



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:35 PM BST

PDB ID : 4DDY  
Title : CTX-M-9 class A beta-lactamase complexed with compound 10  
Authors : Nichols, D.A.; Chen, Y.  
Deposited on : 2012-01-19  
Resolution : 1.36 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](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.

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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) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

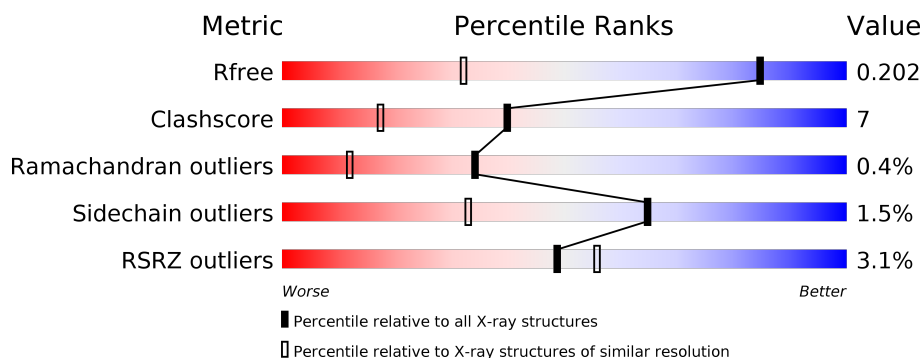
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.36 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))
$R_{free}$	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	263	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5% ..</div> </div> </div>
1	B	263	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>6% .</div> </div> </div>

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	DN6	B	306	-	-	X	-
2	DN6	B	307	-	-	X	X

## 2 Entry composition [i](#)

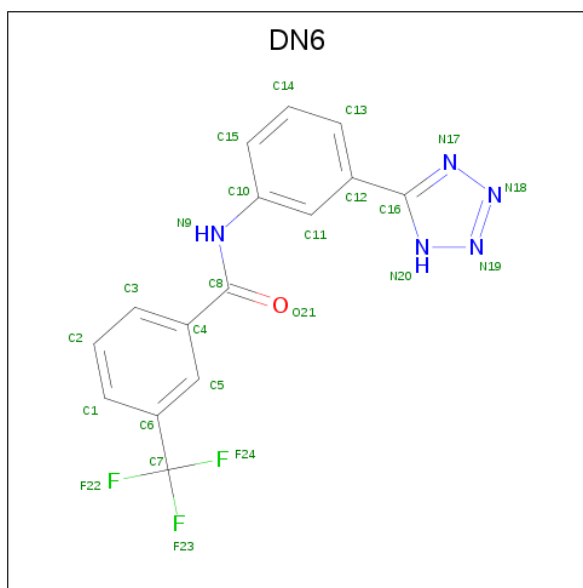
There are 4 unique types of molecules in this entry. The entry contains 4760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	12	6	0
			1981	1228	356	391	6			
1	B	261	Total	C	N	O	S	0	3	0
			1960	1217	352	385	6			

- Molecule 2 is N-[3-(1H-tetrazol-5-yl)phenyl]-3-(trifluoromethyl)benzamide (three-letter code: DN6) (formula: C<sub>15</sub>H<sub>10</sub>F<sub>3</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	15	3	5	1		
2	A	1	Total	C	F	N	O	0	0
			24	15	3	5	1		
2	A	1	Total	C	F	N	O	0	0
			24	15	3	5	1		
2	A	1	Total	C	F	N	O	0	0
			24	15	3	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			24	15	3	5	1		
2	B	1	Total	C	F	N	O	0	0
			24	15	3	5	1		
2	B	1	Total	C	F	N	O	0	0
			24	15	3	5	1		
2	B	1	Total	C	F	N	O	0	0
			24	15	3	5	1		
2	B	1	Total	C	F	N	O	0	0
			24	15	3	5	1		
2	B	1	Total	C	F	N	O	0	0
			24	15	3	5	1		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	250	Total 250	O 250	0	0
4	B	269	Total 269	O 269	0	0

### 3 Residue-property plots [i](#)

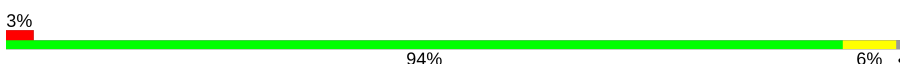
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-lactamase

Chain A: 



#### • Molecule 1: Beta-lactamase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.01Å 107.11Å 47.51Å 90.00° 102.11° 90.00°	Depositor
Resolution (Å)	50.00 – 1.36 25.33 – 1.36	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.36) 98.7 (25.33-1.36)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.171 , 0.205 0.169 , 0.202	Depositor DCC
$R_{free}$ test set	4627 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.1	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 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: DN6, DMS

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	0.75	2/2019 (0.1%)	0.83	1/2747 (0.0%)
1	B	0.71	0/1998	0.81	2/2717 (0.1%)
All	All	0.73	2/4017 (0.0%)	0.82	3/5464 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158[A]	GLU	CG-CD	-5.34	1.44	1.51
1	A	158[B]	GLU	CG-CD	-5.34	1.44	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	184	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	204	ARG	NE-CZ-NH2	5.37	122.99	120.30

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	1981	0	2000	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1960	0	1988	33	0
2	A	96	0	40	0	0
2	B	192	0	80	34	0
3	A	8	0	12	2	0
3	B	4	0	6	3	0
4	A	250	0	0	6	0
4	B	269	0	0	10	0
All	All	4760	0	4126	61	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.

All (61) 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:B:88:LYS:HD2	2:B:306:DN6:C5	1.40	1.49
1:B:88:LYS:CD	2:B:306:DN6:C5	2.28	1.12
1:A:230[B]:THR:HG22	4:A:616:HOH:O	1.54	1.07
1:B:88:LYS:HE3	2:B:306:DN6:F24	1.47	1.04
1:B:88:LYS:HD2	2:B:306:DN6:H2	1.02	0.98
1:B:88:LYS:CD	2:B:306:DN6:H2	1.95	0.94
1:B:61:ARG:H	2:B:307:DN6:C1	1.82	0.92
1:B:61:ARG:HA	2:B:307:DN6:H1	1.50	0.91
1:B:61:ARG:HA	2:B:307:DN6:C1	2.03	0.89
1:B:89:GLN:H	2:B:306:DN6:H10	1.24	0.86
1:B:186:MET:HE1	4:B:582:HOH:O	1.76	0.84
1:B:61:ARG:N	2:B:307:DN6:C1	2.43	0.79
1:B:61:ARG:CA	2:B:307:DN6:C1	2.62	0.78
1:B:269:GLN:HG2	4:B:605:HOH:O	1.83	0.77
2:B:307:DN6:H4	4:B:424:HOH:O	1.86	0.74
1:B:110:GLU:HG3	1:B:111[A]:LYS:HD3	1.70	0.73
1:B:88:LYS:HE3	2:B:306:DN6:C7	2.20	0.70
1:B:62:GLY:H	2:B:307:DN6:C2	2.06	0.69
1:B:61:ARG:N	2:B:307:DN6:C2	2.57	0.68
2:B:301:DN6:H2	4:B:596:HOH:O	1.95	0.66
3:B:309:DMS:H21	4:B:426:HOH:O	1.96	0.66
1:B:88:LYS:CE	2:B:306:DN6:C7	2.74	0.66
2:B:304:DN6:H9	2:B:304:DN6:O21	1.95	0.66
1:A:230[B]:THR:CG2	4:A:616:HOH:O	2.24	0.65
1:A:284:ARG:NH2	1:A:288:GLU:OE2	2.30	0.65
1:B:88:LYS:CE	2:B:306:DN6:F24	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLY:N	2:B:307:DN6:H4	2.12	0.64
1:A:284:ARG:HH21	1:A:284:ARG:CG	2.12	0.62
1:B:62:GLY:H	2:B:307:DN6:H4	1.62	0.62
1:B:88:LYS:CD	2:B:306:DN6:C6	2.78	0.61
1:B:186:MET:CE	4:B:582:HOH:O	2.43	0.60
3:B:309:DMS:H23	4:B:562:HOH:O	2.00	0.60
1:B:61:ARG:CA	2:B:307:DN6:C2	2.79	0.60
2:B:308:DN6:H6	2:B:308:DN6:O21	2.05	0.57
1:B:61:ARG:H	2:B:307:DN6:C6	2.18	0.56
1:A:284:ARG:HG3	1:A:284:ARG:NH2	2.20	0.56
1:A:284:ARG:HH21	1:A:284:ARG:HG3	1.73	0.54
2:B:302:DN6:O21	2:B:302:DN6:H6	2.07	0.53
1:A:111:LYS:NZ	4:A:606:HOH:O	2.38	0.53
1:B:27:SER:N	1:B:30:GLN:HB2	2.24	0.51
1:B:61:ARG:HA	2:B:307:DN6:C2	2.41	0.51
2:B:307:DN6:C2	4:B:424:HOH:O	2.52	0.50
1:B:62:GLY:N	2:B:307:DN6:C2	2.73	0.50
1:A:91:LEU:HB3	1:A:120:ALA:HB2	1.93	0.49
3:B:309:DMS:C2	4:B:562:HOH:O	2.58	0.49
1:B:88:LYS:HE2	2:B:306:DN6:F23	2.02	0.49
1:A:284:ARG:CG	1:A:284:ARG:NH2	2.73	0.49
1:B:88:LYS:CE	2:B:306:DN6:F23	2.50	0.49
2:B:302:DN6:O21	2:B:302:DN6:C15	2.60	0.48
1:A:188[A]:GLN:NE2	3:A:306:DMS:S	2.86	0.48
2:B:304:DN6:O21	2:B:304:DN6:C11	2.62	0.47
1:A:271[A]:ASN:ND2	4:A:527:HOH:O	2.48	0.47
1:A:254:GLN:NE2	4:A:573:HOH:O	2.44	0.46
1:A:188[A]:GLN:CG	4:A:600:HOH:O	2.64	0.46
1:B:91:LEU:HB3	1:B:120:ALA:HB2	1.97	0.45
1:B:61:ARG:H	2:B:307:DN6:C2	2.20	0.42
1:A:271[A]:ASN:H	1:A:271[A]:ASN:HD22	1.66	0.42
1:B:269:GLN:HG2	4:B:489:HOH:O	2.20	0.41
1:A:188[A]:GLN:CD	3:A:306:DMS:S	2.99	0.41
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.76	0.41

