WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 06:48 PM EDT

PDB ID	:	6U8W
Title	:	Crystal structure of DNMT3B(K777A)-DNMT3L in complex with CpGpT DNA
Authors	:	Gao, L.; Zhang, Z.M.; Song, J.
Deposited on	:	2019-09-06
Resolution	:	2.95 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

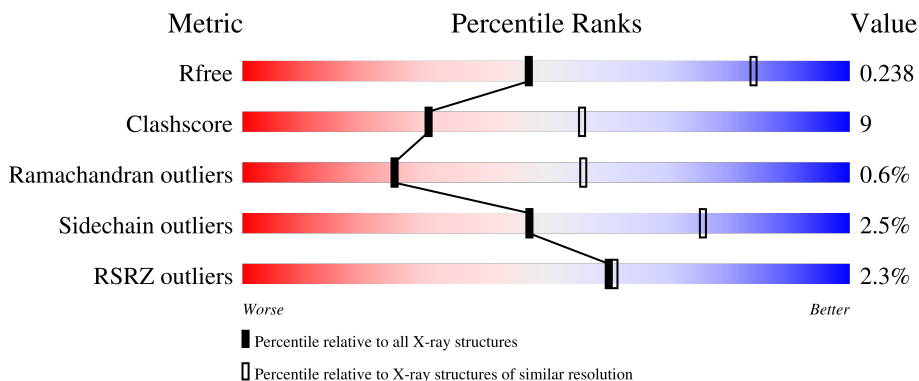|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.95 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	Percentile Ranks	Value
Rfree		0.238
Clashscore		9
Ramachandran outliers		0.6%
Sidechain outliers		2.5%
RSRZ outliers		2.3%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 >=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 <=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	291	76% — 24%
1	D	291	77% — 22% ·
2	B	209	4% / 73% — 18% — 8%
2	C	209	7% / 65% — 21% · 14%
3	E	25	56% — 44%

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Mol	Chain	Length	Quality of chain
3	F	25	64% 32% •

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8431 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 DNA (cytosine-5)-methyltransferase 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	1	0
			2298	1474	401	411	12			
1	D	291	Total	C	N	O	S	0	1	0
			2301	1479	401	409	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	777	ALA	LYS	engineered mutation	UNP Q9UBC3
D	777	ALA	LYS	engineered mutation	UNP Q9UBC3

- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	192	Total	C	N	O	S	0	0	0
			1404	920	239	242	3			
2	C	180	Total	C	N	O	S	0	0	0
			1343	878	230	232	3			

- Molecule 3 is a DNA chain called CpGpT DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	25	Total	C	N	O	P	0	0	0
			510	245	93	148	24			
3	F	25	Total	C	N	O	P	0	0	0
			510	245	93	148	24			

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).
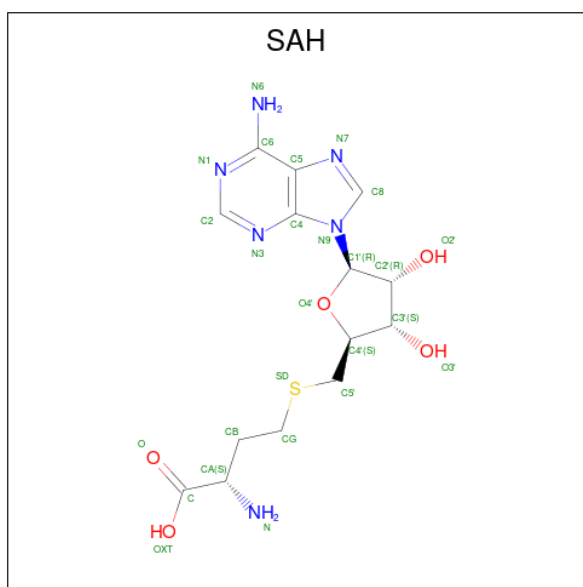
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
4	D	1	Total 26	C 14	N 6	O 5	S 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0
5	D	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total 6	O 6	0	0
6	D	4	Total 4	O 4	0	0
6	F	1	Total 1	O 1	0	0

