



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 04:05 AM BST

PDB ID : 1L9H  
Title : Crystal structure of bovine rhodopsin at 2.6 angstroms RESOLUTION  
Authors : Okada, T.; Fujiyoshi, Y.; Silow, M.; Navarro, J.; Landau, E.M.; Shichida, Y.  
Deposited on : 2002-03-23  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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) : **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

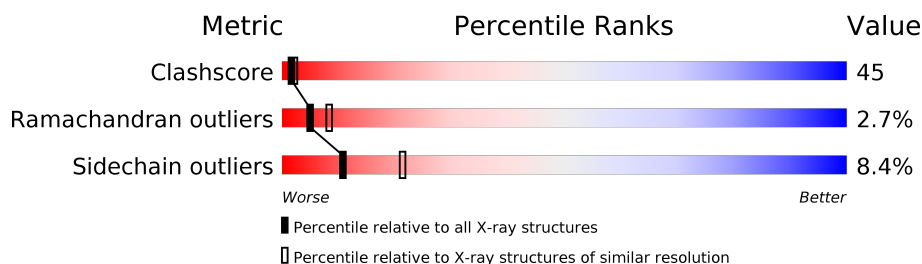
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	349	
1	B	349	
2	C	3	
3	D	2	
3	F	2	
4	E	4	

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	NAG	C	1	-	-	X	-
2	NAG	C	2	X	-	-	-
2	MAN	C	3	X	-	-	-
3	NAG	D	2	X	-	-	-
3	NAG	F	2	X	-	-	-
4	NAG	E	1	-	-	X	-
4	NAG	E	2	X	-	-	-
9	PLM	A	1410	-	X	-	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5584 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 rhodopsin.

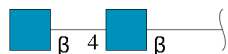
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2685	1783	413	463	26			
1	B	302	Total	C	N	O	S	0	0	0
			2398	1603	366	404	25			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			41	22	2	17			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



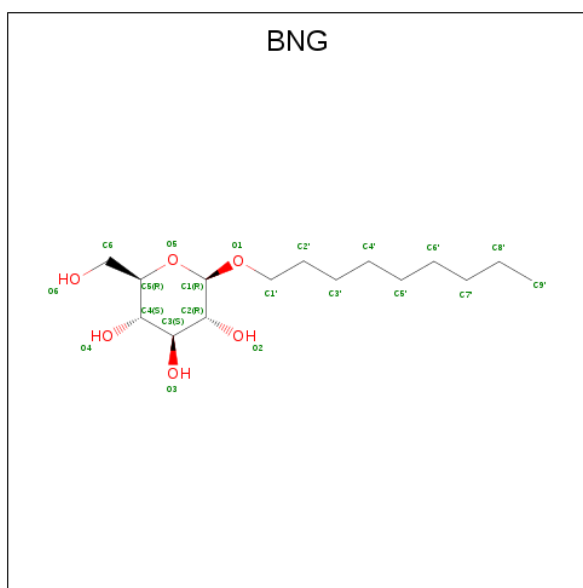
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			29	16	2	11			
3	F	2	Total	C	N	O	0	0	0
			29	16	2	11			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			53	28	2	23			

- Molecule 5 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	B	1	Total	C	O	0	0
			21	15	6		
5	B	1	Total	C	O	0	0
			21	15	6		

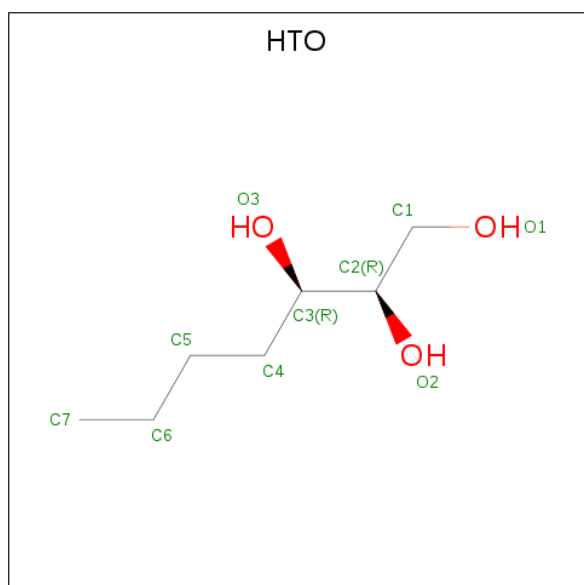
- Molecule 6 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total Hg 3 3	0	0
6	A	3	Total Hg 3 3	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

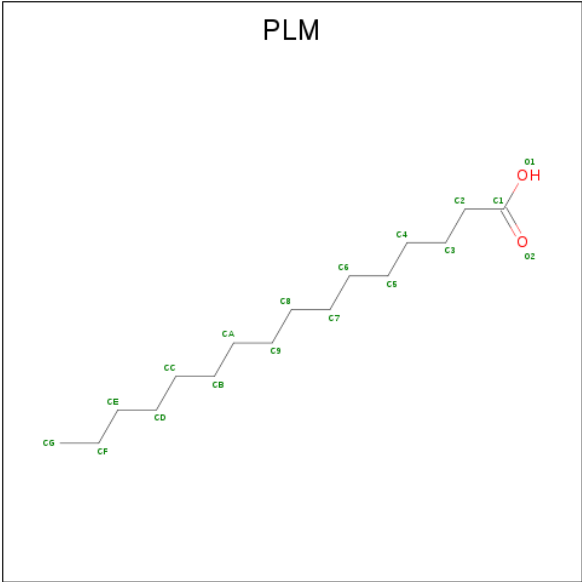
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	3	Total Zn 3 3	0	0
7	A	4	Total Zn 4 4	0	0

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



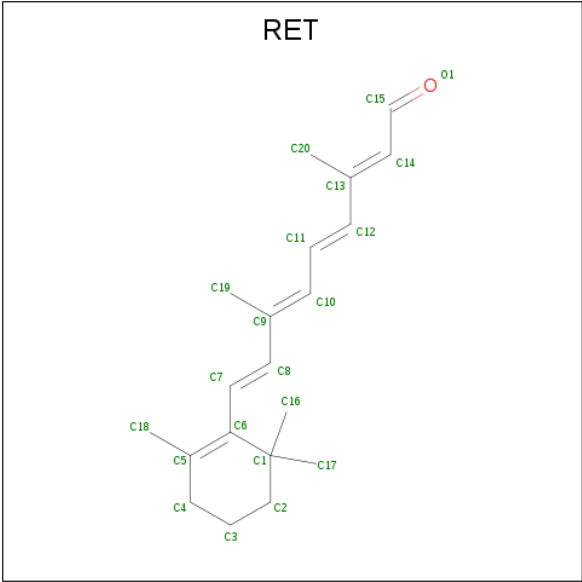
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 10 7 3	0	0
8	A	1	Total C O 10 7 3	0	0
8	A	1	Total C O 10 7 3	0	0
8	A	1	Total C O 10 7 3	0	0

- Molecule 9 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C 16 16	0	0
9	A	1	Total C O 17 16 1	0	0
9	A	1	Total C O 17 16 1	0	0
9	B	1	Total C 16 16	0	0
9	B	1	Total C O 17 16 1	0	0

- Molecule 10 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C 20 20	0	0
10	B	1	Total C 20 20	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	13	Total O 13 13	0	0
11	B	13	Total O 13 13	0	0

