



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5ONC / pdb_00005onc
Title : Catabolism of the Cholesterol Side Chain in Mycobacterium tuberculosis is Controlled by a Redox-Sensitive Thiol Switch
Authors : Schaefer, C.; Kuper, J.; Sampson, N.S.; Kisker, C.
Deposited on : 2017-08-03
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

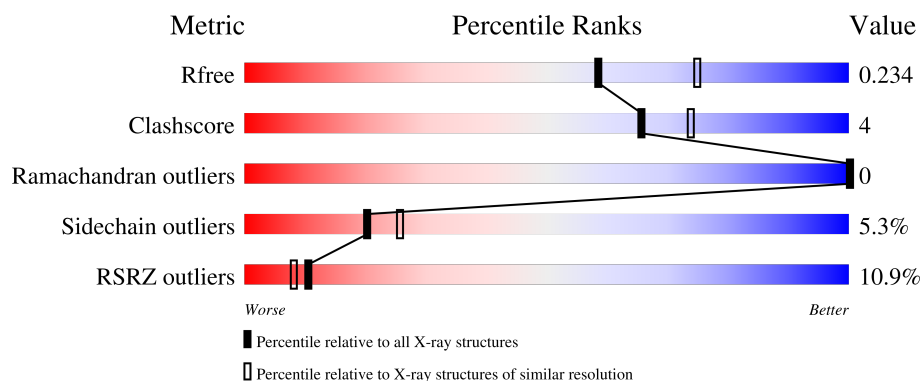
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	399	
1	B	399	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5606 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 Steroid 3-ketoacyl-CoA thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	4	0
			2737	1694	508	522	13			
1	B	359	Total	C	N	O	S	0	0	0
			2651	1643	485	510	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP I6XHI4
A	-6	HIS	-	expression tag	UNP I6XHI4
A	-5	HIS	-	expression tag	UNP I6XHI4
A	-4	HIS	-	expression tag	UNP I6XHI4
A	-3	HIS	-	expression tag	UNP I6XHI4
A	-2	HIS	-	expression tag	UNP I6XHI4
A	-1	GLY	-	expression tag	UNP I6XHI4
A	0	SER	-	expression tag	UNP I6XHI4
B	-7	HIS	-	expression tag	UNP I6XHI4
B	-6	HIS	-	expression tag	UNP I6XHI4
B	-5	HIS	-	expression tag	UNP I6XHI4
B	-4	HIS	-	expression tag	UNP I6XHI4
B	-3	HIS	-	expression tag	UNP I6XHI4
B	-2	HIS	-	expression tag	UNP I6XHI4
B	-1	GLY	-	expression tag	UNP I6XHI4
B	0	SER	-	expression tag	UNP I6XHI4

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cl	0	0
			4	4		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	192	Total 193	O 193	0	1
3	B	19	Total 20	O 20	0	1

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.29Å 120.29Å 206.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.17 – 2.19 46.17 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.17-2.19) 99.9 (46.17-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.182 , 0.226 0.196 , 0.234	Depositor DCC
R_{free} test set	2320 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5606	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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:
CL

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	1.16	2/2784 (0.1%)	1.05	1/3771 (0.0%)
1	B	0.81	2/2688 (0.1%)	0.93	0/3643
All	All	1.00	4/5472 (0.1%)	0.99	1/7414 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	VAL	C-O	-7.46	1.16	1.24
1	A	330	GLU	C-O	-6.36	1.20	1.23
1	A	45	SER	C-O	-5.35	1.17	1.23
1	B	7	VAL	C-O	-5.21	1.19	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	GLU	N-CA-C	7.01	119.96	111.82

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	2737	0	2748	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2651	0	2648	22	1
2	A	4	0	0	1	0
2	B	1	0	0	0	0
3	A	193	0	0	1	0
3	B	20	0	0	0	0
All	All	5606	0	5396	41	1

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 4.

