



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:36 AM GMT

PDB ID : 2XSN  
Title : Crystal Structure of Human Tyrosine Hydroxylase Catalytic Domain  
Authors : Muniz, J.R.C.; Cooper, C.D.O.; Yue, W.W.; Kryzstofinska, E.; Von Delft, F.; Knapp, S.; Gileadi, O.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Kavanagh, K.L.; Oppermann, U.  
Deposited on : 2010-10-29  
Resolution : 2.68 Å(reported)

This is a full wwPDB validation 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>

---

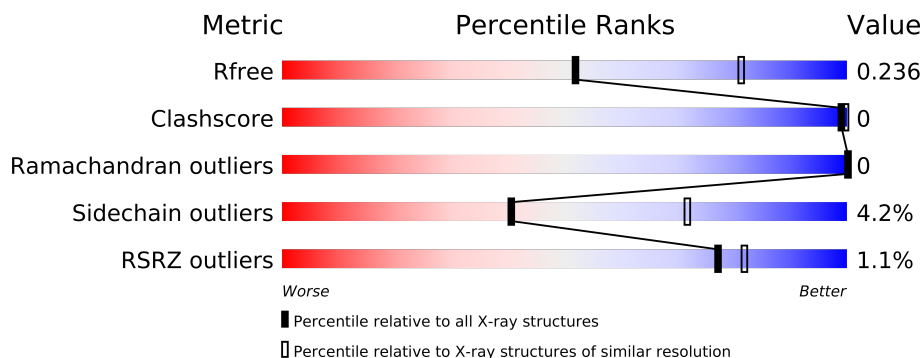
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.68 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	2010 (2.70-2.66)
Clashscore	79885	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)
RSRZ outliers	66119	2013 (2.70-2.66)

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	343	
1	B	343	
1	C	343	
1	D	343	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10951 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 TYROSINE 3-MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	1	0
			2691	1715	460	506	10			
1	B	336	Total	C	N	O	S	0	3	0
			2709	1726	460	513	10			
1	C	328	Total	C	N	O	S	0	1	0
			2626	1674	448	494	10			
1	D	342	Total	C	N	O	S	0	1	0
			2694	1721	452	511	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	MET	LYS	ENGINEERED MUTATION	UNP P07101
A	529	ALA	-	EXPRESSION TAG	UNP P07101
A	530	GLU	-	EXPRESSION TAG	UNP P07101
A	531	ASN	-	EXPRESSION TAG	UNP P07101
A	532	LEU	-	EXPRESSION TAG	UNP P07101
A	533	TYR	-	EXPRESSION TAG	UNP P07101
A	534	PHE	-	EXPRESSION TAG	UNP P07101
A	535	GLN	-	EXPRESSION TAG	UNP P07101
B	193	MET	LYS	ENGINEERED MUTATION	UNP P07101
B	529	ALA	-	EXPRESSION TAG	UNP P07101
B	530	GLU	-	EXPRESSION TAG	UNP P07101
B	531	ASN	-	EXPRESSION TAG	UNP P07101
B	532	LEU	-	EXPRESSION TAG	UNP P07101
B	533	TYR	-	EXPRESSION TAG	UNP P07101
B	534	PHE	-	EXPRESSION TAG	UNP P07101
B	535	GLN	-	EXPRESSION TAG	UNP P07101
C	193	MET	LYS	ENGINEERED MUTATION	UNP P07101
C	529	ALA	-	EXPRESSION TAG	UNP P07101
C	530	GLU	-	EXPRESSION TAG	UNP P07101
C	531	ASN	-	EXPRESSION TAG	UNP P07101
C	532	LEU	-	EXPRESSION TAG	UNP P07101

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	533	TYR	-	EXPRESSION TAG	UNP P07101
C	534	PHE	-	EXPRESSION TAG	UNP P07101
C	535	GLN	-	EXPRESSION TAG	UNP P07101
D	193	MET	LYS	ENGINEERED MUTATION	UNP P07101
D	529	ALA	-	EXPRESSION TAG	UNP P07101
D	530	GLU	-	EXPRESSION TAG	UNP P07101
D	531	ASN	-	EXPRESSION TAG	UNP P07101
D	532	LEU	-	EXPRESSION TAG	UNP P07101
D	533	TYR	-	EXPRESSION TAG	UNP P07101
D	534	PHE	-	EXPRESSION TAG	UNP P07101
D	535	GLN	-	EXPRESSION TAG	UNP P07101

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	68	Total O 68 68	0	0
3	C	57	Total O 57 57	0	0
3	D	35	Total O 35 35	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.

