



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AHU
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH P-CRESOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.70 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

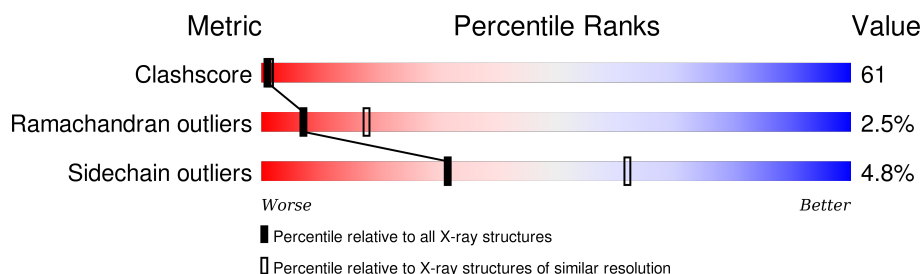
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	 26% 56% 16% ..
1	B	560	 25% 57% 16% ..

2 Entry composition [i](#)

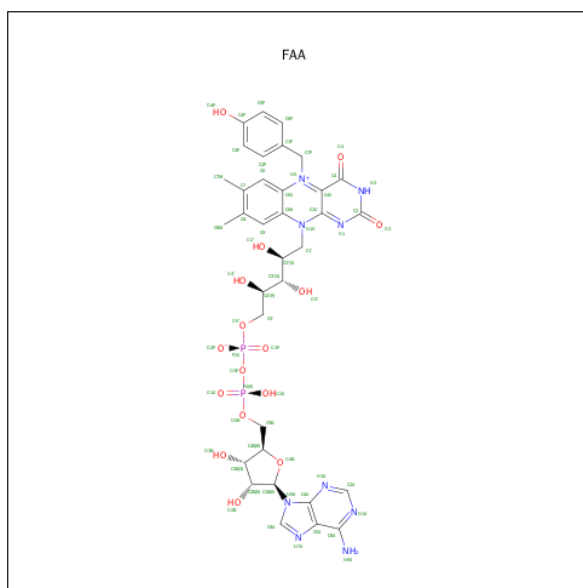
There are 3 unique types of molecules in this entry. The entry contains 9011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	37	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	37	0	0
			4391	2817	751	799	24			

- Molecule 2 is N5-(4-HYDROXYBENZYL)FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAA) (formula: C₃₄H₃₉N₉O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			61	34	9	16	2		
2	B	1	Total	C	N	O	P	0	0
			61	34	9	16	2		

- Molecule 3 is water.

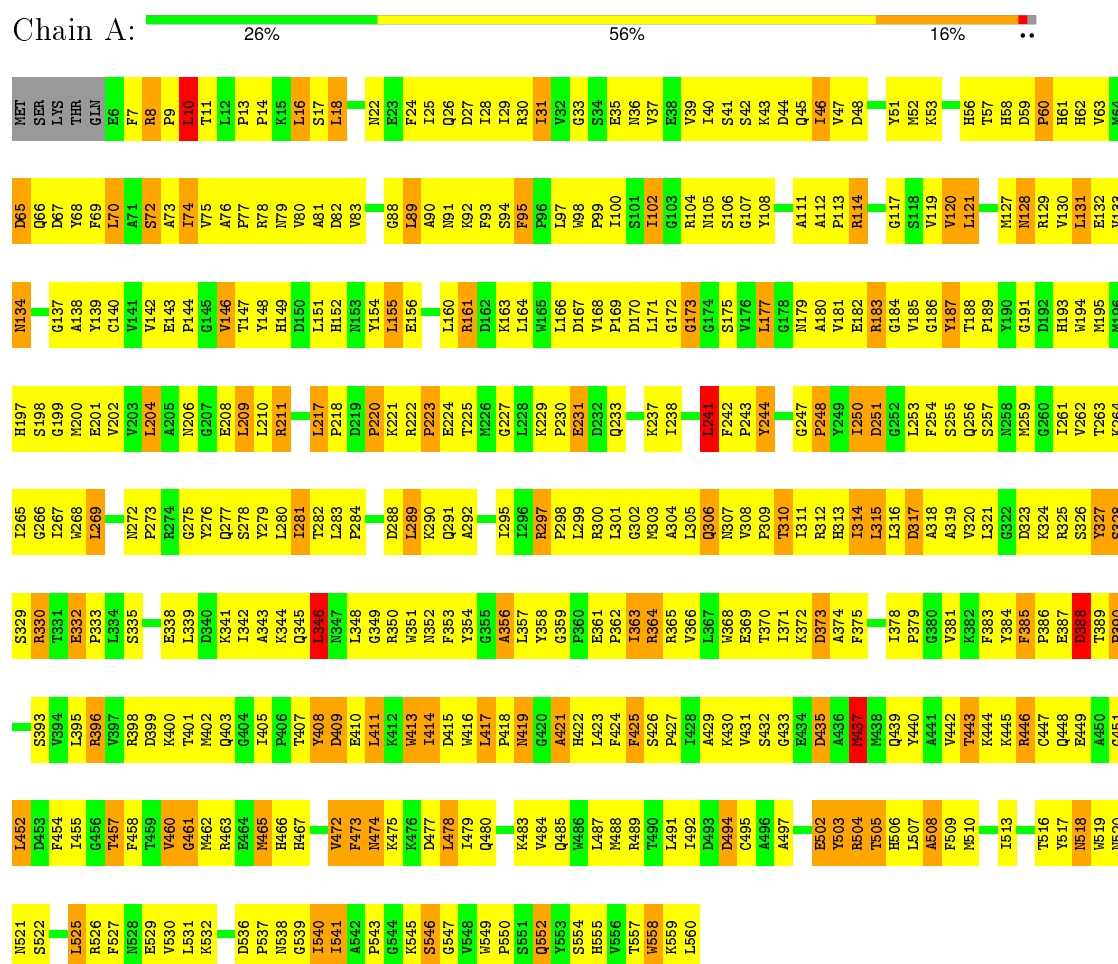
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	52	Total 52	O 52	1	0

