



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:58 am BST

PDB ID : 2ORE
Title : Binary Structure of Escherichia coli DNA Adenine Methyltransferase and S-adenosylhomocysteine
Authors : Horton, J.R.; Cheng, X.
Deposited on : 2007-02-02
Resolution : 2.99 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 ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

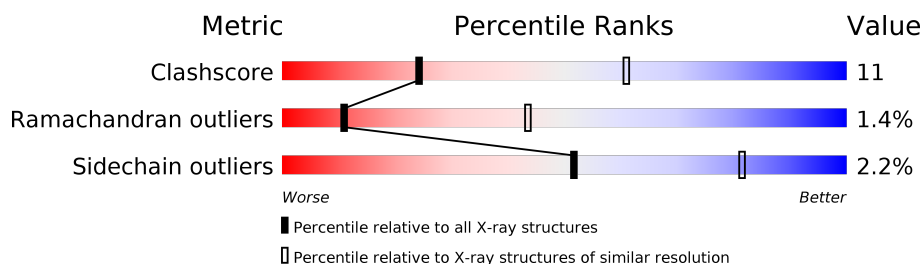
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	298	
1	E	298	
1	F	298	

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
2	SAH	E	302[A]	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6014 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 adenine methylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	243	Total	C	N	O	S	0	0	0
			1954	1266	325	355	8			
1	E	244	Total	C	N	O	S	0	0	0
			1941	1256	325	352	8			
1	F	244	Total	C	N	O	S	3	0	0
			1961	1271	328	354	8			

There are 60 discrepancies between the modelled and reference sequences:

