



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 01:33 pm BST

PDB ID : 5U1T  
Title : Crystal structure of the *Saccharomyces cerevisiae* separase-securin complex at 2.6 angstrom resolution  
Authors : Luo, S.; Tong, L.  
Deposited on : 2016-11-29  
Resolution : 2.60 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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

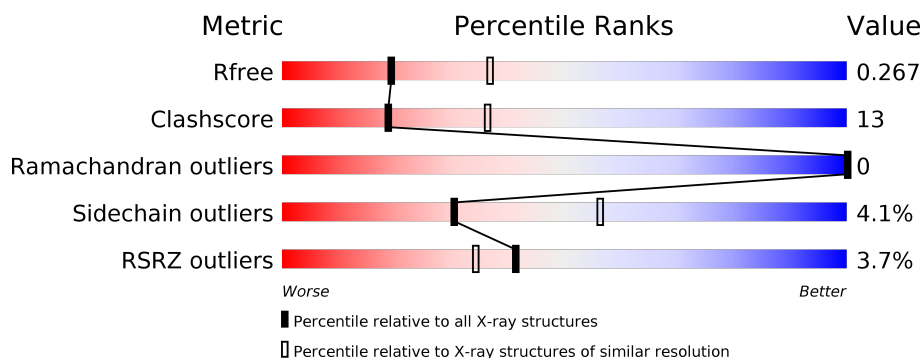
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 respectively. 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	1596	
2	B	117	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12633 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 Separin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1486	Total	C	N	O	S	0	0	0
			12078	7811	1979	2220	68			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP Q03018
A	36	HIS	-	expression tag	UNP Q03018
A	37	HIS	-	expression tag	UNP Q03018
A	38	HIS	-	expression tag	UNP Q03018
A	39	HIS	-	expression tag	UNP Q03018
A	40	HIS	-	expression tag	UNP Q03018
A	41	HIS	-	expression tag	UNP Q03018
A	42	SER	-	expression tag	UNP Q03018
A	43	GLY	-	expression tag	UNP Q03018
A	44	GLY	-	expression tag	UNP Q03018
A	45	SER	-	expression tag	UNP Q03018
A	46	ARG	-	expression tag	UNP Q03018
A	47	SER	-	expression tag	UNP Q03018
A	48	GLU	-	expression tag	UNP Q03018
A	49	ALA	-	expression tag	UNP Q03018
A	50	HIS	-	expression tag	UNP Q03018

- Molecule 2 is a protein called Securin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	66	Total	C	N	O	S	0	0	0
			539	346	79	113	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	257	MET	-	initiating methionine	UNP P40316

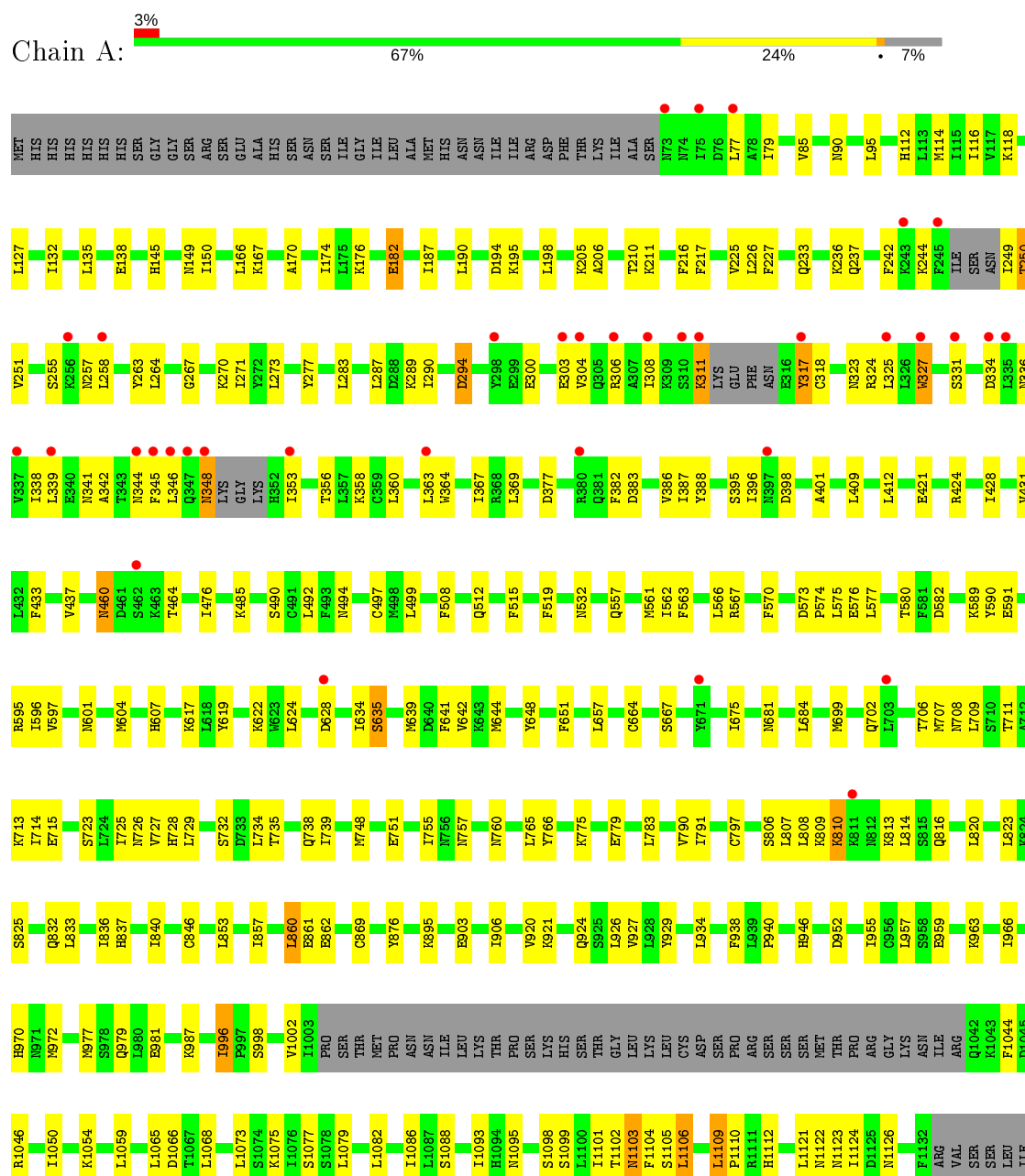
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		

