



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:57 PM UTC

PDB ID : 4BI9 / pdb_00004bi9
Title : Crystal structure of wild-type SCP2 thiolase from Trypanosoma brucei.
Authors : Harijan, R.K.; Kiema, T.-R.; Weiss, M.S.; Michels, P.A.M.; Wierenga, R.K.
Deposited on : 2013-04-10
Resolution : 2.45 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

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

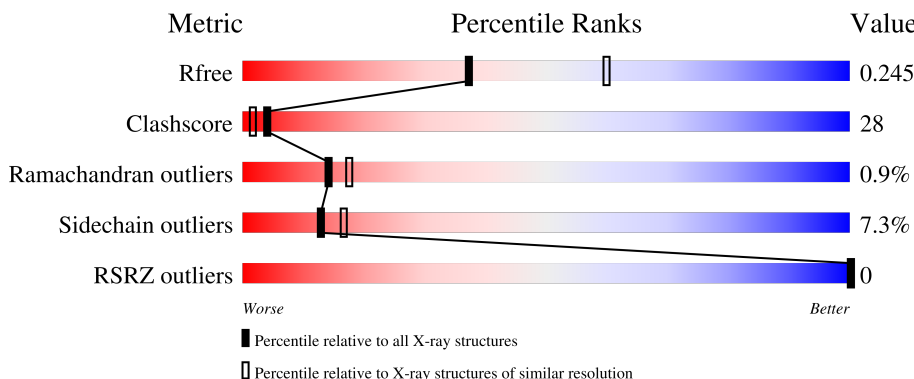
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	454	
1	B	454	
1	C	454	
1	D	454	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12349 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 3-KETOACYL-COA THIOLASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3073	1924	540	592	17			
1	B	416	Total	C	N	O	S	0	0	0
			3069	1921	542	589	17			
1	C	419	Total	C	N	O	S	0	0	0
			3087	1931	545	594	17			
1	D	416	Total	C	N	O	S	0	0	0
			3066	1920	541	588	17			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q57XD5
A	-14	HIS	-	expression tag	UNP Q57XD5
A	-13	HIS	-	expression tag	UNP Q57XD5
A	-12	HIS	-	expression tag	UNP Q57XD5
A	-11	HIS	-	expression tag	UNP Q57XD5
A	-10	HIS	-	expression tag	UNP Q57XD5
A	-9	SER	-	expression tag	UNP Q57XD5
A	-8	SER	-	expression tag	UNP Q57XD5
A	-7	GLY	-	expression tag	UNP Q57XD5
A	-6	LEU	-	expression tag	UNP Q57XD5
A	-5	VAL	-	expression tag	UNP Q57XD5
A	-4	PRO	-	expression tag	UNP Q57XD5
A	-3	ARG	-	expression tag	UNP Q57XD5
A	-2	GLY	-	expression tag	UNP Q57XD5
A	-1	SER	-	expression tag	UNP Q57XD5
A	0	HIS	-	expression tag	UNP Q57XD5
B	-15	HIS	-	expression tag	UNP Q57XD5
B	-14	HIS	-	expression tag	UNP Q57XD5
B	-13	HIS	-	expression tag	UNP Q57XD5
B	-12	HIS	-	expression tag	UNP Q57XD5
B	-11	HIS	-	expression tag	UNP Q57XD5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q57XD5
B	-9	SER	-	expression tag	UNP Q57XD5
B	-8	SER	-	expression tag	UNP Q57XD5
B	-7	GLY	-	expression tag	UNP Q57XD5
B	-6	LEU	-	expression tag	UNP Q57XD5
B	-5	VAL	-	expression tag	UNP Q57XD5
B	-4	PRO	-	expression tag	UNP Q57XD5
B	-3	ARG	-	expression tag	UNP Q57XD5
B	-2	GLY	-	expression tag	UNP Q57XD5
B	-1	SER	-	expression tag	UNP Q57XD5
B	0	HIS	-	expression tag	UNP Q57XD5
C	-15	HIS	-	expression tag	UNP Q57XD5
C	-14	HIS	-	expression tag	UNP Q57XD5
C	-13	HIS	-	expression tag	UNP Q57XD5
C	-12	HIS	-	expression tag	UNP Q57XD5
C	-11	HIS	-	expression tag	UNP Q57XD5
C	-10	HIS	-	expression tag	UNP Q57XD5
C	-9	SER	-	expression tag	UNP Q57XD5
C	-8	SER	-	expression tag	UNP Q57XD5
C	-7	GLY	-	expression tag	UNP Q57XD5
C	-6	LEU	-	expression tag	UNP Q57XD5
C	-5	VAL	-	expression tag	UNP Q57XD5
C	-4	PRO	-	expression tag	UNP Q57XD5
C	-3	ARG	-	expression tag	UNP Q57XD5
C	-2	GLY	-	expression tag	UNP Q57XD5
C	-1	SER	-	expression tag	UNP Q57XD5
C	0	HIS	-	expression tag	UNP Q57XD5
D	-15	HIS	-	expression tag	UNP Q57XD5
D	-14	HIS	-	expression tag	UNP Q57XD5
D	-13	HIS	-	expression tag	UNP Q57XD5
D	-12	HIS	-	expression tag	UNP Q57XD5
D	-11	HIS	-	expression tag	UNP Q57XD5
D	-10	HIS	-	expression tag	UNP Q57XD5
D	-9	SER	-	expression tag	UNP Q57XD5
D	-8	SER	-	expression tag	UNP Q57XD5
D	-7	GLY	-	expression tag	UNP Q57XD5
D	-6	LEU	-	expression tag	UNP Q57XD5
D	-5	VAL	-	expression tag	UNP Q57XD5
D	-4	PRO	-	expression tag	UNP Q57XD5
D	-3	ARG	-	expression tag	UNP Q57XD5
D	-2	GLY	-	expression tag	UNP Q57XD5
D	-1	SER	-	expression tag	UNP Q57XD5