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	264/263 (100%)	257 (97%)	6 (2%)	1 (0%)	34	12
1	B	262/263 (100%)	257 (98%)	4 (2%)	1 (0%)	34	12
All	All	526/526 (100%)	514 (98%)	10 (2%)	2 (0%)	34	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	B	103	VAL

### 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	208/204 (102%)	202 (97%)	6 (3%)	42	10
1	B	206/204 (101%)	205 (100%)	1 (0%)	88	74
All	All	414/408 (102%)	407 (98%)	7 (2%)	65	28

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	130	SER
1	A	271[A]	ASN
1	A	271[B]	ASN

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Mol	Chain	Res	Type
1	A	273	GLU
1	A	284	ARG
1	B	130	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	254	GLN
1	B	30	GLN
1	B	89	GLN
1	B	141	GLN
1	B	269	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 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	DN6	B	308	-	26,26,26	1.93	6 (23%)	37,37,37	2.02	8 (21%)
2	DN6	A	302	-	26,26,26	1.65	4 (15%)	37,37,37	2.10	7 (18%)
2	DN6	B	304	-	26,26,26	1.62	4 (15%)	37,37,37	1.75	6 (16%)
2	DN6	B	307	-	26,26,26	1.90	6 (23%)	37,37,37	2.50	15 (40%)
2	DN6	B	303	-	26,26,26	1.36	4 (15%)	37,37,37	1.96	8 (21%)
2	DN6	B	306	-	26,26,26	1.66	4 (15%)	37,37,37	1.91	7 (18%)
2	DN6	A	304	-	26,26,26	1.76	5 (19%)	37,37,37	1.74	5 (13%)
2	DN6	A	303	-	26,26,26	1.77	5 (19%)	37,37,37	1.66	6 (16%)
3	DMS	B	309	-	3,3,3	2.60	1 (33%)	3,3,3	0.76	0
2	DN6	B	302	-	26,26,26	1.67	4 (15%)	37,37,37	1.88	6 (16%)
2	DN6	B	305	-	26,26,26	1.78	6 (23%)	37,37,37	1.59	5 (13%)
3	DMS	A	305	-	3,3,3	2.71	1 (33%)	3,3,3	0.45	0
2	DN6	B	301	-	26,26,26	1.81	5 (19%)	37,37,37	1.66	6 (16%)
2	DN6	A	301	-	26,26,26	1.63	5 (19%)	37,37,37	2.62	9 (24%)
3	DMS	A	306	-	3,3,3	2.70	1 (33%)	3,3,3	0.26	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	DN6	B	308	-	-	0/18/18/18	0/3/3/3
2	DN6	A	302	-	-	0/18/18/18	0/3/3/3
2	DN6	B	304	-	-	0/18/18/18	0/3/3/3
2	DN6	B	307	-	-	2/18/18/18	0/3/3/3
2	DN6	B	303	-	-	0/18/18/18	0/3/3/3
2	DN6	B	306	-	-	0/18/18/18	0/3/3/3
2	DN6	A	304	-	-	1/18/18/18	0/3/3/3
2	DN6	A	303	-	-	0/18/18/18	0/3/3/3
2	DN6	B	302	-	-	0/18/18/18	0/3/3/3
2	DN6	B	305	-	-	0/18/18/18	0/3/3/3
2	DN6	B	301	-	-	0/18/18/18	0/3/3/3
2	DN6	A	301	-	-	0/18/18/18	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	308	DN6	N18-N19	5.17	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	307	DN6	N18-N19	4.94	1.41	1.32
2	B	301	DN6	N18-N19	4.92	1.41	1.32
2	B	308	DN6	N17-N18	4.83	1.42	1.34
2	A	303	DN6	N18-N19	4.79	1.40	1.32
2	A	304	DN6	N18-N19	4.71	1.40	1.32
2	B	305	DN6	N20-N19	4.68	1.41	1.34
2	B	302	DN6	C12-C16	-4.65	1.36	1.48
3	A	305	DMS	O-S	4.61	1.81	1.50
2	A	301	DN6	N18-N19	4.60	1.40	1.32
3	A	306	DMS	O-S	4.54	1.80	1.50
2	B	304	DN6	N18-N19	4.49	1.40	1.32
2	A	304	DN6	N17-N18	4.46	1.41	1.34
2	B	308	DN6	N20-N19	4.39	1.41	1.34
2	B	305	DN6	N17-N18	4.39	1.41	1.34
2	B	305	DN6	N18-N19	4.39	1.40	1.32
3	B	309	DMS	O-S	4.36	1.79	1.50
2	A	302	DN6	N18-N19	4.35	1.40	1.32
2	B	306	DN6	N18-N19	4.33	1.40	1.32
2	A	303	DN6	N17-N18	4.31	1.41	1.34
2	B	301	DN6	N20-N19	4.29	1.41	1.34
2	B	307	DN6	N17-N18	4.26	1.41	1.34
2	B	303	DN6	N20-N19	4.26	1.41	1.34
2	B	307	DN6	N20-N19	4.11	1.41	1.34
2	A	302	DN6	N17-N18	4.09	1.41	1.34
2	B	301	DN6	N17-N18	4.08	1.41	1.34
2	B	306	DN6	N20-N19	4.00	1.40	1.34
2	B	302	DN6	N18-N19	3.97	1.39	1.32
2	B	304	DN6	N20-N19	3.84	1.40	1.34
2	A	302	DN6	N20-N19	3.75	1.40	1.34
2	B	304	DN6	N17-N18	3.69	1.40	1.34
2	B	302	DN6	N20-N19	3.67	1.40	1.34
2	A	304	DN6	N20-N19	3.67	1.40	1.34
2	A	302	DN6	C12-C16	-3.56	1.39	1.48
2	A	303	DN6	C12-C16	-3.53	1.39	1.48
2	B	306	DN6	N17-N18	3.52	1.40	1.34
2	B	301	DN6	C12-C16	-3.45	1.39	1.48
2	A	301	DN6	C16-N17	3.44	1.37	1.33
2	A	301	DN6	N20-N19	3.31	1.39	1.34
2	A	303	DN6	N20-N19	3.27	1.39	1.34
2	B	307	DN6	C12-C16	-3.24	1.40	1.48
2	B	304	DN6	C12-C16	-3.22	1.40	1.48
2	B	303	DN6	N18-N19	3.17	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	304	DN6	C12-C16	-3.05	1.40	1.48
2	B	308	DN6	C12-C16	-3.01	1.40	1.48
2	A	301	DN6	C12-C16	-3.01	1.40	1.48
2	B	305	DN6	C12-C16	-2.98	1.40	1.48
2	A	304	DN6	C16-N17	2.93	1.37	1.33
2	B	306	DN6	C12-C16	-2.86	1.41	1.48
2	B	308	DN6	C16-N20	2.78	1.37	1.33
2	B	303	DN6	C12-C16	-2.78	1.41	1.48
2	A	303	DN6	C16-N20	2.78	1.37	1.33
2	B	302	DN6	N17-N18	2.65	1.38	1.34
2	B	301	DN6	C16-N17	2.54	1.36	1.33
2	B	307	DN6	C16-N17	2.39	1.36	1.33
2	B	308	DN6	C16-N17	2.21	1.36	1.33
2	A	301	DN6	N17-N18	2.17	1.38	1.34
2	B	307	DN6	C16-N20	2.16	1.36	1.33
2	B	305	DN6	C16-N20	2.16	1.36	1.33
2	B	305	DN6	C16-N17	2.09	1.36	1.33
2	B	303	DN6	N17-N18	2.04	1.38	1.34

