



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:09 am BST

PDB ID : 452D
Title : ACRIDINE BINDING TO DNA
Authors : Thorpe, J.H.; Todd, A.K.; Cardin, C.J.
Deposited on : 1999-02-18
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

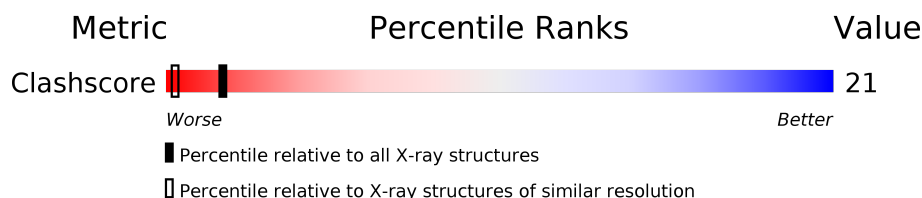
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

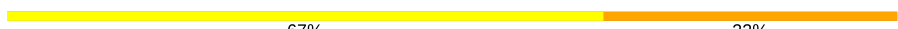
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3665 (1.60-1.60)

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	A	6	 67% 33%

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	9AD	A	3013	-	X	-	-
2	9AD	A	3015	-	X	-	-
3	MPD	A	3016	-	X	-	-

2 Entry composition [i](#)

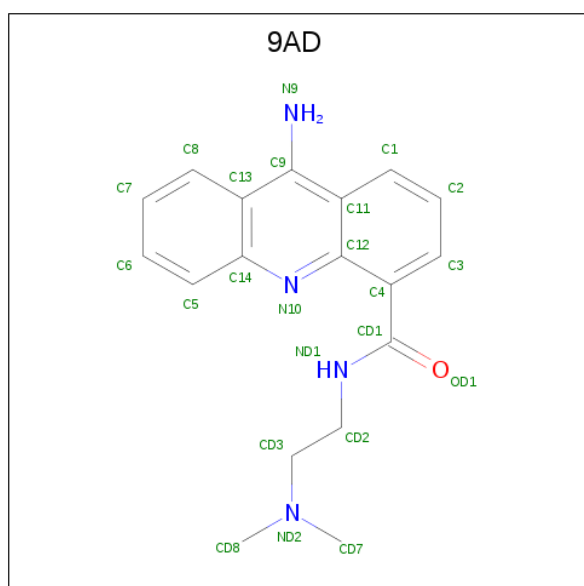
There are 4 unique types of molecules in this entry. The entry contains 321 atoms, of which 119 are hydrogens and 0 are deuteriums.

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 DNA chain called DNA (5'-D(*CP*GP*TP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	6	Total	C	H	N	O	P	0	0
			188	58	68	23	34	5		0

- Molecule 2 is 9-AMINO-(N-(2-DIMETHYLAMINO)ETHYL)ACRIDINE-4-CARBOXAMIDE (three-letter code: 9AD) (formula: C₁₈H₂₀N₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			44	18	21	4	1		
2	A	1	Total	C	H	N	O	0	0
			43	18	20	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(*CP*GP*TP*AP*CP*G)-3')

Chain A: 

G1001
G1002
T1003
A1004
C1005
G1006

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	30.16 Å 30.16 Å 39.69 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (16.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.202 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	321	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 9AD, MPD

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	2.20	2/134 (1.5%)	3.83	16/205 (7.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1002	DG	C1'-N9	9.32	1.61	1.49
1	A	1006	DG	C1'-N9	8.49	1.60	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1003	DT	C6-C5-C7	26.34	138.70	122.90
1	A	1003	DT	C4-C5-C7	-24.54	104.27	119.00
1	A	1002	DG	O4'-C1'-N9	-12.25	99.42	108.00
1	A	1006	DG	O4'-C1'-N9	-11.75	99.77	108.00
1	A	1004	DA	O4'-C1'-N9	-9.18	101.58	108.00
1	A	1003	DT	C2-N3-C4	8.70	132.42	127.20
1	A	1003	DT	N3-C2-O2	7.95	127.07	122.30
1	A	1005	DC	O4'-C1'-N1	7.29	113.10	108.00
1	A	1003	DT	C5-C6-N1	6.12	127.37	123.70
1	A	1006	DG	O4'-C4'-C3'	-5.77	102.19	104.50
1	A	1003	DT	N3-C4-C5	-5.39	111.97	115.20
1	A	1003	DT	C6-N1-C2	-5.36	118.62	121.30
1	A	1001	DC	C5'-C4'-O4'	5.29	119.35	109.30
1	A	1001	DC	N3-C4-N4	5.16	121.61	118.00
1	A	1003	DT	O4'-C1'-N1	-5.09	104.43	108.00
1	A	1001	DC	O4'-C1'-N1	-5.07	104.45	108.00

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	A	120	68	69	3	0
2	A	46	41	40	4	0
3	A	7	10	6	1	0
4	A	29	0	0	2	0
All	All	202	119	115	6	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 21.

