



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 30, 2020 – 02:12 pm BST

PDB ID : 198D  
Title : A TRIGONAL FORM OF THE IDARUBICIN-D(CGATCG) COMPLEX:  
CRYSTAL AND MOLECULAR STRUCTURE AT 2.0 ANGSTROMS RES-  
OLUTION  
Authors : Dautant, A.; Langlois D'Estaintot, B.; Gallois, B.; Brown, T.; Hunter, W.N.  
Deposited on : 1994-11-28  
Resolution : 1.97 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 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)  
Xtrriage (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

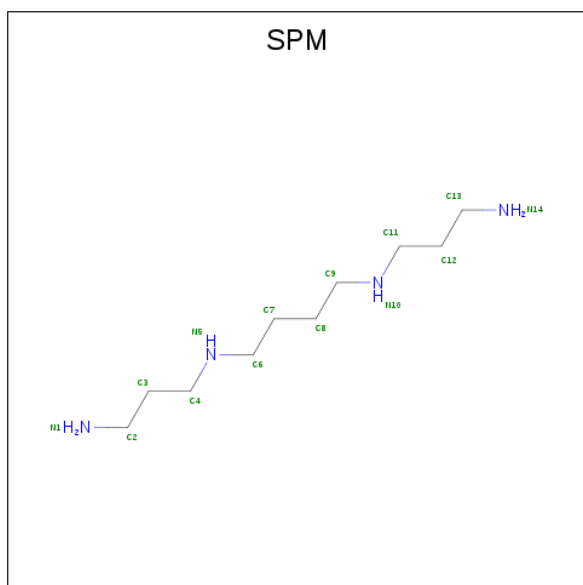




Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			36	26	1	9		
2	D	1	Total	C	N	O	0	0
			36	26	1	9		

- Molecule 3 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	10	4		

- Molecule 4 is water.

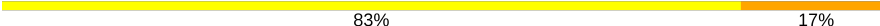
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	38	Total	O	0	0
			38	38		
4	C	37	Total	O	0	0
			37	37		
4	D	38	Total	O	0	0
			38	38		

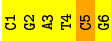
### 3 Residue-property plots

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.

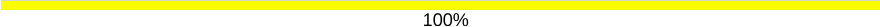
Note EDS was not executed.

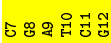
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*TP\*CP\*G)-3')

Chain A:  83% 17%


 C1  
C2  
A3  
T4  
C5  
G6

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

Chain B:  100%


 C7  
G8  
A9  
T10  
C11  
G12

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

Chain C:  83% 17%

 C13  
G14  
A15  
T16  
C17  
G18

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

Chain D:  83% 17%

 C19  
G20  
A21  
T22  
C23  
G24

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.00Å 53.00Å 33.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.00 – 1.97	Depositor
% Data completeness (in resolution range)	(Not available) (18.00-1.97)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	NUCLSQ	Depositor
R, $R_{free}$	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: DM5, SPM

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	2.57	7/134 (5.2%)	2.87	15/205 (7.3%)
1	B	2.18	6/134 (4.5%)	3.24	25/205 (12.2%)
1	C	2.54	8/134 (6.0%)	4.03	37/205 (18.0%)
1	D	2.34	6/134 (4.5%)	3.24	23/205 (11.2%)
All	All	2.41	27/536 (5.0%)	3.37	100/820 (12.2%)

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	C	0	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	DG	C5'-C4'	7.17	1.59	1.51
1	A	2	DG	C6-N1	-7.10	1.34	1.39
1	A	6	DG	N1-C2	-6.85	1.32	1.37
1	C	16	DT	C2-O2	6.84	1.27	1.22
1	C	16	DT	C4-O4	6.64	1.29	1.23

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	DC	O4'-C1'-N1	24.58	125.21	108.00
1	B	12	DG	O4'-C1'-N9	15.12	118.58	108.00
1	C	14	DG	O4'-C1'-N9	14.04	117.83	108.00
1	A	5	DC	O4'-C1'-N1	13.33	117.33	108.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	23	DC	O4'-C1'-N1	12.46	116.72	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	17	DC	Sidechain

## 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	0	69	3	0
1	B	120	0	69	0	0
1	C	120	0	69	0	0
1	D	120	0	69	1	0
2	A	36	0	25	0	0
2	B	36	0	25	1	0
2	D	72	0	50	1	0
3	A	14	0	26	4	0
4	A	47	0	0	1	0
4	B	38	0	0	0	0
4	C	37	0	0	0	0
4	D	38	0	0	2	0
All	All	798	0	402	7	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 7.

