Full wwPDB NMR Structure Validation Report (i)

Jul 3, 2024 – 05:14 PM EDT

PDB ID	:	2MH5
BMRB ID	:	19619
Title	:	Structure and NMR assignments of lantibiotic NAI-107 in DPC micelles
Authors	:	Munch, D.; Muller, A.; Schneider, T.; Kohl, B.; Wenzel, M.; Bandow, J.; Maffioli, S.; Sosio, M.; Donadio, S.; Wimmer, R.; Sahl, H.
Deposited on	:	2013-11-18

This is a Full wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

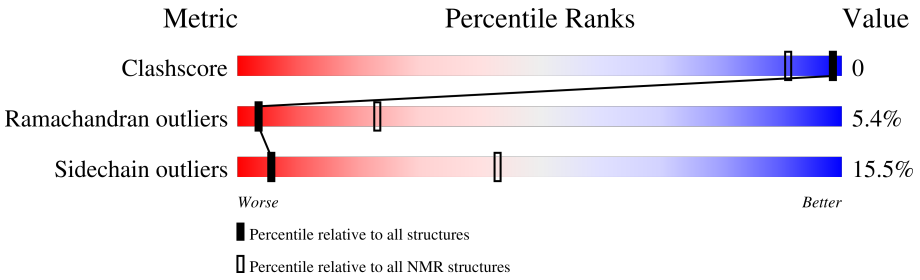
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 70%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	24	75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
1	A	DHA	5	-	6

2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (5) was below the domain threshold value (8).

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 6, 8, 11, 15, 16, 17, 19
2	2, 7, 9, 13, 18, 20
3	4, 10
4	12, 14

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4245 atoms, of which 2598 are hydrogens and 0 are deuteriums.

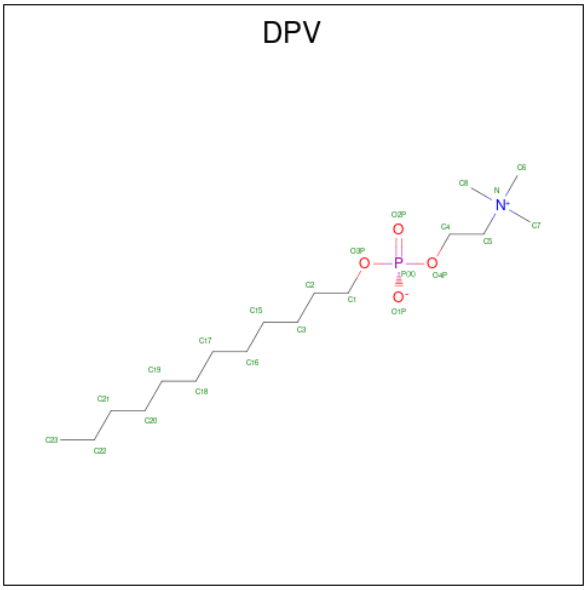
- Molecule 1 is a protein called Lantibiotic 107891.

Mol	Chain	Residues	Atoms							Trace
1	A	24	Total	C	Cl	H	N	O	S	0
			280	94	1	128	26	26	5	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	DAL	SER	conflict	UNP P85065
A	8	DBB	THR	conflict	UNP P85065
A	13	DAL	SER	conflict	UNP P85065
A	18	DAL	SER	conflict	UNP P85065
A	21	DAL	SER	conflict	UNP P85065
A	24	TEE	CYS	conflict	UNP P85065

- Molecule 2 is dodecyl 2-(trimethylammonio)ethyl phosphate (three-letter code: DPV) (formula: $C_{17}H_{38}NO_4P$).



Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1

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Mol	Chain	Residues	Atoms					
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1
2	A	1	Total 61	C 17	H 38	N 1	O 4	P 1

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Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
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			61	17	38	1	4	1
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			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1

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Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1
2	A	1	Total	C	H	N	O	P
			61	17	38	1	4	1

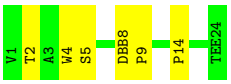
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Lantibiotic 107891

Chain A: 



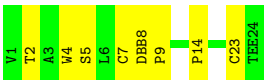
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Lantibiotic 107891

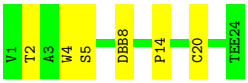
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Lantibiotic 107891

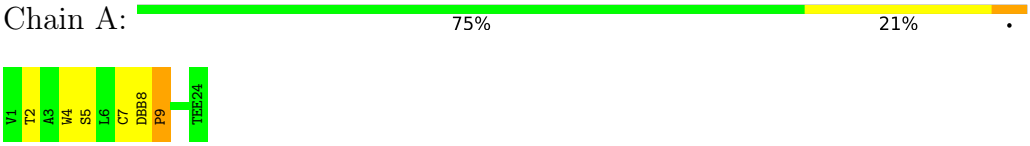
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: Lantibiotic 107891

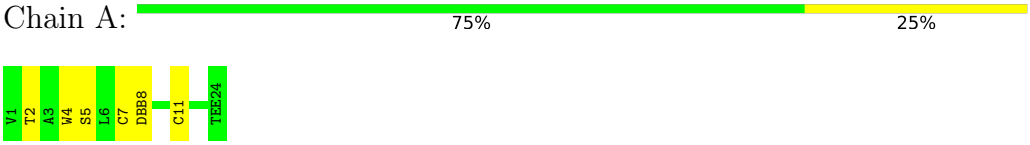
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Lantibiotic 107891

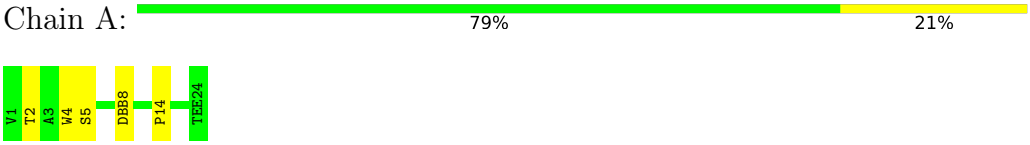
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Lantibiotic 107891

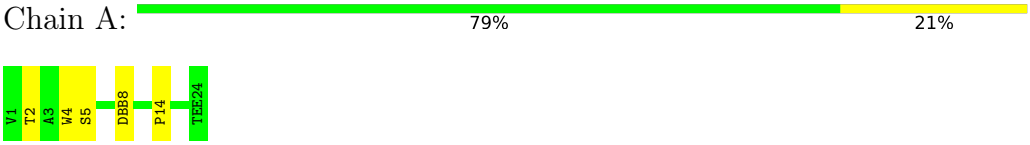
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Lantibiotic 107891

Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Lantibiotic 107891

Chain A:

4.2.8 Score per residue for model 8

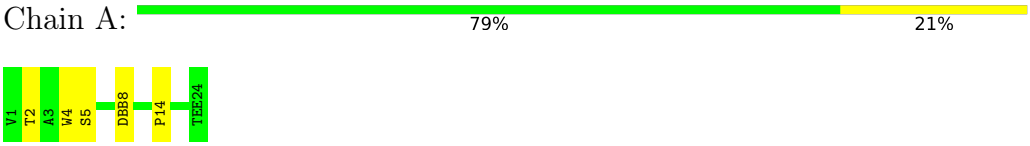
• Molecule 1: Lantibiotic 107891

Chain A:

4.2.9 Score per residue for model 9

• Molecule 1: Lantibiotic 107891

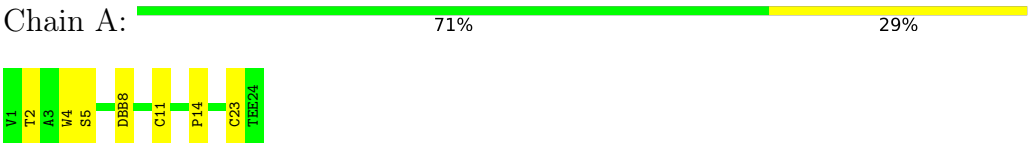
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Lantibiotic 107891

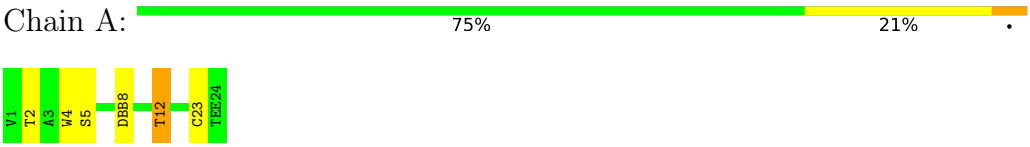
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Lantibiotic 107891

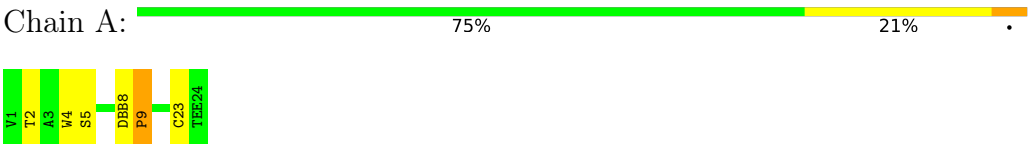
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Lantibiotic 107891

Chain A:



4.2.13 Score per residue for model 13

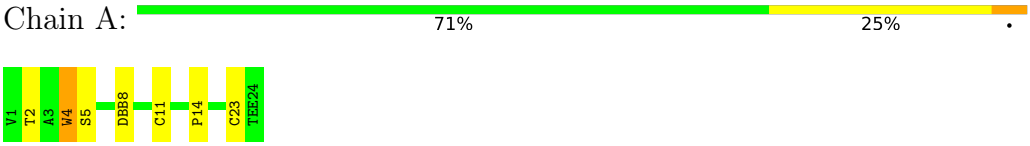
• Molecule 1: Lantibiotic 107891

Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: Lantibiotic 107891

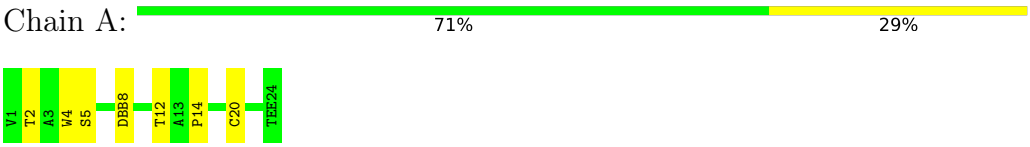
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Lantibiotic 107891

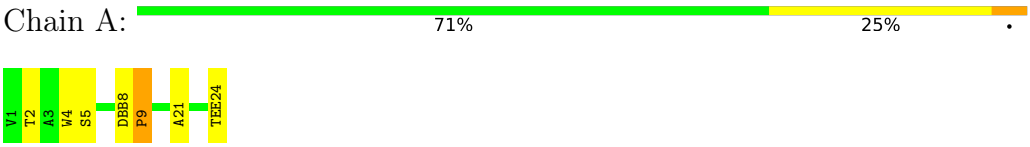
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Lantibiotic 107891

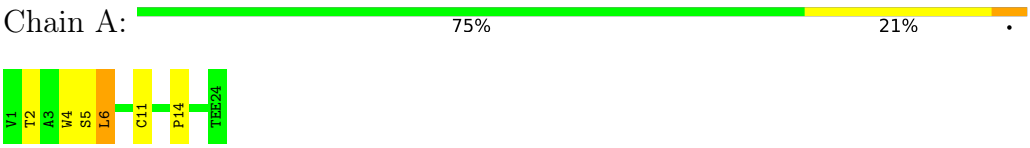
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Lantibiotic 107891

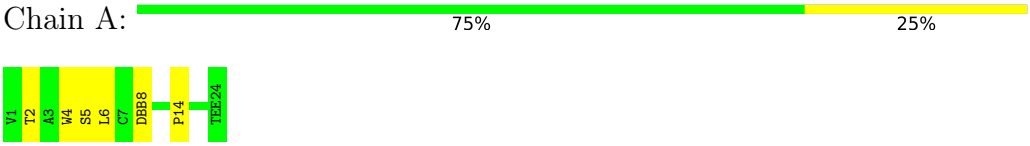
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Lantibiotic 107891

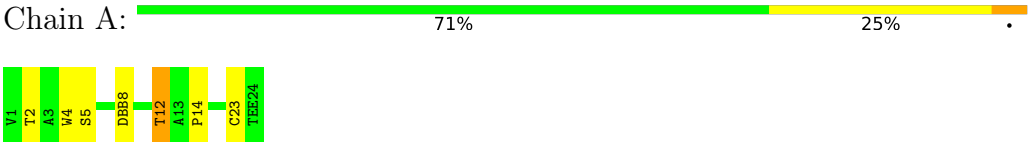
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Lantibiotic 107891

Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Lantibiotic 107891

Chain A:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	3.0
YASARA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	156
Number of shifts mapped to atoms	156
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	70%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, DHA, 5CW, DAL, DBU, DBB, DPV, TEE

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 (average) 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	0.70±0.06	0±0/84 (0.0± 0.0%)	0.77±0.13	0±0/103 (0.0± 0.2%)
All	All	0.70	0/1680 (0.0%)	0.78	1/2060 (0.0%)

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	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	22	PHE	N-CA-C	-5.00	97.49	111.00	7	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	23	CYS	Peptide	1

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	152	128	120	0±1
All	All	32940	51960	51827	6

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 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:DAL:C	1:A:4:5CW:HD1	0.50	2.36	13	1
1:A:21:DAL:C	1:A:24:TEE:HB2	0.49	2.37	8	1
1:A:20:CYS:O	1:A:24:TEE:HB2	0.47	2.09	8	1
1:A:13:DAL:C	1:A:20:CYS:HB3	0.46	2.41	20	1
1:A:4:5CW:CD1	1:A:4:5CW:N	0.42	2.81	14	1
1:A:21:DAL:N	1:A:24:TEE:HB2	0.41	2.30	16	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	13/24 (54%)	10±1 (74±11%)	3±1 (20±10%)	1±1 (5±6%)	3	23
All	All	260/480 (54%)	193 (74%)	53 (20%)	14 (5%)	3	23

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	9	PRO	7
1	A	12	THR	2
1	A	6	LEU	2
1	A	20	CYS	1
1	A	19	ASN	1
1	A	22	PHE	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	10/10 (100%)	8±1 (84±9%)	2±1 (16±9%)	5 43
All	All	200/200 (100%)	169 (84%)	31 (16%)	5 43

All 7 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	23	CYS	7
1	A	7	CYS	6
1	A	9	PRO	6
1	A	11	CYS	5
1	A	12	THR	3
1	A	20	CYS	2
1	A	6	LEU	2

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	5CW	A	4	1	14,16,17	1.51±0.04	3±1 (21±4%)
1	DHA	A	5	1	4,4,5	3.07±0.34	2±0 (50±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	DBB	A	8	1	4,5,6	1.49±0.20	1±0 (23±5%)
1	HYP	A	14	1	6,8,9	1.18±0.25	1±0 (10±8%)
1	DBU	A	2	1	4,5,6	3.30±0.33	2±0 (50±0%)
1	TEE	A	24	1	2,3,3	1.26±0.14	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	5CW	A	4	1	14,22,24	1.82±0.24	3±0 (22±2%)
1	DHA	A	5	1	2,4,6	2.24±0.88	1±1 (42±42%)
1	DBB	A	8	1	1,5,7	0.41±0.30	0±0 (0±0%)
1	HYP	A	14	1	5,10,12	1.01±0.19	0±0 (3±7%)
1	DBU	A	2	1	2,5,7	2.87±0.36	2±0 (82±23%)
1	TEE	A	24	1	0,2,2	0.00±0.00	-

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
1	5CW	A	4	1	-	0±0,4,6,8	0±0,2,2,2
1	TEE	A	24	1	-	0±0,0,1,1	-
1	DBU	A	2	1	-	0±0,1,4,6	-
1	DBB	A	8	1	-	0±0,3,4,6	-
1	HYP	A	14	1	-	0±0,0,11,13	0±0,1,1,1
1	DHA	A	5	1	-	0±0,0,2,4	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	2	DBU	C-CA	6.18	1.55	1.45	20	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	5	DHA	C-CA	5.96	1.54	1.45	17	20
1	A	5	DHA	CA-N	5.26	1.48	1.35	13	20
1	A	2	DBU	CA-N	4.84	1.47	1.35	5	20
1	A	14	HYP	CB-CG	4.00	1.44	1.52	6	12
1	A	8	DBB	CB-CA	3.40	1.62	1.52	13	19
1	A	4	5CW	CD2-CE2	3.27	1.33	1.42	18	20
1	A	4	5CW	CE3-CD2	2.90	1.36	1.42	20	1
1	A	4	5CW	CE3-CZ3	2.34	1.41	1.36	5	16
1	A	4	5CW	CD1-NE1	2.27	1.41	1.36	8	12
1	A	4	5CW	CZ2-CH2	2.20	1.41	1.36	11	12

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	4	5CW	CG-CB-CA	8.56	101.29	114.53	18	20
1	A	5	DHA	CB-CA-N	4.60	114.91	125.81	9	9
1	A	2	DBU	O-C-CA	4.17	120.09	125.39	1	18
1	A	2	DBU	CG-CB-CA	3.36	122.03	126.38	14	15
1	A	4	5CW	CH2-CZ2-CE2	3.25	116.74	120.84	20	20
1	A	4	5CW	CE3-CD2-CE2	3.04	122.42	118.26	20	20
1	A	4	5CW	CB-CA-C	3.01	105.83	111.47	13	2
1	A	5	DHA	O-C-CA	2.72	120.47	125.54	9	8
1	A	14	HYP	CB-CG-CD	2.68	106.55	103.27	20	3

