



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:43 PM GMT

PDB ID : 4ZOY  
Title : Crystal structure of the Chaetomium thermophilum Sqt1  
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Deposited on : 2015-05-07  
Resolution : 1.50 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

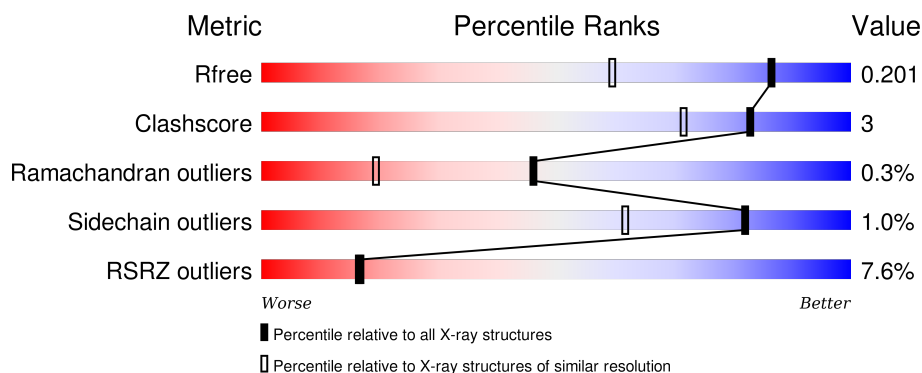
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	491	<div> <div>6%</div> <div>77%</div> <div>5%</div> <div>17%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3569 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 Sqt1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	2	0
			3009	1893	520	589	7			

There are 9 discrepancies between the modelled and reference sequences:

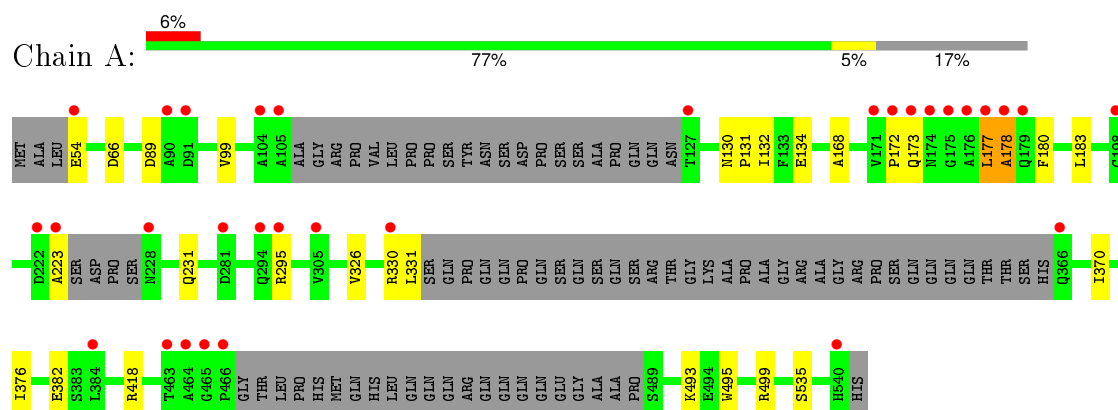
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	MET	-	initiating methionine	UNP G0S0R0
A	534	GLY	-	expression tag	UNP G0S0R0
A	535	SER	-	expression tag	UNP G0S0R0
A	536	HIS	-	expression tag	UNP G0S0R0
A	537	HIS	-	expression tag	UNP G0S0R0
A	538	HIS	-	expression tag	UNP G0S0R0
A	539	HIS	-	expression tag	UNP G0S0R0
A	540	HIS	-	expression tag	UNP G0S0R0
A	541	HIS	-	expression tag	UNP G0S0R0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	560	Total	O	0	0
			560	560		



- Molecule 1: Sqt1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.44Å 73.02Å 113.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.38 – 1.50 37.38 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (37.38-1.50) 96.3 (37.38-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1685)	Depositor
R, $R_{free}$	0.184 , 0.202 0.183 , 0.201	Depositor DCC
$R_{free}$ test set	4388 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 89214 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.41	1/3076 (0.0%)	0.60	2/4189 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	376	ILE	C-O	-6.89	1.10	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	499	ARG	NE-CZ-NH1	6.39	123.50	120.30

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	3009	0	2891	18	2
2	A	560	0	0	8	2
All	All	3569	0	2891	18	2

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 (18) 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:172:PRO:HD2	1:A:177:LEU:HA	1.74	0.69
1:A:535:SER:OG	2:A:602:HOH:O	2.16	0.60
1:A:54:GLU:N	2:A:612:HOH:O	2.36	0.59
1:A:418:ARG:NH1	2:A:607:HOH:O	2.30	0.56
1:A:223:ALA:HB2	2:A:893:HOH:O	2.08	0.52
1:A:168:ALA:HB2	1:A:183:LEU:HD11	1.91	0.51
1:A:132:ILE:HD12	1:A:178:ALA:HB3	1.95	0.49
1:A:493:LYS:HG2	1:A:495:TRP:CZ2	2.49	0.48
1:A:178:ALA:HB1	1:A:180:PHE:CE1	2.50	0.46
1:A:99:VAL:HG11	1:A:180:PHE:CZ	2.51	0.45
1:A:295:ARG:HG3	1:A:370:ILE:HG13	1.99	0.43
1:A:134:GLU:OE1	2:A:604:HOH:O	2.21	0.43
1:A:326:VAL:HG22	1:A:370:ILE:HD13	2.02	0.41
1:A:130:ASN:HA	1:A:131:PRO:HD3	1.97	0.41
1:A:331:LEU:O	2:A:605:HOH:O	2.22	0.41
1:A:177:LEU:HB3	1:A:178:ALA:H	1.54	0.41
1:A:231:GLN:NE2	2:A:603:HOH:O	2.18	0.41
1:A:382:GLU:HG3	2:A:1027:HOH:O	2.21	0.40

All (2) 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)
1:A:66:ASP:OD2	2:A:601:HOH:O[4_545]	2.04	0.16
1:A:89:ASP:OD2	2:A:601:HOH:O[4_545]	2.04	0.16

## 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	398/491 (81%)	384 (96%)	13 (3%)	1 (0%)	46 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	ALA

### 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	317/386 (82%)	314 (99%)	3 (1%)	84	65

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	177	LEU
1	A	330	ARG

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

### 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 carbohydrates 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	406/491 (82%)	0.38	31 (7%) 17 16	13, 19, 41, 52	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	LEU	12.6
1	A	176	ALA	12.3
1	A	174	ASN	9.2
1	A	175	GLY	8.4
1	A	173	GLN	6.9
1	A	223	ALA	6.6
1	A	104	ALA	6.1
1	A	540	HIS	5.1
1	A	466	PRO	4.9
1	A	105	ALA	4.6
1	A	178	ALA	4.3
1	A	465	GLY	4.3
1	A	172	PRO	4.2
1	A	366	GLN	4.2
1	A	330	ARG	3.9
1	A	198	CYS	3.9
1	A	464	ALA	3.7
1	A	228	ASN	3.4
1	A	171	VAL	3.3
1	A	294	GLN	3.2
1	A	295	ARG	3.2
1	A	90	ALA	2.8
1	A	222	ASP	2.5
1	A	127	THR	2.4
1	A	91	ASP	2.4
1	A	305	VAL	2.3
1	A	281	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	384	LEU	2.3
1	A	179	GLN	2.1
1	A	54	GLU	2.1
1	A	463	THR	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 carbohydrates 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.