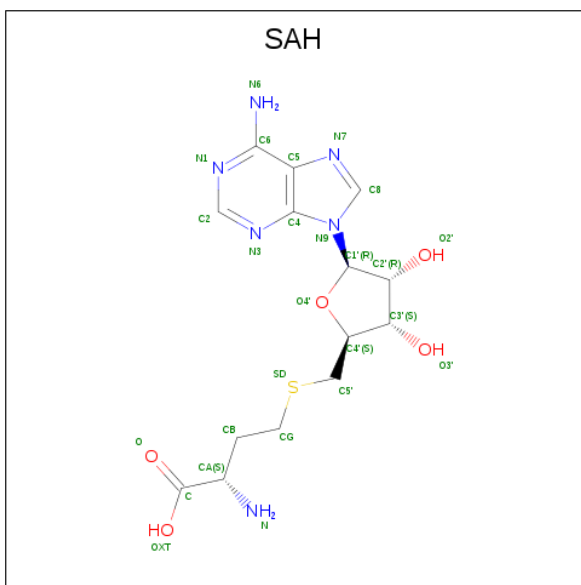
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	CLONING ARTIFACT	UNP P0AEE8
D	-18	GLY	-	CLONING ARTIFACT	UNP P0AEE8
D	-17	SER	-	CLONING ARTIFACT	UNP P0AEE8
D	-16	SER	-	CLONING ARTIFACT	UNP P0AEE8
D	-15	HIS	-	EXPRESSION TAG	UNP P0AEE8
D	-14	HIS	-	EXPRESSION TAG	UNP P0AEE8
D	-13	HIS	-	EXPRESSION TAG	UNP P0AEE8
D	-12	HIS	-	EXPRESSION TAG	UNP P0AEE8
D	-11	HIS	-	EXPRESSION TAG	UNP P0AEE8
D	-10	HIS	-	EXPRESSION TAG	UNP P0AEE8
D	-9	SER	-	EXPRESSION TAG	UNP P0AEE8
D	-8	SER	-	CLONING ARTIFACT	UNP P0AEE8
D	-7	GLY	-	CLONING ARTIFACT	UNP P0AEE8
D	-6	LEU	-	CLONING ARTIFACT	UNP P0AEE8
D	-5	VAL	-	CLONING ARTIFACT	UNP P0AEE8
D	-4	PRO	-	CLONING ARTIFACT	UNP P0AEE8
D	-3	ARG	-	CLONING ARTIFACT	UNP P0AEE8
D	-2	GLY	-	CLONING ARTIFACT	UNP P0AEE8
D	-1	SER	-	CLONING ARTIFACT	UNP P0AEE8
D	0	HIS	-	CLONING ARTIFACT	UNP P0AEE8
E	-19	MET	-	CLONING ARTIFACT	UNP P0AEE8
E	-18	GLY	-	CLONING ARTIFACT	UNP P0AEE8
E	-17	SER	-	CLONING ARTIFACT	UNP P0AEE8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	SER	-	CLONING ARTIFACT	UNP P0AEE8
E	-15	HIS	-	EXPRESSION TAG	UNP P0AEE8
E	-14	HIS	-	EXPRESSION TAG	UNP P0AEE8
E	-13	HIS	-	EXPRESSION TAG	UNP P0AEE8
E	-12	HIS	-	EXPRESSION TAG	UNP P0AEE8
E	-11	HIS	-	EXPRESSION TAG	UNP P0AEE8
E	-10	HIS	-	EXPRESSION TAG	UNP P0AEE8
E	-9	SER	-	CLONING ARTIFACT	UNP P0AEE8
E	-8	SER	-	CLONING ARTIFACT	UNP P0AEE8
E	-7	GLY	-	CLONING ARTIFACT	UNP P0AEE8
E	-6	LEU	-	CLONING ARTIFACT	UNP P0AEE8
E	-5	VAL	-	CLONING ARTIFACT	UNP P0AEE8
E	-4	PRO	-	CLONING ARTIFACT	UNP P0AEE8
E	-3	ARG	-	CLONING ARTIFACT	UNP P0AEE8
E	-2	GLY	-	CLONING ARTIFACT	UNP P0AEE8
E	-1	SER	-	CLONING ARTIFACT	UNP P0AEE8
E	0	HIS	-	CLONING ARTIFACT	UNP P0AEE8
F	-19	MET	-	CLONING ARTIFACT	UNP P0AEE8
F	-18	GLY	-	CLONING ARTIFACT	UNP P0AEE8
F	-17	SER	-	CLONING ARTIFACT	UNP P0AEE8
F	-16	SER	-	CLONING ARTIFACT	UNP P0AEE8
F	-15	HIS	-	EXPRESSION TAG	UNP P0AEE8
F	-14	HIS	-	EXPRESSION TAG	UNP P0AEE8
F	-13	HIS	-	EXPRESSION TAG	UNP P0AEE8
F	-12	HIS	-	EXPRESSION TAG	UNP P0AEE8
F	-11	HIS	-	EXPRESSION TAG	UNP P0AEE8
F	-10	HIS	-	EXPRESSION TAG	UNP P0AEE8
F	-9	SER	-	CLONING ARTIFACT	UNP P0AEE8
F	-8	SER	-	CLONING ARTIFACT	UNP P0AEE8
F	-7	GLY	-	CLONING ARTIFACT	UNP P0AEE8
F	-6	LEU	-	CLONING ARTIFACT	UNP P0AEE8
F	-5	VAL	-	CLONING ARTIFACT	UNP P0AEE8
F	-4	PRO	-	CLONING ARTIFACT	UNP P0AEE8
F	-3	ARG	-	CLONING ARTIFACT	UNP P0AEE8
F	-2	GLY	-	CLONING ARTIFACT	UNP P0AEE8
F	-1	SER	-	CLONING ARTIFACT	UNP P0AEE8
F	0	HIS	-	CLONING ARTIFACT	UNP P0AEE8

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total	C	N	O	S	0	1
			52	28	12	10	2		
2	F	1	Total	C	N	O	S	0	1
			52	28	12	10	2		

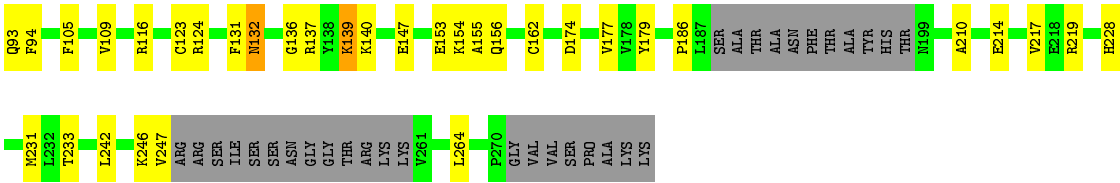
- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	9	Total 9	O 9	0	0
4	E	4	Total 4	O 4	0	0
4	F	10	Total 10	O 10	0	0