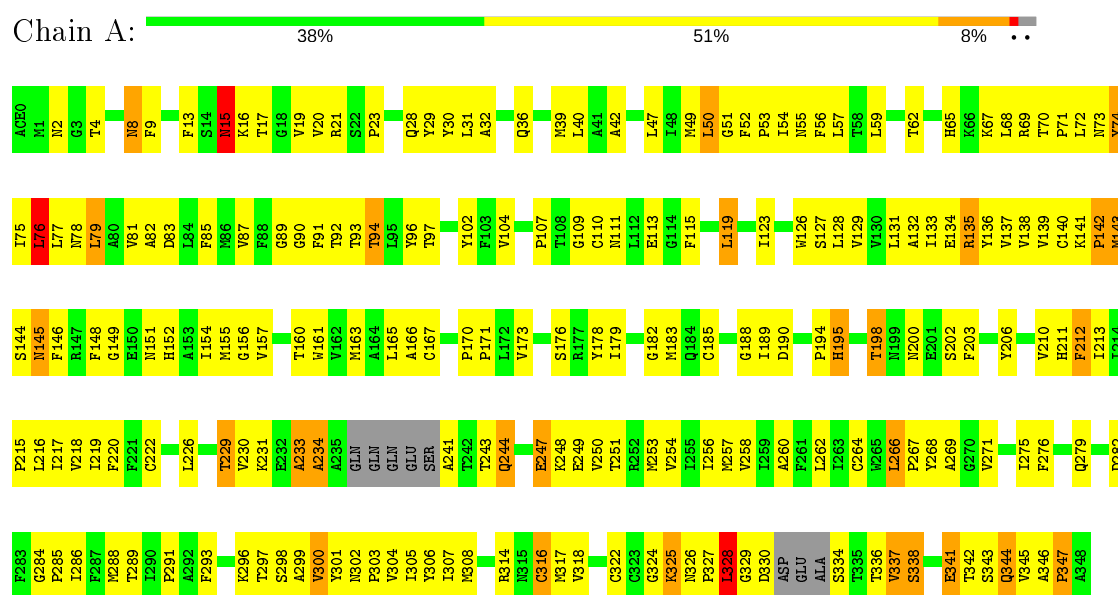


### 3 Residue-property plots

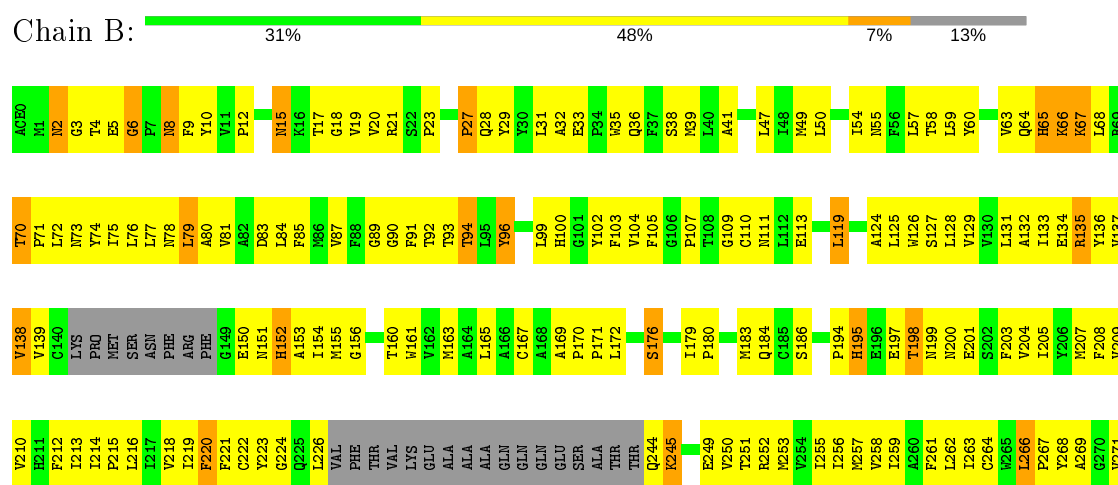
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

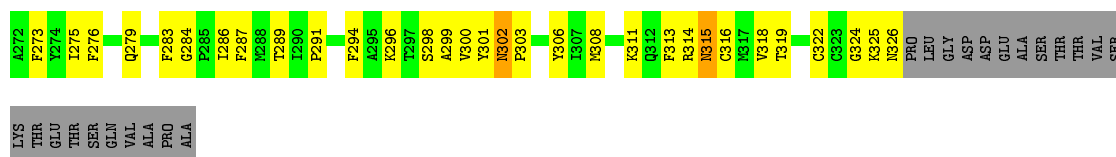
Note EDS was not executed.

#### • Molecule 1: rhodopsin



#### • Molecule 1: rhodopsin





- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  67% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%



- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 25% 25%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.75Å 96.75Å 149.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	71.0 (30.00-2.60)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.188 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, ACE, HTO, RET, PLM, BNG, HG, MAN

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	0.68	2/2765 (0.1%)	0.76	6/3767 (0.2%)
1	B	0.68	0/2472	0.77	6/3368 (0.2%)
All	All	0.68	2/5237 (0.0%)	0.76	12/7135 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ASN	CG-ND2	7.93	1.52	1.32
1	A	15	ASN	CA-CB	5.82	1.68	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ASN	CB-CA-C	-11.05	88.31	110.40
1	A	15	ASN	CB-CG-ND2	-11.00	90.29	116.70
1	B	15	ASN	N-CA-CB	7.56	124.21	110.60
1	A	15	ASN	CB-CA-C	-6.83	96.73	110.40
1	B	296	LYS	CD-CE-NZ	6.79	127.31	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ASN	Sidechain
1	B	96	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	2685	0	2657	263	0
1	B	2398	0	2369	242	0
2	C	41	0	36	11	0
3	D	29	0	26	6	0
3	F	29	0	26	1	0
4	E	53	0	45	7	0
5	A	105	0	150	11	0
5	B	42	0	60	7	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	4	0	0	0	0
7	B	3	0	0	0	0
8	A	40	0	64	4	0
9	A	50	0	89	3	0
9	B	33	0	58	2	0
10	A	20	0	27	1	0
10	B	20	0	27	3	0
11	A	13	0	0	2	0
11	B	13	0	0	5	0
All	All	5584	0	5634	496	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 45.

The worst 5 of 496 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:2:ASN:HD21	3:F:1:NAG:C1	1.13	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:HD21	3:D:1:NAG:C1	1.29	1.41
1:A:15:ASN:HD21	2:C:1:NAG:C1	1.29	1.40
1:A:65:HIS:HB3	1:A:337:VAL:HG22	1.26	1.12
1:A:75:ILE:HG21	1:A:131:LEU:HD21	1.32	1.10

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	335/349 (96%)	284 (85%)	37 (11%)	14 (4%)	3	3
1	B	296/349 (85%)	253 (86%)	40 (14%)	3 (1%)	15	32
All	All	631/698 (90%)	537 (85%)	77 (12%)	17 (3%)	5	8

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	LYS
1	A	328	LEU
1	A	347	PRO
1	A	142	PRO
1	A	195	HIS

### 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	289/296 (98%)	266 (92%)	23 (8%)	12	24
1	B	257/296 (87%)	234 (91%)	23 (9%)	9	19
All	All	546/592 (92%)	500 (92%)	46 (8%)	11	21

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	GLU
1	B	64	GLN
1	B	300	VAL
1	A	343	SER
1	B	8	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	A	344	GLN
1	B	64	GLN
1	A	302	ASN
1	B	8	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

11 monosaccharides 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	NAG	C	1	1,2	14,14,15	0.67	0	17,19,21	0.71	0
2	NAG	C	2	2	15,15,15	0.58	0	21,21,21	1.08	2 (9%)
2	MAN	C	3	2	12,12,12	0.57	0	17,17,17	0.63	0
3	NAG	D	1	1,3	14,14,15	0.54	0	17,19,21	0.78	0
3	NAG	D	2	3	15,15,15	0.73	0	21,21,21	1.09	2 (9%)
4	NAG	E	1	1,4	14,14,15	0.47	0	17,19,21	0.82	0
4	NAG	E	2	4	15,15,15	0.41	0	21,21,21	1.67	1 (4%)
4	MAN	E	3	4	12,12,12	0.71	0	17,17,17	0.61	0
4	MAN	E	4	4	12,12,12	0.56	0	17,17,17	0.54	0
3	NAG	F	1	1,3	14,14,15	0.66	0	17,19,21	0.71	0
3	NAG	F	2	3	15,15,15	0.70	0	21,21,21	0.83	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	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	1/1/6/7	4/6/26/26	0/1/1/1
2	MAN	C	3	2	1/1/5/5	2/2/22/22	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	1/1/6/7	4/6/26/26	0/1/1/1
4	NAG	E	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	1/1/6/7	5/6/26/26	0/1/1/1
4	MAN	E	3	4	-	2/2/22/22	0/1/1/1
4	MAN	E	4	4	-	2/2/22/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	1/1/6/7	4/6/26/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C2-N2-C7	7.31	140.95	123.18
2	C	2	NAG	C1-C2-N2	-2.63	107.68	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C4-C3-C2	2.39	113.84	110.34
3	D	2	NAG	C4-C3-C2	2.21	113.58	110.34
3	D	2	NAG	O5-C1-C2	2.04	111.56	109.52

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	2	NAG	C1
3	D	2	NAG	C1
4	E	2	NAG	C1
2	C	2	NAG	C1
2	C	3	MAN	C1

5 of 37 torsion outliers are listed below:

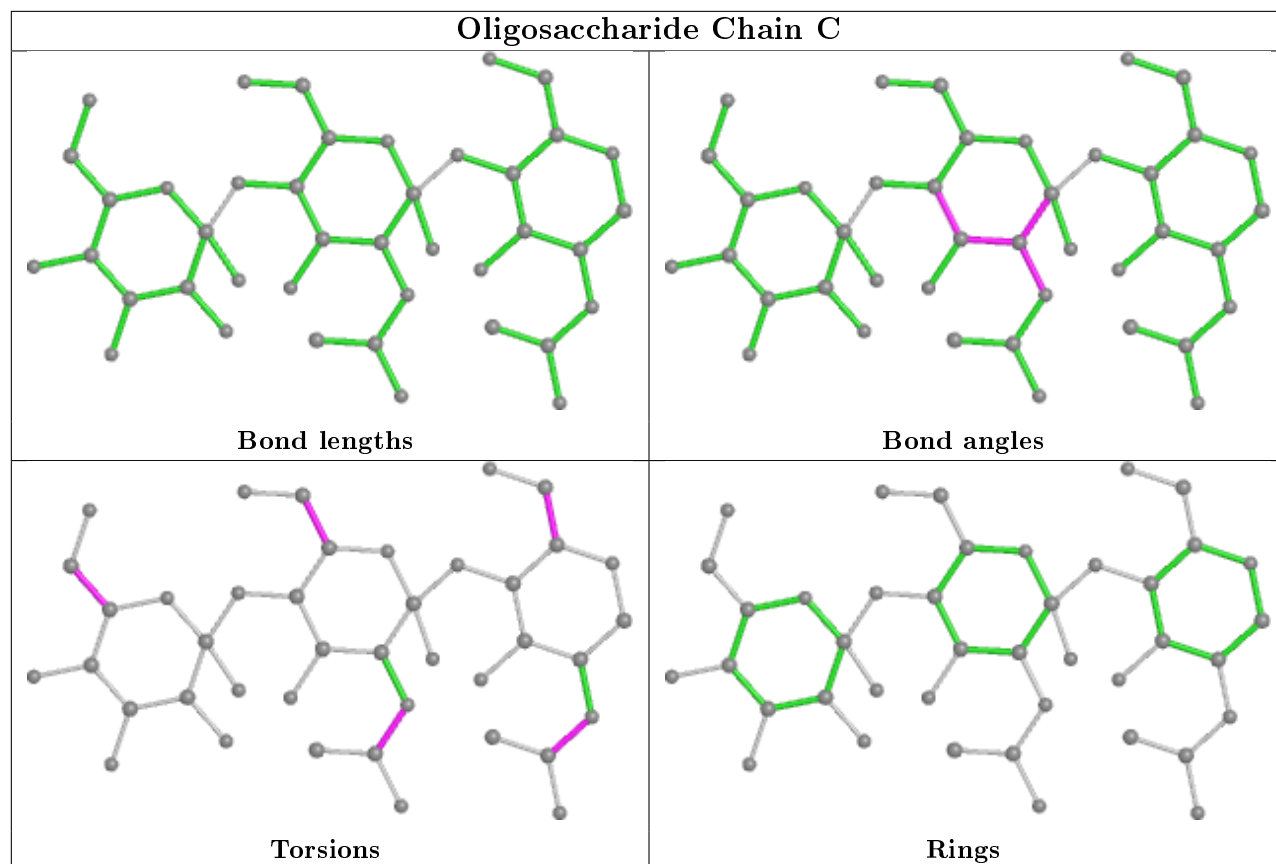
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2

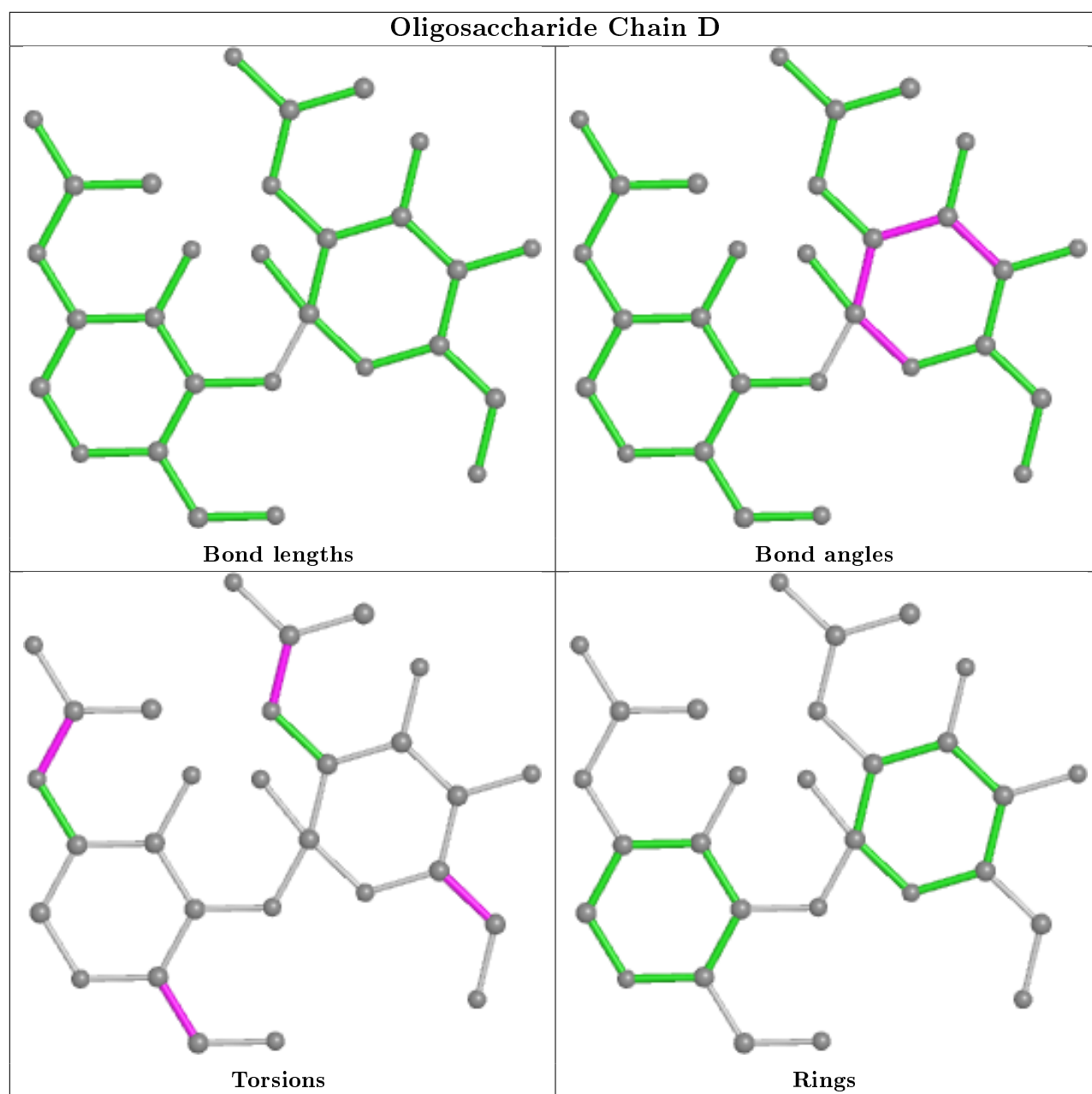
There are no ring outliers.

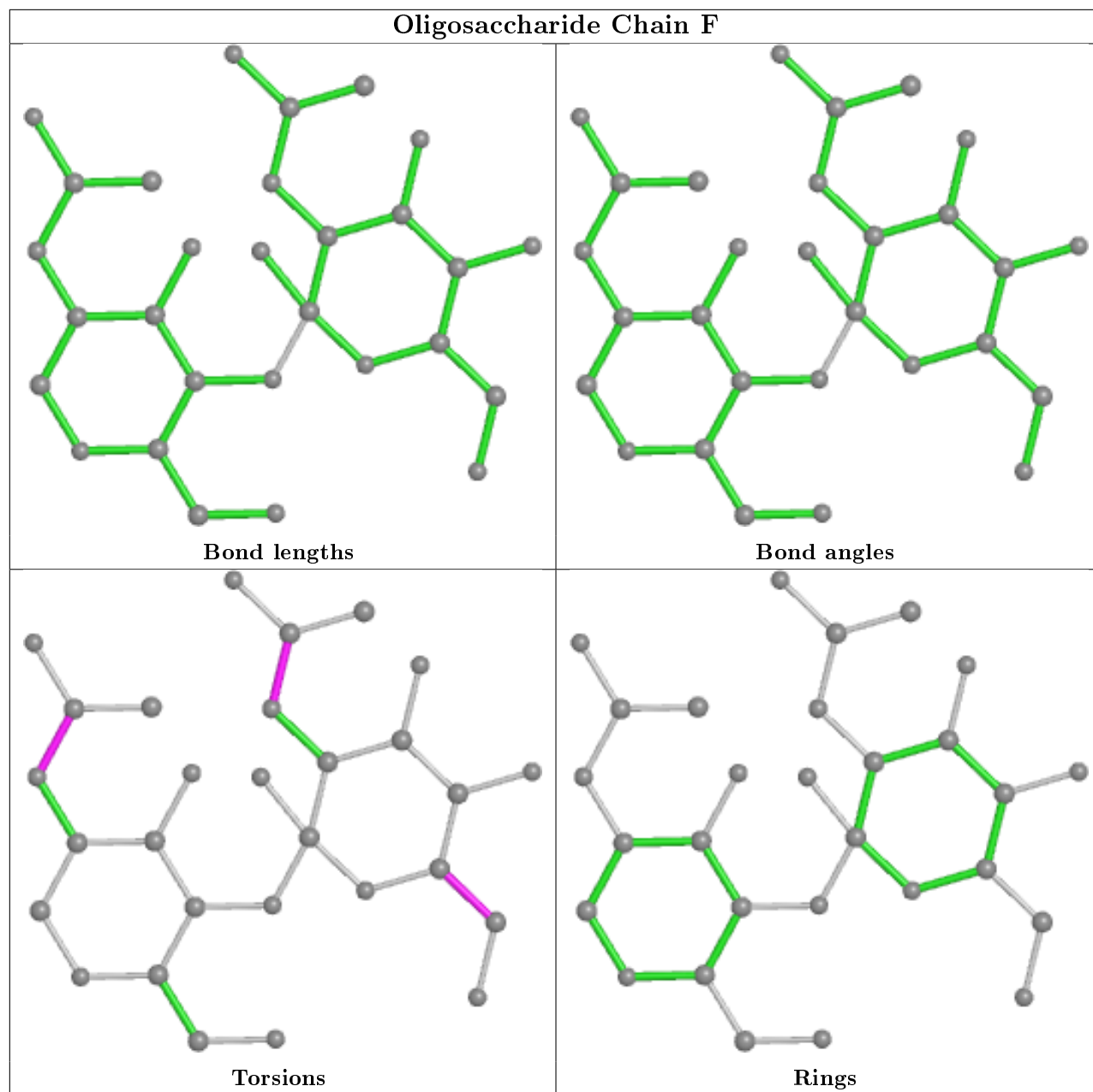
7 monomers are involved in 25 short contacts:

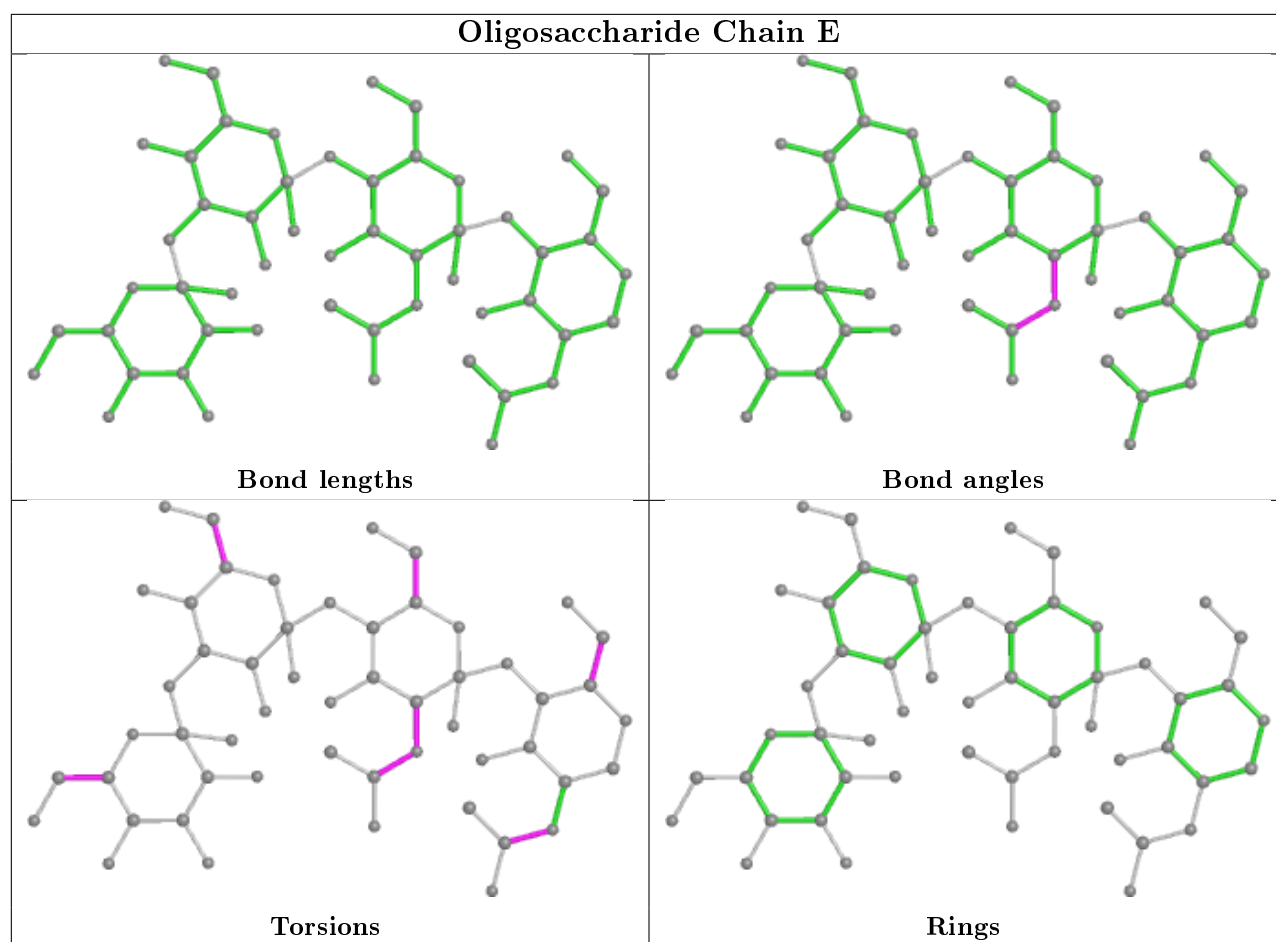
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	6	0
2	C	1	NAG	8	0
3	F	1	NAG	1	0
4	E	1	NAG	7	0
4	E	2	NAG	2	0
2	C	2	NAG	4	0
2	C	3	MAN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 13 are monoatomic - leaving 18 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
8	HTO	A	1400	-	9,9,9	2.19	3 (33%)	10,10,10	1.00	0
9	PLM	B	1407	-	15,15,17	1.74	3 (20%)	14,14,17	3.33	7 (50%)
8	HTO	A	1404	-	9,9,9	2.45	3 (33%)	10,10,10	1.00	0
9	PLM	A	1410	-	15,15,17	1.82	3 (20%)	14,14,17	3.34	8 (57%)
10	RET	B	1296	1	20,20,21	1.99	5 (25%)	27,27,28	1.98	9 (33%)
5	BNG	A	1505	-	21,21,21	2.04	7 (33%)	26,26,26	0.93	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BNG	A	1501	-	21,21,21	1.92	7 (33%)	26,26,26	0.71	0
9	PLM	A	1322	1	16,16,17	0.37	0	15,15,17	0.61	0
9	PLM	B	1322	1	16,16,17	0.53	0	15,15,17	0.46	0
5	BNG	B	1506	-	21,21,21	1.88	7 (33%)	26,26,26	0.83	1 (3%)
8	HTO	A	1405	-	9,9,9	2.08	2 (22%)	10,10,10	0.98	0
10	RET	A	1296	1	20,20,21	1.83	5 (25%)	27,27,28	1.97	10 (37%)
9	PLM	A	1323	1	16,16,17	0.37	0	15,15,17	0.58	0
8	HTO	A	1401	-	9,9,9	2.25	3 (33%)	10,10,10	1.17	1 (10%)
5	BNG	A	1503	-	21,21,21	2.14	7 (33%)	26,26,26	0.81	1 (3%)
5	BNG	A	1504	-	21,21,21	1.94	7 (33%)	26,26,26	0.76	1 (3%)
5	BNG	A	1500	-	21,21,21	2.02	6 (28%)	26,26,26	0.79	1 (3%)
5	BNG	B	1502	-	21,21,21	2.22	7 (33%)	26,26,26	0.87	1 (3%)

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
8	HTO	A	1400	-	-	1/10/10/10	-
9	PLM	B	1407	-	-	6/13/13/15	-
8	HTO	A	1404	-	-	0/10/10/10	-
9	PLM	A	1410	-	-	7/13/13/15	-
10	RET	B	1296	1	-	9/13/30/31	0/1/1/1
5	BNG	A	1505	-	-	2/12/32/32	0/1/1/1
5	BNG	A	1501	-	-	4/12/32/32	0/1/1/1
9	PLM	A	1322	1	-	11/13/14/15	-
9	PLM	B	1322	1	-	7/13/14/15	-
5	BNG	B	1506	-	-	9/12/32/32	0/1/1/1
8	HTO	A	1405	-	-	1/10/10/10	-
10	RET	A	1296	1	-	4/13/30/31	0/1/1/1
9	PLM	A	1323	1	-	5/13/14/15	-
8	HTO	A	1401	-	-	0/10/10/10	-
5	BNG	A	1503	-	-	6/12/32/32	0/1/1/1
5	BNG	A	1504	-	-	6/12/32/32	0/1/1/1
5	BNG	A	1500	-	-	8/12/32/32	0/1/1/1
5	BNG	B	1502	-	-	6/12/32/32	0/1/1/1

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1502	BNG	O1-C1	5.64	1.49	1.40
8	A	1404	HTO	C3-C2	5.38	1.66	1.52
5	A	1503	BNG	O5-C1	5.19	1.55	1.41
8	A	1401	HTO	C3-C2	4.97	1.65	1.52
5	B	1502	BNG	O5-C1	4.88	1.54	1.41

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1407	PLM	CD-CC-CB	8.07	155.41	114.42
9	A	1410	PLM	CD-CC-CB	8.04	155.22	114.42
9	A	1410	PLM	CA-C9-C8	7.09	150.40	114.42
9	B	1407	PLM	CA-C9-C8	6.95	149.72	114.42
10	A	1296	RET	C11-C12-C13	4.32	138.55	126.42

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1506	BNG	C2'-C1'-O1-C1
10	A	1296	RET	C7-C8-C9-C10
10	A	1296	RET	C7-C8-C9-C19
10	B	1296	RET	C7-C8-C9-C10
10	B	1296	RET	C7-C8-C9-C19

There are no ring outliers.