### 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: Separin





LEU	D257	GLU	D297	GLU	D298	GLU	D299	GLU	D306	GLU	D313	GLU	D314	GLU	D315	GLU	D316	GLU	D317	GLU	D318	GLU	D319	GLU	D320	GLU	D321	GLU	D322	GLU	D323	GLU	D324	GLU	D325	GLU	D326	GLU	D327	GLU	D328	GLU	D329	GLU	D330	GLU	D331	GLU	D332	GLU	D333	GLU	D334	GLU	D335	GLU	D336	GLU	D337	GLU	D338	GLU	D339	GLU	D340	GLU	D341	GLU	D342	GLU	D343	GLU	D344	GLU	D345	GLU	D346	GLU	D347	GLU	D348	GLU	D349	GLU	D350	GLU	D351	GLU	D352	GLU	D353	GLU	D354	GLU	D355	GLU	D356	GLU	D357	GLU	D358	GLU	D359	GLU	D360	GLU	D361	GLU	D362	GLU	D363	GLU	D364	GLU	D365	GLU	D366	GLU	D367	GLU	D368	GLU	D369	GLU	D370	GLU	D371	GLU	D372	GLU	D373	GLU	D374	GLU	D375	GLU	D376	GLU	D377	GLU	D378	GLU	D379	GLU	D380	GLU	D381	GLU	D382	GLU	D383	GLU	D384	GLU	D385	GLU	D386	GLU	D387	GLU	D388	GLU	D389	GLU	D390	GLU	D391	GLU	D392	GLU	D393	GLU	D394	GLU	D395	GLU	D396	GLU	D397	GLU	D398	GLU	D399	GLU	D400	GLU	D401	GLU	D402	GLU	D403	GLU	D404	GLU	D405	GLU	D406	GLU	D407	GLU	D408	GLU	D409	GLU	D410	GLU	D411	GLU	D412	GLU	D413	GLU	D414	GLU	D415	GLU	D416	GLU	D417	GLU	D418	GLU	D419	GLU	D420	GLU	D421	GLU	D422	GLU	D423	GLU	D424	GLU	D425	GLU	D426	GLU	D427	GLU	D428	GLU	D429	GLU	D430	GLU	D431	GLU	D432	GLU	D433	GLU	D434	GLU	D435	GLU	D436	GLU	D437	GLU	D438	GLU	D439	GLU	D440	GLU	D441	GLU	D442	GLU	D443	GLU	D444	GLU	D445	GLU	D446	GLU	D447	GLU	D448	GLU	D449	GLU	D450	GLU	D451	GLU	D452	GLU	D453	GLU	D454	GLU	D455	GLU	D456	GLU	D457	GLU	D458	GLU	D459	GLU	D460	GLU	D461	GLU	D462	GLU	D463	GLU	D464	GLU	D465	GLU	D466	GLU	D467	GLU	D468	GLU	D469	GLU	D470	GLU	D471	GLU	D472	GLU	D473	GLU	D474	GLU	D475	GLU	D476	GLU	D477	GLU	D478	GLU	D479	GLU	D480	GLU	D481	GLU	D482	GLU	D483	GLU	D484	GLU	D485	GLU	D486	GLU	D487	GLU	D488	GLU	D489	GLU	D490	GLU	D491	GLU	D492	GLU	D493	GLU	D494	GLU	D495	GLU	D496	GLU	D497	GLU	D498	GLU	D499	GLU	D500	GLU	D501	GLU	D502	GLU	D503	GLU	D504	GLU	D505	GLU	D506	GLU	D507	GLU	D508	GLU	D509	GLU	D510	GLU	D511	GLU	D512	GLU	D513	GLU	D514	GLU	D515	GLU	D516	GLU	D517	GLU	D518	GLU	D519	GLU	D520	GLU	D521	GLU	D522	GLU	D523	GLU	D524	GLU	D525	GLU	D526	GLU	D527	GLU	D528	GLU	D529	GLU	D530	GLU	D531	GLU	D532	GLU	D533	GLU	D534	GLU	D535	GLU	D536	GLU	D537	GLU	D538	GLU	D539	GLU	D540	GLU	D541	GLU	D542	GLU	D543	GLU	D544	GLU	D545	GLU	D546	GLU	D547	GLU	D548	GLU	D549	GLU	D550	GLU	D551	GLU	D552	GLU	D553	GLU	D554	GLU	D555	GLU	D556	GLU	D557	GLU	D558	GLU	D559	GLU	D560	GLU	D561	GLU	D562	GLU	D563	GLU	D564	GLU	D565	GLU	D566	GLU	D567	GLU	D568	GLU	D569	GLU	D570	GLU	D571	GLU	D572	GLU	D573	GLU	D574	GLU	D575	GLU	D576	GLU	D577	GLU	D578	GLU	D579	GLU
