



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 02:44 PM EDT

PDB ID : 5DPL  
Title : The structure of PKMT2 from Rickettsia typhi in complex with AdoHcy  
Authors : Noinaj, N.; Abeykoon, A.; He, Y.; Yang, D.C.; Buchanan, S.K.  
Deposited on : 2015-09-12  
Resolution : 3.20 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.

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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

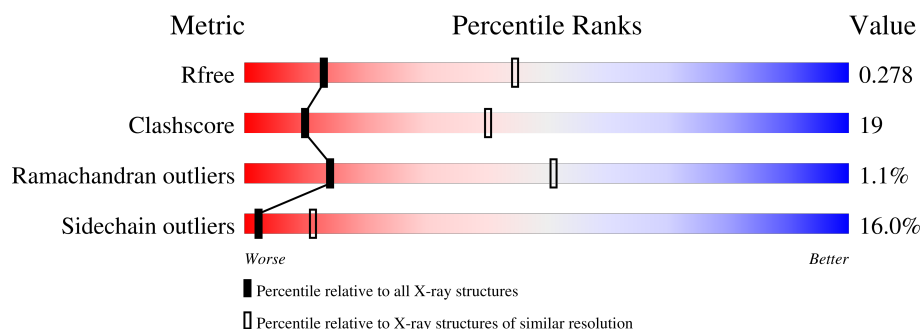
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	535	<div> <div>53%</div> <div>37%</div> <div>6% . .</div> </div>
1	B	535	<div> <div>53%</div> <div>35%</div> <div>7% . .</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8077 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 protein lysine methyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	1	0
			4055	2615	659	768	13			
1	B	512	Total	C	N	O	S	0	1	0
			3970	2566	643	749	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q68XQ5
B	0	GLY	-	expression tag	UNP Q68XQ5

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



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

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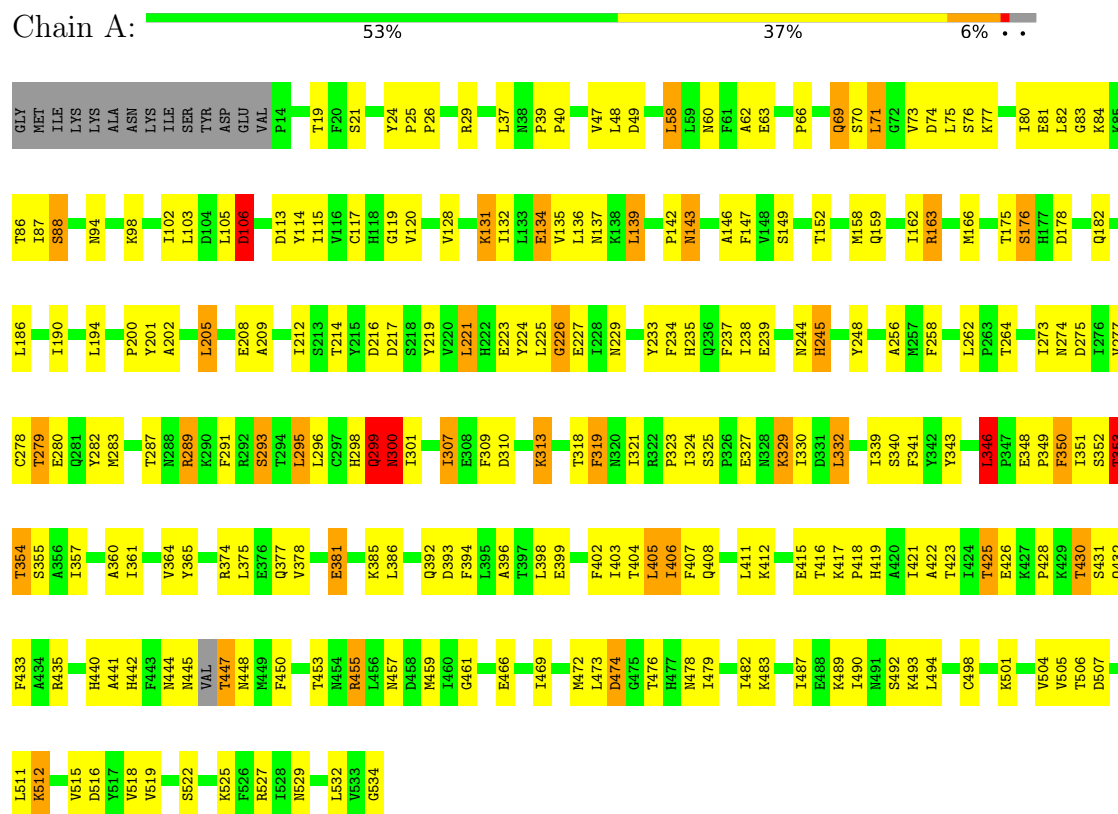
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

