



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:38 PM UTC

PDB ID : 2EHA / pdb\_00002eha  
Title : Crystal structure of goat lactoperoxidase complexed with formate anion at 3.3 Å resolution  
Authors : Singh, A.K.; Ethayathulla, A.S.; Singh, N.; Sharma, S.; Kaur, P.; Singh, T.P.  
Deposited on : 2007-03-06  
Resolution : 3.30 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.

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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

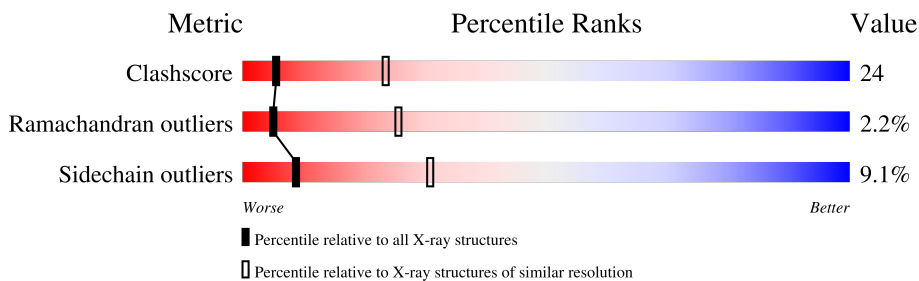
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)



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 of 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	595	
1	B	595	
2	C	3	
2	D	3	
2	G	3	
3	E	3	
3	H	3	
3	I	3	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	J	2	 100%

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
10	OSM	B	3021	-	-	X	-
7	SCN	A	3002	-	-	X	-
9	FMT	A	2001	-	X	-	-
9	FMT	A	2002	-	X	X	-
9	FMT	B	2003	-	X	X	-
9	FMT	B	2004	-	X	-	-

## 2 Entry composition [i](#)

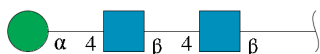
There are 11 unique types of molecules in this entry. The entry contains 10124 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactoperoxidase.

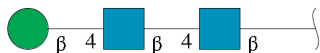
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4753	3021	844	862	26	0	0	0
1	B	595	4753	3021	844	862	26	0	0	0

- 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
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0
2	D	3	39	22	2	15	0	0	0
2	G	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called beta-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
			Total	C	N	O			
3	E	3	39	22	2	15	0	0	0
3	H	3	39	22	2	15	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	3	39	22	2	15	0	0	0

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

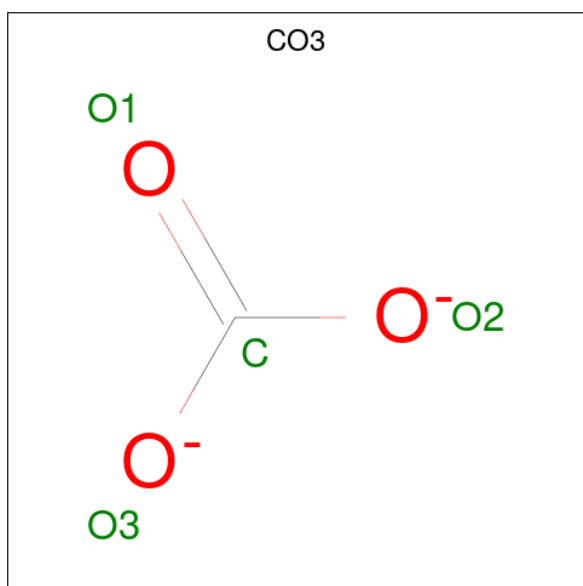


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	2	28	16	2	10	0	0	0
4	J	2	28	16	2	10	0	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

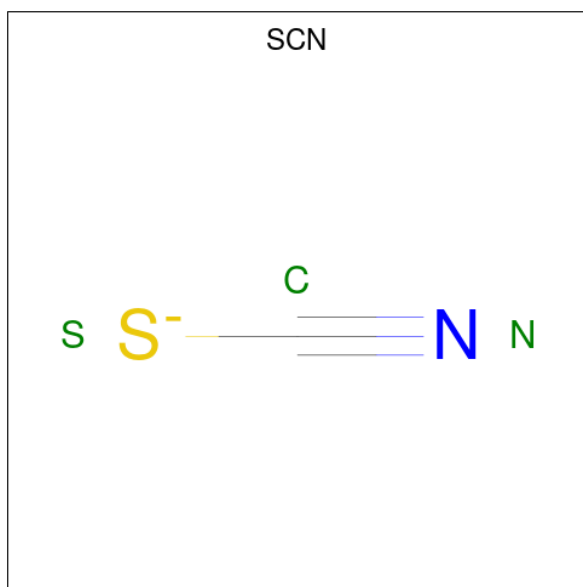
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 7 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		

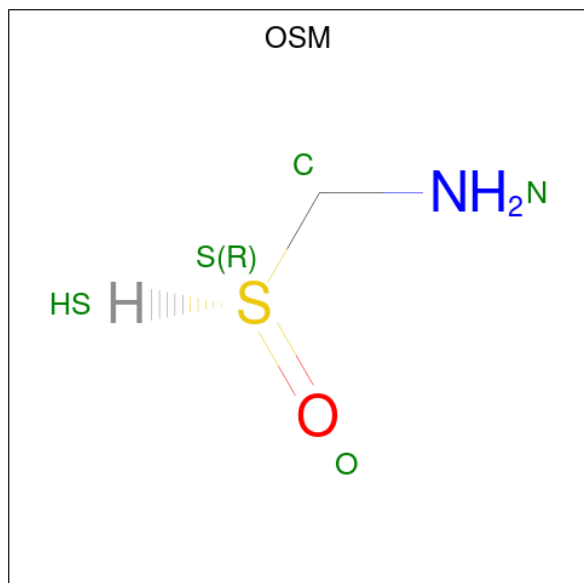
- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			3	1	2		
9	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 10 is 1-(OXIDOSULFANYL)METHANAMINE (CCD ID: OSM) (formula: CH<sub>5</sub>NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			4	1	1	1	1		

- Molecule 11 is water.

