



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 29, 2024 – 08:41 AM EST

PDB ID : 5UFY  
Title : Structure of Streptococcus pneumoniae peptidoglycan O-acetyltransferase A (OatA) C-terminal catalytic domain  
Authors : Sychantha, D.; Jones, C.; Little, D.J.; Moynihan, P.J.; Robinson, H.; Galley, N.F.; Roper, D.I.; Dowson, C.G.; Howell, P.L.; Clarke, A.J.  
Deposited on : 2017-01-06  
Resolution : 1.12 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) : 1.13  
EDS : 2.36  
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) : 2.36

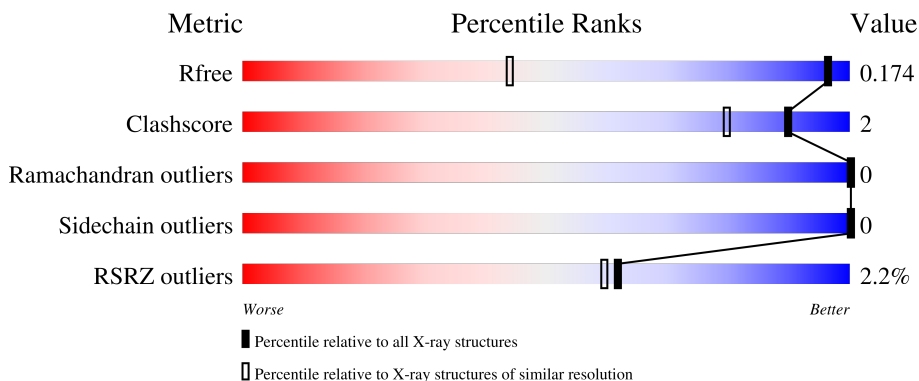
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.12 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))
$R_{free}$	130704	1168 (1.14-1.10)
Clashscore	141614	1205 (1.14-1.10)
Ramachandran outliers	138981	1168 (1.14-1.10)
Sidechain outliers	138945	1165 (1.14-1.10)
RSRZ outliers	127900	1146 (1.14-1.10)

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	224	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2993 atoms, of which 1371 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 Acyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	179	2749	868	1371	232	274	4	0	2	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	MET	-	initiating methionine	UNP A0A0T7JIN8
A	383	GLY	-	expression tag	UNP A0A0T7JIN8
A	384	GLY	-	expression tag	UNP A0A0T7JIN8
A	385	SER	-	expression tag	UNP A0A0T7JIN8
A	386	HIS	-	expression tag	UNP A0A0T7JIN8
A	387	HIS	-	expression tag	UNP A0A0T7JIN8
A	388	HIS	-	expression tag	UNP A0A0T7JIN8
A	389	HIS	-	expression tag	UNP A0A0T7JIN8
A	390	HIS	-	expression tag	UNP A0A0T7JIN8
A	391	HIS	-	expression tag	UNP A0A0T7JIN8
A	392	GLY	-	expression tag	UNP A0A0T7JIN8
A	393	MET	-	expression tag	UNP A0A0T7JIN8
A	394	ALA	-	expression tag	UNP A0A0T7JIN8
A	395	SER	-	expression tag	UNP A0A0T7JIN8
A	396	MET	-	expression tag	UNP A0A0T7JIN8
A	397	THR	-	expression tag	UNP A0A0T7JIN8
A	398	GLY	-	expression tag	UNP A0A0T7JIN8
A	399	GLY	-	expression tag	UNP A0A0T7JIN8
A	400	GLN	-	expression tag	UNP A0A0T7JIN8
A	401	GLN	-	expression tag	UNP A0A0T7JIN8
A	402	MET	-	expression tag	UNP A0A0T7JIN8
A	403	GLY	-	expression tag	UNP A0A0T7JIN8
A	404	ARG	-	expression tag	UNP A0A0T7JIN8
A	405	ASP	-	expression tag	UNP A0A0T7JIN8
A	406	LEU	-	expression tag	UNP A0A0T7JIN8
A	407	TYR	-	expression tag	UNP A0A0T7JIN8
A	408	ASP	-	expression tag	UNP A0A0T7JIN8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	409	ASP	-	expression tag	UNP A0A0T7JIN8
A	410	ASP	-	expression tag	UNP A0A0T7JIN8
A	411	ASP	-	expression tag	UNP A0A0T7JIN8
A	412	LYS	-	expression tag	UNP A0A0T7JIN8
A	413	ASP	-	expression tag	UNP A0A0T7JIN8
A	414	ARG	-	expression tag	UNP A0A0T7JIN8
A	415	TRP	-	expression tag	UNP A0A0T7JIN8
A	416	GLY	-	expression tag	UNP A0A0T7JIN8
A	417	SER	-	expression tag	UNP A0A0T7JIN8
A	418	GLU	-	expression tag	UNP A0A0T7JIN8
A	419	LEU	-	expression tag	UNP A0A0T7JIN8
A	420	GLU	-	expression tag	UNP A0A0T7JIN8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

