A421	H422	L423	F424	I428	A429	K430	V431	S432	G433	Y440	T443	K444	K445	R446	C447	Q448	E449	F454	T457	F458	T459	V460	G461	M462	R463	E464	M465	H466	I471	V472	F473	N474	K475	K476	D477	L478	I479
S328	S329	R330	T331	E332	P333	E337	E338	K341	K344	Q345	L346	N347	L348	G349	R350	N351	N352	F353	A356	L357	T358	G359	P360	E361	P362	T363	R364	R365	T366	N368	L371	K372	P378	P379	F383	T384	F385	P386	E387	D388	T389	P390	R396	V397	R398	D399	K400	T401	M402	Q403		
P243	Y244	G245	F246	G247	P248	Y249	I250	D251	G252	L253	F254	S255	I261	T263	K264	L265	G266	M270	P271	N272	P273	Y276	Q277	S278	T284	K290	I295	I296	R297	P298	L299	R300	L301	G302	M303	A304	L305	Q306	N307	V308	P309	T310	I311	R312	H313	I314	L315	L316	K324	Y327		
N153	Y154	L155	E156	L160	R161	D162	K163	L164	W165	L166	P169	D170	L171	S175	V176	L177	G178	N179	A180	V181	G184	V185	G186	Y187	T188	P189	Y190	M195	H197	S198	G199	M200	E201	V202	L210	R211	R222	P223	E224	K229	P230	E231	D232	Q233	T238	K239	H240	L241	F242			

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	130.24Å 130.24Å 133.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.9 (30.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.88	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, FAD, ACT

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	3/4470 (0.1%)	1.68	89/6075 (1.5%)
1	B	0.76	3/4470 (0.1%)	1.68	89/6075 (1.5%)
All	All	0.76	6/8940 (0.1%)	1.68	178/12150 (1.5%)

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	2	0
1	B	2	0
All	All	4	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	PHE	CE1-CZ	7.54	1.51	1.37
1	B	7	PHE	CE1-CZ	7.50	1.51	1.37
1	A	7	PHE	CD1-CE1	7.35	1.53	1.39
1	B	7	PHE	CD1-CE1	7.35	1.53	1.39
1	A	7	PHE	CD2-CE2	6.36	1.51	1.39

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	ARG	NE-CZ-NH2	-19.95	110.33	120.30
1	A	526	ARG	NE-CZ-NH2	-19.88	110.36	120.30
1	B	526	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	A	526	ARG	NE-CZ-NH1	13.87	127.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ARG	NE-CZ-NH1	12.01	126.31	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	PHE	CA
1	A	332	GLU	CA
1	B	7	PHE	CA
1	B	332	GLU	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4351	0	4288	307	1
1	B	4351	0	4288	286	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	29	6	0
4	B	53	0	29	5	0
5	A	166	0	0	19	0
5	B	150	0	0	11	0
All	All	9134	0	8640	580	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 580 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:600:FAD:H51A	4:B:600:FAD:H8A	1.22	1.16
4:A:600:FAD:H8A	4:A:600:FAD:H51A	1.23	1.11

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.11	1.07
1:A:211:ARG:HG3	1:B:519:TRP:CZ3	1.99	0.98
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.46	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:330:ARG:NH2	1:A:330:ARG:NH2[2.765]	2.15	0.05

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	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	25	42
1	B	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	25	42
All	All	1092/1120 (98%)	1006 (92%)	76 (7%)	10 (1%)	25	42

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	48	ASP
1	A	199	GLY
1	A	388	ASP
1	B	199	GLY

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	470/482 (98%)	449 (96%)	21 (4%)	38	63
1	B	470/482 (98%)	449 (96%)	21 (4%)	38	63
All	All	940/964 (98%)	898 (96%)	42 (4%)	38	63

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	TYR
1	B	64	MET
1	B	464	GLU
1	A	505	THR
1	B	7	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	GLN
1	B	66	GLN
1	B	520	ASN
1	B	56	HIS
1	B	79	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
4	FAD	A	600	1	58,58,58	0.89	1 (1%)	85,89,89	1.30	7 (8%)
2	ACT	A	601	-	1,3,3	3.71	1 (100%)	0,3,3	0.00	-
4	FAD	B	600	1	58,58,58	0.89	1 (1%)	85,89,89	1.30	6 (7%)
2	ACT	B	601	-	1,3,3	3.78	1 (100%)	0,3,3	0.00	-

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
4	FAD	A	600	1	-	0/34/50/50	0/1/6/6
2	ACT	A	601	-	-	0/0/0/0	0/0/0/0
4	FAD	B	600	1	-	0/34/50/50	0/1/6/6
2	ACT	B	601	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ACT	CH3-C	3.78	1.54	1.48
2	A	601	ACT	CH3-C	3.71	1.54	1.48
4	A	600	FAD	O5B-C5B	-3.34	1.31	1.44
4	B	600	FAD	O5B-C5B	-3.33	1.31	1.44

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C2-N1-C10	5.79	120.82	114.98
4	B	600	FAD	C2-N1-C10	5.78	120.81	114.98
4	A	600	FAD	O4B-C1B-N9A	5.11	113.19	108.44
4	B	600	FAD	O4B-C1B-N9A	5.05	113.14	108.44
4	A	600	FAD	C4X-C10-N10	-3.07	118.98	120.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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