W O R L D W I D E
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PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 05:17 AM EDT

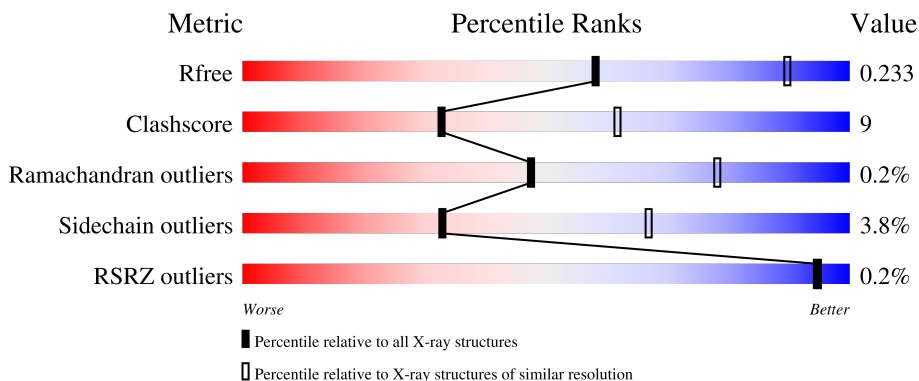|		
PDB ID	:	3RN9
Title	:	Structure of the Toluene/o-Xylene Monooxygenase Hydroxylase T201S/L272E Double Mutant
Authors	:	Gucinski, G.; Song, W.J.; Lippard, S.J.; Sazinsky, M.H.
Deposited on	:	2011-04-22
Resolution	:	2.80 Å(reported)

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 2.80 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	Percentile Ranks	Value
Rfree		0.233
Clashscore		9
Ramachandran outliers		0.2%
Sidechain outliers		3.8%
RSRZ outliers		0.2%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	79% ... 19% ..
2	B	330	77% ... 18% ..
3	C	86	77% ... 20% ..

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7535 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total 4012	C 2560	N 671	O 755	S 26	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	SER	THR	engineered mutation	UNP Q6IV66
A	272	GLU	LEU	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	B	323	Total 2630	C 1669	N 462	O 489	S 10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	84	Total 681	C 428	N 121	O 127	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 2	Fe 2	0	0

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

OH

HO⁻o

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
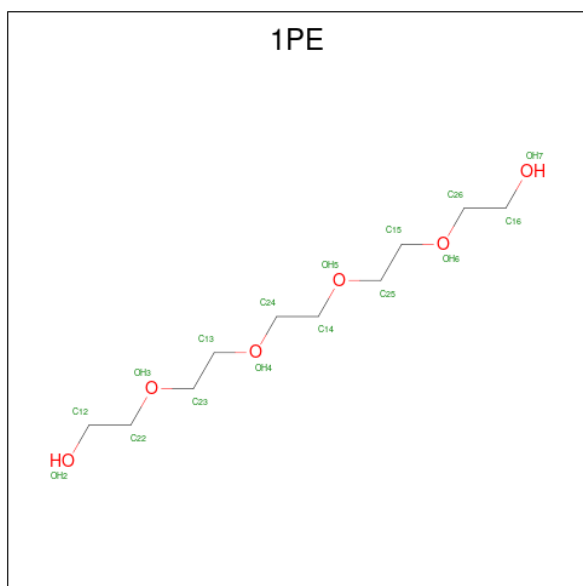
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 16	C 10	O 6	0	0

- Molecule 9 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	101	Total 101	O 101	0	0
9	B	72	Total 72	O 72	0	0
9	C	11	Total 11	O 11	0	0

