



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2025 – 12:39 PM JST

PDB ID : 9J0C  
Title : Site-Specific Introduction of Sulfoxides and Sulfones into Polyketide Scaffold through a Relayed Chemo-Biosynthetic Strategy  
Authors : Zhang, J.; Qu, X.D.  
Deposited on : 2024-08-02  
Resolution : 1.60 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

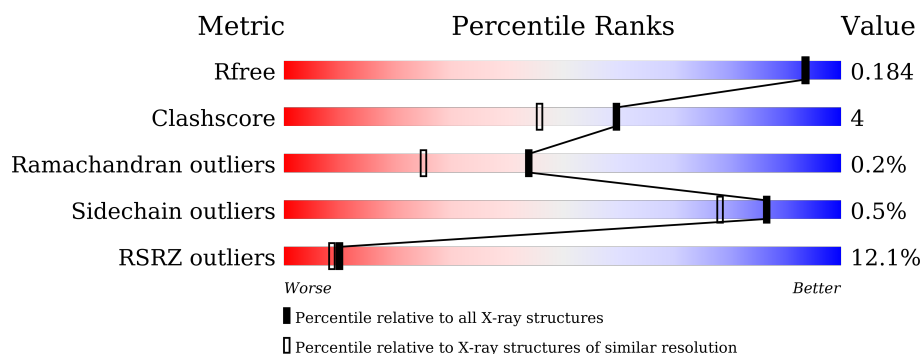
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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 of 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	529	<div> <div>12%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4425 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 Acyl-CoA carboxylase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3831	2389	692	727	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A345XRN6
A	-1	SER	-	expression tag	UNP A0A345XRN6
A	0	HIS	-	expression tag	UNP A0A345XRN6

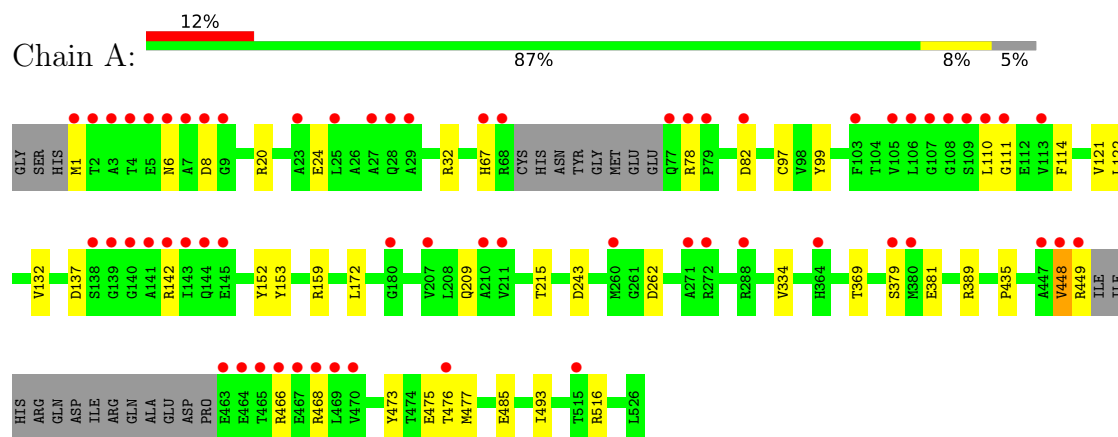
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	594	Total	O	0	0
			594	594		

### 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: Acyl-CoA carboxylase subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.04Å 124.04Å 134.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.76 – 1.60 34.76 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.76-1.60) 99.3 (34.76-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.21.1.5286	Depositor
R, $R_{free}$	0.172 , 0.184 0.173 , 0.184	Depositor DCC
$R_{free}$ test set	78607 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4425	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 13.25% 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	0.35	0/3895	0.61	0/5279

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ARG	Sidechain

### 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	3831	0	3816	32	0
2	A	594	0	0	10	4
All	All	4425	0	3816	32	4

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.

