



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:32 AM UTC

PDB ID : 4ZN4 / pdb_00004zn4
Title : Crystal structure of Sqt1 from Chaetomium thermophilum solved by MR
Authors : Ahmed, Y.L.; Sinning, I.
Deposited on : 2015-05-04
Resolution : 1.94 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

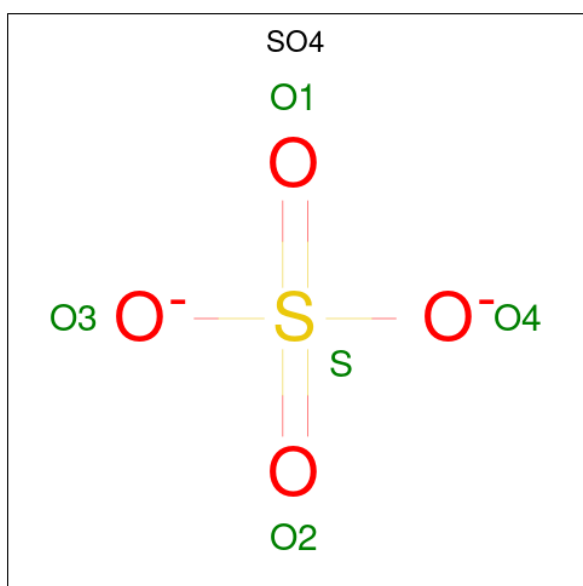
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

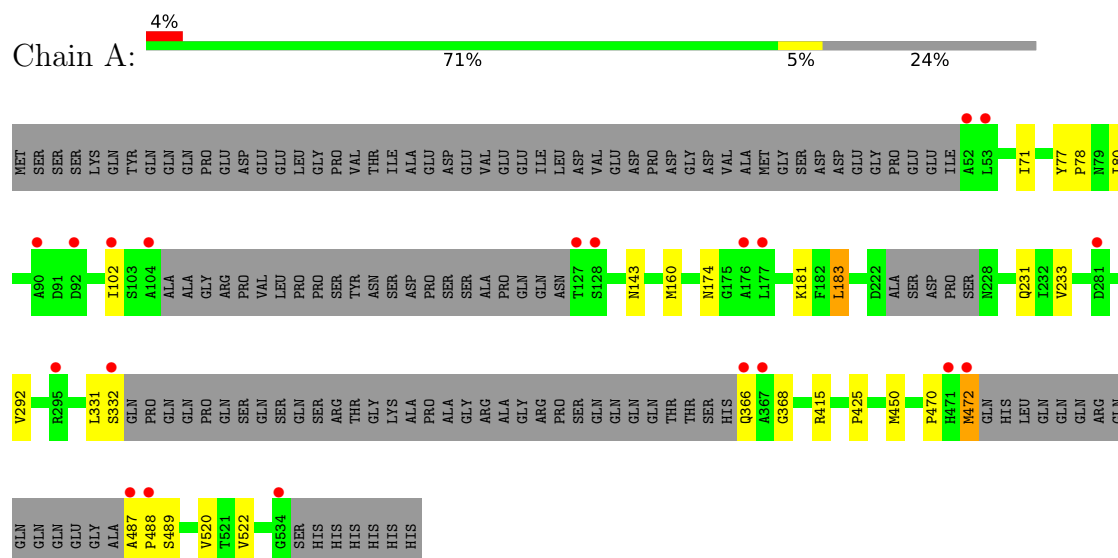
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total 156	O 156	0	0
4	B	149	Total 149	O 149	0	0