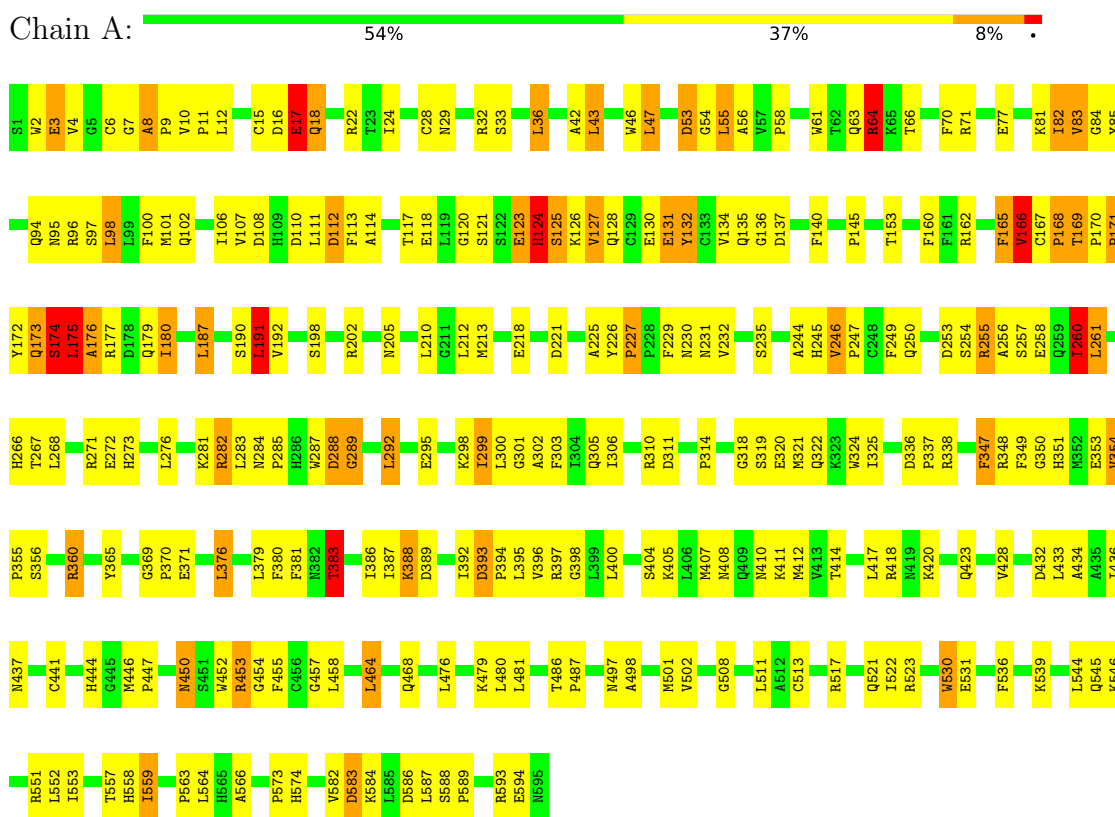
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	116	Total	O	0	0
			116	116		
11	B	97	Total	O	0	0
			97	97		

### 3 Residue-property plots

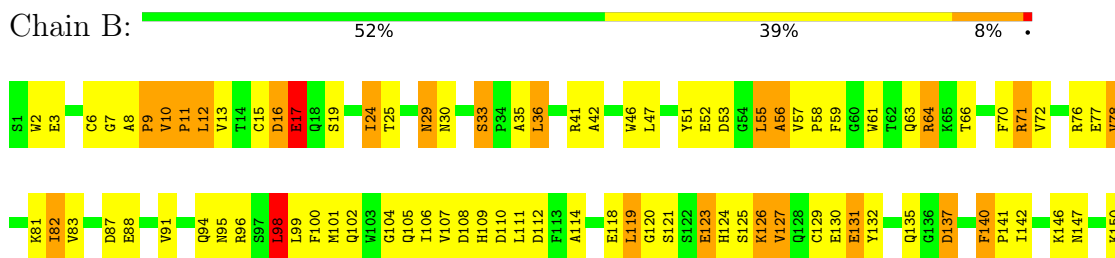
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

