Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 07:57 am BST

PDB ID	:	5ONC
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)

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

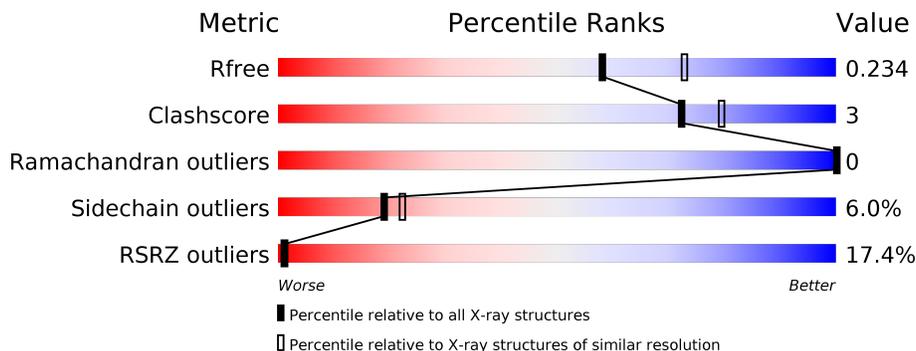|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.234
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		6.0%
RSRZ outliers		17.4%

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	399	6% / 83% / 8% · 8%
1	B	399	25% / 79% / 10% · 10%

2 Entry composition (i)

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 2737	C 1694	N 508	O 522	S 13	0	4	0
1	B	359	Total 2651	C 1643	N 485	O 510	S 13	0	0	0

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Steroid 3-ketoacyl-CoA thiolase

Chain A:

- Molecule 1: Steroid 3-ketoacyl-CoA thiolase

Chain B:

4   Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.05%)	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)	0.33 , 53.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical 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.

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: 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	0.86	0/2784	0.85	0/3771
1	B	0.56	0/2688	0.72	0/3643
All	All	0.73	0/5472	0.79	0/7414

There are no bond length outliers.

There are no bond angle outliers.

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	2737	0	2748	21	0
1	B	2651	0	2648	20	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	37	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 3.

All (37) 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: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: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: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:H	1:A:44:GLN:NE2	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:258:MET:CE	1:B:268:LEU:HD13	2.48	0.43
1:B:45:SER:OG	1:B:268:LEU:HG	2.18	0.43
1:A:148:LEU:HD22	1:A:149:PRO:CD	2.49	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:175:GLU:CD	1:A:178:ARG:NH1	2.73	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:258:MET:HE1	1:B:268:LEU:HD13	2.01	0.42
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:HA	1:A:213:LEU:HD12	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 (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	281/303 (93%)	271 (96%)	10 (4%)	35	45
1	B	272/303 (90%)	249 (92%)	23 (8%)	10	10
All	All	553/606 (91%)	520 (94%)	33 (6%)	19	22

All (33) 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

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Mol	Chain	Res	Type
1	A	72	ARG
1	A	90	ASP
1	A	95	SER
1	A	126	VAL
1	A	150	ASN
1	A	205	ASN
1	A	285	TYR
1	B	1	MET
1	B	47	LEU
1	B	67	SER
1	B	82	GLU
1	B	95	SER
1	B	182	ARG
1	B	201	LEU
1	B	204	GLN
1	B	205	ASN
1	B	206	GLN
1	B	208	THR
1	B	221	ARG
1	B	230	GLU
1	B	236	GLU
1	B	248	ILE
1	B	268	LEU
1	B	269	THR
1	B	273	ARG
1	B	279	LEU
1	B	280	VAL
1	B	293	GLN
1	B	305	LYS
1	B	349	VAL

Some 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	98	GLN
1	A	150	ASN
1	A	181	GLN
1	A	204	GLN
1	B	54	GLN
1	B	62	GLN
1	B	97	GLN

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Mol	Chain	Res	Type
1	B	150	ASN
1	B	177	GLN
1	B	204	GLN
1	B	293	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)