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.13Å 160.13Å 94.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.67 – 2.99	Depositor
% Data completeness (in resolution range)	99.5 (34.67-2.99)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6014	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	D	0.36	0/2008	0.57	0/2731
1	E	0.38	0/1996	0.56	0/2719
1	F	0.36	0/2016	0.56	0/2742
All	All	0.37	0/6020	0.56	0/8192

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 [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	D	1954	0	1836	45	0
1	E	1941	0	1786	43	0
1	F	1961	0	1837	40	0
2	D	26	0	18	0	0
2	E	52	0	36	2	0
2	F	52	0	37	0	0
3	F	5	0	0	0	0
4	D	9	0	0	0	0
4	E	4	0	0	0	0
4	F	10	0	0	0	0
All	All	6014	0	5550	127	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 11.

The worst 5 of 127 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:D:187:LEU:HD11	1:D:261:VAL:HG21	1.36	1.04
1:F:139:LYS:HD3	1:F:139:LYS:H	1.28	0.96
1:D:139:LYS:HD2	1:D:139:LYS:H	1.32	0.93
1:D:126:ASN:HB3	1:D:132:ASN:HD22	1.41	0.84
1:D:10:TRP:HB2	1:D:38:ALA:HB2	1.62	0.79

There are no symmetry-related clashes.

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	D	237/298 (80%)	218 (92%)	16 (7%)	3 (1%)	12	45
1	E	238/298 (80%)	216 (91%)	18 (8%)	4 (2%)	9	39
1	F	238/298 (80%)	211 (89%)	24 (10%)	3 (1%)	12	45
All	All	713/894 (80%)	645 (90%)	58 (8%)	10 (1%)	11	43

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	17	LEU
1	E	18	LEU
1	F	14	LYS
1	E	16	PRO
1	E	139	LYS

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	D	198/256 (77%)	194 (98%)	4 (2%)	55	83
1	E	191/256 (75%)	188 (98%)	3 (2%)	62	86
1	F	197/256 (77%)	191 (97%)	6 (3%)	41	75
All	All	586/768 (76%)	573 (98%)	13 (2%)	52	81

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	262	ASP
1	E	263	GLU
1	F	132	ASN
1	E	174	ASP
1	F	42	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	220	HIS
1	E	150	HIS
1	F	120	ASN
1	D	157	ASN
1	F	102	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	D	301	-	21,28,28	1.93	6 (28%)	20,40,40	2.42	9 (45%)
2	SAH	F	303[B]	-	21,28,28	1.95	6 (28%)	20,40,40	2.61	7 (35%)
2	SAH	E	302[A]	-	21,28,28	1.94	6 (28%)	20,40,40	2.79	6 (30%)
2	SAH	F	303[A]	-	21,28,28	1.95	6 (28%)	20,40,40	2.62	6 (30%)
2	SAH	E	302[B]	-	21,28,28	1.91	5 (23%)	20,40,40	2.49	7 (35%)
3	SO4	F	501	-	4,4,4	0.34	0	6,6,6	0.06	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
2	SAH	F	303[A]	-	-	0/7/31/31	0/3/3/3
2	SAH	D	301	-	-	1/7/31/31	0/3/3/3
2	SAH	F	303[B]	-	-	3/7/31/31	0/3/3/3
2	SAH	E	302[A]	-	1/1/6/6	1/7/31/31	0/3/3/3
2	SAH	E	302[B]	-	-	5/7/31/31	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	302[B]	SAH	C2-N3	4.56	1.39	1.32
2	E	302[A]	SAH	C2-N3	4.54	1.39	1.32
2	F	303[B]	SAH	C2-N3	4.44	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	303[A]	SAH	C2-N3	4.42	1.39	1.32
2	E	302[B]	SAH	O4'-C1'	4.22	1.47	1.41