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

65 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds

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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	DPV	A	111	-	22,22,22	1.05±0.03	1±0 (2±2%)
2	DPV	A	120	-	22,22,22	1.02±0.04	0±1 (1±2%)
2	DPV	A	161	-	22,22,22	1.05±0.04	0±0 (1±2%)
2	DPV	A	157	-	22,22,22	1.03±0.03	0±1 (2±2%)
2	DPV	A	152	-	22,22,22	1.04±0.04	0±0 (1±2%)
2	DPV	A	142	-	22,22,22	1.06±0.03	0±0 (0±1%)
2	DPV	A	119	-	22,22,22	1.05±0.04	0±1 (2±3%)
2	DPV	A	114	-	22,22,22	1.04±0.03	0±0 (1±2%)
2	DPV	A	131	-	22,22,22	1.04±0.03	0±1 (1±3%)
2	DPV	A	148	-	22,22,22	1.05±0.03	0±1 (2±2%)
2	DPV	A	134	-	22,22,22	1.03±0.03	0±0 (1±1%)
2	DPV	A	144	-	22,22,22	1.03±0.05	0±1 (2±3%)
2	DPV	A	165	-	22,22,22	1.05±0.03	0±0 (1±1%)
2	DPV	A	115	-	22,22,22	1.05±0.03	0±1 (1±2%)
2	DPV	A	137	-	22,22,22	1.03±0.07	0±1 (0±2%)
2	DPV	A	102	-	22,22,22	1.04±0.04	0±1 (1±2%)
2	DPV	A	149	-	22,22,22	1.03±0.03	0±0 (1±1%)
2	DPV	A	156	-	22,22,22	1.05±0.04	0±0 (0±1%)
2	DPV	A	116	-	22,22,22	1.05±0.04	0±1 (2±3%)
2	DPV	A	158	-	22,22,22	1.06±0.04	0±1 (2±2%)
2	DPV	A	138	-	22,22,22	1.05±0.04	0±1 (1±3%)
2	DPV	A	163	-	22,22,22	1.04±0.03	0±1 (1±2%)
2	DPV	A	128	-	22,22,22	1.04±0.03	0±1 (1±2%)
2	DPV	A	143	-	22,22,22	1.03±0.03	0±1 (1±2%)
2	DPV	A	153	-	22,22,22	1.07±0.04	1±1 (2±3%)
2	DPV	A	160	-	22,22,22	1.02±0.03	0±0 (0±1%)
2	DPV	A	130	-	22,22,22	1.03±0.03	0±1 (1±2%)
2	DPV	A	147	-	22,22,22	1.04±0.04	0±0 (1±2%)
2	DPV	A	110	-	22,22,22	1.05±0.04	1±1 (2±3%)
2	DPV	A	126	-	22,22,22	1.04±0.04	0±0 (0±1%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	DPV	A	141	-	22,22,22	1.02±0.04	0±1 (1±2%)
2	DPV	A	105	-	22,22,22	1.04±0.03	0±1 (1±2%)
2	DPV	A	121	-	22,22,22	1.03±0.03	0±1 (1±2%)
2	DPV	A	104	-	22,22,22	1.05±0.04	0±1 (1±2%)
2	DPV	A	139	-	22,22,22	1.06±0.03	1±1 (3±3%)
2	DPV	A	151	-	22,22,22	1.02±0.03	0±0 (0±1%)
2	DPV	A	132	-	22,22,22	1.05±0.02	0±1 (1±2%)
2	DPV	A	125	-	22,22,22	1.04±0.04	1±1 (2±3%)
2	DPV	A	162	-	22,22,22	1.03±0.04	0±1 (1±2%)
2	DPV	A	117	-	22,22,22	1.05±0.03	0±1 (1±2%)
2	DPV	A	159	-	22,22,22	1.05±0.04	0±1 (2±3%)
2	DPV	A	101	-	22,22,22	1.04±0.04	0±1 (1±3%)
2	DPV	A	164	-	22,22,22	1.04±0.03	0±0 (0±1%)
2	DPV	A	108	-	22,22,22	1.04±0.03	0±1 (2±3%)
2	DPV	A	122	-	22,22,22	1.05±0.03	0±0 (1±2%)
2	DPV	A	155	-	22,22,22	1.04±0.03	0±1 (1±3%)
2	DPV	A	106	-	22,22,22	1.05±0.03	0±0 (1±2%)
2	DPV	A	113	-	22,22,22	1.05±0.04	0±1 (1±2%)
2	DPV	A	109	-	22,22,22	1.04±0.02	0±1 (1±2%)
2	DPV	A	124	-	22,22,22	1.05±0.04	0±1 (2±3%)
2	DPV	A	135	-	22,22,22	1.06±0.04	0±1 (1±2%)
2	DPV	A	133	-	22,22,22	1.04±0.03	0±1 (1±2%)
2	DPV	A	140	-	22,22,22	1.06±0.03	1±1 (2±3%)
2	DPV	A	107	-	22,22,22	1.05±0.03	0±1 (2±3%)
2	DPV	A	103	-	22,22,22	1.06±0.04	0±1 (1±2%)
2	DPV	A	129	-	22,22,22	1.02±0.02	1±1 (2±2%)
2	DPV	A	150	-	22,22,22	1.05±0.07	0±1 (1±4%)
2	DPV	A	136	-	22,22,22	1.03±0.03	0±0 (0±1%)
2	DPV	A	123	-	22,22,22	1.06±0.04	0±1 (2±3%)
2	DPV	A	146	-	22,22,22	1.04±0.03	0±1 (2±3%)
2	DPV	A	154	-	22,22,22	1.05±0.04	0±0 (1±2%)
2	DPV	A	127	-	22,22,22	1.06±0.03	0±1 (1±2%)
2	DPV	A	145	-	22,22,22	1.05±0.04	0±1 (1±3%)
2	DPV	A	112	-	22,22,22	1.05±0.03	0±0 (2±2%)
2	DPV	A	118	-	22,22,22	1.05±0.03	0±1 (2±3%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DPV	A	111	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	120	-	26,27,27	0.64±0.02	0±0 (0±0%)
2	DPV	A	161	-	26,27,27	0.59±0.03	0±0 (0±0%)
2	DPV	A	157	-	26,27,27	0.62±0.02	0±0 (0±0%)
2	DPV	A	152	-	26,27,27	0.60±0.04	0±0 (0±0%)
2	DPV	A	142	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	119	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	114	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	131	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	148	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	134	-	26,27,27	0.61±0.02	0±0 (0±0%)
2	DPV	A	144	-	26,27,27	0.64±0.03	0±0 (0±0%)
2	DPV	A	165	-	26,27,27	0.61±0.02	0±0 (0±0%)
2	DPV	A	115	-	26,27,27	0.61±0.05	0±0 (0±0%)
2	DPV	A	137	-	26,27,27	0.63±0.02	0±0 (0±0%)
2	DPV	A	102	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	149	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	156	-	26,27,27	0.59±0.02	0±0 (0±0%)
2	DPV	A	116	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	158	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	138	-	26,27,27	0.61±0.02	0±0 (0±0%)
2	DPV	A	163	-	26,27,27	0.61±0.02	0±0 (0±0%)
2	DPV	A	128	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	143	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	153	-	26,27,27	0.59±0.03	0±0 (0±0%)
2	DPV	A	160	-	26,27,27	0.63±0.02	0±0 (0±0%)
2	DPV	A	130	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	147	-	26,27,27	0.59±0.03	0±0 (0±0%)
2	DPV	A	110	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	126	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	141	-	26,27,27	0.63±0.03	0±0 (0±0%)
2	DPV	A	105	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	121	-	26,27,27	0.62±0.03	0±0 (0±0%)
2	DPV	A	104	-	26,27,27	0.59±0.04	0±0 (0±0%)
2	DPV	A	139	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	151	-	26,27,27	0.62±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DPV	A	132	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	125	-	26,27,27	0.61±0.02	0±0 (0±0%)
2	DPV	A	162	-	26,27,27	0.62±0.02	0±0 (0±0%)
2	DPV	A	117	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	159	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	101	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	164	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	108	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	122	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	155	-	26,27,27	0.62±0.04	0±0 (0±0%)
2	DPV	A	106	-	26,27,27	0.61±0.03	0±0 (0±0%)
2	DPV	A	113	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	109	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	124	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	135	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	133	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	140	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	107	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	103	-	26,27,27	0.59±0.02	0±0 (0±0%)
2	DPV	A	129	-	26,27,27	0.62±0.02	0±0 (0±0%)
2	DPV	A	150	-	26,27,27	0.60±0.02	0±0 (0±0%)
2	DPV	A	136	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	123	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	146	-	26,27,27	0.61±0.02	0±0 (0±0%)
2	DPV	A	154	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	127	-	26,27,27	0.59±0.02	0±0 (0±0%)
2	DPV	A	145	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	112	-	26,27,27	0.60±0.03	0±0 (0±0%)
2	DPV	A	118	-	26,27,27	0.61±0.03	0±0 (0±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	DPV	A	157	-	-	0±0,22,22,22	-
2	DPV	A	156	-	-	0±0,22,22,22	-
2	DPV	A	119	-	-	0±0,22,22,22	-
2	DPV	A	104	-	-	0±0,22,22,22	-
2	DPV	A	164	-	-	0±0,22,22,22	-
2	DPV	A	143	-	-	0±0,22,22,22	-
2	DPV	A	147	-	-	0±0,22,22,22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPV	A	109	-	-	0±0,22,22,22	-
2	DPV	A	159	-	-	0±0,22,22,22	-
2	DPV	A	160	-	-	0±0,22,22,22	-
2	DPV	A	151	-	-	0±0,22,22,22	-
2	DPV	A	114	-	-	0±0,22,22,22	-
2	DPV	A	111	-	-	0±0,22,22,22	-
2	DPV	A	131	-	-	0±0,22,22,22	-
2	DPV	A	136	-	-	0±0,22,22,22	-
2	DPV	A	102	-	-	0±0,22,22,22	-
2	DPV	A	155	-	-	0±0,22,22,22	-
2	DPV	A	133	-	-	0±0,22,22,22	-
2	DPV	A	165	-	-	0±0,22,22,22	-
2	DPV	A	134	-	-	0±0,22,22,22	-
2	DPV	A	120	-	-	0±0,22,22,22	-
2	DPV	A	129	-	-	0±0,22,22,22	-
2	DPV	A	152	-	-	0±0,22,22,22	-
2	DPV	A	140	-	-	0±0,22,22,22	-
2	DPV	A	122	-	-	0±0,22,22,22	-
2	DPV	A	145	-	-	0±0,22,22,22	-
2	DPV	A	146	-	-	0±0,22,22,22	-
2	DPV	A	106	-	-	0±0,22,22,22	-
2	DPV	A	135	-	-	0±0,22,22,22	-
2	DPV	A	163	-	-	0±0,22,22,22	-
2	DPV	A	112	-	-	0±0,22,22,22	-
2	DPV	A	108	-	-	0±0,22,22,22	-
2	DPV	A	142	-	-	0±0,22,22,22	-
2	DPV	A	154	-	-	0±0,22,22,22	-
2	DPV	A	103	-	-	0±0,22,22,22	-
2	DPV	A	117	-	-	0±0,22,22,22	-
2	DPV	A	139	-	-	0±0,22,22,22	-
2	DPV	A	144	-	-	0±0,22,22,22	-
2	DPV	A	123	-	-	0±0,22,22,22	-
2	DPV	A	132	-	-	0±0,22,22,22	-
2	DPV	A	150	-	-	0±0,22,22,22	-
2	DPV	A	138	-	-	0±0,22,22,22	-
2	DPV	A	130	-	-	0±0,22,22,22	-
2	DPV	A	158	-	-	0±0,22,22,22	-
2	DPV	A	101	-	-	0±0,22,22,22	-
2	DPV	A	162	-	-	0±0,22,22,22	-
2	DPV	A	127	-	-	0±0,22,22,22	-
2	DPV	A	124	-	-	0±0,22,22,22	-
2	DPV	A	148	-	-	0±0,22,22,22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPV	A	125	-	-	0±0,22,22,22	-
2	DPV	A	110	-	-	0±0,22,22,22	-
2	DPV	A	113	-	-	0±0,22,22,22	-
2	DPV	A	121	-	-	0±0,22,22,22	-
2	DPV	A	105	-	-	0±0,22,22,22	-
2	DPV	A	128	-	-	0±0,22,22,22	-
2	DPV	A	141	-	-	0±0,22,22,22	-
2	DPV	A	116	-	-	0±0,22,22,22	-
2	DPV	A	161	-	-	0±0,22,22,22	-
2	DPV	A	149	-	-	0±0,22,22,22	-
2	DPV	A	153	-	-	0±0,22,22,22	-
2	DPV	A	118	-	-	0±0,22,22,22	-
2	DPV	A	107	-	-	0±0,22,22,22	-
2	DPV	A	137	-	-	0±0,22,22,22	-
2	DPV	A	115	-	-	0±0,22,22,22	-
2	DPV	A	126	-	-	0±0,22,22,22	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	125	DPV	C5-N	3.26	1.62	1.51	20	5
2	A	150	DPV	C5-C4	3.14	1.61	1.51	20	2
2	A	125	DPV	C5-C4	3.02	1.60	1.51	20	7
2	A	116	DPV	C5-C4	3.01	1.60	1.51	20	4
2	A	157	DPV	C5-C4	3.01	1.60	1.51	20	5
2	A	105	DPV	C5-C4	2.85	1.60	1.51	20	2
2	A	141	DPV	C7-N	2.79	1.58	1.50	20	1
2	A	128	DPV	C7-N	2.76	1.58	1.50	20	1
2	A	138	DPV	C5-N	2.67	1.60	1.51	20	4
2	A	127	DPV	C5-C4	2.64	1.59	1.51	20	4
2	A	135	DPV	C5-C4	2.64	1.59	1.51	20	4
2	A	153	DPV	C5-C4	2.61	1.59	1.51	20	6
2	A	137	DPV	C6-N	2.56	1.57	1.50	20	1
2	A	131	DPV	C5-N	2.56	1.59	1.51	20	5
2	A	101	DPV	C6-N	2.56	1.57	1.50	20	1
2	A	126	DPV	C5-C4	2.55	1.59	1.51	20	3
2	A	149	DPV	C5-C4	2.54	1.59	1.51	20	5
2	A	137	DPV	C5-C4	2.53	1.59	1.51	20	2
2	A	121	DPV	C5-C4	2.51	1.59	1.51	20	6
2	A	119	DPV	C5-C4	2.49	1.59	1.51	20	7
2	A	102	DPV	C7-N	2.47	1.57	1.50	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	110	DPV	C5-C4	2.46	1.59	1.51	20	7
2	A	144	DPV	C5-N	2.44	1.59	1.51	20	2
2	A	159	DPV	C5-C4	2.44	1.59	1.51	20	5
2	A	113	DPV	C5-N	2.40	1.59	1.51	20	2
2	A	160	DPV	C5-N	2.40	1.59	1.51	20	1
2	A	117	DPV	C5-C4	2.39	1.58	1.51	11	6
2	A	162	DPV	C5-C4	2.38	1.58	1.51	20	3
2	A	108	DPV	C8-N	2.36	1.56	1.50	20	1
2	A	129	DPV	C5-C4	2.36	1.58	1.51	20	11
2	A	129	DPV	C5-N	2.35	1.59	1.51	20	1
2	A	144	DPV	C5-C4	2.35	1.58	1.51	16	5
2	A	123	DPV	C5-C4	2.34	1.58	1.51	20	4
2	A	130	DPV	C5-C4	2.33	1.58	1.51	3	1
2	A	112	DPV	C5-C4	2.33	1.58	1.51	20	6
2	A	108	DPV	C5-C4	2.32	1.58	1.51	12	6
2	A	144	DPV	C6-N	2.32	1.56	1.50	20	1
2	A	164	DPV	C5-N	2.32	1.59	1.51	20	2
2	A	104	DPV	C5-C4	2.31	1.58	1.51	8	2
2	A	107	DPV	C5-C4	2.30	1.58	1.51	2	6
2	A	115	DPV	C7-N	2.30	1.56	1.50	20	1
2	A	132	DPV	C6-N	2.29	1.56	1.50	20	1
2	A	138	DPV	C5-C4	2.30	1.58	1.51	12	3
2	A	142	DPV	C7-N	2.30	1.56	1.50	20	1
2	A	140	DPV	C5-C4	2.29	1.58	1.51	20	8
2	A	134	DPV	C5-C4	2.29	1.58	1.51	20	2
2	A	131	DPV	C5-C4	2.29	1.58	1.51	14	3
2	A	102	DPV	C5-C4	2.28	1.58	1.51	20	5
2	A	106	DPV	C7-N	2.28	1.56	1.50	20	1
2	A	142	DPV	C5-N	2.27	1.58	1.51	14	1
2	A	118	DPV	C5-C4	2.24	1.58	1.51	14	6
2	A	144	DPV	C7-N	2.24	1.56	1.50	20	1
2	A	148	DPV	C5-N	2.24	1.58	1.51	20	2
2	A	113	DPV	C6-N	2.24	1.56	1.50	20	1
2	A	139	DPV	C5-C4	2.23	1.58	1.51	20	6
2	A	158	DPV	C8-N	2.23	1.56	1.50	20	1
2	A	150	DPV	C6-N	2.23	1.56	1.50	20	1
2	A	150	DPV	C5-N	2.22	1.58	1.51	20	2
2	A	157	DPV	C5-N	2.22	1.58	1.51	8	4
2	A	154	DPV	C5-C4	2.22	1.58	1.51	20	6
2	A	114	DPV	C5-C4	2.22	1.58	1.51	16	4
2	A	123	DPV	C6-N	2.22	1.56	1.50	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	161	DPV	C5-C4	2.22	1.58	1.51	8	4
2	A	124	DPV	C5-C4	2.21	1.58	1.51	18	6
2	A	139	DPV	C5-N	2.21	1.58	1.51	4	8
2	A	146	DPV	C5-N	2.21	1.58	1.51	14	5
2	A	158	DPV	C5-N	2.21	1.58	1.51	5	2
2	A	132	DPV	C5-C4	2.21	1.58	1.51	12	5
2	A	152	DPV	C5-C4	2.20	1.58	1.51	4	6
2	A	136	DPV	C5-C4	2.20	1.58	1.51	2	4
2	A	145	DPV	C5-C4	2.19	1.58	1.51	1	4
2	A	103	DPV	C5-N	2.19	1.58	1.51	13	3
2	A	163	DPV	C5-C4	2.19	1.58	1.51	20	4
2	A	130	DPV	C7-N	2.17	1.56	1.50	20	1
2	A	155	DPV	C5-C4	2.17	1.58	1.51	13	3
2	A	148	DPV	C5-C4	2.17	1.58	1.51	6	8
2	A	128	DPV	C5-C4	2.16	1.58	1.51	8	4
2	A	101	DPV	C5-N	2.16	1.58	1.51	6	2
2	A	119	DPV	C8-N	2.16	1.56	1.50	20	1
2	A	146	DPV	C5-C4	2.16	1.58	1.51	20	5
2	A	159	DPV	C5-N	2.16	1.58	1.51	19	5
2	A	147	DPV	C5-C4	2.16	1.58	1.51	5	5
2	A	140	DPV	C5-N	2.16	1.58	1.51	2	4
2	A	120	DPV	C5-C4	2.15	1.58	1.51	13	2
2	A	156	DPV	C5-C4	2.15	1.58	1.51	17	2
2	A	103	DPV	C5-C4	2.15	1.58	1.51	20	5
2	A	109	DPV	C5-C4	2.15	1.58	1.51	14	2
2	A	115	DPV	C5-C4	2.14	1.58	1.51	10	5
2	A	133	DPV	C5-C4	2.14	1.58	1.51	13	4
2	A	124	DPV	C5-N	2.14	1.58	1.51	11	4
2	A	116	DPV	C5-N	2.14	1.58	1.51	9	4
2	A	151	DPV	C5-C4	2.14	1.58	1.51	8	4
2	A	145	DPV	C7-N	2.13	1.56	1.50	20	1
2	A	114	DPV	C5-N	2.13	1.58	1.51	20	2
2	A	162	DPV	C8-N	2.12	1.56	1.50	20	1
2	A	105	DPV	C5-N	2.12	1.58	1.51	18	3
2	A	143	DPV	C5-C4	2.12	1.58	1.51	20	4
2	A	133	DPV	C5-N	2.12	1.58	1.51	11	4
2	A	111	DPV	C5-N	2.12	1.58	1.51	20	5
2	A	128	DPV	C5-N	2.12	1.58	1.51	3	2
2	A	141	DPV	C6-N	2.12	1.56	1.50	20	1
2	A	101	DPV	C5-C4	2.12	1.57	1.51	20	5
2	A	118	DPV	C7-N	2.11	1.56	1.50	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	132	DPV	C5-N	2.11	1.58	1.51	2	2
2	A	163	DPV	C5-N	2.11	1.58	1.51	16	3
2	A	115	DPV	C8-N	2.11	1.56	1.50	20	1
2	A	120	DPV	C5-N	2.11	1.58	1.51	14	2
2	A	155	DPV	C6-N	2.11	1.56	1.50	20	1
2	A	135	DPV	C8-N	2.10	1.56	1.50	20	1
2	A	110	DPV	C5-N	2.10	1.58	1.51	11	5
2	A	111	DPV	C5-C4	2.09	1.57	1.51	1	6
2	A	116	DPV	C6-N	2.09	1.56	1.50	20	1
2	A	130	DPV	C5-N	2.09	1.58	1.51	13	2
2	A	164	DPV	C5-C4	2.09	1.57	1.51	3	2
2	A	160	DPV	C5-C4	2.09	1.57	1.51	5	3
2	A	106	DPV	C5-C4	2.08	1.57	1.51	9	5
2	A	120	DPV	C8-N	2.08	1.56	1.50	20	1
2	A	127	DPV	C5-N	2.08	1.58	1.51	20	2
2	A	150	DPV	C8-N	2.08	1.56	1.50	20	1
2	A	165	DPV	C5-C4	2.08	1.57	1.51	1	5
2	A	123	DPV	C5-N	2.08	1.58	1.51	9	4
2	A	153	DPV	C5-N	2.08	1.58	1.51	17	5
2	A	104	DPV	C5-N	2.08	1.58	1.51	18	4
2	A	109	DPV	C6-N	2.08	1.56	1.50	20	1
2	A	107	DPV	C5-N	2.07	1.58	1.51	20	3
2	A	112	DPV	C5-N	2.07	1.58	1.51	15	3
2	A	122	DPV	C5-N	2.07	1.58	1.51	14	3
2	A	158	DPV	C5-C4	2.07	1.57	1.51	20	7
2	A	113	DPV	C5-C4	2.07	1.57	1.51	4	4
2	A	155	DPV	C5-N	2.07	1.58	1.51	20	3
2	A	118	DPV	C5-N	2.07	1.58	1.51	14	3
2	A	106	DPV	C5-N	2.07	1.58	1.51	19	2
2	A	119	DPV	C5-N	2.07	1.58	1.51	9	2
2	A	109	DPV	C5-N	2.06	1.58	1.51	5	4
2	A	135	DPV	C5-N	2.06	1.58	1.51	4	1
2	A	108	DPV	C5-N	2.06	1.58	1.51	12	3
2	A	134	DPV	C5-N	2.06	1.58	1.51	10	3
2	A	141	DPV	C5-C4	2.05	1.57	1.51	8	2
2	A	122	DPV	C5-C4	2.05	1.57	1.51	8	3
2	A	130	DPV	P-O1P	2.04	1.45	1.55	20	1
2	A	161	DPV	C5-N	2.04	1.58	1.51	19	2
2	A	117	DPV	C7-N	2.04	1.56	1.50	20	1
2	A	147	DPV	C5-N	2.04	1.58	1.51	17	1
2	A	141	DPV	C5-N	2.04	1.58	1.51	18	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	142	DPV	C5-C4	2.03	1.57	1.51	12	2
2	A	143	DPV	C5-N	2.03	1.58	1.51	13	3
2	A	162	DPV	C5-N	2.03	1.58	1.51	13	1
2	A	138	DPV	P-O1P	2.02	1.45	1.55	20	1
2	A	137	DPV	C5-N	2.02	1.58	1.51	11	1
2	A	109	DPV	C7-N	2.01	1.55	1.50	20	1
2	A	121	DPV	C5-N	2.01	1.58	1.51	18	1
2	A	145	DPV	C5-N	2.01	1.58	1.51	17	1
2	A	154	DPV	C5-N	2.01	1.58	1.51	12	1
2	A	102	DPV	C5-N	2.01	1.58	1.51	3	1
2	A	126	DPV	C5-N	2.01	1.58	1.51	16	1
2	A	115	DPV	C5-N	2.00	1.58	1.51	4	1
2	A	145	DPV	C6-N	2.00	1.55	1.50	20	1

