



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 07:41 PM GMT

PDB ID : 2RDB
Title : X-ray Crystal Structure of Toluene/o-Xylene Monooxygenase Hydroxylase I100W Mutant
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Deposited on : 2007-09-21
Resolution : 2.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

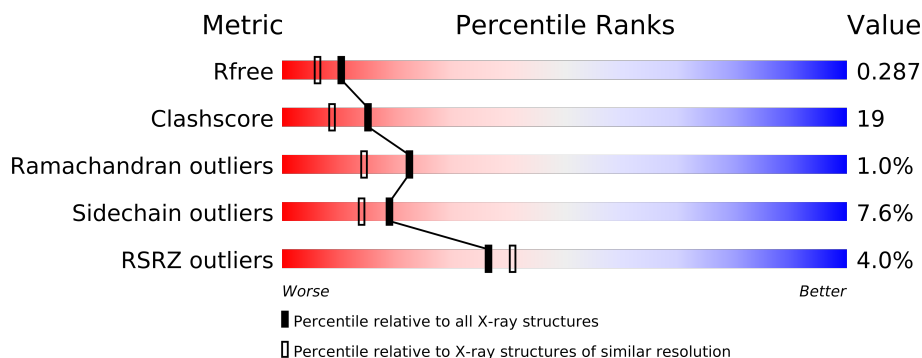
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. 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	498	
2	B	330	
3	C	86	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	P6G	A	4974	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7556 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 Toluene, o-xylene monooxygenase oxygenase subunit;alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	1	0
			4035	2580	676	753	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	TRP	ILE	ENGINEERED	UNP O87798

- Molecule 2 is a protein called Toluene, o-xylene monooxygenase oxygenase subunit;beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2641	1674	467	490	10			

- Molecule 3 is a protein called Toluene, o-xylene monooxygenase oxygenase subunit;gamma.

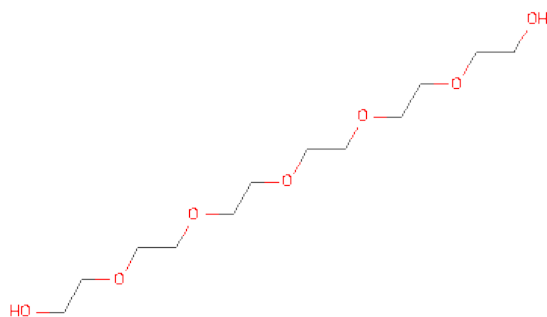
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total	C	N	O	S	0	0	0
			676	425	120	126	5			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).

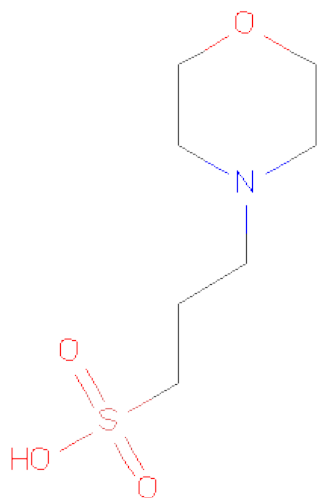


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 7 is 3[N-MORPHOLINO]PROPANESULFONIC ACID (three-letter code: MPO) (formula: C₇H₁₅NO₄S).



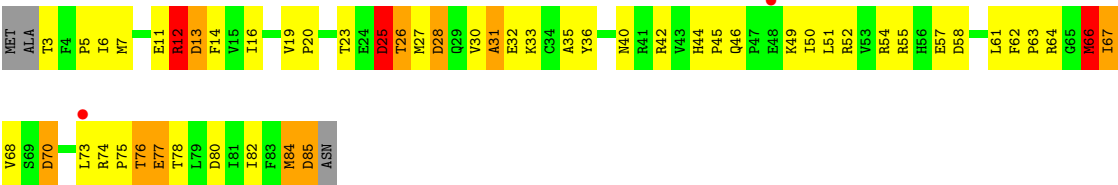
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	82	Total	O	0	0
			82	82		
8	B	72	Total	O	0	0
			72	72		
8	C	4	Total	O	0	0
			4	4		

● Molecule 3: Toluene, o-xylene monooxygenase oxygenase subunit;gamma

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.42Å 182.42Å 67.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.84 – 2.10 36.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.7 (36.84-2.10) 84.4 (36.83-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.284 0.227 , 0.287	Depositor DCC
R_{free} test set	3687 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.952	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.8	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 73939 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7556	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GOL, FE, P6G, MPO

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	1.61	29/4166 (0.7%)	1.34	32/5664 (0.6%)
2	B	1.69	27/2713 (1.0%)	1.43	27/3688 (0.7%)
3	C	1.45	2/690 (0.3%)	1.42	7/934 (0.7%)
All	All	1.63	58/7569 (0.8%)	1.38	66/10286 (0.6%)

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 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	TYR	CD1-CE1	13.31	1.59	1.39
1	A	64	GLU	CB-CG	10.37	1.71	1.52
2	B	43	GLU	CG-CD	10.24	1.67	1.51
2	B	283	GLU	CG-CD	10.23	1.67	1.51
1	A	146	TYR	CD1-CE1	-9.87	1.24	1.39

