



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 01:54 PM BST

PDB ID : 1PTH
Title : The Structural Basis of Aspirin Activity Inferred from the Crystal Structure of Inactivated Prostaglandin H2 Synthase
Authors : Loll, P.J.; Picot, D.; Garavito, R.M.
Deposited on : 1995-04-11
Resolution : 3.40 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

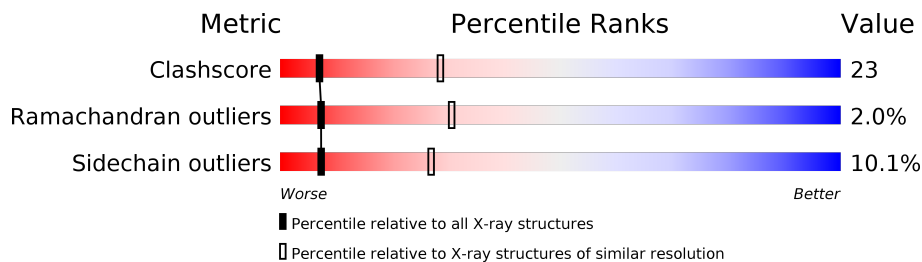
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 ≥ 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	576	
1	B	576	
2	C	2	
2	D	2	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 9221 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 PROSTAGLANDIN H2 SYNTHASE-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	S			
1	A	551	4481	1	2905	758	789	28	0	0	0
1	B	551	4481	1	2905	758	789	28	0	0	0

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



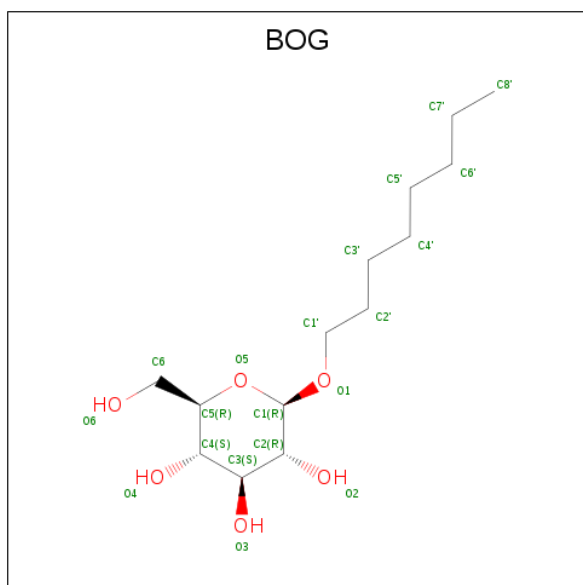
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

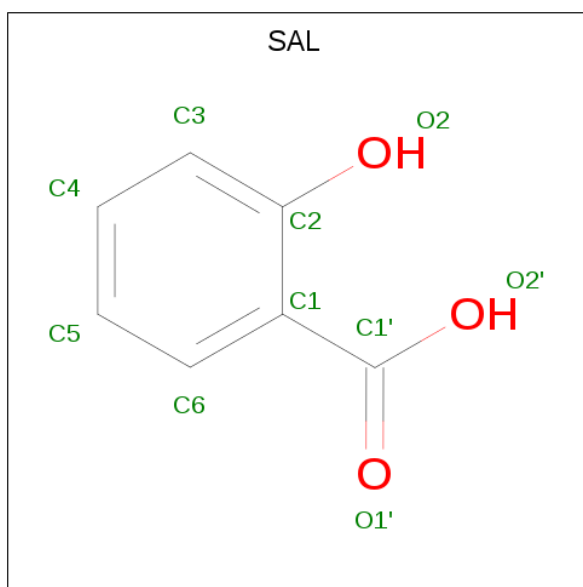
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).