All (6) 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:1002:DG:P	4:A:4027:HOH:O	2.27	0.92
2:A:3015:9AD:N10	2:A:3015:9AD:OD1	2.23	0.65
2:A:3013:9AD:N10	2:A:3013:9AD:OD1	2.50	0.44
1:A:1006:DG:N7	2:A:3015:9AD:ND2	2.66	0.44
2:A:3015:9AD:H3	3:A:3016:MPD:O4	2.19	0.43
1:A:1002:DG:H5''	4:A:4024:HOH:O	2.18	0.43

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	9AD	A	3015	-	25,25,25	1.78	6 (24%)	34,35,35	2.93	19 (55%)
3	MPD	A	3016	-	6,6,7	6.91	4 (66%)	7,8,10	5.38	5 (71%)
2	9AD	A	3013	-	25,25,25	2.02	9 (36%)	34,35,35	3.97	15 (44%)

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	9AD	A	3015	-	-	9/10/10/10	0/3/3/3
3	MPD	A	3016	-	-	3/4/4/5	-
2	9AD	A	3013	-	-	8/10/10/10	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3016	MPD	C3-C4	-14.25	1.24	1.52
3	A	3016	MPD	C3-C2	-6.73	1.30	1.53
2	A	3013	9AD	CD1-ND1	5.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3016	MPD	O2-C2	-5.20	1.31	1.44
2	A	3015	9AD	C4-CD1	-4.39	1.43	1.50
2	A	3013	9AD	CD3-CD2	3.36	1.61	1.51
2	A	3015	9AD	OD1-CD1	3.32	1.30	1.23
2	A	3015	9AD	C7-C6	3.19	1.46	1.38
2	A	3013	9AD	C9-N9	3.08	1.43	1.33
2	A	3013	9AD	C4-CD1	-2.79	1.45	1.50
2	A	3015	9AD	CD3-CD2	-2.78	1.43	1.51
2	A	3013	9AD	CD7-ND2	2.75	1.54	1.46
2	A	3015	9AD	C5-C14	-2.65	1.37	1.41
2	A	3013	9AD	C7-C6	2.56	1.44	1.38
3	A	3016	MPD	O4-C4	-2.50	1.29	1.42
2	A	3015	9AD	C3-C4	-2.21	1.34	1.38
2	A	3013	9AD	C4-C12	-2.13	1.40	1.43
2	A	3013	9AD	C12-N10	-2.06	1.31	1.35
2	A	3013	9AD	CD8-ND2	2.01	1.52	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3016	MPD	O4-C4-C3	10.08	138.34	111.39
2	A	3013	9AD	C12-N10-C14	8.69	126.92	117.02
2	A	3013	9AD	C13-C14-N10	-7.94	115.92	123.35
2	A	3013	9AD	CD7-ND2-CD3	7.55	140.67	110.74
2	A	3013	9AD	CD3-CD2-ND1	7.51	125.97	111.60
3	A	3016	MPD	O2-C2-C3	7.13	134.39	107.88
2	A	3013	9AD	CD2-CD3-ND2	6.34	135.15	113.08
2	A	3015	9AD	C12-N10-C14	6.16	124.04	117.02
2	A	3013	9AD	C5-C14-N10	6.14	126.82	119.09
2	A	3013	9AD	OD1-CD1-ND1	-5.47	111.70	122.61
2	A	3013	9AD	CD2-ND1-CD1	5.34	134.26	122.08
2	A	3013	9AD	C11-C9-N9	-5.28	114.99	120.59
2	A	3013	9AD	C1-C11-C9	5.19	129.89	122.83
2	A	3015	9AD	C1-C11-C9	5.16	129.84	122.83
2	A	3015	9AD	C13-C14-N10	-4.94	118.72	123.35
2	A	3013	9AD	C7-C8-C13	4.72	127.44	120.89
3	A	3016	MPD	O2-C2-CM	-4.71	92.95	108.08
2	A	3015	9AD	C6-C5-C14	4.60	126.70	120.08
2	A	3015	9AD	C7-C8-C13	4.55	127.21	120.89
2	A	3013	9AD	C13-C9-C11	4.52	123.73	118.73
2	A	3015	9AD	CD3-CD2-ND1	4.52	120.25	111.60
3	A	3016	MPD	O2-C2-C1	-4.37	94.07	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3015	9AD	C4-CD1-ND1	4.19	121.96	116.30
2	A	3015	9AD	C6-C7-C8	-3.66	115.31	120.44
2	A	3015	9AD	C5-C14-N10	3.59	123.61	119.09
2	A	3015	9AD	C13-C9-C11	3.56	122.67	118.73
2	A	3015	9AD	C3-C4-C12	3.38	122.52	118.37
2	A	3015	9AD	C8-C13-C9	3.18	127.15	122.83
2	A	3013	9AD	C6-C5-C14	2.95	124.33	120.08
2	A	3013	9AD	C6-C7-C8	-2.90	116.37	120.44
2	A	3015	9AD	CD2-CD3-ND2	2.78	122.77	113.08
2	A	3015	9AD	OD1-CD1-ND1	-2.74	117.14	122.61
2	A	3015	9AD	C3-C4-CD1	2.68	122.92	118.52
2	A	3015	9AD	C8-C13-C14	-2.61	115.40	118.33
2	A	3015	9AD	C13-C9-N9	-2.43	118.01	120.59
2	A	3013	9AD	C11-C12-N10	-2.31	120.12	123.31
3	A	3016	MPD	CM-C2-C3	-2.28	104.39	111.42
2	A	3015	9AD	C4-C12-N10	-2.18	117.61	120.30
2	A	3015	9AD	C1-C11-C12	-2.05	114.72	118.98

