



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:08 AM GMT

PDB ID : 3O6T  
Title : Mycobacterium tuberculosis thioredoxin C C40S mutant in Complex with  
Quinol Inhibitor PMX464  
Authors : Hall, G.; Emsley, J.  
Deposited on : 2010-07-29  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

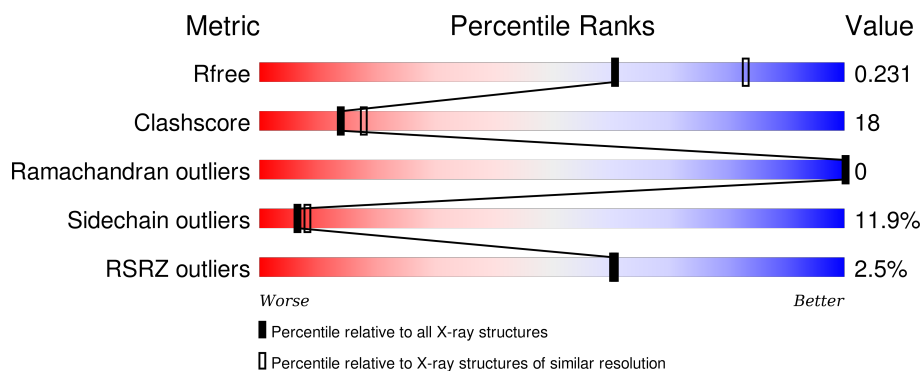
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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  $\leq 5\%$ . 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	118	<div> <div>2%</div> <div>62% 26% 8%</div> </div>
1	B	118	<div> <div>2%</div> <div>64% 26% 7%</div> </div>
1	C	118	<div> <div>3%</div> <div>58% 32% 8%</div> </div>
1	D	118	<div> <div>3%</div> <div>53% 34% 6% 8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PGE	C	118	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3491 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.

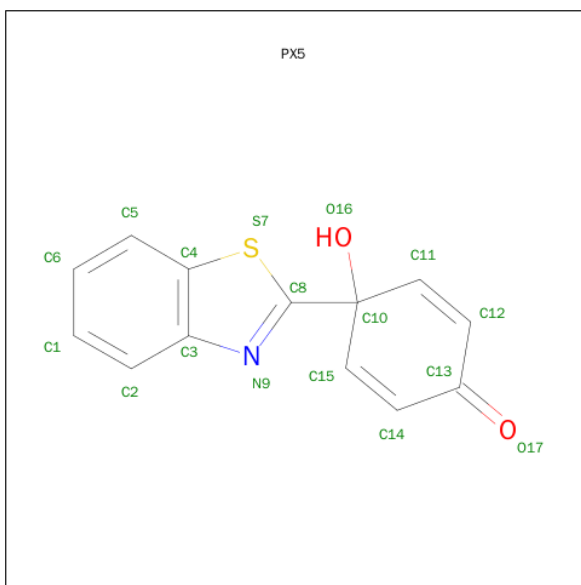
- Molecule 1 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			816	521	136	157	2			
1	B	110	Total	C	N	O	S	0	0	0
			832	531	139	160	2			
1	C	108	Total	C	N	O	S	0	0	0
			816	521	136	157	2			
1	D	109	Total	C	N	O	S	0	0	0
			824	527	137	158	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P0A616
A	0	SER	-	EXPRESSION TAG	UNP P0A616
A	40	SER	CYS	ENGINEERED MUTATION	UNP P0A616
B	-1	GLY	-	EXPRESSION TAG	UNP P0A616
B	0	SER	-	EXPRESSION TAG	UNP P0A616
B	40	SER	CYS	ENGINEERED MUTATION	UNP P0A616
C	-1	GLY	-	EXPRESSION TAG	UNP P0A616
C	0	SER	-	EXPRESSION TAG	UNP P0A616
C	40	SER	CYS	ENGINEERED MUTATION	UNP P0A616
D	-1	GLY	-	EXPRESSION TAG	UNP P0A616
D	0	SER	-	EXPRESSION TAG	UNP P0A616
D	40	SER	CYS	ENGINEERED MUTATION	UNP P0A616

- Molecule 2 is 4-(1,3-BENZOTHAZOL-2-YL)-4-HYDROXYCYCLOHEXA-2,5-DIEN-1-ONE (three-letter code: PX5) (formula: C<sub>13</sub>H<sub>9</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			17	13	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			17	13	1	2	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).

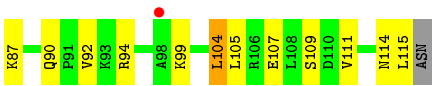


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total 51	O 51	0	0
4	B	26	Total 26	O 26	0	0
4	C	37	Total 37	O 37	0	0
4	D	35	Total 35	O 35	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.22Å 75.09Å 65.24Å 90.00° 107.31° 90.00°	Depositor
Resolution (Å)	40.29 – 2.40 40.29 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.3 (40.29-2.40) 97.2 (40.29-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, $R_{free}$	0.199 , 0.260 0.206 , 0.231	Depositor DCC
$R_{free}$ test set	1001 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19458 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PGE, PX5