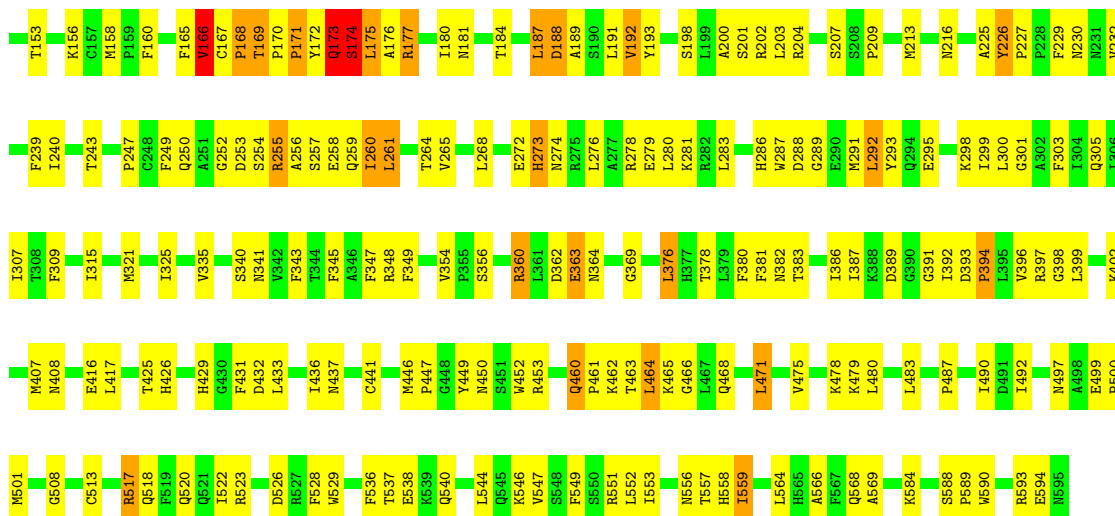
Note EDS was not executed.

- Molecule 1: Lactoperoxidase



- Molecule 1: Lactoperoxidase





- 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: 33% 67%

MAG1  
MAG2  
MAN3

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

Chain D: 33% 67%

MAG1  
MAG2  
MAN3

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

Chain G: 67% 33%

MAG1  
MAG2  
MAN3

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

Chain E: 33% 67%

MAG1  
MAG2  
BWA3

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

Chain H:  33% 67%

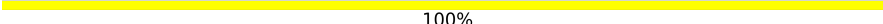
MAG1  
MAG2  
BMA3

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

Chain I:  33% 67%

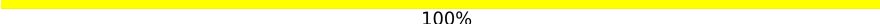
MAG1  
MAG2  
BMA3

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

Chain F:  100%

MAG1  
MAG2

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

Chain J:  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	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.99Å 72.27Å 83.65Å 85.45° 84.04° 75.89°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.196 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10124	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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: SCN, OSM, BMA, HEM, FMT, CO3, CA, NAG, 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	0.55	0/4882	1.26	73/6632 (1.1%)
1	B	0.57	2/4882 (0.0%)	1.25	66/6632 (1.0%)
All	All	0.56	2/9764 (0.0%)	1.25	139/13264 (1.0%)

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 outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	GLN	CA-C	6.04	1.60	1.52
1	B	174	SER	N-CA	5.61	1.53	1.46

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	SER	CA-C-N	12.76	135.79	119.84
1	A	33	SER	C-N-CA	12.76	135.79	119.84
1	B	166	VAL	N-CA-C	11.29	132.83	109.34
1	B	12	LEU	N-CA-C	10.09	125.22	111.90
1	B	125	SER	N-CA-C	-10.08	101.07	113.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4753	0	4646	241	0
1	B	4753	0	4646	230	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
2	G	39	0	34	7	0
3	E	39	0	34	0	0
3	H	39	0	34	1	0
3	I	39	0	34	1	0
4	F	28	0	25	0	0
4	J	28	0	25	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	3	0	0	3	0
8	A	43	0	30	11	0
8	B	43	0	30	5	0
9	A	6	0	4	3	0
9	B	6	0	4	3	0
10	B	4	0	5	2	0
11	A	116	0	0	19	0
11	B	97	0	0	8	0
All	All	10124	0	9619	463	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 24.

The worst 5 of 463 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:167:CYS:HB2	1:B:168:PRO:HD3	1.26	1.14

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.28	1.13
1:B:108:ASP:OD2	8:B:1003:HEM:HMD1	1.51	1.09
1:A:124:HIS:HB2	1:B:137:ASP:CG	1.80	1.06
1:A:132:TYR:OH	1:B:120:GLY:HA2	1.58	1.04

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	593/595 (100%)	526 (89%)	54 (9%)	13 (2%)	5	26
1	B	593/595 (100%)	529 (89%)	51 (9%)	13 (2%)	5	26
All	All	1186/1190 (100%)	1055 (89%)	105 (9%)	26 (2%)	5	26

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	VAL
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	594	GLU

### 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	517/517 (100%)	468 (90%)	49 (10%)	8	29
1	B	517/517 (100%)	472 (91%)	45 (9%)	9	32
All	All	1034/1034 (100%)	940 (91%)	94 (9%)	9	31

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	ARG
1	B	255	ARG
1	B	121	SER
1	B	166	VAL
1	B	279	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	ASN
1	B	250	GLN
1	B	520	GLN
1	B	179	GLN
1	B	341	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](#)

