



wwPDB X-ray Structure Validation Summary Report

Feb 14, 2017 – 08:00 pm GMT

PDB ID : 3PSI
Title : Crystal Structure of the Spt6 core domain from *Saccharomyces cerevisiae*,
Form Spt6(239-1451)
Authors : Close, D.; Hill, C.P.; Johnson, S.J.
Deposited on : 2010-12-01
Resolution : 3.30 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

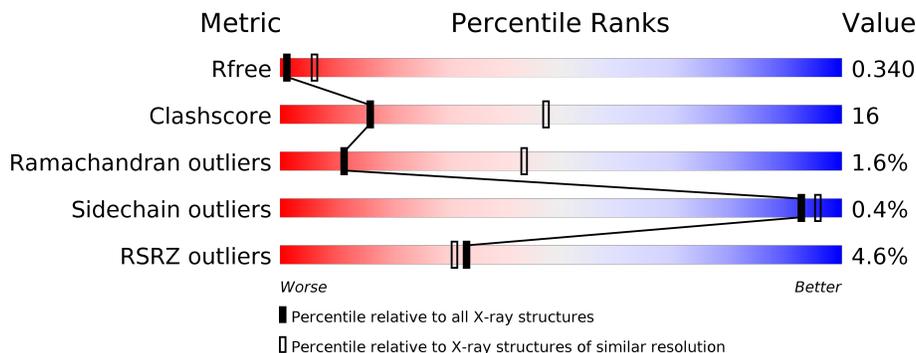
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	1219	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13677 atoms, of which 6800 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 Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	843	13677	4370	6800	1164	1326	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLY	-	EXPRESSION TAG	UNP P23615
A	234	ILE	-	EXPRESSION TAG	UNP P23615
A	235	ASP	-	EXPRESSION TAG	UNP P23615
A	236	PRO	-	EXPRESSION TAG	UNP P23615
A	237	PHE	-	EXPRESSION TAG	UNP P23615
A	238	THR	-	EXPRESSION TAG	UNP P23615

VAL
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ARG
GLN
ASN
GLN
SER
VAL
SER
SER
ARG
GLY
ASP
ASP
HIS
HIS
LEU
VAL
ILE
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SER
ASN
SER
SER
SER
LYS
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ASN
TYR
TYR
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.75Å 118.75Å 214.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.67 – 3.30 45.67 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.67-3.30) 99.4 (45.67-3.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 3.32Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.265 , 0.308 0.247 , 0.340	Depositor DCC
R_{free} test set	2827 reflections (10.53%)	DCC
Wilson B-factor (Å ²)	111.6	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 136.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13677	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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	0.62	0/7015	0.77	2/9487 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1020	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	1101	LEU	CB-CG-CD1	-5.88	101.00	111.00

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	6877	6800	6777	221	0
All	All	6877	6800	6777	221	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 16.

The worst 5 of 221 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:A:980:ILE:HD12	1:A:981:THR:N	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LEU:HD11	1:A:658:HIS:HB2	1.61	0.83
1:A:980:ILE:HD12	1:A:981:THR:H	1.41	0.81
1:A:641:PHE:CE1	1:A:713:LEU:HD23	2.21	0.75
1:A:653:LEU:HD12	1:A:653:LEU:C	2.07	0.74

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	831/1219 (68%)	760 (92%)	58 (7%)	13 (2%)	11 43

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1117	GLY
1	A	742	VAL
1	A	551	SER
1	A	628	ASN
1	A	762	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	762/1108 (69%)	759 (100%)	3 (0%)	93 96

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

Mol	Chain	Res	Type
1	A	689	PHE
1	A	726	ARG
1	A	1204	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	909	ASN
1	A	1147	HIS
1	A	982	HIS
1	A	429	ASN
1	A	1074	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	843/1219 (69%)	0.27	39 (4%) 33 31	74, 150, 305, 453	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	ILE	7.3
1	A	638	PRO	5.4
1	A	519	ILE	5.3
1	A	679	THR	4.8
1	A	569	LEU	4.3

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.