

wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 12:36 PM EDT

PDB ID : 3RNA

 $\label{thm:total} \hbox{Title} \quad : \quad \hbox{Structure of the Toluene/o-Xylene Monooxygenase Hydroxylase } \hbox{T201S/I100W}$

Double Mutant

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Deposited on : 2011-04-22

Resolution : 3.00 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

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467 Xtriage (Phenix): 1.13

EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

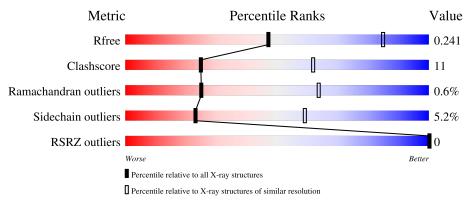
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 3.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\mathring{A}))$		
R_{free}	130704	2092 (3.00-3.00)		
Clashscore	141614	2416 (3.00-3.00)		
Ramachandran outliers	138981	2333 (3.00-3.00)		
Sidechain outliers	138945	2336 (3.00-3.00)		
RSRZ outliers	127900	1990 (3.00-3.00)		

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	498	74%	23%	
2	В	330	74%	22%	· · ·
3	С	86	66%	26%	5% •



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7390 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 Toluene o-xylene monooxygenase component.

\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	491	Total 4023	C 2569	N 675	O 753	S 26	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	TRP	ILE	engineered mutation	UNP Q6IV66
A	201	SER	THR	engineered mutation	UNP Q6IV66
A	445	LYS	GLU	engineered mutation	UNP Q6IV66

• Molecule 2 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	322	Total	С	N	O	S	0	0	0
_			2641	1674	467	490	10			

• Molecule 3 is a protein called Toluene o-xylene monooxygenase component.

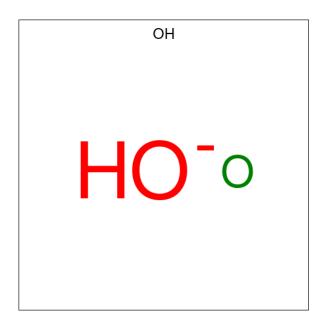
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	83	Total 676	C 425	N 120	O 126	S 5	0	0	0

• Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Fe 2 2	0	0

• Molecule 5 is HYDROXIDE ION (three-letter code: OH) (formula: HO).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0

• Molecule 6 is water.

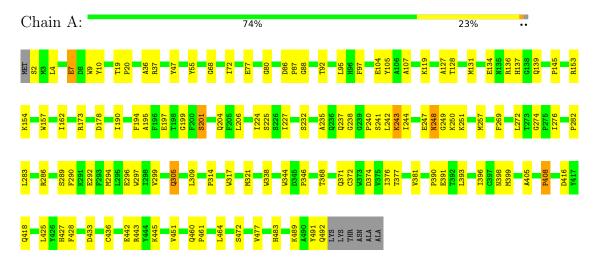
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	В	16	Total O 16 16	0	0
6	С	6	Total O 6 6	0	0



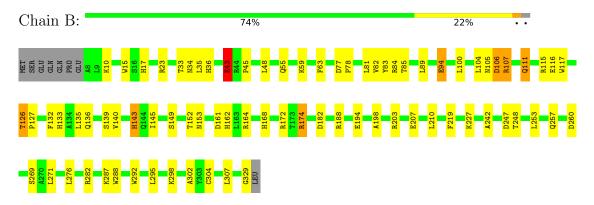
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

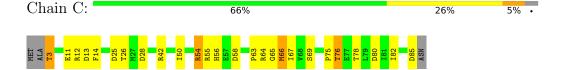
• Molecule 1: Toluene o-xylene monooxygenase component