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	DN6	N20-N19-N18	-8.78	103.80	109.53
2	A	301	DN6	C16-N20-N19	8.62	112.54	104.87
2	A	302	DN6	N20-N19-N18	-7.46	104.66	109.53
2	B	308	DN6	N20-N19-N18	-6.87	105.04	109.53
2	B	303	DN6	C16-N17-N18	6.21	110.39	104.87
2	B	308	DN6	C16-N20-N19	5.94	110.16	104.87
2	A	302	DN6	C16-N20-N19	5.87	110.09	104.87
2	B	303	DN6	N17-N18-N19	-5.81	105.74	109.53
2	B	307	DN6	C1-C6-C7	5.71	129.04	119.97
2	B	306	DN6	C16-N17-N18	5.66	109.91	104.87
2	A	304	DN6	N17-N18-N19	-5.64	105.85	109.53
2	B	302	DN6	N17-N18-N19	-5.63	105.85	109.53
2	B	306	DN6	C16-N20-N19	5.31	109.60	104.87
2	B	307	DN6	C2-C3-C4	-5.12	114.28	120.34
2	B	306	DN6	N17-N18-N19	-5.10	106.20	109.53
2	A	303	DN6	C16-N20-N19	4.75	109.09	104.87
2	A	301	DN6	C16-N17-N18	4.70	109.05	104.87
2	B	307	DN6	N17-N18-N19	-4.67	106.48	109.53
2	A	303	DN6	N20-N19-N18	-4.64	106.50	109.53
2	B	304	DN6	C16-N20-N19	4.61	108.97	104.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	306	DN6	N20-N19-N18	-4.58	106.54	109.53
2	A	304	DN6	C16-N17-N18	4.55	108.92	104.87
2	A	304	DN6	C16-N20-N19	4.54	108.91	104.87
2	B	304	DN6	C16-N17-N18	4.51	108.88	104.87
2	A	301	DN6	N17-C16-N20	-4.50	106.36	111.39
2	B	304	DN6	N20-N19-N18	-4.44	106.63	109.53
2	B	305	DN6	C16-N17-N18	4.39	108.78	104.87
2	B	307	DN6	C16-N17-N18	4.33	108.72	104.87
2	B	305	DN6	N20-N19-N18	-4.32	106.71	109.53
2	B	301	DN6	N17-N18-N19	-4.30	106.72	109.53
2	A	303	DN6	C16-N17-N18	4.28	108.68	104.87
2	B	304	DN6	N17-N18-N19	-4.26	106.75	109.53
2	B	305	DN6	C16-N20-N19	4.24	108.64	104.87
2	B	307	DN6	C16-N20-N19	4.14	108.55	104.87
2	A	303	DN6	N17-N18-N19	-4.14	106.83	109.53
2	B	302	DN6	C16-N17-N18	4.12	108.54	104.87
2	B	305	DN6	N17-N18-N19	-4.08	106.87	109.53
2	A	302	DN6	C16-N17-N18	3.99	108.42	104.87
2	B	301	DN6	N20-N19-N18	-3.98	106.94	109.53
2	B	301	DN6	C16-N20-N19	3.92	108.35	104.87
2	B	301	DN6	C16-N17-N18	3.91	108.35	104.87
2	B	307	DN6	N20-N19-N18	-3.81	107.04	109.53
2	B	308	DN6	C16-N17-N18	3.69	108.16	104.87
2	B	303	DN6	N20-N19-N18	-3.54	107.22	109.53
2	B	307	DN6	O21-C8-C4	-3.51	114.67	120.94
2	B	307	DN6	C5-C4-C8	-3.46	108.98	120.44
2	B	306	DN6	N17-C16-N20	-3.33	107.67	111.39
2	B	303	DN6	C16-N20-N19	3.26	107.77	104.87
2	B	307	DN6	C5-C6-C7	-3.20	115.25	119.58
2	B	307	DN6	C4-C8-N9	3.00	122.53	115.92
2	A	304	DN6	N20-N19-N18	-2.99	107.58	109.53
2	B	302	DN6	C5-C6-C7	-2.89	115.67	119.58
2	B	307	DN6	C3-C4-C8	2.83	129.80	120.62
2	B	307	DN6	C4-C5-C6	2.82	124.89	121.07
2	A	301	DN6	F24-C7-C6	-2.75	106.89	112.93
2	B	301	DN6	F23-C7-C6	-2.73	106.93	112.93
2	B	308	DN6	C11-C12-C16	-2.72	116.05	120.05
2	A	301	DN6	F22-C7-F24	2.71	115.64	105.72
2	A	302	DN6	F23-C7-C6	-2.67	107.06	112.93
2	B	307	DN6	C10-N9-C8	-2.65	119.70	126.58
2	B	302	DN6	F22-C7-C6	-2.63	107.16	112.93
2	A	302	DN6	N17-N18-N19	-2.53	107.88	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	DN6	C12-C16-N17	2.49	128.34	124.12
2	A	301	DN6	O21-C8-C4	-2.48	116.51	120.94
2	B	303	DN6	C14-C15-C10	-2.47	116.77	119.72
2	B	308	DN6	N17-C16-N20	-2.46	108.64	111.39
2	A	304	DN6	N17-C16-N20	-2.41	108.70	111.39
2	B	304	DN6	N17-C16-N20	-2.35	108.76	111.39
2	B	308	DN6	N17-N18-N19	-2.35	108.00	109.53
2	B	307	DN6	C3-C2-C1	2.33	123.55	120.25
2	A	303	DN6	N17-C16-N20	-2.27	108.86	111.39
2	B	303	DN6	N17-C16-N20	-2.25	108.88	111.39
2	A	302	DN6	N17-C16-N20	-2.25	108.88	111.39
2	B	308	DN6	C13-C12-C16	2.24	124.59	120.79
2	B	308	DN6	C12-C16-N17	2.23	127.90	124.12
2	B	302	DN6	C14-C15-C10	-2.20	117.09	119.72
2	A	303	DN6	F22-C7-C6	-2.20	108.09	112.93
2	B	303	DN6	C2-C3-C4	-2.19	117.76	120.34
2	B	305	DN6	N17-C16-N20	-2.16	108.98	111.39
2	B	303	DN6	O21-C8-C4	-2.13	117.15	120.94
2	B	306	DN6	F24-C7-C6	-2.12	108.26	112.93
2	B	304	DN6	F24-C7-C6	-2.11	108.30	112.93
2	A	301	DN6	N17-N18-N19	-2.10	108.16	109.53
2	B	301	DN6	C10-N9-C8	-2.07	121.20	126.58
2	B	302	DN6	N20-N19-N18	-2.06	108.19	109.53
2	B	307	DN6	F23-C7-C6	2.04	117.41	112.93
2	B	306	DN6	C12-C16-N17	2.03	127.55	124.12
2	A	302	DN6	C2-C3-C4	2.02	122.73	120.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	307	DN6	C11-C10-N9-C8
2	B	307	DN6	C15-C10-N9-C8
2	A	304	DN6	C11-C10-N9-C8

There are no ring outliers.

8 monomers are involved in 39 short contacts:

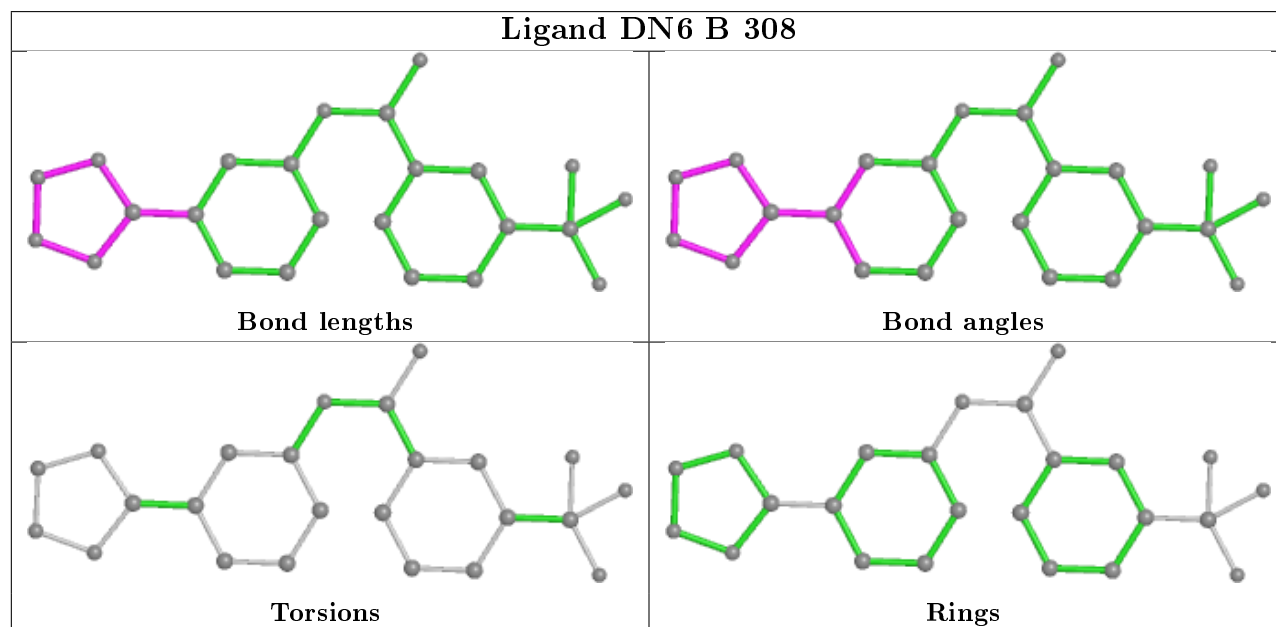
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	308	DN6	1	0
2	B	304	DN6	2	0

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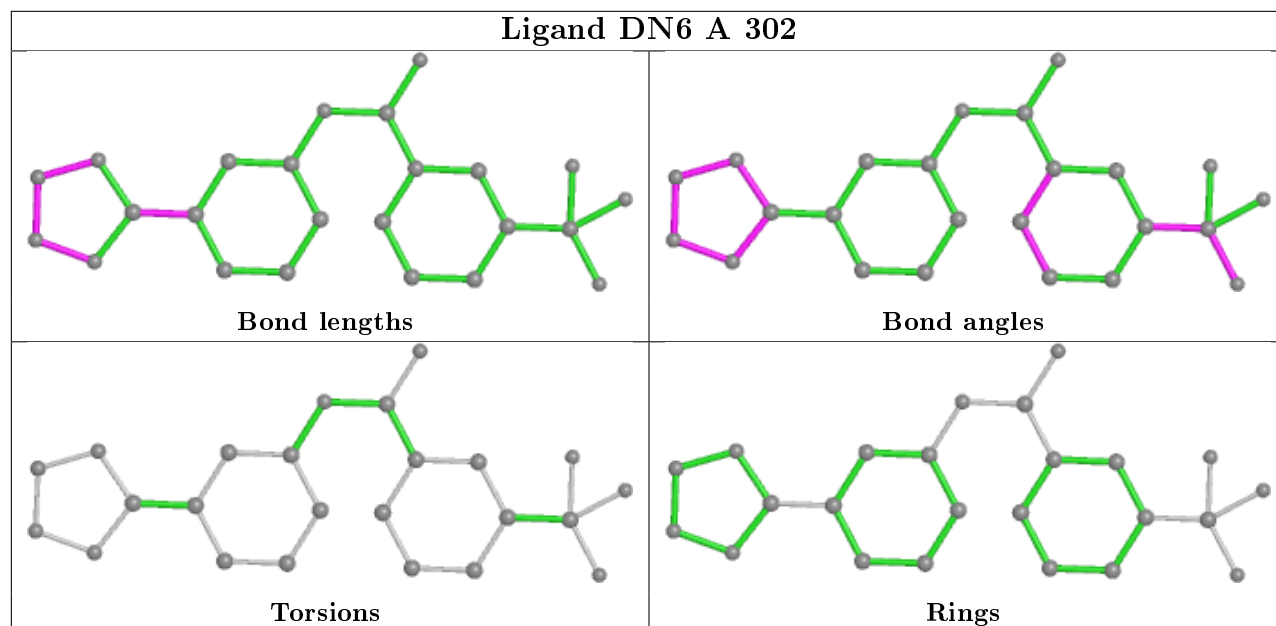
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	307	DN6	16	0
2	B	306	DN6	12	0
3	B	309	DMS	3	0
2	B	302	DN6	2	0
2	B	301	DN6	1	0
3	A	306	DMS	2	0

