



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:34 PM BST

PDB ID : 1NNB  
Title : THREE-DIMENSIONAL STRUCTURE OF INFLUENZA A N9 NEURAMINIDASE AND ITS COMPLEX WITH THE INHIBITOR 2-DEOXY 2,3-DEHYDRO-N-ACETYL NEURAMINIC ACID  
Authors : Bossart-Whitaker, P.; Carson, M.; Babu, Y.S.; Smith, C.D.; Laver, W.G.; Air, G.M.  
Deposited on : 1993-03-08  
Resolution : 2.80 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)  
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) : 2.13.1

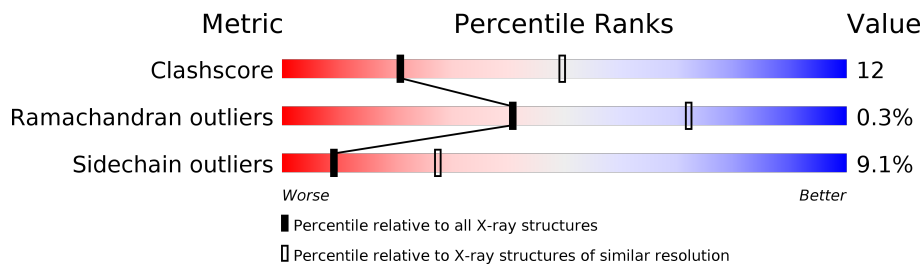
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	387	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3799 atoms, of which 722 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.

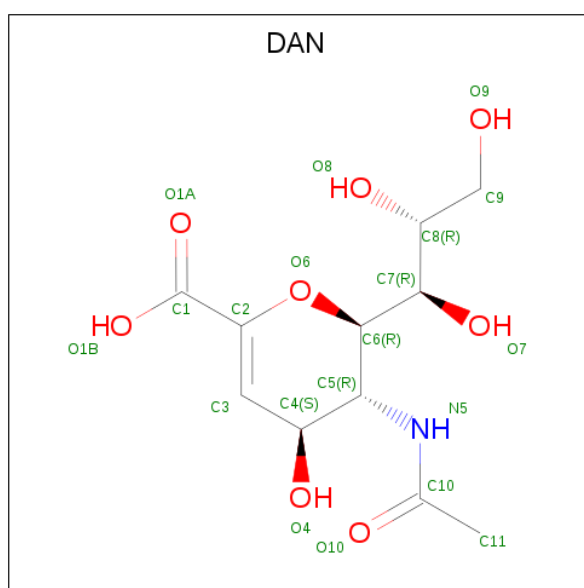
- Molecule 1 is a protein called NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	387	3765	1908	709	534	591	23	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (three-letter code: DAN) (formula: C<sub>11</sub>H<sub>17</sub>NO<sub>8</sub>).



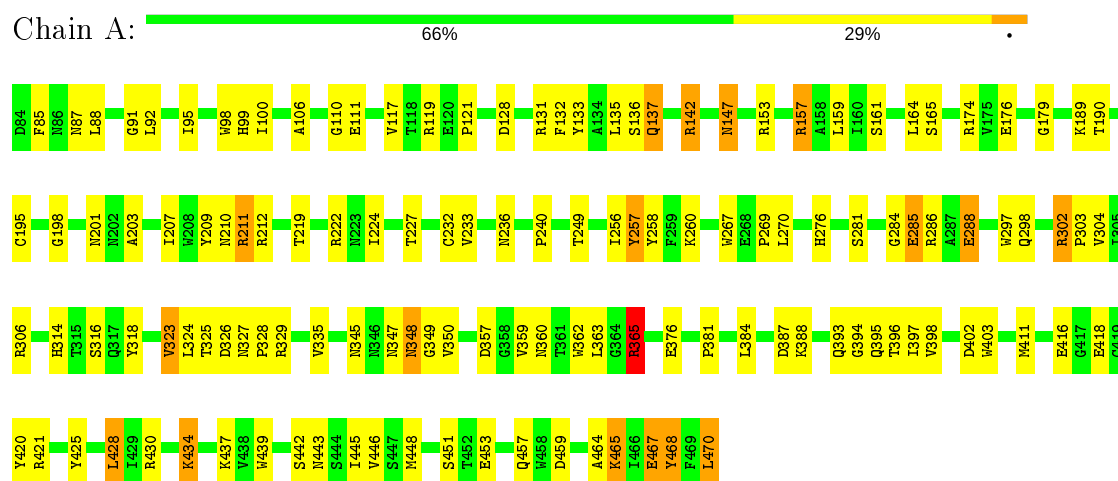
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	33	11	13	1	8	0	0

