



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:30 am GMT

PDB ID : 4ZOV
Title : Crystal structure of the Saccharomyces cerevisiae Sqt1
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Deposited on : 2015-05-07
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

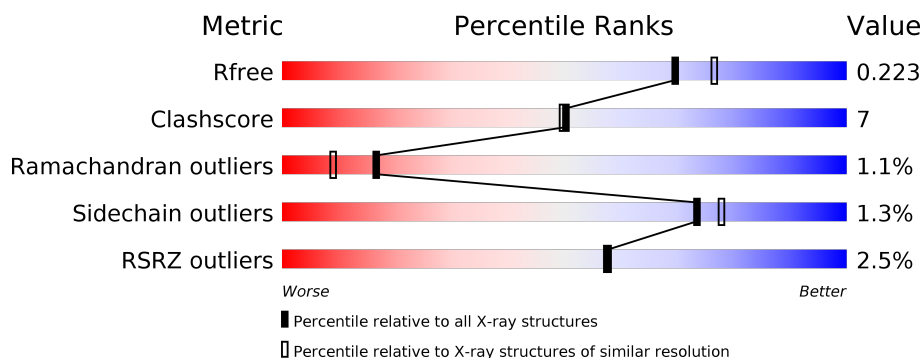
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 ≥ 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	387	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>••</div> </div> </div>
1	B	387	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>•</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6367 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 Ribosome assembly protein SQT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2889	1826	481	562	20			
1	B	373	Total	C	N	O	S	0	0	0
			2838	1794	473	551	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	GLY	-	expression tag	UNP P35184
A	433	SER	-	expression tag	UNP P35184
A	434	HIS	-	expression tag	UNP P35184
A	435	HIS	-	expression tag	UNP P35184
A	436	HIS	-	expression tag	UNP P35184
A	437	HIS	-	expression tag	UNP P35184
A	438	HIS	-	expression tag	UNP P35184
A	439	HIS	-	expression tag	UNP P35184
B	432	GLY	-	expression tag	UNP P35184
B	433	SER	-	expression tag	UNP P35184
B	434	HIS	-	expression tag	UNP P35184
B	435	HIS	-	expression tag	UNP P35184
B	436	HIS	-	expression tag	UNP P35184
B	437	HIS	-	expression tag	UNP P35184
B	438	HIS	-	expression tag	UNP P35184
B	439	HIS	-	expression tag	UNP P35184

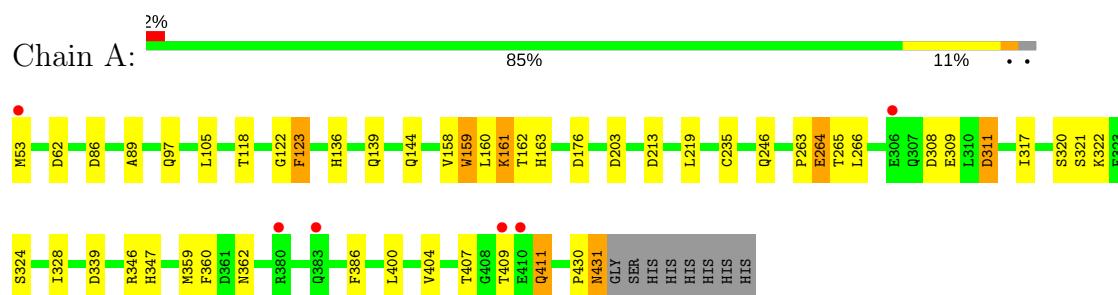
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	332	Total	O	0	0
			332	332		
2	B	308	Total	O	0	0
			308	308		

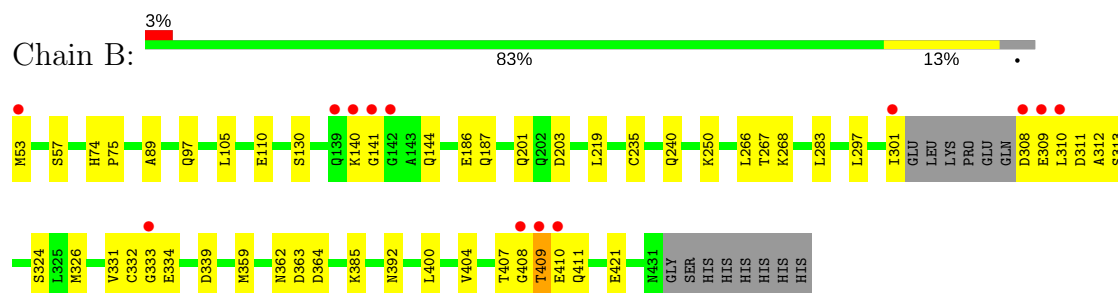
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Ribosome assembly protein SQT1



• Molecule 1: Ribosome assembly protein SQT1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.79Å 75.17Å 101.25Å 90.00° 104.42° 90.00°	Depositor
Resolution (Å)	42.56 – 2.00 42.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (42.56-2.00) 98.0 (42.82-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.02 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1685)	Depositor
R, R_{free}	0.187 , 0.223 0.188 , 0.223	Depositor DCC
R_{free} test set	1991 reflections (3.84%)	DCC
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6367	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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	0.42	0/2950	0.62	0/4003
1	B	0.40	0/2897	0.59	1/3930 (0.0%)
All	All	0.41	0/5847	0.60	1/7933 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLY	N-CA-C	-5.04	100.51	113.10

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	2889	0	2810	35	0
1	B	2838	0	2758	44	0
2	A	332	0	0	11	2
2	B	308	0	0	10	2
All	All	6367	0	5568	75	3

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 7.

The worst 5 of 75 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:240:GLN:NE2	2:B:504:HOH:O	2.10	0.83
1:A:86:ASP:OD1	2:A:501:HOH:O	1.97	0.82
1:A:118:THR:OG1	1:A:122:GLY:O	1.99	0.80
1:A:53:MET:SD	2:A:530:HOH:O	2.39	0.79
1:B:186:GLU:OE2	2:B:501:HOH:O	2.04	0.76

All (3) 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)
2:A:504:HOH:O	2:A:658:HOH:O[2_656]	1.79	0.41
2:B:705:HOH:O	2:B:712:HOH:O[1_455]	2.13	0.07
2:A:665:HOH:O	2:B:646:HOH:O[2_747]	2.16	0.04

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	377/387 (97%)	357 (95%)	14 (4%)	6 (2%)	11	5
1	B	369/387 (95%)	353 (96%)	14 (4%)	2 (0%)	32	26
All	All	746/774 (96%)	710 (95%)	28 (4%)	8 (1%)	17	9

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	TRP
1	A	163	HIS
1	B	408	GLY
1	A	411	GLN
1	A	123	PHE

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	320/327 (98%)	315 (98%)	5 (2%)	68	72
1	B	314/327 (96%)	311 (99%)	3 (1%)	80	84
All	All	634/654 (97%)	626 (99%)	8 (1%)	73	78

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	ASP
1	B	409	THR
1	B	144	GLN
1	A	264	GLU
1	A	431	ASN

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

Mol	Chain	Res	Type
1	B	240	GLN
1	B	431	ASN

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 [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	379/387 (97%)	-0.36	6 (1%) 72 71	14, 26, 41, 58	0
1	B	373/387 (96%)	-0.33	13 (3%) 44 45	14, 26, 45, 60	0
All	All	752/774 (97%)	-0.34	19 (2%) 58 57	14, 26, 43, 60	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	LEU	5.8
1	B	141	GLY	5.4
1	B	409	THR	4.2
1	B	309	GLU	3.8
1	B	142	GLY	3.5

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.