14 monomers are involved in 31 short contacts:

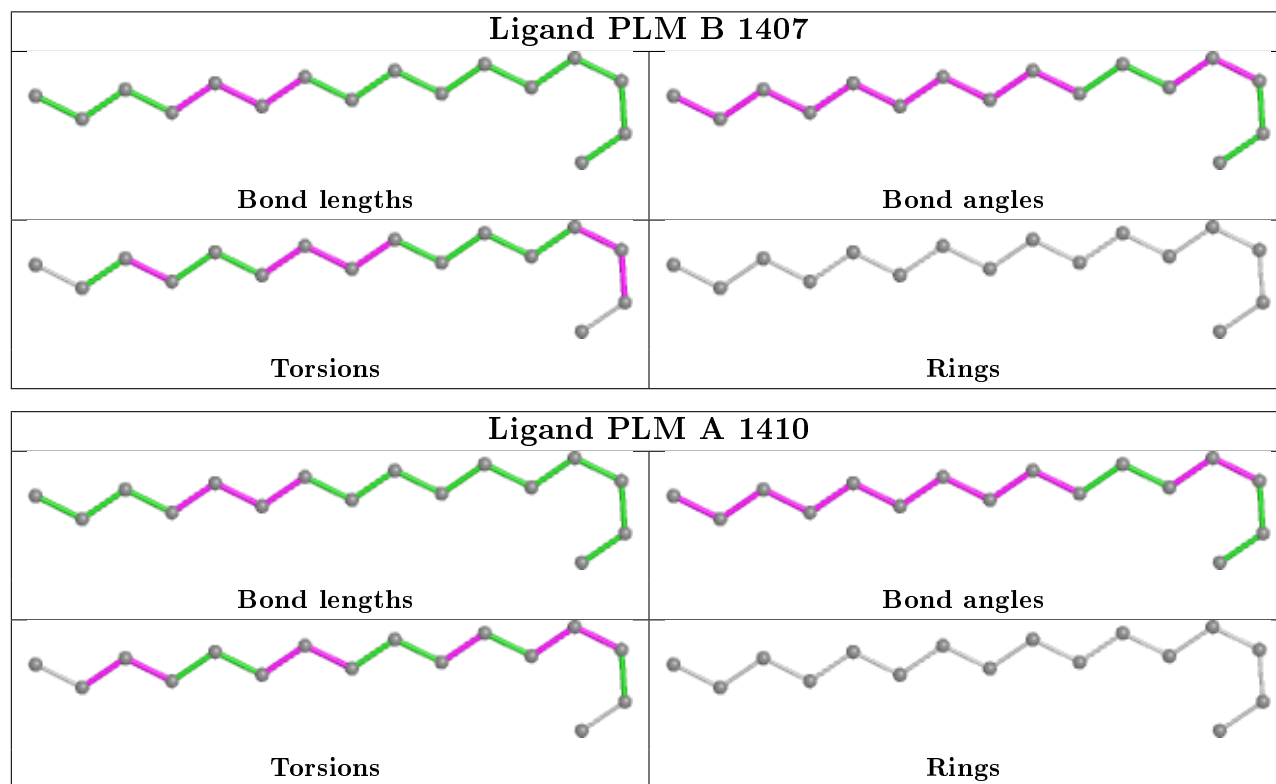
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1407	PLM	1	0
8	A	1404	HTO	1	0
10	B	1296	RET	3	0
5	A	1505	BNG	2	0
5	A	1501	BNG	1	0
9	A	1322	PLM	3	0
9	B	1322	PLM	1	0
5	B	1506	BNG	7	0
8	A	1405	HTO	1	0
10	A	1296	RET	1	0
8	A	1401	HTO	2	0

*Continued on next page...*

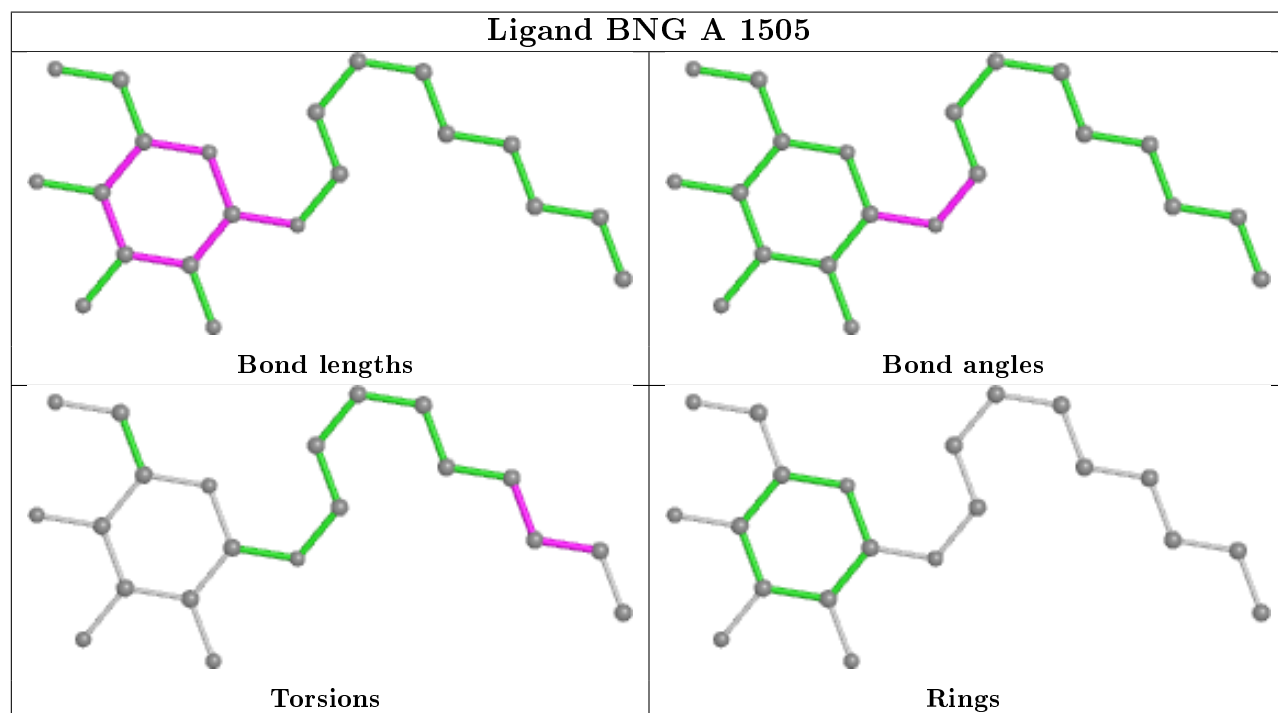
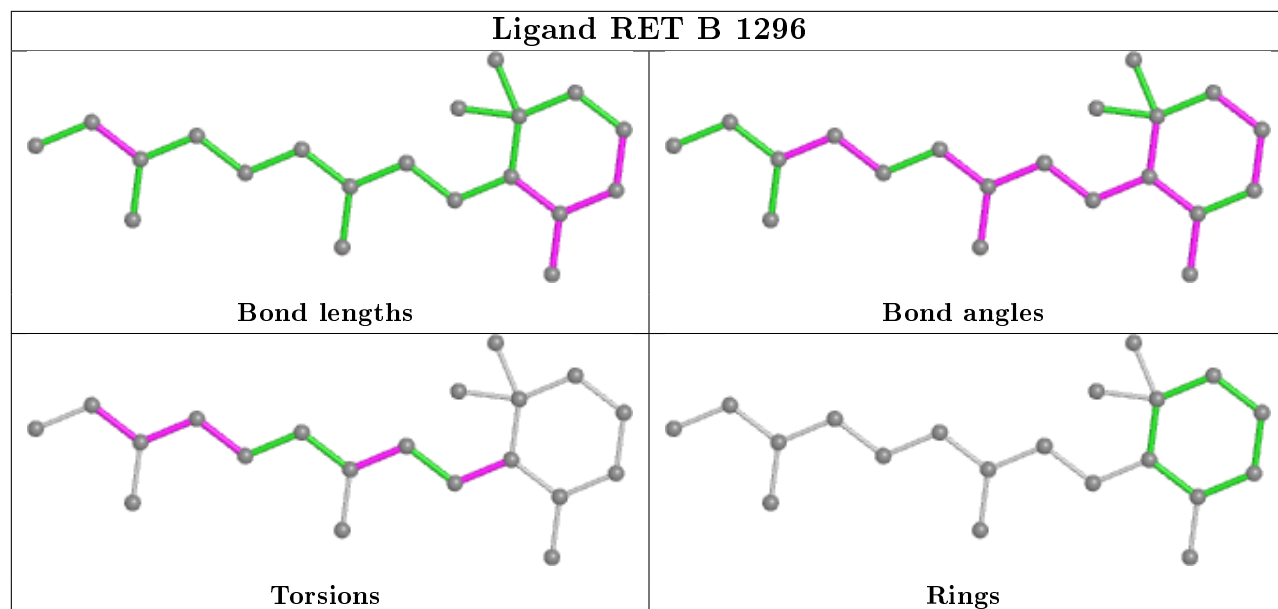
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1503	BNG	1	0
5	A	1504	BNG	1	0
5	A	1500	BNG	6	0