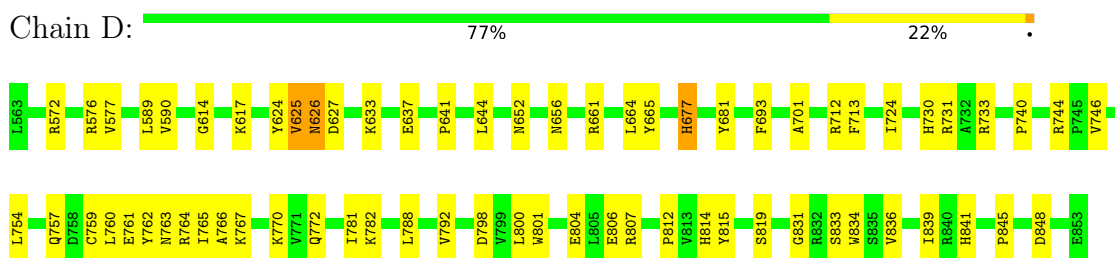# 3 Residue-property plots ⓘ

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 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.
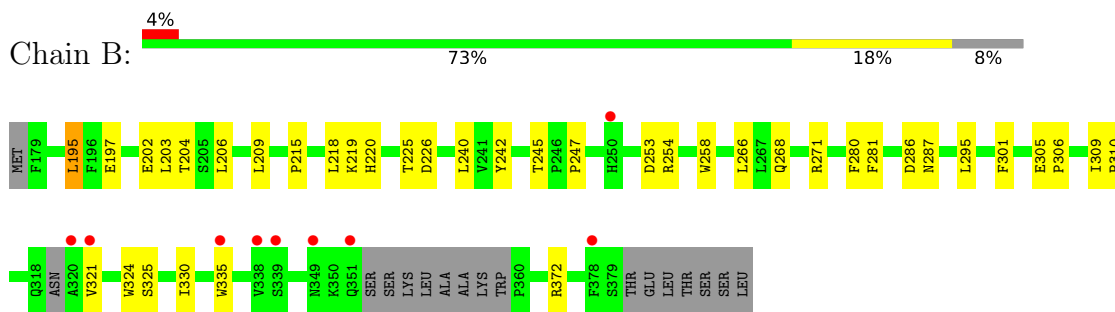
- Molecule 1: DNA (cytosine-5)-methyltransferase 3B

Chain A:

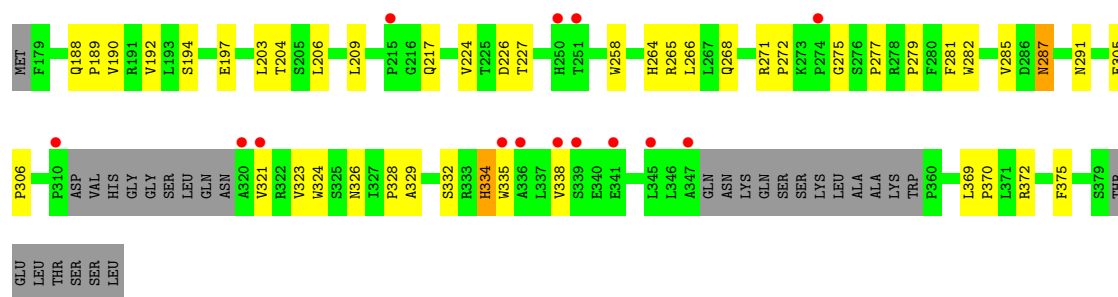- Molecule 1: DNA (cytosine-5)-methyltransferase 3B

Chain D:

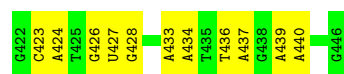- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

Chain B:

- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

Chain C:

MET F179 Q188 P189 V190 R191 V192 L193 S194 E197 L203 T204 S205 L206 L209 P215 G216 Q217 V224 T225 D226 T227 H250 T251 W258 H264 R265 L266 L267 Q268 R271 R272 K273 P274 G275 S276 P277 R278 P279 F280 F281 W282 V285 D286 N287 N291 E305

P306 P310 ASP VAL HIS GLY GLY SER LEU GLN ASN A320 V321 R322 V323 W324 S325 N326 I327 P328 A329 S332 R333 H334 W335 A336 L337 V338 S339 E340 E341 L345 L346 A347 GLN ASN LYS GLN SER SER LYS LEU ALA ALA LYS TRP P360 L369 P370 L371 R372 F375 S379 THR