• Molecule 2: Toluene o-xylene monooxygenase component



• Molecule 3: Toluene o-xylene monooxygenase component





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	182.79Å 182.79Å 67.70Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.70 - 3.00	Depositor
resolution (A)	45.70 - 3.00	EDS
% Data completeness	96.7 (45.70-3.00)	Depositor
(in resolution range)	96.7 (45.70-3.00)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	10.16 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.177 , 0.241	Depositor
it, it _{free}	0.181 , 0.241	DCC
R_{free} test set	1283 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 24.1	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7390	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: FE, OH

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	Bo	nd lengths	Bond angles		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.73	0/4149	0.78	1/5639~(0.0%)	
2	В	0.84	3/2713 (0.1%)	0.82	1/3688 (0.0%)	
3	С	0.73	0/690	0.83	0/934	
All	All	0.77	$3/7552 \ (0.0\%)$	0.80	$2/10261 \ (0.0\%)$	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	В	43	GLU	CG-CD	5.93	1.60	1.51
2	В	182	ASP	CB-CG	5.41	1.63	1.51
2	В	116	GLU	CG-CD	5.21	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	115	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	80	GLY	N-CA-C	5.12	125.89	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4023	0	3770	83	0
2	В	2641	0	2537	70	0
3	С	676	0	667	26	0
4	A	2	0	0	0	0
5	A	1	0	0	1	0
6	A	25	0	0	1	0
6	В	16	0	0	1	0
6	С	6	0	0	1	0
All	All	7390	0	6974	155	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 11.

The worst 5 of 155 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap (Å)} \end{array}$
1:A:2:SER:N	2:B:105:ASN:HD22	1.30	1.27
1:A:2:SER:N	2:B:105:ASN:ND2	1.99	1.09
1:A:2:SER:HB2	2:B:105:ASN:HD21	1.16	1.06
2:B:174:ARG:HG2	2:B:174:ARG:HH21	1.27	0.97
2:B:111:GLN:HE21	2:B:111:GLN:H	1.09	0.97

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 C		Outliers	Percent	tiles	
1	A	489/498 (98%)	438 (90%)	48 (10%)	3 (1%)	25	64
2	В	320/330 (97%)	302 (94%)	16 (5%)	2 (1%)	25	64
3	С	81/86 (94%)	69 (85%)	12 (15%)	0	100	100
All	All	890/914 (97%)	809 (91%)	76 (8%)	5 (1%)	25	64



All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	ASN
1	A	489	LYS
2	В	106	ASP
1	A	408	PRO
2	В	126	THR

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	417/422~(99%)	399 (96%)	18 (4%)	29 66		
2	В	274/282 (97%)	259 (94%)	15 (6%)	21 57		
3	С	77/79 (98%)	70 (91%)	7 (9%)	9 34		
All	All	768/783 (98%)	728 (95%)	40 (5%)	23 59		

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	188	ARG
3	С	66	MET
2	В	248	THR
2	В	298	LYS
3	С	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	111	GLN
2	В	162	HIS
3	С	56	HIS
2	В	168	HIS
1	A	427	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - 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.

No monomer is involved in short contacts.

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)

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^{th} 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	$\langle { m RSRZ} \rangle$	#RSRZ>2		$\mathbb{Z}>2$	$OWAB(Å^2)$	Q<0.9
1	A	491/498 (98%)	-0.53	0	100	100	38, 52, 67, 75	0
2	В	322/330 (97%)	-0.57	0	100	100	36, 47, 69, 94	0
3	С	83/86 (96%)	-0.54	0	100	100	53, 62, 71, 78	0
All	All	896/914 (98%)	-0.55	0	100	100	36, 52, 69, 94	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	RSCC	RSR	$\operatorname{B-factors}(\mathrm{\AA}^2)$	Q<0.9
4	FE	A	499	1/1	0.98	0.17	60,60,60,60	0
5	ОН	A	501	1/1	0.99	0.19	55,55,55,55	0
4	FE	A	500	1/1	1.00	0.14	47,47,47,47	0



6.5 Other polymers (i)

There are no such residues in this entry.