The worst 5 of 7 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
3:A:29:SPM:H22	4:A:95:HOH:O	1.83	0.78
1:A:5:DC:H6	3:A:29:SPM:HN0	1.33	0.76
1:A:5:DC:H2'	3:A:29:SPM:H122	1.72	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:DM5:H4	4:D:81:HOH:O	2.02	0.60
1:A:5:DC:C2'	3:A:29:SPM:H122	2.36	0.55

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](#)

5 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
3	SPM	A	29	-	13,13,13	0.90	0	12,12,12	0.48	0
2	DM5	A	25	-	38,40,40	2.25	17 (44%)	51,63,63	2.00	16 (31%)
2	DM5	B	26	-	38,40,40	2.15	14 (36%)	51,63,63	2.08	16 (31%)
2	DM5	D	28	-	38,40,40	2.48	20 (52%)	51,63,63	2.03	16 (31%)
2	DM5	D	27	-	38,40,40	2.34	15 (39%)	51,63,63	2.08	15 (29%)

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	SPM	A	29	-	-	6/11/11/11	-
2	DM5	A	25	-	-	0/10/56/56	0/5/5/5
2	DM5	B	26	-	-	1/10/56/56	0/5/5/5
2	DM5	D	28	-	-	0/10/56/56	0/5/5/5
2	DM5	D	27	-	-	2/10/56/56	0/5/5/5

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	28	DM5	C15-C16	-5.82	1.43	1.51
2	B	26	DM5	O13-C13	5.67	1.33	1.21
2	D	28	DM5	O13-C13	5.59	1.33	1.21
2	A	25	DM5	O4'-C4'	-5.47	1.30	1.43
2	D	27	DM5	O4'-C4'	-5.00	1.31	1.43

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	27	DM5	C4-C5-C20	5.71	125.61	119.26
2	B	26	DM5	O4'-C4'-C5'	5.24	121.27	109.67
2	A	25	DM5	C2'-C3'-C4'	-4.92	102.61	110.04
2	D	28	DM5	C4-C5-C20	4.72	124.51	119.26
2	B	26	DM5	O13-C13-C12	-4.69	109.61	119.88

