



# Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2026 – 06:04 PM EDT

PDB ID : 10YN / pdb\_000010yn  
Title : Joint X-ray/neutron structure of E53Q mutant of *Thermus thermophilus* serine hydroxymethyltransferase (TthSHMT)  
Authors : Kovalevsky, A.; Drago, V.N.; Phillips, R.S.  
Deposited on : 2026-02-12  
Resolution : 2.40 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	<b>FAILED</b>
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

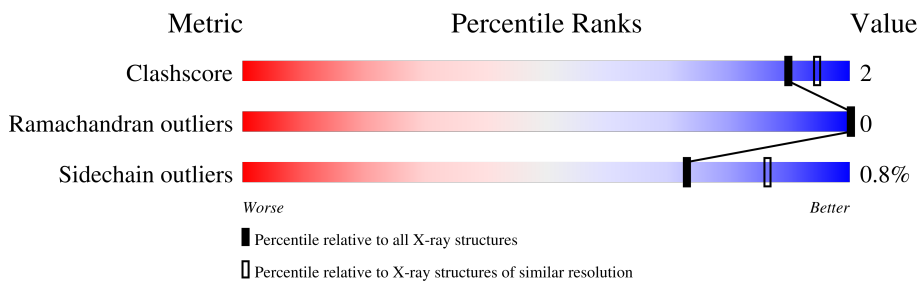
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION, NEUTRON 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	405	97% ..
1	B	405	95% ..

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15044 atoms, of which 5966 are hydrogens and 2313 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 Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	402	Total	C	D	H	N	O	P	S	0	309	0
			6762	1984	648	2989	557	574	1	9			
1	B	402	Total	C	D	H	N	O	P	S	0	293	0
			6757	1984	655	2977	557	574	1	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	GLN	GLU	engineered mutation	UNP A0AAD1KUU5
B	1053	GLN	GLU	engineered mutation	UNP A0AAD1KUU5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	257	Total	D	O	0	0
			771	514	257		
3	B	248	Total	D	O	0	0
			744	496	248		

### 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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Serine hydroxymethyltransferase

Chain A:  97%



- Molecule 1: Serine hydroxymethyltransferase

Chain B:  95%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.82Å 83.52Å 95.42Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40	Depositor
% Data completeness (in resolution range)	65.1 (40.00-2.40)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 1.65Å)	Xtriage
Refinement program	nCNS 1.0.8	Depositor
R, $R_{free}$	0.236 , 0.263	Depositor
Wilson B-factor (Å <sup>2</sup> )	3.9	Xtriage
Anisotropy	0.362	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
Total number of atoms	15044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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, 0.333 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: SO4, LLP, DOD

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	0.59	0/5635	0.95	7/7623 (0.1%)
1	B	0.62	2/5525 (0.0%)	0.91	9/7474 (0.1%)
All	All	0.61	2/11160 (0.0%)	0.93	16/15097 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1032[A]	GLU	CD-OE2	-5.48	1.22	1.33
1	B	1032[B]	GLU	CD-OE2	-5.48	1.22	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223[A]	THR	N-CA-C	-7.09	99.97	110.46
1	A	223[B]	THR	N-CA-C	-7.09	99.97	110.46
1	B	1138[A]	VAL	N-CA-C	6.14	116.70	108.11
1	B	1138[B]	VAL	N-CA-C	6.14	116.70	108.11
1	A	352[A]	ARG	N-CA-C	-6.08	105.82	113.72
1	A	352[B]	ARG	N-CA-C	-6.08	105.82	113.72
1	A	30[A]	ALA	N-CA-C	5.87	119.26	111.75
1	A	30[B]	ALA	N-CA-C	5.87	119.26	111.75
1	B	1107	GLU	N-CA-C	-5.83	102.06	110.40
1	B	1243	LEU	N-CA-C	-5.76	105.09	111.36
1	B	1341[A]	LYS	N-CA-C	-5.72	101.93	110.23
1	B	1341[B]	LYS	N-CA-C	-5.72	101.93	110.23
1	B	1030	ALA	N-CA-C	5.25	117.75	111.71
1	B	1223[A]	THR	N-CA-C	-5.14	102.46	110.42
1	B	1223[B]	THR	N-CA-C	-5.14	102.46	110.42
1	A	405	PRO	N-CA-C	5.10	119.31	111.21

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	3773	2989	665	4	0
1	B	3780	2977	749	6	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	771	0	0	2	1
3	B	744	0	0	2	1
All	All	9078	5966	1414	14	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 2.