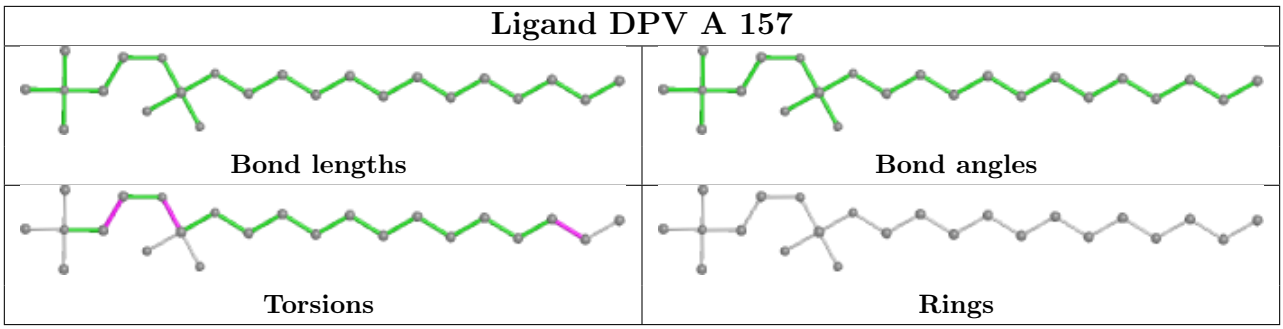
There are no bond-angle outliers.

There are no chirality outliers.

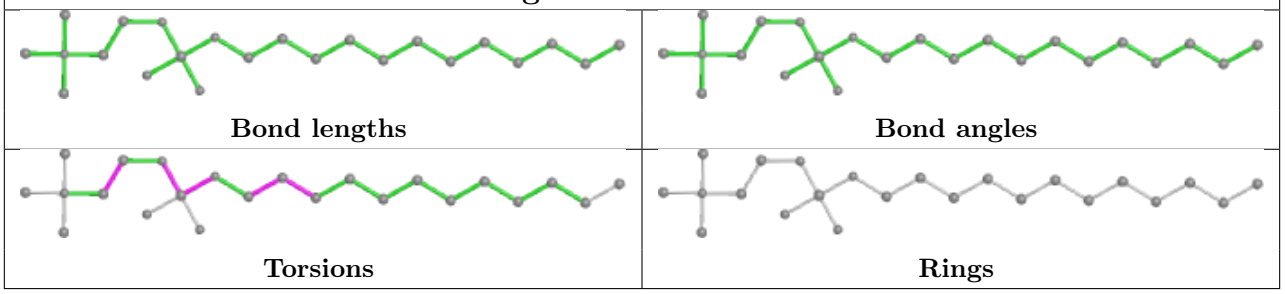
There are no torsion outliers.

There are no ring outliers.

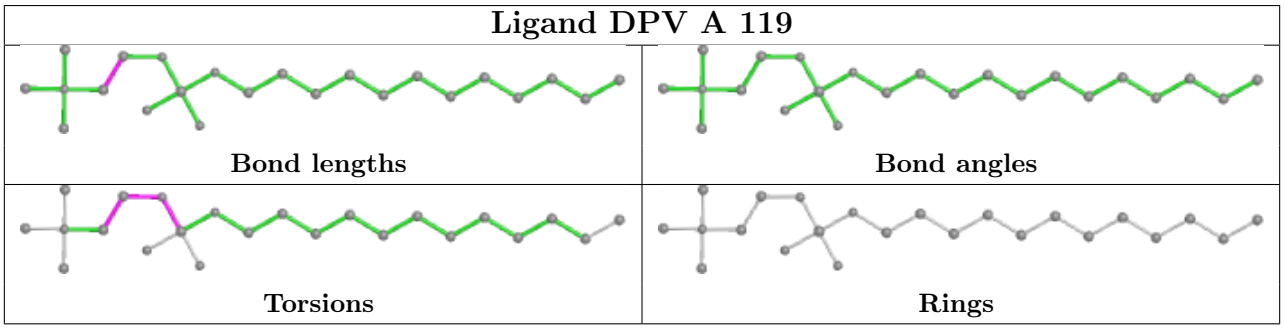
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