### 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. 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: NEURAMINIDASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.78Å 183.78Å 183.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	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: CA, DAN

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	0.56	0/3139	0.70	0/4276

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	A	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	153	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	257	TYR	Sidechain
1	A	258	TYR	Sidechain
1	A	302	ARG	Sidechain
1	A	323	VAL	Mainchain
1	A	365	ARG	Sidechain
1	A	421	ARG	Sidechain
1	A	425	TYR	Sidechain
1	A	468	TYR	Sidechain

## 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	3056	709	2883	73	0
2	A	1	0	0	0	0
3	A	20	13	16	0	0
All	All	3077	722	2899	73	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 12.

All (73) 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:437:LYS:HD3	1:A:470:LEU:HD21	1.71	0.73
1:A:276:HIS:HB2	1:A:297:TRP:CD1	2.26	0.69
1:A:276:HIS:HB2	1:A:297:TRP:HD1	1.57	0.69
1:A:345:ASN:HD21	1:A:348:ASN:HB3	1.62	0.65
1:A:465:LYS:HB3	1:A:467:GLU:OE2	1.98	0.64
1:A:403:TRP:CH2	1:A:434:LYS:HG2	2.33	0.63
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.63	0.62
1:A:147:ASN:ND2	1:A:439:TRP:HB3	2.14	0.62
1:A:451:SER:OG	1:A:453:GLU:HB2	2.00	0.61
1:A:95:ILE:HG21	1:A:98:TRP:CZ2	2.36	0.60
1:A:119:ARG:HA	1:A:443:ASN:ND2	2.18	0.59
1:A:359:VAL:HA	1:A:381:PRO:HB3	1.85	0.58
1:A:87:ASN:OD1	1:A:236:ASN:HB2	2.03	0.58
1:A:397:ILE:HD12	1:A:448:MET:HE1	1.86	0.58
1:A:132:PHE:CE1	1:A:164:LEU:HD12	2.41	0.56
1:A:398:VAL:CG1	1:A:402:ASP:HB2	2.37	0.55
1:A:276:HIS:CB	1:A:297:TRP:HD1	2.19	0.54
1:A:397:ILE:HD12	1:A:448:MET:CE	2.38	0.54
1:A:326:ASP:O	1:A:329:ARG:HD3	2.06	0.54
1:A:136:SER:O	1:A:157:ARG:HD2	2.08	0.53
1:A:179:GLY:HA3	1:A:195:CYS:HB3	1.91	0.53
1:A:465:LYS:HB2	1:A:468:TYR:CD2	2.44	0.52
1:A:302:ARG:NH2	1:A:350:VAL:O	2.38	0.52
1:A:147:ASN:HD21	1:A:439:TRP:HE3	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLN:HG3	1:A:457:GLN:HE21	1.75	0.51
1:A:133:TYR:CE2	1:A:161:SER:HB3	2.46	0.51
1:A:207:ILE:N	1:A:207:ILE:HD12	2.26	0.51
1:A:303:PRO:HA	1:A:318:TYR:HA	1.93	0.51
1:A:190:THR:HG22	1:A:209:TYR:CZ	2.45	0.51
1:A:85:PHE:CD1	1:A:189:LYS:HD2	2.46	0.50
1:A:106:ALA:O	1:A:110:GLY:N	2.45	0.50
1:A:240:PRO:HA	1:A:257:TYR:O	2.12	0.50
1:A:111:GLU:O	1:A:142:ARG:NH1	2.44	0.50
1:A:465:LYS:HZ2	1:A:465:LYS:HB3	1.77	0.50
1:A:285:GLU:HB3	1:A:420:TYR:HD2	1.76	0.49
1:A:393:GLN:HG2	1:A:394:GLY:N	2.27	0.49
1:A:85:PHE:CE2	1:A:260:LYS:NZ	2.80	0.49
1:A:357:ASP:HB3	1:A:360:ASN:O	2.14	0.47
1:A:249:THR:HG22	1:A:347:ASN:HB3	1.97	0.47
1:A:396:THR:H	1:A:457:GLN:NE2	2.13	0.47
1:A:362:TRP:O	1:A:363:LEU:HD23	2.15	0.47
1:A:121:PRO:HA	1:A:133:TYR:O	2.16	0.46
1:A:201:ASN:O	1:A:222:ARG:NH2	2.48	0.46
1:A:284:GLY:HA2	1:A:288:GLU:O	2.17	0.45
1:A:327:ASN:HA	1:A:328:PRO:C	2.36	0.45
1:A:398:VAL:HG12	1:A:402:ASP:HB2	1.97	0.45
1:A:302:ARG:NH1	1:A:325:THR:O	2.50	0.45
1:A:445:ILE:HG22	1:A:446:VAL:N	2.31	0.45
1:A:430:ARG:NH2	1:A:464:ALA:O	2.50	0.45
1:A:198:GLY:HA3	1:A:203:ALA:HA	1.99	0.44
1:A:323:VAL:HG13	1:A:365:ARG:NH2	2.32	0.44
1:A:190:THR:CG2	1:A:209:TYR:CZ	3.01	0.44
1:A:117:VAL:HG12	1:A:137:GLN:HG3	2.00	0.44
1:A:411:MET:SD	1:A:420:TYR:HB3	2.58	0.44
1:A:267:TRP:CZ3	1:A:269:PRO:HD3	2.53	0.44
1:A:393:GLN:HG2	1:A:394:GLY:H	1.83	0.44
1:A:91:GLY:HA2	1:A:285:GLU:HB2	2.00	0.43
1:A:135:LEU:HD22	1:A:179:GLY:O	2.19	0.43
1:A:88:LEU:HD13	1:A:284:GLY:HA3	2.00	0.42
1:A:174:ARG:HD2	1:A:211:ARG:CZ	2.50	0.42
1:A:304:VAL:O	1:A:316:SER:HA	2.19	0.42
1:A:159:LEU:HD23	1:A:176:GLU:HB2	2.02	0.42
1:A:365:ARG:HD2	1:A:376:GLU:OE2	2.19	0.42
1:A:428:LEU:O	1:A:443:ASN:HA	2.20	0.42
1:A:286:ARG:CG	1:A:286:ARG:HH11	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASN:ND2	1:A:349:GLY:H	2.18	0.42
1:A:329:ARG:NH2	1:A:365:ARG:HD3	2.35	0.42
1:A:233:VAL:O	1:A:240:PRO:HD2	2.21	0.41
1:A:164:LEU:O	1:A:165:SER:HB2	2.20	0.41
1:A:92:LEU:HG	1:A:285:GLU:HG2	2.03	0.41
1:A:99:HIS:HD2	1:A:100:ILE:O	2.03	0.41
1:A:388:LYS:HZ2	1:A:388:LYS:HB3	1.85	0.41
1:A:270:LEU:HA	1:A:314:HIS:CE1	2.57	0.40