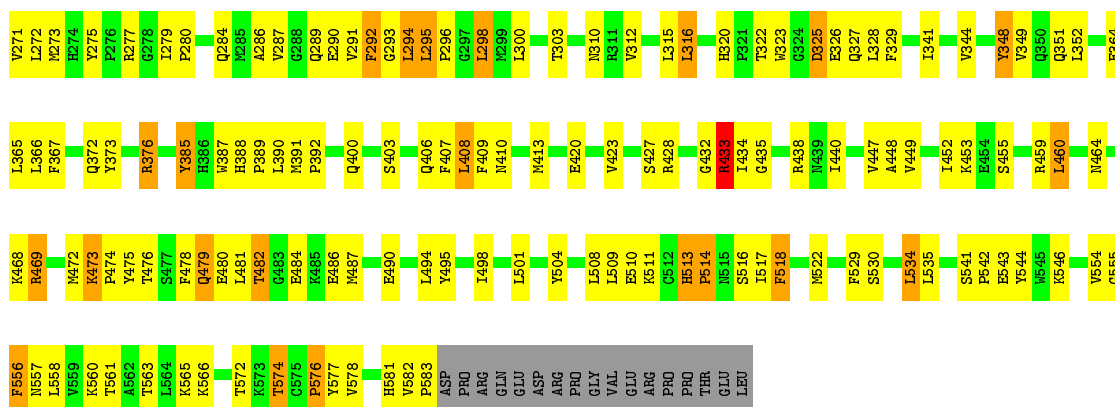




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		



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

Chain C: 100%

MAG1
MAG2

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

Chain D: 100%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.57Å 209.80Å 235.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40	Depositor
% Data completeness (in resolution range)	75.5 (8.00-3.40)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9221	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0AH, HEM, BOG, NAG, SAL

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	0.61	0/4608	0.81	5/6253 (0.1%)
1	B	0.61	0/4608	0.81	5/6253 (0.1%)
All	All	0.61	0/9216	0.81	10/12506 (0.1%)

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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	433	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	408	LEU	N-CA-C	5.31	125.33	111.00
1	B	408	LEU	N-CA-C	5.29	125.30	111.00
1	A	224	LEU	CA-CB-CG	-5.12	103.52	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	348	TYR	Sidechain
1	B	136	TYR	Sidechain
1	B	348	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	4481	0	4381	212	1
1	B	4481	0	4381	213	1
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	28	0	26	2	0
3	B	28	0	26	2	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0
5	A	43	0	30	6	0
5	B	43	0	30	6	0
6	A	10	0	4	1	0
6	B	10	0	4	1	0
7	A	1	0	0	0	0
All	All	9221	0	8988	417	1

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 23.

The worst 5 of 417 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:156:PRO:HG2	1:B:159:CYS:SG	1.79	1.23
1:A:156:PRO:HG2	1:A:159:CYS:SG	1.79	1.22
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.42	1.01
1:B:203:GLN:HG2	1:B:298:LEU:HD11	1.43	1.00
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.54	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:PHE:CE1	1:B:277:ARG:NH1[8_456]	2.18	0.02

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	548/576 (95%)	488 (89%)	49 (9%)	11 (2%)	7	30
1	B	548/576 (95%)	488 (89%)	49 (9%)	11 (2%)	7	30
All	All	1096/1152 (95%)	976 (89%)	98 (9%)	22 (2%)	7	30

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	295	LEU
1	A	408	LEU
1	A	514	PRO
1	B	54	ARG

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	485/505 (96%)	436 (90%)	49 (10%)	7	27
1	B	485/505 (96%)	436 (90%)	49 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	970/1010 (96%)	872 (90%)	98 (10%)	7 27

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	LEU
1	B	120	ARG
1	B	513	HIS
1	A	535	LEU
1	B	53	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	GLN
1	B	95	HIS
1	B	372	GLN
1	A	375	ASN
1	B	375	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	0AH	A	530	1	8,9,10	0.91	0	5,10,12	5.80	1 (20%)
1	0AH	B	530	1	8,9,10	0.91	0	5,10,12	5.80	1 (20%)

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	0AH	A	530	1	-	2/7/9/11	-
1	0AH	B	530	1	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	0AH	O2-CB-CA	12.85	144.81	108.48
1	A	530	0AH	O2-CB-CA	12.85	144.79	108.48

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	530	0AH	O2-C1-C2-BR2
1	B	530	0AH	O2-C1-C2-BR2
1	A	530	0AH	O1-C1-C2-BR2
1	B	530	0AH	O1-C1-C2-BR2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

4 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	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.67	0	17,19,21	1.22	1 (5%)
2	NAG	D	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.17	2 (11%)

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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C4-C5	2.04	1.57	1.53
2	C	2	NAG	C4-C5	2.02	1.57	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	-2.65	119.13	122.90
2	C	1	NAG	C2-N2-C7	-2.62	119.17	122.90
2	C	2	NAG	C4-C3-C2	-2.54	107.29	111.02
2	D	2	NAG	C4-C3-C2	-2.53	107.31	111.02
2	C	2	NAG	O5-C1-C2	-2.07	108.01	111.29

There are no chirality outliers.