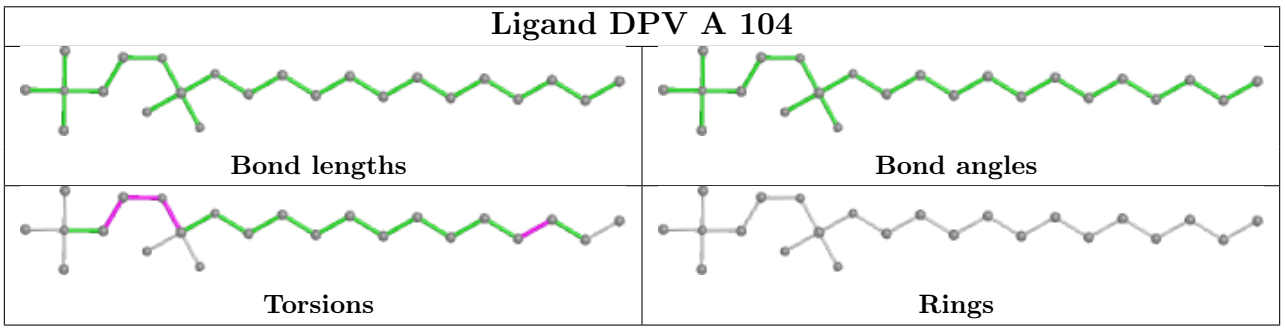
Ligand DPV A 156



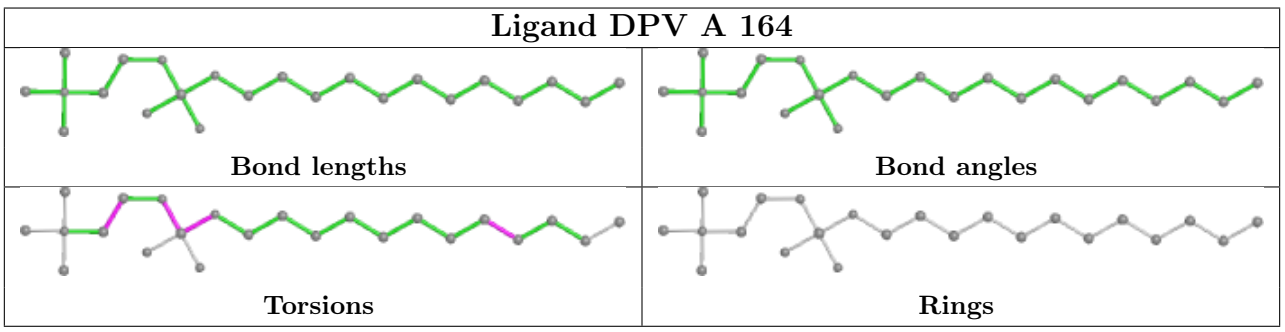
Ligand DPV A 119



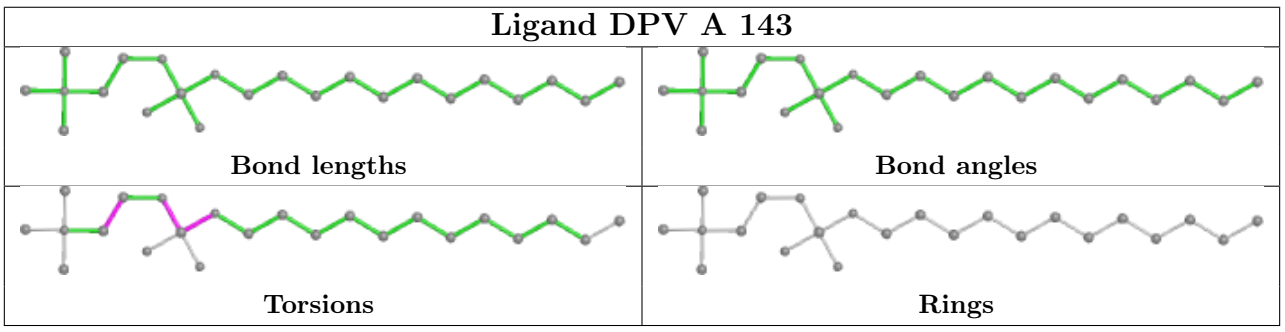
Ligand DPV A 104



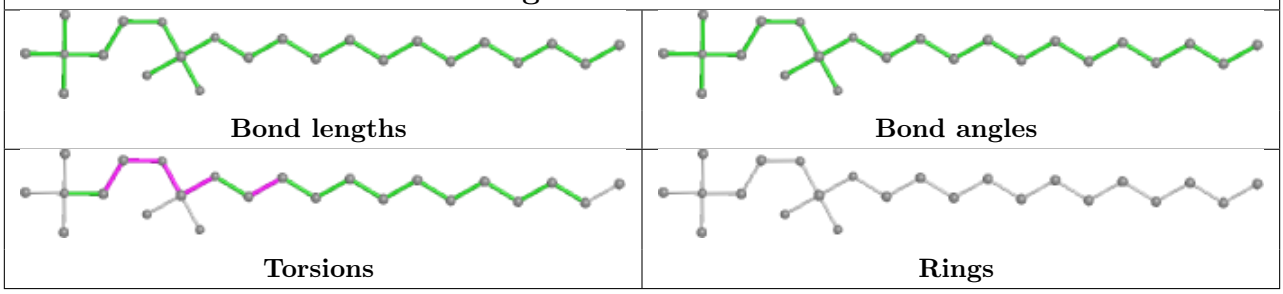
Ligand DPV A 164



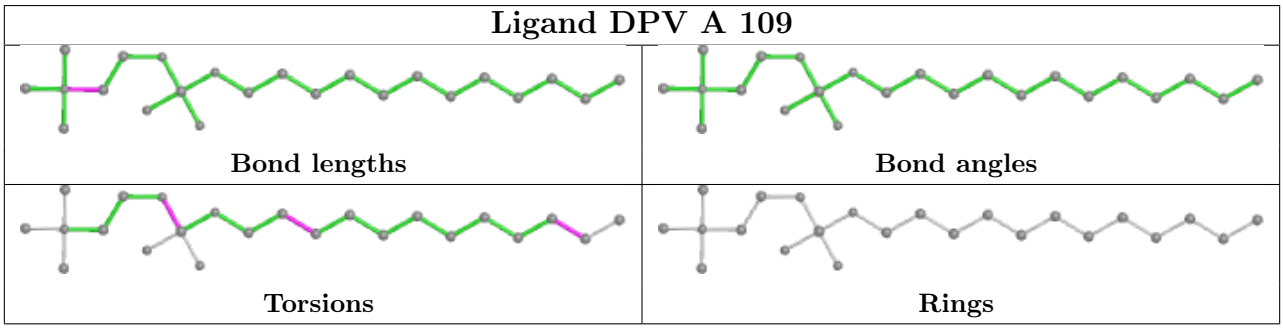
Ligand DPV A 143



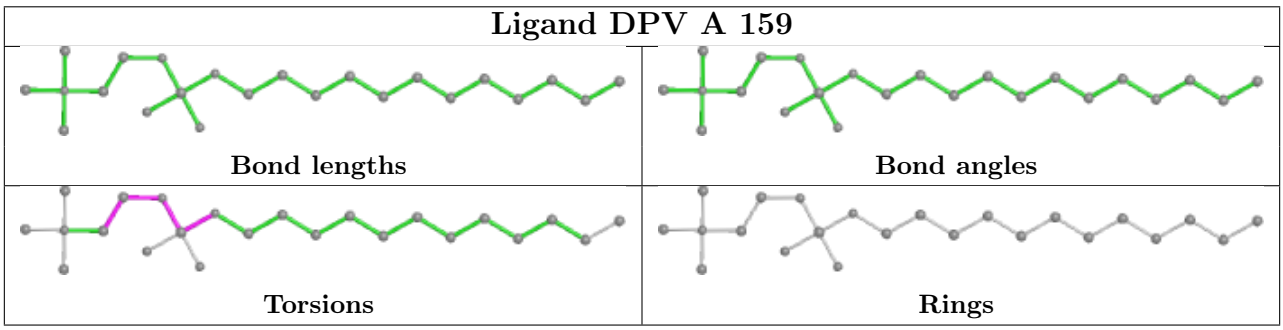
Ligand DPV A 147



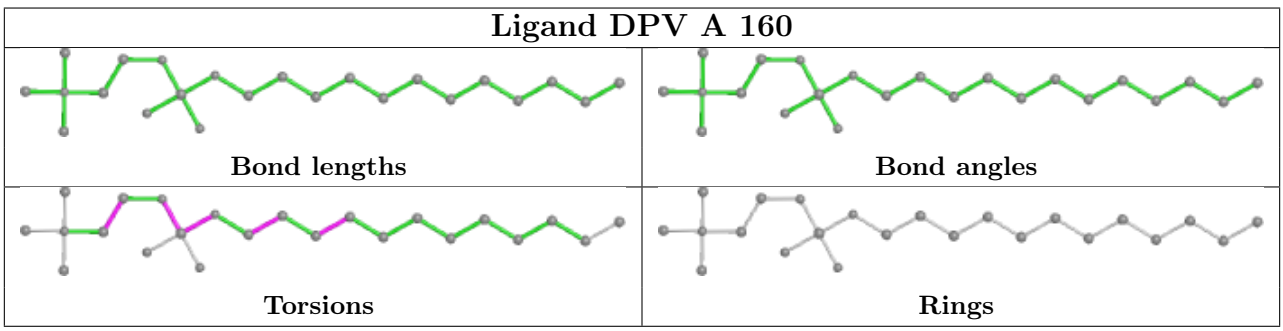
Ligand DPV A 109



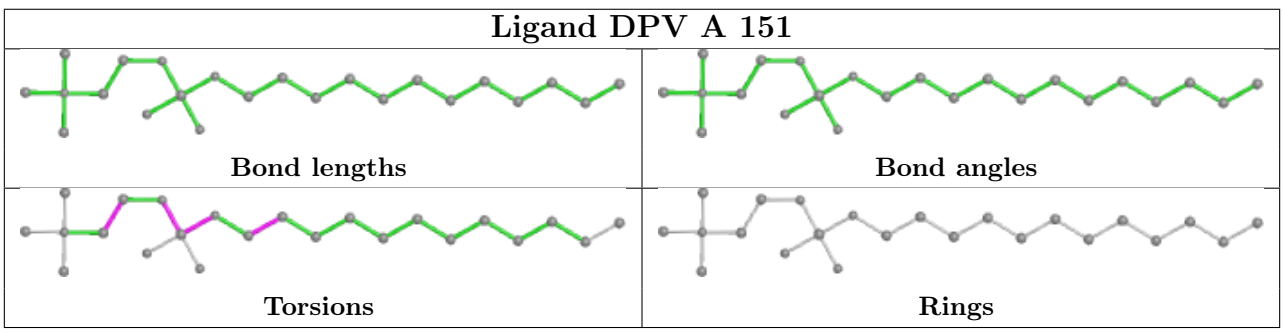
Ligand DPV A 159



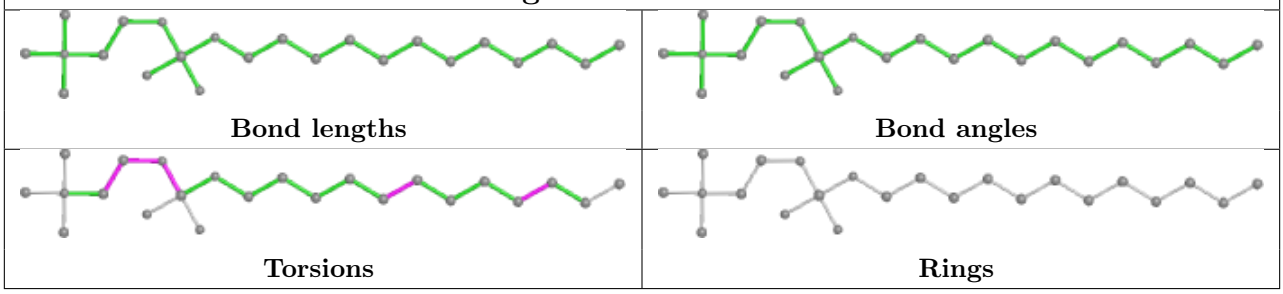
Ligand DPV A 160



Ligand DPV A 151



Ligand DPV A 114



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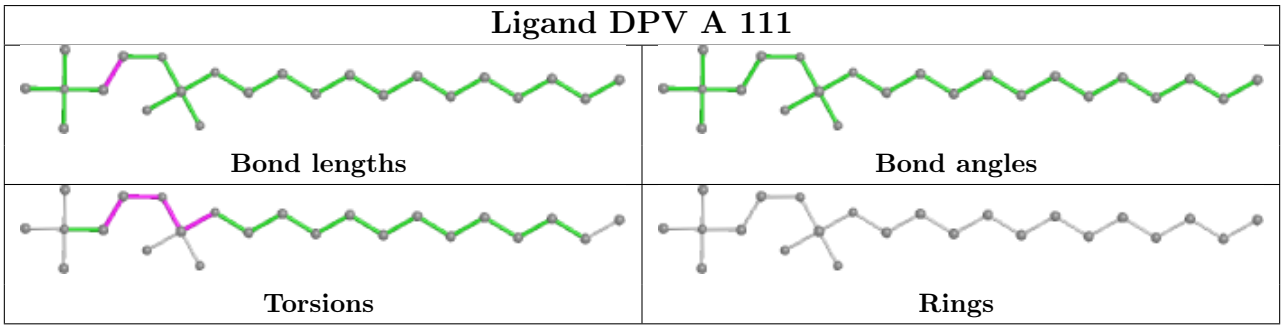

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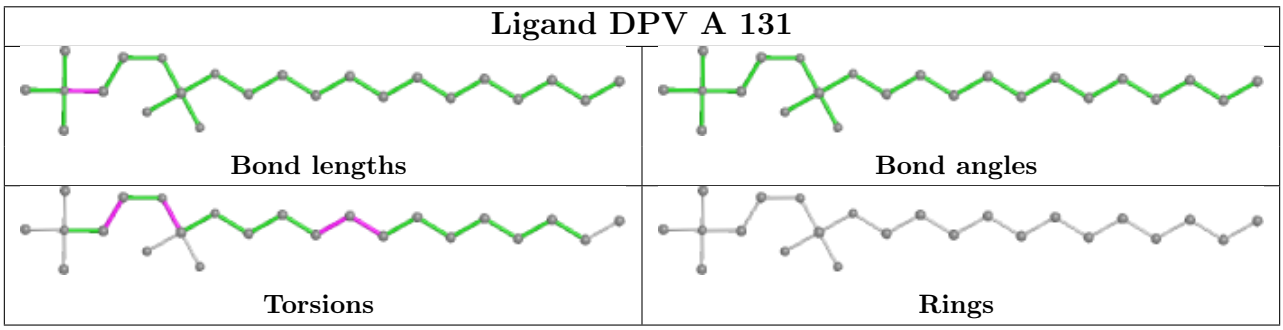

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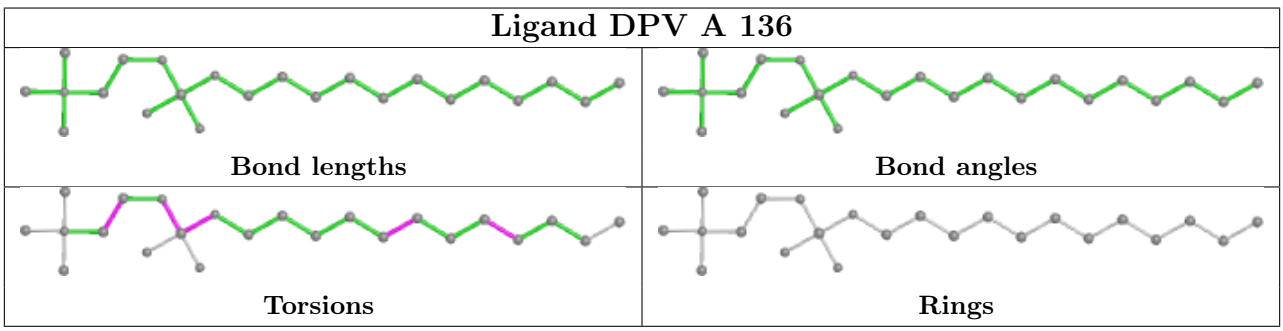

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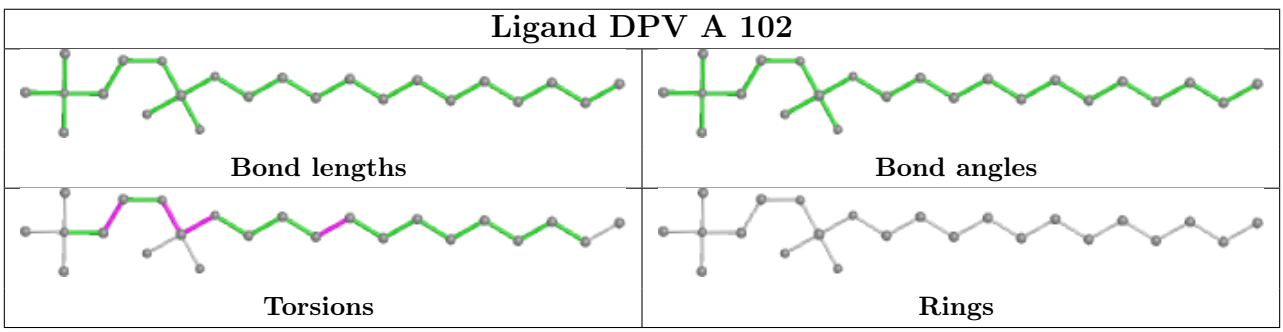

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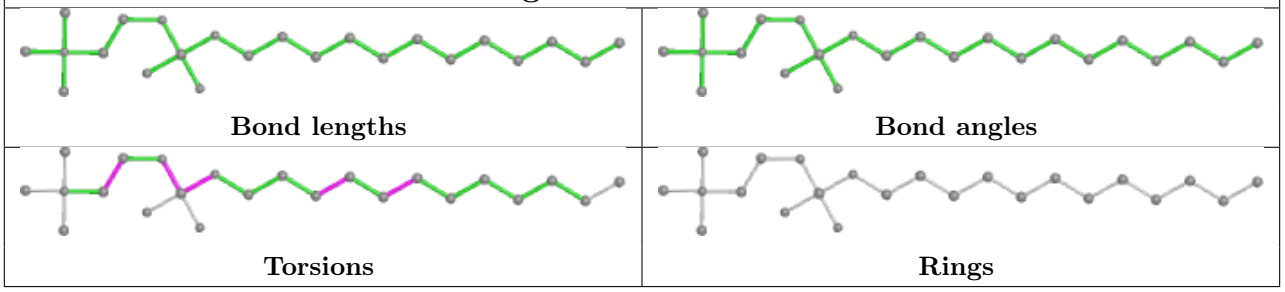

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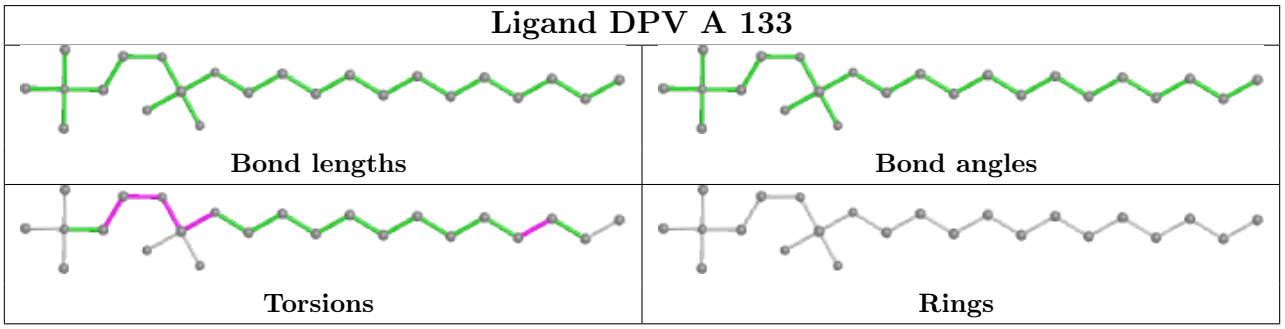

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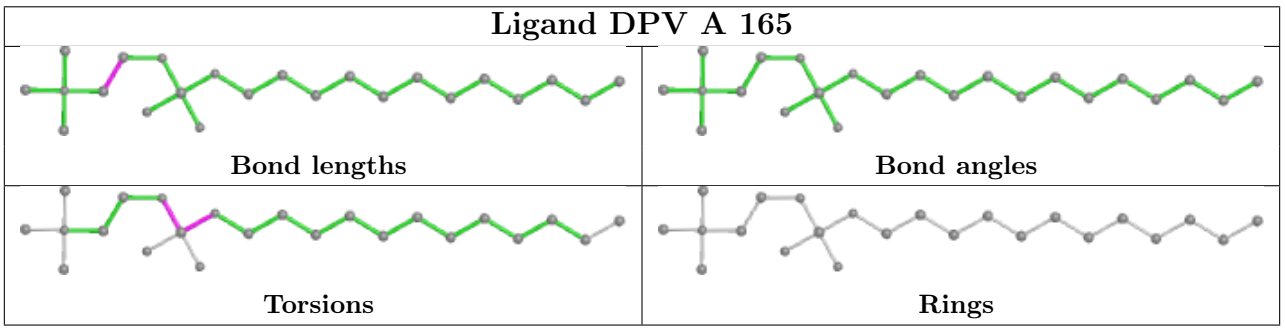

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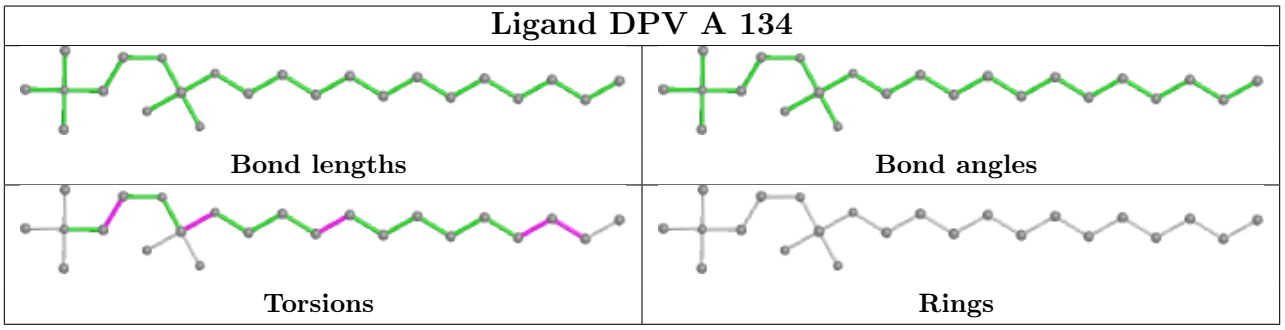

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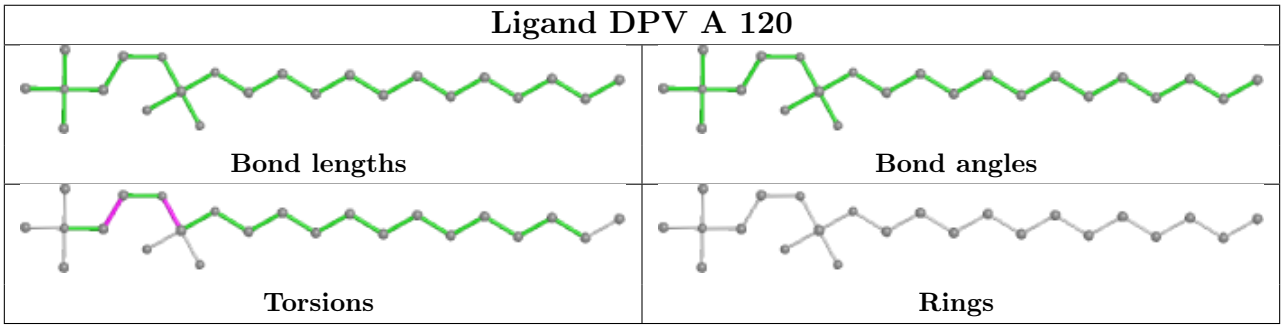

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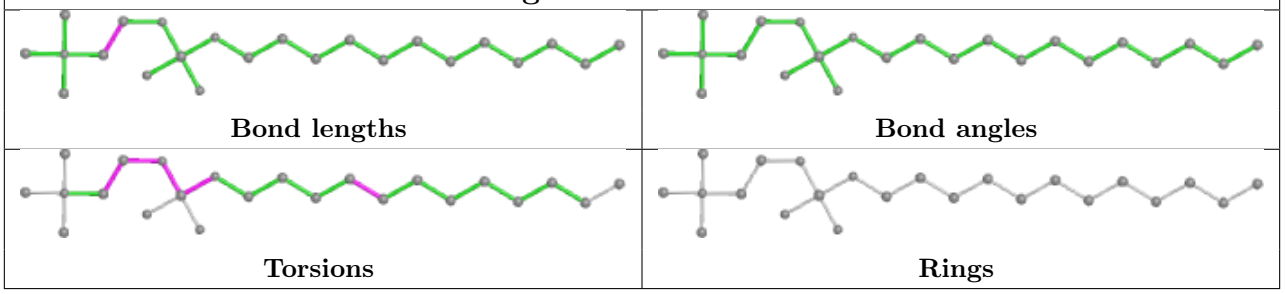

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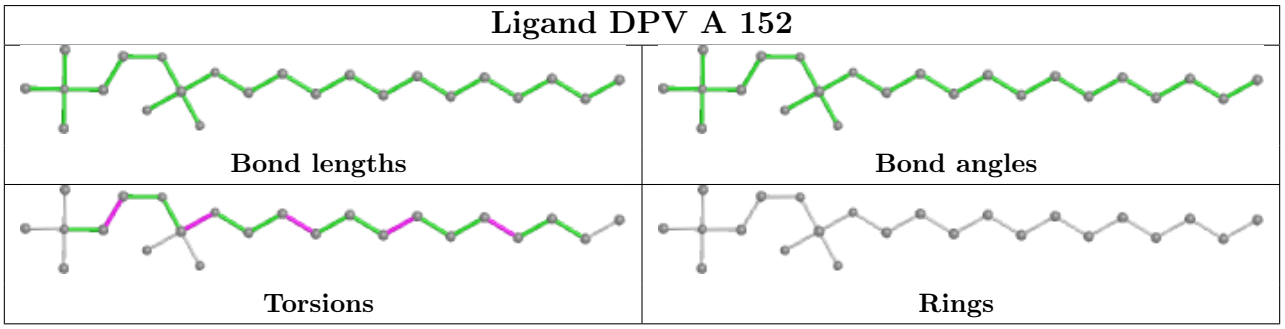

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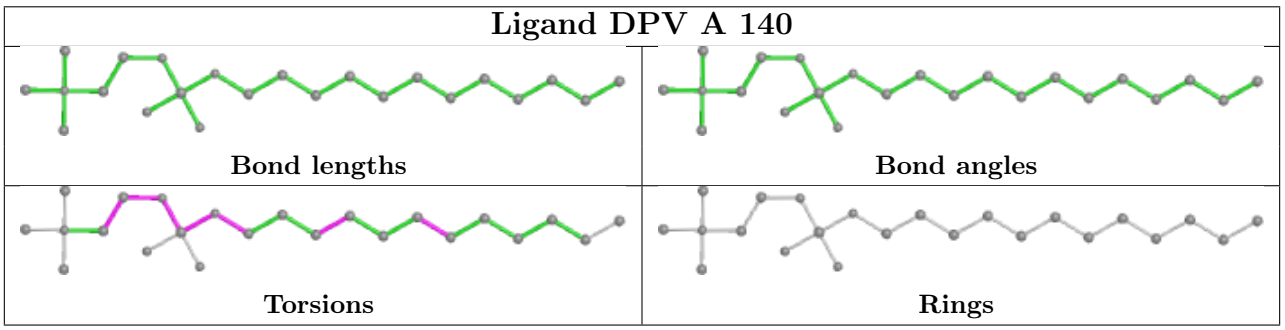