All (14) 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:1226:LLP:NZ	1:B:1226:LLP:O3	2.48	0.46
1:B:1120:GLY:O	1:B:1171:ALA:HB1	2.13	0.42
1:B:1372:GLU:CD	1:B:1372:GLU:H	2.21	0.42

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)
3:A:812:DOD:D1	3:B:1738:DOD:O[2_546]	1.54	0.66



## 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	707/405 (175%)	684 (97%)	23 (3%)	0	100	100
1	B	691/405 (171%)	672 (97%)	19 (3%)	0	100	100
All	All	1398/810 (173%)	1356 (97%)	42 (3%)	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	565/322 (176%)	561 (99%)	4 (1%)	76	88
1	B	556/322 (173%)	550 (99%)	6 (1%)	65	82
All	All	1121/644 (174%)	1111 (99%)	10 (1%)	73	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6[A]	LYS
1	A	6[B]	LYS
1	A	51[A]	TYR
1	A	51[B]	TYR
1	B	1051[A]	TYR
1	B	1051[B]	TYR
1	B	1340[A]	ASN
1	B	1340[B]	ASN

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Mol	Chain	Res	Type
1	B	1406[A]	MET
1	B	1406[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	B	1226	1	23,24,25	1.39	6 (26%)	25,32,34	2.13	8 (32%)
1	LLP	A	226	1	23,24,25	1.39	5 (21%)	25,32,34	2.21	7 (28%)

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
1	LLP	B	1226	1	-	3/16/17/19	0/1/1/1
1	LLP	A	226	1	-	1/16/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1226	LLP	C6-N1	-2.82	1.28	1.34
1	A	226	LLP	C6-N1	-2.65	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	LLP	C4-C3	2.54	1.45	1.41
1	A	226	LLP	OP4-C5'	-2.39	1.36	1.44
1	B	1226	LLP	CD-CE	2.32	1.59	1.51
1	B	1226	LLP	OP4-C5'	-2.26	1.36	1.44
1	B	1226	LLP	CB-CA	2.22	1.56	1.53
1	B	1226	LLP	C3-C2	2.13	1.43	1.41
1	A	226	LLP	CD-CE	2.08	1.58	1.51
1	B	1226	LLP	C4-C3	2.07	1.44	1.41
1	A	226	LLP	CB-CA	2.03	1.56	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	LLP	OP4-C5'-C5	6.11	120.82	109.36
1	B	1226	LLP	OP4-C5'-C5	5.35	119.39	109.36
1	A	226	LLP	C6-N1-C2	4.19	126.80	119.20
1	B	1226	LLP	C6-N1-C2	4.03	126.51	119.20
1	B	1226	LLP	C5-C4-C4'	3.65	127.09	121.47
1	A	226	LLP	C3-C4-C5	-3.51	115.46	118.28
1	B	1226	LLP	C3-C4-C5	-3.29	115.63	118.28
1	A	226	LLP	C5-C4-C4'	3.23	126.45	121.47
1	A	226	LLP	C3-C2-N1	-3.08	117.07	120.96
1	B	1226	LLP	C3-C2-N1	-2.98	117.20	120.96
1	A	226	LLP	O3-C3-C4	2.38	125.85	119.44
1	B	1226	LLP	C5-C6-N1	-2.15	120.33	123.83
1	B	1226	LLP	O3-C3-C4	2.13	125.17	119.44
1	A	226	LLP	C5-C6-N1	-2.08	120.45	123.83
1	B	1226	LLP	CE-NZ-C4'	2.04	125.24	118.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	226	LLP	O-C-CA-CB
1	B	1226	LLP	C6-C5-C5'-OP4
1	B	1226	LLP	O-C-CA-CB
1	B	1226	LLP	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1226	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	SO4	B	1501	-	4,4,4	0.32	0	6,6,6	0.21	0
2	SO4	A	501	-	4,4,4	0.37	0	6,6,6	0.15	0

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

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.