GLU LEU THR SER SER LEU

● Molecule 3: CpGpT DNA (25-MER)

Chain E:

56%   44%

G422 C423 A424 T425 G426 U427 G428 A433 A434 T435 T436 A437 G438 A439 A440 G446

● Molecule 3: CpGpT DNA (25-MER)

Chain F:

64%   32%   •

G422 G426 U427 G428 A433 A434 T435 T436 A437 G438 G446

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	193.51Å 193.51Å 49.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.38 – 2.95 48.38 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.38-2.95) 99.6 (48.38-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.216 , 0.236 0.216 , 0.238	Depositor DCC
R_{free} test set	1977 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	78.7	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 38.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l 0.468 for h,-h-k,-l 0.032 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8431	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PYO, MG, 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	0.27	0/2353	0.46	0/3189
1	D	0.26	0/2356	0.44	0/3192
2	B	0.26	0/1450	0.45	0/1992
2	C	0.25	0/1389	0.45	0/1907
3	E	0.50	0/550	0.90	0/846
3	F	0.51	0/550	0.96	1/846 (0.1%)
All	All	0.30	0/8648	0.54	1/11972 (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	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	434	DA	OP2-P-O3'	5.19	116.62	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	625	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	D	625	VAL	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	2298	0	2248	42	0
1	D	2301	0	2264	45	0
2	B	1404	0	1216	27	0
2	C	1343	0	1183	30	0
3	E	510	0	279	6	0
3	F	510	0	279	6	0
4	A	26	0	19	0	0
4	D	26	0	19	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	0	0	0
6	D	4	0	0	0	0
6	F	1	0	0	0	0
All	All	8431	0	7507	147	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 9.

The worst 5 of 147 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)
2:C:224:VAL:HG21	2:C:266:LEU:HD11	1.51	0.91
1:A:754:LEU:O	1:A:770:LYS:NZ	2.17	0.78
1:D:781:ILE:HD11	1:D:800:LEU:HB2	1.71	0.73
1:A:576:ARG:HH21	1:A:641:PRO:HB2	1.53	0.72
1:D:576:ARG:HH21	1:D:641:PRO:HB2	1.56	0.71

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	290/291 (100%)	281 (97%)	7 (2%)	2 (1%)	22	52
1	D	290/291 (100%)	284 (98%)	4 (1%)	2 (1%)	22	52
2	B	186/209 (89%)	176 (95%)	8 (4%)	2 (1%)	14	40
2	C	174/209 (83%)	164 (94%)	10 (6%)	0	100	100
All	All	940/1000 (94%)	905 (96%)	29 (3%)	6 (1%)	25	56

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	ASN
1	D	626	ASN
1	A	627	ASP
1	D	627	ASP
2	B	215	PRO

5.3.2 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	238/251 (95%)	232 (98%)	6 (2%)	47	76
1	D	239/251 (95%)	234 (98%)	5 (2%)	53	79
2	B	123/191 (64%)	120 (98%)	3 (2%)	49	77
2	C	124/191 (65%)	120 (97%)	4 (3%)	39	70
All	All	724/884 (82%)	706 (98%)	18 (2%)	47	76

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	664	LEU
1	D	782	LYS
1	D	733	ARG
2	B	305	GLU
1	D	577	VAL

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

Mol	Chain	Res	Type
1	D	626	ASN
1	D	677	HIS
1	D	698	ASN
1	D	757	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
3	PYO	E	427	1,3	16,20,21	2.55	5 (31%)	22,28,31	1.02	1 (4%)
3	PYO	F	427	1,3	16,20,21	2.56	5 (31%)	22,28,31	1.01	1 (4%)

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	PYO	E	427	1,3	-	4/7/25/26	0/2/2/2
3	PYO	F	427	1,3	-	4/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	427	PYO	C6-C5	6.62	1.50	1.35
3	E	427	PYO	C6-C5	6.61	1.50	1.35
3	E	427	PYO	C5-C4	4.56	1.49	1.40
3	F	427	PYO	C5-C4	4.54	1.49	1.40
3	F	427	PYO	C6-N1	3.79	1.47	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	427	PYO	C5-C4-N3	-3.84	119.58	124.29
3	F	427	PYO	C5-C4-N3	-3.78	119.66	124.29