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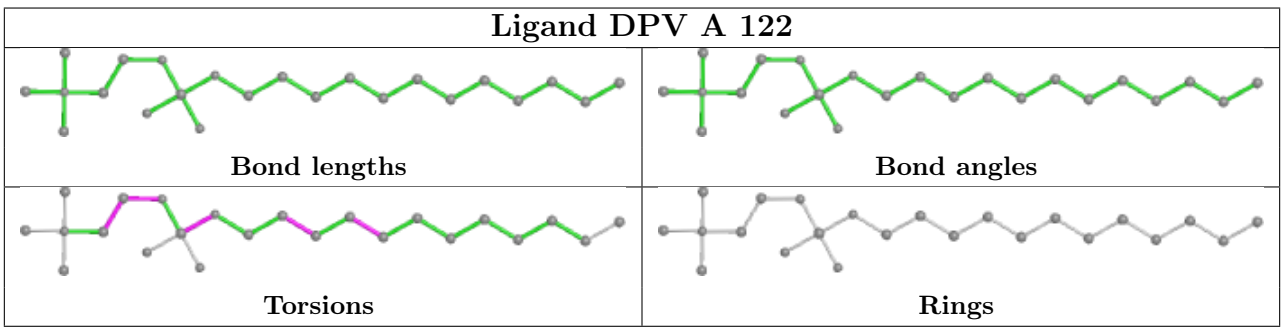

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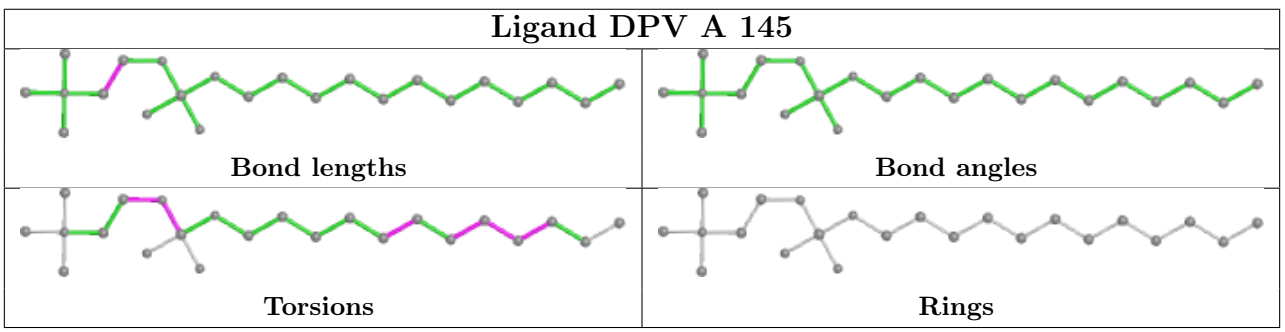

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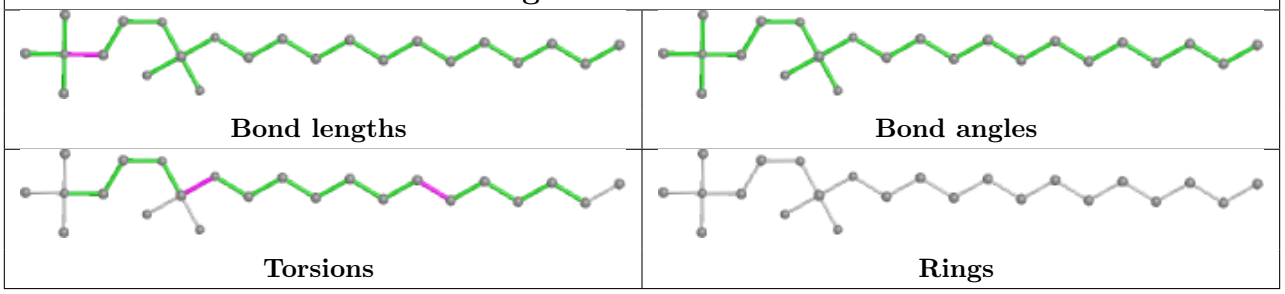
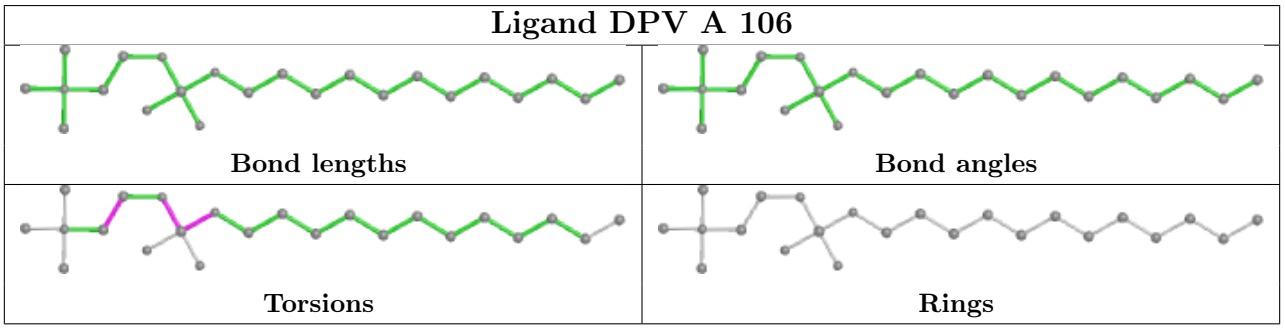


Ligand DPV A 106



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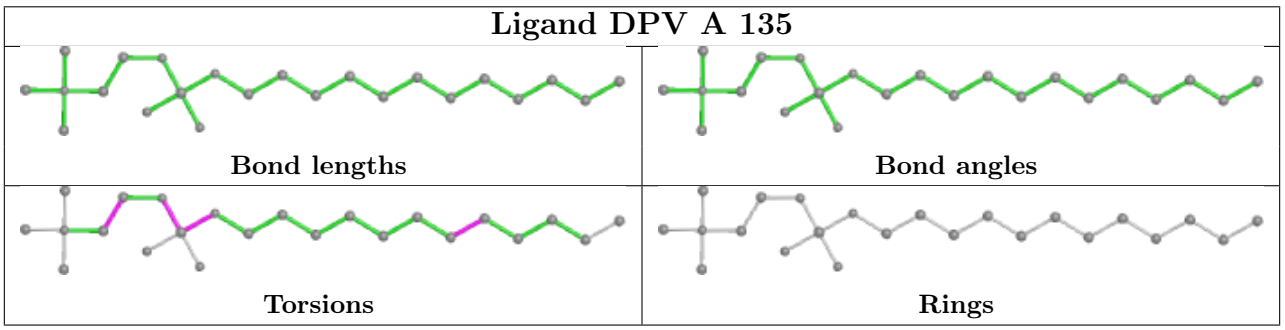
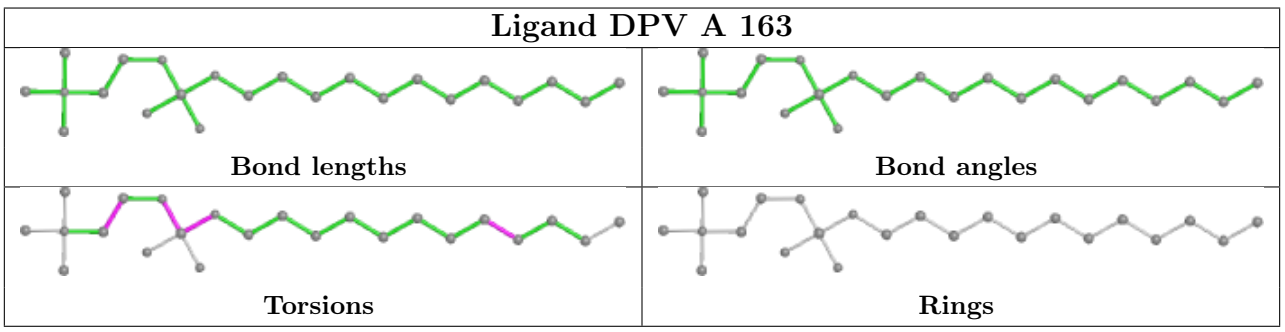
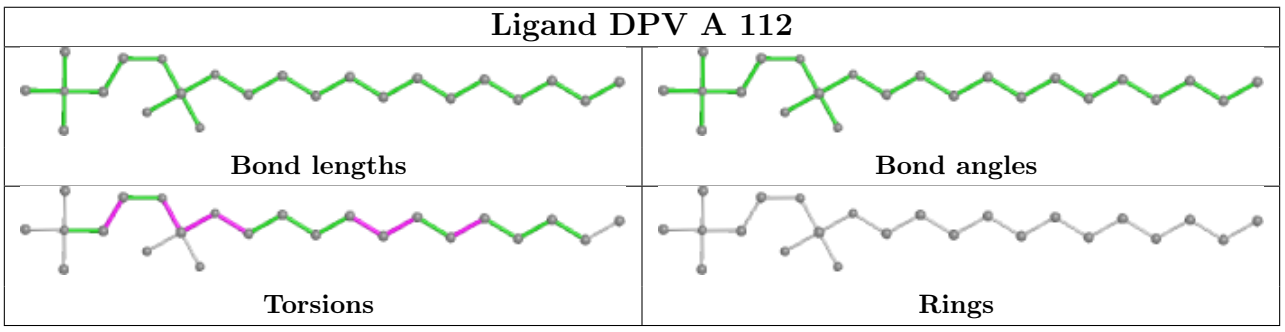


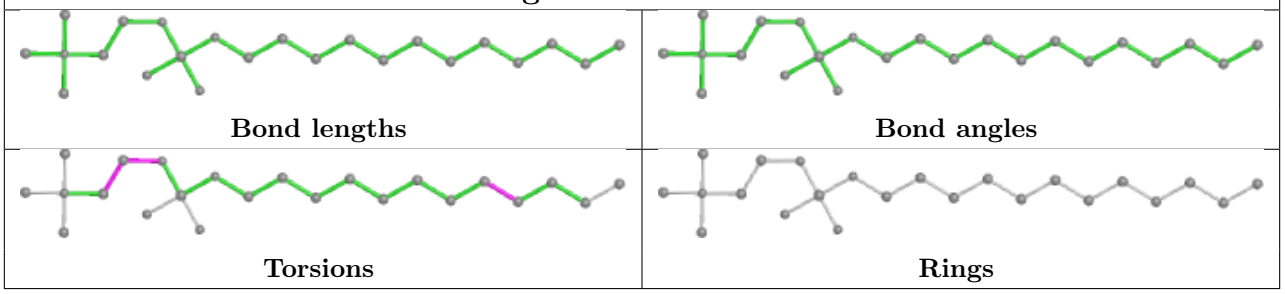
Ligand DPV A 163



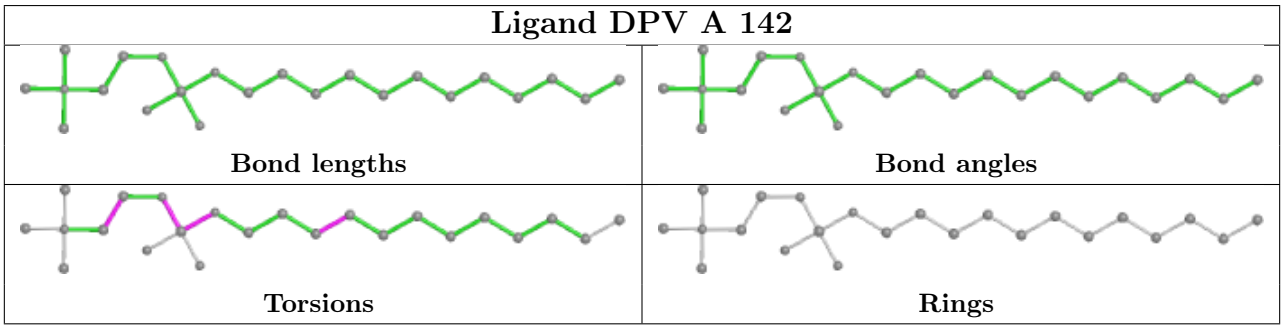
Ligand DPV A 112



Ligand DPV A 108



Ligand DPV A 142



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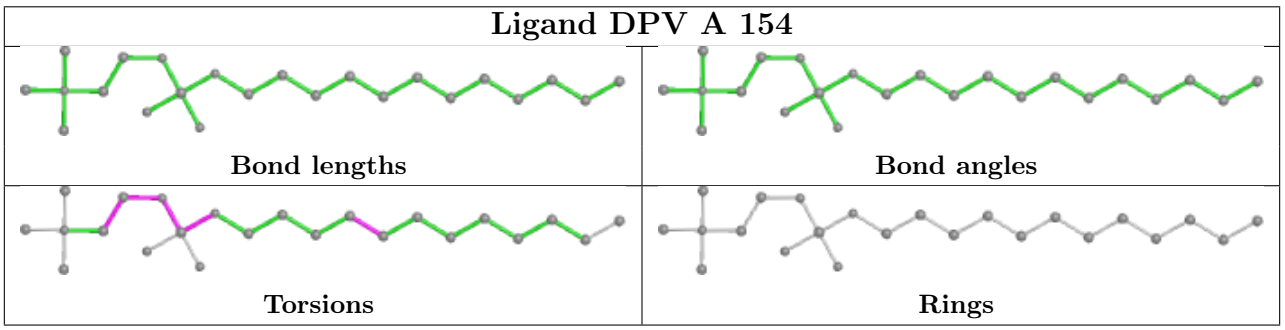

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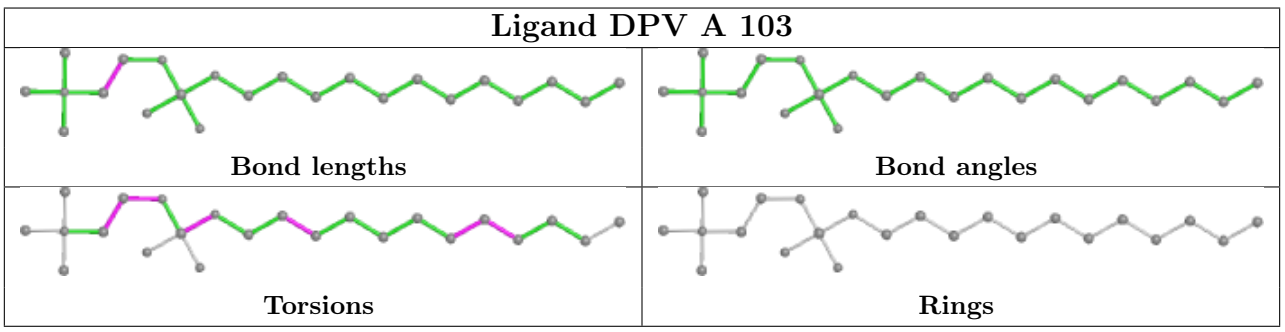
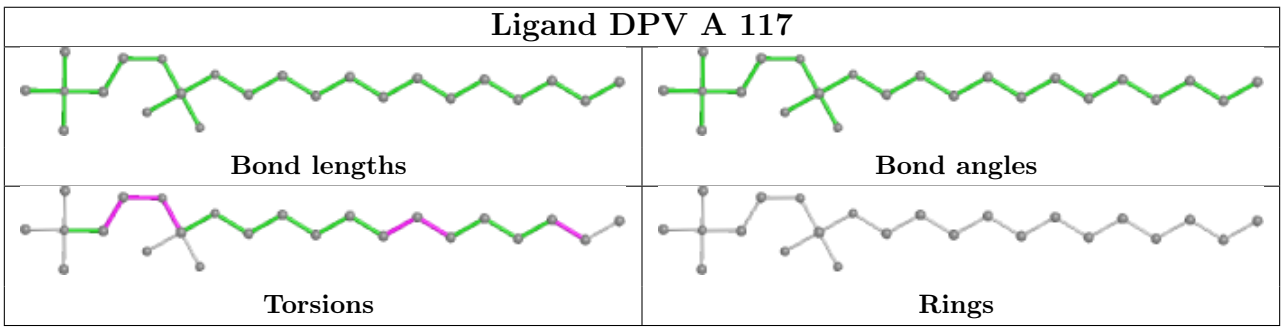


Ligand DPV A 117



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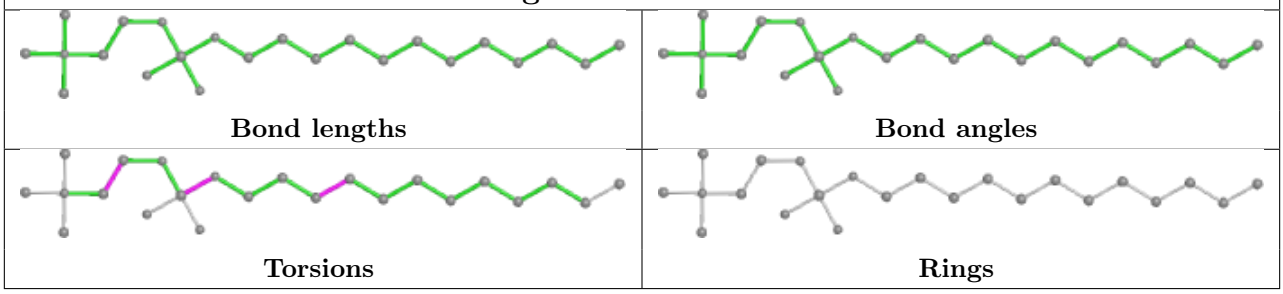

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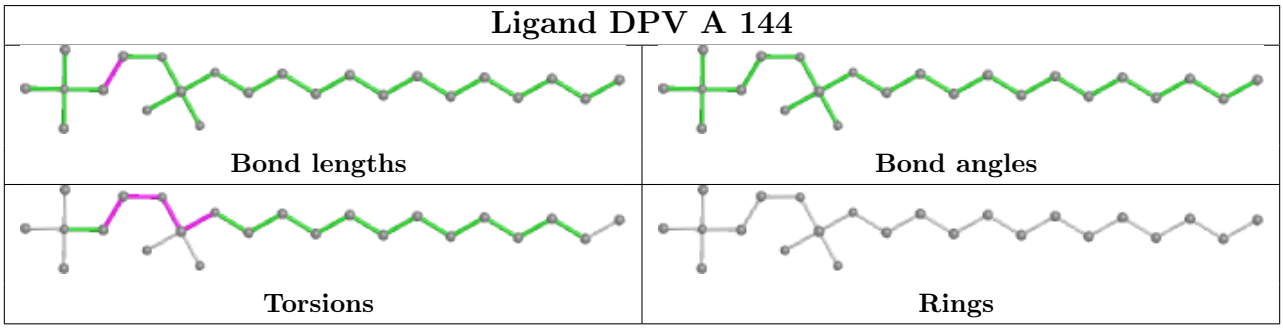

