



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:53 AM UTC

PDB ID : 9SHR / pdb\_00009shr  
Title : Alpha-Hemolysin of S.aureus (monomer) in complex with the small molecule  
N-(3-(Diethylamino)propyl)-1-(6-(p-tolyl)imidazo[2,1-b][1,3,4]thiadiazol-2-yl)  
piperidine-4-carboxamide  
Authors : Lukat, P.; Blankenfeldt, W.; Broenstrup, M.  
Deposited on : 2025-08-27  
Resolution : 2.08 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

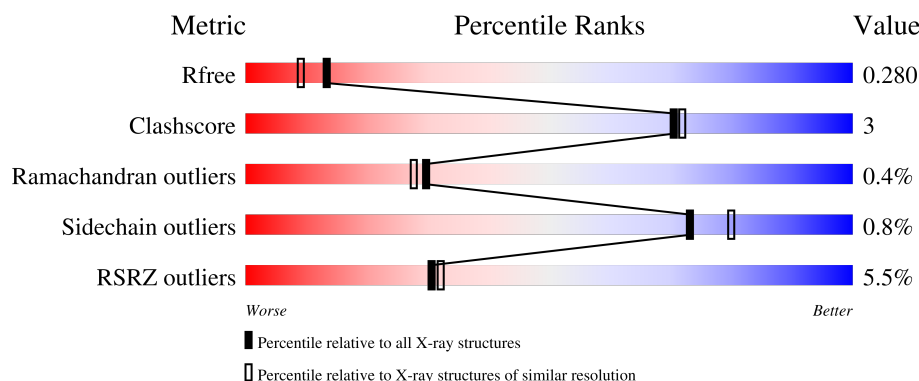
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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))
$R_{free}$	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	304	<div> <div>5%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4935 atoms, of which 2295 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.

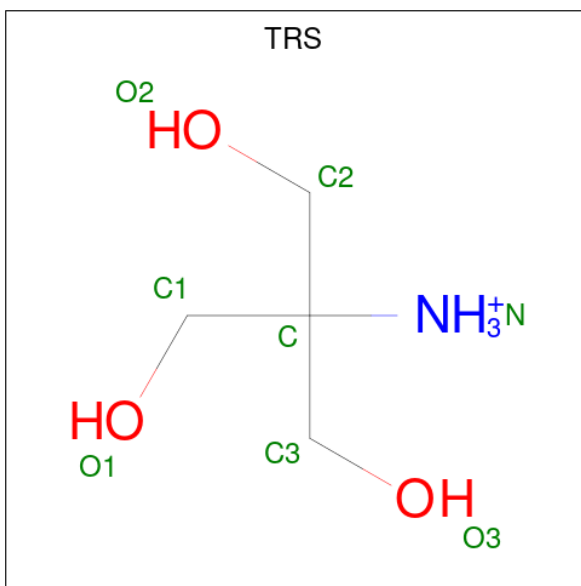
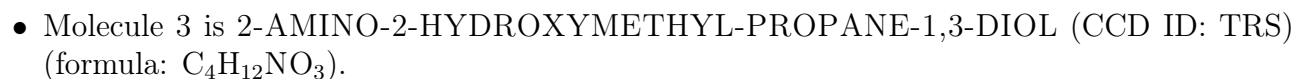
- Molecule 1 is a protein called Alpha-hemolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	H	N	O	S	0	3	0
			4589	1473	2248	400	461	7			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q2G1X0
A	294	SER	-	expression tag	UNP Q2G1X0
A	295	ALA	-	expression tag	UNP Q2G1X0
A	296	TRP	-	expression tag	UNP Q2G1X0
A	297	SER	-	expression tag	UNP Q2G1X0
A	298	HIS	-	expression tag	UNP Q2G1X0
A	299	PRO	-	expression tag	UNP Q2G1X0
A	300	GLN	-	expression tag	UNP Q2G1X0
A	301	PHE	-	expression tag	UNP Q2G1X0
A	302	GLU	-	expression tag	UNP Q2G1X0
A	303	LYS	-	expression tag	UNP Q2G1X0