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	427	PYO	C2'-C1'-N1-C6
3	F	427	PYO	C2'-C1'-N1-C6
3	E	427	PYO	C2'-C1'-N1-C2
3	F	427	PYO	C2'-C1'-N1-C2
3	E	427	PYO	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	SAH	A	901	-	24,28,28	1.18	3 (12%)	25,40,40	1.71	4 (16%)
4	SAH	D	901	-	24,28,28	1.17	3 (12%)	25,40,40	1.67	4 (16%)

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	SAH	A	901	-	-	4/11/31/31	0/3/3/3
4	SAH	D	901	-	-	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)
4	A	901	SAH	C2-N3	3.89	1.38	1.32
4	D	901	SAH	C2-N3	3.89	1.38	1.32
4	D	901	SAH	C2-N1	2.42	1.38	1.33
4	A	901	SAH	C2-N1	2.41	1.38	1.33
4	A	901	SAH	OXT-C	-2.03	1.23	1.30

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	901	SAH	N3-C2-N1	-5.44	120.18	128.68
4	A	901	SAH	N3-C2-N1	-5.42	120.20	128.68
4	A	901	SAH	C5'-SD-CG	-3.87	90.65	102.27
4	D	901	SAH	C5'-SD-CG	-3.44	91.96	102.27
4	A	901	SAH	OXT-C-O	-2.82	117.68	124.09

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	SAH	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
4	D	901	SAH	N-CA-CB-CG
4	A	901	SAH	C-CA-CB-CG
4	D	901	SAH	C-CA-CB-CG
4	A	901	SAH	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand SAH A 901

