



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 10:30 pm GMT

PDB ID : 1S3H
Title : Propionibacterium shermanii transcarboxylase 5S subunit A59T
Authors : Hall, P.R.; Zheng, R.; Antony, L.; Pusztai-Carey, M.; Carey, P.R.; Yee, V.C.
Deposited on : 2004-01-13
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

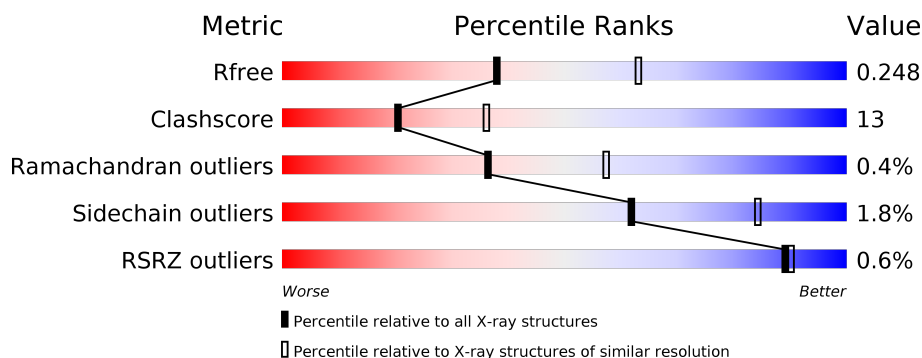
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	539	<div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3667 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 transcarboxylase 5S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3665	2301	633	703	28			

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	CLONING ARTIFACT	UNP Q70AC7
A	-9	ALA	-	CLONING ARTIFACT	UNP Q70AC7
A	-8	ILE	-	CLONING ARTIFACT	UNP Q70AC7
A	-7	SER	-	CLONING ARTIFACT	UNP Q70AC7
A	-6	ARG	-	CLONING ARTIFACT	UNP Q70AC7
A	-5	GLU	-	CLONING ARTIFACT	UNP Q70AC7
A	-4	LEU	-	CLONING ARTIFACT	UNP Q70AC7
A	-3	VAL	-	CLONING ARTIFACT	UNP Q70AC7
A	-2	ASP	-	CLONING ARTIFACT	UNP Q70AC7
A	-1	PRO	-	CLONING ARTIFACT	UNP Q70AC7
A	0	ASN	-	CLONING ARTIFACT	UNP Q70AC7
A	1	SER	-	CLONING ARTIFACT	UNP Q70AC7
A	59	THR	ALA	ENGINEERED	UNP Q70AC7
A	184	KCX	LYS	MODIFIED RESIDUE	UNP Q70AC7
A	506	THR	-	CLONING ARTIFACT	UNP Q70AC7
A	507	ARG	-	CLONING ARTIFACT	UNP Q70AC7
A	508	ALA	-	CLONING ARTIFACT	UNP Q70AC7
A	509	SER	-	CLONING ARTIFACT	UNP Q70AC7
A	510	GLN	-	CLONING ARTIFACT	UNP Q70AC7
A	511	PRO	-	CLONING ARTIFACT	UNP Q70AC7
A	512	GLU	-	CLONING ARTIFACT	UNP Q70AC7
A	513	LEU	-	CLONING ARTIFACT	UNP Q70AC7
A	514	ALA	-	CLONING ARTIFACT	UNP Q70AC7
A	515	PRO	-	CLONING ARTIFACT	UNP Q70AC7
A	516	GLU	-	CLONING ARTIFACT	UNP Q70AC7
A	517	ASP	-	CLONING ARTIFACT	UNP Q70AC7
A	518	PRO	-	CLONING ARTIFACT	UNP Q70AC7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	519	GLU	-	CLONING ARTIFACT	UNP Q70AC7
A	520	ASP	-	CLONING ARTIFACT	UNP Q70AC7
A	521	LEU	-	CLONING ARTIFACT	UNP Q70AC7
A	522	GLU	-	CLONING ARTIFACT	UNP Q70AC7
A	523	HIS	-	CLONING ARTIFACT	UNP Q70AC7
A	524	HIS	-	CLONING ARTIFACT	UNP Q70AC7
A	525	HIS	-	CLONING ARTIFACT	UNP Q70AC7
A	526	HIS	-	CLONING ARTIFACT	UNP Q70AC7
A	527	HIS	-	CLONING ARTIFACT	UNP Q70AC7
A	528	HIS	-	CLONING ARTIFACT	UNP Q70AC7

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.26Å 146.32Å 78.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.19 – 2.50 41.06 – 1.91	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.19-2.50) 94.7 (41.06-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.250 0.205 , 0.248	Depositor DCC
R_{free} test set	905 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3667	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	0/3726	0.65	0/5037

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	3665	0	3625	97	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
All	All	3667	0	3625	97	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 97 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:335:VAL:HB	1:A:336:PRO:HD3	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:PHE:CE1	1:A:434:GLY:HA2	2.16	0.81
1:A:365:MET:HB3	1:A:369:LYS:HE3	1.68	0.76
1:A:365:MET:HE3	1:A:370:ARG:HB3	1.67	0.76
1:A:420:GLU:HG3	1:A:424:LYS:NZ	2.01	0.75

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	469/539 (87%)	445 (95%)	22 (5%)	2 (0%)	36 57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ALA
1	A	326	ASP

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	391/448 (87%)	384 (98%)	7 (2%)	62 84

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	470	LEU
1	A	353	GLN
1	A	56	TRP
1	A	420	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	461	HIS
1	A	353	GLN
1	A	208	GLN
1	A	447	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	KCX	A	184	1,2	8,11,12	1.00	1 (12%)	6,12,14	1.10	0

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
1	KCX	A	184	1,2	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	KCX	CA-C	2.39	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	471/539 (87%)	-0.93	3 (0%) 89 90	6, 17, 45, 59	5 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	ARG	2.9
1	A	325	GLU	2.3
1	A	324	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
1	KCX	A	184	12/13	0.94	0.09	12,18,26,29	0

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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	CO	A	529	1/1	0.99	0.02	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.