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.86Å 125.86Å 271.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 2.60 48.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.67-2.60) 91.5 (48.67-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.221 , 0.264 0.227 , 0.267	Depositor DCC
$R_{free}$ test set	2016 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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, 0.333 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	0.53	0/12316	0.59	2/16621 (0.0%)
2	B	0.56	0/549	0.61	0/745
All	All	0.53	0/12865	0.59	2/17366 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	813	LYS	N-CA-C	-5.18	97.02	111.00
1	A	860	LEU	CB-CG-CD1	-5.11	102.31	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	996	ILE	Peptide

### 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	12078	0	12320	325	0
2	B	539	0	518	21	0
3	A	16	0	0	1	0
All	All	12633	0	12838	333	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 13.

The worst 5 of 333 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:353:ILE:CD1	1:A:395:SER:OG	1.66	1.43
1:A:734:LEU:HD11	1:A:738:GLN:NE2	1.42	1.33
1:A:353:ILE:HD12	1:A:395:SER:OG	1.12	1.28
1:A:591:GLU:OE2	1:A:595:ARG:NE	1.71	1.23
1:A:255:SER:HB3	1:A:290:ILE:HD11	1.15	1.12

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	1470/1596 (92%)	1394 (95%)	76 (5%)	0	100	100
2	B	60/117 (51%)	58 (97%)	2 (3%)	0	100	100
All	All	1530/1713 (89%)	1452 (95%)	78 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	1391/1491 (93%)	1337 (96%)	54 (4%)	32	58
2	B	63/108 (58%)	58 (92%)	5 (8%)	12	24
All	All	1454/1599 (91%)	1395 (96%)	59 (4%)	30	56

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	797	CYS
1	A	1066	ASP
2	B	258	ASP
1	A	810	LYS
1	A	903	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	708	ASN
1	A	837	HIS
1	A	1495	GLN
1	A	738	GLN
1	A	882	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	1486/1596 (93%)	0.12	55 (3%) 41 34	42, 67, 107, 139	0
2	B	66/117 (56%)	0.28	2 (3%) 50 43	57, 79, 101, 119	0
All	All	1552/1713 (90%)	0.13	57 (3%) 41 34	42, 68, 108, 139	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	ILE	6.2
1	A	348	ASN	5.0
1	A	245	PHE	4.9
1	A	1471	ILE	4.7
1	A	1594	ASN	4.6

### 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.