wwPDB X-ray Structure Validation Summary Report (i)

Dec 4, 2023 – 04:00 am GMT

PDB ID	:	2WDE
Title	:	Termus thermophilus Sulfate thiohydrolase SoxB in complex with thiosulfate
Authors	:	Sauve, V.; Roversi, P.; Leath, K.J.; Garman, E.F.; Antrobus, R.; Lea, S.M.; Berks, B.C.
Deposited on	:	2009-03-24
Resolution	:	1.85 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 (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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	FAILED
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

PERCENTILES INFOmissingINFO

1 Entry composition

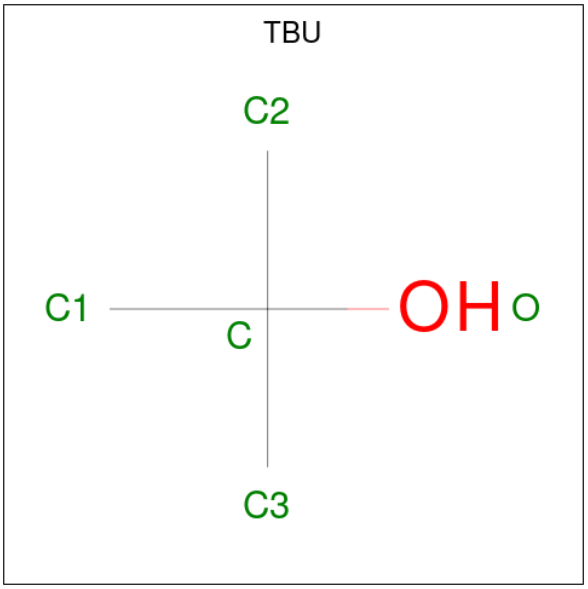
There are 5 unique types of molecules in this entry. The entry contains 4840 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SULFUR OXIDATION PROTEIN SOXB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	11	0
			4374	2822	766	780	6			

- Molecule 2 is TERTIARY-BUTYL ALCOHOL (three-letter code: TBU) (formula: $C_4H_{10}O$).

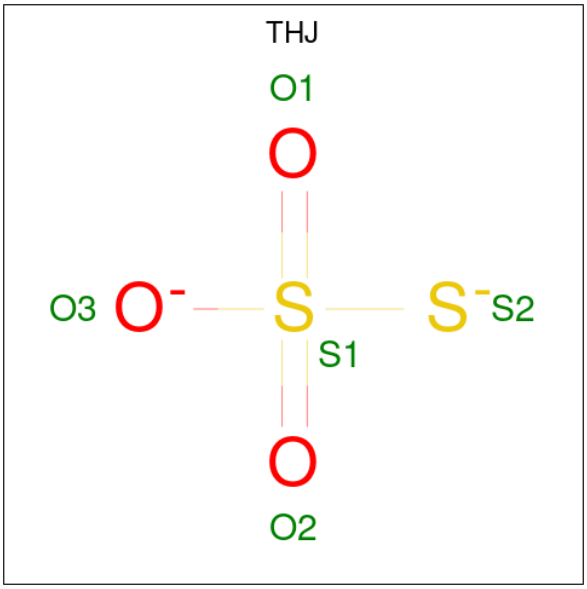


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			5	4	1			
2	A	1	Total	C	O		0	0
			5	4	1			
2	A	1	Total	C	O		0	0
			5	4	1			
2	A	1	Total	C	O		0	0
			5	4	1			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mn 2 2	0	0

- Molecule 4 is THIOSULFATE (three-letter code: THJ) (formula: O_3S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 3 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	439	Total O 439 439	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.80Å 86.74Å 95.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.15 – 1.85 64.17 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (64.15-1.85) 100.0 (64.17-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 1.86Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, R_{free}	0.185 , 0.224 0.189 , 0.229	Depositor DCC
R_{free} test set	2581 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4840	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

3 Model quality

3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TBU, MN, THJ

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	0.35	0/4525	0.62	1/6160 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	ASP	N-CA-C	5.55	125.97	111.00

There are no chirality outliers.

There are no planarity outliers.

3.2 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	4374	0	4388	57	0
2	A	20	0	40	1	0
3	A	2	0	0	0	0
4	A	5	0	0	0	0
5	A	439	0	0	3	0
All	All	4840	0	4428	57	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 6.

The worst 5 of 57 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:472:GLN:HB2	1:A:473:GLN:HG3	1.41	1.02
1:A:472:GLN:HB2	1:A:473:GLN:CG	2.04	0.86
1:A:472:GLN:HB2	1:A:473:GLN:CA	2.12	0.80
1:A:472:GLN:CB	1:A:473:GLN:HG3	2.12	0.80
1:A:406:GLU:OE1	1:A:529:LYS:HE3	1.88	0.72

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

3.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

3.3.3 RNA (i)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains (i)

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

3.5 Carbohydrates (i)

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

3.6 Ligand geometry (i)

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

3.7 Other polymers (i)

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

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 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, 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	OWAB(Å^2)	Q<0.9
1	A	545/562 (96%)	-0.25	10 (1%) 68 68	9, 18, 38, 69	6 (1%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475[A]	GLY	6.1
1	A	472	GLN	4.7
1	A	469	PRO	4.6
1	A	470	PHE	3.5
1	A	31	LEU	3.5

4.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.3 Carbohydrates

There are no monosaccharides in this entry.

4.4 Ligands

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	B-factors(Å^2)	Q<0.9
2	TBU	A	1575	5/5	0.78	0.23	71,72,73,73	0
2	TBU	A	1574	5/5	0.80	0.21	39,39,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TBU	A	1573	5/5	0.86	0.15	28,28,30,31	0
2	TBU	A	1576	5/5	0.88	0.17	40,42,43,44	0
4	THJ	A	1579	5/5	0.99	0.07	19,20,23,23	0
3	MN	A	1578	1/1	1.00	0.07	12,12,12,12	0
3	MN	A	1577	1/1	1.00	0.07	13,13,13,13	0

4.5 Other polymers

There are no such residues in this entry.