All (32) 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:466:ARG:HH11	1:A:468:ARG:HB3	1.39	0.87
1:A:32:ARG:NH2	2:A:606:HOH:O	2.18	0.77
1:A:243:ASP:OD2	2:A:601:HOH:O	2.08	0.70
1:A:262:ASP:OD1	2:A:602:HOH:O	2.11	0.68
1:A:209:GLN:NE2	1:A:215:THR:OG1	2.27	0.68
1:A:379:SER:O	2:A:604:HOH:O	2.15	0.64
1:A:381:GLU:N	1:A:381:GLU:OE1	2.31	0.64
1:A:99:TYR:OH	2:A:603:HOH:O	2.13	0.62
1:A:389:ARG:NH2	2:A:605:HOH:O	2.17	0.61
1:A:6:ASN:ND2	1:A:8:ASP:OD2	2.33	0.61
1:A:20:ARG:NH1	1:A:24:GLU:OE2	2.36	0.59
1:A:466:ARG:NH1	1:A:468:ARG:HB3	2.16	0.57
1:A:1:MET:SD	1:A:1:MET:N	2.79	0.54
1:A:435:PRO:HD3	1:A:493:ILE:O	2.09	0.53
1:A:110:LEU:HD13	1:A:153:TYR:CD1	2.46	0.51
1:A:110:LEU:HD21	1:A:152:TYR:HB2	1.93	0.50
1:A:485:GLU:OE2	2:A:607:HOH:O	2.21	0.46
1:A:97:CYS:HB3	1:A:121:VAL:HG22	1.98	0.45
1:A:122:LEU:HD23	1:A:132:VAL:HG21	1.98	0.45
1:A:110:LEU:HD12	1:A:114:PHE:HE1	1.82	0.45
1:A:516:ARG:HB3	2:A:677:HOH:O	2.18	0.44
1:A:466:ARG:HG2	1:A:468:ARG:H	1.82	0.44
1:A:473:TYR:O	1:A:477:MET:HB2	2.18	0.43
1:A:67:HIS:O	1:A:78:ARG:HD2	2.17	0.42
1:A:448:VAL:O	2:A:608:HOH:O	2.21	0.42
1:A:475:GLU:O	1:A:476:THR:OG1	2.31	0.42
1:A:110:LEU:HD12	1:A:114:PHE:CE1	2.55	0.41
1:A:334:VAL:O	1:A:369:THR:HA	2.20	0.41
1:A:82:ASP:CG	1:A:142:ARG:HH12	2.24	0.41
1:A:448:VAL:HG23	1:A:449:ARG:H	1.85	0.41
1:A:466:ARG:NH2	2:A:617:HOH:O	2.32	0.40
1:A:111:GLY:H	1:A:114:PHE:HB3	1.86	0.40

All (4) 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:1010:HOH:O	2:A:1100:HOH:O[11_655]	2.18	0.02
2:A:1124:HOH:O	2:A:1189:HOH:O[2_545]	2.18	0.02
2:A:698:HOH:O	2:A:1161:HOH:O[11_655]	2.19	0.01
2:A:983:HOH:O	2:A:1063:HOH:O[11_655]	2.19	0.01

## 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	499/529 (94%)	486 (97%)	12 (2%)	1 (0%)	44 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	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	396/417 (95%)	394 (100%)	2 (0%)	86 78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	LEU
1	A	448	VAL



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

Mol	Chain	Res	Type
1	A	209	GLN

### 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 oligosaccharides 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 ⓘ

### 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	505/529 (95%)	0.24	61 (12%) 10 8	12, 18, 52, 114	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ALA	7.6
1	A	141	ALA	7.2
1	A	466	ARG	6.8
1	A	4	THR	6.6
1	A	3	ALA	6.4
1	A	106	LEU	6.2
1	A	143	ILE	6.0
1	A	448	VAL	5.9
1	A	2	THR	5.9
1	A	110	LEU	5.6
1	A	6	ASN	5.5
1	A	68	ARG	5.2
1	A	140	GLY	5.1
1	A	8	ASP	5.1
1	A	105	VAL	5.0
1	A	467	GLU	4.9
1	A	139	GLY	4.8
1	A	107	GLY	4.8
1	A	465	THR	4.6
1	A	380	MET	4.6
1	A	470	VAL	4.4
1	A	103	PHE	4.4
1	A	1	MET	4.3
1	A	5	GLU	4.2
1	A	79	PRO	3.9
1	A	449	ARG	3.7
1	A	476	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	464	GLU	3.4
1	A	469	LEU	3.3
1	A	144	GLN	3.3
1	A	211	VAL	3.2
1	A	78	ARG	3.1
1	A	145	GLU	3.1
1	A	27	ALA	3.1
1	A	463	GLU	2.9
1	A	9	GLY	2.8
1	A	67	HIS	2.7
1	A	210	ALA	2.7
1	A	515	THR	2.7
1	A	108	GLY	2.7
1	A	447	ALA	2.6
1	A	77	GLN	2.6
1	A	109	SER	2.6
1	A	272	ARG	2.6
1	A	271	ALA	2.6
1	A	260	MET	2.5
1	A	28	GLN	2.5
1	A	25	LEU	2.4
1	A	29	ALA	2.4
1	A	82	ASP	2.4
1	A	468	ARG	2.3
1	A	111	GLY	2.3
1	A	364	HIS	2.3
1	A	180	GLY	2.3
1	A	138	SER	2.3
1	A	142	ARG	2.2
1	A	23	ALA	2.2
1	A	379	SER	2.1
1	A	113	VAL	2.1
1	A	207	VAL	2.1
1	A	288	ARG	2.0

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

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.