### 3 Residue-property plots

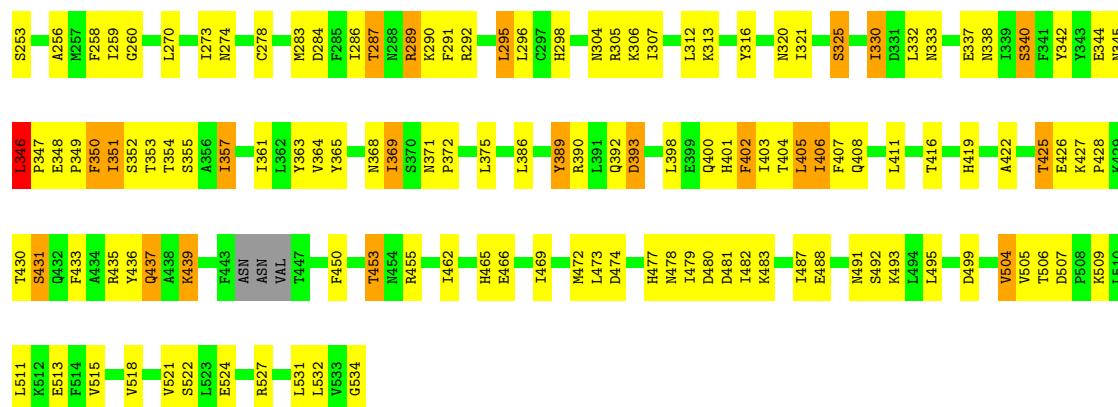
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: protein lysine methyltransferase 2



#### • Molecule 1: protein lysine methyltransferase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.35Å 91.03Å 105.83Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	48.95 – 3.20 48.96 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.95-3.20) 93.5 (48.96-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10_2142)	Depositor
R, $R_{free}$	0.244 , 0.280 0.245 , 0.278	Depositor DCC
$R_{free}$ test set	2000 reflections (8.36%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , -13.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.080 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: SAH

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	0.32	0/4145	0.62	3/5643 (0.1%)
1	B	0.32	0/4059	0.63	2/5530 (0.0%)
All	All	0.32	0/8204	0.63	5/11173 (0.0%)

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	6
1	B	0	5
All	All	0	11

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	LEU	CA-CB-CG	7.28	132.05	115.30
1	B	118	HIS	C-N-CA	-6.63	108.38	122.30
1	B	180	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	205	LEU	CA-CB-CG	5.06	126.95	115.30
1	A	353	THR	C-N-CA	5.02	134.25	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	176	SER	Peptide
1	A	226	GLY	Peptide
1	A	299	GLN	Peptide
1	A	501	LYS	Peptide

## 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	4055	0	3881	151	0
1	B	3970	0	3781	151	0
2	A	26	0	19	2	0
2	B	26	0	19	2	0
All	All	8077	0	7700	300	0

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 19.

The worst 5 of 300 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:B:320:ASN:HA	1:B:369:ILE:HD11	1.36	1.03
1:A:435:ARG:NH1	1:A:473:LEU:O	2.01	0.92
1:B:186:LEU:O	1:B:189:PHE:HB3	1.68	0.92
1:B:393:ASP:OD1	1:B:393:ASP:N	2.05	0.89
1:A:421:ILE:HG22	1:A:423:THR:H	1.42	0.84

There are no symmetry-related clashes.