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	302[A]	SAH	CB-CG-SD	-7.39	96.74	113.31
2	E	302[A]	SAH	O4'-C1'-C2'	-6.39	97.59	106.93
2	F	303[A]	SAH	O4'-C1'-C2'	-6.25	97.79	106.93
2	F	303[A]	SAH	CB-CG-SD	-6.00	99.86	113.31
2	F	303[B]	SAH	O4'-C1'-C2'	-5.90	98.30	106.93

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	302[A]	SAH	CA

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	303[B]	SAH	N-CA-CB-CG
2	F	303[B]	SAH	C-CA-CB-CG
2	F	303[B]	SAH	CB-CG-SD-C5'
2	E	302[A]	SAH	N-CA-CB-CG
2	E	302[B]	SAH	N-CA-CB-CG

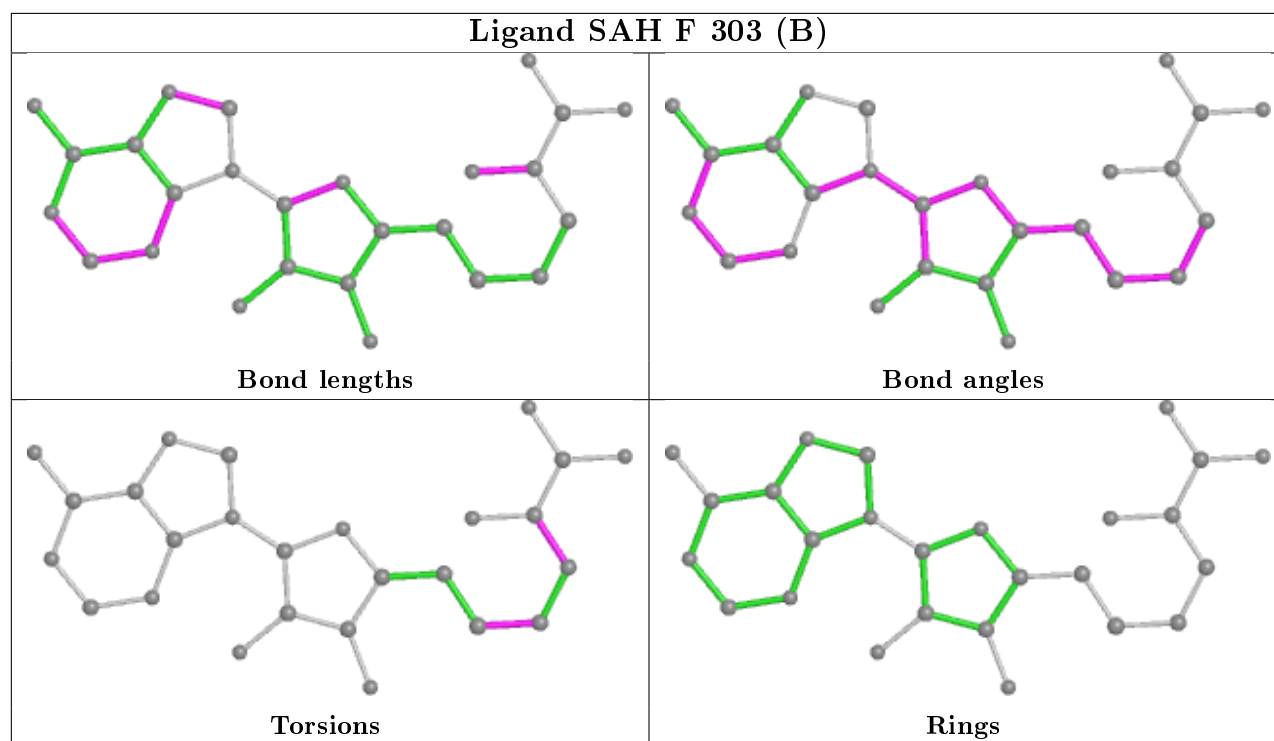
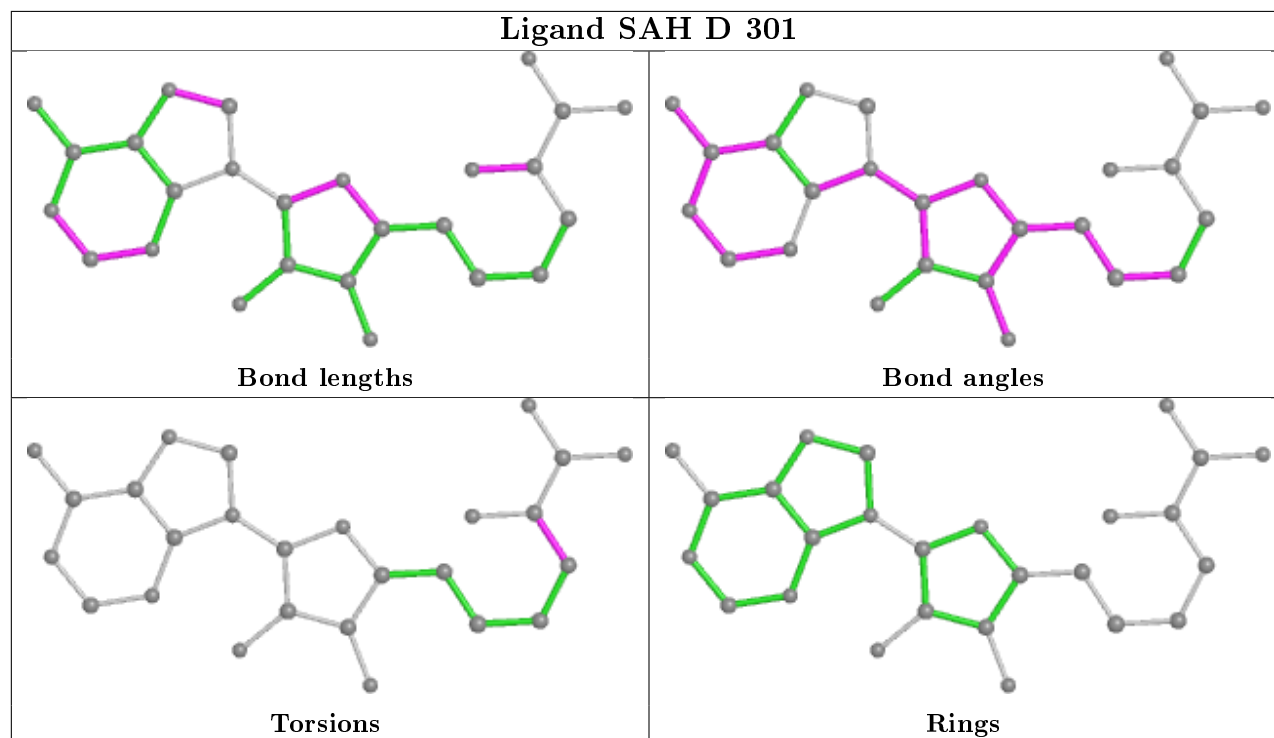
There are no ring outliers.