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	1.79	1/830 (0.1%)	0.98	4/1134 (0.4%)
1	B	1.75	2/846 (0.2%)	1.00	1/1156 (0.1%)
1	C	1.75	2/830 (0.2%)	0.95	2/1134 (0.2%)
1	D	1.74	8/838 (1.0%)	1.02	2/1145 (0.2%)
All	All	1.76	13/3344 (0.4%)	0.99	9/4569 (0.2%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	PHE	CD1-CE1	-5.77	1.27	1.39
1	B	21	VAL	CB-CG2	-5.69	1.40	1.52
1	D	77	VAL	CB-CG2	-5.59	1.41	1.52
1	D	28	VAL	CB-CG2	-5.52	1.41	1.52
1	D	36	TRP	CB-CG	-5.52	1.40	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	104	LEU	CA-CB-CG	5.69	128.39	115.30
1	C	64	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	63	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	63	LEU	CA-CB-CG	5.43	127.78	115.30

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	816	0	843	23	0
1	B	832	0	861	37	0
1	C	816	0	843	30	0
1	D	824	0	855	48	0
2	A	17	0	8	0	0
2	C	17	0	8	3	0
3	A	10	0	14	1	0
3	C	10	0	14	0	0
4	A	51	0	0	1	0
4	B	26	0	0	0	0
4	C	37	0	0	1	0
4	D	35	0	0	2	0
All	All	3491	0	3446	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 18.

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:B:36:TRP:CZ3	1:B:37:CYS:HB2	1.89	1.06
1:D:37:CYS:SG	4:D:142:HOH:O	2.20	0.99
1:A:74:ASN:HD22	1:D:90:GLN:NE2	1.71	0.89
1:D:63:LEU:HD13	1:D:64:ASP:N	1.89	0.86
1:D:63:LEU:C	1:D:63:LEU:HD13	1.97	0.83

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	106/118 (90%)	104 (98%)	2 (2%)	0	100	100
1	B	108/118 (92%)	107 (99%)	1 (1%)	0	100	100
1	C	106/118 (90%)	104 (98%)	2 (2%)	0	100	100
1	D	107/118 (91%)	106 (99%)	1 (1%)	0	100	100
All	All	427/472 (90%)	421 (99%)	6 (1%)	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	92/101 (91%)	82 (89%)	10 (11%)	8	11
1	B	94/101 (93%)	82 (87%)	12 (13%)	5	6
1	C	92/101 (91%)	82 (89%)	10 (11%)	8	11
1	D	93/101 (92%)	81 (87%)	12 (13%)	5	6
All	All	371/404 (92%)	327 (88%)	44 (12%)	6	8

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	VAL
1	C	19	THR
1	D	87	LYS
1	B	99	LYS
1	C	7	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	GLN
1	D	90	GLN
1	C	90	GLN
1	A	90	GLN
1	D	76	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	$\# Z  > 2$
2	PX5	A	117	1	17,19,19	3.02	5 (29%)	14,28,28	2.65	3 (21%)
3	PGE	A	118	-	9,9,9	0.64	0	8,8,8	0.68	0
2	PX5	C	117	1	17,19,19	2.98	6 (35%)	14,28,28	3.56	5 (35%)
3	PGE	C	118	-	9,9,9	0.50	0	8,8,8	0.65	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
2	PX5	A	117	1	-	0/0/18/18	0/3/3/3
3	PGE	A	118	-	-	0/7/7/7	0/0/0/0
2	PX5	C	117	1	-	0/0/18/18	0/3/3/3
3	PGE	C	118	-	-	0/7/7/7	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	117	PX5	C10-C11	-3.71	1.47	1.51
2	A	117	PX5	O16-C10	-3.29	1.38	1.43
2	A	117	PX5	C2-C3	-3.19	1.36	1.41
2	C	117	PX5	O16-C10	-2.85	1.39	1.43
2	C	117	PX5	C8-S7	-2.44	1.65	1.73

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	117	PX5	C15-C14-C13	-11.13	110.97	121.44
2	A	117	PX5	C15-C14-C13	-7.65	114.24	121.44
2	C	117	PX5	C11-C12-C13	-5.11	116.63	121.44
2	C	117	PX5	O16-C10-C11	-2.36	102.67	108.02
2	C	117	PX5	C6-C1-C2	-2.26	117.17	120.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	118	PGE	1	0
2	C	117	PX5	3	0

## 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<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	108/118 (91%)	-0.12	2 (1%) 70 69	15, 25, 42, 56	0
1	B	110/118 (93%)	-0.15	2 (1%) 71 71	16, 27, 46, 51	0
1	C	108/118 (91%)	-0.03	4 (3%) 45 46	17, 27, 46, 61	0
1	D	109/118 (92%)	0.08	3 (2%) 56 55	14, 28, 47, 52	0
All	All	435/472 (92%)	-0.06	11 (2%) 61 60	14, 26, 47, 61	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	ALA	4.3
1	D	7	SER	3.1
1	A	114	ASN	3.0
1	C	7	SER	2.9
1	C	105	LEU	2.4

### 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PGE	C	118	10/10	0.89	0.16	3.03	26,30,44,47	0
3	PGE	A	118	10/10	0.95	0.16	1.63	18,23,27,27	0
2	PX5	C	117	17/17	0.94	0.18	0.27	22,27,40,42	0
2	PX5	A	117	17/17	0.96	0.13	-0.40	22,27,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.