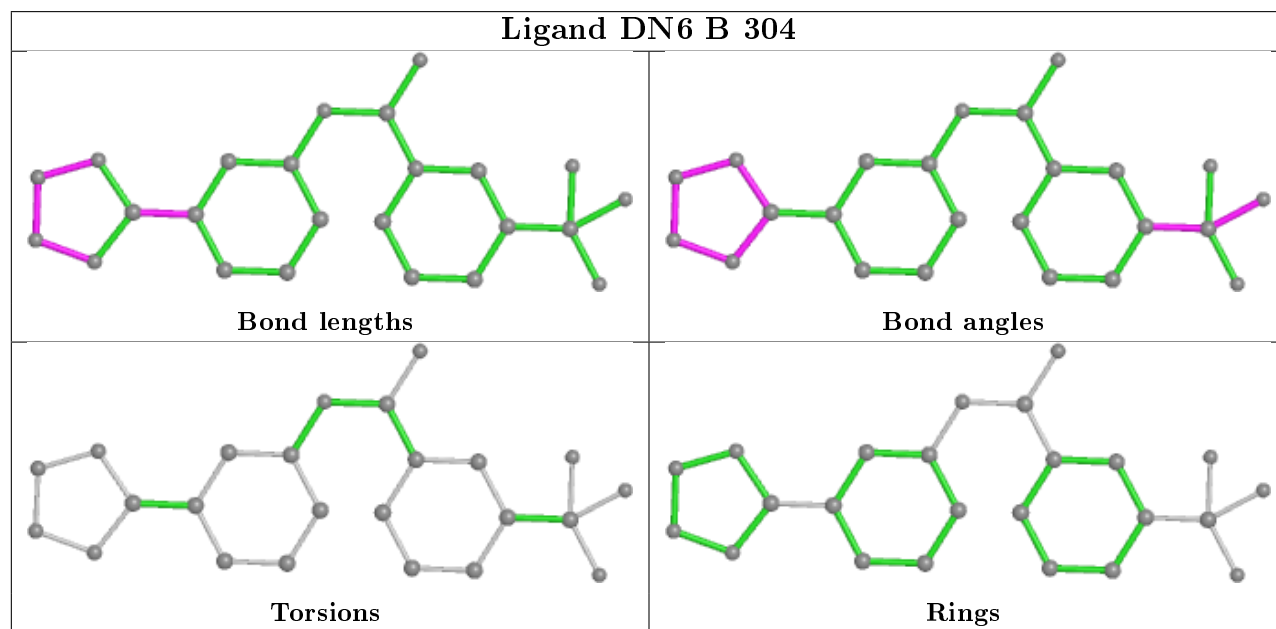
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



