



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 07:02 pm BST

PDB ID : 3EGV  
Title : Ribosomal protein L11 methyltransferase (PrmA) in complex with trimethylated ribosomal protein L11  
Authors : Demirci, H.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2008-09-11  
Resolution : 1.75 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](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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

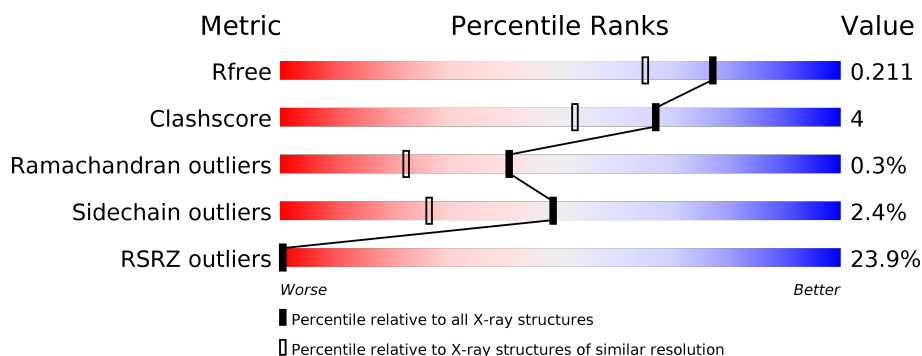
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2997 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 Ribosomal protein L11 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1958	1270	339	345	4			

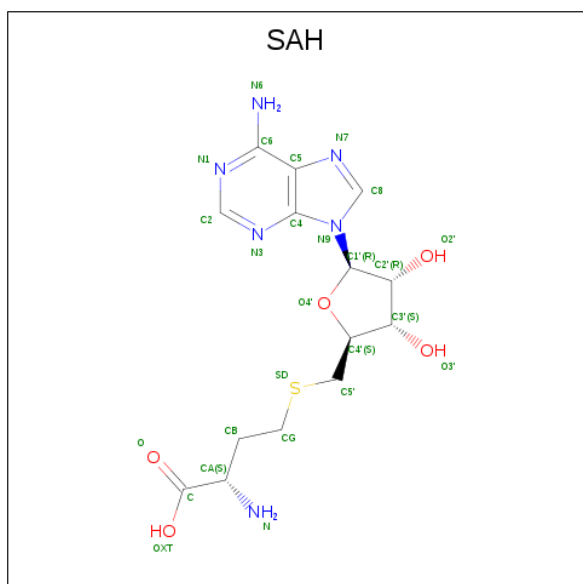
- Molecule 2 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			572	375	93	101	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	ALA	LYS	ENGINEERED MUTATION	UNP Q5SLP6

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	I	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	356	Total 356	O 356	0	0
7	B	59	Total 59	O 59	0	0

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.55Å 134.55Å 48.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.75 29.13 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-1.75) 98.6 (29.13-1.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.183 , 0.213 0.181 , 0.211	Depositor DCC
$R_{free}$ test set	2577 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IOD, SAH, 4MM, CL

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	0.84	4/2015 (0.2%)	0.77	5/2747 (0.2%)
2	B	0.52	0/575	0.57	0/788
All	All	0.78	4/2590 (0.2%)	0.73	5/3535 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	TYR	CG-CD2	11.53	1.54	1.39
1	A	47	TYR	CE1-CZ	10.19	1.51	1.38
1	A	47	TYR	CG-CD1	6.17	1.47	1.39
1	A	47	TYR	CE2-CZ	6.03	1.46	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	TYR	CB-CG-CD1	-5.99	117.40	121.00
1	A	226	LEU	CA-CB-CG	5.97	129.02	115.30
1	A	170	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	170	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	122	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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	1958	0	1955	14	0
2	B	572	0	600	7	0
3	A	26	0	19	1	0
4	A	24	0	32	0	1
5	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	356	0	0	7	1
7	B	59	0	0	0	0
All	All	2997	0	2606	19	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 4.

The worst 5 of 19 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:187:LEU:HD13	1:A:213:ARG:HB2	1.47	0.93
2:B:1:4MM:CAJ	2:B:2:LYS:CA	2.57	0.80
1:A:203:ARG:HG2	7:A:418:HOH:O	1.85	0.75
1:A:187:LEU:CD1	1:A:213:ARG:HB2	2.17	0.74
2:B:74:ALA:O	2:B:78:ILE:HB	1.92	0.69

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)
4:A:303:GOL:O3	7:A:612:HOH:O[2_454]	1.91	0.29

## 4.3 Torsion angles [i](#)

### 4.3.1 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	252/254 (99%)	245 (97%)	7 (3%)	0	100	100
2	B	75/147 (51%)	70 (93%)	4 (5%)	1 (1%)	12	2
All	All	327/401 (82%)	315 (96%)	11 (3%)	1 (0%)	41	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	76	TYR

#### 4.3.2 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	189/189 (100%)	185 (98%)	4 (2%)	53	31
2	B	58/109 (53%)	56 (97%)	2 (3%)	37	14
All	All	247/298 (83%)	241 (98%)	6 (2%)	49	26