3 Residue-property plots

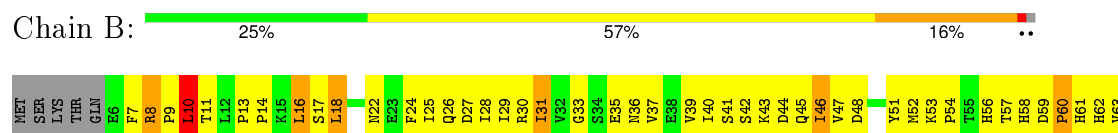
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



T516	E449	D388	S326	T263	H197	M134	M64
T517	A450	T389	Y327	K264	S198	G137	D65
M518	G451	P390	S328	I265	G199		Q66
M519	L452		S329	G266	M200		D67
M520	D453	S393	R330	I267	E201	Y139	Y68
M521	F454	V394	T331	W268	V202	C140	F69
S522	L455	L395	E332	L269	V203	W141	L70
	G456	R396	E333	M270	L204	V142	A71
	T457	V397	L334	P271	A205	E143	S72
L525	F458	R398	S335	M272	G207	P144	A73
R526	T459	D399		P273	G145	G146	G147
F527	V460	K400	E338	R274	E208	V147	V75
M528	G461	T401	L339	G275	L209	A147	A76
E529	M462	M402	E340	Y276	L210	Y148	F77
V530	R463	Q403	K341	Q277	R211	H149	R78
L531	E464	G404	I342	S278		D150	M79
K532	M465	I405	A343	Y279	W214	L151	W80
	H466	P406	K344	L280		H152	A81
D536	H467	T407	Q345	I281	L217	M153	D82
P537		Y408	E346	T282	P218	Y154	W83
M538	V472	D409	K347	L283	D219	E156	
G539	F473	E410	L348	P284	K221		L89
I540	M474	L411	G349		R222		A90
I541	K475	K412	R350	D288	R223	L160	M91
A542	V476	M413	R351	L289	E224	R161	Q92
P543	D477	I414	R352	K290	T225	D162	F93
G544	L478	D415	F353	Q291	W226	K163	S94
K545	L479	W416	Y354	A292	G227	L164	F95
S546	Q480	L417	G355		L295	W165	P96
		P418	A356	I296	L228	L166	L97
W549	K483	M419	L357	R297	K229	D167	W98
P550	V484	G420	Y358	R298	P230	V168	P99
S551	Q485	A421	G359	E231	E231	P169	I100
Q552	D486	R422	P360	L299	D232	D170	S101
Y553	L487	L423	P361	R300	Q233	L171	I102
M554	M488	F424	P362	L301		G172	G103
H555	R489	F425	I363	G302	K237	G173	R104
W556	T490	S426	R364	K303	L238	G174	M105
T557	L491	P427	R365	A304		S175	S106
W558	L492	I428	Y366	L305	L241	V176	G107
K559	D493	A429	L367	Q306	F242	L177	Y108
	C495	V431	K368	K307	P243	G178	
	L496	S432	T370	V308	Y244	M179	A111
	A497	G433	I371	P309		A180	A112
		E434	K372	T310	G247	V181	P113
M500		D435	D373	I311	P248	E182	R114
G501	G501	A436	A374	R312	Y249	R183	
B502	Y503	K437	F375	H313	I250	G184	G117
Y503	R504	M438		I314	D251	V185	S118
R504	T505	Q439	I378	L315	G252	G186	V119
H506	H506	A441	P379	L316	L253	Y187	L121
L507	V507	K441	G380	D317	F254	T188	
A508	V507	T443	V381	A318	S255	P189	M127
F509	M508	K444	K382	A319	Q256	Y190	N128
M510	F509	K445	F383	V320	S257	G191	R129
B511	M510	R446	V384	L321	W258	D192	M129
Q512	P511	C447	K385	G322	K259	H193	V130
I513	I513	Q448	P386	K323	G260	W194	L131
				K324	L261	M195	E132
				R325	V262	M196	V133