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

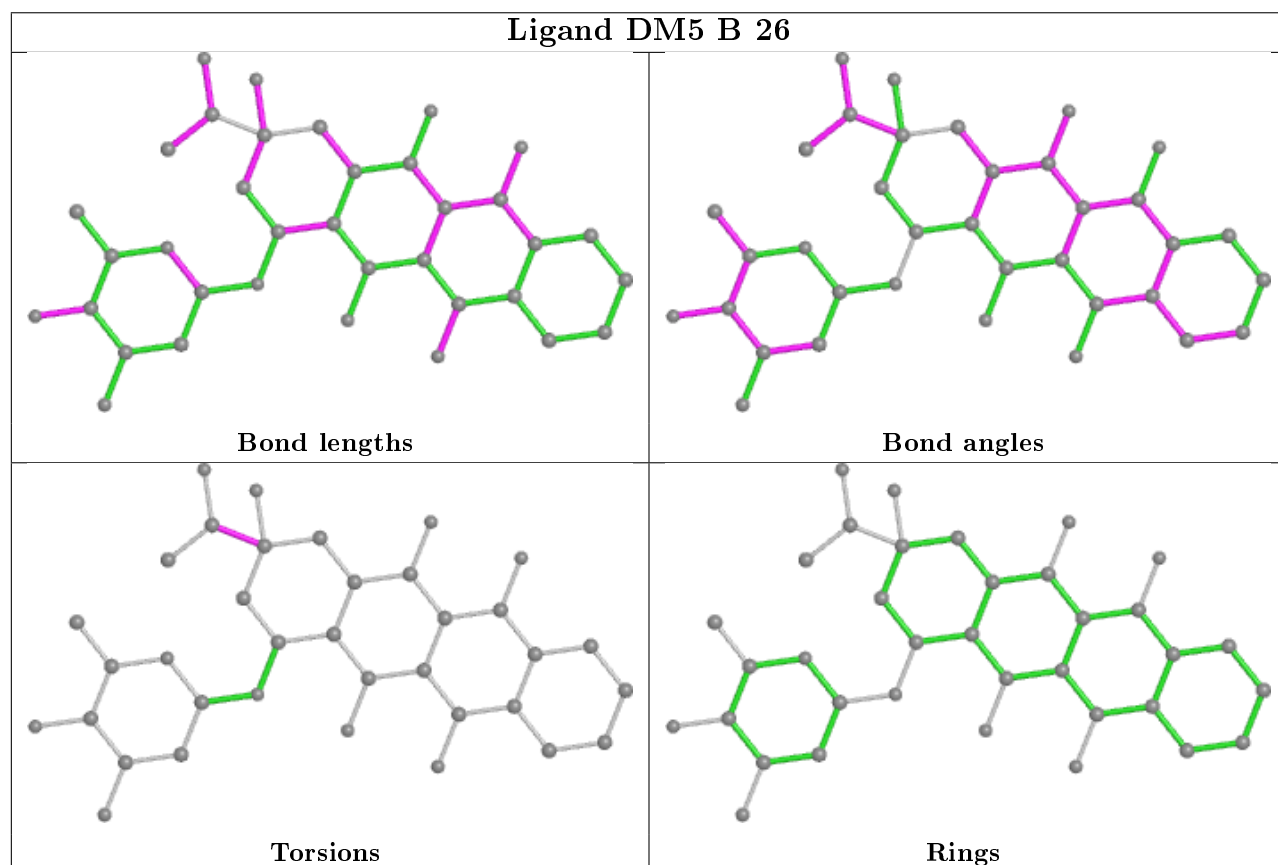
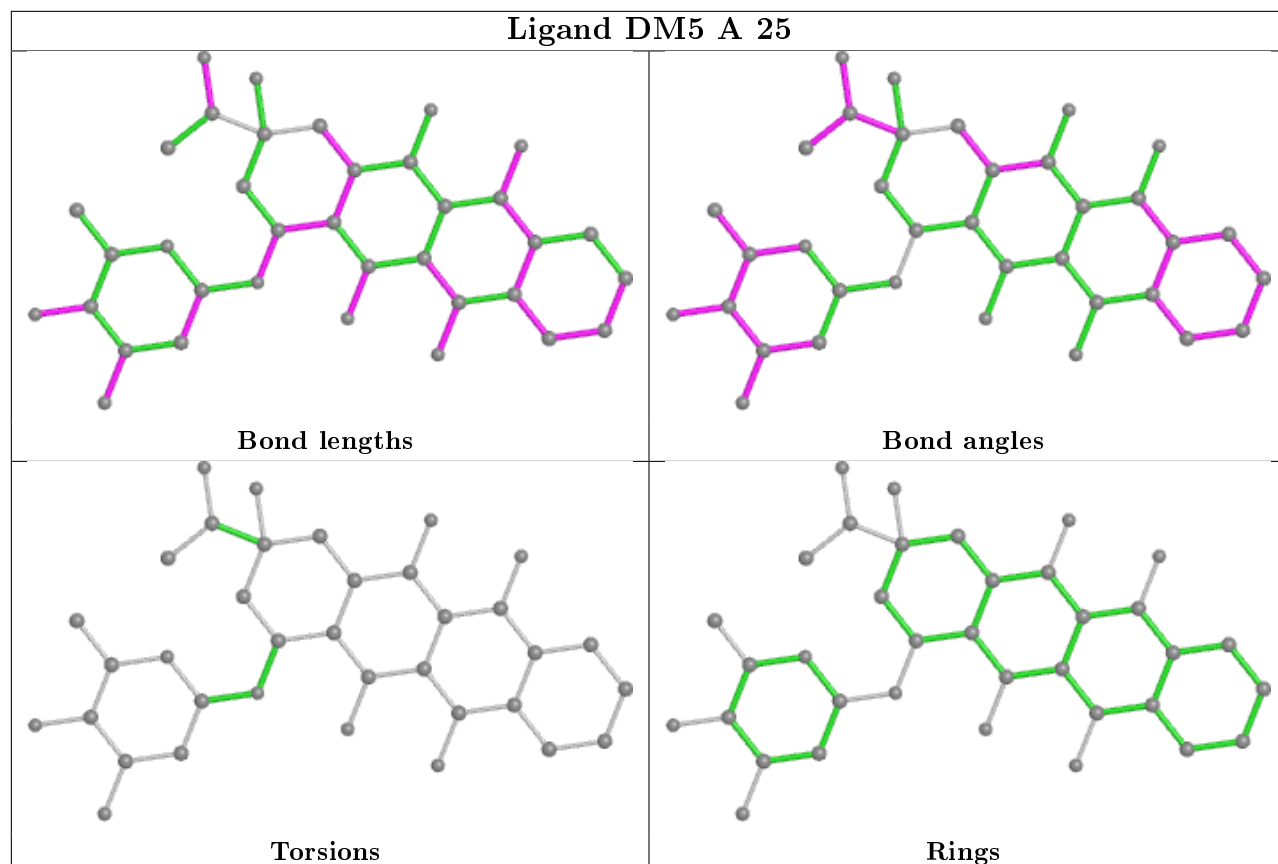
Mol	Chain	Res	Type	Atoms
3	A	29	SPM	C7-C8-C9-N10
3	A	29	SPM	C6-C7-C8-C9
3	A	29	SPM	C8-C9-N10-C11
3	A	29	SPM	C2-C3-C4-N5
2	B	26	DM5	O12-C12-C13-C14