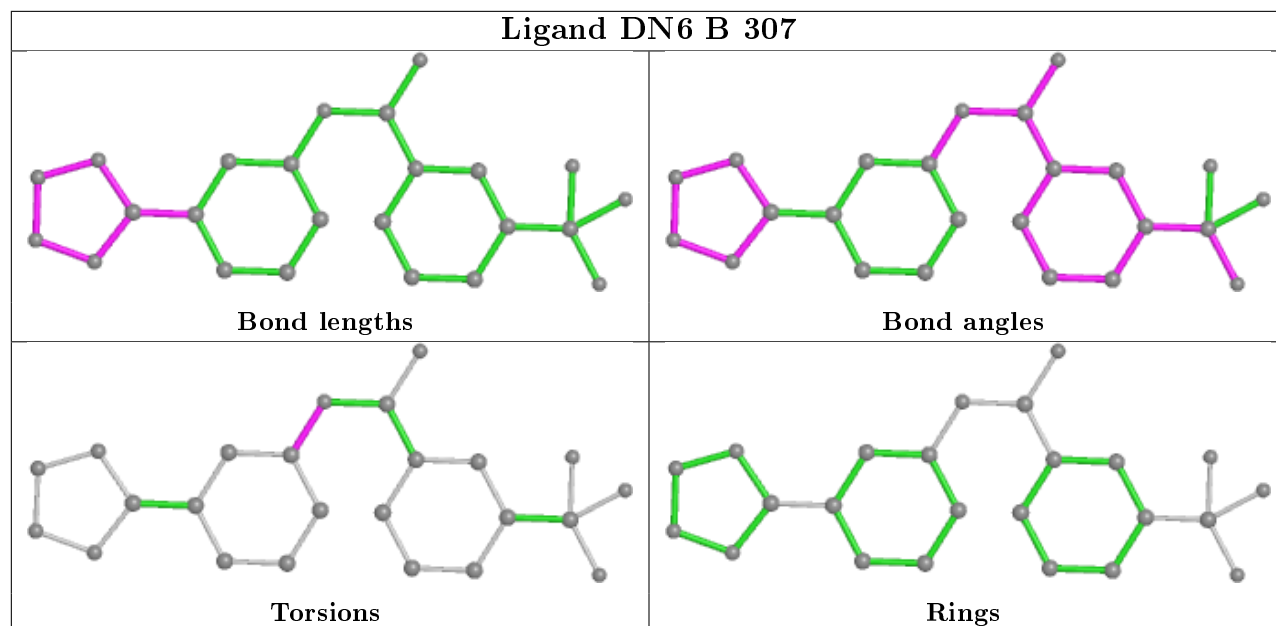
## Ligand DN6 A 302



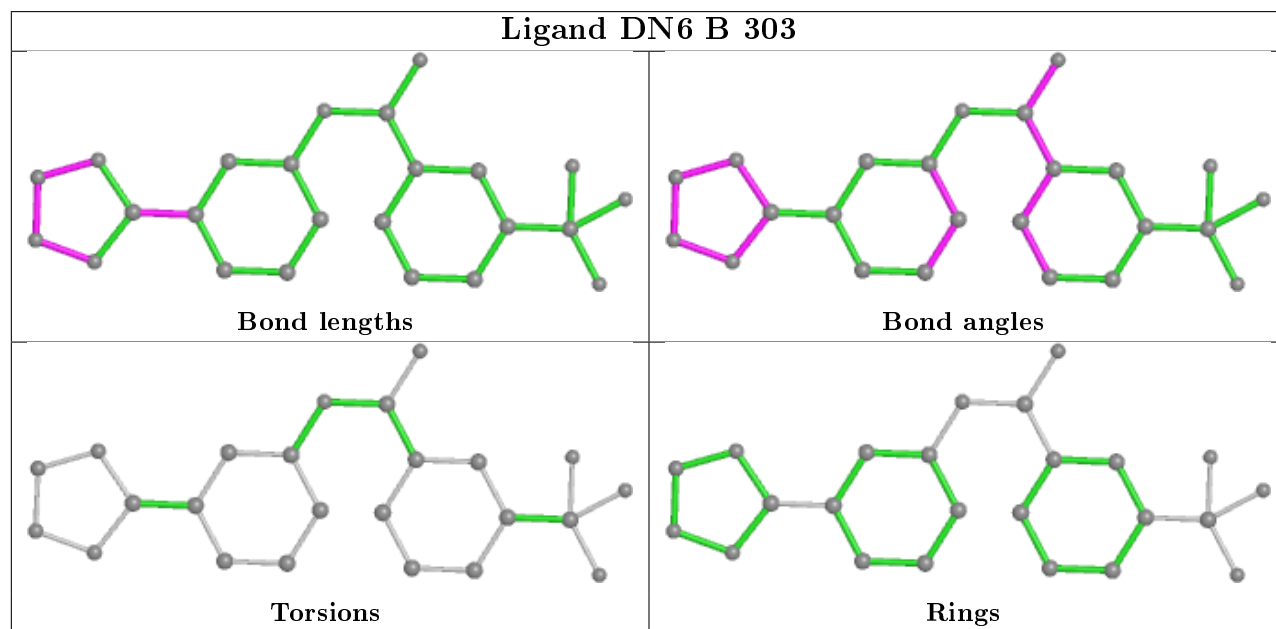
## Ligand DN6 B 304



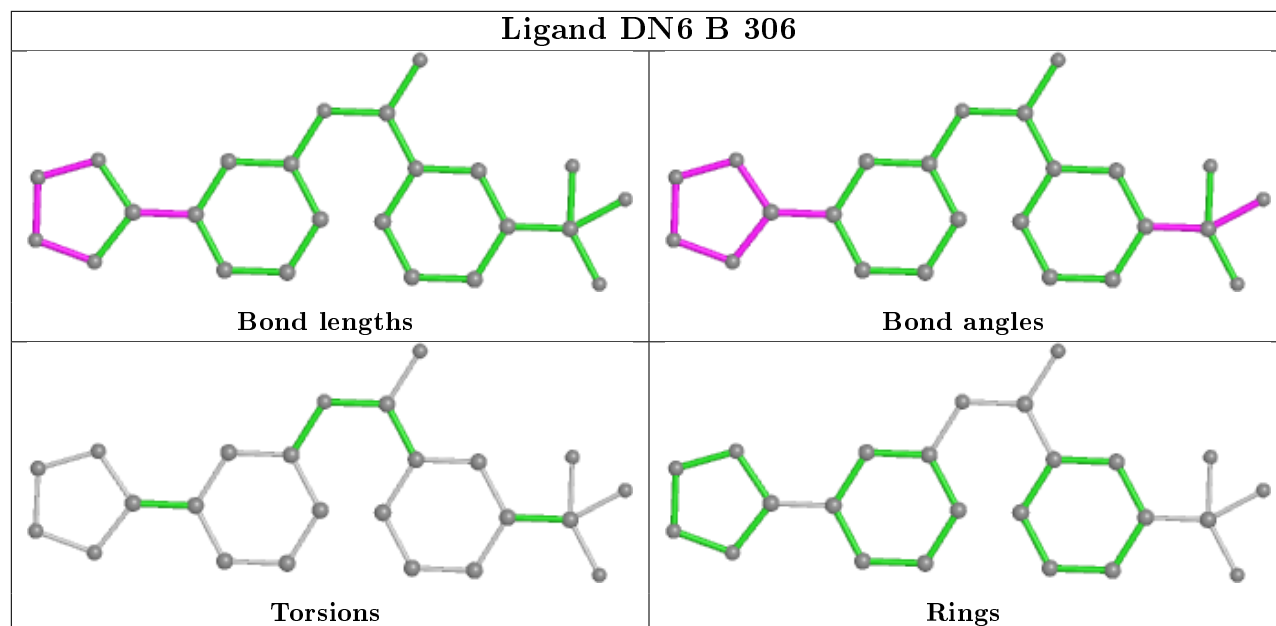
## Ligand DN6 B 307



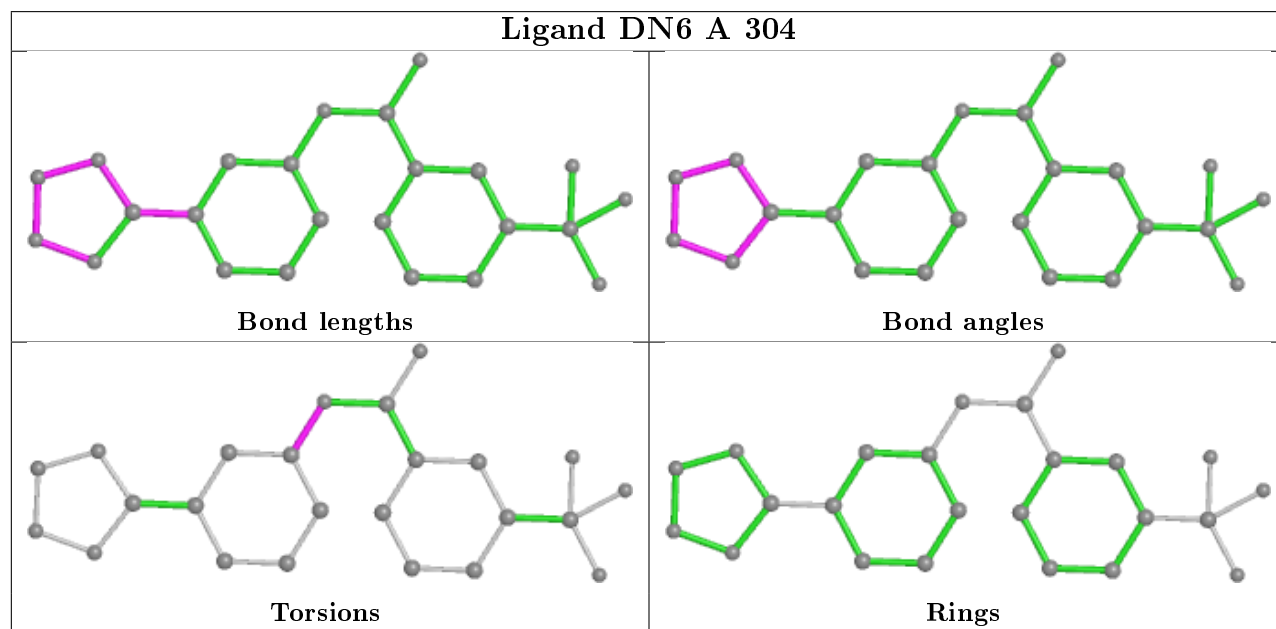
## Ligand DN6 B 303



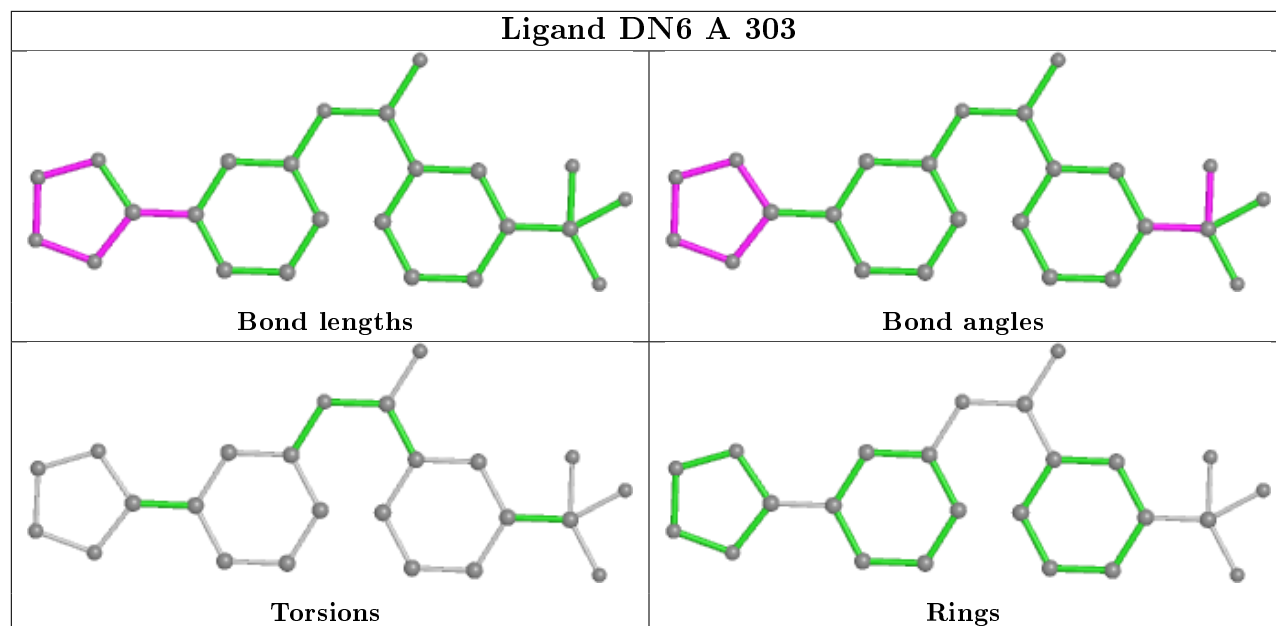
## Ligand DN6 B 306



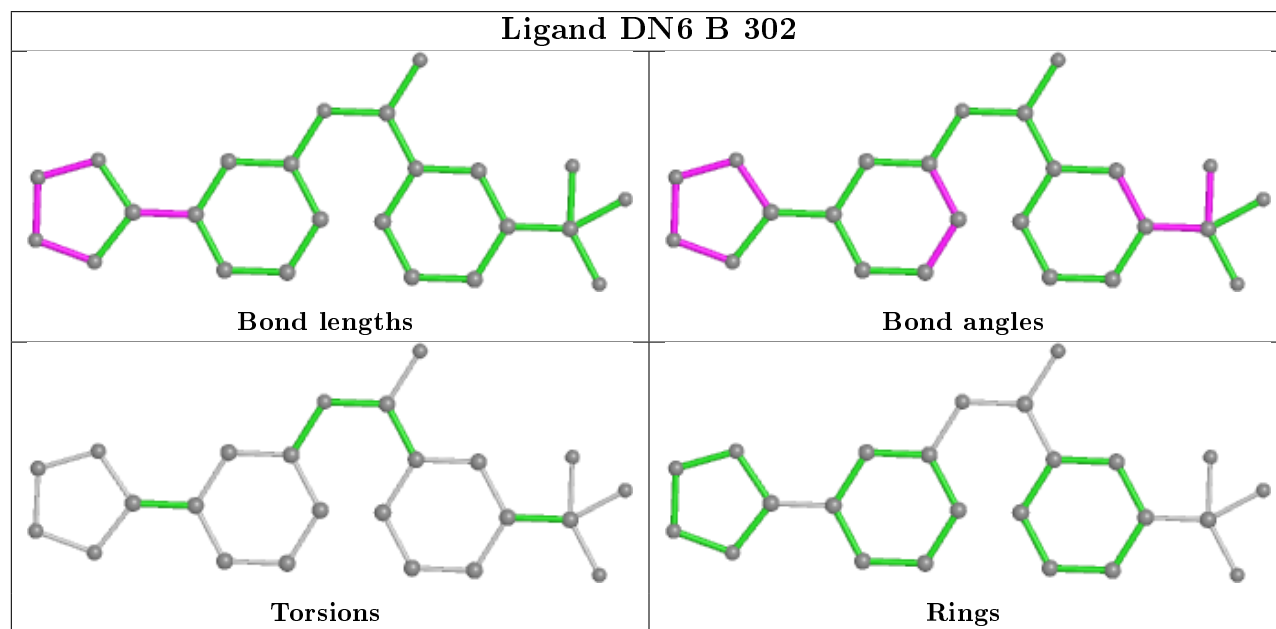
## Ligand DN6 A 304



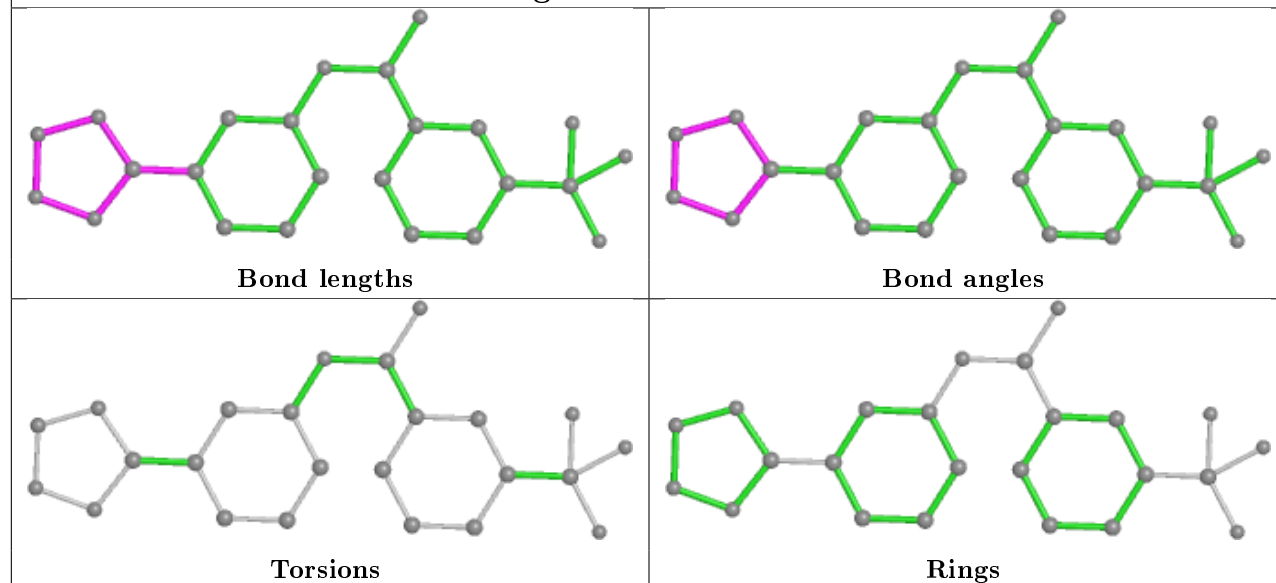
## Ligand DN6 A 303



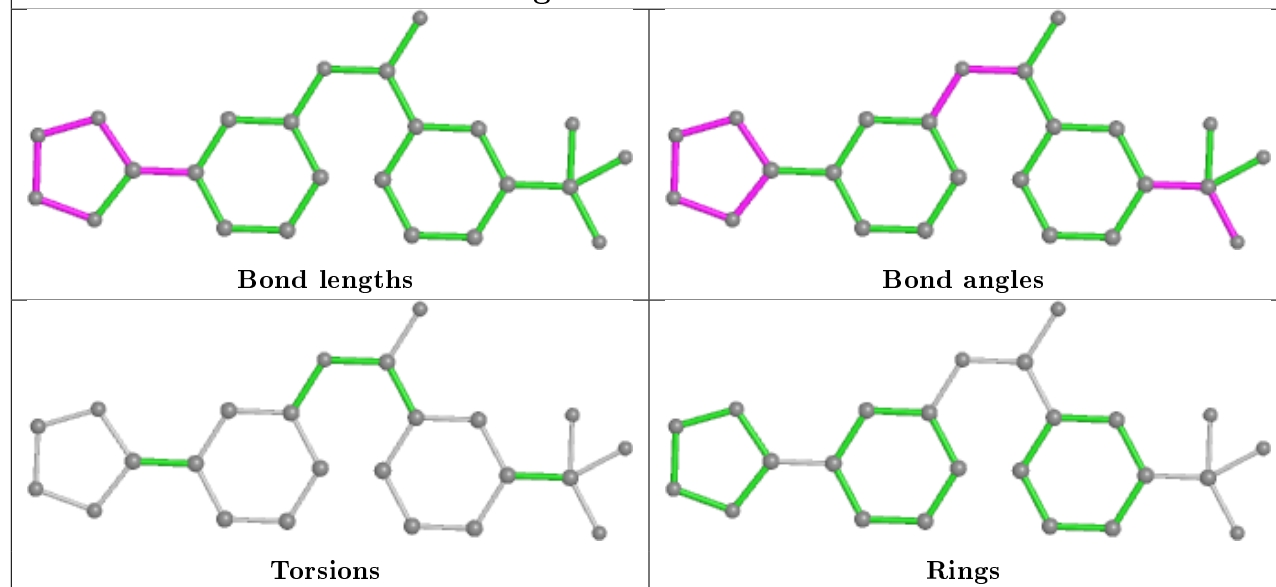
## Ligand DN6 B 302



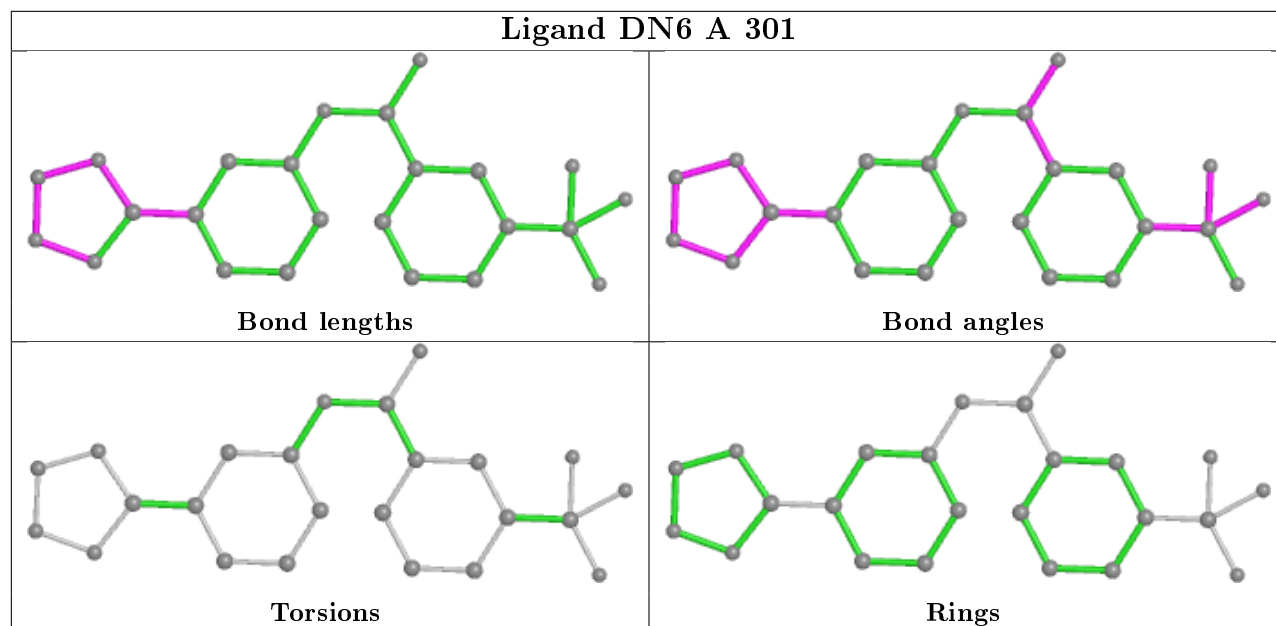
## Ligand DN6 B 305



## Ligand DN6 B 301







## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/263 (98%)	0.22	8 (3%)	49	56	9, 11, 18, 24	7 (2%)
1	B	261/263 (99%)	0.14	8 (3%)	49	56	9, 12, 18, 27	10 (3%)
All	All	521/526 (99%)	0.18	16 (3%)	49	56	9, 12, 18, 27	17 (3%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	SER	6.6
1	B	290	LEU	4.9
1	A	88	LYS	4.5
1	A	227	THR	3.9
1	A	229	TRP	3.6
1	B	28	ALA	3.5
1	A	55	THR	3.4
