WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 10, 2025 – 06:05 PM EDT

PDB ID	:	9MVY / pdb_00009mvy
Title	:	Crystal structure of ZMET2 in complex with unmethylated CTG DNA and a histone H3Kc9me2 peptide
Authors	:	Herle, G.; Fang, J.; Song, J.
Deposited on	:	2025-01-16
Resolution	:	2.71 Å(reported)

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

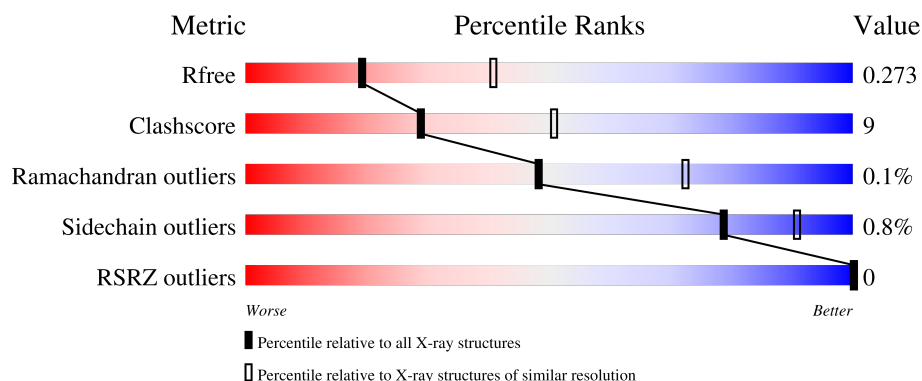|		
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
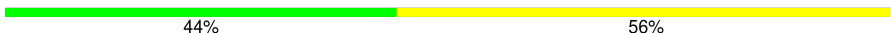*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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		0.273
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		0.8%
RSRZ outliers		0

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$_{free}$	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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	758	72% 18% 9%
1	D	758	74% 17% 9%
2	B	18	44% 56%
2	E	18	28% 61% 11%
3	C	18	39% 50% 6% 6%

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Mol	Chain	Length	Quality of chain
3	F	18	44%　　　　　　　39%　　　6%　　11%
4	G	32	59%　　　　　　　41%
4	H	32	12%　　6%　　　81%
4	I	32	12%　　9%　　　78%
4	P	32	50%　　·　　47%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C49	F	10	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13299 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total 5427	C 3468	N 929	O 998	S 32	0	0	0
1	D	689	Total 5423	C 3464	N 923	O 1003	S 33	0	0	0

- Molecule 2 is a DNA chain called ssDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total 370	C 179	N 70	O 104	P 17	0	0	0
2	E	16	Total 333	C 159	N 66	O 92	P 16	0	0	0

- Molecule 3 is a DNA chain called C49 ssDNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	17	Total 346	C 168	F 1	N 55	O 105	P 17	0	0	0
3	F	16	Total 326	C 158	F 1	N 53	O 98	P 16	0	0	0

- Molecule 4 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	19	Total 135	C 83	N 27	O 24	S 1	0	0	0
4	H	6	Total 49	C 28	N 11	O 9	S 1	0	0	0
4	I	7	Total 48	C 28	N 9	O 10	S 1	0	0	0
4	P	17	Total 123	C 75	N 25	O 22	S 1	0	0	0

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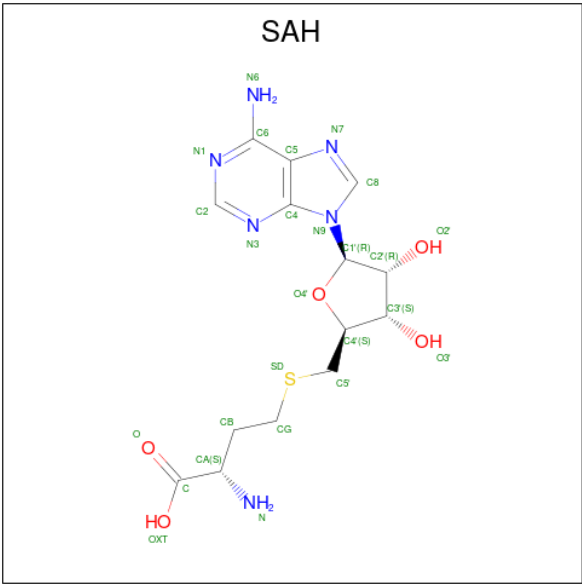
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	291	Total	O	0	0
			291	291		
6	B	20	Total	O	0	0
			20	20		
6	C	21	Total	O	0	0
			21	21		
6	D	285	Total	O	0	0
			285	285		
6	E	22	Total	O	0	0
			22	22		
6	F	11	Total	O	0	0
			11	11		
6	G	6	Total	O	0	0
			6	6		
6	H	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total 2	O 2	0	0
6	P	3	Total 3	O 3	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 1