Bond lengths   Bond angles

Torsions   Rings

Ligand SAH D 901

Bond lengths

Bond angles

Torsions

Rings
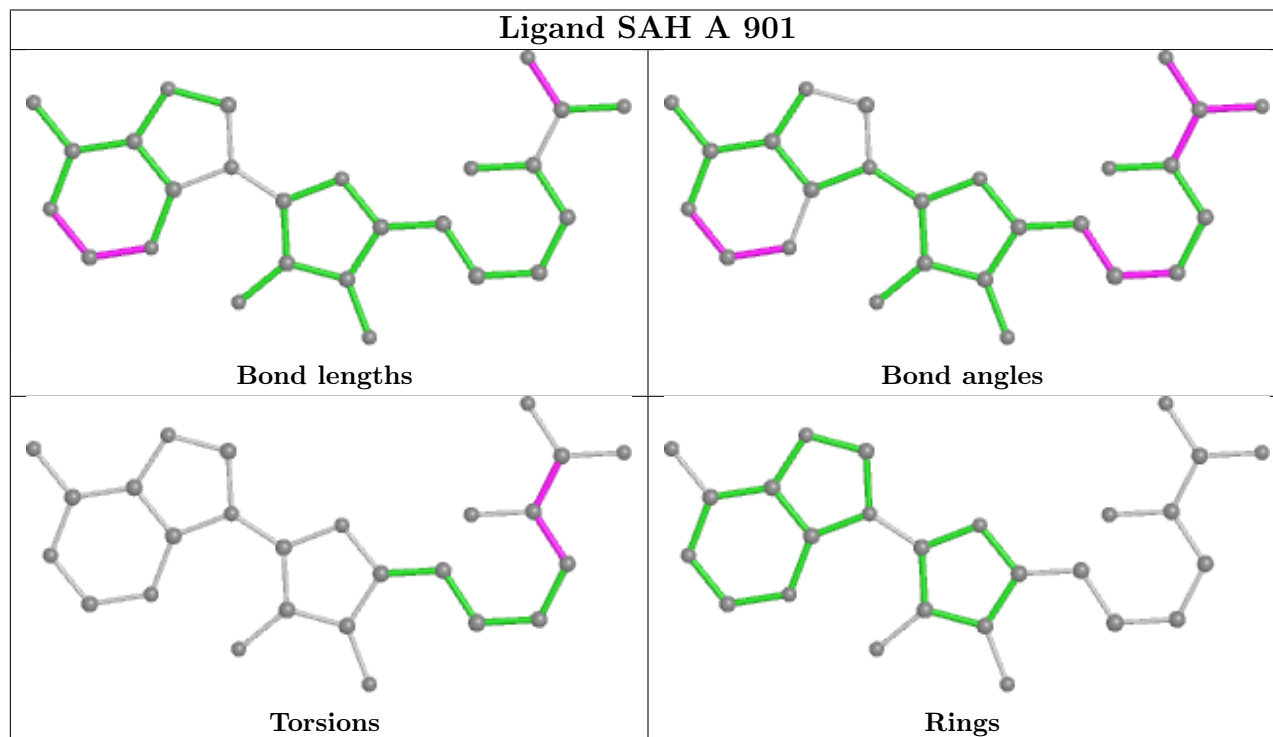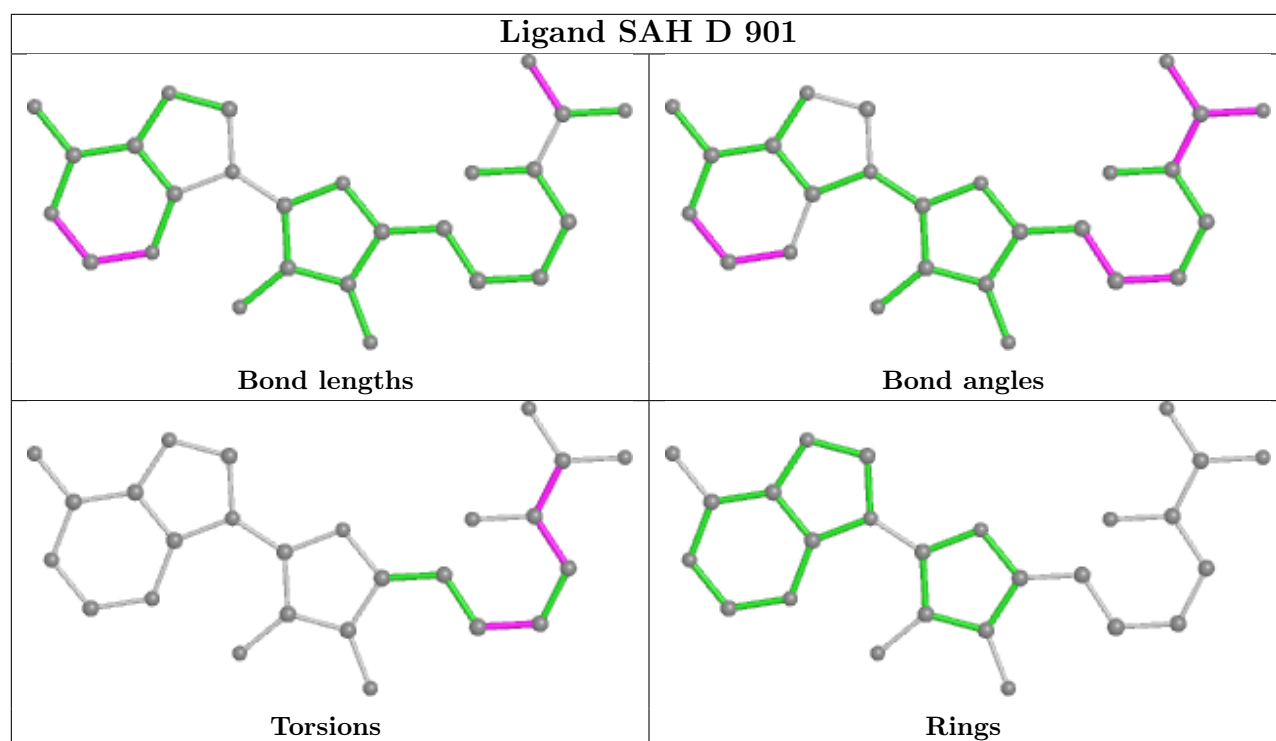
5.7 Other polymers ⓘ