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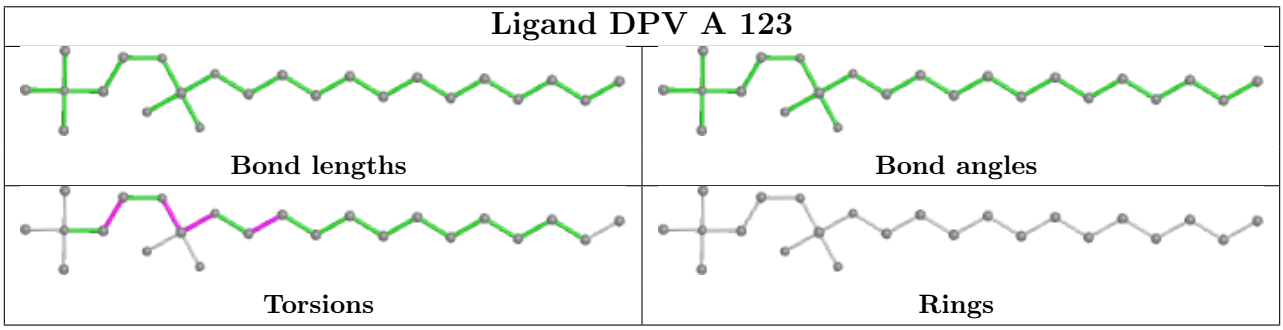
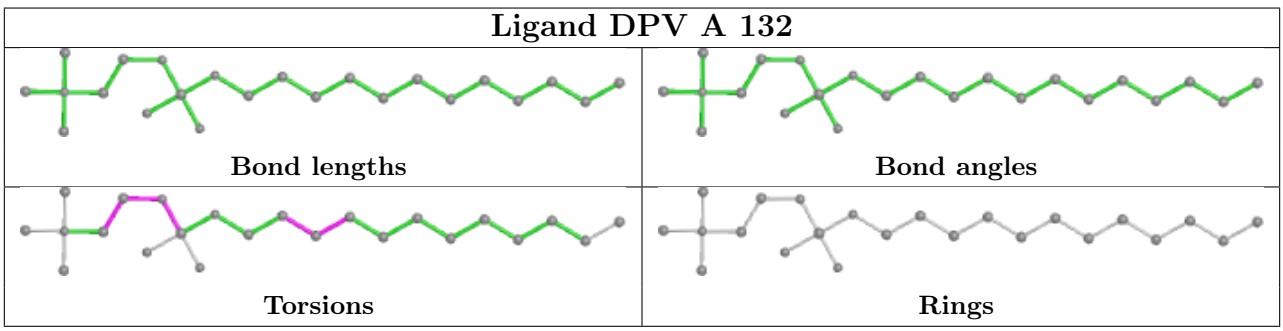
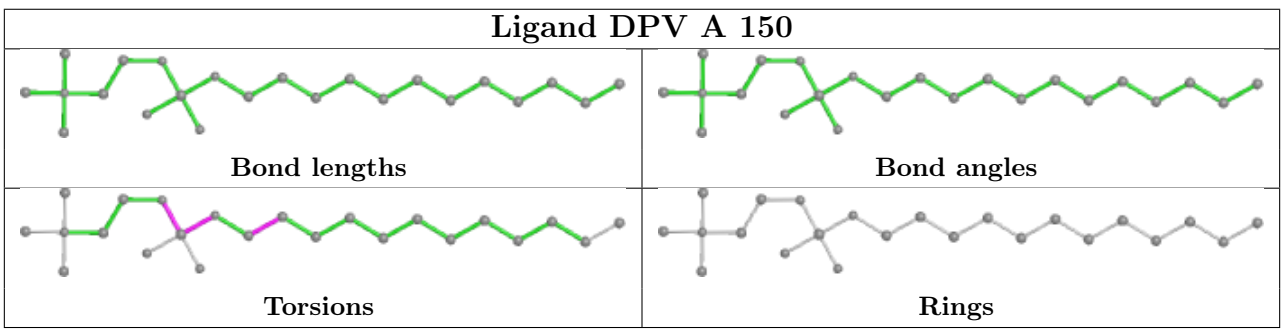


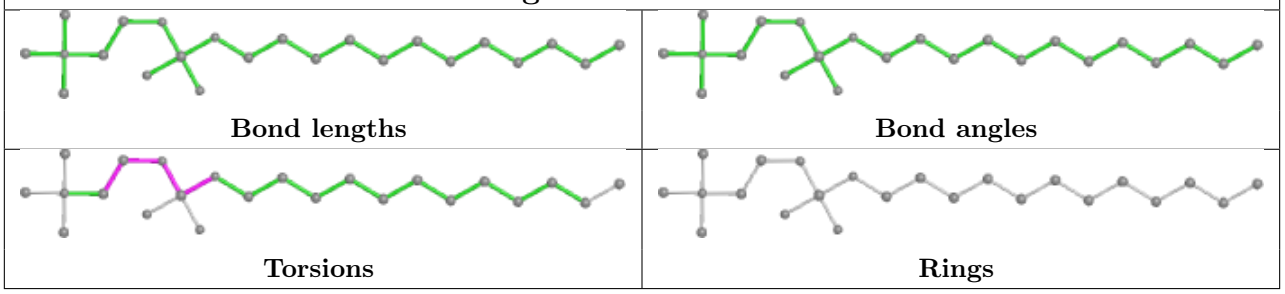
Ligand DPV A 132



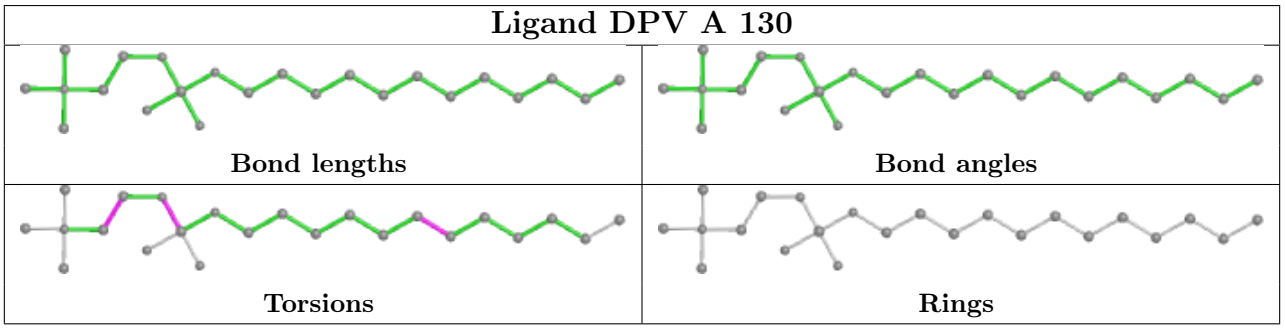
Ligand DPV A 150



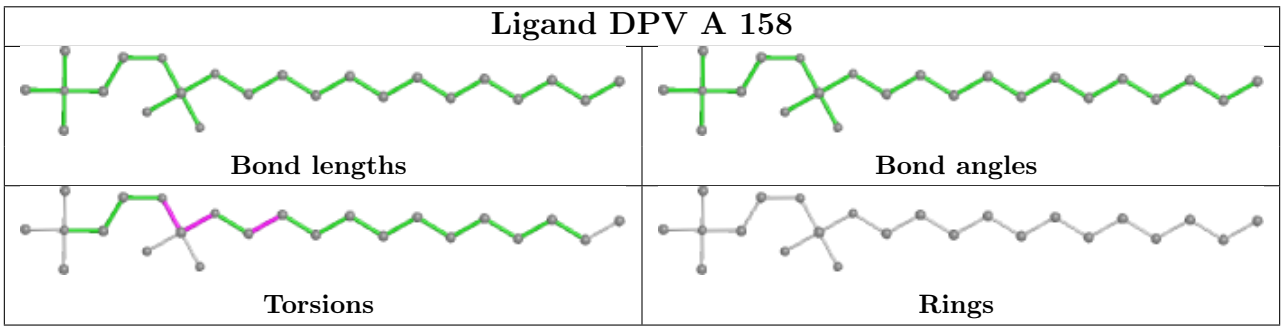
Ligand DPV A 138



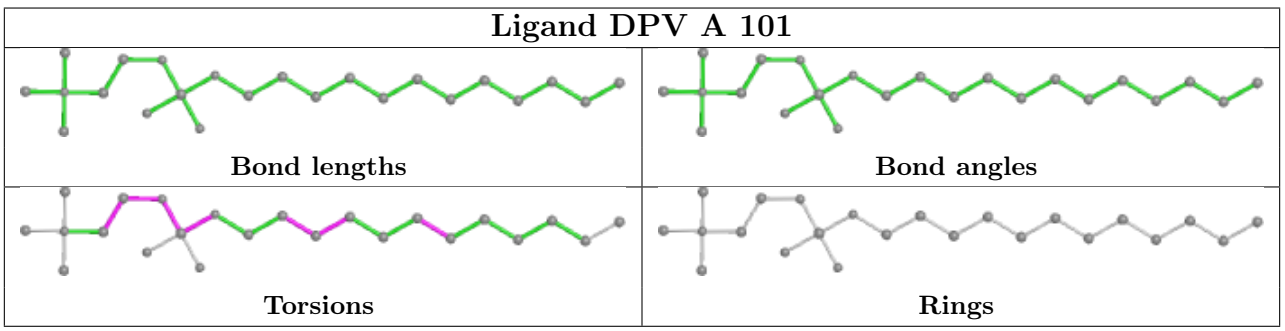
Ligand DPV A 130



Ligand DPV A 158



Ligand DPV A 101



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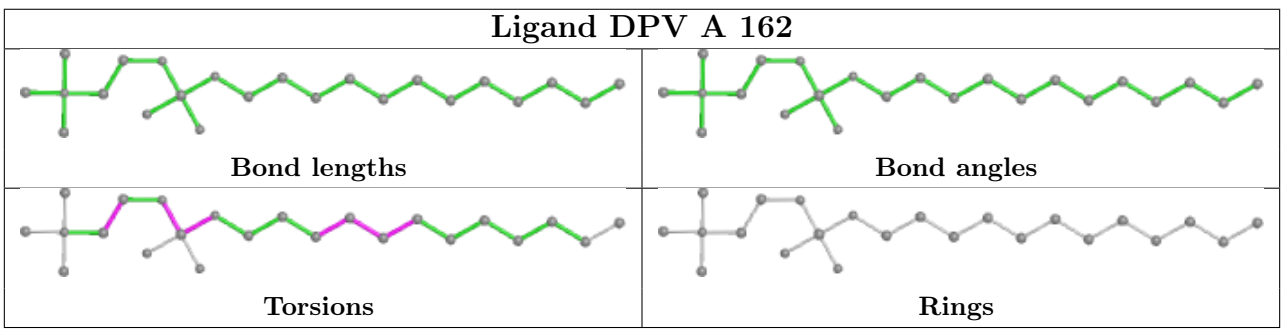
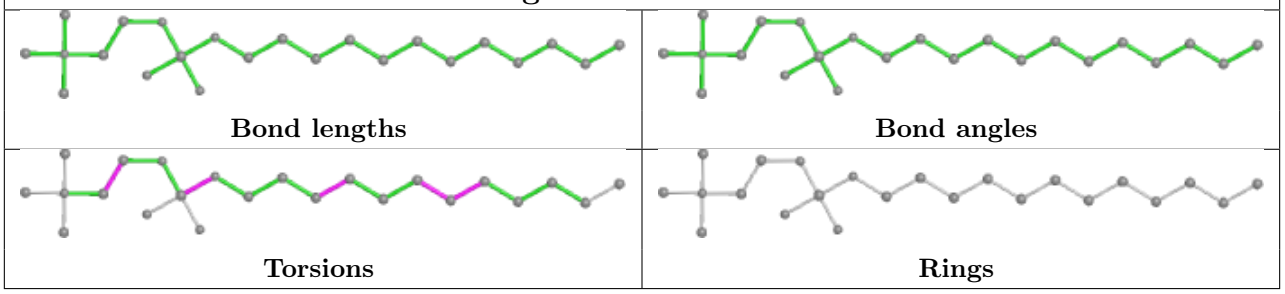


Ligand DPV A 127



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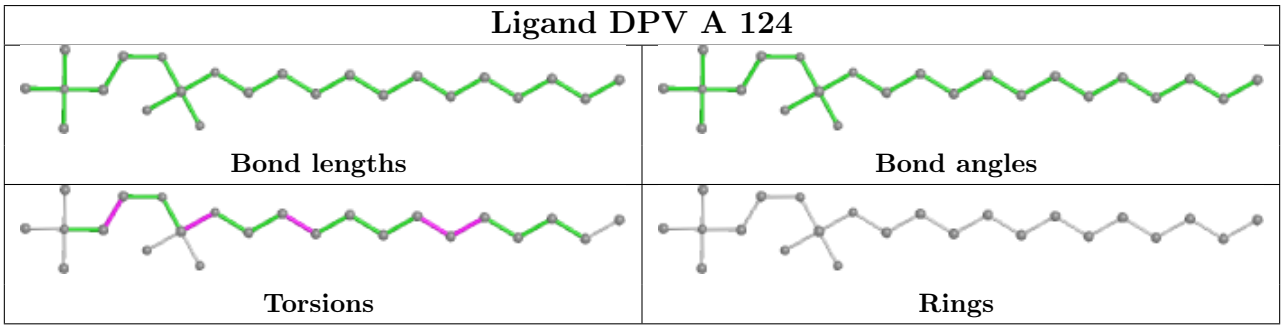

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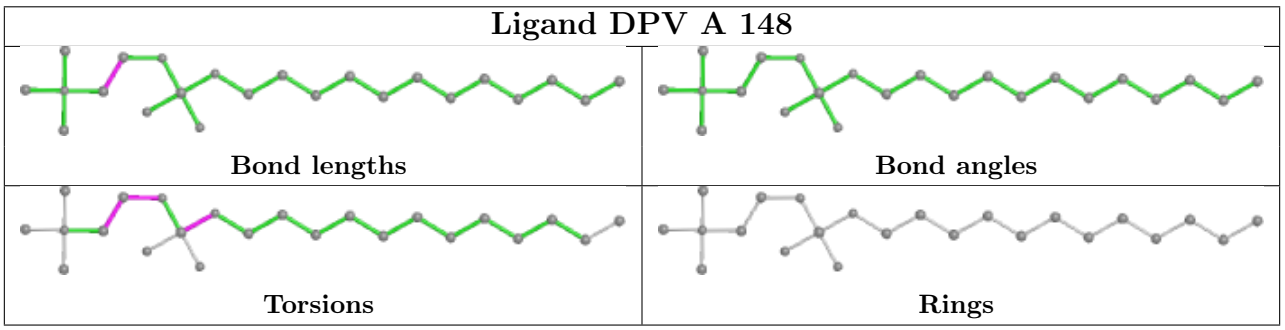

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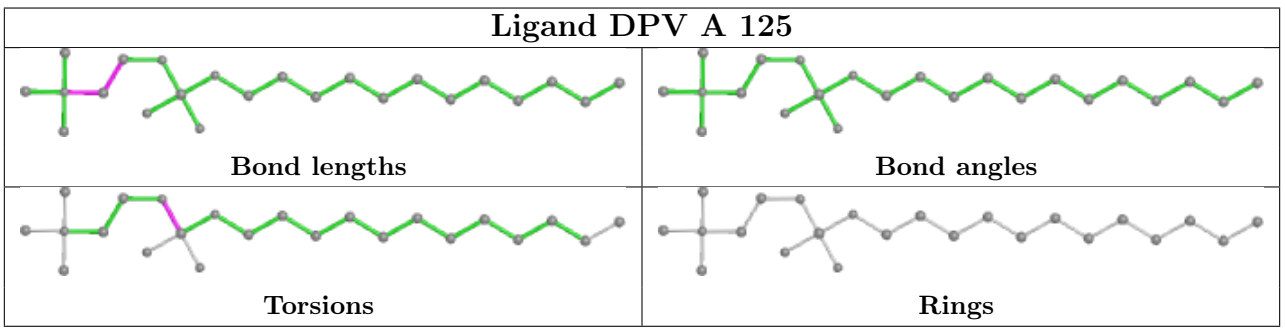

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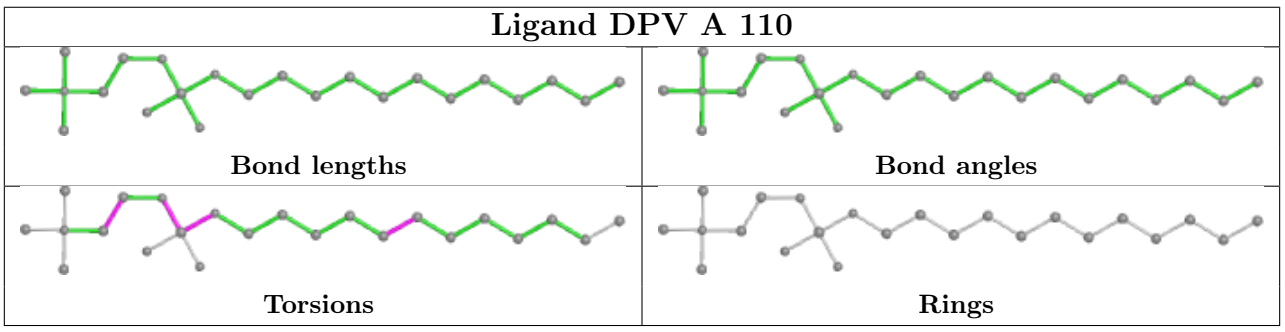

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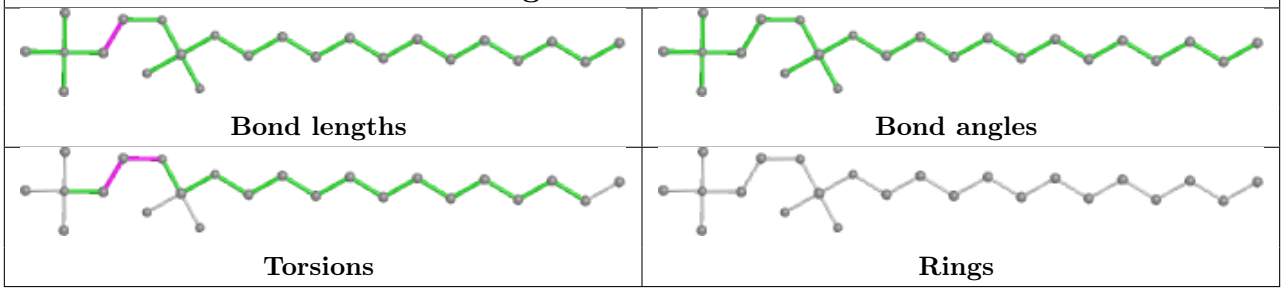