• Molecule 1: DNA (cytosine-5)-methyltransferase 1

P663 K684 T685 Q688 R689 Y690 I691 D710 L715 P719 N723 N724 D725 E728 I733 V747 L766 K770 P771 Y776 G790 R791 L792 E796 P807 V811 P815 V820 L821 T822 I823 R828 L829 D834 G840 P841 I842 K845 Y846

I847 N851 V855 P856 V857 G866 L879 Y880 T887

• Molecule 2: ssDNA

Chain B:

44%   56%

T1 A2 A3 A4 T5 T6 C7 T12 A13 G14 G15 T18

• Molecule 2: ssDNA

Chain E:

28%   61%   11%

DT A2 A3 A4 T5 T6 C7 T12 A13 G14 G15 A16 A17 DT

• Molecule 3: C49 ssDNA

Chain C:

39%   50%   6%   6%

DA T2 T3 C4 C5 T6 A7 A8 T9 C10 T11 G12 A18

• Molecule 3: C49 ssDNA

Chain F:

44%   39%   6%   11%

DA DT T3 C4 C5 T6 A7 A8 T9 C10 T11 G12 A18

• Molecule 4: Histone H3.2

Chain G:

59%   41%

ALA ARG THR K4 T11 GLY GLY K14 A24 ALA ARG LYS SER ALA PRO ALA THR

• Molecule 4: Histone H3.2

Chain H:

12% 6%   81%

ALA ARG THR LYS Q5 R8 K9 S10 THR GLY GLY LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO ALA THR

• Molecule 4: Histone H3.2

Chain I:

12%   9%   78%

ALA ARG THR LYS **Q5** **K9** **S10** **T11** GLY GLY LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO ALA THR

● Molecule 4: Histone H3.2

Chain P:

50%   ·   47%

ALA ARG THR **K4** **S10** THR GLY GLY LYS **A15** **A24** ALA ARG LYS SER ALA PRO ALA THR
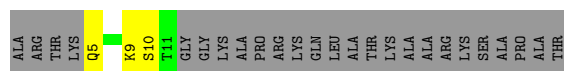
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.52Å 277.30Å 64.48Å 90.00° 97.26° 90.00°	Depositor
Resolution (Å)	48.40 – 2.71 48.40 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.40-2.71) 98.0 (48.40-2.71)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.227 , 0.271 0.228 , 0.273	Depositor DCC
R_{free} test set	57192 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.5	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.436 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13299	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: M2L, C49, 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	0.14	0/5561	0.33	0/7536
1	D	0.14	0/5556	0.31	0/7534
2	B	0.25	0/416	0.55	0/641
2	E	0.23	0/375	0.51	0/577
3	C	0.27	0/361	0.53	0/552
3	F	0.26	0/339	0.50	0/518
4	G	0.09	0/122	0.23	0/160
4	H	0.19	0/36	0.28	0/45
4	I	0.16	0/35	0.43	0/45
4	P	0.10	0/110	0.36	0/144
All	All	0.15	0/12911	0.35	0/17752

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
4	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	9	M2L	Mainchain

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	5427	0	5312	93	0
1	D	5423	0	5287	92	0
2	B	370	0	206	7	0
2	E	333	0	181	9	0
3	C	346	0	196	12	0
3	F	326	0	184	10	0
4	G	135	0	141	0	0
4	H	49	0	50	3	0
4	I	48	0	41	2	0
4	P	123	0	127	1	0
5	A	26	0	19	3	0
5	D	26	0	19	1	0
6	A	291	0	0	6	0
6	B	20	0	0	0	0
6	C	21	0	0	1	0
6	D	285	0	0	7	0
6	E	22	0	0	0	0
6	F	11	0	0	0	0
6	G	6	0	0	0	0
6	H	6	0	0	0	0
6	I	2	0	0	0	0
6	P	3	0	0	0	0
All	All	13299	0	11763	209	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 209 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:517:CYS:SG	3:C:10:C49:C6	2.08	1.41
1:D:517:CYS:SG	3:F:10:C49:C6	2.09	1.40
1:D:517:CYS:HG	3:F:10:C49:C6	1.70	0.95
1:D:517:CYS:SG	3:F:10:C49:C5	2.56	0.93
1:A:517:CYS:SG	3:C:10:C49:C5	2.60	0.89