## 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	517/535 (97%)	445 (86%)	67 (13%)	5 (1%)	15	54
1	B	507/535 (95%)	443 (87%)	58 (11%)	6 (1%)	13	49
All	All	1024/1070 (96%)	888 (87%)	125 (12%)	11 (1%)	14	51

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	504	VAL
1	B	505	VAL
1	A	299	GLN
1	B	200	PRO

### 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	426/484 (88%)	358 (84%)	68 (16%)	2	11
1	B	414/484 (86%)	348 (84%)	66 (16%)	2	12
All	All	840/968 (87%)	706 (84%)	134 (16%)	2	11

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	386	LEU
1	B	402	PHE
1	B	495	LEU
1	A	351	ILE
1	A	350	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	137	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are 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	SAH	A	601	-	24,28,28	1.20	3 (12%)	25,40,40	1.69	5 (20%)
2	SAH	B	601	-	24,28,28	1.20	3 (12%)	25,40,40	1.73	5 (20%)

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	SAH	A	601	-	-	3/11/31/31	0/3/3/3
2	SAH	B	601	-	-	5/11/31/31	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	SAH	C2-N3	4.02	1.38	1.32
2	A	601	SAH	C2-N3	4.01	1.38	1.32
2	A	601	SAH	C2-N1	2.45	1.38	1.33
2	B	601	SAH	C2-N1	2.41	1.38	1.33
2	B	601	SAH	OXT-C	-2.11	1.23	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	SAH	N3-C2-N1	-5.37	120.29	128.68
2	A	601	SAH	N3-C2-N1	-5.30	120.39	128.68
2	B	601	SAH	C5'-SD-CG	-4.33	89.29	102.27
2	A	601	SAH	C5'-SD-CG	-3.68	91.22	102.27
2	A	601	SAH	OXT-C-O	-2.69	117.99	124.09

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	SAH	N-CA-CB-CG
2	A	601	SAH	C-CA-CB-CG
2	B	601	SAH	N-CA-CB-CG
2	B	601	SAH	C-CA-CB-CG
2	B	601	SAH	O-C-CA-N

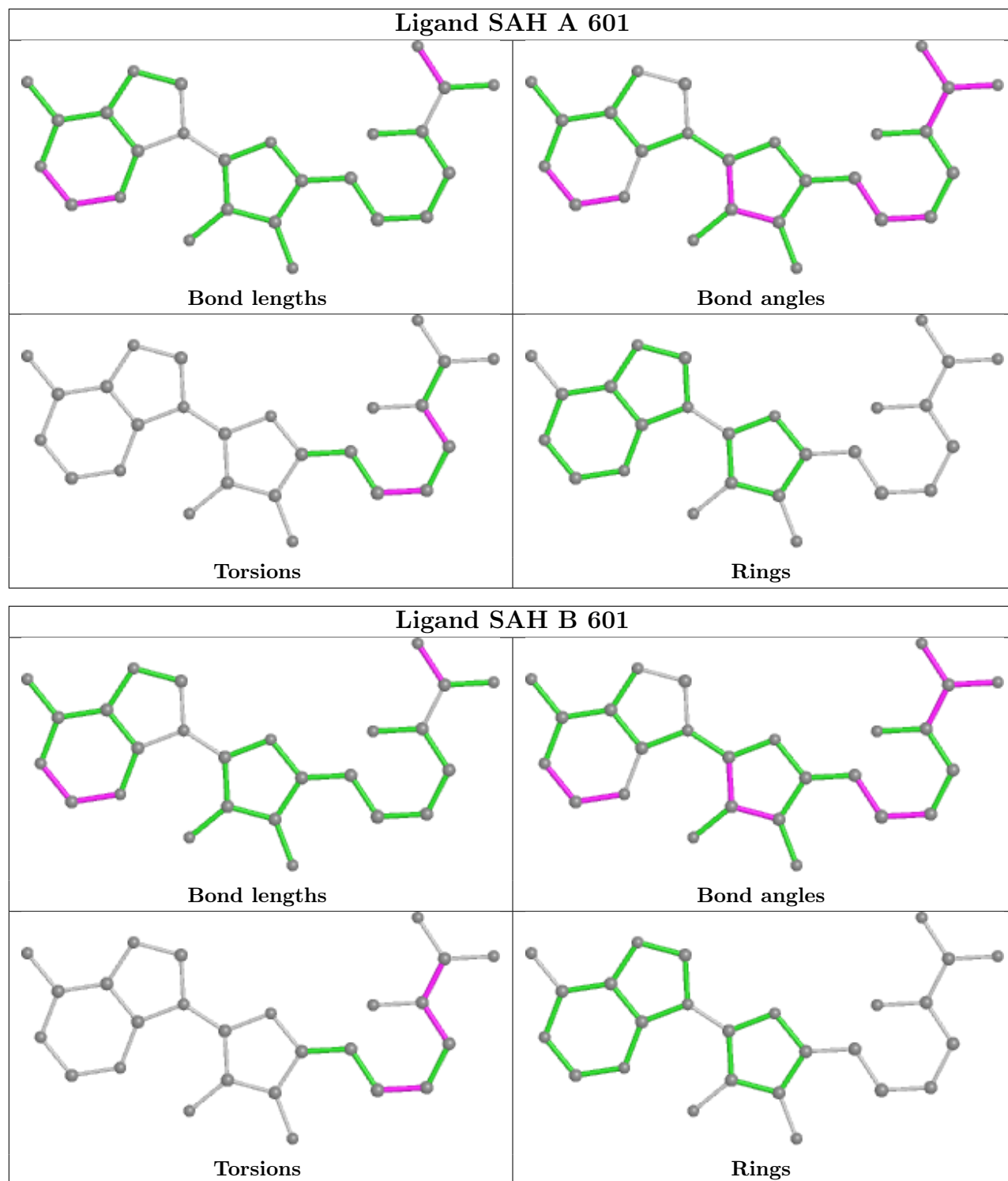
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SAH	2	0
2	B	601	SAH	2	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 ⓘ