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	128.82Å 128.82Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.4 (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.97	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.221 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9011	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: FAA

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	0.73	0/4511	1.74	110/6131 (1.8%)
1	B	0.73	0/4511	1.74	108/6131 (1.8%)
All	All	0.73	0/9022	1.74	218/12262 (1.8%)

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

There are no bond length outliers.

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	B	330	ARG	NE-CZ-NH1	-11.24	114.68	120.30
1	A	536	ASP	C-N-CD	-9.85	98.92	120.60
1	B	536	ASP	C-N-CD	-9.85	98.93	120.60
1	B	417	LEU	CA-CB-CG	-9.34	93.83	115.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	187	TYR	CA
1	A	332	GLU	CA
1	B	187	TYR	CA

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Mol	Chain	Res	Type	Atom
1	B	332	GLU	CA

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	531	0
1	B	4391	0	4330	548	0
2	A	61	0	35	13	0
2	B	61	0	35	13	0
3	A	55	0	0	9	0
3	B	52	0	0	9	0
All	All	9011	0	8730	1058	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 61.

The worst 5 of 1058 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:A:600:FAA:H8A	2:A:600:FAA:H51A	1.21	1.13
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.32	1.11
2:B:600:FAA:H51A	2:B:600:FAA:H8A	1.21	1.10
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.32	1.07
1:A:507:LEU:HA	1:A:510:MET:HE3	1.37	1.06

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%)	470 (85%)	69 (12%)	14 (2%)	7	18
1	B	553/560 (99%)	470 (85%)	69 (12%)	14 (2%)	7	18
All	All	1106/1120 (99%)	940 (85%)	138 (12%)	28 (2%)	7	18

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	B	44	ASP
1	A	30	ARG
1	A	46	ILE
1	A	328	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	475/482 (98%)	452 (95%)	23 (5%)	31	62
1	B	475/482 (98%)	452 (95%)	23 (5%)	31	62
All	All	950/964 (98%)	904 (95%)	46 (5%)	31	62

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	466	HIS

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Mol	Chain	Res	Type
1	B	65	ASP
1	B	443	THR
1	A	478	LEU
1	B	10	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	520	ASN
1	B	66	GLN
1	B	520	ASN
1	A	552	GLN
1	B	58	HIS

5.3.3 RNA [i](#)

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](#)

2 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	FAA	A	600	1	55,67,67	0.90	1 (1%)	61,102,102	2.08	5 (8%)
2	FAA	B	600	1	55,67,67	0.89	1 (1%)	61,102,102	2.08	5 (8%)

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	FAA	A	600	1	-	0/34/54/54	0/7/7/7
2	FAA	B	600	1	-	0/34/54/54	0/7/7/7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAA	C4-N3	3.38	1.39	1.33
2	B	600	FAA	C4-N3	3.40	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAA	C7P-N5-C5X	-11.46	102.71	120.13
2	B	600	FAA	C7P-N5-C5X	-11.46	102.72	120.13
2	B	600	FAA	C4X-C4-N3	-5.62	115.91	123.59
2	A	600	FAA	C4X-C4-N3	-5.59	115.94	123.59
2	A	600	FAA	C2B-C1B-N9A	-2.78	110.05	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAA	13	0
2	B	600	FAA	13	0

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 [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.