



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:12 pm GMT

PDB ID : 1E8F
Title : STRUCTURE OF THE H61T MUTANT OF THE FLAVOENZYME
VANILLYL-ALCOHOL OXIDASE IN THE APO FORM
Authors : Mattevi, A.; Fraaije, M.W.
Deposited on : 2000-09-20
Resolution : 2.90 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

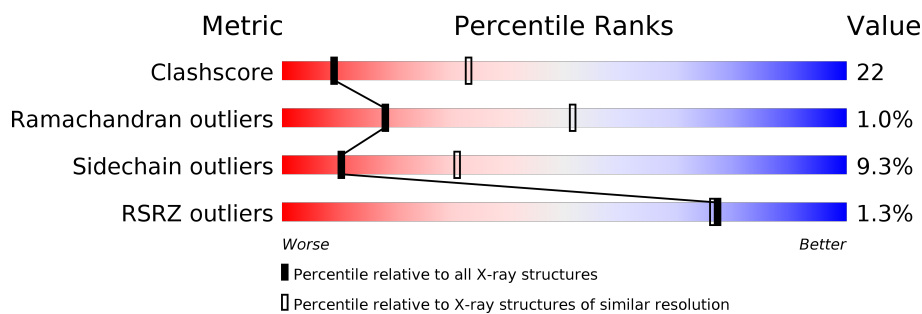
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	560	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>41%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	560	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>40%</div> <div>8%</div> <div>..</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8642 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	545	Total	C	N	O	S	136	0	0
			4311	2768	737	782	24			
1	B	545	Total	C	N	O	S	136	0	0
			4311	2768	737	782	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	HIS	ENGINEERED	UNP P56216
B	61	THR	HIS	ENGINEERED	UNP P56216

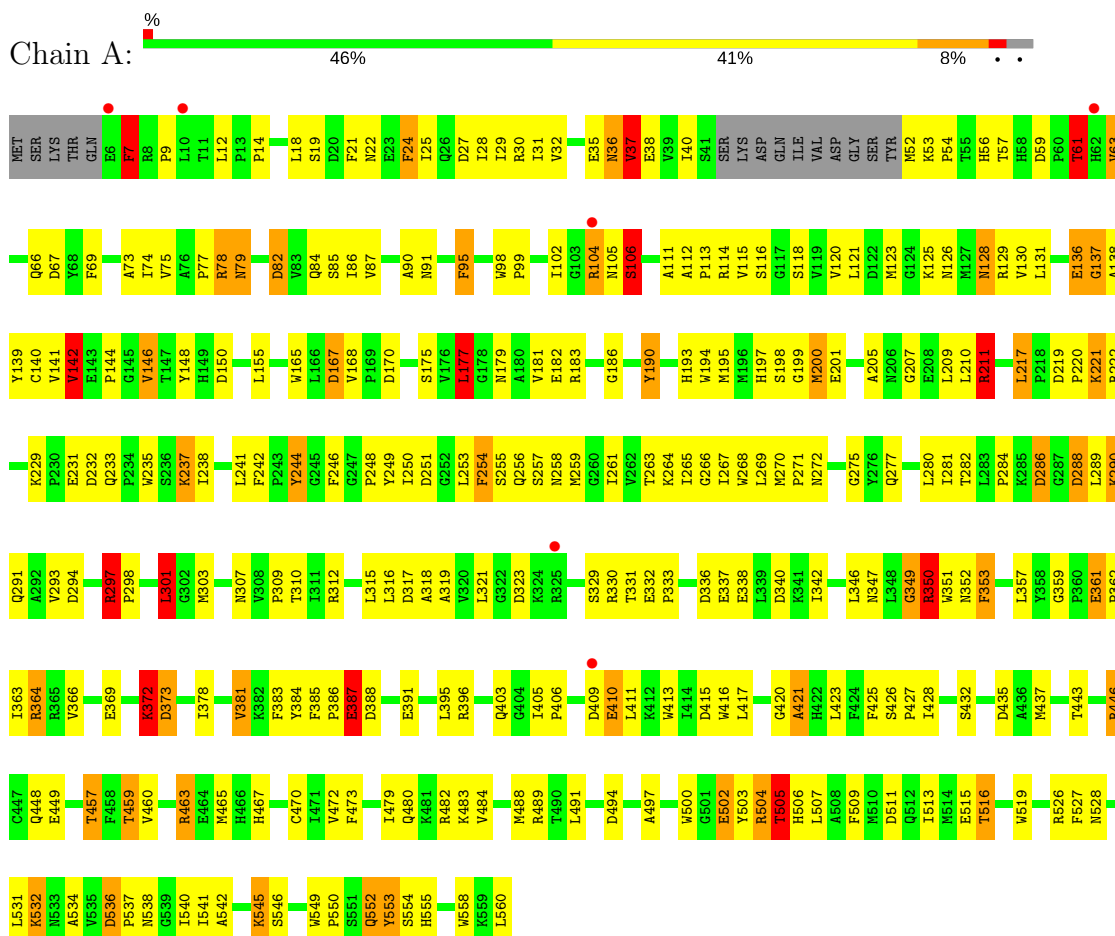
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	8	Total	O	0	0
			8	8		