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

## 5.5 Carbohydrates [i](#)

22 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	2,1	14,14,15	0.67	0	17,19,21	0.59	0
2	NAG	C	2	2	14,14,15	0.80	0	17,19,21	1.05	1 (5%)
2	MAN	C	3	2	11,11,12	0.71	0	15,15,17	0.68	1 (6%)
2	NAG	D	1	2,1	14,14,15	0.58	0	17,19,21	0.83	1 (5%)
2	NAG	D	2	2	14,14,15	0.67	0	17,19,21	1.23	1 (5%)
2	MAN	D	3	2	11,11,12	0.57	0	15,15,17	0.39	0
3	NAG	E	1	3,1	14,14,15	0.57	0	17,19,21	0.81	0
3	NAG	E	2	3	14,14,15	0.83	0	17,19,21	1.28	1 (5%)
3	BMA	E	3	3	11,11,12	0.70	0	15,15,17	1.17	2 (13%)
4	NAG	F	1	4,1	14,14,15	0.64	0	17,19,21	1.38	2 (11%)
4	NAG	F	2	4	14,14,15	0.63	0	17,19,21	1.39	2 (11%)
2	NAG	G	1	2,1	14,14,15	0.65	0	17,19,21	0.56	0
2	NAG	G	2	2	14,14,15	0.54	0	17,19,21	1.48	4 (23%)
2	MAN	G	3	2	11,11,12	0.68	0	15,15,17	0.90	1 (6%)
3	NAG	H	1	3,1	14,14,15	0.52	0	17,19,21	0.93	1 (5%)
3	NAG	H	2	3	14,14,15	0.95	1 (7%)	17,19,21	0.96	1 (5%)
3	BMA	H	3	3	11,11,12	0.87	0	15,15,17	1.75	3 (20%)
3	NAG	I	1	3,1	14,14,15	0.50	0	17,19,21	0.73	0