1	B	92	ASN	3.0
1	A	290	LEU	2.9
1	A	271[A]	ASN	2.9
1	A	289	GLY	2.7
1	B	256	ARG	2.7
1	A	228	SER	2.3
1	B	247	ILE	2.2
1	B	269	GLN	2.1
1	B	271	ASN	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

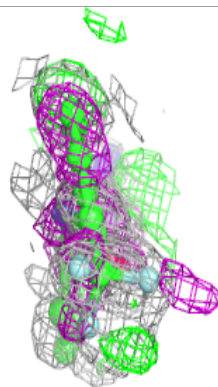
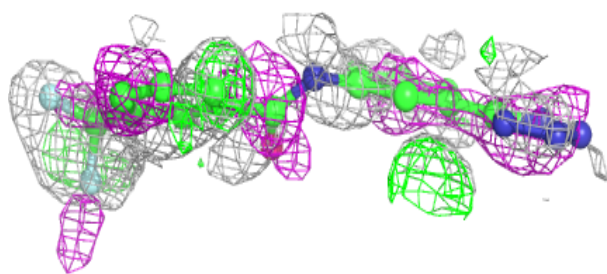
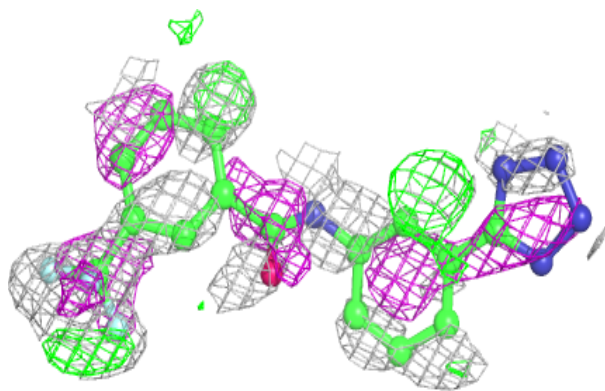
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DN6	B	307	24/24	0.53	0.48	30,40,52,53	0
2	DN6	B	308	24/24	0.57	0.31	27,29,33,34	0
2	DN6	B	304	24/24	0.62	0.29	23,27,38,38	0
2	DN6	B	301	24/24	0.81	0.22	26,28,31,31	0
2	DN6	B	305	24/24	0.82	0.24	18,23,26,28	0
3	DMS	A	306	4/4	0.82	0.25	31,32,32,32	0
2	DN6	B	302	24/24	0.87	0.12	18,19,23,23	0
2	DN6	A	304	24/24	0.87	0.26	16,19,27,27	0
3	DMS	A	305	4/4	0.90	0.23	19,22,22,22	0
2	DN6	A	303	24/24	0.91	0.24	18,20,22,22	0
2	DN6	A	302	24/24	0.92	0.12	14,17,25,26	0
2	DN6	B	306	24/24	0.93	0.19	17,20,26,27	0
3	DMS	B	309	4/4	0.94	0.18	24,24,25,25	0
2	DN6	B	303	24/24	0.95	0.07	10,11,13,15	0
2	DN6	A	301	24/24	0.96	0.07	9,10,13,15	0