- Molecule 2 is {N}-[3-(diethylamino)propyl]-1-[6-(4-methylphenyl)imidazo[2,1-b][1,3,4]thiadiazol-2-yl]piperidine-4-carboxamide (CCD ID: A1JN0) (formula: C<sub>24</sub>H<sub>34</sub>N<sub>6</sub>OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula:  $\text{O}_4\text{S}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

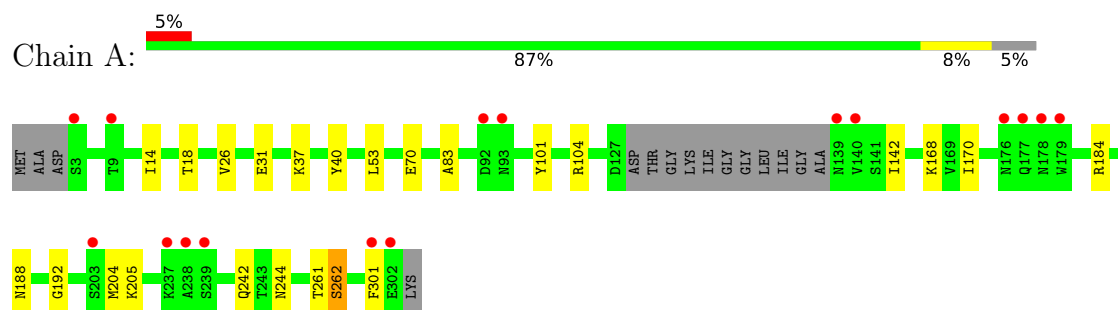
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	203	Total 203	O 203	0	0



- Molecule 1: Alpha-hemolysin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.77Å 95.77Å 157.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.14 – 2.08 57.14 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.14-2.08) 99.9 (57.14-2.08)	Depositor EDS
$R_{merge}$	0.50	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.239 , 0.279 0.240 , 0.280	Depositor DCC
$R_{free}$ test set	1273 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.5	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	4935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, A1JN0, NA, TRS

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	0.08	0/2408	0.26	0/3262

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	2341	2248	2241	16	0
2	A	32	35	0	0	0
3	A	8	12	12	0	0
4	A	55	0	0	1	0
5	A	1	0	0	0	0
6	A	203	0	0	5	1
All	All	2640	2295	2253	16	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 3.

All (16) 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:301:PHE:O	6:A:501:HOH:O	2.03	0.75
1:A:242:GLN:NE2	6:A:507:HOH:O	2.28	0.65
1:A:26:VAL:HG22	1:A:37:LYS:HG2	1.84	0.58
1:A:204:MET:O	6:A:503:HOH:O	2.18	0.57
1:A:244:ASN:ND2	6:A:515:HOH:O	2.36	0.57
1:A:168:LYS:HG2	1:A:170[B]:ILE:HG23	1.87	0.56
1:A:40:TYR:HB2	1:A:53:LEU:HD11	1.86	0.56
1:A:83:ALA:HB2	1:A:170[B]:ILE:HG22	1.93	0.50
1:A:31:GLU:O	6:A:504:HOH:O	2.20	0.49
1:A:14:ILE:HD11	1:A:18:THR:CG2	2.45	0.46
1:A:184:ARG:NH1	4:A:406:SO4:O4	2.47	0.45
1:A:261:THR:O	1:A:262:SER:CB	2.66	0.44
1:A:83:ALA:CB	1:A:170[B]:ILE:HG22	2.48	0.43
1:A:188:ASN:O	1:A:192:GLY:N	2.53	0.41
1:A:101:TYR:O	1:A:104:ARG:HD2	2.20	0.41

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)
6:A:590:HOH:O	6:A:590:HOH:O[11_455]	1.98	0.22

## 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	288/304 (95%)	276 (96%)	11 (4%)	1 (0%)	36	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	SER

### 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	261/269 (97%)	258 (99%)	3 (1%)	65 73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70[A]	GLU
1	A	70[B]	GLU
1	A	142	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	89	GLN
1	A	201	ASN
1	A	293	ASN

