



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:24 pm GMT

PDB ID : 1AHV
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH 2-NITRO-P-CRESOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 3.10 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

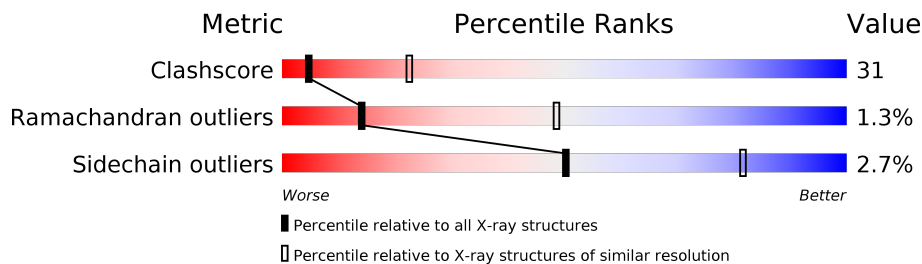
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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
3	NCR	A	601	-	-	X	-
3	NCR	B	601	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8910 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.

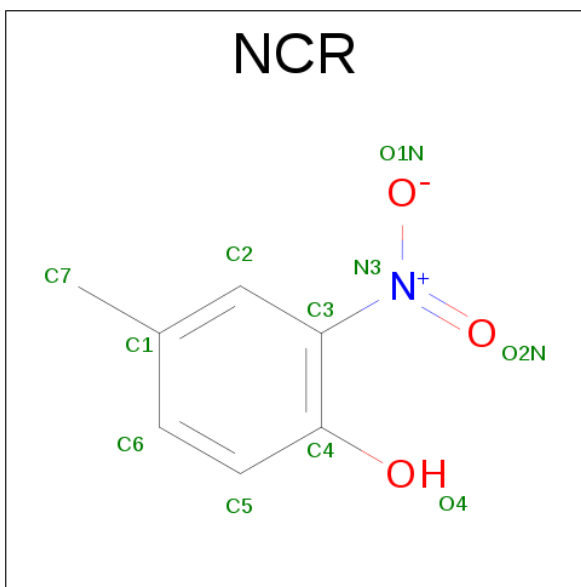
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			

- Molecule 2 is 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-NITRO-P-CRESOL (three-letter code: NCR) (formula: $C_7H_7NO_3$).



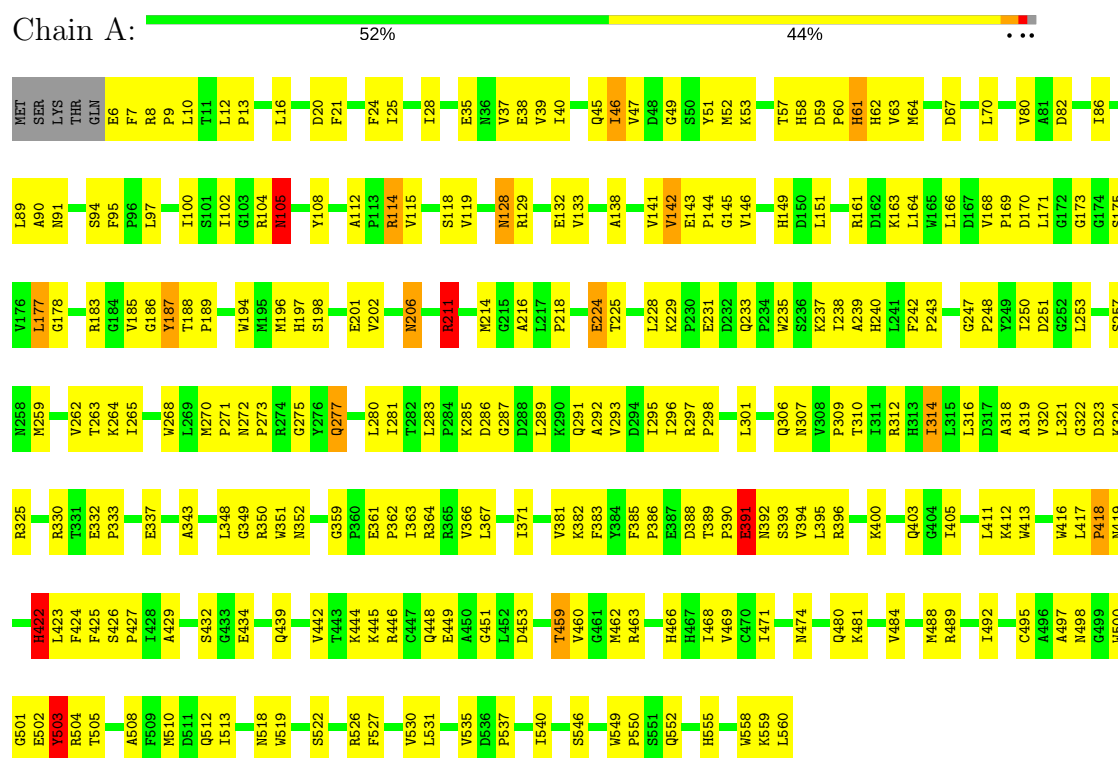
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		

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 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.

