

Full wwPDB X-ray Structure Validation Report (i)

Oct 29, 2023 – 12:04 PM EDT

PDB ID	:	8S9D
Title	:	C143S variant of Citrate Synthase (CitA) in Mycobacterium tuberculosis
Authors	:	Pathirage, R.; Ronning, D.
Deposited on		
Resolution	:	2.57 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 (i) 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 (1)) were used in the production of this report:

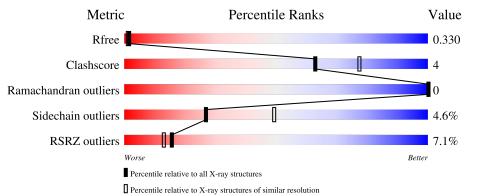
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.57 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	
			7%	
1	А	379	86%	10% ••

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	А	404	-	-	-	Х



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2848 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.

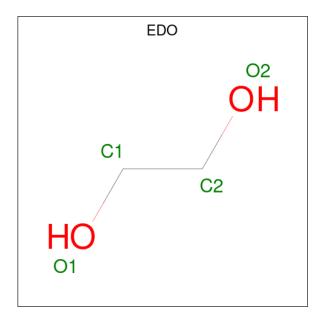
• Molecule 1 is a protein called citrate synthase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	368	Total 2788	C 1754	N 506	0 516	S 12	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

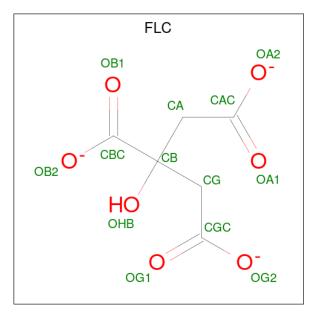
Chain	Residue	Modelled	Actual	Comment	Reference
А	143	SER	CYS	engineered mutation	UNP A0A045JB88
А	374	HIS	-	expression tag	UNP A0A045JB88
А	375	HIS	-	expression tag	UNP A0A045JB88
А	376	HIS	-	expression tag	UNP A0A045JB88
А	377	HIS	-	expression tag	UNP A0A045JB88
А	378	HIS	-	expression tag	UNP A0A045JB88
А	379	HIS	-	expression tag	UNP A0A045JB88

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 13	С 6	O 7	0	0

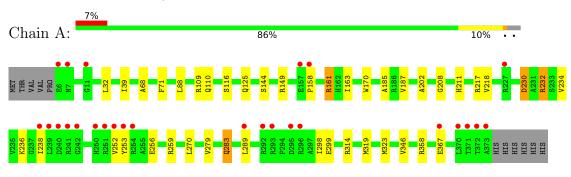
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	27	TotalO2727	0	0



3 Residue-property plots (i)

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: citrate synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants	150.25Å 150.25Å 231.66Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.85 - 2.57	Depositor
Resolution (A)	53.12 - 2.50	EDS
% Data completeness	99.6 (50.85-2.57)	Depositor
(in resolution range)	87.6 (53.12-2.50)	EDS
R _{merge}	0.18	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.23 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158:000	Depositor
D D.	0.313 , 0.329	Depositor
R, R_{free}	0.313 , 0.330	DCC
R_{free} test set	2003 reflections $(4.36%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35 , 68.5	EDS
L-test for twinning ²	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	2848	wwPDB-VP
Average B, all atoms $(Å^2)$	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 22.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5266e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: FLC, EDO

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.28	0/2851	0.53	0/3883	

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	А	2788	0	2759	23	0
2	А	20	0	30	3	0
3	А	13	0	5	2	0
4	А	27	0	0	1	0
All	All	2848	0	2794	24	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 4.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



A + a 1	A 4 a ma 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:110:GLN:NE2	4:A:501:HOH:O	2.20	0.74
1:A:289:LEU:HB3	1:A:298:ILE:HD13	1.73	0.70
1:A:125:GLN:HG2	2:A:406:EDO:H12	1.71	0.69
1:A:158:PRO:HB2	1:A:163:ILE:HD11	1.74	0.68
1:A:149:ARG:HD2	2:A:403:EDO:H21	1.77	0.64
1:A:259:ARG:HH22	3:A:404:FLC:HG1	1.63	0.62
1:A:230:ASP:OD1	1:A:230:ASP:N	2.27	0.61
1:A:279:VAL:O	1:A:283:GLN:HG3	2.08	0.53
1:A:170:TRP:HE1	1:A:323:MET:HE3	1.73	0.53
1:A:208:GLY:O	1:A:211:HIS:ND1	2.37	0.53
3:A:404:FLC:OA2	3:A:404:FLC:OHB	2.25	0.51
1:A:161:ARG:NH1	1:A:270:LEU:O	2.43	0.49
1:A:170:TRP:NE1	1:A:323:MET:HE3	2.29	0.47
1:A:234:VAL:O	1:A:238:ILE:HG13	2.16	0.46
1:A:256:GLU:HA	1:A:299:GLU:HG2	1.99	0.45
1:A:252:VAL:HG23	1:A:253:TYR:H	1.82	0.44
1:A:185:ALA:HB2	1:A:202:ALA:HB2	2.00	0.44
1:A:252:VAL:HG23	1:A:253:TYR:N	2.33	0.43
1:A:187:VAL:HG22	1:A:346:VAL:HG21	2.01	0.43
1:A:314:ARG:HD3	1:A:314:ARG:HA	1.79	0.43
1:A:367:GLU:H	1:A:367:GLU:CD	2.21	0.43
1:A:68:ALA:H	2:A:403:EDO:H22	1.85	0.41
1:A:32:LEU:HD23	1:A:39:ILE:HD13	2.03	0.41
1:A:232:ARG:NH1	1:A:236:LYS:HZ3	2.19	0.40