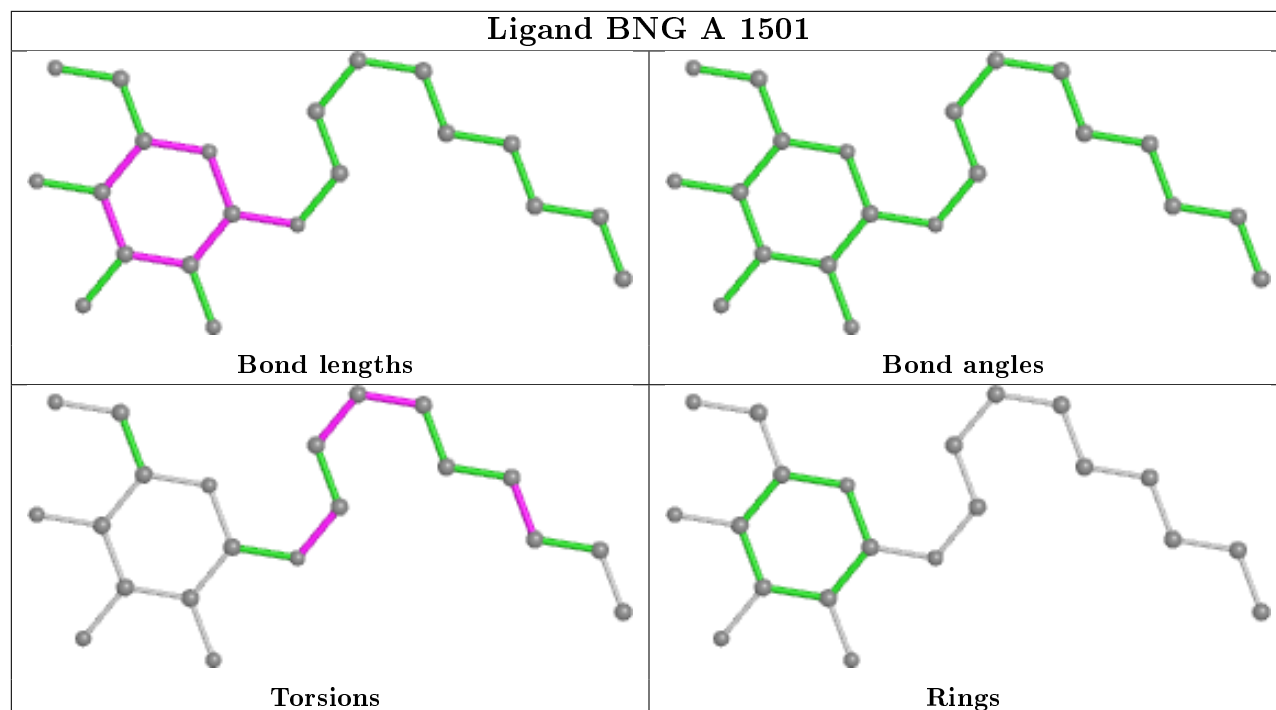
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