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	A	385/387 (100%)	351 (91%)	33 (9%)	1 (0%)	41 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ILE

### 5.3.2 Protein sidechains [i](#)

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	340/340 (100%)	309 (91%)	31 (9%)	9 27

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ASP
1	A	131	ARG
1	A	137	GLN
1	A	147	ASN
1	A	157	ARG
1	A	210	ASN
1	A	211	ARG
1	A	219	THR
1	A	227	THR
1	A	232	CYS
1	A	256	ILE
1	A	281	SER
1	A	285	GLU
1	A	288	GLU
1	A	298	GLN
1	A	306	ARG
1	A	324	LEU
1	A	335	VAL
1	A	348	ASN
1	A	365	ARG
1	A	384	LEU
1	A	387	ASP
1	A	416	GLU
1	A	418	GLU
1	A	428	LEU
1	A	434	LYS
1	A	442	SER
1	A	459	ASP
1	A	465	LYS
1	A	467	GLU
1	A	470	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	147	ASN
1	A	200	ASN
1	A	314	HIS
1	A	345	ASN
1	A	348	ASN
1	A	443	ASN
1	A	457	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	DAN	A	500	-	17,20,20	4.35	5 (29%)	18,28,28	2.82	10 (55%)

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	DAN	A	500	-	-	0/14/34/34	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	DAN	C3-C2	16.71	1.52	1.32
3	A	500	DAN	O6-C2	3.91	1.44	1.37
3	A	500	DAN	C9-C8	2.86	1.59	1.52
3	A	500	DAN	C4-C5	2.44	1.55	1.53
3	A	500	DAN	C8-C7	2.15	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	500	DAN	O6-C2-C3	-6.35	115.75	124.33
3	A	500	DAN	O4-C4-C3	5.57	121.86	109.31
3	A	500	DAN	C8-C7-C6	-3.82	105.80	113.03
3	A	500	DAN	O8-C8-C7	-3.10	101.56	109.10
3	A	500	DAN	C4-C3-C2	-2.87	116.75	121.60
3	A	500	DAN	O10-C10-C11	-2.81	116.83	122.06
3	A	500	DAN	C6-C5-N5	-2.73	106.39	110.91
3	A	500	DAN	C5-N5-C10	2.55	129.38	123.18
3	A	500	DAN	C5-C4-C3	-2.42	102.10	108.74
3	A	500	DAN	C11-C10-N5	2.02	119.53	116.10

