



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 09:59 am GMT

PDB ID : 3QO8  
Title : Crystal Structure of seryl-tRNA synthetase from *Candida albicans*  
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Deposited on : 2011-02-09  
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](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	:	1.7.2 (RC1), CSD as538be (2017)
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

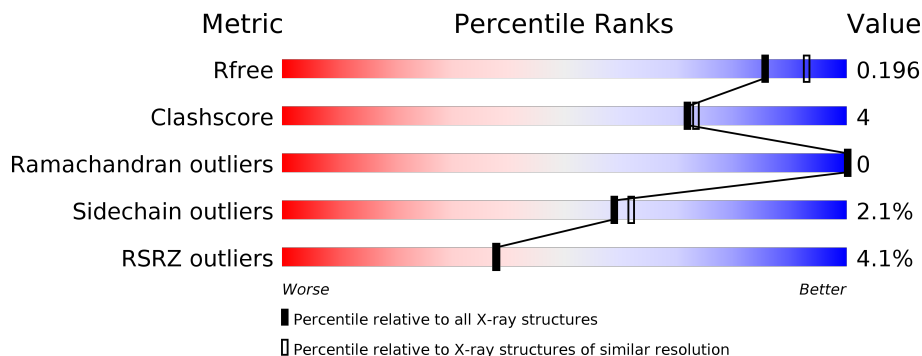
# 1 Overall quality at a glance

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  $\geq 3$ , 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	485	<div> <div>4%</div> <div>82%</div> <div>9%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	489	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3913 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.

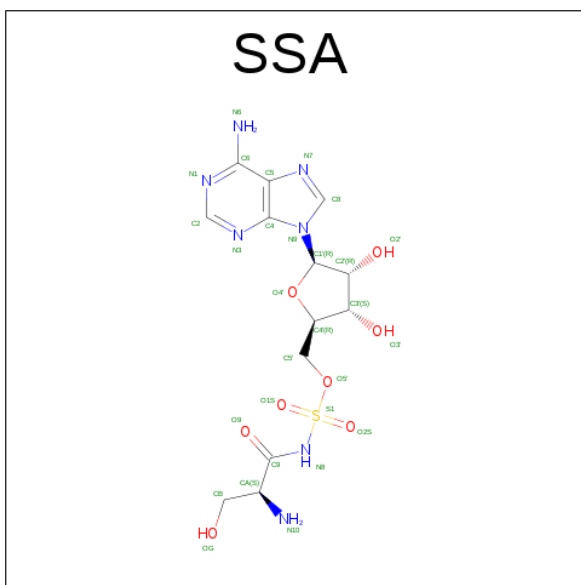
- Molecule 1 is a protein called Seryl-tRNA synthetase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	5	0
			3598	2291	606	688	13			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	PRO	-	EXPRESSION TAG	UNP Q9HGT6
A	464	LYS	-	EXPRESSION TAG	UNP Q9HGT6
A	465	ASN	-	EXPRESSION TAG	UNP Q9HGT6
A	466	THR	-	EXPRESSION TAG	UNP Q9HGT6
A	467	THR	-	EXPRESSION TAG	UNP Q9HGT6
A	468	SER	-	EXPRESSION TAG	UNP Q9HGT6
A	469	VAL	-	EXPRESSION TAG	UNP Q9HGT6
A	470	LYS	-	EXPRESSION TAG	UNP Q9HGT6
A	471	LYS	-	EXPRESSION TAG	UNP Q9HGT6
A	472	ALA	-	EXPRESSION TAG	UNP Q9HGT6
A	473	LYS	-	EXPRESSION TAG	UNP Q9HGT6
A	474	GLY	-	EXPRESSION TAG	UNP Q9HGT6
A	475	LYS	-	EXPRESSION TAG	UNP Q9HGT6
A	476	ASN	-	EXPRESSION TAG	UNP Q9HGT6
A	477	GLY	-	EXPRESSION TAG	UNP Q9HGT6
A	478	SER	-	EXPRESSION TAG	UNP Q9HGT6
A	479	ARG	-	EXPRESSION TAG	UNP Q9HGT6
A	480	HIS	-	EXPRESSION TAG	UNP Q9HGT6
A	481	HIS	-	EXPRESSION TAG	UNP Q9HGT6
A	482	HIS	-	EXPRESSION TAG	UNP Q9HGT6
A	483	HIS	-	EXPRESSION TAG	UNP Q9HGT6
A	484	HIS	-	EXPRESSION TAG	UNP Q9HGT6
A	485	HIS	-	EXPRESSION TAG	UNP Q9HGT6