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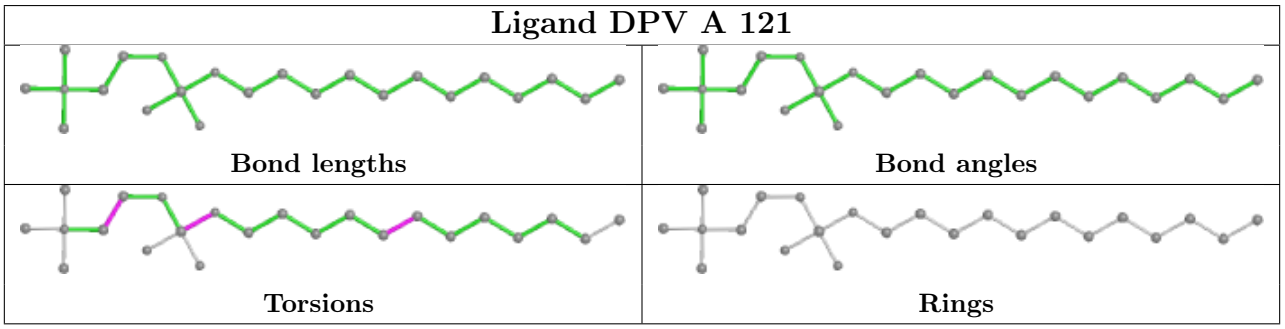

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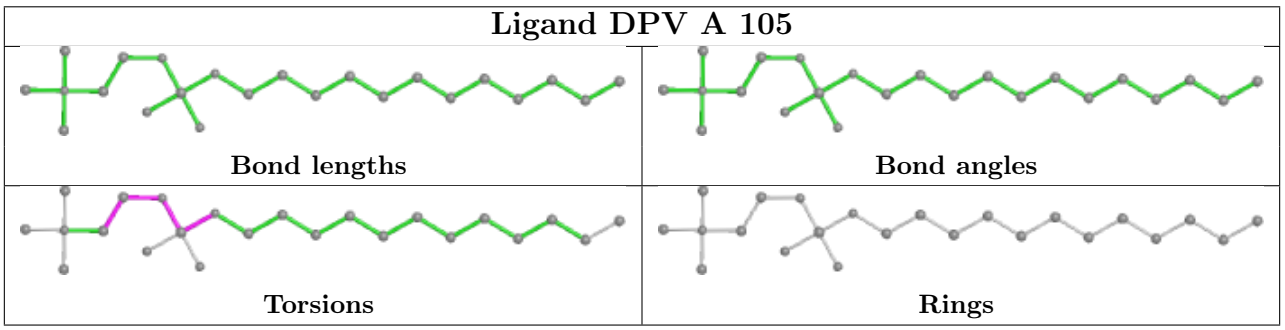
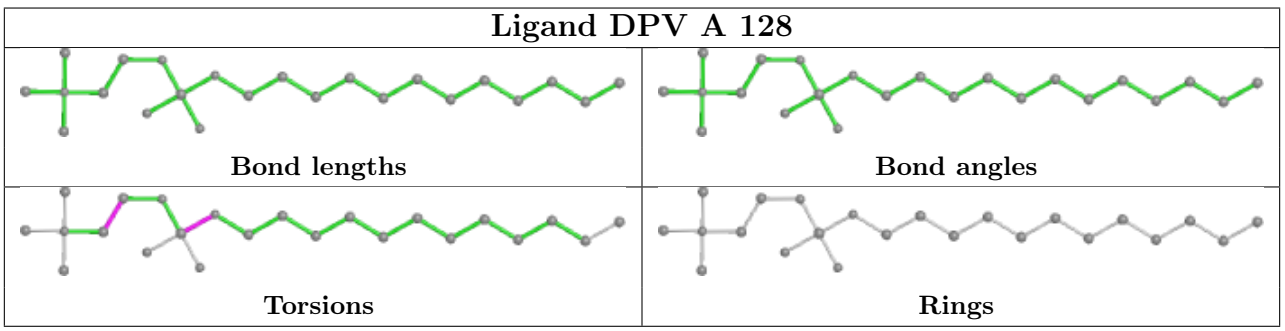


Ligand DPV A 128



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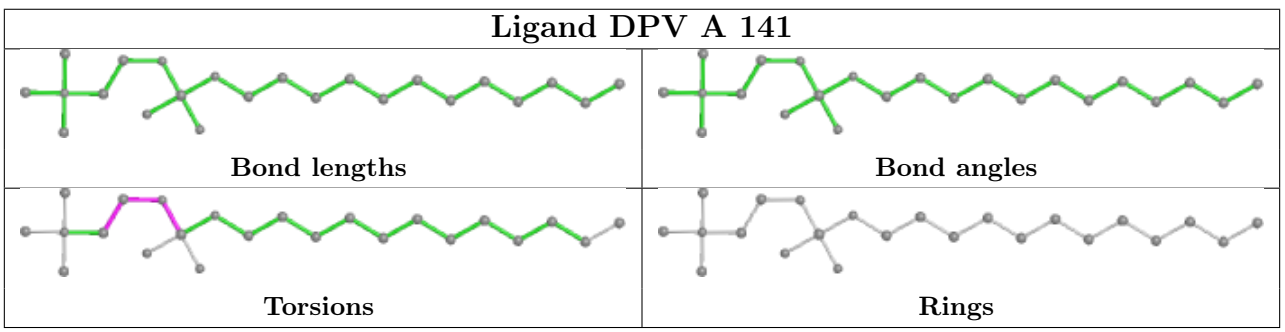

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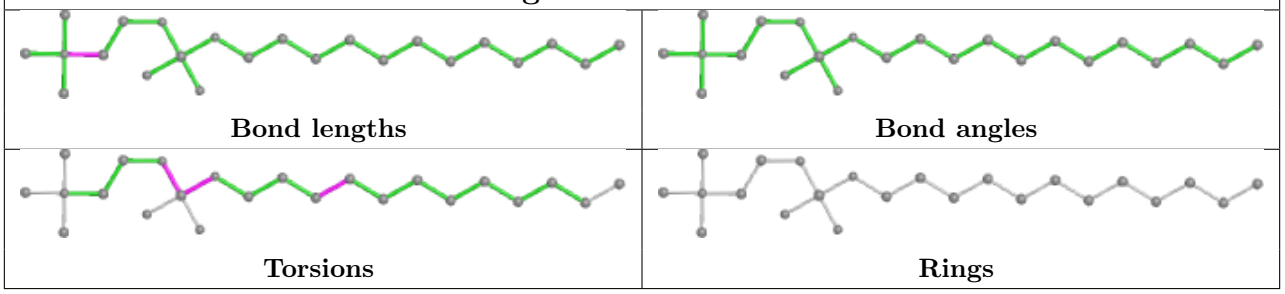

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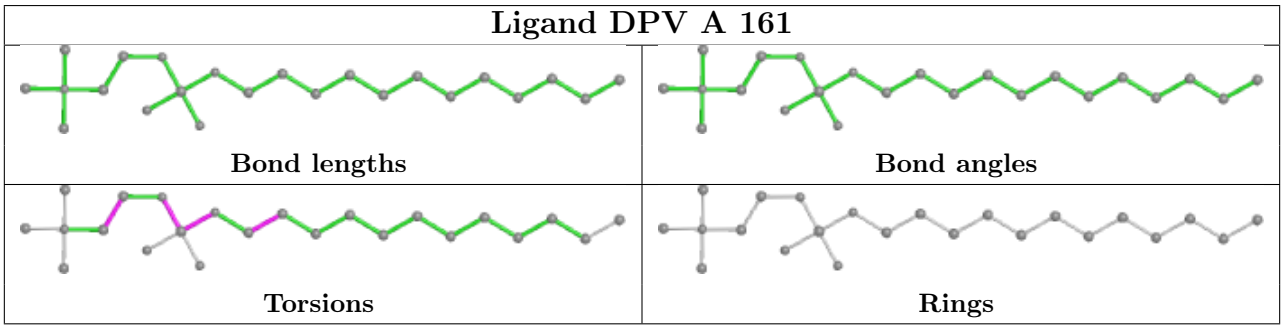

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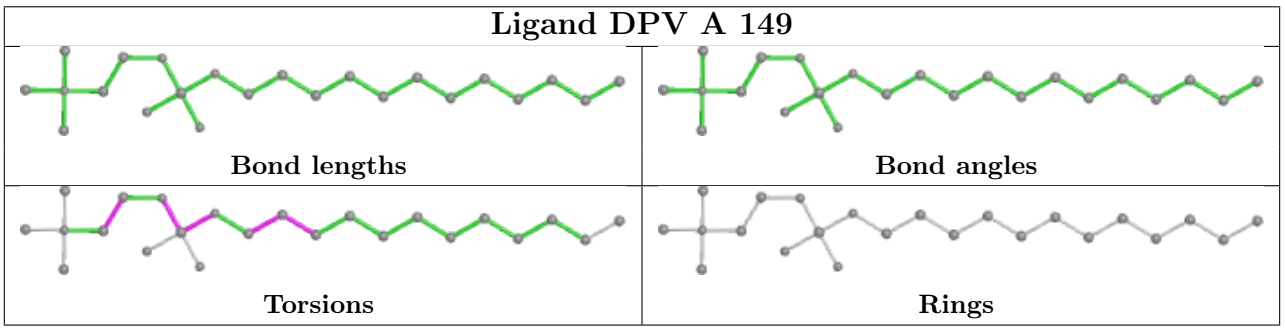
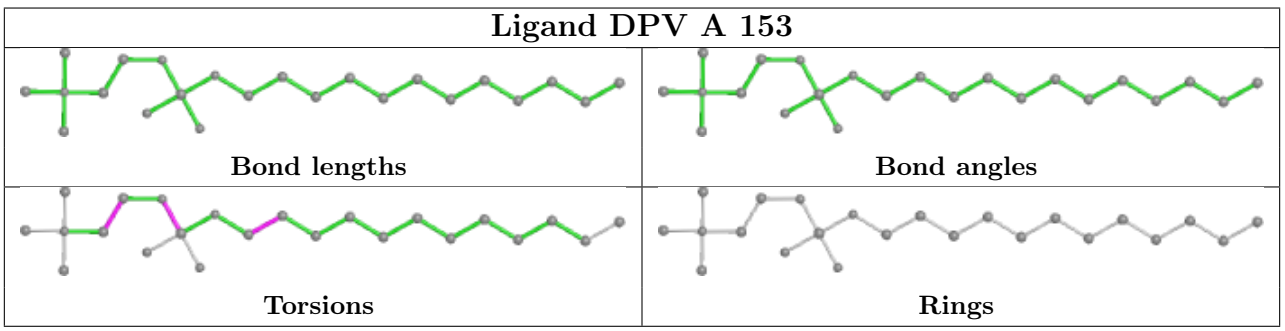
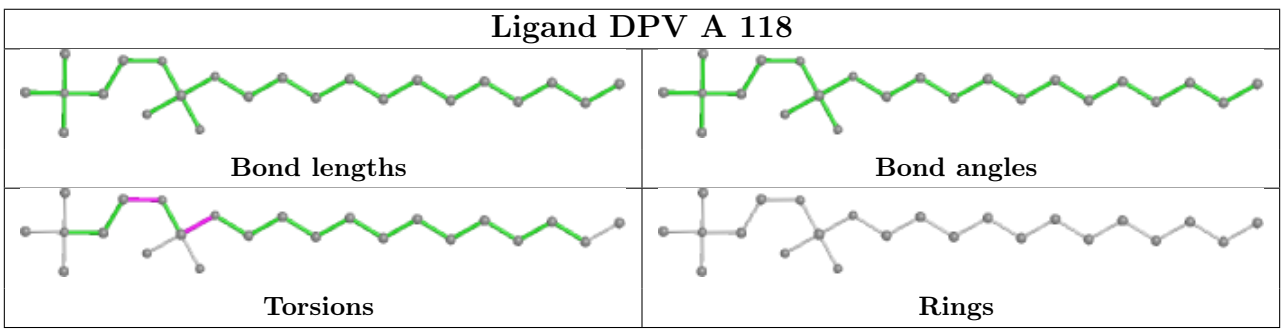
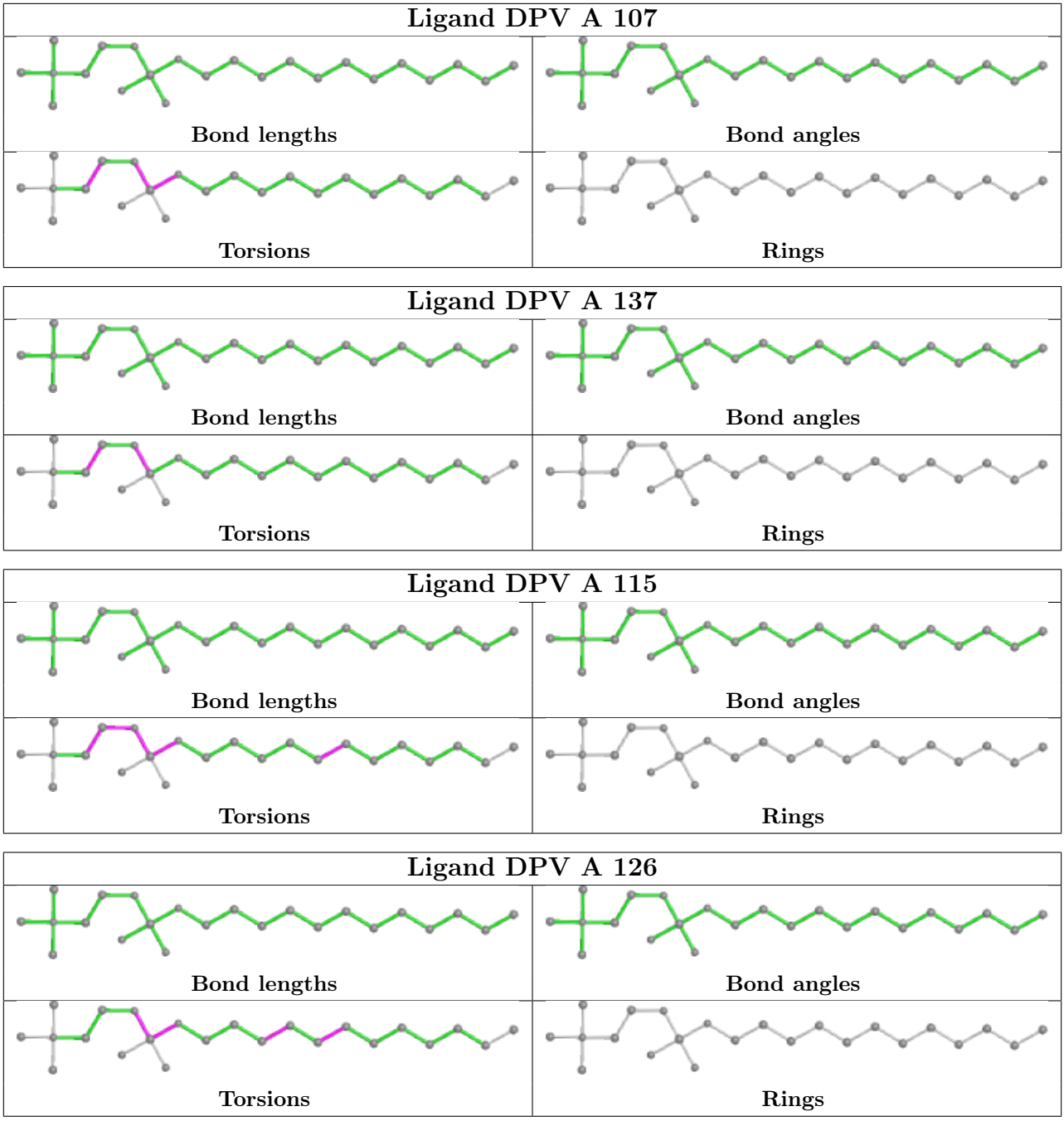


Ligand DPV A 153



Ligand DPV A 118





6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 70% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	156
Number of shifts mapped to atoms	156
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 70%, i.e. 99 atoms were assigned a chemical shift out of a possible 142. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	37/72 (51%)	29/31 (94%)	8/28 (29%)	0/13 (0%)
Sidechain	54/60 (90%)	40/40 (100%)	14/19 (74%)	0/1 (0%)
Aromatic	8/10 (80%)	4/5 (80%)	4/5 (80%)	0/0 (—%)
Overall	99/142 (70%)	73/76 (96%)	26/52 (50%)	0/14 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 99 atoms were assigned a chemical shift out of a possible 142. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	37/72 (51%)	29/31 (94%)	8/28 (29%)	0/13 (0%)
Sidechain	54/60 (90%)	40/40 (100%)	14/19 (74%)	0/1 (0%)
Aromatic	8/10 (80%)	4/5 (80%)	4/5 (80%)	0/0 (—%)
Overall	99/142 (70%)	73/76 (96%)	26/52 (50%)	0/14 (0%)

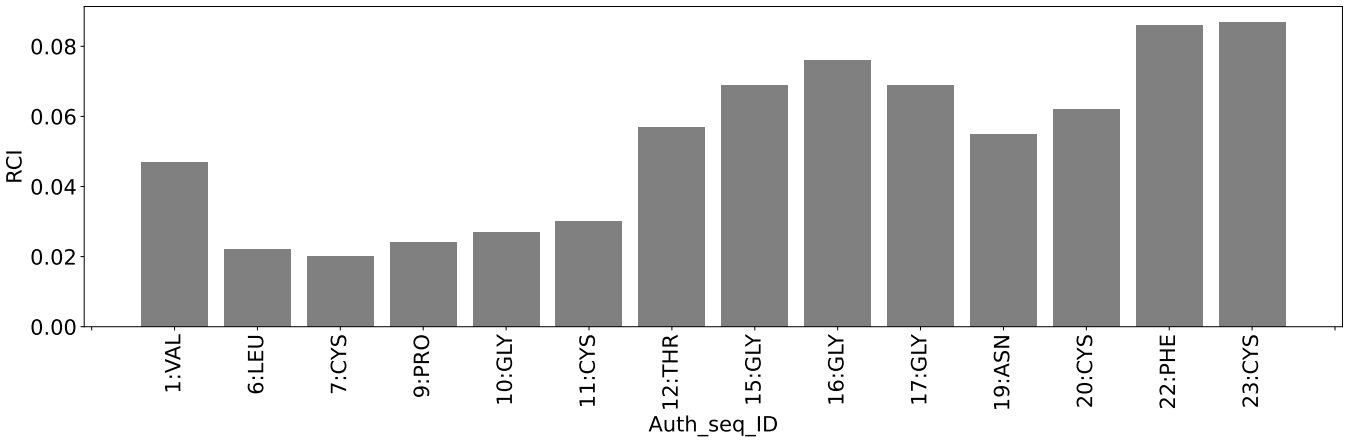
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	35
Intra-residue (|i-j|=0)	23
Sequential (|i-j|=1)	1
Medium range (|i-j|>1 and |i-j|<5)	5
Long range (|i-j|≥5)	6
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	18
Number of unmapped restraints	0
Number of restraints per residue	0.6
Number of long range restraints per residue[1]	0.1