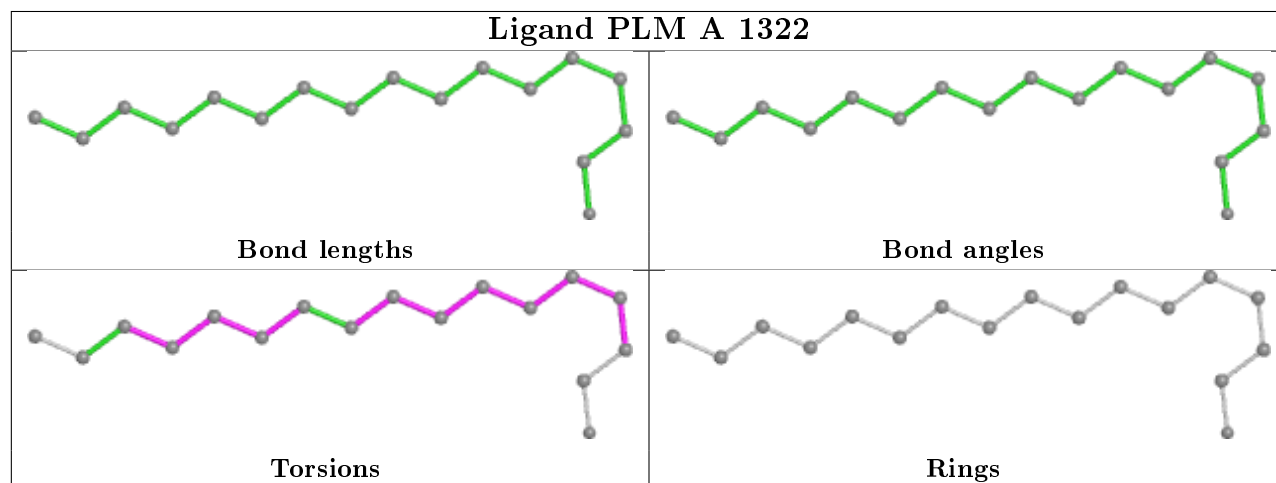




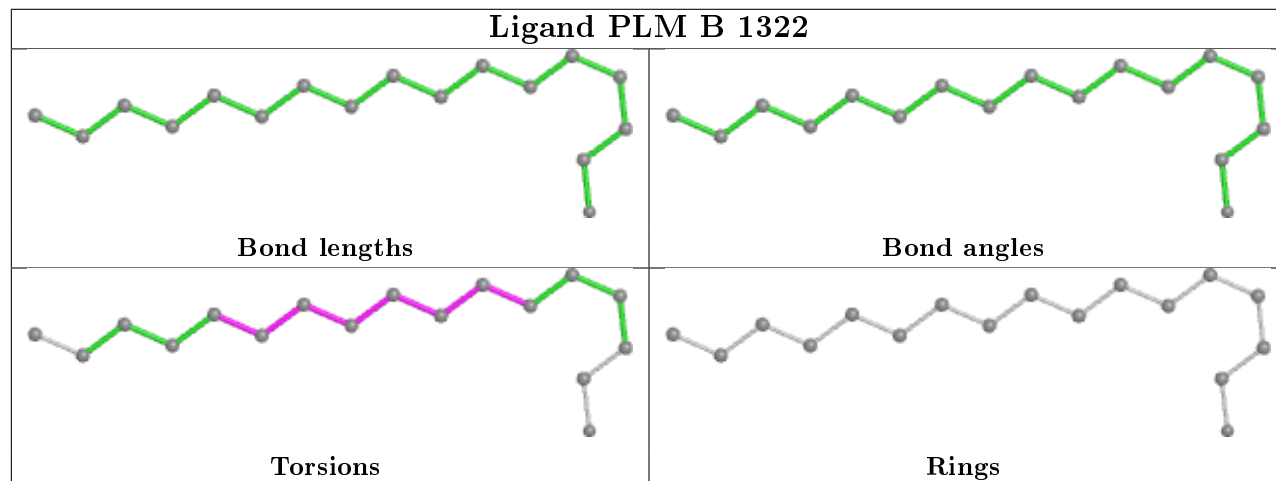
## Ligand BNG A 1501



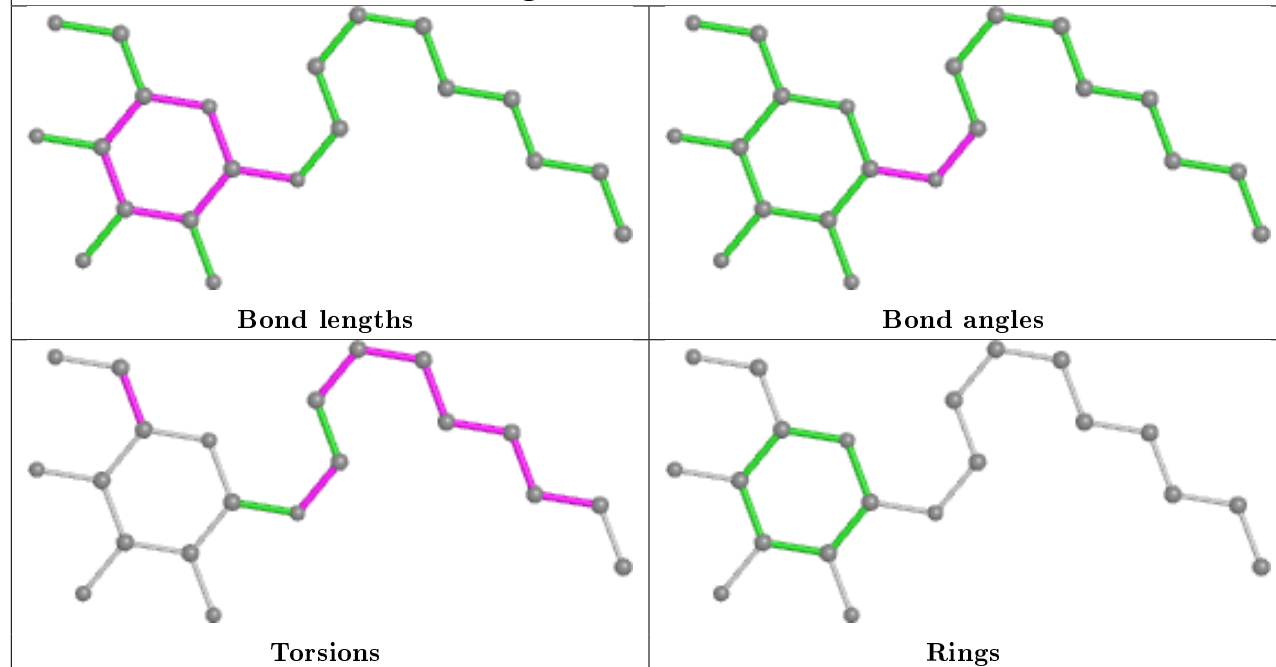
## Ligand PLM A 1322



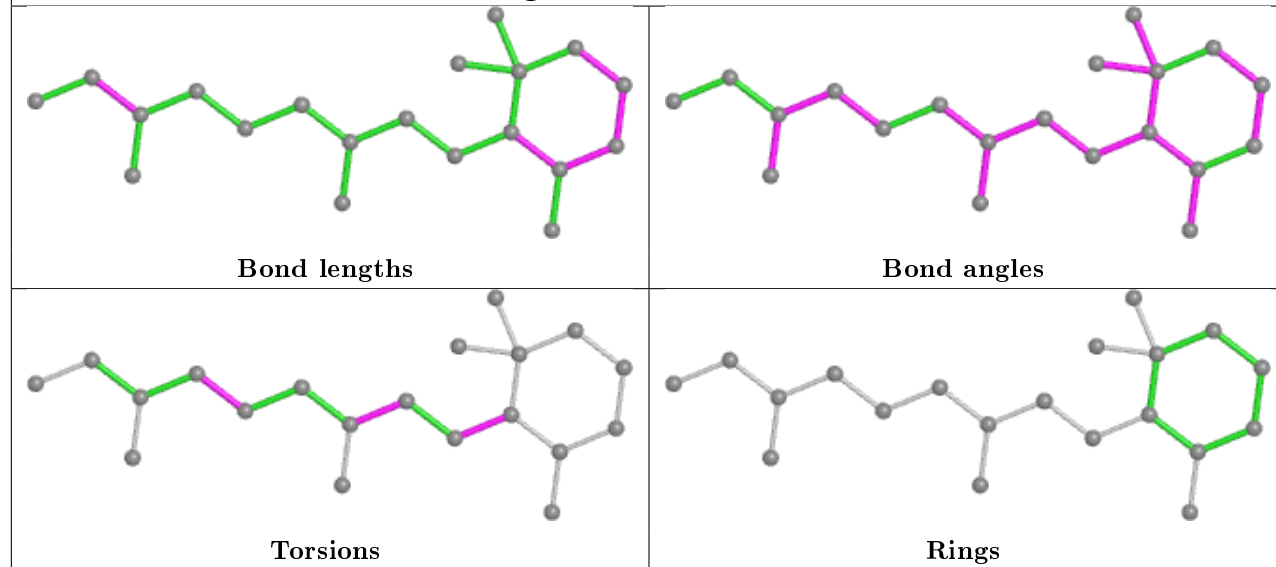
## Ligand PLM B 1322

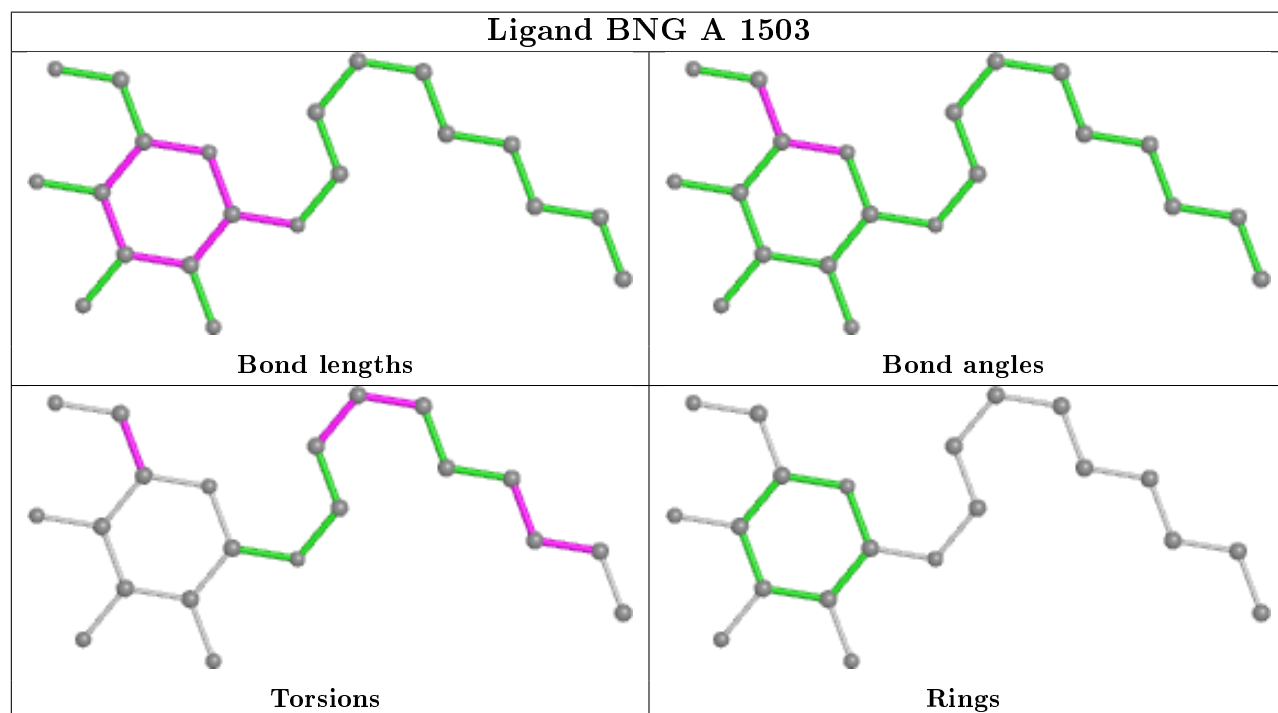
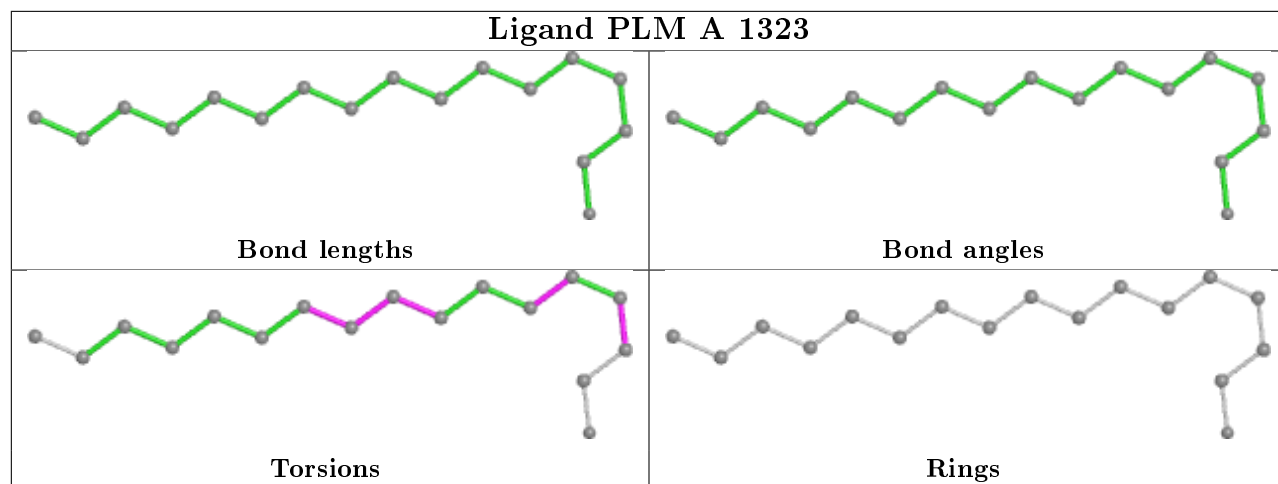