2 monomers are involved in 2 short contacts:

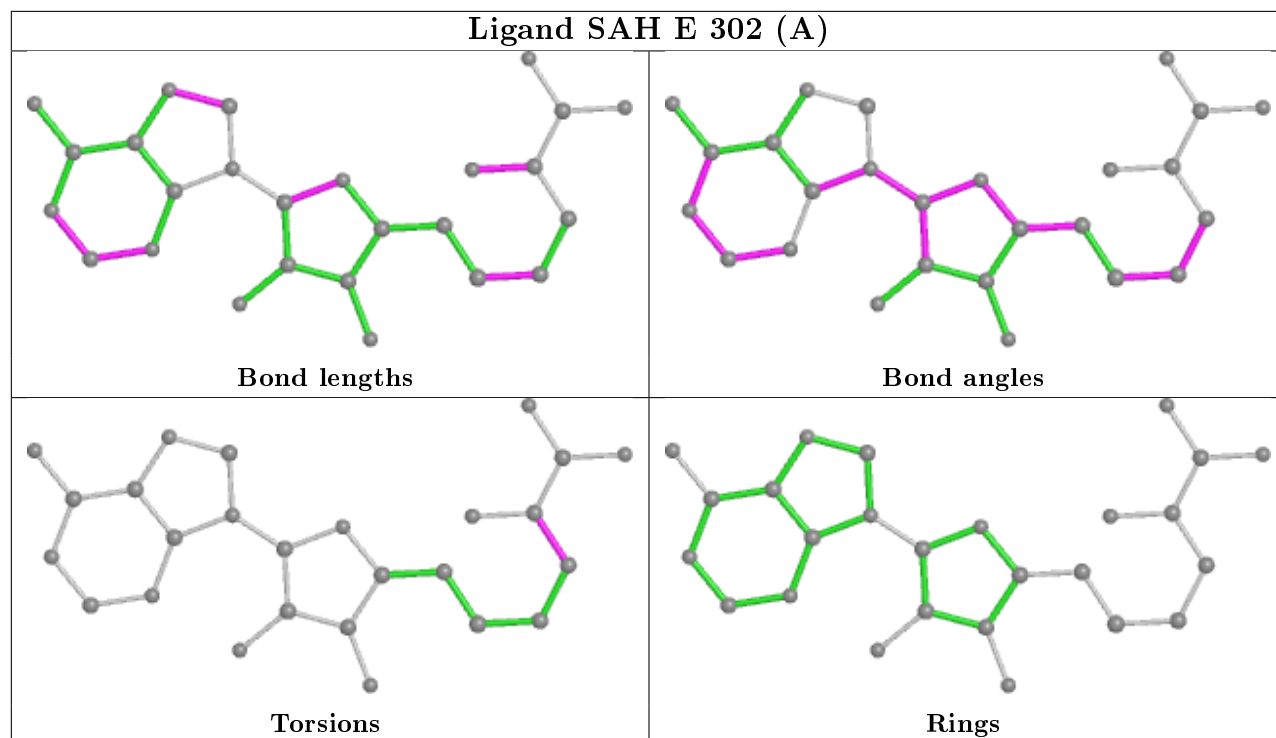
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	302[A]	SAH	1	0
2	E	302[B]	SAH	1	0

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

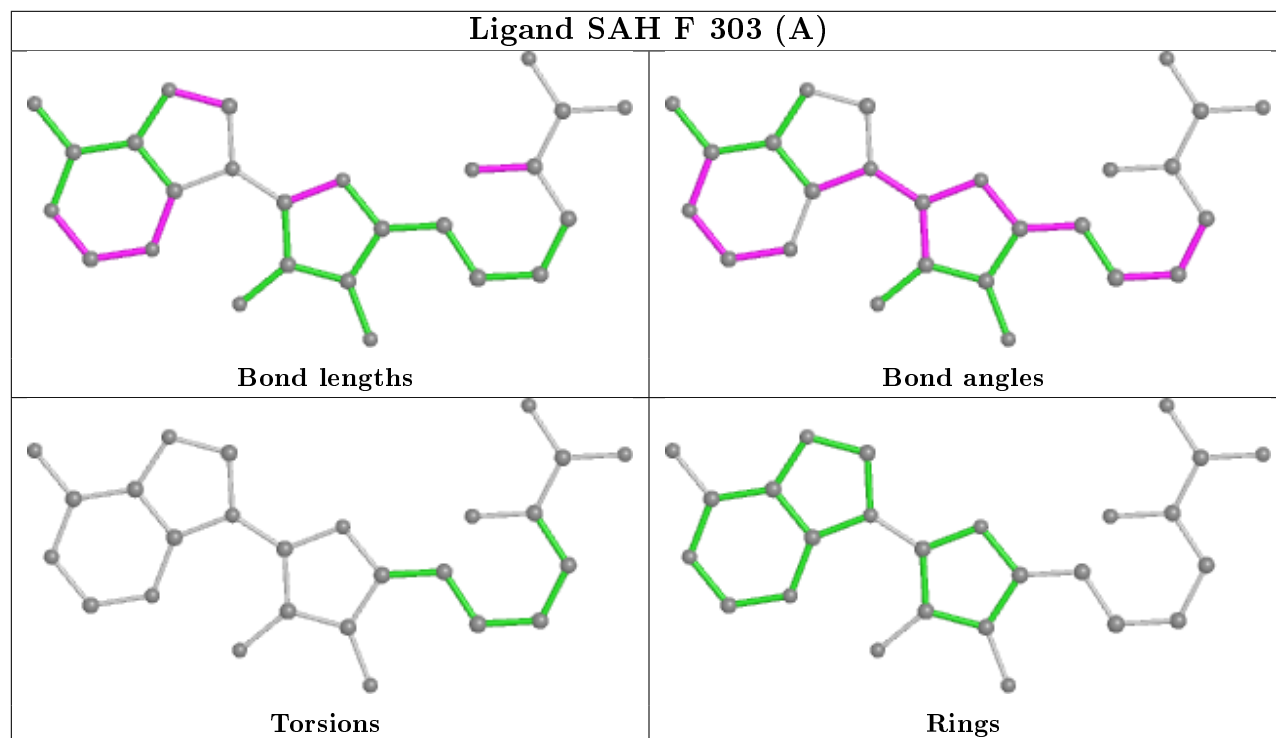
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