There are no chirality outliers.

All (20) torsion outliers are listed below:

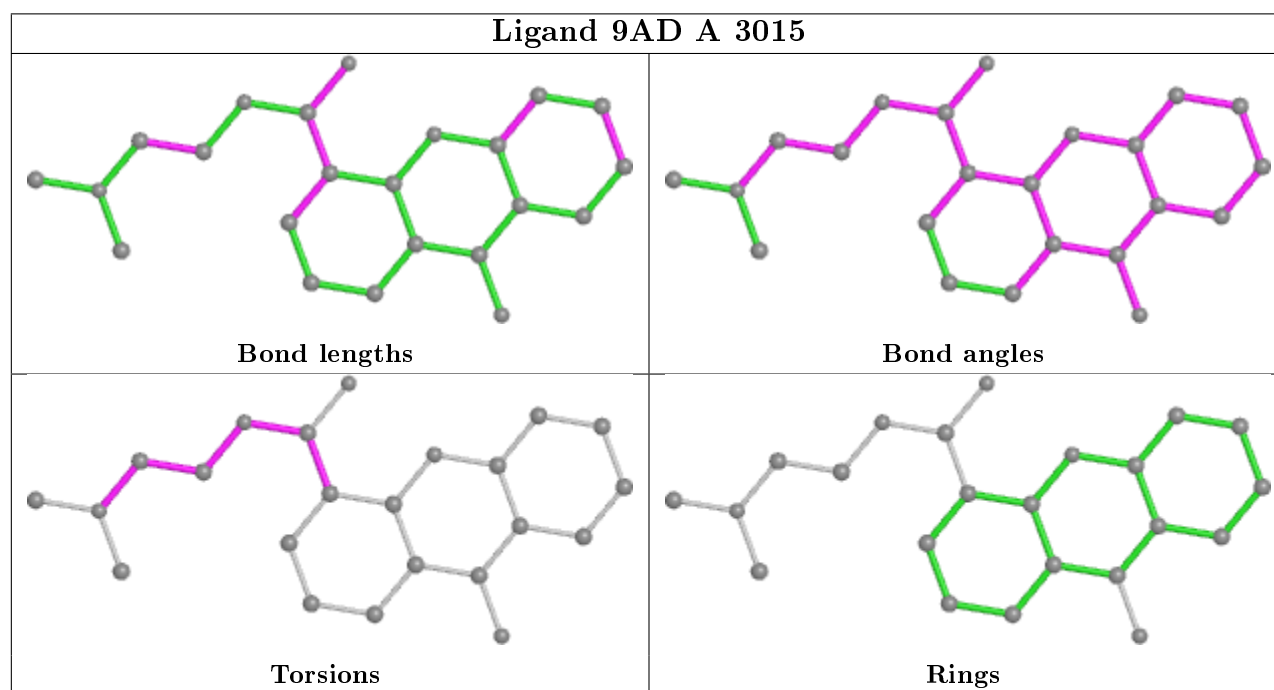
Mol	Chain	Res	Type	Atoms
2	A	3015	9AD	C3-C4-CD1-OD1
2	A	3015	9AD	C3-C4-CD1-ND1
2	A	3015	9AD	C12-C4-CD1-OD1
2	A	3015	9AD	C12-C4-CD1-ND1
2	A	3015	9AD	C4-CD1-ND1-CD2
2	A	3015	9AD	CD3-CD2-ND1-CD1
2	A	3015	9AD	ND1-CD2-CD3-ND2
3	A	3016	MPD	O2-C2-C3-C4
2	A	3013	9AD	C4-CD1-ND1-CD2
2	A	3013	9AD	CD3-CD2-ND1-CD1
2	A	3013	9AD	CD2-CD3-ND2-CD8
2	A	3015	9AD	OD1-CD1-ND1-CD2
2	A	3015	9AD	CD2-CD3-ND2-CD7
2	A	3013	9AD	ND1-CD2-CD3-ND2
2	A	3013	9AD	C3-C4-CD1-OD1
2	A	3013	9AD	C12-C4-CD1-OD1
3	A	3016	MPD	C1-C2-C3-C4
2	A	3013	9AD	C3-C4-CD1-ND1
3	A	3016	MPD	CM-C2-C3-C4
2	A	3013	9AD	C12-C4-CD1-ND1