### 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

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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
3	TRS	A	402	-	7,7,7	0.22	0	9,9,9	0.35	0
4	SO4	A	409	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	A	411	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	408	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	404	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	A	403	-	4,4,4	0.22	0	6,6,6	0.10	0
2	A1JN0	A	401	-	35,35,35	0.35	0	46,48,48	0.69	1 (2%)
4	SO4	A	413	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	A	410	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	406	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	405	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	A	412	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	407	-	4,4,4	0.24	0	6,6,6	0.09	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
3	TRS	A	402	-	-	6/9/9/9	-
2	A1JN0	A	401	-	-	4/23/33/33	0/4/4/4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1JN0	N12-C11-N29	3.97	123.34	116.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

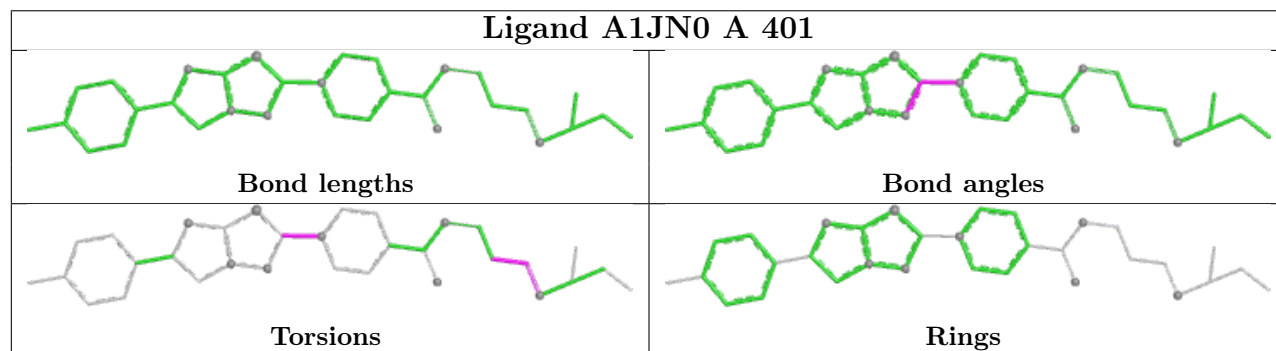
Mol	Chain	Res	Type	Atoms
3	A	402	TRS	C1-C-C3-O3
3	A	402	TRS	C2-C-C3-O3
3	A	402	TRS	N-C-C3-O3
2	A	401	A1JN0	C18-C19-C20-N21
2	A	401	A1JN0	C19-C20-N21-C24
2	A	401	A1JN0	C19-C20-N21-C22
3	A	402	TRS	C2-C-C1-O1
2	A	401	A1JN0	N29-C11-N12-C28
3	A	402	TRS	C3-C-C1-O1
3	A	402	TRS	N-C-C1-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	406	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	289/304 (95%)	0.22	16 (5%) 30 32	3, 15, 37, 57	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ASN	4.6
1	A	302	GLU	4.3
1	A	177	GLN	4.2
1	A	301	PHE	3.9
1	A	93	ASN	3.8
1	A	92	ASP	3.2
1	A	179	TRP	3.1
1	A	176	ASN	3.1
1	A	203	SER	3.0
1	A	140	VAL	2.9
1	A	178	ASN	2.9
1	A	239	SER	2.6
1	A	237	LYS	2.5
1	A	238	ALA	2.3
1	A	9	THR	2.1
1	A	3	SER	2.1