3 Residue-property plots ⓘ

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.
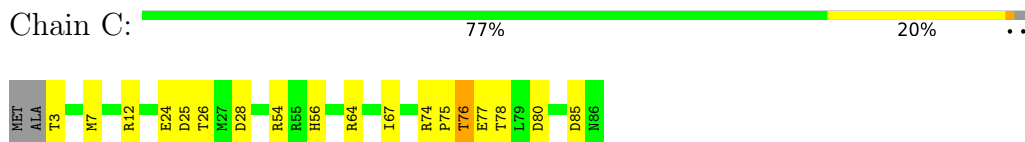
• Molecule 1: Toluene o-xylene monooxygenase component

Chain A:
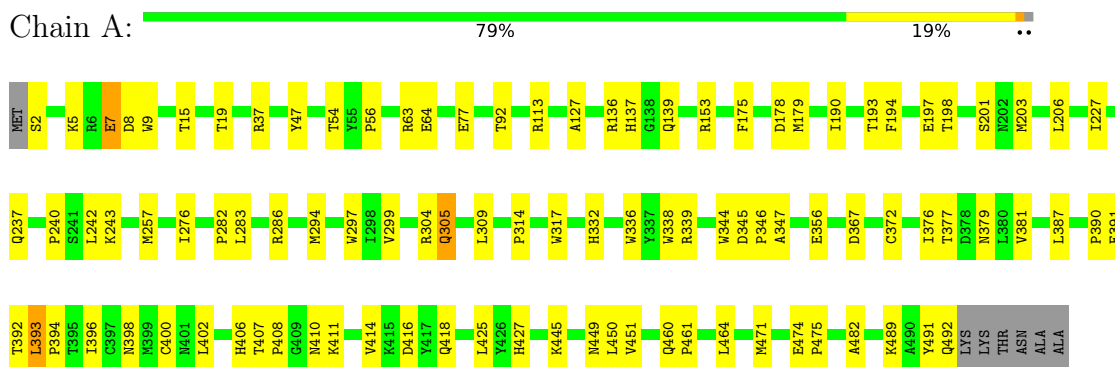
• Molecule 2: Toluene o-xylene monooxygenase component

Chain B:
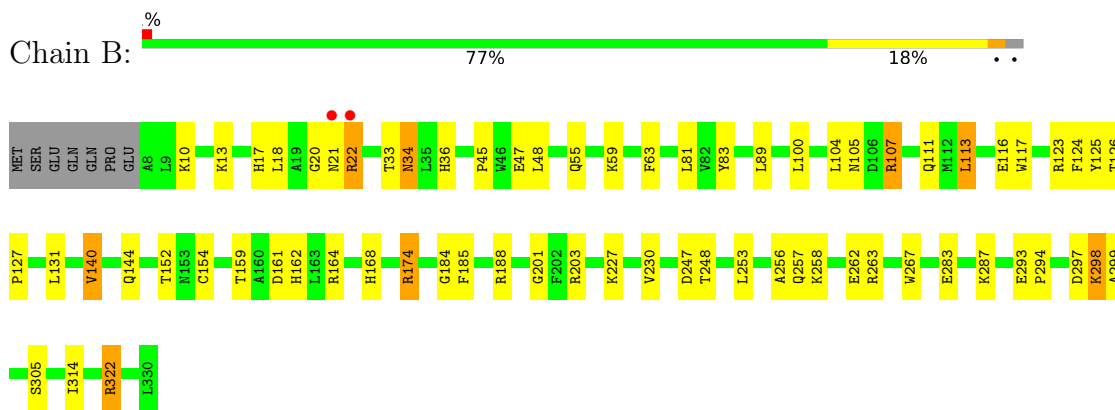
• Molecule 3: Toluene o-xylene monooxygenase component

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.41Å 182.41Å 67.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.60 – 2.80 45.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.60-2.80) 99.7 (45.60-2.80)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	5.73 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.161 , 0.230 0.166 , 0.233	Depositor DCC
R_{free} test set	1609 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.7	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7535	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OH, 1PE, FE, EDO, SO4

