



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:48 PM GMT

PDB ID : 1RQB  
Title : Propionibacterium shermanii transcarboxylase 5S subunit  
Authors : Hall, P.R.; Zheng, R.; Antony, L.; Pusztai-Carey, M.; Carey, P.R.; Yee, V.C.  
Deposited on : 2003-12-04  
Resolution : 1.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

---

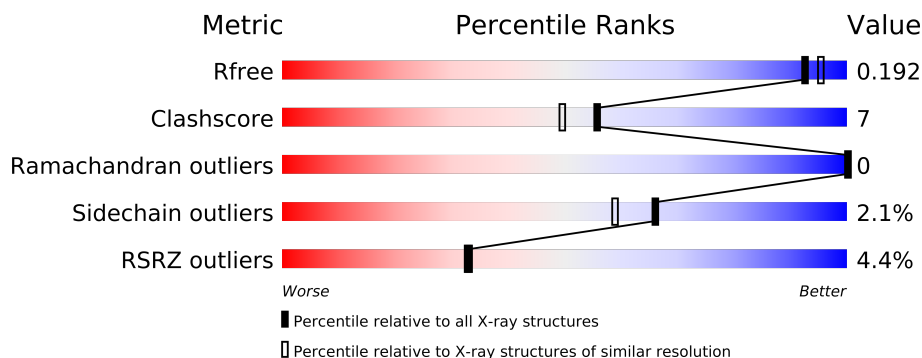
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	539	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4036 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			Total	C	N	O	S	Se			
1	A	472	3663	2300	633	702	5	23	0	0	0

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	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	29	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	33	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	35	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	38	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	83	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	90	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	120	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	129	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	135	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	139	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	176	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	184	KCX	LYS	MODIFIED RESIDUE	UNP Q70AC7
A	186	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	228	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	245	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	311	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	315	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	328	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	332	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	364	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	365	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	371	MSE	MET	MODIFIED RESIDUE	UNP Q70AC7
A	379	MSE	MET	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
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	372	Total 372	O 372	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.46Å 145.94Å 79.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.12 – 1.90 41.17 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (33.12-1.90) 95.6 (41.17-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.162 , 0.191 0.163 , 0.192	Depositor DCC
$R_{free}$ test set	1961 reflections (4.66%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 44329 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.41	0/3701	0.61	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3663	0	3623	48	1
2	A	1	0	0	0	0
3	A	372	0	0	2	0
All	All	4036	0	3623	48	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 48 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:MSE:HG3	1:A:332:MSE:HE2	1.59	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:GLU:O	1:A:424:LYS:HG2	1.78	0.83
1:A:327:LYS:HD2	1:A:364:MSE:HE1	1.65	0.79
1:A:371:MSE:HE3	1:A:375:PHE:HD2	1.52	0.73
1:A:328:MSE:HE2	1:A:332:MSE:HG3	1.72	0.71

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	Distance(Å)	Clash(Å)
1:A:393:LYS:NZ	1:A:393:LYS:NZ[3_654]	1.97	0.23

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	460 (98%)	9 (2%)	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	390/423 (92%)	382 (98%)	8 (2%)	66	59

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

Mol	Chain	Res	Type
1	A	129	MSE
1	A	420	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	322	GLN
1	A	56	TRP
1	A	213	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	213	ASN
1	A	322	GLN
1	A	401	GLN
1	A	447	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	11,11,12	5.38	2 (18%)	10,12,14	2.13	3 (30%)

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	-	0/8/10/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	KCX	O-C	17.49	1.23	1.11
1	A	184	KCX	CA-C	2.75	1.53	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	KCX	OQ2-CX-OQ1	-3.89	117.31	122.17
1	A	184	KCX	OQ2-CX-NZ	3.64	120.86	116.33
1	A	184	KCX	C-CA-N	-2.98	110.85	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	472/539 (87%)	-0.13	21 (4%) 33 33	8, 20, 63, 89	5 (1%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	ALA	5.2
1	A	3	PRO	3.8
1	A	369	LYS	3.7
1	A	320	ARG	3.7
1	A	323	GLY	3.7

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	A	184	12/13	0.09	-0.11	10,13,15,18	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CO	A	529	1/1	0.07	-3.20	12,12,12,12	0

## 6.5 Other polymers

There are no such residues in this entry.