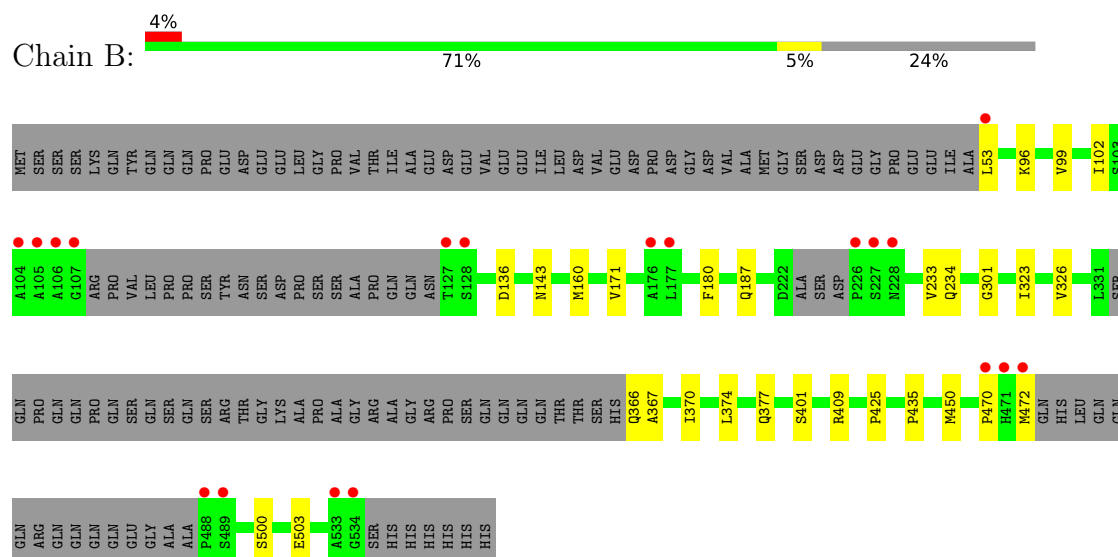
3 Residue-property plots [i](#)

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: sqt1



• Molecule 1: sqt1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.57Å 94.82Å 94.95Å 90.00° 109.90° 90.00°	Depositor
Resolution (Å)	47.41 – 1.94 47.41 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.41-1.94) 97.6 (47.41-1.94)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.171 , 0.205 0.176 , 0.207	Depositor DCC
R_{free} test set	3398 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6362	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	156	0	0	3	0
4	B	149	0	0	0	0
All	All	6362	0	5861	30	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 3.

All (30) 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:470:PRO:HB2	1:B:472:MET:HB3	1.64	0.79
1:B:500:SER:OG	1:B:503:GLU:OE1	2.02	0.77
1:A:470:PRO:HB2	1:A:472:MET:HB3	1.68	0.75
1:A:415:ARG:HD2	4:A:734:HOH:O	1.99	0.61
1:B:143:ASN:ND2	1:B:160:MET:SD	2.70	0.59
1:B:366:GLN:HG2	1:B:367:ALA:N	2.18	0.57
1:A:366:GLN:N	4:A:702:HOH:O	2.43	0.51
1:A:102:ILE:HD13	1:A:520:VAL:HG21	1.93	0.51
1:A:470:PRO:C	1:A:472:MET:H	2.16	0.51
1:A:143:ASN:ND2	1:A:160:MET:SD	2.79	0.48
1:A:470:PRO:C	1:A:472:MET:N	2.72	0.47
1:A:425:PRO:HD2	1:A:450:MET:HB2	1.96	0.47
1:A:174:ASN:OD1	1:A:174:ASN:N	2.45	0.47
1:A:487:ALA:HB3	1:A:488:PRO:HD3	1.96	0.47
1:B:233:VAL:HG12	1:B:234[B]:GLN:HG2	1.97	0.46
1:A:71:ILE:HD12	1:A:522:VAL:HG13	1.98	0.45
1:B:99:VAL:HG11	1:B:180:PHE:CZ	2.51	0.45
1:A:331:LEU:O	1:A:332:SER:HB3	2.17	0.44
1:B:326:VAL:HG22	1:B:370:ILE:HD13	2.01	0.43
1:A:77:TYR:HB2	1:A:80:ILE:HD12	2.01	0.43
1:B:96:LYS:NZ	1:B:136:ASP:OD1	2.41	0.42
1:A:368:GLY:HA3	4:A:841:HOH:O	2.19	0.41
1:B:160:MET:HE3	1:B:160:MET:HB3	1.92	0.41
1:B:377:GLN:HG2	1:B:401:SER:OG	2.21	0.41
1:A:233:VAL:O	1:B:409:ARG:HD2	2.21	0.41
1:B:323:ILE:HB	1:B:374:LEU:HB2	2.02	0.41
1:B:470:PRO:C	1:B:472:MET:H	2.27	0.41
1:A:181:LYS:O	1:A:183:LEU:HD13	2.21	0.41
1:B:425:PRO:HD2	1:B:450:MET:HB2	2.02	0.41
1:A:77:TYR:HA	1:A:78:PRO:HD2	1.96	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	Percentiles	
1	A	401/541 (74%)	391 (98%)	10 (2%)	0	100	100
1	B	402/541 (74%)	393 (98%)	9 (2%)	0	100	100
All	All	803/1082 (74%)	784 (98%)	19 (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	319/430 (74%)	314 (98%)	5 (2%)	55	46
1	B	319/430 (74%)	316 (99%)	3 (1%)	70	67
All	All	638/860 (74%)	630 (99%)	8 (1%)	65	54