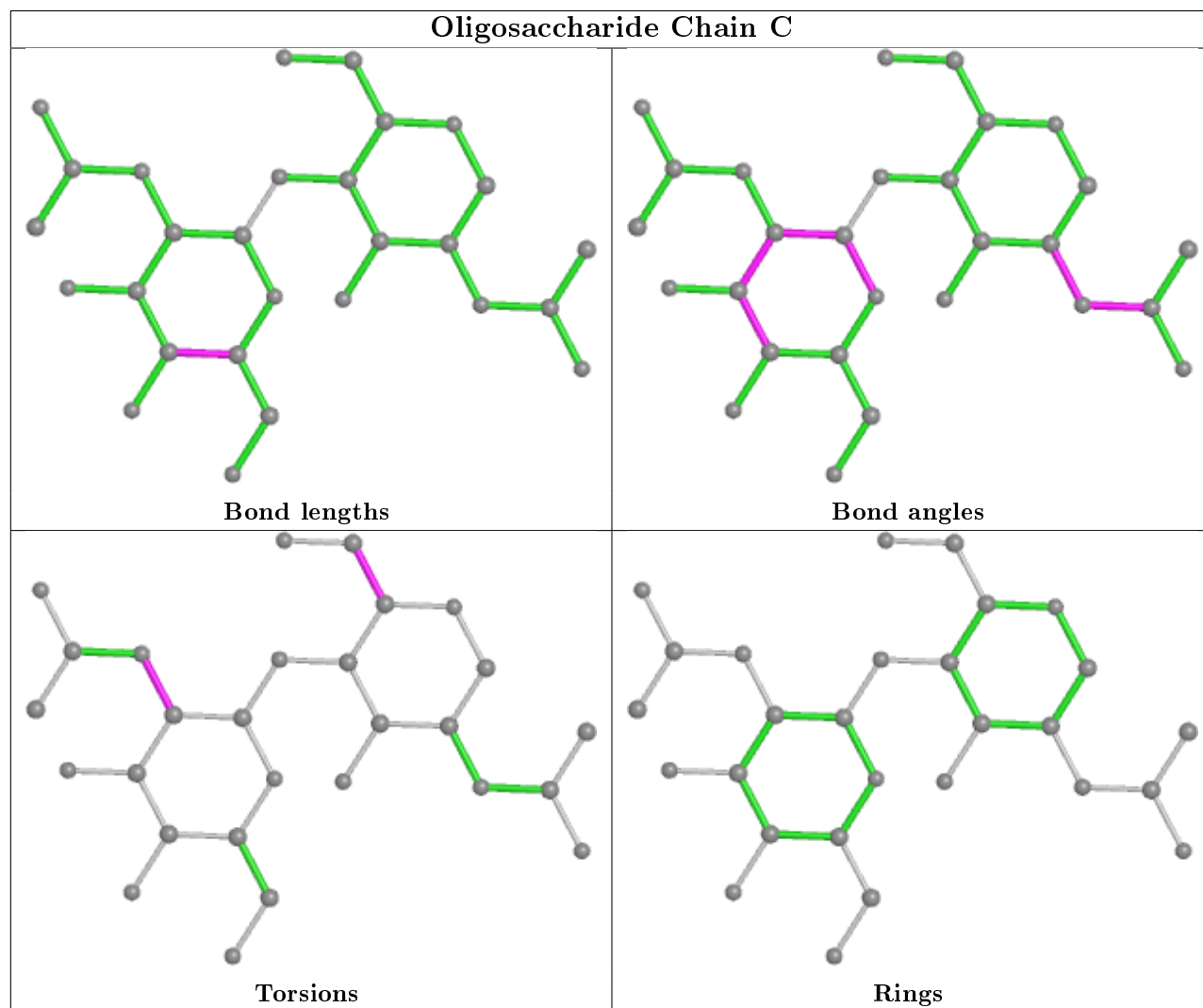
5 of 6 torsion outliers are listed below:

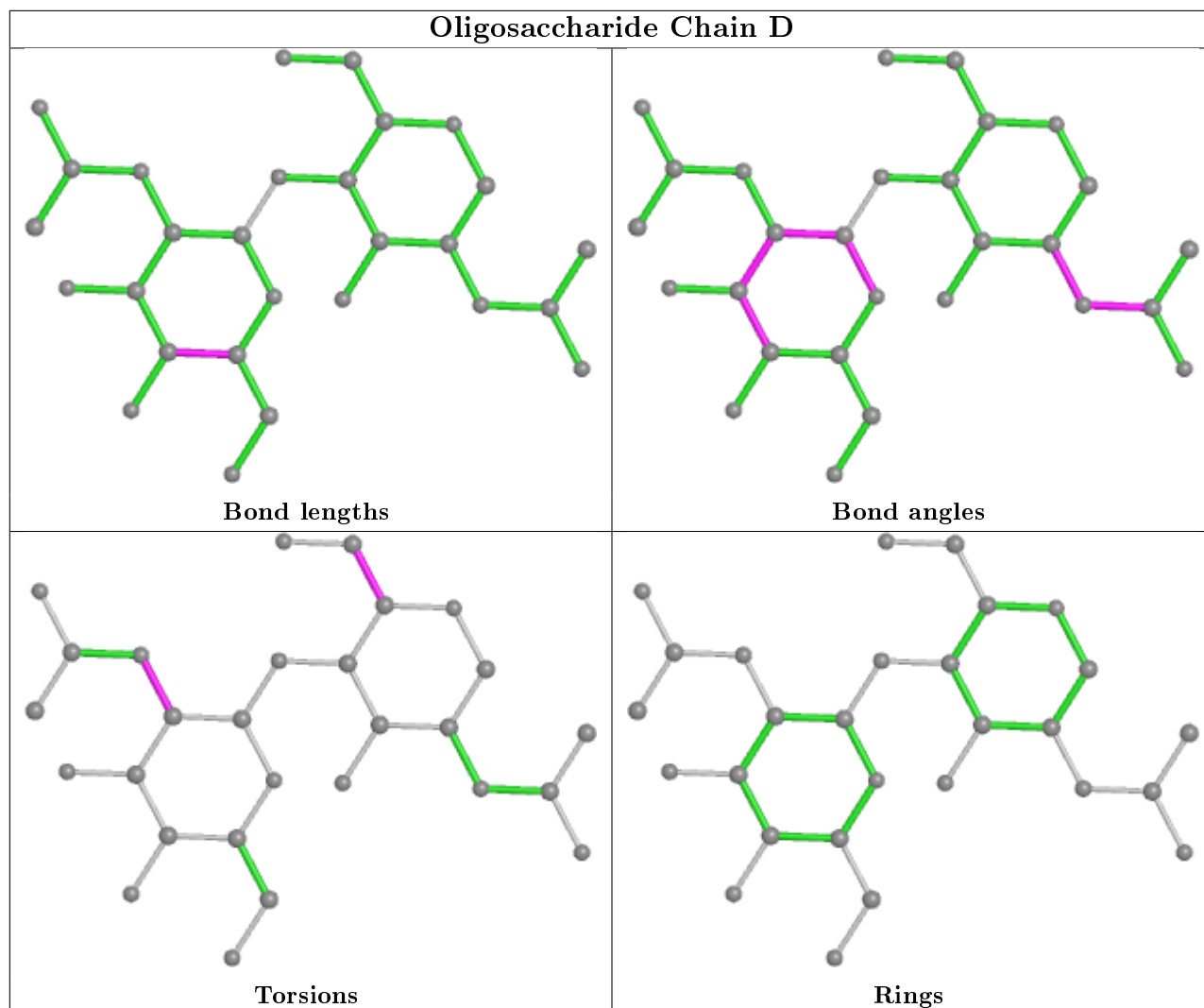
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C1-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	B	661	1	14,14,15	0.50	0	17,19,21	0.79	0
3	NAG	B	681	1	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
5	HEM	B	602	1	27,50,50	2.23	9 (33%)	17,82,82	2.31	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BOG	B	702	-	20,20,20	0.63	0	25,25,25	0.79	1 (4%)
6	SAL	A	710	-	8,10,10	0.54	0	9,13,13	0.58	0
4	BOG	A	702	-	20,20,20	0.64	0	25,25,25	0.79	1 (4%)
5	HEM	A	601	1	27,50,50	2.23	9 (33%)	17,82,82	2.31	5 (29%)
6	SAL	B	711	-	8,10,10	0.56	0	9,13,13	0.58	0
3	NAG	A	661	1	14,14,15	0.51	0	17,19,21	0.79	0
3	NAG	A	681	1	14,14,15	0.53	0	17,19,21	1.06	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	661	1	-	0/6/23/26	0/1/1/1
3	NAG	B	681	1	-	0/6/23/26	0/1/1/1
5	HEM	B	602	1	-	0/6/54/54	-
4	BOG	B	702	-	-	2/11/31/31	0/1/1/1
6	SAL	A	710	-	-	0/0/4/4	0/1/1/1
4	BOG	A	702	-	-	2/11/31/31	0/1/1/1
5	HEM	A	601	1	-	0/6/54/54	-
6	SAL	B	711	-	-	0/0/4/4	0/1/1/1
3	NAG	A	661	1	-	0/6/23/26	0/1/1/1
3	NAG	A	681	1	-	0/6/23/26	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEM	C3C-CAC	-6.30	1.34	1.47
5	B	602	HEM	C3C-CAC	-6.28	1.34	1.47
5	B	602	HEM	C3C-C2C	-5.37	1.32	1.40
5	A	601	HEM	C3C-C2C	-5.35	1.32	1.40
5	A	601	HEM	C1B-C2B	3.54	1.50	1.42