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å
are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.1	0.14
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

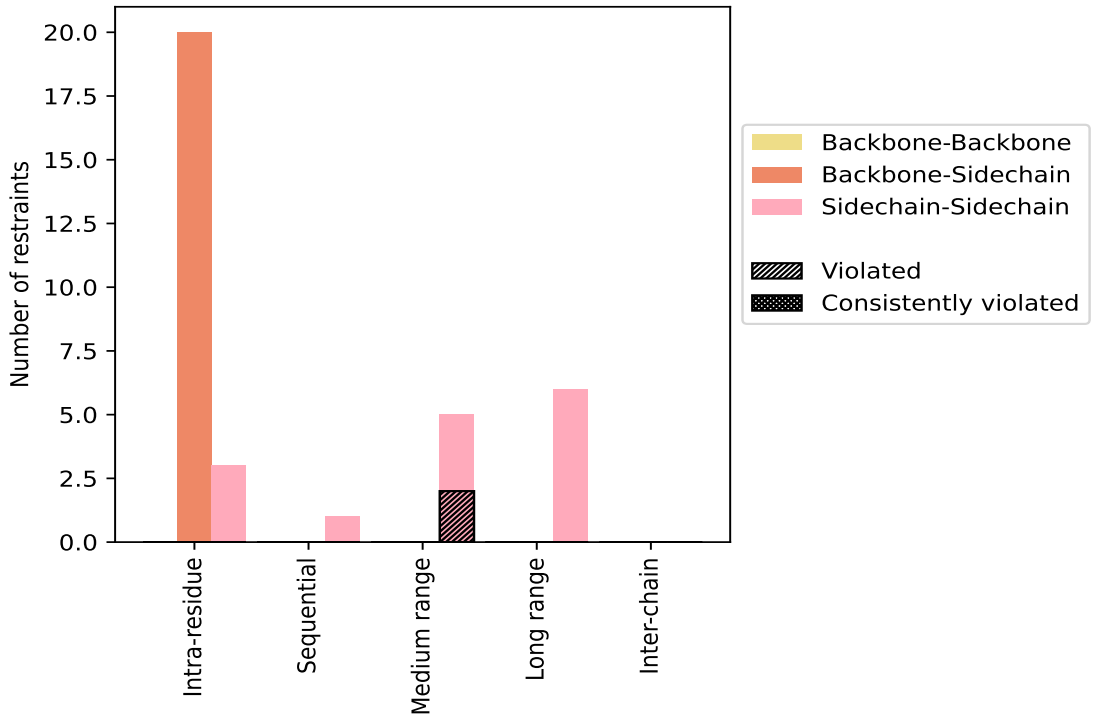
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	23	65.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	20	57.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	3	8.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	2.9	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	5	14.3	2	40.0	5.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	5	14.3	2	40.0	5.7	0	0.0	0.0
Long range (|i-j|≥5)	6	17.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	6	17.1	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	35	100.0	2	5.7	5.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	20	57.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	15	42.9	2	13.3	5.7	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å
are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	1	0	0	1	0.1	0.1	0.0	0.1
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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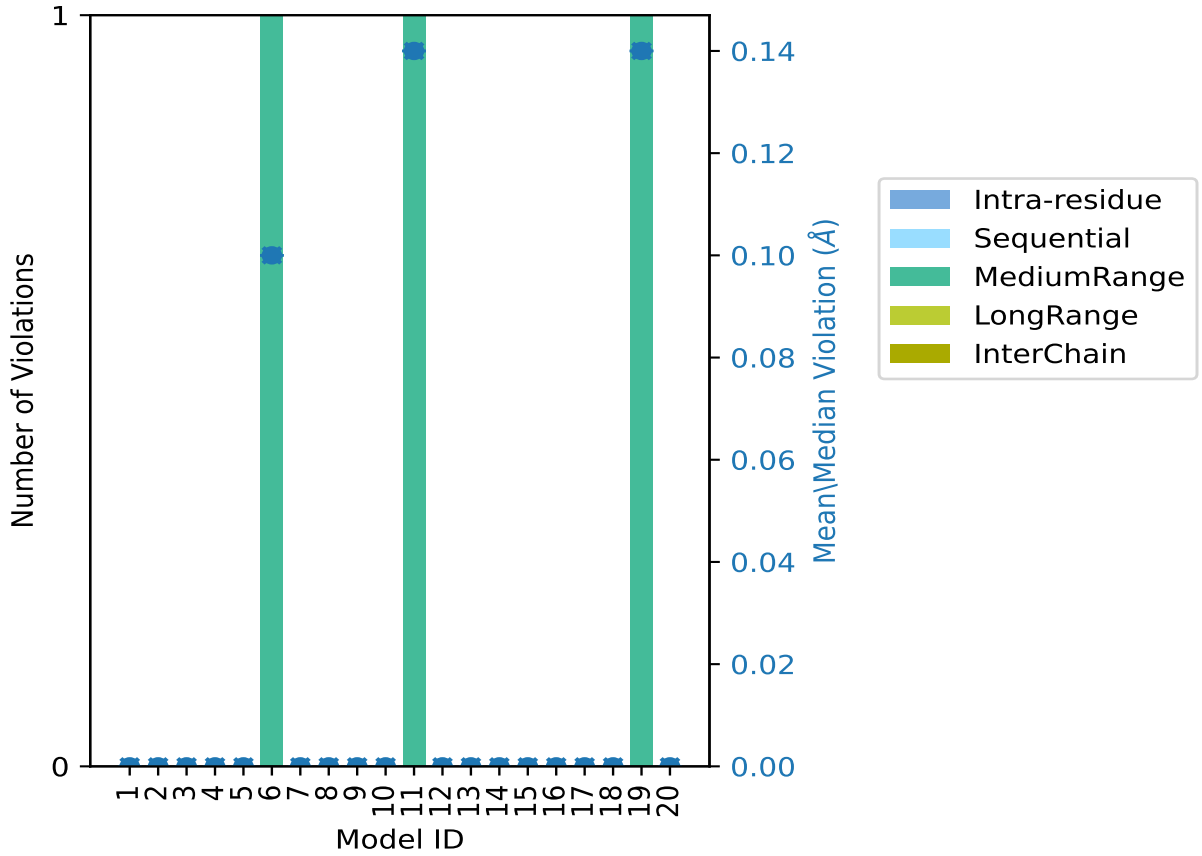
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	0	1	0	0	1	0.14	0.14	0.0	0.14
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	1	0	0	1	0.14	0.14	0.0	0.14
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

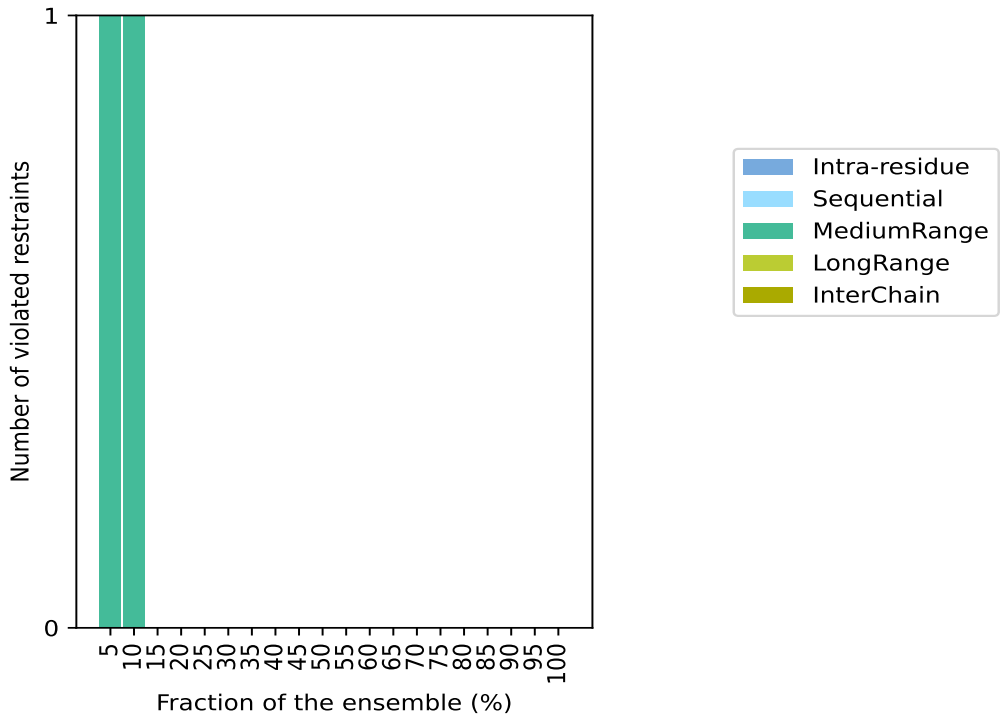
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 33(IR:23, SQ:1, MR:3, LR:6, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	1	0	0	1	1	5.0
0	0	1	0	0	1	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

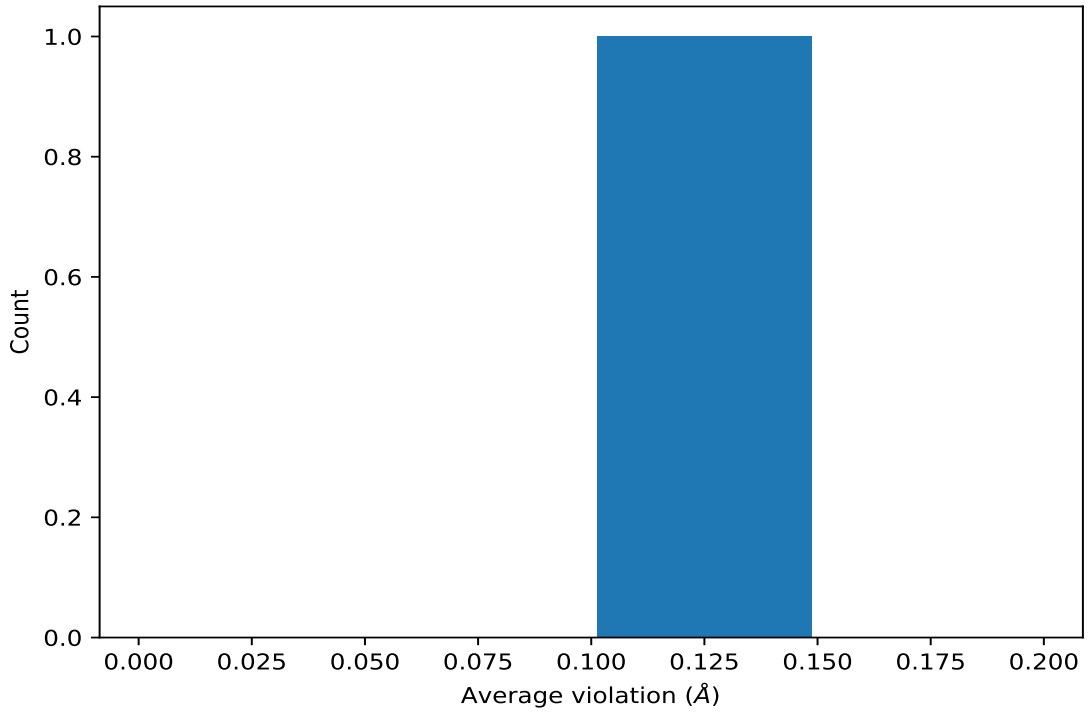
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

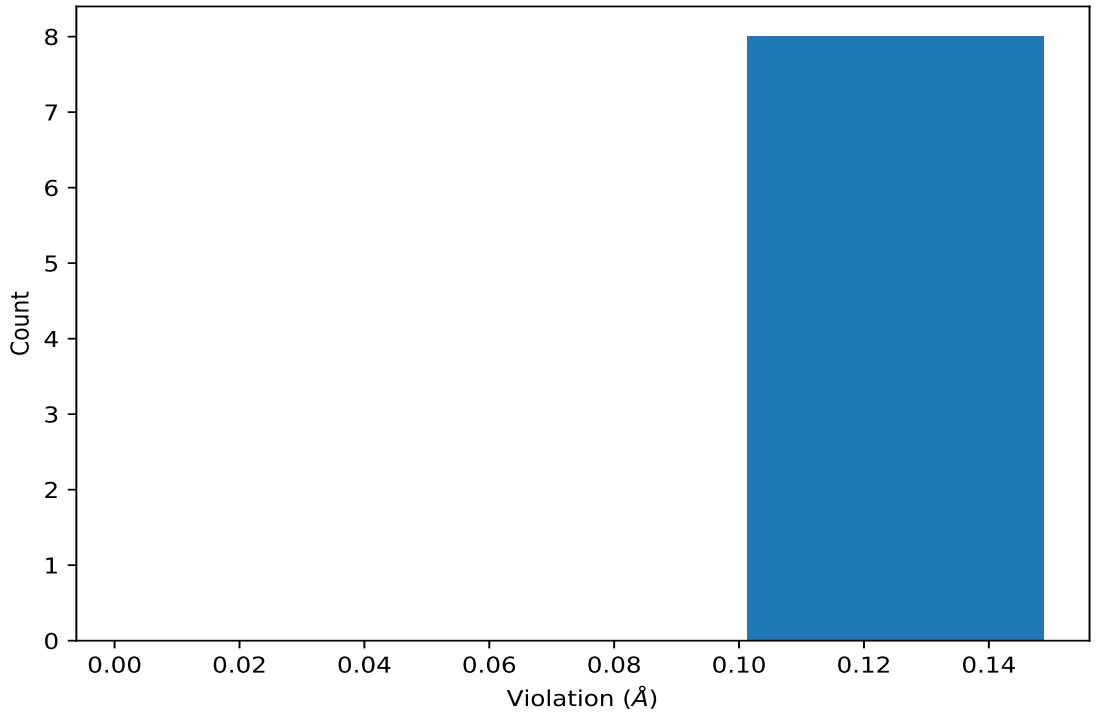
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,6)	1:2:A:DBU:HB	1:4:A:5CW:HE1	2	0.14	0.0	0.14

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:2:A:DBU:HB	1:4:A:5CW:HE1	11	0.14
(1,6)	1:2:A:DBU:HB	1:4:A:5CW:HE1	19	0.14
(1,23)	1:1:A:VAL:HG11	1:4:A:5CW:HE1	6	0.1
(1,23)	1:1:A:VAL:HG12	1:4:A:5CW:HE1	6	0.1
(1,23)	1:1:A:VAL:HG13	1:4:A:5CW:HE1	6	0.1
(1,23)	1:1:A:VAL:HG21	1:4:A:5CW:HE1	6	0.1
(1,23)	1:1:A:VAL:HG22	1:4:A:5CW:HE1	6	0.1
(1,23)	1:1:A:VAL:HG23	1:4:A:5CW:HE1	6	0.1

10 Dihedral-angle violation analysis

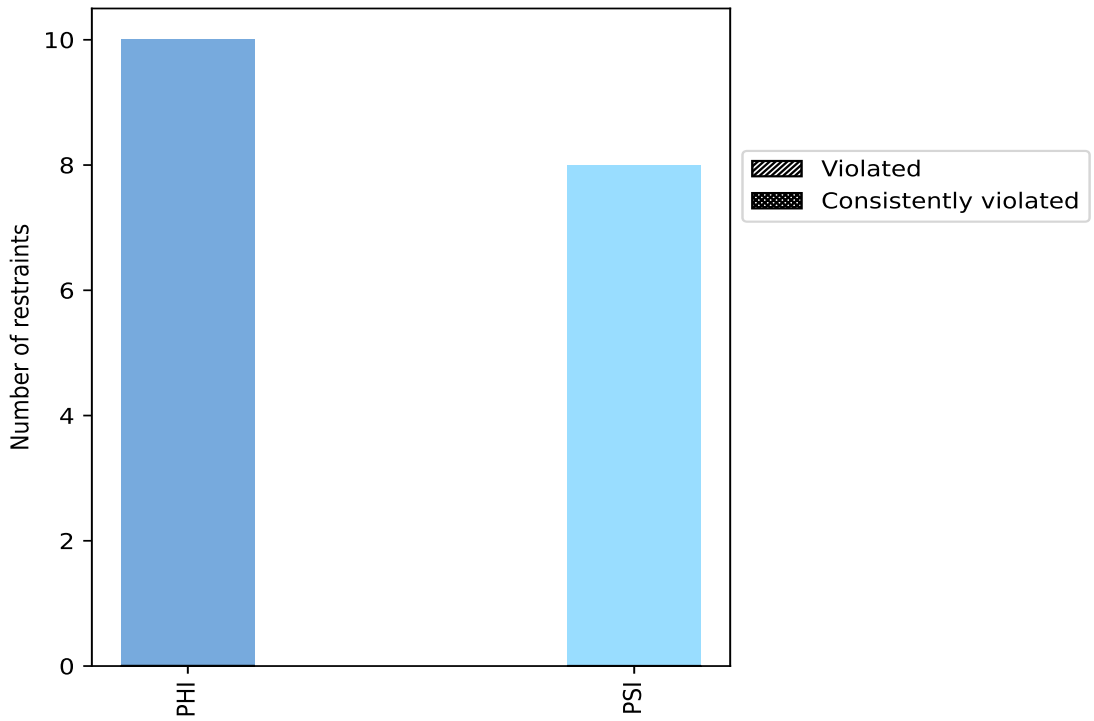
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	10	55.6	0	0.0	0.0	0	0.0	0.0
PSI	8	44.4	0	0.0	0.0	0	0.0	0.0
Total	18	100.0	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

No violations found

10.3 Dihedral-angle violation statistics for the ensemble (i)

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble (i)

No violations found

10.5 All violated dihedral-angle restraints (i)

No violations found