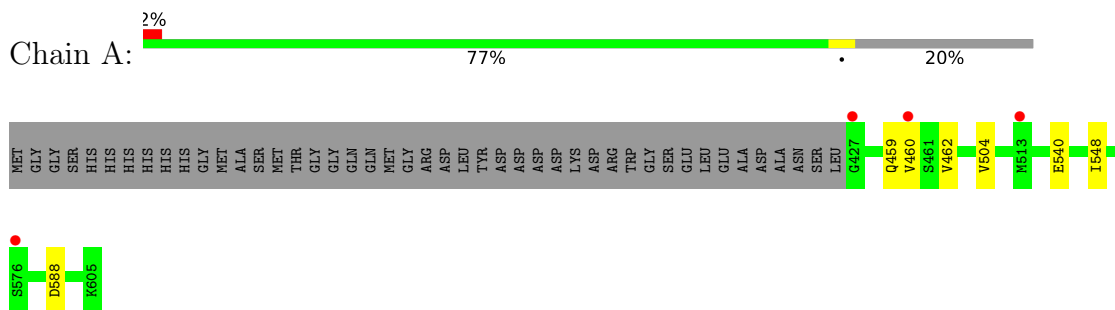
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	243	Total O 243 243	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: Acyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.20Å 70.20Å 135.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.05 – 1.12 40.05 – 1.12	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.05-1.12) 98.3 (40.05-1.12)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.40 (at 1.12Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.150 , 0.168 0.157 , 0.174	Depositor DCC
$R_{free}$ test set	2000 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	2993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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](#)

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

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	0.38	0/1409	0.62	0/1916

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	A	1378	1371	1382	5	0
2	A	1	0	0	0	0
3	A	243	0	0	3	4
All	All	1622	1371	1382	5	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 2.

All (5) 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:460:VAL:HG23	3:A:942:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLU:OE2	3:A:801:HOH:O	2.07	0.72
1:A:588:ASP:OD1	3:A:802:HOH:O	2.10	0.68
1:A:459:GLN:HB2	1:A:462:VAL:HG23	2.01	0.41
1:A:504:VAL:HG13	1:A:548:ILE:HD11	2.03	0.41

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)
3:A:826:HOH:O	3:A:940:HOH:O[6_565]	1.98	0.22
3:A:877:HOH:O	3:A:895:HOH:O[3_565]	2.01	0.19
3:A:997:HOH:O	3:A:1019:HOH:O[15_454]	2.07	0.13
3:A:1012:HOH:O	3:A:1012:HOH:O[6_565]	2.18	0.02

## 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	179/224 (80%)	173 (97%)	6 (3%)	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	148/181 (82%)	148 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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](#)

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, 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	179/224 (79%)	-0.01	4 (2%) 62 59	8, 12, 31, 44	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	MET	5.2
1	A	576	SER	2.5
1	A	427	GLY	2.1
1	A	460	VAL	2.0

### 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](#)

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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	A	701	1/1	1.00	0.15	9,9,9,9	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.