### 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](#)

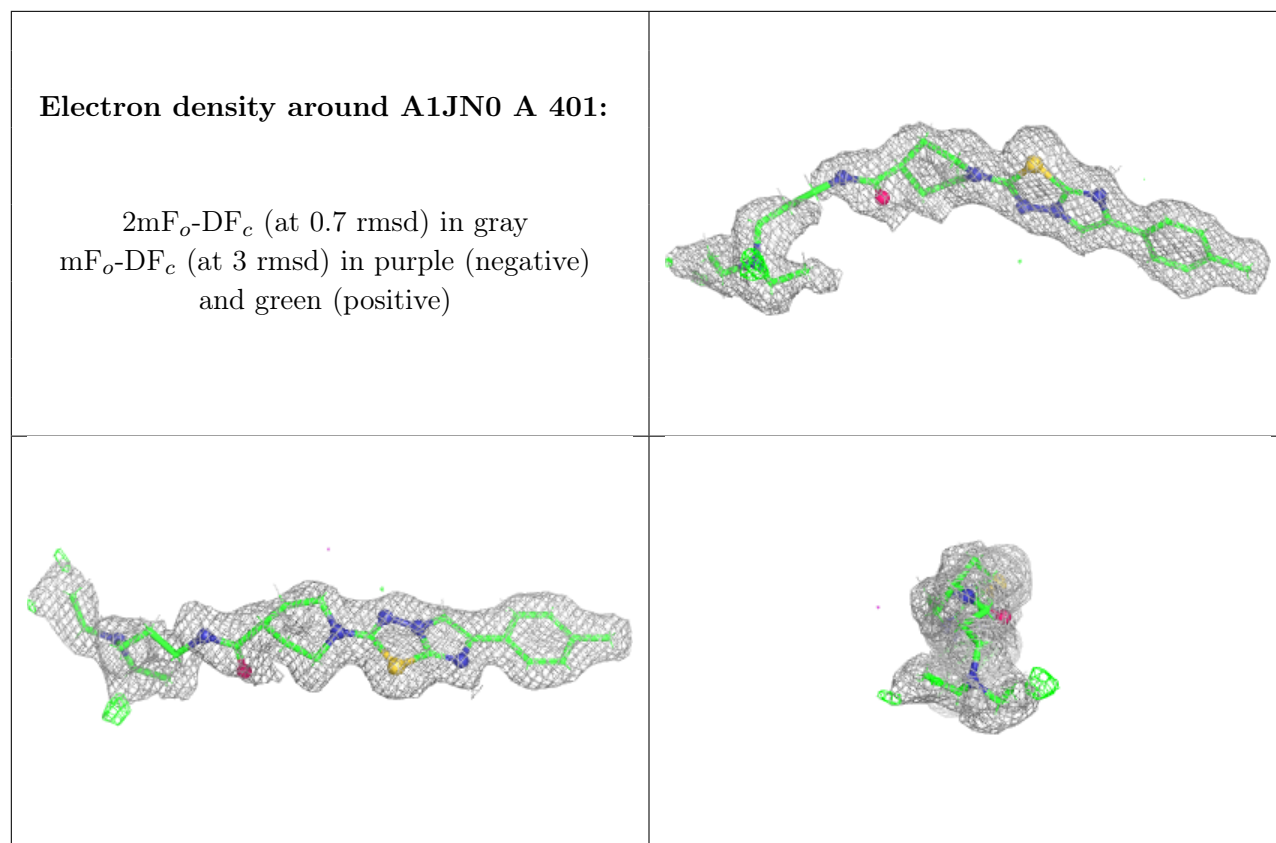
There are no oligosaccharides in this entry.

## 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. 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
4	SO4	A	412	5/5	0.76	0.17	34,34,38,50	5
4	SO4	A	408	5/5	0.82	0.13	27,31,39,58	5
4	SO4	A	411	5/5	0.83	0.16	21,28,41,54	5
4	SO4	A	405	5/5	0.86	0.11	26,27,37,52	5
3	TRS	A	402	8/8	0.86	0.13	8,17,31,33	0
4	SO4	A	407	5/5	0.88	0.10	15,16,29,51	5
4	SO4	A	410	5/5	0.88	0.14	18,23,24,34	5
4	SO4	A	413	5/5	0.88	0.15	30,32,36,39	4
4	SO4	A	409	5/5	0.90	0.10	12,13,23,33	5
4	SO4	A	404	5/5	0.92	0.13	14,31,35,49	5
2	A1JN0	A	401	32/32	0.93	0.11	6,26,45,51	0
4	SO4	A	406	5/5	0.94	0.09	18,20,31,32	5
4	SO4	A	403	5/5	0.96	0.09	8,17,22,33	0
5	NA	A	414	1/1	0.98	0.13	18,18,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.