All (41) 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:382:LEU:HD21	1:B:279:LEU:HD13	1.58	0.81
1:B:157:ARG:NH1	1:B:285:TYR:O	2.15	0.78
1:B:258:MET:HE1	1:B:268:LEU:HD13	1.78	0.66
1:B:7:VAL:HG21	1:B:258:MET:HE3	1.84	0.57
1:A:382:LEU:HD21	1:B:279:LEU:CD1	2.32	0.57
1:A:382:LEU:CD2	1:B:279:LEU:HD13	2.32	0.57
1:A:175:GLU:OE2	1:A:178:ARG:NH1	2.41	0.54
1:A:258:MET:HE2	1:A:262:VAL:HG12	1.89	0.53
1:A:114:VAL:HG22	1:A:258:MET:HE3	1.92	0.52
1:A:148:LEU:HD22	1:A:149:PRO:HD2	1.93	0.51
1:A:11:ARG:O	1:A:193:ILE:HA	2.13	0.48
1:A:264[B]:ARG:NH2	3:A:506:HOH:O	2.46	0.48
1:A:175:GLU:OE1	1:A:178:ARG:NH1	2.46	0.48
1:B:201:LEU:HD13	1:B:202:ASP:H	1.78	0.47
1:B:279:LEU:HG	1:B:384:THR:HG22	1.95	0.47
1:A:175:GLU:CD	1:A:178:ARG:NH1	2.73	0.47
1:A:203:GLU:HB3	1:A:204:GLN:NE2	2.29	0.47
1:B:205:ASN:N	1:B:205:ASN:OD1	2.48	0.47
1:B:23:GLY:HA3	1:B:199:PRO:HG2	1.97	0.46
1:A:44:GLN:NE2	1:A:44:GLN:H	2.14	0.46
1:B:177:GLN:HE21	1:B:221:ARG:H	1.64	0.46
1:B:200:VAL:HG21	1:B:207:PRO:HB2	1.98	0.45
1:B:206:GLN:N	1:B:207:PRO:CD	2.79	0.45
1:B:311:ILE:O	1:B:372:ALA:HA	2.17	0.44
1:B:213:LEU:HD22	1:B:215:PHE:CE1	2.52	0.43
1:A:311:ILE:O	1:A:372:ALA:HA	2.19	0.43
1:B:62:GLN:NE2	1:B:90:ASP:OD2	2.52	0.43
1:B:45:SER:OG	1:B:268:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD22	1:A:149:PRO:CD	2.49	0.42
1:B:258:MET:CE	1:B:268:LEU:HD13	2.48	0.42
1:A:278:ALA:HB1	1:A:297:LYS:HD3	2.01	0.42
1:B:90:ASP:HB3	1:B:91:CYS:H	1.52	0.42
1:A:12:SER:HB2	1:A:196:ILE:HG13	2.02	0.42
1:A:148:LEU:HD13	1:A:150:ASN:HD21	1.85	0.42
1:B:367:THR:C	1:B:368:ASP:OD1	2.63	0.41
1:A:105:GLY:HA3	1:B:284:PRO:HG2	2.02	0.41
1:B:47:LEU:HD13	1:B:51:ASP:HB2	2.02	0.41
1:A:315:ASN:HB3	2:A:403:CL:CL	2.58	0.41
1:A:213:LEU:HD12	1:A:213:LEU:HA	1.93	0.41
1:A:258:MET:CE	1:A:262:VAL:HG12	2.51	0.41
1:A:22:SER:O	1:A:125:ARG:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLY:O	1:B:44:GLN:NE2[12_554]	2.06	0.14

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	Outliers	Percentiles	
1	A	364/399 (91%)	360 (99%)	4 (1%)	0	100	100
1	B	351/399 (88%)	342 (97%)	9 (3%)	0	100	100
All	All	715/798 (90%)	702 (98%)	13 (2%)	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	281/303 (93%)	273 (97%)	8 (3%)	38	52
1	B	272/303 (90%)	251 (92%)	21 (8%)	12	13
All	All	553/606 (91%)	524 (95%)	29 (5%)	20	26