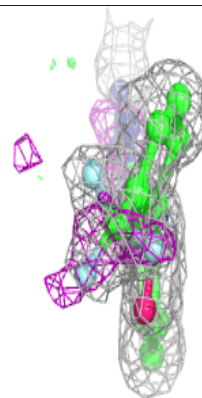
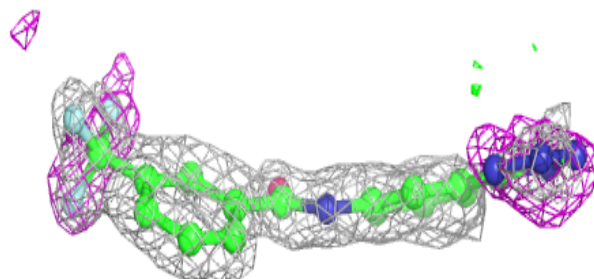
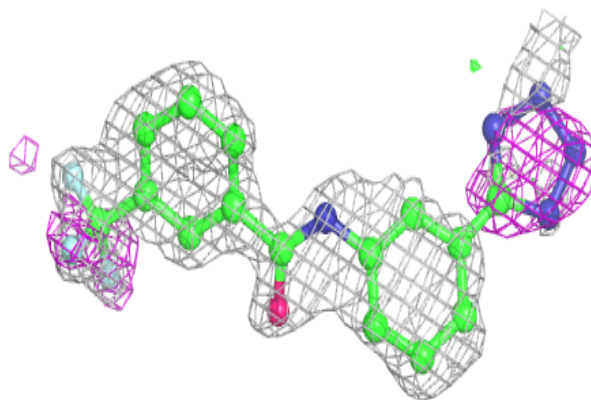
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around DN6 B 307:**

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

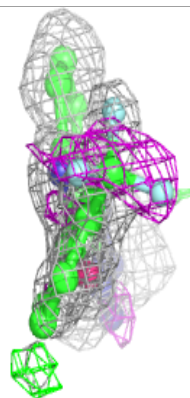
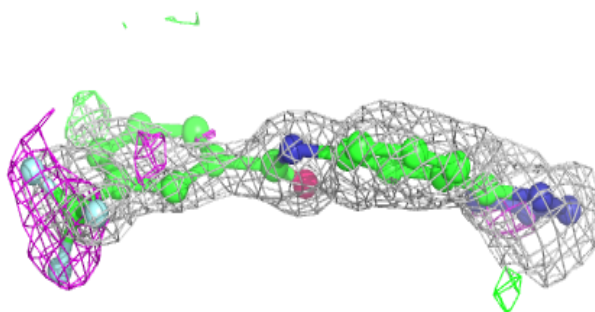
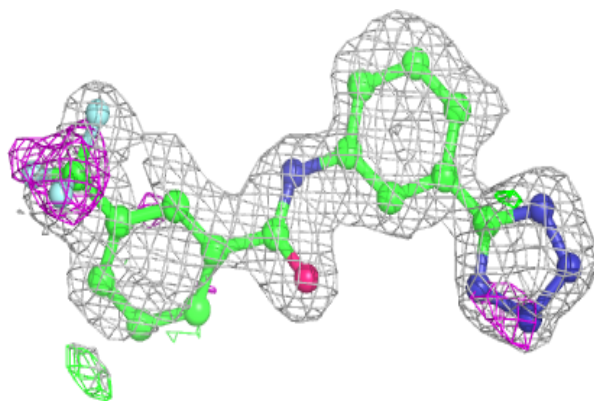
**Electron density around DN6 B 308:**

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

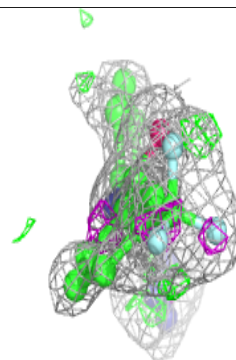
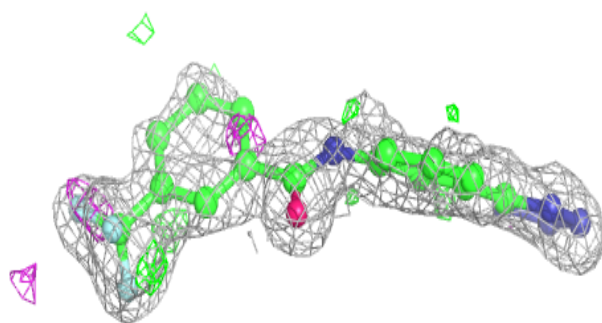
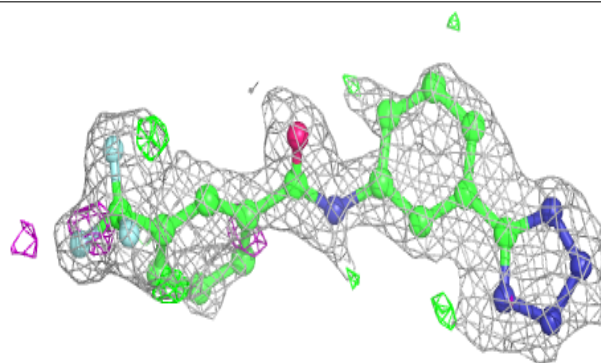


**Electron density around DN6 B 304:**

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

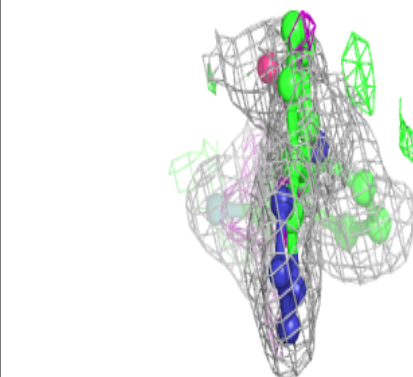
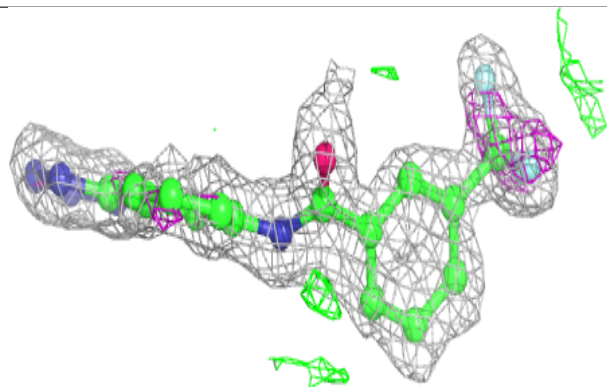
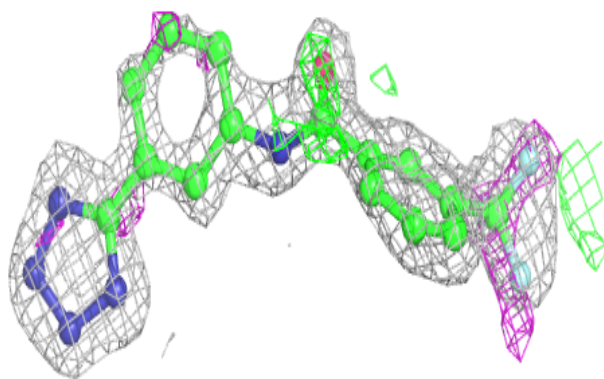
**Electron density around DN6 B 301:**

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

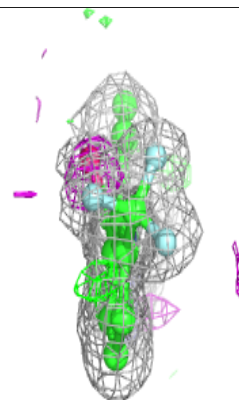
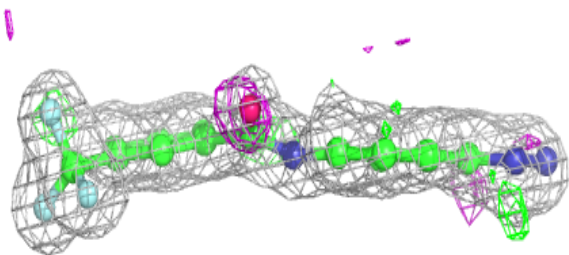
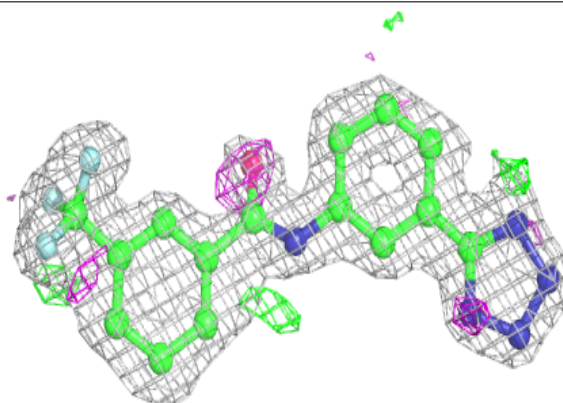


**Electron density around DN6 B 305:**

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

**Electron density around DN6 B 302:**

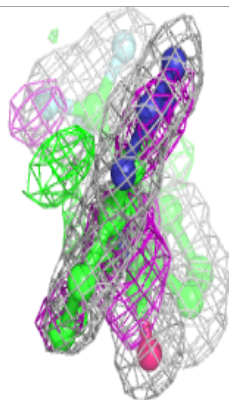
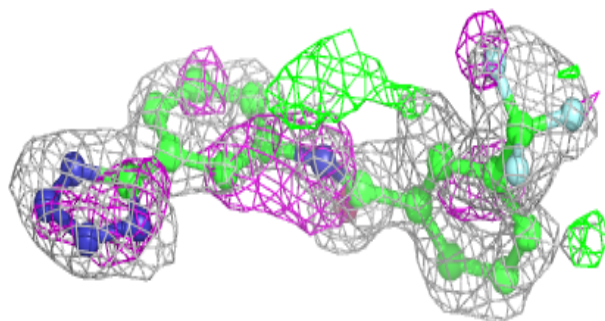
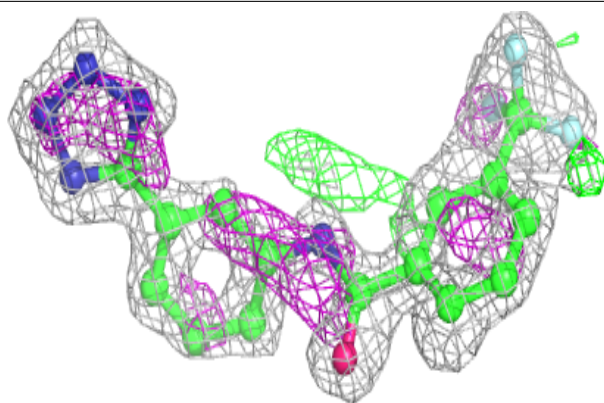
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