- Molecule 2 is 5'-O-(N-(L-SERYL)-SULFAMOYL)ADENOSINE (three-letter code: SSA) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>7</sub>O<sub>8</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 29	C 13	N 7	O 8	S 1	0	0
2	A	1	Total 29	C 13	N 7	O 8	S 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

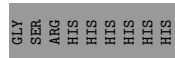
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	255	Total O 255 255	0	0



- Molecule 1: Seryl-tRNA synthetase, cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.00Å 91.00Å 275.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.83 – 2.00 75.77 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (59.83-2.00) 99.2 (75.77-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.83 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.181 , 0.206 0.167 , 0.196	Depositor DCC
$R_{free}$ test set	2334 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SSA

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	0.37	0/3684	0.50	0/4965

There are no bond length outliers.

There are no bond angle outliers.

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	3598	0	3555	29	0
2	A	58	0	38	1	0
3	A	2	0	0	0	0
4	A	255	0	0	0	0
All	All	3913	0	3593	29	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 4.

The worst 5 of 29 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:432:ARG:NH2	2:A:488:SSA:H2	2.02	0.75
1:A:215:LYS:HG2	1:A:242:TYR:CE2	2.31	0.66
1:A:450:LYS:HG3	1:A:451:ASN:N	2.13	0.63
1:A:269[B]:VAL:HG23	1:A:306:LEU:HD13	1.82	0.61
1:A:28:SER:HB3	1:A:31:LEU:HD13	1.84	0.59

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	440/485 (91%)	433 (98%)	7 (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	390/424 (92%)	382 (98%)	8 (2%)	59	62

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

Mol	Chain	Res	Type
1	A	164	TYR
1	A	433	LYS

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Mol	Chain	Res	Type
1	A	265	GLU
1	A	74	LYS
1	A	246	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	SSA	A	486	3	27,31,31	0.96	1 (3%)	28,46,46	2.87	3 (10%)
2	SSA	A	488	-	27,31,31	1.11	3 (11%)	28,46,46	2.80	3 (10%)

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	SSA	A	486	3	-	0/16/37/37	0/3/3/3
2	SSA	A	488	-	-	0/16/37/37	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	488	SSA	O5'-S1	-3.32	1.54	1.59
2	A	486	SSA	O5'-S1	-3.24	1.54	1.59
2	A	488	SSA	O1S-S1	2.01	1.44	1.42
2	A	488	SSA	O2S-S1	2.38	1.44	1.42

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	486	SSA	O2S-S1-O1S	-11.08	109.98	121.30
2	A	488	SSA	O2S-S1-O1S	-10.72	110.35	121.30
2	A	488	SSA	N3-C2-N1	-8.81	121.18	128.86
2	A	486	SSA	N3-C2-N1	-8.71	121.28	128.86
2	A	488	SSA	C4-C5-N7	-2.32	107.17	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	488	SSA	1	0

## 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	441/485 (90%)	0.05	18 (4%) 38 38	13, 28, 72, 124	1 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	PHE	5.6
1	A	64	GLY	5.0
1	A	283	GLY	4.9
1	A	285	HIS	4.8
1	A	290	TRP	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	489	1/1	0.97	0.33	10.78	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SSA	A	488	29/29	0.81	0.19	1.45	33,45,65,71	29
2	SSA	A	486	29/29	0.97	0.11	-0.61	14,18,20,23	0
3	MG	A	487	1/1	0.99	0.09	-	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.