

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 10, 2023 – 06:52 AM EDT

PDB ID	:	7T1C
Title	:	Crystal structure of RUBISCO from Sulfurivirga caldicuralii
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Deposited on		
Resolution	:	1.73  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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

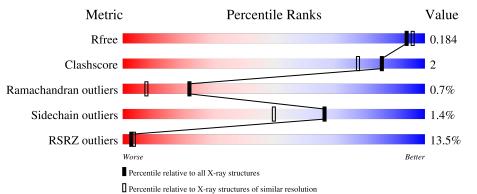
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.73 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3764(1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	Δ	466	91%	6% •
1	11	400	91%	070 •



#### 7T1C

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7235 atoms, of which 3397 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 Ribulose-bisphosphate carboxylase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	453	Total 6935	C 2263	Н 3397	N 603	O 649	S 23	0	0	0

• Molecule 2 is water.

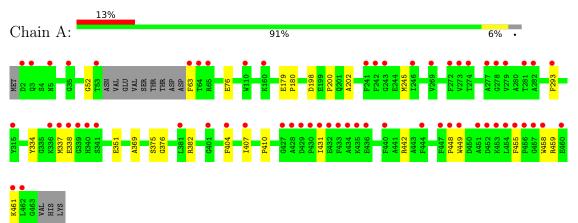
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	300	Total O 300 300	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Ribulose-bisphosphate carboxylase





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants	133.06Å 133.06Å 112.46Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	43.55 - 1.73	Depositor
Resolution (A)	43.55 - 1.73	EDS
% Data completeness	89.5(43.55-1.73)	Depositor
(in resolution range)	87.8 (43.55-1.73)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.83 (at 1.73 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.166 , $0.184$	Depositor
$R, R_{free}$	0.165 , $0.184$	DCC
$R_{free}$ test set	2000 reflections $(3.25\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	27.6	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.40 , $42.8$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.51, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7235	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.28	0/3636	0.53	0/4912

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 (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	А	3538	3397	3396	15	0
2	А	300	0	0	1	1
All	All	3838	3397	3396	15	1

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 2.

All (15) 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:431:ILE:HG21	1:A:461:LYS:HD3	1.87	0.55
1:A:76:GLU:OE2	2:A:501:HOH:O	2.18	0.55
1:A:407:ILE:HD11	1:A:442:ARG:HB3	1.95	0.47
1:A:351:GLU:HA	1:A:369:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ARG:HH11	1:A:459:ARG:HG2	1.82	0.44
1:A:179:GLU:HB2	1:A:180:PRO:HD3	1.99	0.44
1:A:334:TYR:O	1:A:382:ARG:HD3	2.18	0.44
1:A:431:ILE:HD11	1:A:455:PHE:HB3	1.99	0.44
1:A:63:PHE:O	1:A:63:PHE:CG	2.71	0.43
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.32	0.43
1:A:404:PHE:CD1	1:A:410:PRO:HB3	2.53	0.43
1:A:198:ASP:CG	1:A:200:PRO:HD2	2.40	0.42
1:A:198:ASP:OD2	1:A:200:PRO:HD2	2.20	0.41
1:A:448:PRO:HD2	1:A:449:TRP:H	1.84	0.41
1:A:458:TRP:CE2	1:A:459:ARG:HG3	2.55	0.41

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All (1) 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:753:HOH:O	2:A:753:HOH:O[12_556]	2.06	0.14

### 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	А	449/466~(96%)	432 (96%)	14 (3%)	3 (1%)	22 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	52	GLY
1	А	202	ALA
1	А	376	GLY



#### 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	А	356/369~(96%)	351~(99%)	5(1%)	67 50	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	245	MET
1	А	293	PHE
1	А	337	MET
1	А	338	GLU
1	А	375	SER

Sometimes 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 monosaccharides 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,  $95^{th}$  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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	453/466~(97%)	0.41	61 (13%) 3 4	21, 34, 74, 150	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	63	PHE	8.7
1	А	455	PHE	6.7
1	А	64	THR	6.7
1	А	338	GLU	6.5
1	А	337	MET	6.1
1	А	462	LEU	5.9
1	А	449	TRP	5.2
1	А	2	ASP	5.1
1	А	404	PHE	5.0
1	А	381	LEU	4.7
1	А	65	ARG	4.6
1	А	454	LEU	4.4
1	А	336	LYS	4.2
1	А	53	THR	4.1
1	А	431	ILE	4.1
1	А	435	LYS	3.8
1	А	272	PHE	3.7
1	А	339	GLY	3.6
1	А	460	GLU	3.6
1	А	429	ASP	3.5
1	А	407	ILE	3.5
1	А	451	ALA	3.3
1	А	447	PHE	3.3
1	А	457	GLY	3.1
1	А	433	PHE	3.1
1	А	427	GLY	3.1
1	A	242	PHE	3.1

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7]	Γ1	С
( ]	LI	U

Mol	Chain	Res	Type	RSRZ
1	А	436	GLU	3.0
1	А	315	TYR	3.0
1	А	110	TRP	3.0
1	А	277	ALA	2.8
1	А	273	VAL	2.8
1	А	3	GLN	2.8
1	А	341	SER	2.8
1	А	444	PHE	2.7
1	А	448	PRO	2.7
1	А	432	GLU	2.7
1	А	340	HIS	2.7
1	А	434	ALA	2.6
1	А	461	LYS	2.6
1	А	281	THR	2.6
1	А	241	PHE	2.5
1	А	456	PRO	2.4
1	А	269	VAL	2.4
1	А	458	TRP	2.4
1	А	452	ASP	2.4
1	А	428	ALA	2.4
1	А	293	PHE	2.4
1	А	430	PRO	2.3
1	А	279	VAL	2.3
1	А	453	LYS	2.3
1	А	5	ASN	2.2
1	А	401	GLY	2.2
1	А	35	GLY	2.1
1	А	278	GLY	2.1
1	А	274	THR	2.1
1	А	282	ALA	2.1
1	А	440	PHE	2.1
1	А	246	ILE	2.1
1	А	160	LYS	2.0
1	А	243	GLY	2.0

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### 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 monosaccharides 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.