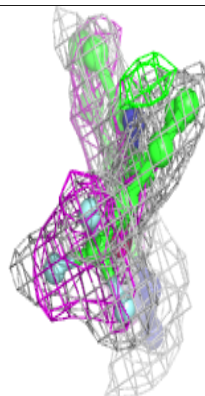
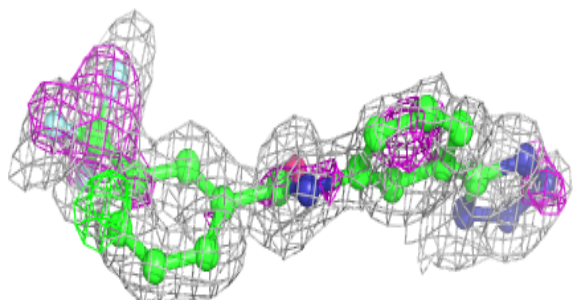
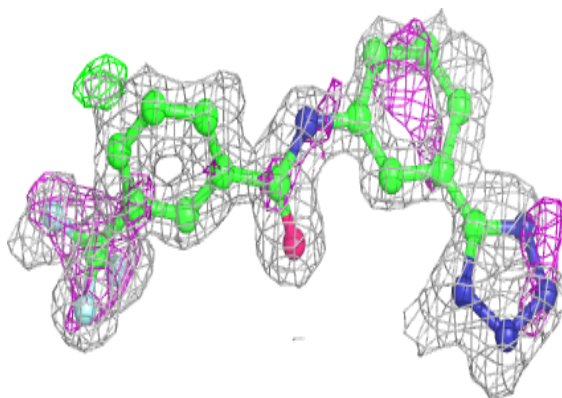


**Electron density around DN6 A 304:**

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

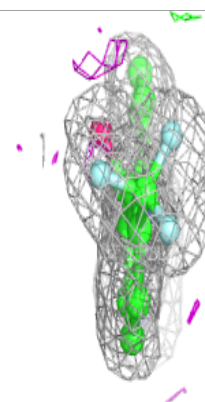
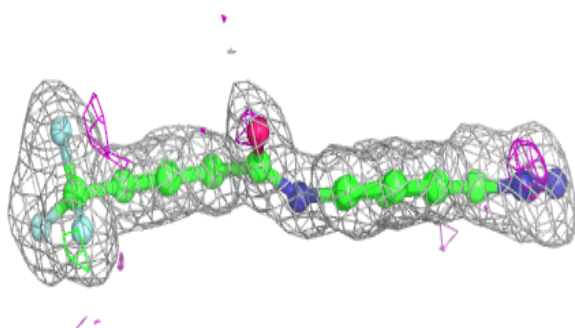
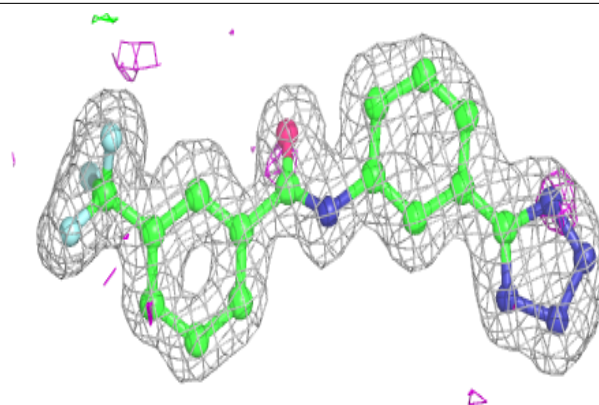
**Electron density around DN6 A 303:**

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

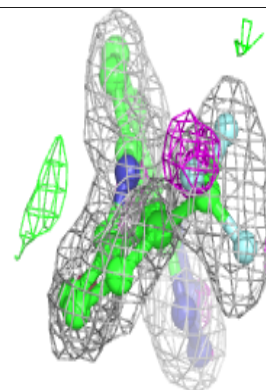
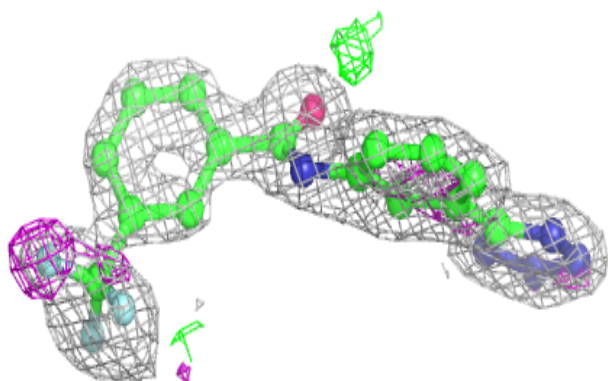
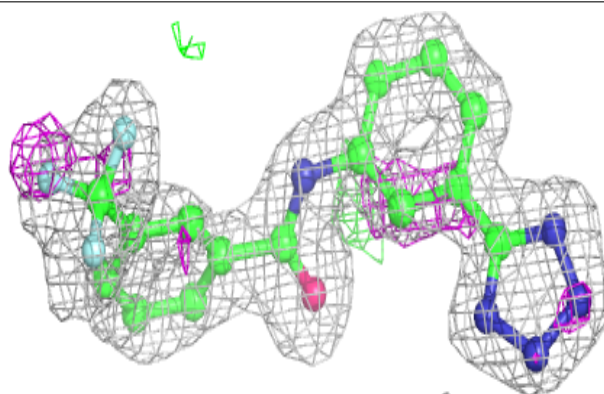


**Electron density around DN6 A 302:**

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

**Electron density around DN6 B 306:**

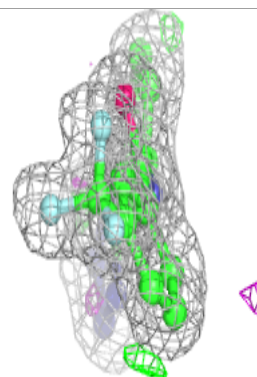
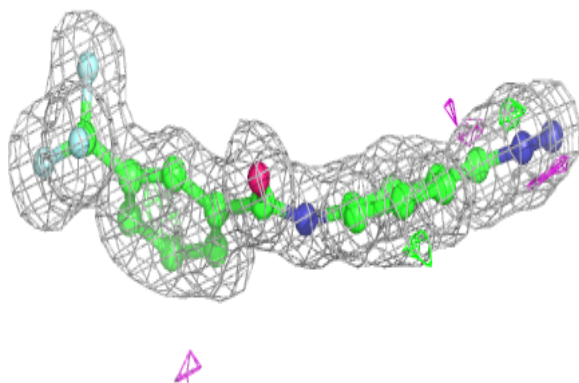
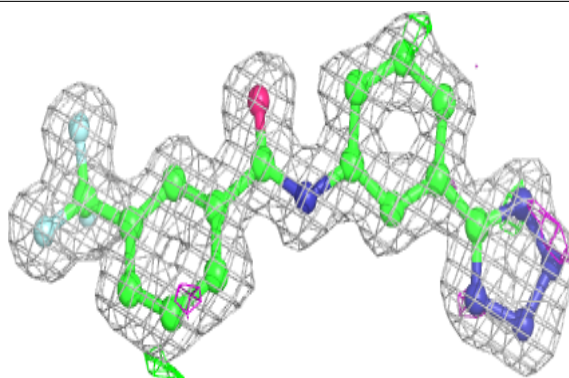
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



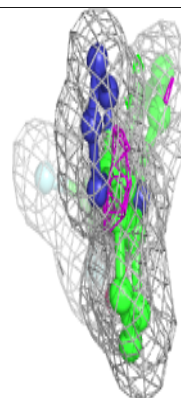
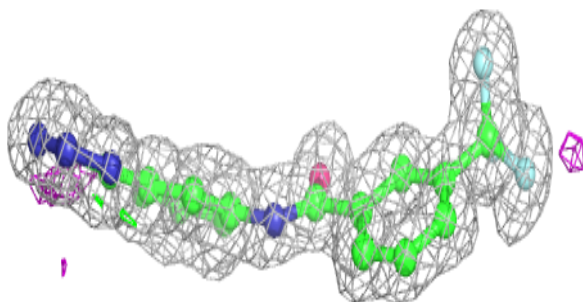
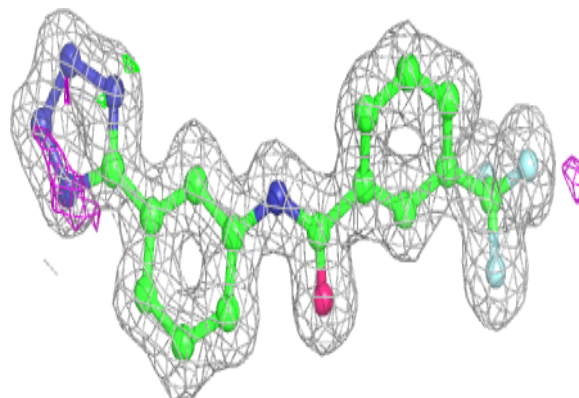


**Electron density around DN6 B 303:**

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

**Electron density around DN6 A 301:**

$2mF_o-DF_c$  (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.