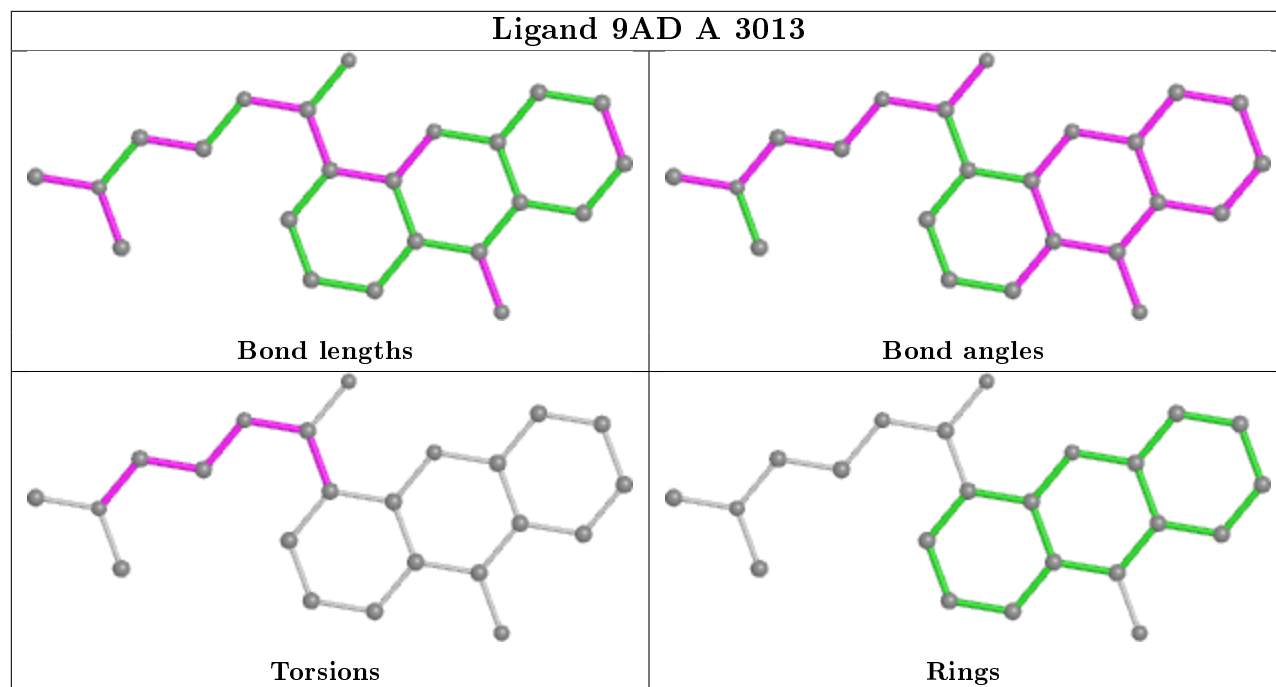
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3015	9AD	3	0
3	A	3016	MPD	1	0
2	A	3013	9AD	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.





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.