There are no symmetry-related clashes.

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	Percentil	es
1	А	366/379~(97%)	352~(96%)	14 (4%)	0	100 10	0

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	280/291~(96%)	267~(95%)	13~(5%)	27 49	

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	71	PHE
1	А	88	LEU
1	А	109	ARG
1	А	116	SER
1	А	144	SER
1	А	161	ARG
1	А	217	ARG
1	А	218	VAL
1	А	230	ASP
1	А	232	ARG
1	А	283	GLN
1	А	319	MET
1	А	358	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	155	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	Turne	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
INIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	EDO	А	406	-	$3,\!3,\!3$	0.40	0	2,2,2	0.27	0
2	EDO	А	401	-	$3,\!3,\!3$	0.48	0	2,2,2	0.28	0
3	FLC	А	404	-	12,12,12	1.11	2 (16%)	$17,\!17,\!17$	1.15	2 (11%)
2	EDO	А	403	-	3,3,3	0.55	0	2,2,2	0.22	0
2	EDO	А	405	-	3,3,3	0.42	0	2,2,2	0.50	0
2	EDO	А	402	-	3,3,3	0.52	0	2,2,2	0.28	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	EDO	А	406	-	-	1/1/1/1	-
2	EDO	А	401	-	-	0/1/1/1	-
3	FLC	А	404	-	-	9/16/16/16	-
2	EDO	А	403	-	-	0/1/1/1	-
2	EDO	А	405	-	-	0/1/1/1	-
2	EDO	А	402	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	404	FLC	OA2-CAC	-2.73	1.21	1.30
3	А	404	FLC	OA1-CAC	2.63	1.30	1.22



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	404	FLC	OA1-CAC-CA	-3.43	112.91	122.94
3	А	404	FLC	OA2-CAC-CA	2.83	123.44	114.35

All (2) bond angle outliers are listed below:

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	404	FLC	CAC-CA-CB-CG
3	А	404	FLC	CAC-CA-CB-OHB
3	А	404	FLC	CG-CB-CBC-OB1
3	А	404	FLC	CG-CB-CBC-OB2
3	А	404	FLC	OHB-CB-CBC-OB1
3	А	404	FLC	OHB-CB-CBC-OB2
3	А	404	FLC	CAC-CA-CB-CBC
2	А	406	EDO	O1-C1-C2-O2
3	А	404	FLC	CB-CA-CAC-OA1
3	А	404	FLC	CB-CA-CAC-OA2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	406	EDO	1	0
3	А	404	FLC	2	0
2	А	403	EDO	2	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^{th} 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	368/379~(97%)	0.29	26 (7%) 16 13	43, 65, 112, 148	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	372	THR	10.7
1	А	371	THR	6.6
1	А	373	ALA	5.3
1	А	370	LEU	5.1
1	А	254	ARG	5.1
1	А	252	VAL	5.0
1	А	7	ASN	4.7
1	А	295	ASP	3.9
1	А	158	PRO	3.8
1	А	367	GLU	3.7
1	А	6	GLU	3.3
1	А	250	HIS	3.3
1	А	253	TYR	3.1
1	А	238	ILE	2.8
1	А	296	ARG	2.8
1	А	292	ARG	2.7
1	А	239	LEU	2.7
1	А	293	ARG	2.7
1	А	242	GLY	2.6
1	А	241	ARG	2.6
1	А	240	ASP	2.6
1	А	227	ARG	2.3
1	А	11	GLY	2.2
1	А	251	ARG	2.2
1	А	289	LEU	2.2
1	А	157	GLU	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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	EDO	А	402	4/4	0.64	0.28	20,20,20,20	4
3	FLC	А	404	13/13	0.68	0.64	$15,\!16,\!19,\!21$	13
2	EDO	А	406	4/4	0.79	0.33	20,20,20,20	4
2	EDO	А	405	4/4	0.79	0.33	20,20,20,20	4
2	EDO	А	403	4/4	0.81	0.30	20,20,20,20	4
2	EDO	А	401	4/4	0.94	0.27	20,20,20,20	4

6.5 Other polymers (i)

There are no such residues in this entry.