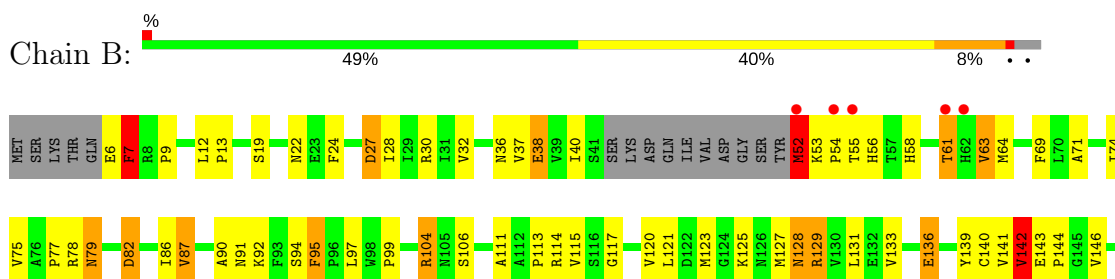
3 Residue-property plots

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.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



S551	Q552	H555	V558	K559	L560	Q480	K481	R482	K483	V484	Q485	M488	R489	T490	L491	I492	A497	W500	G501	E502	Y503	R504	T505	H506	L507	A508	F509	M510	D511	Q512	I513	T516	N517	W518	W519	N520	N521	S522	S523	F524	L525	R526	F527	N528	E529	V530	L531	K532	N533	A534	V535	D536	P537	N538	I541	A542	V548	W549	P550	R398	M402	Q403	G404	T405	P406	D409	E410	L411	K412	W413	I414	D415	W416	L417	P418	M419	G420	A421	H422	L423	F424	F425	S426	P427	L428	V431	S432	M437	T443	R446	D453	T457	F458	T459	V460	G461	M462	R463	E464	M465	H466	H467	I468	V469	C470	F473	K476	I479	L315	A318	A319	V320	L321	R325	S329	R330	T331	E332	P333	D336	D340	A343	K344	Q345	L346	G349	R350	W351	N352	F353	Y354	L357	T358	G359	P362	I363	R364	R365	Y366	K372	D373	I378	V381	K382	F383	Y384	F385	P386	E387	E391	V394	L395	R396	V397	L241	Y244	P248	Y249	L250	L253	F254	S255	Q256	S257	N258	I261	K264	L265	G266	L267	W268	L269	M270	P271	M195	H196	H197	S198	G199	M200	E201	W202	V203	W206	G207	E208	R211	L217	P218	D219	P220	K221	E224	T225	M226	K229	P230	E231	D232	Q233	K237	L238	A239	H240	D150	Y154	L155	D167	V168	P169	D170	L177	V181	E182	R183	G184	V185	G186	Y187	T188	P189	Y190	W194	M195	H196	H197	S198	G199	M200	E201	W202	V203	W206	G207	E208	R211	L217	P218	D219	P220	K221	E224	T225	M226	K229	P230	E231	D232	Q233	K237	L238	A239	H240
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4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	129.28Å 129.28Å 130.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.90) 98.1 (19.95-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.312 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.005 for -l,-k,-h 0.015 for -h,-l,-k 0.000 for -h,l,k 0.039 for -h,k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	4/4428 (0.1%)	1.88	123/6018 (2.0%)
1	B	0.80	10/4428 (0.2%)	1.81	92/6018 (1.5%)
All	All	0.78	14/8856 (0.2%)	1.85	215/12036 (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	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	LYS	CG-CD	-24.75	0.68	1.52
1	B	53	LYS	CB-CG	18.00	2.01	1.52
1	B	52	MET	CA-CB	15.90	1.89	1.53
1	B	476	LYS	CG-CD	12.89	1.96	1.52
1	B	325	ARG	CB-CG	-9.83	1.26	1.52