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	679/758 (90%)	648 (95%)	30 (4%)	1 (0%)	48	72
1	D	681/758 (90%)	650 (95%)	31 (5%)	0	100	100
4	G	14/32 (44%)	14 (100%)	0	0	100	100
4	H	3/32 (9%)	2 (67%)	1 (33%)	0	100	100
4	I	4/32 (12%)	4 (100%)	0	0	100	100
4	P	12/32 (38%)	12 (100%)	0	0	100	100
All	All	1393/1644 (85%)	1330 (96%)	62 (4%)	1 (0%)	48	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	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	578/651 (89%)	574 (99%)	4 (1%)	81	92
1	D	577/651 (89%)	572 (99%)	5 (1%)	75	89
4	G	11/21 (52%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	4/21 (19%)	4 (100%)	0	100	100
4	I	3/21 (14%)	3 (100%)	0	100	100
4	P	10/21 (48%)	10 (100%)	0	100	100
All	All	1183/1386 (85%)	1174 (99%)	9 (1%)	79	91

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	664	ASP
1	D	747	VAL
1	A	855	VAL
1	D	173	ARG
1	D	376	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	718	GLN
1	D	277	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	C49	C	10	3	17,22,24	5.20	11 (64%)	17,33,38	2.08	5 (29%)
4	M2L	G	9	4	9,10,11	0.56	0	7,11,13	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	M2L	I	9	4	9,10,11	0.54	0	7,11,13	0.48	0
4	M2L	P	9	4	9,10,11	0.55	0	7,11,13	0.53	0
3	C49	F	10	3	17,22,24	5.20	11 (64%)	17,33,38	2.24	6 (35%)
4	M2L	H	9	4	9,10,11	0.56	0	7,11,13	0.60	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	C49	C	10	3	-	6/7/40/46	0/2/2/2
4	M2L	G	9	4	-	2/7/9/11	-
4	M2L	I	9	4	-	4/7/9/11	-
4	M2L	P	9	4	-	1/7/9/11	-
3	C49	F	10	3	-	6/7/40/46	0/2/2/2
4	M2L	H	9	4	-	1/7/9/11	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	10	C49	C2-N1	11.16	1.51	1.35
3	C	10	C49	C2-N1	11.09	1.51	1.35
3	C	10	C49	C3'-C4'	-8.97	1.29	1.53
3	F	10	C49	C3'-C4'	-8.94	1.29	1.53
3	C	10	C49	C2-N3	7.99	1.51	1.38

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	10	C49	N3-C2-N1	5.27	121.94	116.65
3	C	10	C49	N3-C2-N1	4.84	121.51	116.65
3	C	10	C49	O2-C2-N1	-4.10	118.17	123.10
3	F	10	C49	O2-C2-N1	-3.88	118.44	123.10
3	F	10	C49	CM5-C5-C4	-3.60	103.55	109.11

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	9	M2L	SG-CD-CE-NZ
4	I	9	M2L	CD-CE-NZ-CM1
3	C	10	C49	O4'-C4'-C5'-O5'
3	C	10	C49	C3'-C4'-C5'-O5'
3	C	10	C49	O4'-C1'-N1-C6

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	10	C49	4	0
3	F	10	C49	7	0
4	H	9	M2L	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#|Z| > 2$
5	SAH	D	1000	-	23,28,28	0.98	2 (8%)	22,40,40	1.06	2 (9%)
5	SAH	A	1000	-	23,28,28	0.97	2 (8%)	22,40,40	1.16	2 (9%)

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
5	SAH	D	1000	-	-	5/11/31/31	0/3/3/3
5	SAH	A	1000	-	-	2/11/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1000	SAH	C8-N7	-2.38	1.30	1.34
5	A	1000	SAH	C8-N7	-2.30	1.30	1.34
5	A	1000	SAH	C1'-N9	-2.25	1.44	1.49
5	D	1000	SAH	C1'-N9	-2.25	1.44	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1000	SAH	C4'-O4'-C1'	-3.19	107.00	109.92
5	A	1000	SAH	CB-CG-SD	-2.67	107.50	113.45
5	D	1000	SAH	CB-CG-SD	-2.59	107.67	113.45
5	D	1000	SAH	C4'-O4'-C1'	-2.49	107.64	109.92