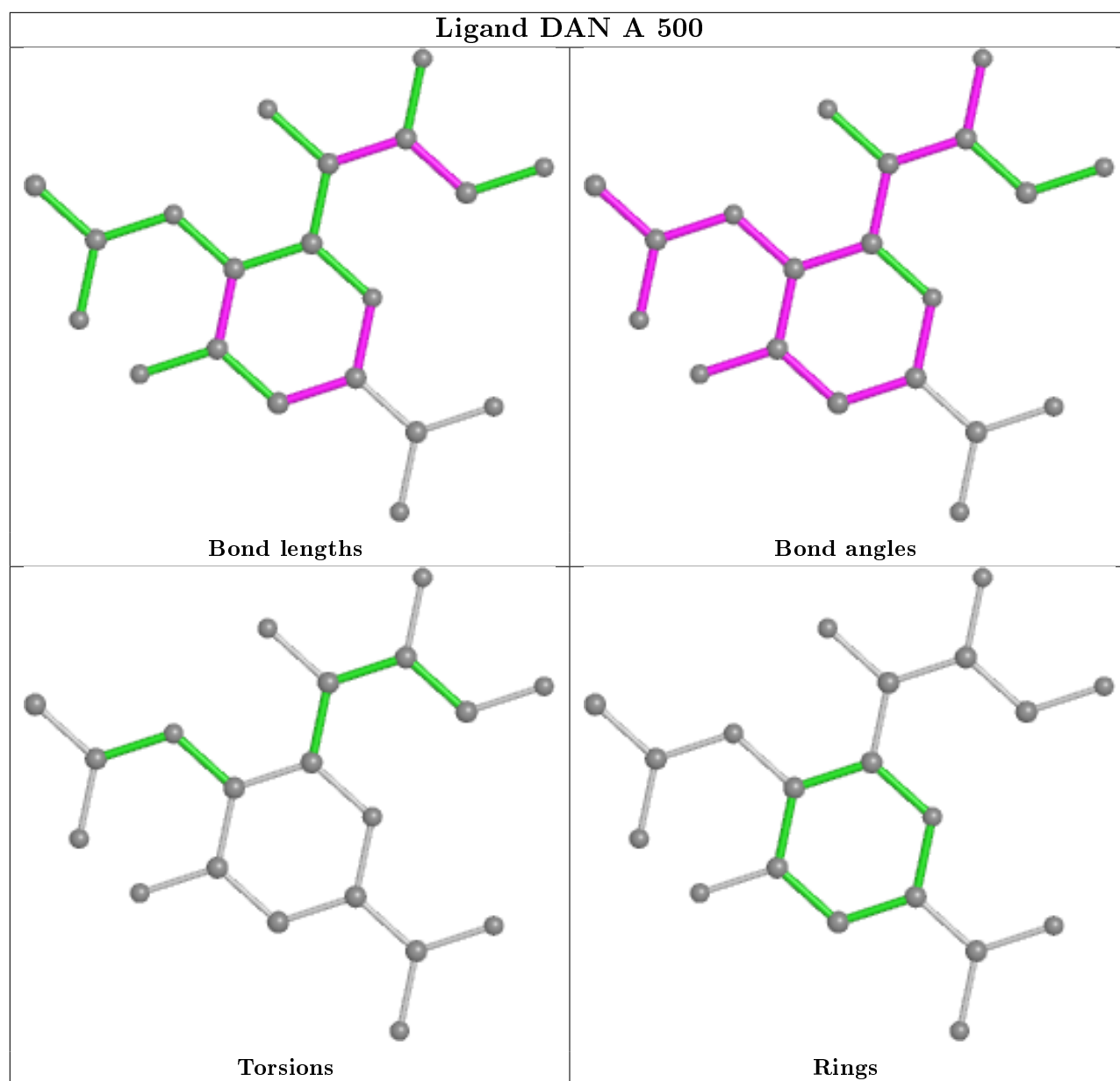
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.