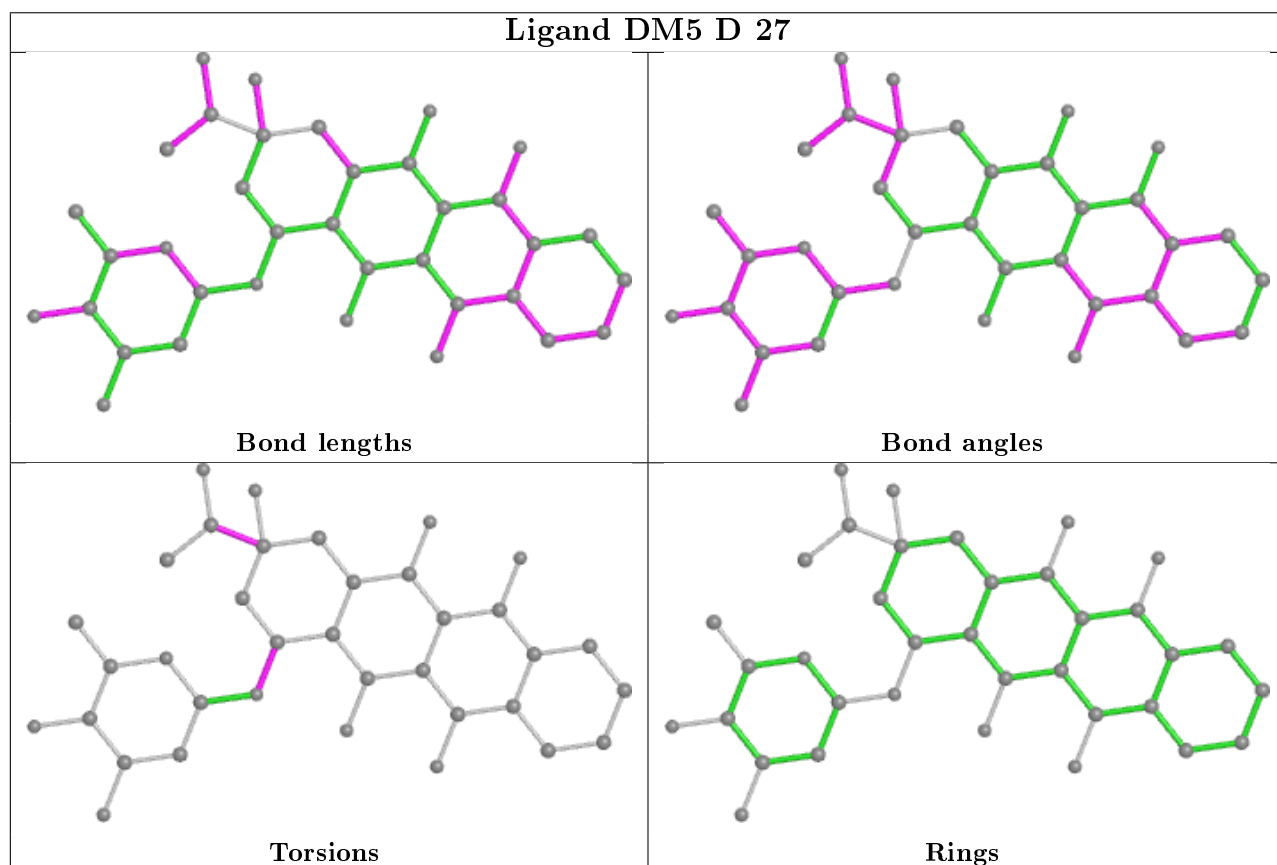
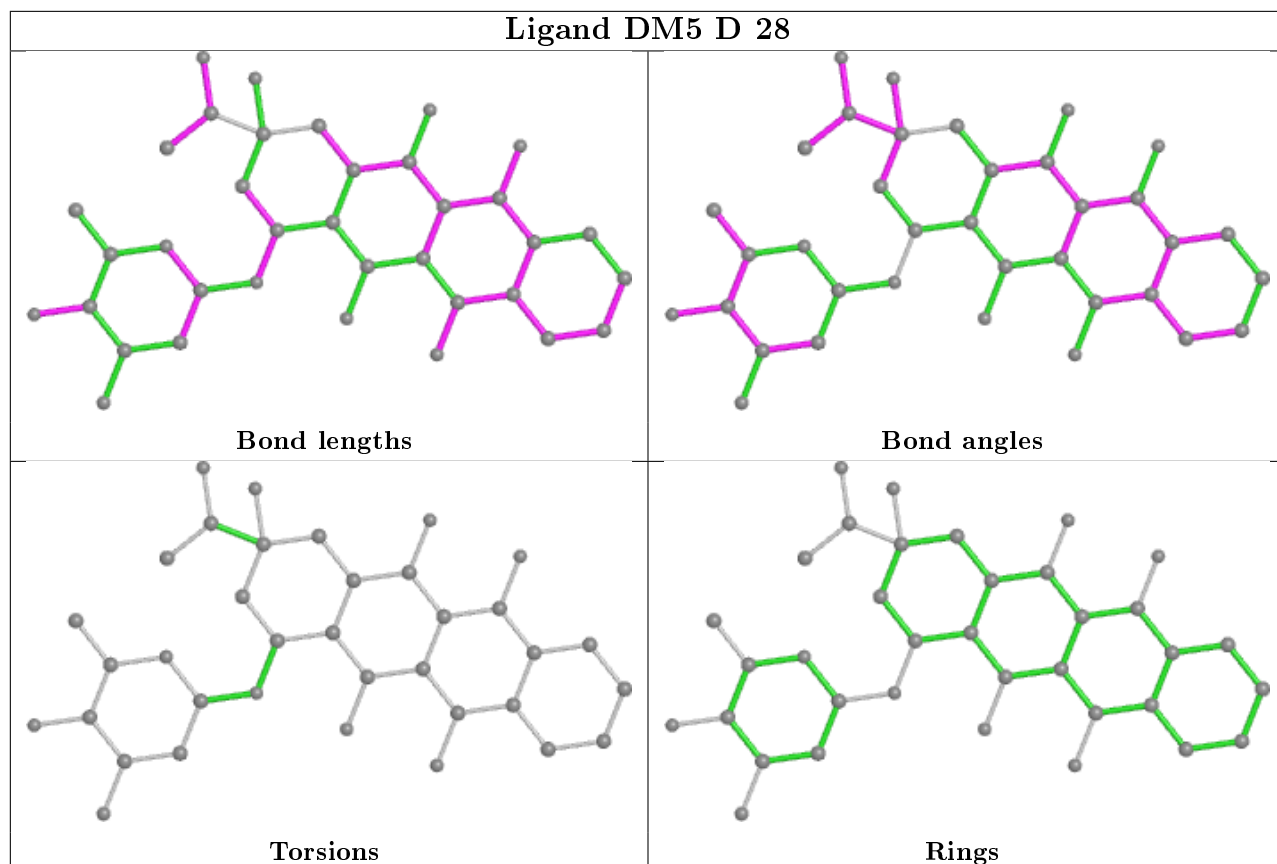
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	29	SPM	4	0
2	B	26	DM5	1	0
2	D	27	DM5	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

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

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.