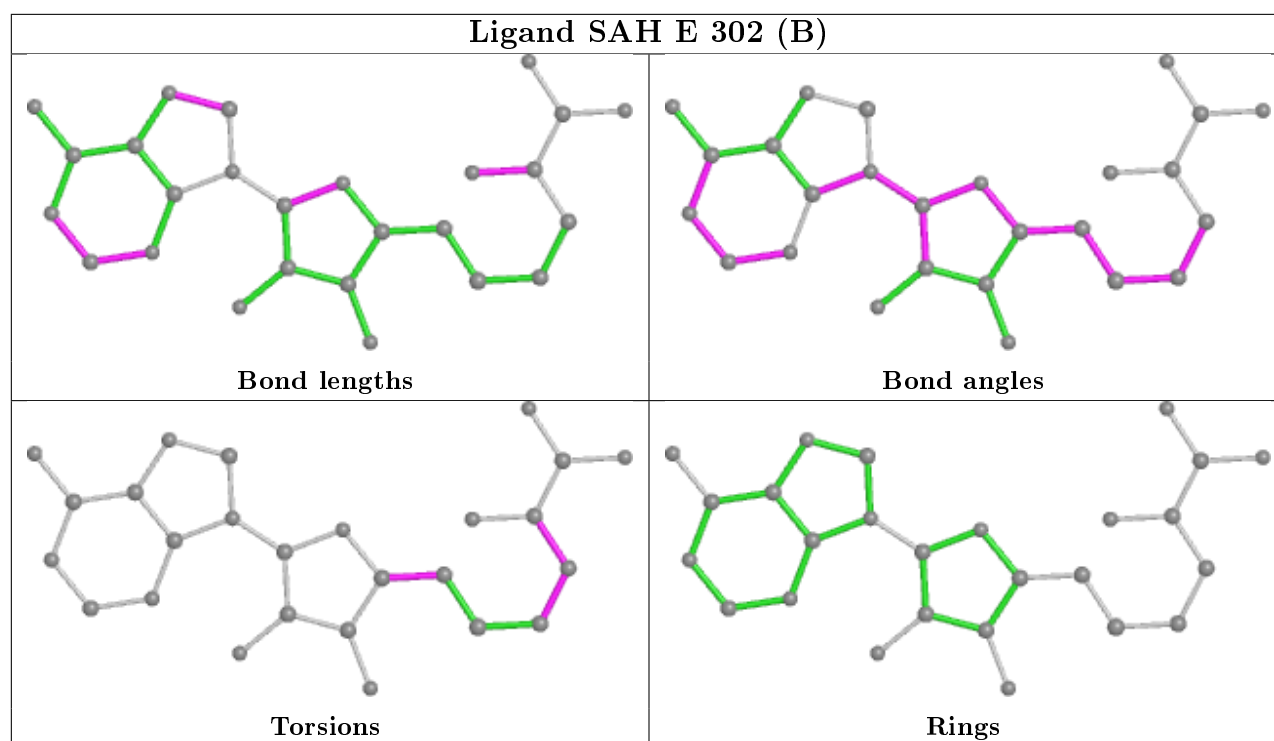


Ligand SAH E 302 (A)



Ligand SAH F 303 (A)





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.