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1000	SAH	N-CA-CB-CG
5	D	1000	SAH	C-CA-CB-CG
5	D	1000	SAH	O-C-CA-CB
5	D	1000	SAH	CB-CG-SD-C5'
5	D	1000	SAH	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1000	SAH	1	0
5	A	1000	SAH	3	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 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 D 1000

Ligand SAH A 1000
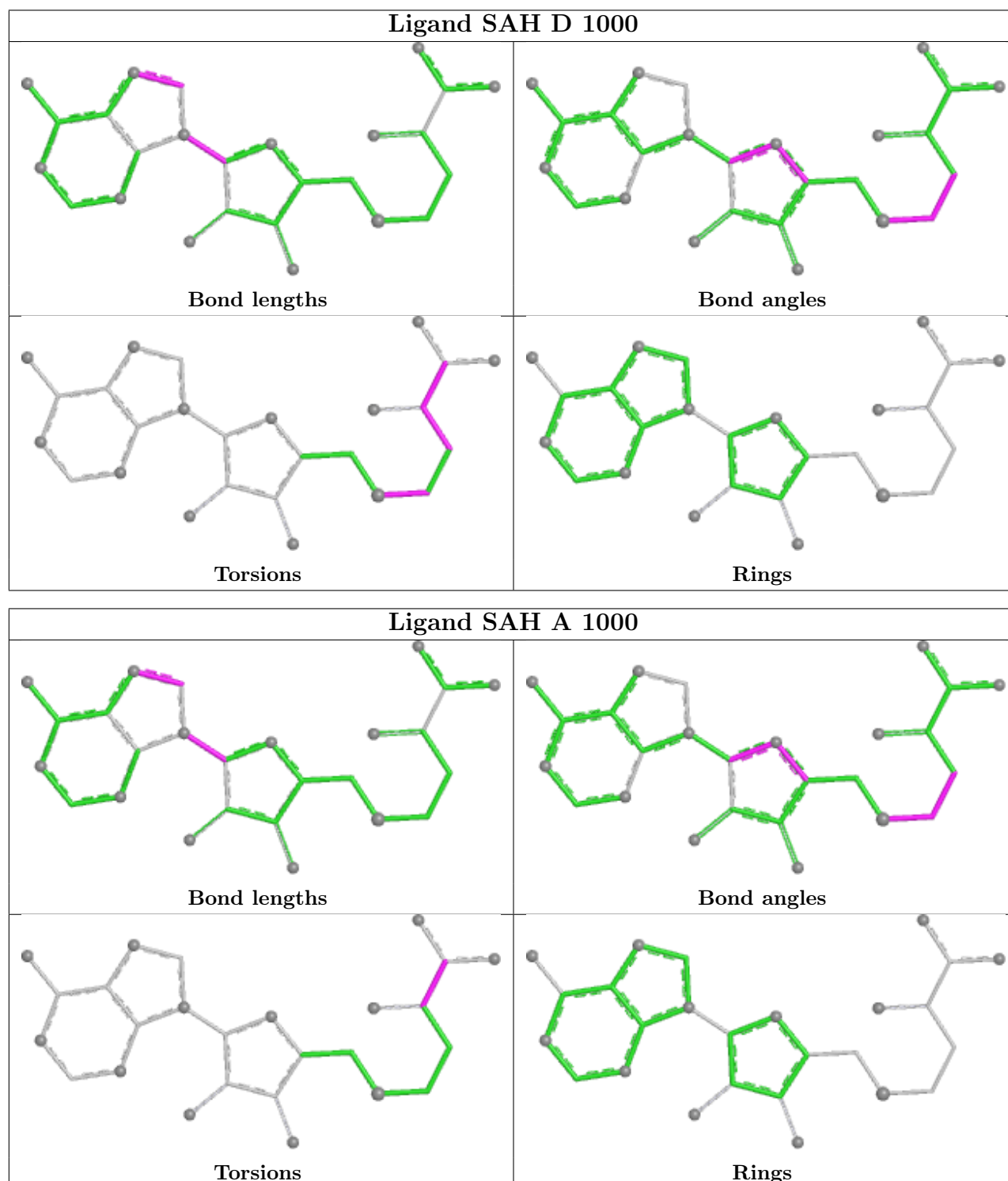
5.7 Other polymers ⓘ

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	687/758 (90%)	-1.91	0	100	100	22, 38, 83, 129	0
1	D	689/758 (90%)	-1.93	0	100	100	21, 37, 84, 122	0
2	B	18/18 (100%)	-2.22	0	100	100	42, 56, 136, 136	0
2	E	16/18 (88%)	-2.17	0	100	100	37, 49, 128, 157	0
3	C	16/18 (88%)	-2.21	0	100	100	36, 62, 118, 121	0