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	0.75	2/4136 (0.0%)	0.78	1/5621 (0.0%)
2	B	0.86	2/2702 (0.1%)	0.80	2/3676 (0.1%)
3	C	0.73	0/695	0.83	0/941
All	All	0.79	4/7533 (0.1%)	0.79	3/10238 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	GLU	CB-CG	5.66	1.62	1.52
2	B	283	GLU	CG-CD	5.05	1.59	1.51
2	B	125	TYR	CD2-CE2	-5.02	1.31	1.39
1	A	64	GLU	CG-CD	5.02	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	B	113	LEU	CA-CB-CG	5.06	126.95	115.30
2	B	174	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4012	0	3755	69	0
2	B	2630	0	2513	53	0
3	C	681	0	669	21	0
4	A	2	0	0	0	0
5	A	1	0	0	1	0
6	A	5	0	0	0	0
7	A	4	0	5	0	0
8	A	16	0	22	3	0
9	A	101	0	0	0	0
9	B	72	0	0	2	0
9	C	11	0	0	2	0
All	All	7535	0	6964	125	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 9.

The worst 5 of 125 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:A:393:LEU:HD22	8:A:504:1PE:H142	1.21	1.15
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.18	1.07
1:A:139:GLN:HE22	2:B:83:TYR:H	1.06	1.02
1:A:9:TRP:HB3	2:B:174:ARG:HG3	1.46	0.97
1:A:427:HIS:CE1	3:C:76:THR:HG23	2.02	0.94

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	489/498 (98%)	455 (93%)	32 (6%)	2 (0%)	34	66
2	B	321/330 (97%)	306 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	82/86 (95%)	72 (88%)	10 (12%)	0	100	100
All	All	892/914 (98%)	833 (93%)	57 (6%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	PRO
1	A	489	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	416/422 (99%)	401 (96%)	15 (4%)	35	69
2	B	271/282 (96%)	260 (96%)	11 (4%)	30	64
3	C	77/79 (98%)	74 (96%)	3 (4%)	32	66
All	All	764/783 (98%)	735 (96%)	29 (4%)	33	67

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	LYS
3	C	76	THR
2	B	34	ASN
2	B	298	LYS
2	B	22	ARG

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	B	144	GLN
2	B	168	HIS
3	C	56	HIS

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Mol	Chain	Res	Type
2	B	326	GLN
1	A	398	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 3 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	$\#|Z| > 2$
8	1PE	A	504	-	15,15,15	0.80	0	14,14,14	0.69	0
7	EDO	A	503	4	3,3,3	0.43	0	2,2,2	0.28	0
6	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.27	0

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
7	EDO	A	503	4	-	0/1/1/1	-
8	1PE	A	504	-	-	6/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	504	1PE	OH5-C14-C24-OH4
8	A	504	1PE	OH6-C15-C25-OH5
8	A	504	1PE	C25-C15-OH6-C26
8	A	504	1PE	C15-C25-OH5-C14
8	A	504	1PE	OH4-C13-C23-OH3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	504	1PE	3	0

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(Å²)	Q<0.9
1	A	491/498 (98%)	-0.55	0	100	100	15, 26, 42, 51	0
2	B	323/330 (97%)	-0.62	2 (0%)	89	86	12, 23, 42, 63	0
3	C	84/86 (97%)	-0.46	0	100	100	24, 36, 46, 53	0
All	All	898/914 (98%)	-0.57	2 (0%)	95	94	12, 26, 43, 63	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	22	ARG	2.7
2	B	21	ASN	2.2

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 monosaccharides 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. 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	RSCC	RSR	B-factors(Å²)	Q<0.9
6	SO4	A	502	5/5	0.89	0.22	79,80,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	1PE	A	504	16/16	0.94	0.19	41,49,60,60	0
7	EDO	A	503	4/4	0.97	0.28	46,49,49,50	0
4	FE	A	499	1/1	0.99	0.11	24,24,24,24	0
5	OH	A	501	1/1	1.00	0.13	30,30,30,30	0
4	FE	A	500	1/1	1.00	0.12	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.