3	NAG	I	2	3	14,14,15	0.71	0	17,19,21	1.80	2 (11%)
3	BMA	I	3	3	11,11,12	0.68	0	15,15,17	0.93	2 (13%)
4	NAG	J	1	4,1	14,14,15	0.51	0	17,19,21	1.47	4 (23%)
4	NAG	J	2	4	14,14,15	0.52	0	17,19,21	0.88	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
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	1/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	MAN	D	3	2	-	2/2/19/22	1/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	1/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	1/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	1/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	C1-C2	2.10	1.55	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C4-C3-C2	-5.54	102.90	111.02
3	H	3	BMA	C1-O5-C5	4.72	118.51	112.19
4	F	2	NAG	C4-C3-C2	4.14	117.09	111.02
4	J	1	NAG	C4-C3-C2	4.01	116.90	111.02
4	F	1	NAG	C4-C3-C2	3.56	116.23	111.02

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2

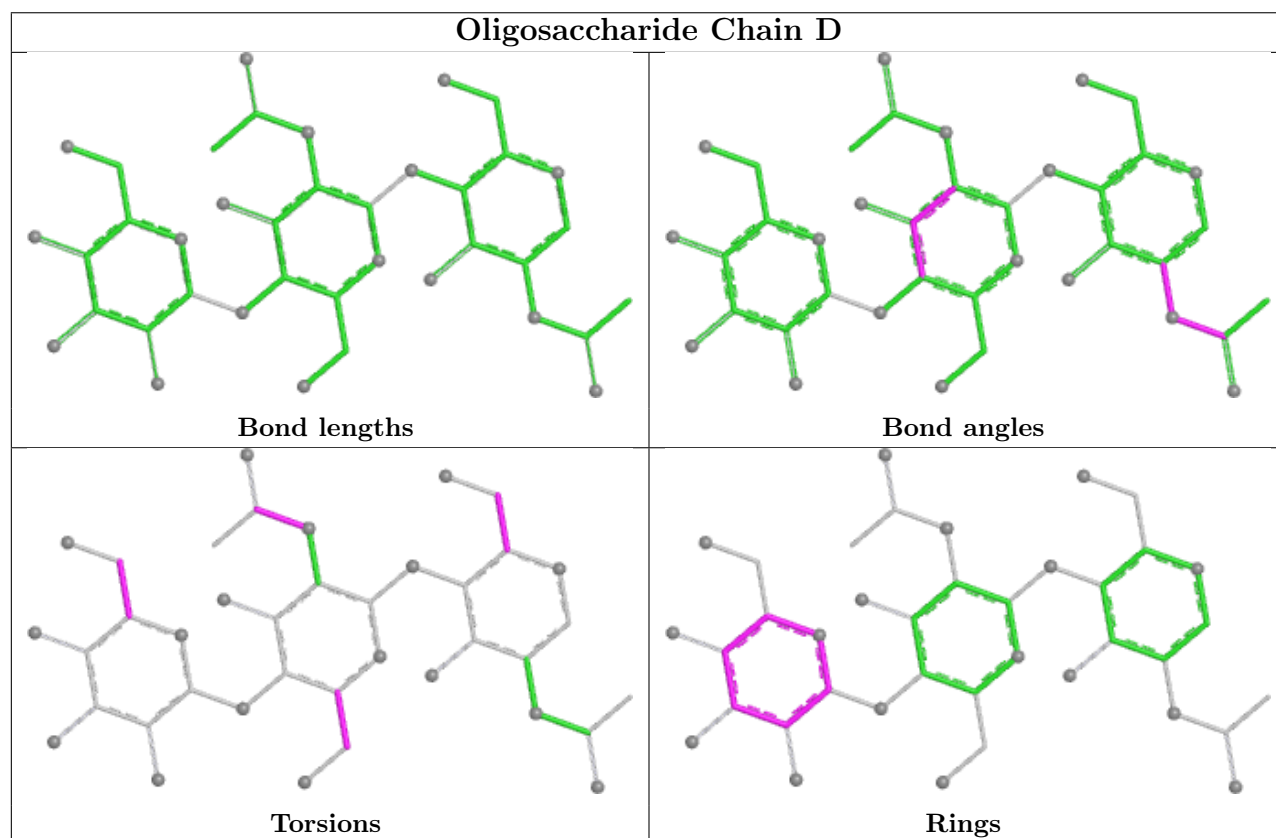
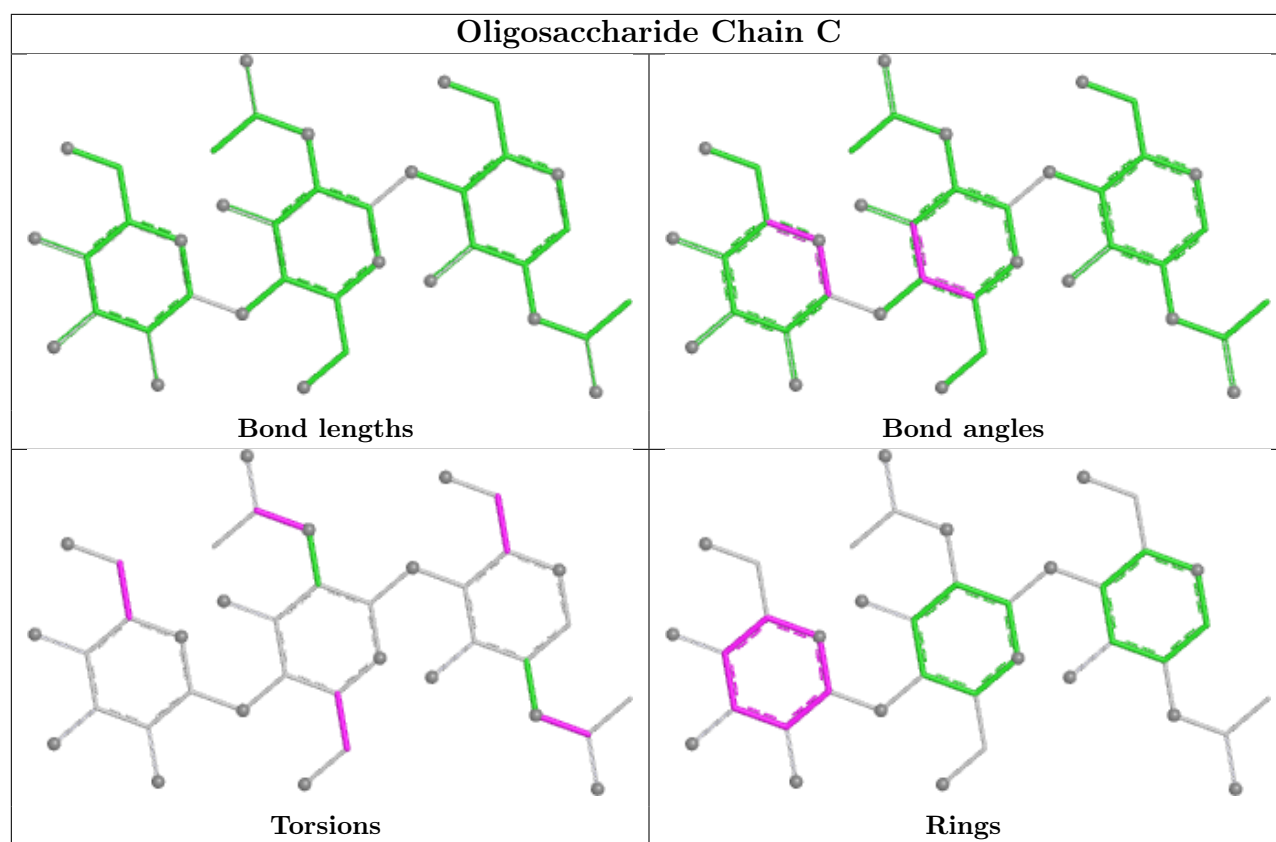
All (5) ring outliers are listed below:

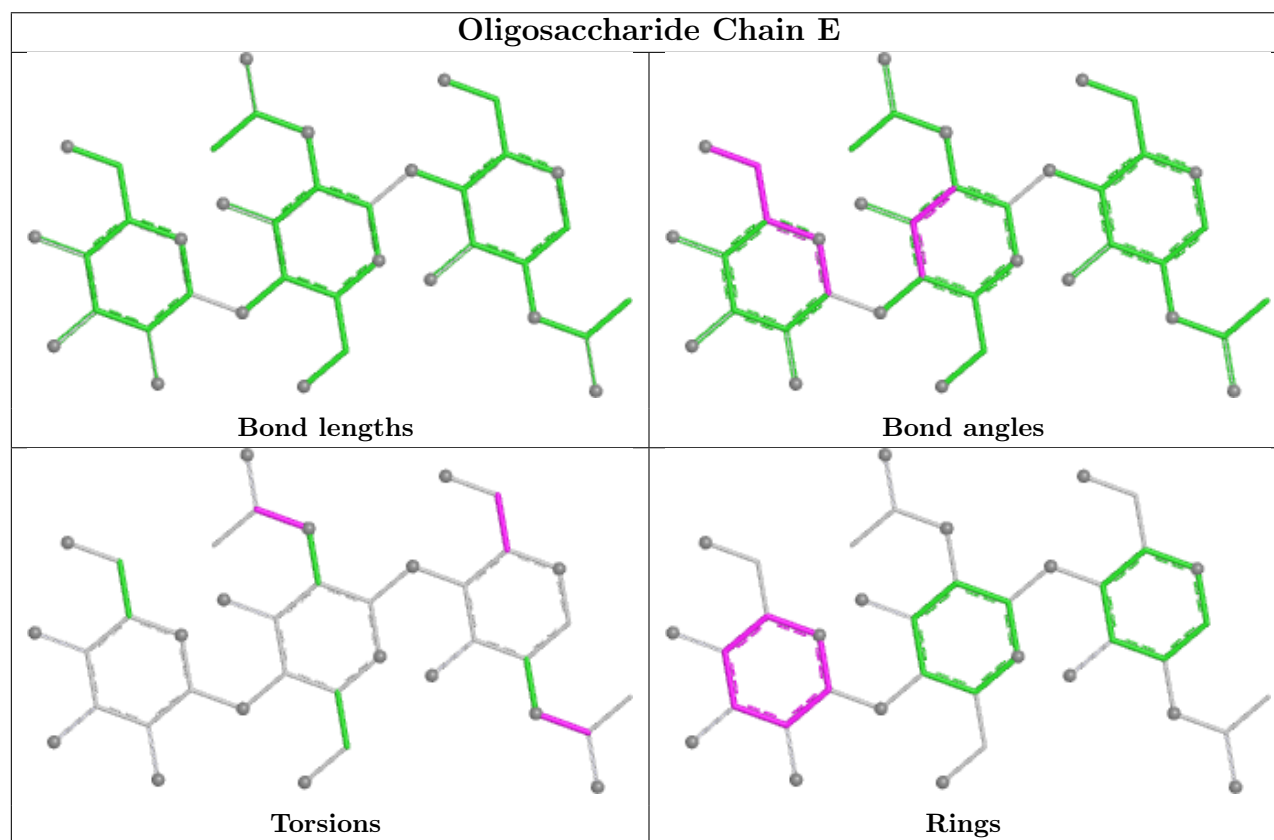
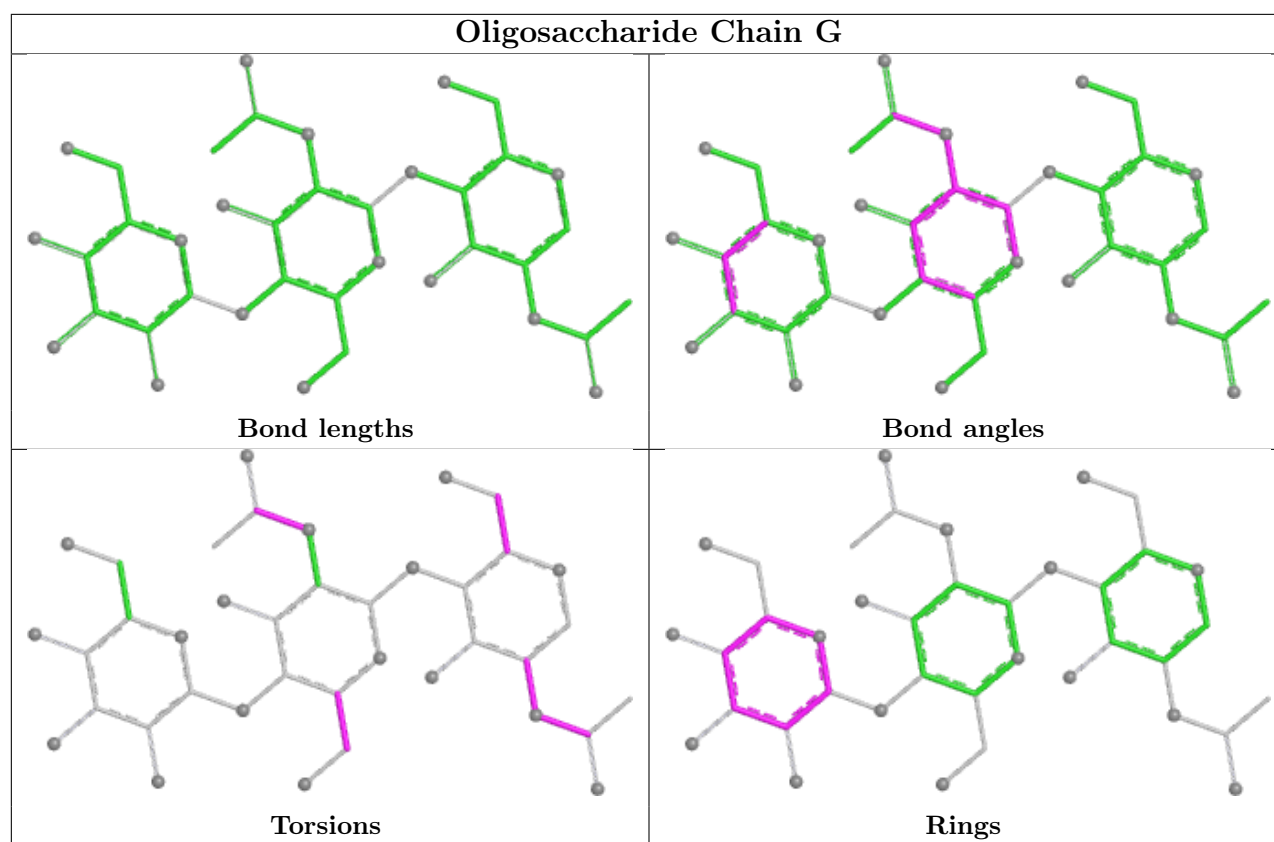
Mol	Chain	Res	Type	Atoms
2	D	3	MAN	C1-C2-C3-C4-C5-O5
2	C	3	MAN	C1-C2-C3-C4-C5-O5
3	I	3	BMA	C1-C2-C3-C4-C5-O5
2	G	3	MAN	C1-C2-C3-C4-C5-O5
3	E	3	BMA	C1-C2-C3-C4-C5-O5