## Ligand BNG B 1506

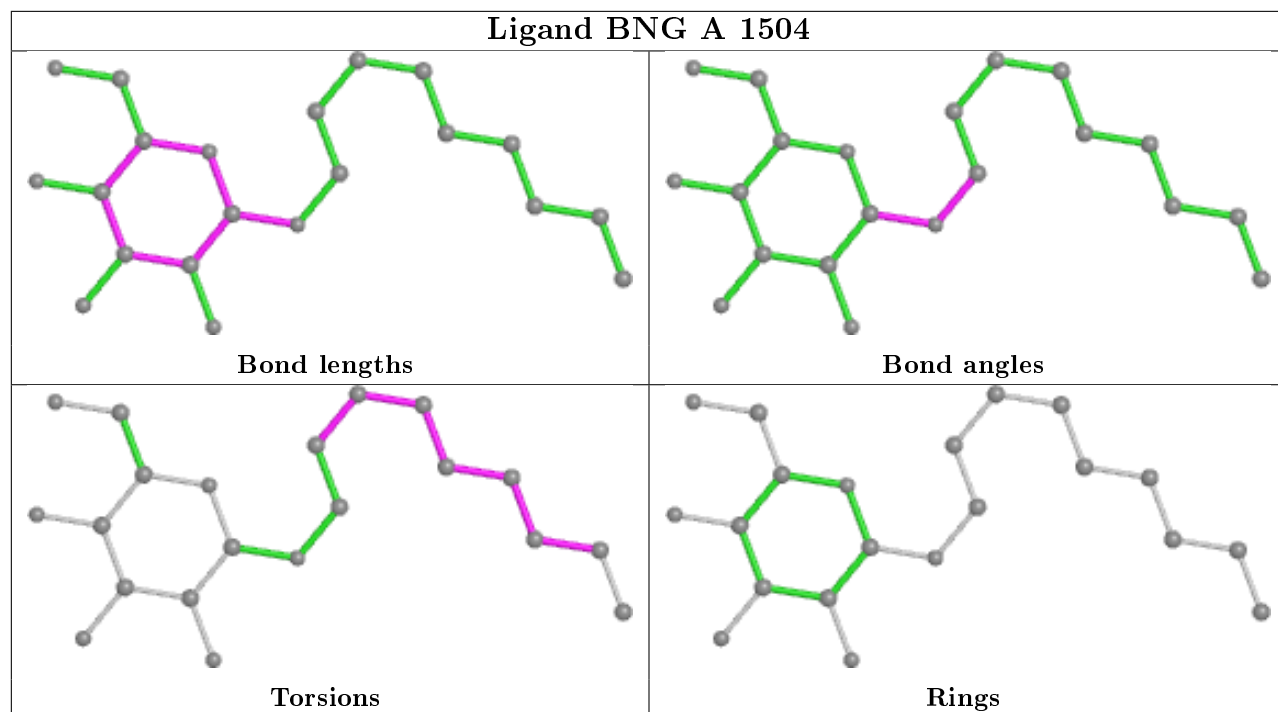


## Ligand RET A 1296

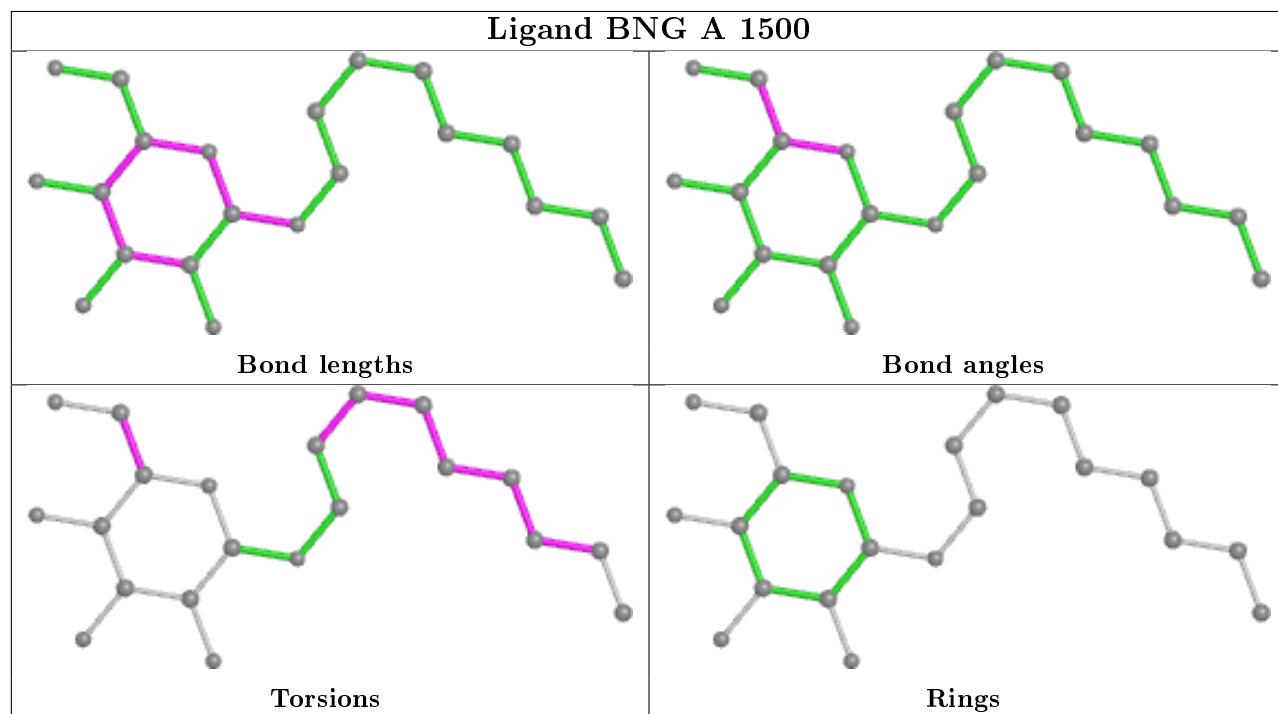


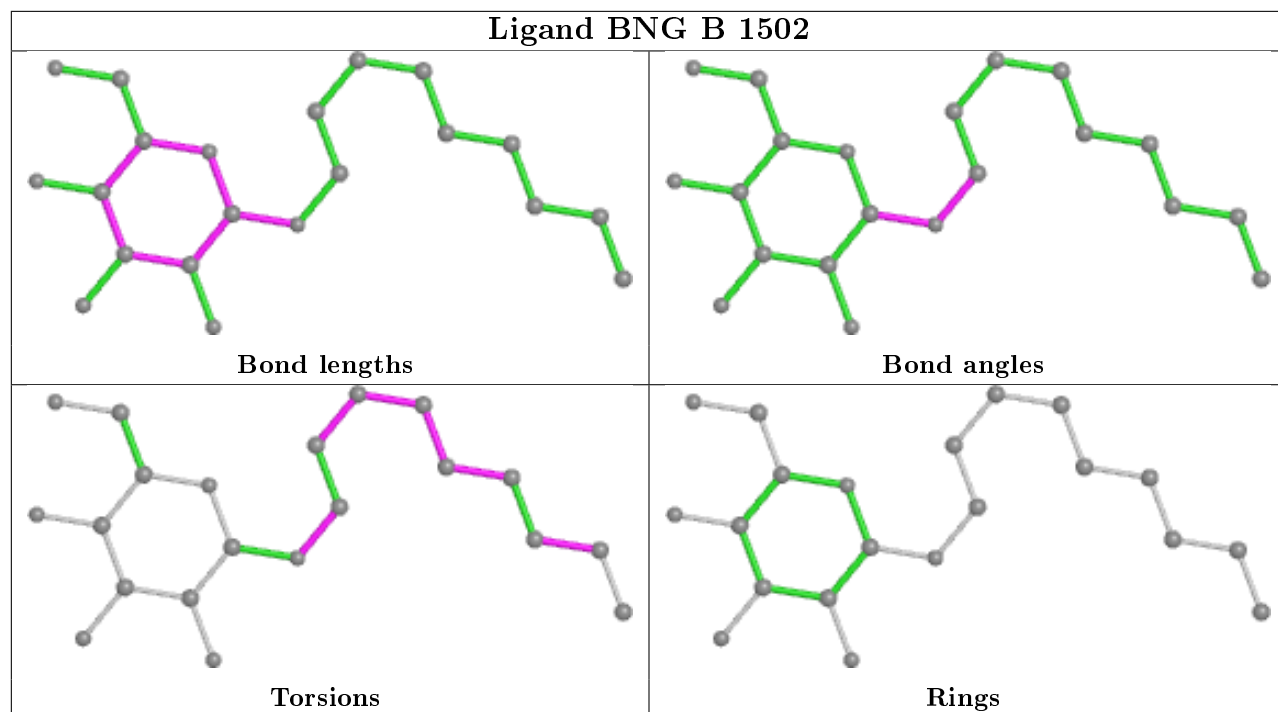


## Ligand BNG A 1504



## Ligand BNG A 1500





## 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.