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEM	C4A-C3A-C2A	5.81	111.04	107.00
5	B	602	HEM	C4A-C3A-C2A	5.79	111.02	107.00
5	B	602	HEM	CBA-CAA-C2A	5.34	122.33	112.49
5	A	601	HEM	CBA-CAA-C2A	5.33	122.31	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEM	CMA-C3A-C2A	-3.44	118.46	124.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

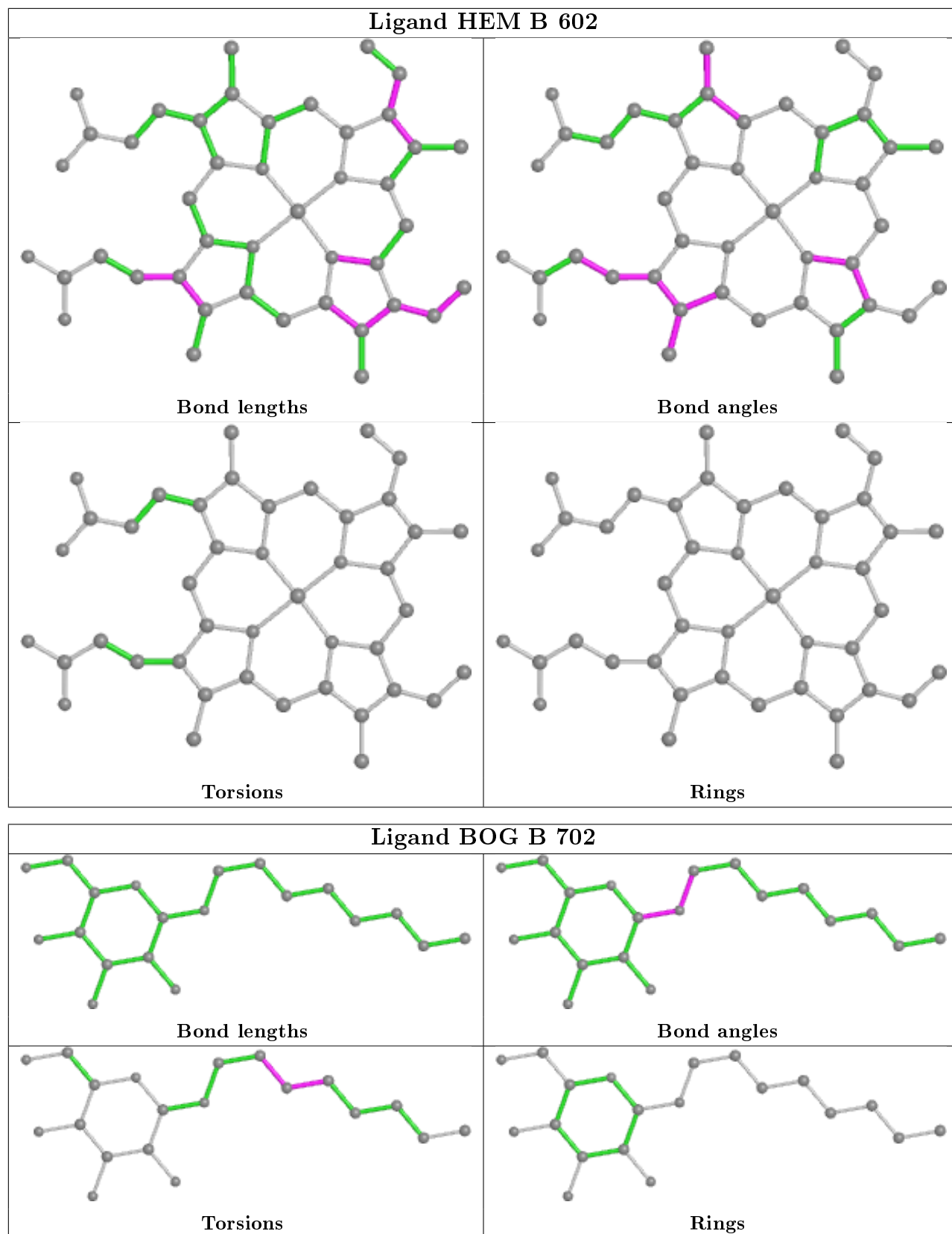
Mol	Chain	Res	Type	Atoms
4	B	702	BOG	C1'-C2'-C3'-C4'
4	A	702	BOG	C1'-C2'-C3'-C4'
4	B	702	BOG	C2'-C3'-C4'-C5'
4	A	702	BOG	C2'-C3'-C4'-C5'