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	17	ARG
1	A	44	GLN
1	A	95	SER
1	A	126	VAL
1	A	150	ASN
1	A	181	GLN
1	A	205	ASN
1	B	1	MET
1	B	45	SER
1	B	47	LEU
1	B	82	GLU
1	B	95	SER
1	B	174	LEU
1	B	201	LEU
1	B	204	GLN
1	B	205	ASN
1	B	206	GLN
1	B	208	THR
1	B	230	GLU
1	B	236	GLU
1	B	248	ILE
1	B	268	LEU
1	B	269	THR
1	B	279	LEU
1	B	280	VAL
1	B	293	GLN

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Mol	Chain	Res	Type
1	B	305	LYS
1	B	349	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	48	HIS
1	A	98	GLN
1	A	150	ASN
1	A	204	GLN
1	A	206	GLN
1	A	277	GLN
1	B	62	GLN
1	B	151	GLN
1	B	177	GLN
1	B	247	GLN
1	B	293	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 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.

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

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	366/399 (91%)	0.01	12 (3%)	49 46	23, 41, 99, 123	4 (1%)
1	B	359/399 (89%)	1.19	67 (18%)	3 2	28, 99, 152, 187	0
All	All	725/798 (90%)	0.60	79 (10%)	10 8	23, 70, 138, 187	4 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94[A]	GLY	8.2
1	B	200	VAL	4.9
1	B	149	PRO	4.9
1	B	201	LEU	4.6
1	B	235	LEU	4.0
1	B	21	LEU	3.9
1	B	96	GLY	3.6
1	A	148	LEU	3.6
1	A	126	VAL	3.5
1	B	208	THR	3.3
1	B	306	ILE	3.3
1	B	228	LEU	3.3
1	B	123	MET	3.3
1	B	93	CYS	3.2
1	B	378	ALA	3.2
1	B	89	VAL	3.2
1	A	61	THR	3.2
1	B	348	PRO	3.2
1	B	207	PRO	3.1
1	B	169	VAL	2.9
1	B	174	LEU	2.8
1	B	163	GLY	2.8
1	B	239	ILE	2.8
1	B	377	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	223	THR	2.7
1	B	364	LEU	2.7
1	A	93	CYS	2.7
1	B	345	LEU	2.6
1	B	185	ALA	2.6
1	B	196	ILE	2.5
1	A	147	ASP	2.5
1	B	92	GLN	2.5
1	B	220	LEU	2.5
1	A	282	ALA	2.5
1	B	272	ALA	2.5
1	B	47	LEU	2.5
1	B	268	LEU	2.5
1	B	161	ARG	2.5
1	B	248	ILE	2.5
1	B	361	LEU	2.4
1	B	1	MET	2.4
1	A	91	CYS	2.4
1	B	373	LEU	2.3
1	A	281	GLY	2.3
1	B	120	ILE	2.3
1	B	262	VAL	2.3
1	B	206	GLN	2.3
1	B	91	CYS	2.3
1	B	226	ALA	2.3
1	B	170	ASP	2.3
1	A	89	VAL	2.3
1	B	338	VAL	2.3
1	B	265	ALA	2.3
1	A	60	VAL	2.2
1	B	286	TYR	2.2
1	B	97	GLN	2.2
1	B	124	SER	2.2
1	B	90	ASP	2.2
1	B	234	VAL	2.2
1	B	159	ALA	2.2
1	B	4	PRO	2.1
1	B	229	GLY	2.1
1	B	180	ALA	2.1
1	B	213	LEU	2.1
1	B	269	THR	2.1
1	B	270	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	19	GLY	2.1
1	B	37	VAL	2.1
1	B	173	GLY	2.1
1	B	39	ASP	2.1
1	B	184	TRP	2.1
1	B	214	VAL	2.1
1	B	32	ALA	2.1
1	B	104	ALA	2.1
1	B	244	THR	2.1
1	B	103	ILE	2.1
1	B	231	LEU	2.0
1	A	285	TYR	2.0
1	B	164	ILE	2.0

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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
2	CL	A	403	1/1	0.96	0.08	68,68,68,68	0
2	CL	B	401	1/1	0.96	0.15	73,73,73,73	0
2	CL	A	404	1/1	0.97	0.16	67,67,67,67	0
2	CL	A	402	1/1	0.97	0.11	52,52,52,52	0
2	CL	A	401	1/1	0.99	0.13	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.