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	LEU
2	B	78	ILE
1	A	237	ARG
1	A	221	LYS
2	B	77	LEU

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

Mol	Chain	Res	Type
1	A	103	HIS

#### 4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 4.4 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	$\# Z  > 2$
2	4MM	B	1	2	7,10,11	0.92	0	9,13,15	1.18	1 (11%)

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
2	4MM	B	1	2	-	1/11/12/14	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	4MM	CAA-SAI-CAG	2.91	110.39	100.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	4MM	CAH-CAG-SAI-CAA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	4MM	2	0

## 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 4.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
4	GOL	A	304	-	5,5,5	0.52	0	5,5,5	0.39	0
3	SAH	A	301	-	21,28,28	1.17	2 (9%)	20,40,40	1.61	2 (10%)
4	GOL	A	302	-	5,5,5	0.26	0	5,5,5	0.85	0
4	GOL	A	305	-	5,5,5	0.35	0	5,5,5	0.38	0
4	GOL	A	303	-	5,5,5	0.68	0	5,5,5	0.21	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
4	GOL	A	304	-	-	0/4/4/4	-
3	SAH	A	301	-	-	1/7/31/31	0/3/3/3
4	GOL	A	302	-	-	0/4/4/4	-
4	GOL	A	305	-	-	4/4/4/4	-
4	GOL	A	303	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	SAH	C2-N3	3.55	1.37	1.32
3	A	301	SAH	C2-N1	2.56	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	SAH	N3-C2-N1	-5.45	120.17	128.68
3	A	301	SAH	C1'-N9-C4	-2.39	122.45	126.64

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

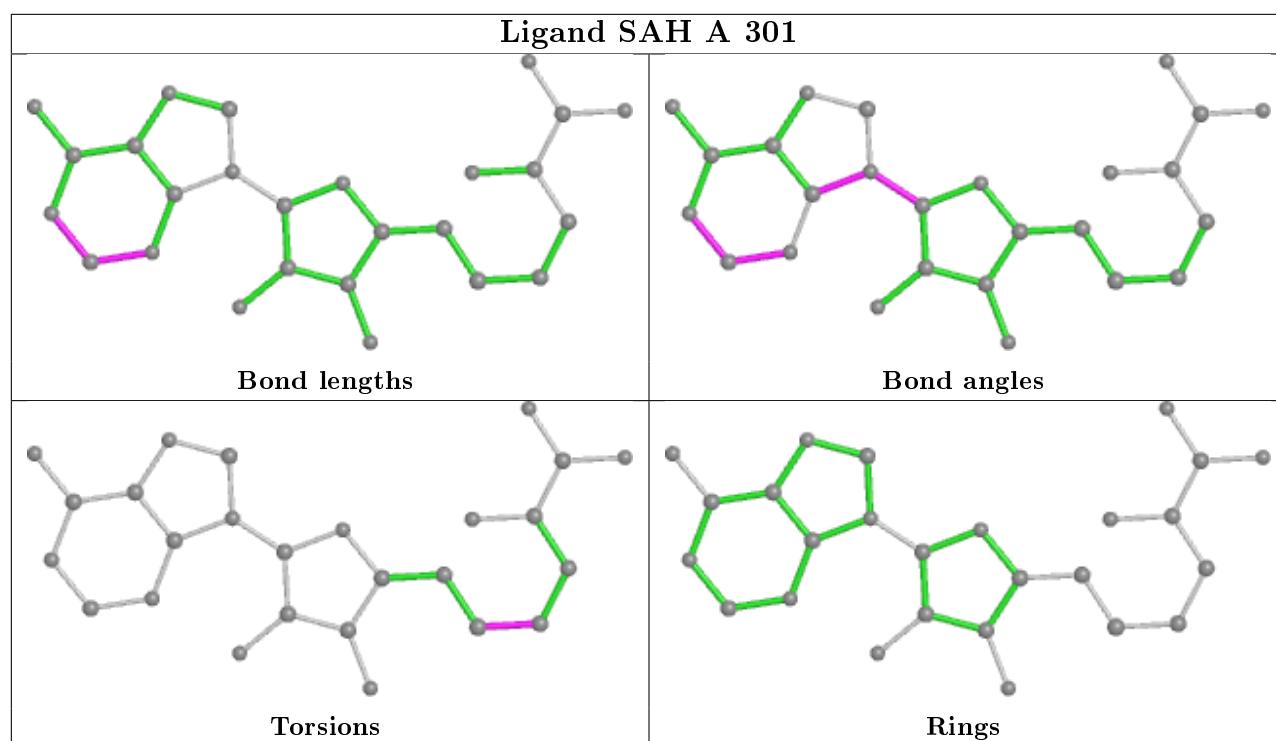
Mol	Chain	Res	Type	Atoms
4	A	305	GOL	C1-C2-C3-O3
4	A	303	GOL	C1-C2-C3-O3
4	A	305	GOL	O1-C1-C2-C3
4	A	305	GOL	O1-C1-C2-O2
4	A	305	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	SAH	1	0
4	A	303	GOL	0	1

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.