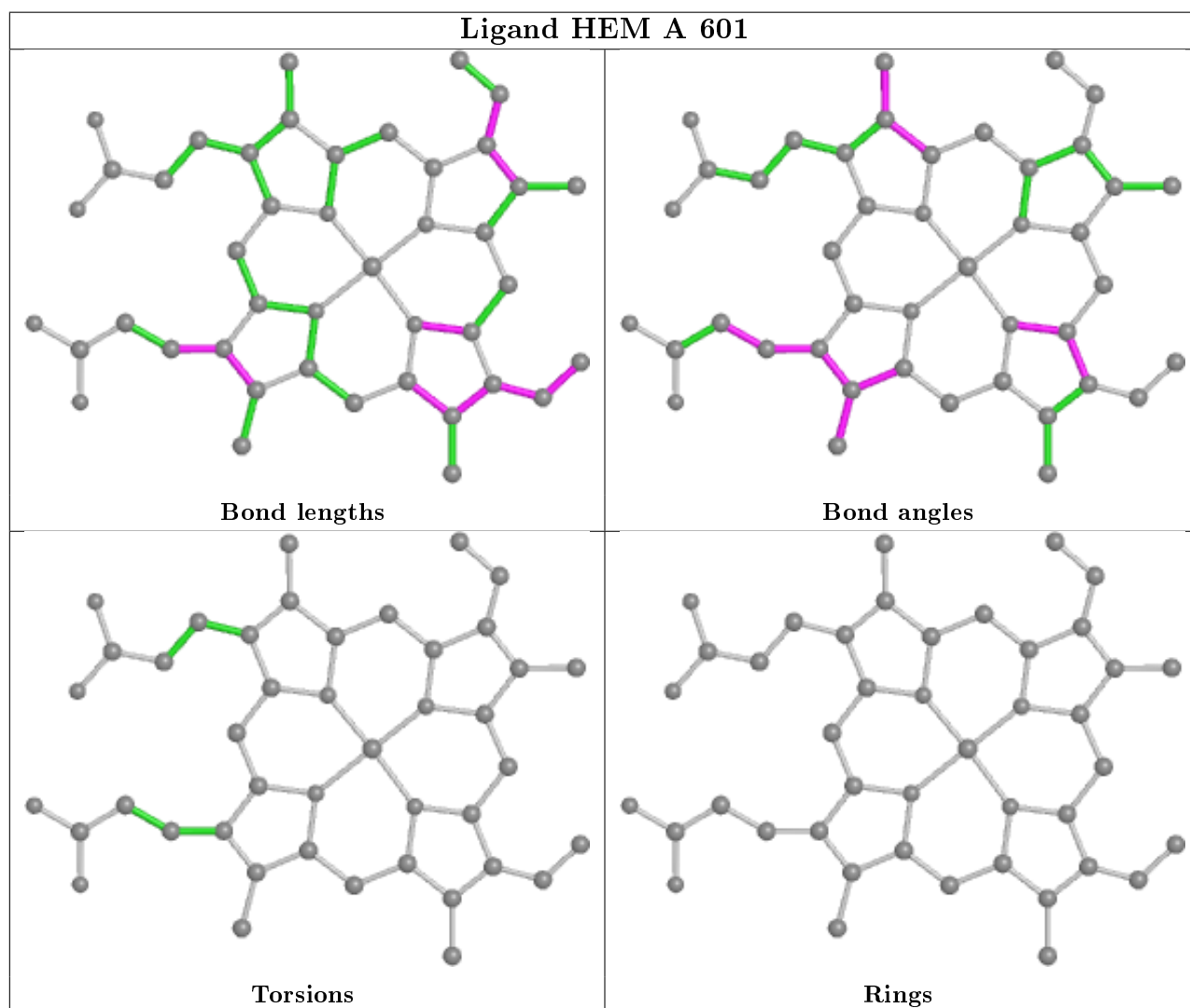
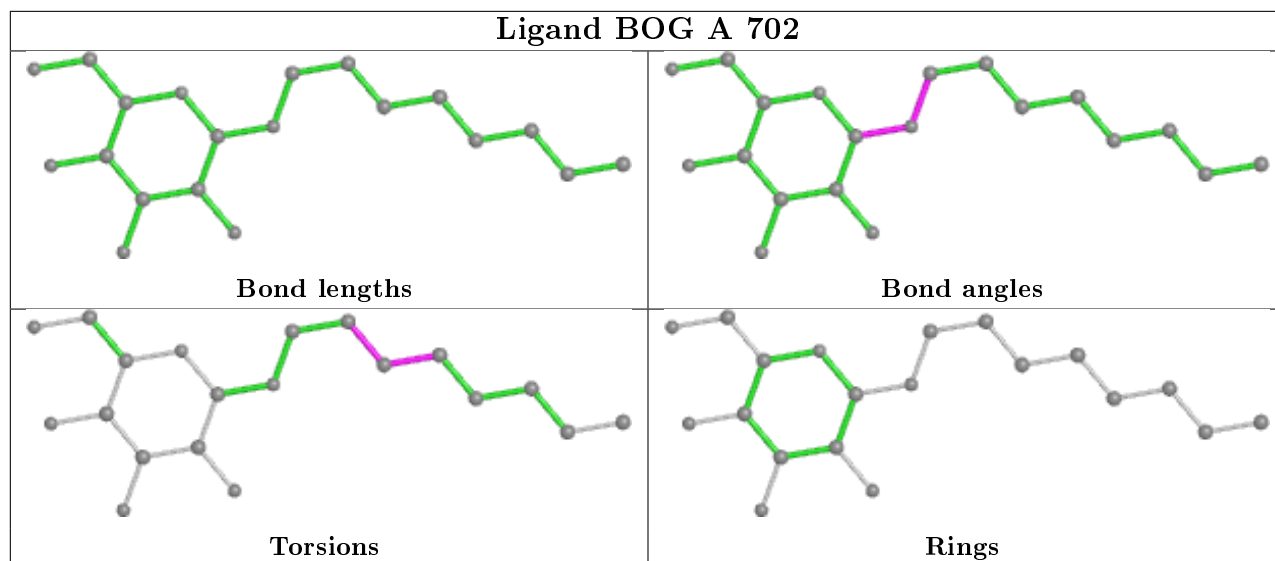
There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	661	NAG	1	0
3	B	681	NAG	1	0
5	B	602	HEM	6	0
6	A	710	SAL	1	0
5	A	601	HEM	6	0
6	B	711	SAL	1	0
3	A	661	NAG	1	0
3	A	681	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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.