



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:35 PM GMT

PDB ID : 1E5R  
Title : PROLINE 3-HYDROXYLASE (TYPE II) -APO FORM  
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Deposited on : 2000-07-28  
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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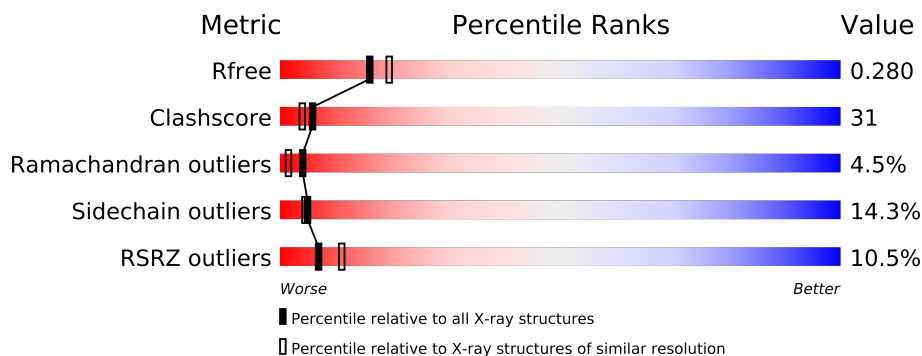
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	290	
1	B	290	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4474 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 PROLINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2110	1357	363	384	6			
1	B	262	Total	C	N	O	S	0	0	0
			2106	1354	363	383	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	110	Total	O	0	0
			110	110		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.54Å 72.54Å 223.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.53 – 2.30 28.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.53-2.30) 99.3 (28.51-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.69 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.225 , 0.275 0.223 , 0.280	Depositor DCC
$R_{free}$ test set	1252 reflections (4.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.7	EDS
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 31127 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.94	2/2167 (0.1%)	1.00	6/2941 (0.2%)
1	B	0.91	2/2161 (0.1%)	0.94	4/2933 (0.1%)
All	All	0.92	4/4328 (0.1%)	0.97	10/5874 (0.2%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	LYS	CD-CE	5.71	1.65	1.51
1	A	210	GLU	CG-CD	5.63	1.60	1.51
1	A	161	VAL	CB-CG1	5.59	1.64	1.52
1	B	237	VAL	CB-CG2	5.26	1.63	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	LEU	CA-CB-CG	8.45	134.72	115.30
1	A	75	VAL	C-N-CD	-6.50	106.29	120.60
1	B	263	LYS	CD-CE-NZ	6.37	126.34	111.70
1	A	76	PRO	N-CA-C	6.28	128.41	112.10
1	A	36	PHE	N-CA-C	-5.83	95.26	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	TYR	Sidechain

## 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	2110	0	2040	143	0
1	B	2106	0	2036	117	0
2	A	148	0	0	9	0
2	B	110	0	0	9	0
All	All	4474	0	4076	260	0

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 31.

The worst 5 of 260 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:19:ASP:OD1	1:A:75:VAL:HG12	1.62	0.99
1:A:92:GLN:HE21	1:A:176:ALA:HB2	1.23	0.97
1:A:274:PHE:HB2	1:A:281:LEU:HD13	1.46	0.96
1:A:90:HIS:CD2	1:A:90:HIS:H	1.79	0.95
1:A:90:HIS:HD2	1:A:90:HIS:H	1.14	0.95

There are no symmetry-related clashes.

## 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	252/290 (87%)	219 (87%)	17 (7%)	16 (6%)	2	1
1	B	254/290 (88%)	228 (90%)	19 (8%)	7 (3%)	8	4
All	All	506/580 (87%)	447 (88%)	36 (7%)	23 (4%)	4	1

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PHE
1	A	122	ARG
1	A	180	PRO
1	A	185	GLU
1	A	284	ARG

### 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	226/256 (88%)	194 (86%)	32 (14%)	5	4
1	B	223/256 (87%)	191 (86%)	32 (14%)	5	4
All	All	449/512 (88%)	385 (86%)	64 (14%)	5	4

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	HIS
1	B	84	THR
1	B	279	ARG
1	A	231	LEU
1	B	2	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	GLN
1	B	38	ASN
1	B	211	HIS

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Mol	Chain	Res	Type
1	A	162	ASN
1	B	220	GLN

### 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 ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/290 (89%)	0.33	29 (11%) 6 9	21, 42, 89, 110	0
1	B	262/290 (90%)	0.28	26 (9%) 8 13	22, 48, 98, 111	0
All	All	522/580 (90%)	0.31	55 (10%) 7 11	21, 45, 95, 111	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	GLY	6.8
1	A	178	ASP	6.5
1	A	284	ARG	5.7
1	B	176	ALA	5.5
1	B	49	ALA	5.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.