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	A	292	VAL
1	A	472	MET
1	A	489[A]	SER
1	A	489[B]	SER

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Mol	Chain	Res	Type
1	B	53	LEU
1	B	102	ILE
1	B	187	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	HIS
1	B	187	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](#)

3 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	GOL	A	601	-	5,5,5	0.44	0	5,5,5	0.61	0
2	GOL	A	602	-	5,5,5	0.44	0	5,5,5	0.46	0
3	SO4	A	603	-	4,4,4	0.26	0	6,6,6	0.14	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	GOL	A	601	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-C3
2	A	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3

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

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	409/541 (75%)	0.12	20 (4%) 35 39	21, 35, 65, 94	2 (0%)
1	B	411/541 (75%)	0.03	19 (4%) 37 42	11, 35, 64, 87	1 (0%)
All	All	820/1082 (75%)	0.07	39 (4%) 35 40	11, 35, 65, 94	3 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	THR	5.7
1	A	471	HIS	5.4
1	B	471	HIS	5.3
1	B	226	PRO	5.2
1	B	53	LEU	5.1
1	A	487	ALA	5.0
1	A	53	LEU	4.5
1	A	127	THR	4.4
1	B	105	ALA	4.2
1	B	488	PRO	4.2
1	A	472	MET	3.9
1	A	104	ALA	3.8
1	A	52	ALA	3.5
1	B	534	GLY	3.5
1	A	128[A]	SER	3.5
1	A	366	GLN	3.3
1	A	488	PRO	3.1
1	B	472	MET	2.8
1	B	128	SER	2.8
1	B	104	ALA	2.7
1	A	281	ASP	2.6
1	A	176	ALA	2.6
1	A	102	ILE	2.5
1	B	470	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	533	ALA	2.5
1	B	176	ALA	2.4
1	A	332	SER	2.3
1	B	489	SER	2.3
1	B	227	SER	2.3
1	A	295	ARG	2.2
1	A	90	ALA	2.2
1	A	534	GLY	2.2
1	A	92	ASP	2.2
1	B	106	ALA	2.2
1	B	107	GLY	2.1
1	A	177	LEU	2.1
1	B	177	LEU	2.1
1	A	367	ALA	2.1
1	B	228	ASN	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 oligosaccharides 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
3	SO4	A	603	5/5	0.81	0.12	55,55,56,57	0
2	GOL	A	601	6/6	0.95	0.07	26,29,33,35	0
2	GOL	A	602	6/6	0.96	0.06	28,31,35,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.