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 ⓘ

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, 95th 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^2)	Q<0.9
1	A	291/291 (100%)	-0.12	0	100	100	37, 69, 114, 140	0
1	D	291/291 (100%)	-0.16	0	100	100	38, 69, 115, 138	0
2	B	192/209 (91%)	0.18	9 (4%)	31	31	78, 127, 209, 230	0
2	C	180/209 (86%)	0.19	14 (7%)	13	11	76, 122, 197, 210	0
3	E	24/25 (96%)	-0.05	0	100	100	107, 160, 185, 187	0
3	F	24/25 (96%)	-0.06	0	100	100	108, 162, 182, 189	0
All	All	1002/1050 (95%)	-0.02	23 (2%)	60	61	37, 89, 186, 230	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	320	ALA	8.5
2	B	250	HIS	8.5
2	B	320	ALA	5.9
2	C	250	HIS	5.2
2	B	338	VAL	5.2

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

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, 95th 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.

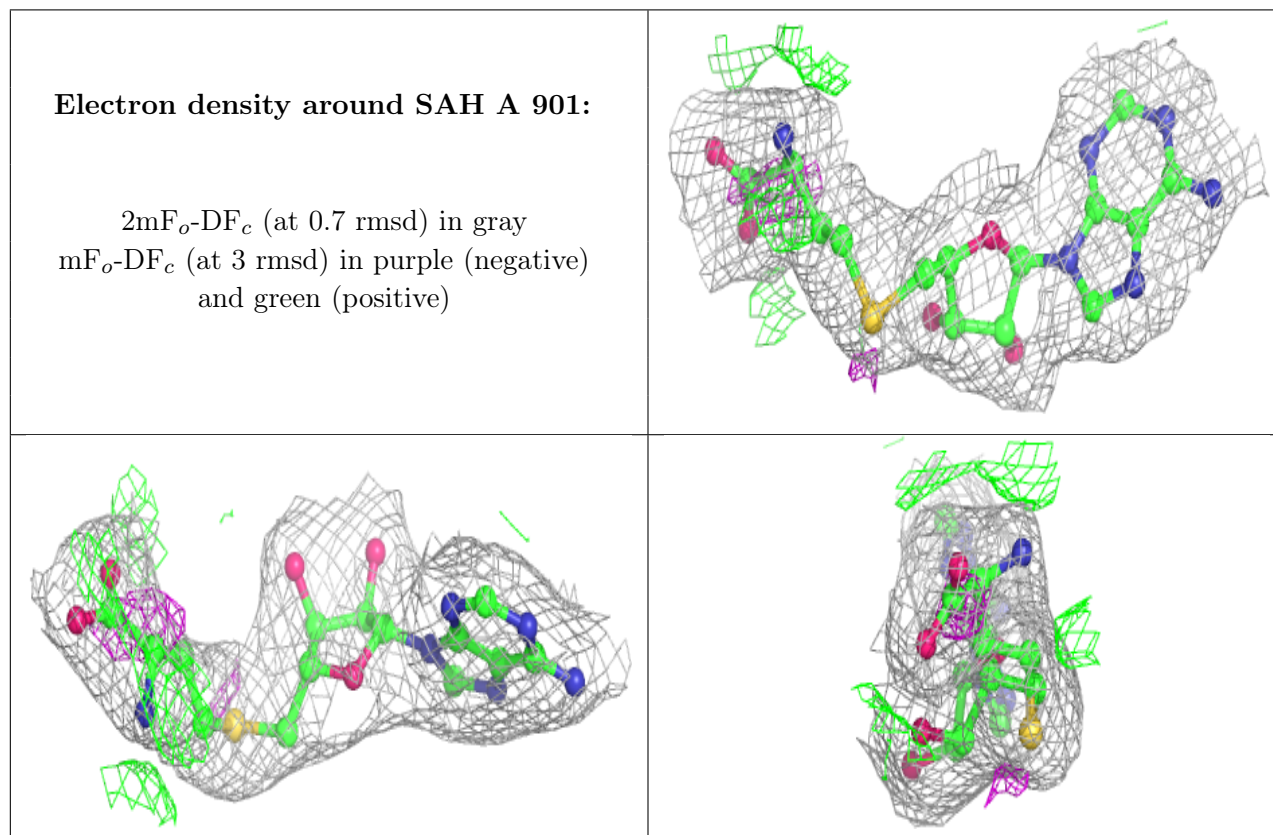| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PYO	E	427	19/20	0.95	0.12	78,85,95,99	0
3	PYO	F	427	19/20	0.96	0.14	78,84,95,101	0