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASN	N-CA-C	8.92	135.08	111.00
1	A	233	ARG	NE-CZ-NH1	8.24	124.42	120.30
3	C	25	ASP	CB-CG-OD2	-8.13	110.99	118.30
2	B	191	ASP	CB-CG-OD1	-8.11	111.00	118.30
2	B	238	LEU	CB-CG-CD2	-7.67	97.97	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	ARG	Peptide

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	4035	0	3782	163	0
2	B	2641	0	2537	92	0
3	C	676	0	667	50	0
4	A	12	0	15	4	0
5	A	19	0	25	20	0
6	A	2	0	0	0	0
7	B	13	0	15	2	0
8	A	82	0	0	7	0
8	B	72	0	0	2	0
8	C	4	0	0	0	0
All	All	7556	0	7041	273	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 19.

The worst 5 of 273 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:162:HIS:HE1	2:B:227:LYS:NZ	1.33	1.23
1:A:372:CYS:HB3	3:C:42:ARG:HG2	1.25	1.11
2:B:162:HIS:CE1	2:B:227:LYS:NZ	2.20	1.10
2:B:72:TRP:H	7:B:4401:MPO:H71	1.19	1.05
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.19	1.02

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	490/498 (98%)	442 (90%)	44 (9%)	4 (1%)	27	20
2	B	320/330 (97%)	292 (91%)	25 (8%)	3 (1%)	25	17
3	C	81/86 (94%)	70 (86%)	9 (11%)	2 (2%)	9	3
All	All	891/914 (98%)	804 (90%)	78 (9%)	9 (1%)	22	14

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	GLU
1	A	287	ASN
2	B	310	GLY
1	A	408	PRO
1	A	445	LYS

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	418/422 (99%)	393 (94%)	25 (6%)	27	22
2	B	274/282 (97%)	252 (92%)	22 (8%)	17	12
3	C	77/79 (98%)	66 (86%)	11 (14%)	5	2
All	All	769/783 (98%)	711 (92%)	58 (8%)	19	14

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	22	ARG

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Mol	Chain	Res	Type
2	B	111	GLN
3	C	67	ILE
2	B	23	ARG
2	B	89	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	HIS
2	B	36	HIS
2	B	153	ASN
1	A	418	GLN
2	B	162	HIS

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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
4	GOL	A	3287	-	5,5,5	0.37	0	5,5,5	0.87	0
5	P6G	A	4974	-	18,18,18	1.46	3 (16%)	17,17,17	1.21	3 (17%)
4	GOL	A	4975	6	5,5,5	0.93	0	5,5,5	1.79	2 (40%)
7	MPO	B	4401	-	13,13,13	2.89	8 (61%)	17,17,17	5.11	10 (58%)

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
4	GOL	A	3287	-	-	0/4/4/4	0/0/0/0
5	P6G	A	4974	-	-	0/16/16/16	0/0/0/0
4	GOL	A	4975	6	-	0/4/4/4	0/0/0/0
7	MPO	B	4401	-	-	0/7/15/15	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4401	MPO	C4-N1	-5.37	1.32	1.47
7	B	4401	MPO	O2-S1	4.65	1.60	1.45
7	B	4401	MPO	C4-C5	-3.69	1.34	1.50
5	A	4974	P6G	O19-C18	-3.58	1.22	1.42
7	B	4401	MPO	O1-S1	3.45	1.56	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4401	MPO	O2-S1-C1	13.47	118.35	106.81
7	B	4401	MPO	C5-C4-N1	7.86	121.54	110.04
7	B	4401	MPO	O3-S1-O2	-7.41	95.76	111.78
7	B	4401	MPO	C3-C2-C1	6.56	127.90	112.42
7	B	4401	MPO	C2-C1-S1	4.79	119.42	113.24

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, 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	491/498 (98%)	0.07	19 (3%) 37 42	33, 50, 65, 81	0
2	B	322/330 (97%)	-0.08	15 (4%) 30 33	33, 45, 65, 92	0
3	C	83/86 (96%)	0.08	2 (2%) 56 61	48, 63, 78, 85	0
All	All	896/914 (98%)	0.02	36 (4%) 36 41	33, 49, 69, 92	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	8	ALA	5.6
2	B	23	ARG	5.4
1	A	100[A]	TRP	4.8
2	B	22	ARG	4.1
1	A	268	LEU	3.5

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, 95th 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(\AA^2)	Q<0.9
5	P6G	A	4974	19/19	0.19	4.03	47,56,72,76	0
4	GOL	A	3287	6/6	0.34	1.69	83,87,88,89	0
7	MPO	B	4401	13/13	0.15	1.46	60,66,72,77	0
4	GOL	A	4975	6/6	0.28	1.30	43,57,61,65	0
6	FE	A	499	1/1	0.12	-1.02	39,39,39,39	0
6	FE	A	500	1/1	0.13	-1.05	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.