Note EDS was not executed.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



K264	E337	P427	T505
L265		I428	
	A343	A429	A508
W268		K430	F509
		V431	M510
P271	L348	S432	B511
N272	G349	G433	Q512
P273	R350	E434	I513
R274	W351		
G275	N352	Q439	M518
V276			W519
Q277	G359	V442	
	P360	T443	S522
L280	E361	K444	
L281	P362	K445	R526
T282	I363	R446	F527
L283	R364	C447	
P284	R365	Q448	V530
K285	V366	E449	L531
D286	L367	A450	
G287		G451	V535
D288	I371	L452	D536
L289		D453	P537
	V381	T459	
K290	K382	V460	I540
Q291	F383		
A292	Y384	G461	S546
D293	F385	N462	
V294	P386	R463	W549
I295	E387	E464	P550
I296	D388	M465	S551
I297	T389	H466	Q552
P298	P390	H467	
	E391	I468	H555
L301	N392	V469	
	S393	C470	W558
Q306	V394	I471	K559
N307	L395		L560
V308	R396	N474	
P309			
T310	K400	Q480	
I311		K481	
R312			
H313	Q403	V484	
I314	G404		
L315	I405		
L316		M488	
D317	L411	R489	
A318	K412		
A319	W413	I492	
V320			
L321	W416	C495	
G322	L417	A496	
D323	P418	A497	
K324	N419	N498	
R325		G499	
	R422	V500	
	L423	G501	
R330	F424	E502	
T331	F425	Y503	
E332	S426	R504	

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	140.62Å 140.62Å 132.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
% Data completeness (in resolution range)	94.3 (30.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.62	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.205 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8910	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: NCR, 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	0.33	0/4511	1.02	13/6131 (0.2%)
1	B	0.33	0/4511	1.02	13/6131 (0.2%)
All	All	0.33	0/9022	1.02	26/12262 (0.2%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	TYR	N-CA-C	7.66	131.68	111.00
1	B	187	TYR	N-CA-C	7.65	131.66	111.00
1	B	7	PHE	N-CA-C	7.37	130.89	111.00
1	A	7	PHE	N-CA-C	7.36	130.87	111.00
1	B	129	ARG	N-CA-C	6.96	129.79	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	278	0
1	B	4391	0	4330	278	0
2	A	53	0	29	6	0
2	B	53	0	29	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	6	6	0
3	B	11	0	6	7	0
All	All	8910	0	8730	539	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 31.

The worst 5 of 539 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:A:510:MET:HE1	1:A:546:SER:H	1.16	1.10
1:A:314:ILE:HD11	1:A:350:ARG:HG3	1.32	1.08
1:B:314:ILE:HD11	1:B:350:ARG:HG3	1.32	1.08
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.38	1.02
2:B:600:FAD:H51A	2:B:600:FAD:H8A	1.38	1.02

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%)	510 (92%)	36 (6%)	7 (1%)	14	48
1	B	553/560 (99%)	509 (92%)	37 (7%)	7 (1%)	14	48
All	All	1106/1120 (99%)	1019 (92%)	73 (7%)	14 (1%)	14	48

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	GLY

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Mol	Chain	Res	Type
1	A	170	ASP
1	A	418	PRO
1	B	49	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	475/482 (98%)	462 (97%)	13 (3%)	50	81
1	B	475/482 (98%)	462 (97%)	13 (3%)	50	81
All	All	950/964 (98%)	924 (97%)	26 (3%)	50	81

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	HIS
1	B	105	ASN
1	B	422	HIS
1	A	503	TYR
1	B	61	HIS

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	498	ASN
1	B	84	GLN
1	B	485	GLN
1	B	61	HIS
1	B	91	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	51,58,58	0.93	2 (3%)	54,89,89	1.47	3 (5%)
3	NCR	A	601	-	9,11,11	0.69	0	11,15,15	2.04	1 (9%)
2	FAD	B	600	1	51,58,58	0.92	2 (3%)	54,89,89	1.47	3 (5%)
3	NCR	B	601	-	9,11,11	0.70	0	11,15,15	2.04	1 (9%)

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	-	0/28/50/50	0/6/6/6
3	NCR	A	601	-	-	0/2/4/4	0/1/1/1
2	FAD	B	600	1	-	0/28/50/50	0/6/6/6
3	NCR	B	601	-	-	0/2/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C2-N1	-2.73	1.32	1.38
2	B	600	FAD	C2-N1	-2.70	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C4-N3	3.47	1.39	1.33
2	B	600	FAD	C4-N3	3.49	1.39	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C4X-C4-N3	-5.00	116.36	123.48
2	B	600	FAD	C4X-C4-N3	-4.97	116.41	123.48
2	A	600	FAD	C1'-N10-C9A	2.04	120.22	118.35
2	B	600	FAD	C1'-N10-C9A	2.09	120.26	118.35
3	A	601	NCR	C2-C3-N3	5.79	122.55	115.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	6	0
3	A	601	NCR	6	0
2	B	600	FAD	6	0
3	B	601	NCR	7	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.