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

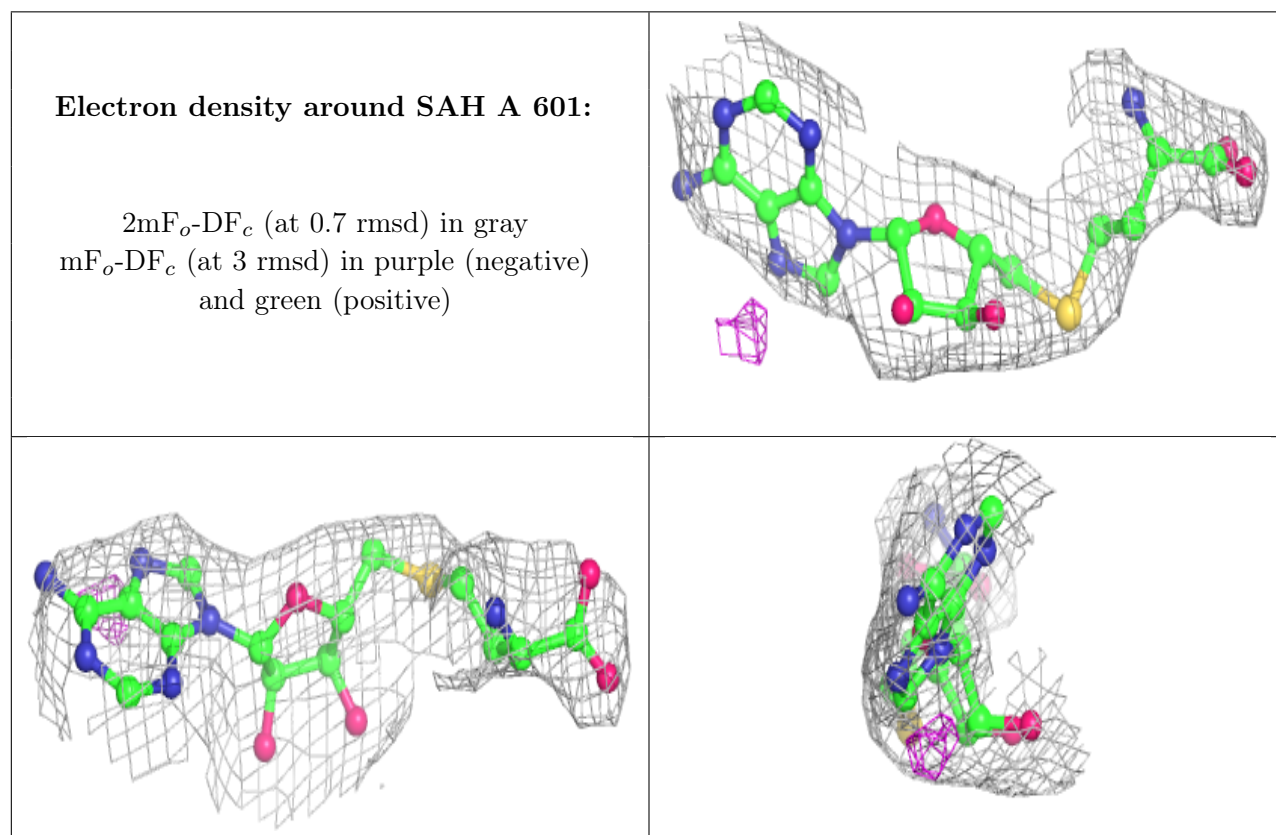
### 6.3 Carbohydrates ⓘ

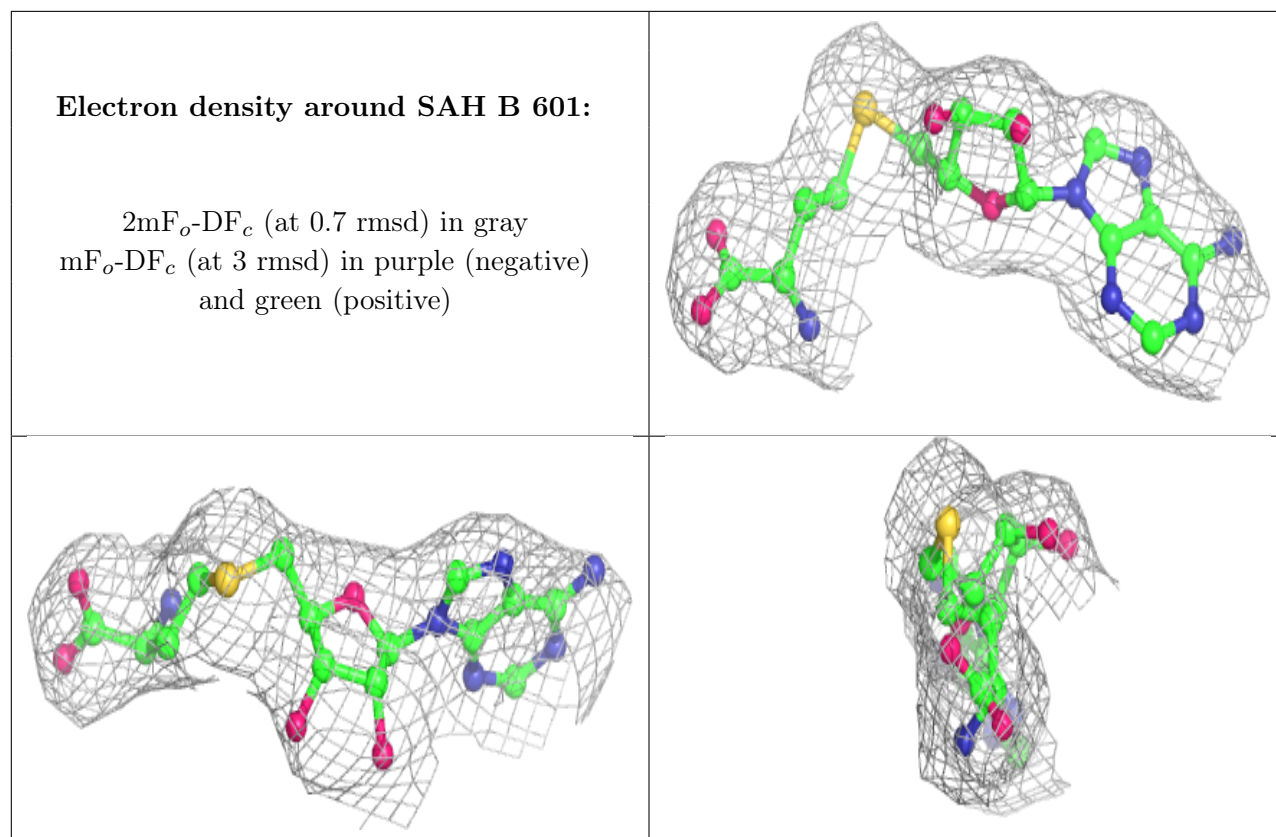
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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](#)

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