3	F	15/18 (83%)	-2.22	0	100	100	32, 52, 105, 133	0
4	G	18/32 (56%)	-1.55	0	100	100	55, 70, 102, 117	0
4	H	5/32 (15%)	-1.82	0	100	100	91, 93, 99, 109	0
4	I	6/32 (18%)	-1.43	0	100	100	83, 92, 117, 131	0
4	P	16/32 (50%)	-1.69	0	100	100	41, 63, 93, 131	0
All	All	1486/1716 (86%)	-1.92	0	100	100	21, 39, 90, 157	0

There are no RSRZ outliers to report.

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.

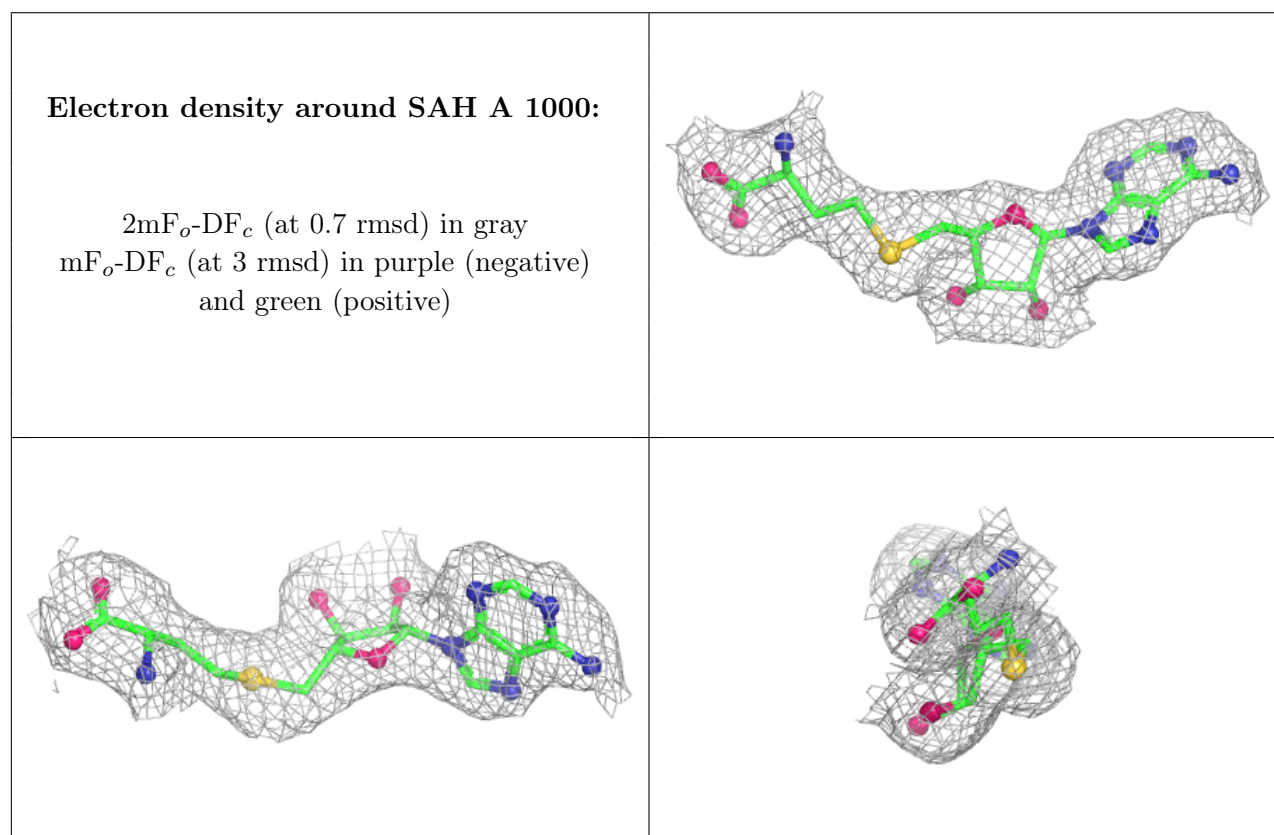| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	M2L	H	9	11/12	0.99	0.06	135,140,152,172	0
4	M2L	I	9	11/12	0.99	0.06	102,117,132,144	0
4	M2L	P	9	11/12	0.99	0.03	33,41,57,59	0
4	M2L	G	9	11/12	1.00	0.03	34,39,71,74	0
3	C49	C	10	21/23	1.00	0.02	31,34,37,44	0
3	C49	F	10	21/23	1.00	0.02	22,27,35,42	0