- Molecule 1: TYROSINE 3-MONOOXYGENASE

Chain A: 



- Molecule 1: TYROSINE 3-MONOOXYGENASE

Chain B: 



- Molecule 1: TYROSINE 3-MONOOXYGENASE

Chain C: 



- Molecule 1: TYROSINE 3-MONOOXYGENASE

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.42Å 191.42Å 168.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.66 – 2.68 62.66 – 2.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.66-2.68) 99.8 (62.66-2.68)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.69Å)	Xtriage
Refinement program	BUSTER-TNT 2.8.0	Depositor
R, $R_{free}$	0.189 , 0.222 0.200 , 0.236	Depositor DCC
$R_{free}$ test set	2604 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 51346 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10951	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.52% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.50	0/2761	0.63	0/3746
1	B	0.51	0/2779	0.63	0/3771
1	C	0.49	0/2692	0.63	0/3651
1	D	0.49	0/2766	0.63	0/3762
All	All	0.50	0/10998	0.63	0/14930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2691	0	0	0	0
1	B	2709	0	0	1	0
1	C	2626	0	0	0	0
1	D	2694	0	0	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	67	0	0	0	0
3	B	68	0	0	0	0
3	C	57	0	0	0	0
3	D	35	0	0	0	0
All	All	10951	0	0	1	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 0.

All (1) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:314:THR:O	1:B:337:ARG:NH1	2.53	0.41

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	334/343 (97%)	325 (97%)	9 (3%)	0	100	100
1	B	337/343 (98%)	329 (98%)	8 (2%)	0	100	100
1	C	325/343 (95%)	316 (97%)	9 (3%)	0	100	100
1	D	341/343 (99%)	331 (97%)	10 (3%)	0	100	100
All	All	1337/1372 (97%)	1301 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	287/295 (97%)	276 (96%)	11 (4%)	44	75
1	B	286/295 (97%)	275 (96%)	11 (4%)	44	75
1	C	275/295 (93%)	259 (94%)	16 (6%)	28	55
1	D	278/295 (94%)	267 (96%)	11 (4%)	42	73
All	All	1126/1180 (95%)	1077 (96%)	49 (4%)	40	70

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	HIS
1	A	298	ASP
1	A	316	PHE
1	A	340	GLN
1	A	345	ILE
1	A	352	MET
1	A	359	CYS
1	A	439	GLU
1	A	469	SER
1	A	484	ARG
1	A	504	GLN
1	B	208	HIS
1	B	228	GLN
1	B	291	ARG
1	B	316	PHE
1	B	319	ARG
1	B	345	ILE
1	B	352	MET
1	B	439	GLU
1	B	469	SER
1	B	507[A]	ARG
1	B	507[B]	ARG
1	C	208	HIS
1	C	243	GLN
1	C	291	ARG
1	C	298	ASP
1	C	316	PHE
1	C	319	ARG
1	C	345	ILE
1	C	351	PRO
1	C	358	ASP
1	C	429	GLU
1	C	439	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	459	GLN
1	C	469	SER
1	C	507	ARG
1	C	508	ARG
1	C	525	SER
1	D	208	HIS
1	D	220	LEU
1	D	298	ASP
1	D	316	PHE
1	D	345	ILE
1	D	352	MET
1	D	359[A]	CYS
1	D	359[B]	CYS
1	D	439	GLU
1	D	469	SER
1	D	507	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	335/343 (97%)	-0.28	2 (0%) 86 90	27, 48, 75, 92	0
1	B	336/343 (97%)	-0.31	1 (0%) 91 95	28, 47, 75, 93	0
1	C	328/343 (95%)	-0.27	4 (1%) 75 80	26, 52, 90, 119	0
1	D	342/343 (99%)	-0.15	8 (2%) 57 62	31, 56, 102, 132	0
All	All	1341/1372 (97%)	-0.25	15 (1%) 77 82	26, 51, 92, 132	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	414	GLY	4.5
1	C	352	MET	3.7
1	D	427	TYR	3.3
1	D	486	PHE	3.3
1	C	353	HIS	3.0
1	C	355	PRO	2.8
1	D	415	GLU	2.7
1	A	214	PHE	2.6
1	D	468	PHE	2.3
1	A	416	VAL	2.3
1	D	461	VAL	2.3
1	D	434	LEU	2.1
1	B	440	ILE	2.1
1	D	194	VAL	2.1
1	C	533	TYR	2.1

### 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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	D	1536	1/1	0.12	-0.06	84,84,84,84	0
2	ZN	A	1528	1/1	0.08	-2.19	60,60,60,60	0
2	ZN	B	1529	1/1	0.08	-4.41	57,57,57,57	0
2	ZN	C	1536	1/1	0.07	-5.01	77,77,77,77	0

### 6.5 Other polymers

There are no such residues in this entry.