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	TYR	CB-CG-CD1	21.52	133.91	121.00
1	B	463	ARG	NE-CZ-NH1	20.52	130.56	120.30
1	A	221	LYS	CG-CD-CE	-19.44	53.59	111.90
1	B	325	ARG	CB-CG-CD	19.04	161.11	111.60
1	B	53	LYS	CB-CA-C	18.17	146.73	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	VAL	Mainchain

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	4311	0	4260	210	18
1	B	4311	0	4260	192	10
2	A	12	0	0	2	0
2	B	8	0	0	1	0
All	All	8642	0	8520	364	18

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 22.

The worst 5 of 364 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:B:63:VAL:HG11	1:B:423:LEU:HD11	1.44	1.00
1:B:310:THR:HG22	1:B:459:THR:HG22	1.45	0.96
1:A:357:LEU:HB3	1:A:364:ARG:HG2	1.55	0.89
1:A:310:THR:HG22	1:A:459:THR:HG22	1.55	0.88
1:B:79:ASN:ND2	1:B:82:ASP:H	1.74	0.86

The worst 5 of 18 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:NH2	1:A:332:GLU:CB[2_765]	0.47	1.73
1:A:52:MET:SD	1:B:415:ASP:OD1[6_655]	0.77	1.43
1:A:18:LEU:CD2	1:A:30:ARG:NH1[3_655]	1.13	1.07
1:A:330:ARG:NH2	1:A:332:GLU:CA[2_765]	1.17	1.03
1:A:53:LYS:CA	1:B:412:LYS:NZ[6_655]	1.35	0.85

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	541/560 (97%)	494 (91%)	40 (7%)	7 (1%)	14	43
1	B	541/560 (97%)	490 (91%)	47 (9%)	4 (1%)	25	60
All	All	1082/1120 (97%)	984 (91%)	87 (8%)	11 (1%)	18	51

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	PHE
1	A	7	PHE
1	A	67	ASP
1	B	410	GLU
1	A	410	GLU

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	466/481 (97%)	422 (91%)	44 (9%)	10	30
1	B	466/481 (97%)	423 (91%)	43 (9%)	11	32
All	All	932/962 (97%)	845 (91%)	87 (9%)	10	31

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	THR

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Mol	Chain	Res	Type
1	B	79	ASN
1	B	503	TYR
1	A	516	THR
1	B	19	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	GLN
1	B	79	ASN
1	B	467	HIS
1	A	520	ASN
1	B	520	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 ⓘ

There are no ligands in this entry.

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](#)

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, 95th 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 ²)	Q<0.9
1	A	545/560 (97%)	-0.32	6 (1%) 80 79	3, 14, 38, 49	30 (5%)
1	B	545/560 (97%)	-0.28	8 (1%) 74 72	3, 14, 38, 50	30 (5%)
All	All	1090/1120 (97%)	-0.30	14 (1%) 77 76	3, 14, 38, 50	60 (5%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	MET	4.2
1	A	409	ASP	3.8
1	B	55	THR	3.0
1	B	418	PRO	3.0
1	B	409	ASP	3.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.