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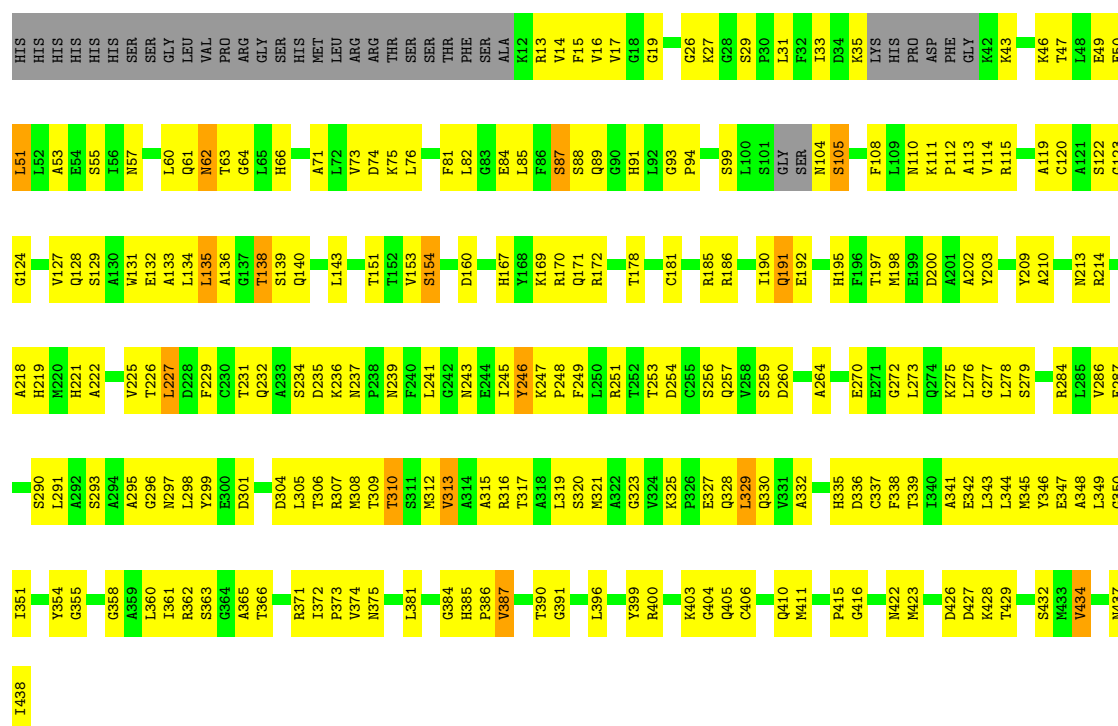
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q57XD5

- Molecule 2 is water.

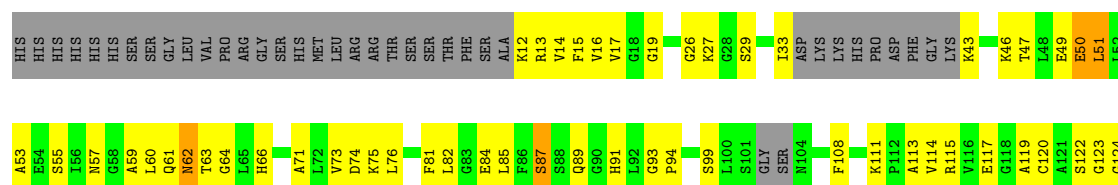
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	9	Total	O	0	0
			9	9		
2	C	15	Total	O	0	0
			15	15		
2	D	13	Total	O	0	0
			13	13		



• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE



• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE



G355	G358	A359	L360	I361	R362	S363	G364	A365	T366	R371	I372	P373	V374	N375	L381	S382	F383	G384	H385	P386	V387	T390	G391	L396	Y399	R400	K403	G404	Q405	C406	Q410	M411	P415	G416	N422	M423	D426	T427	K428	T429	S432	H433	V434	N437	I438										
S290	L291	A292	S293	A294	A295	G296	N297	L298	Y299	E300	D301	D304	L305	T306	R307	M308	T309	T310	S311	M312	V313	A314	A315	R316	T317	A318	L319	S320	M321	K325	F326	E327	Q328	L329	Q330	V331	A332	H335	D336	C337	F338	T339	I340	A341	E342	L343	L344	M345	Y346	E347	A348	L349	G350	I351	Y354
A218	H219	M220	H221	V225	T226	L227	D228	F229	C230	T231	Q232	A233	S234	D235	K236	N237	P238	N239	N243	E244	I245	Y246	K247	P248	F249	L250	R251	T252	T253	D254	Q257	V258	S259	D260	A264	S269	E270	E271	G272	L273	Q274	K275	L276	G277	L278	S279	P280	N283	R284	L285	V286	E287			
V127	Q128	S129	W131	E132	A133	L134	L135	A136	G137	T138	S139	Q140	L143	T151	T152	V153	S154	D160	H167	Y168	K169	R170	Q171	R172	T178	C181	R185	R186	I190	Q191	E192	H195	F196	T197	M198	E199	D200	A201	A202	Y203	V204	Y209	A210	N213	R214										

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	59.14Å 59.14Å 377.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.75 – 2.45 50.75 – 2.45	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.75-2.45) 88.5 (50.75-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.224 , 0.242 0.224 , 0.245	Depositor DCC
R_{free} test set	2493 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 107.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.449 for -h,-k,l 0.183 for h,-h-k,-l 0.177 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 49663 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12349	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.64	0/3119	1.04	11/4218 (0.3%)
1	B	0.62	0/3115	1.06	14/4211 (0.3%)
1	C	0.65	0/3133	1.03	11/4236 (0.3%)
1	D	0.63	0/3112	1.05	15/4207 (0.4%)
All	All	0.63	0/12479	1.05	51/16872 (0.3%)

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	ARG	NE-CZ-NH2	-9.56	110.59	119.20
1	B	307	ARG	NE-CZ-NH1	8.67	130.17	121.50
1	D	66	HIS	CA-C-N	8.21	136.47	121.70
1	D	66	HIS	C-N-CA	8.21	136.47	121.70
1	B	307	ARG	CD-NE-CZ	8.00	135.60	124.40

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	3073	0	3058	181	0
1	B	3069	0	3067	179	0
1	C	3087	0	3075	194	0
1	D	3066	0	3063	188	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	17	0	0	3	0
2	B	9	0	0	1	0
2	C	15	0	0	3	0
2	D	13	0	0	1	0
All	All	12349	0	12263	680	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 28.

The worst 5 of 680 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:C:94:PRO:HB3	1:D:295:ALA:HB1	1.46	0.97
1:C:138:THR:HG21	1:D:132:GLU:HG2	1.53	0.90
1:B:290:SER:HB2	1:B:434:VAL:HB	1.54	0.90
1:C:132:GLU:HG2	1:D:138:THR:HG21	1.51	0.90
1:C:290:SER:HB2	1:C:434:VAL:HB	1.54	0.89

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	Percentiles	
1	A	412/454 (91%)	362 (88%)	45 (11%)	5 (1%)	10	11
1	B	410/454 (90%)	363 (88%)	44 (11%)	3 (1%)	18	24
1	C	413/454 (91%)	361 (87%)	48 (12%)	4 (1%)	12	14
1	D	410/454 (90%)	363 (88%)	44 (11%)	3 (1%)	18	24
All	All	1645/1816 (91%)	1449 (88%)	181 (11%)	15 (1%)	14	17

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	43	LYS
1	B	27	LYS
1	C	27	LYS
1	C	105	SER

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	315/350 (90%)	291 (92%)	24 (8%)	12	15
1	B	316/350 (90%)	293 (93%)	23 (7%)	13	17
1	C	317/350 (91%)	295 (93%)	22 (7%)	14	19
1	D	315/350 (90%)	292 (93%)	23 (7%)	13	17
All	All	1263/1400 (90%)	1171 (93%)	92 (7%)	13	17

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	191	GLN
1	D	62	ASN
1	C	225	VAL
1	C	310	THR
1	D	129	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	167	HIS
1	D	191	GLN
1	B	239	ASN
1	B	422	ASN
1	C	191	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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(Å ²)	Q<0.9
1	A	418/454 (92%)	-1.43	0 100 100	34, 65, 86, 105	0
1	B	416/454 (91%)	-1.42	0 100 100	34, 65, 85, 104	0
1	C	419/454 (92%)	-1.43	0 100 100	34, 65, 86, 108	0
1	D	416/454 (91%)	-1.43	0 100 100	34, 64, 86, 105	0
All	All	1669/1816 (91%)	-1.43	0 100 100	34, 65, 86, 108	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.