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 (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, 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	366/399 (91%)	0.34	25 (6%)	17	16	26, 42, 99, 123	0
1	B	359/399 (89%)	1.41	101 (28%)	0	0	28, 99, 152, 187	0
All	All	725/798 (90%)	0.87	126 (17%)	1	1	26, 70, 138, 187	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	LEU	13.1
1	B	232	LYS	7.9
1	B	235	LEU	7.8
1	B	200	VAL	7.7
1	A	147	ASP	6.7
1	B	47	LEU	6.4
1	B	231	LEU	6.3
1	B	215	PHE	6.2
1	B	206	GLN	6.1
1	B	24	LEU	6.0
1	A	126	VAL	6.0
1	B	202	ASP	5.9
1	B	152	PHE	5.8
1	B	268	LEU	5.8
1	B	234	VAL	5.8
1	B	17	ARG	5.4
1	B	208	THR	5.4
1	B	21	LEU	5.2
1	B	233	PRO	4.8
1	B	228	LEU	4.8
1	B	207	PRO	4.8
1	B	43	ILE	4.5
1	B	330	GLU	4.5
1	B	159	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	237	GLY	4.4
1	B	124	SER	4.4
1	A	75	TRP	4.2
1	B	331	PRO	4.2
1	B	184	TRP	4.2
1	B	345	LEU	4.2
1	B	163	GLY	4.1
1	B	239	ILE	4.0
1	B	32	ALA	4.0
1	B	306	ILE	4.0
1	B	198	ALA	4.0
1	B	169	VAL	3.9
1	B	199	PRO	3.9
1	B	368	ASP	3.9
1	B	171	VAL	3.9
1	B	60	VAL	3.8
1	B	204	GLN	3.8
1	B	227	GLY	3.8
1	B	170	ASP	3.8
1	B	45	SER	3.6
1	B	164	ILE	3.6
1	B	19	GLY	3.6
1	B	238	GLY	3.5
1	B	29	LEU	3.5
1	B	213	LEU	3.4
1	B	3	TYR	3.4
1	B	319	ALA	3.4
1	B	172	PHE	3.3
1	A	357	ILE	3.2
1	A	356	LEU	3.1
1	B	35	LYS	3.1
1	B	49	ALA	3.1
1	B	305	LYS	3.1
1	A	78	ALA	3.1
1	A	86	ALA	3.0
1	B	89	VAL	3.0
1	B	23	GLY	2.9
1	A	378	ALA	2.9
1	B	226	ALA	2.9
1	B	196	ILE	2.9
1	B	299	LEU	2.9
1	B	205	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	223	THR	2.8
1	B	44	GLN	2.8
1	B	48	HIS	2.8
1	B	39	ASP	2.8
1	B	191	ARG	2.8
1	B	174	LEU	2.8
1	B	33	VAL	2.7
1	B	167	GLU	2.7
1	A	382	LEU	2.7
1	B	195	PRO	2.7
1	B	307	GLY	2.7
1	B	25	HIS	2.7
1	A	377	CYS	2.7
1	B	241	THR	2.7
1	B	18	ASN	2.7
1	A	358	THR	2.6
1	B	323	LEU	2.6
1	B	230	GLU	2.5
1	B	320	SER	2.5
1	A	82	GLU	2.5
1	B	304	MET	2.5
1	B	31	GLY	2.4
1	B	391	ILE	2.4
1	A	30	LEU	2.4
1	B	340	GLY	2.4
1	B	120	ILE	2.4
1	A	91	CYS	2.3
1	B	338	VAL	2.3
1	B	273	ARG	2.3
1	A	56	ILE	2.3
1	B	270	PRO	2.3
1	A	384	THR	2.3
1	B	269	THR	2.3
1	B	311	ILE	2.3
1	B	222	GLU	2.3
1	A	70	ILE	2.3
1	B	300	GLU	2.3
1	A	352	THR	2.3
1	B	165	THR	2.3
1	A	84	VAL	2.2
1	B	52	VAL	2.2
1	B	166	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	22	SER	2.2
1	B	176	SER	2.2
1	A	351	CYS	2.2
1	B	214	VAL	2.2
1	B	41	ALA	2.2
1	B	302	ALA	2.2
1	B	236	GLU	2.2
1	B	51	ASP	2.2
1	B	190	ASP	2.1
1	B	90	ASP	2.1
1	A	353	GLY	2.1
1	B	220	LEU	2.1
1	A	79	GLY	2.1
1	B	38	VAL	2.1
1	A	76	LEU	2.1
1	B	263	ALA	2.1
1	A	374	ILE	2.1
1	A	90	ASP	2.1

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. 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(Å^2)	Q<0.9
2	CL	B	401	1/1	0.86	0.07	73,73,73,73	0
2	CL	A	403	1/1	0.93	0.20	68,68,68,68	0
2	CL	A	402	1/1	0.96	0.09	52,52,52,52	0
2	CL	A	404	1/1	0.97	0.11	67,67,67,67	0
2	CL	A	401	1/1	0.99	0.15	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.