6.3 Carbohydrates (i)
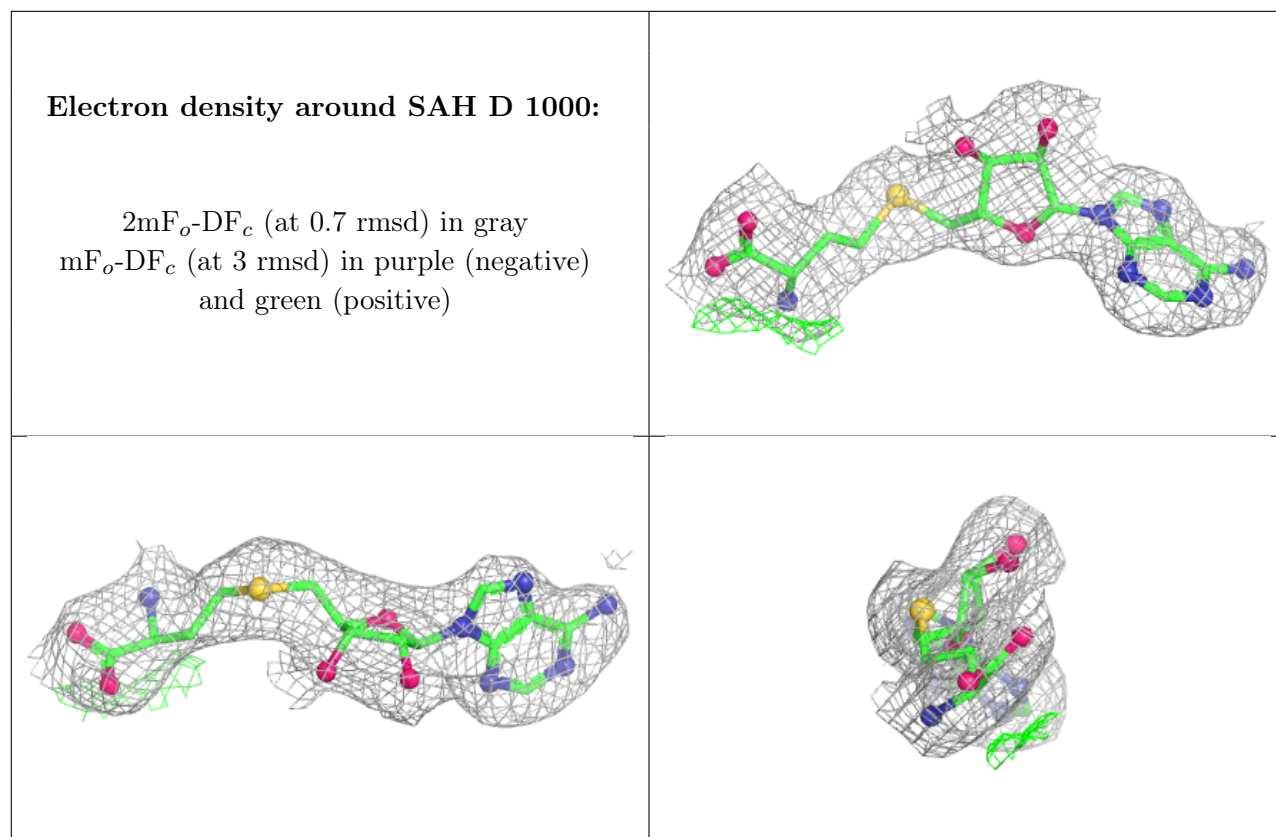
There are no monosaccharides in this entry.

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, 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	SAH	A	1000	26/26	1.00	0.02	18,29,43,48	0
5	SAH	D	1000	26/26	1.00	0.02	18,29,39,44	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 1000:

$2mF_o\text{-}DF_c$ (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 1000:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.