#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 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	254/254 (100%)	1.07	60 (23%) 0 0	20, 25, 46, 49	0
2	B	77/147 (52%)	1.59	19 (24%) 0 0	28, 34, 52, 53	5 (6%)
All	All	331/401 (82%)	1.19	79 (23%) 0 0	20, 29, 48, 53	5 (1%)

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	78	ILE	14.4
2	B	77	LEU	14.1
2	B	47	ASN	6.7
2	B	46	ALA	6.5
2	B	74	ALA	5.8

### 5.2 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, 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	4MM	B	1	11/12	0.83	0.15	30,31,38,45	0

### 5.3 Carbohydrates [i](#)

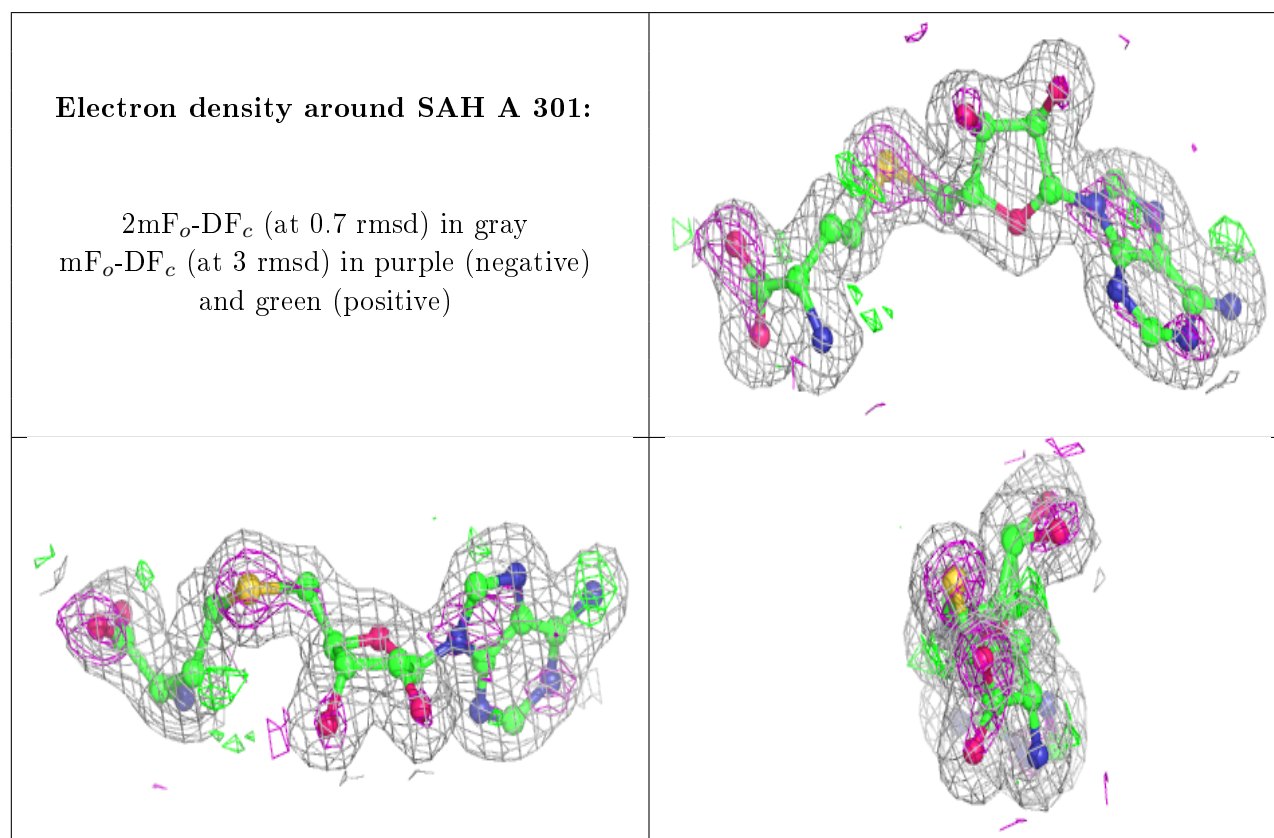
There are no carbohydrates in this entry.

## 5.4 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	GOL	A	305	6/6	0.71	0.30	63,67,67,68	0
4	GOL	A	303	6/6	0.85	0.24	29,29,32,33	0
4	GOL	A	304	6/6	0.93	0.19	23,26,29,30	0
4	GOL	A	302	6/6	0.95	0.25	26,35,37,39	0
3	SAH	A	301	26/26	0.96	0.08	18,23,25,26	0
5	CL	A	306	1/1	0.96	0.08	34,34,34,34	0
6	IOD	B	201	1/1	0.98	0.04	29,29,29,29	1

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.



## 5.5 Other polymers ⓘ

There are no such residues in this entry.