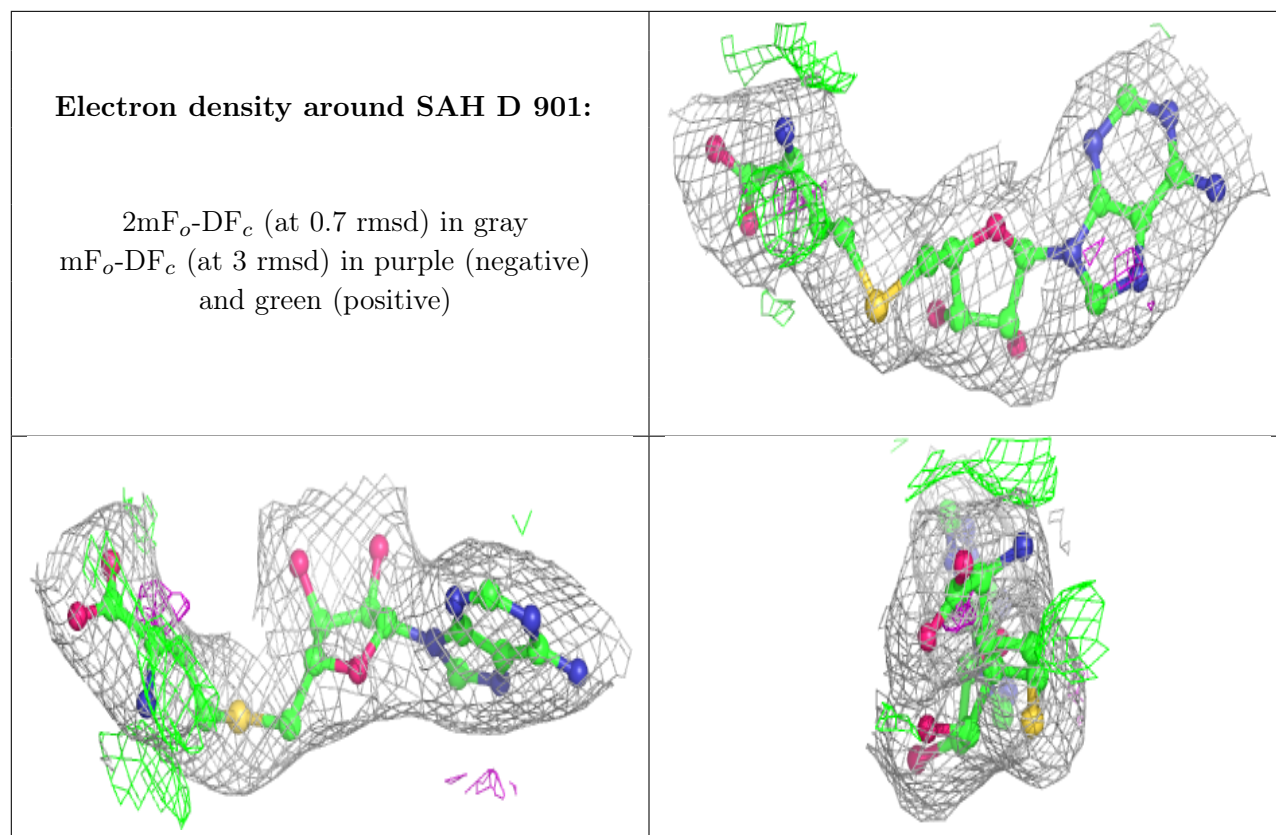## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 95th 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^2)	Q<0.9
5	MG	D	902	1/1	0.87	0.15	75,75,75,75	0
5	MG	A	902	1/1	0.91	0.21	81,81,81,81	0
4	SAH	A	901	26/26	0.96	0.17	42,52,59,64	0
4	SAH	D	901	26/26	0.97	0.16	43,53,61,67	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.

Electron density around SAH A 901:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around SAH D 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.