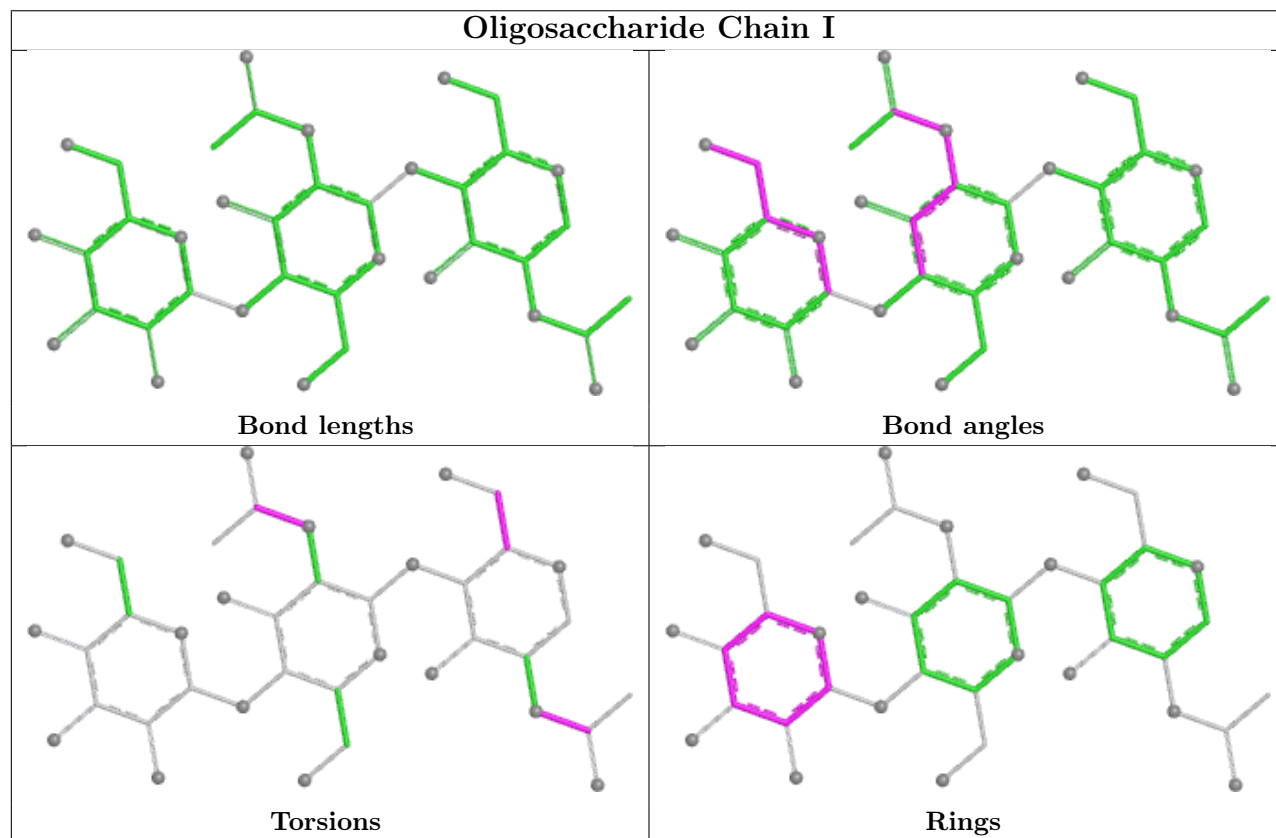
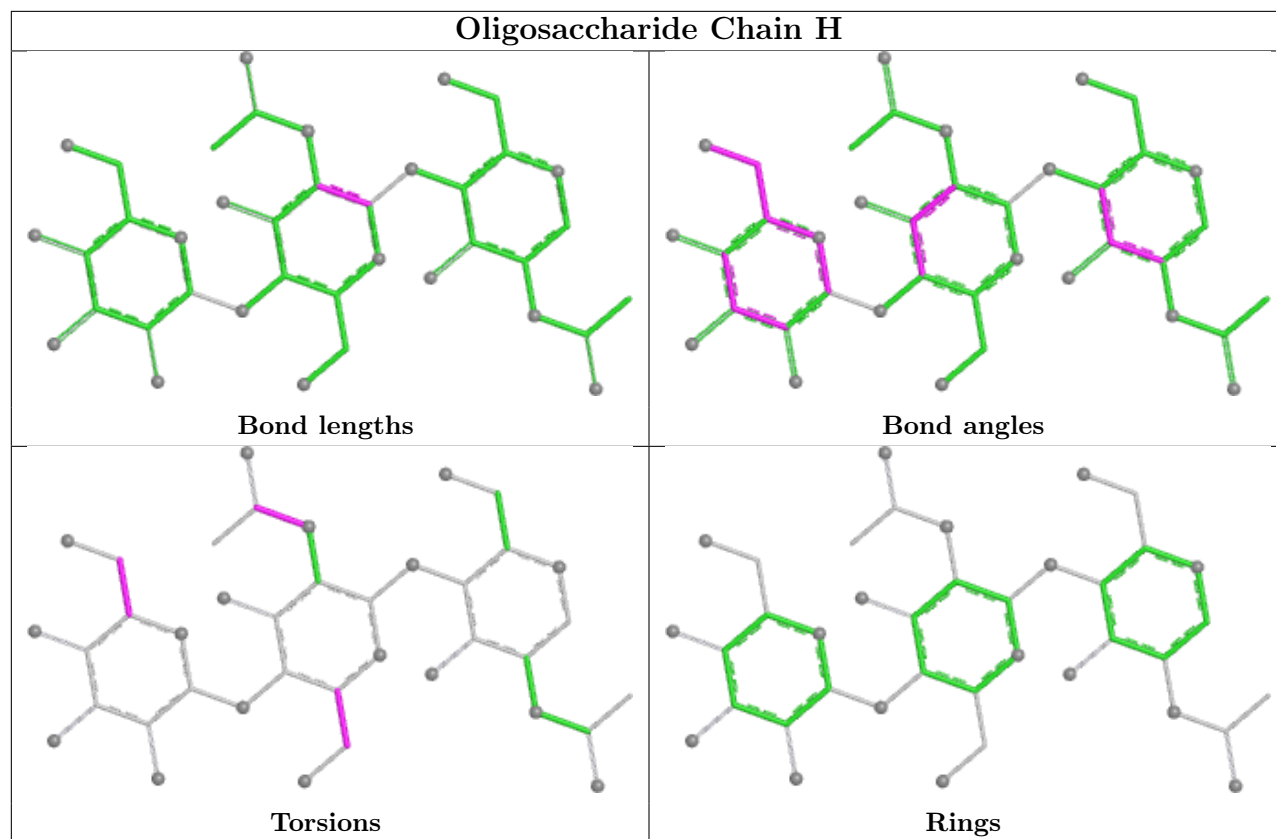
6 monomers are involved in 9 short contacts:

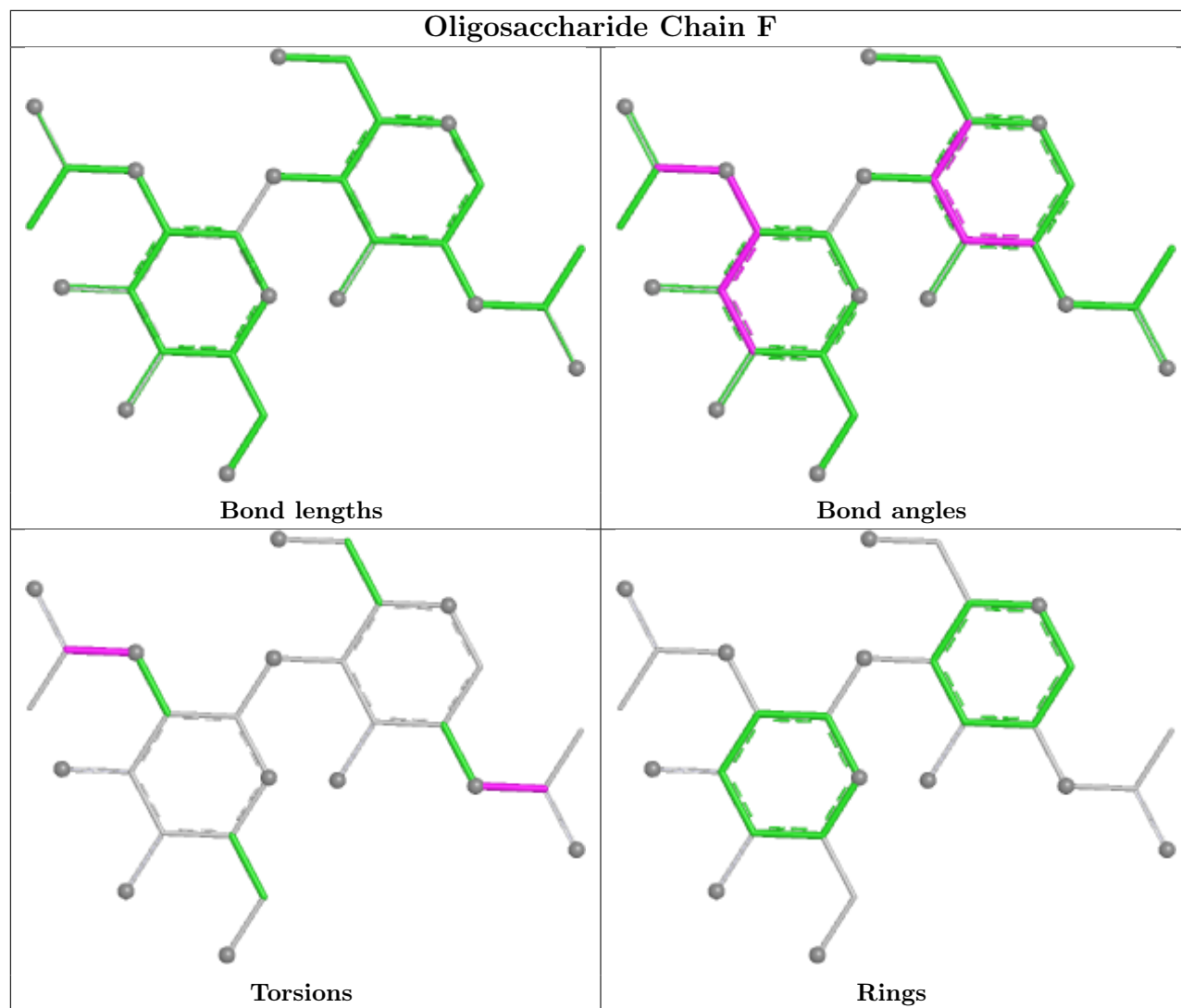
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	NAG	1	0
2	G	1	NAG	1	0
3	H	1	NAG	1	0
3	I	3	BMA	1	0
3	H	2	NAG	1	0
2	G	2	NAG	6	0

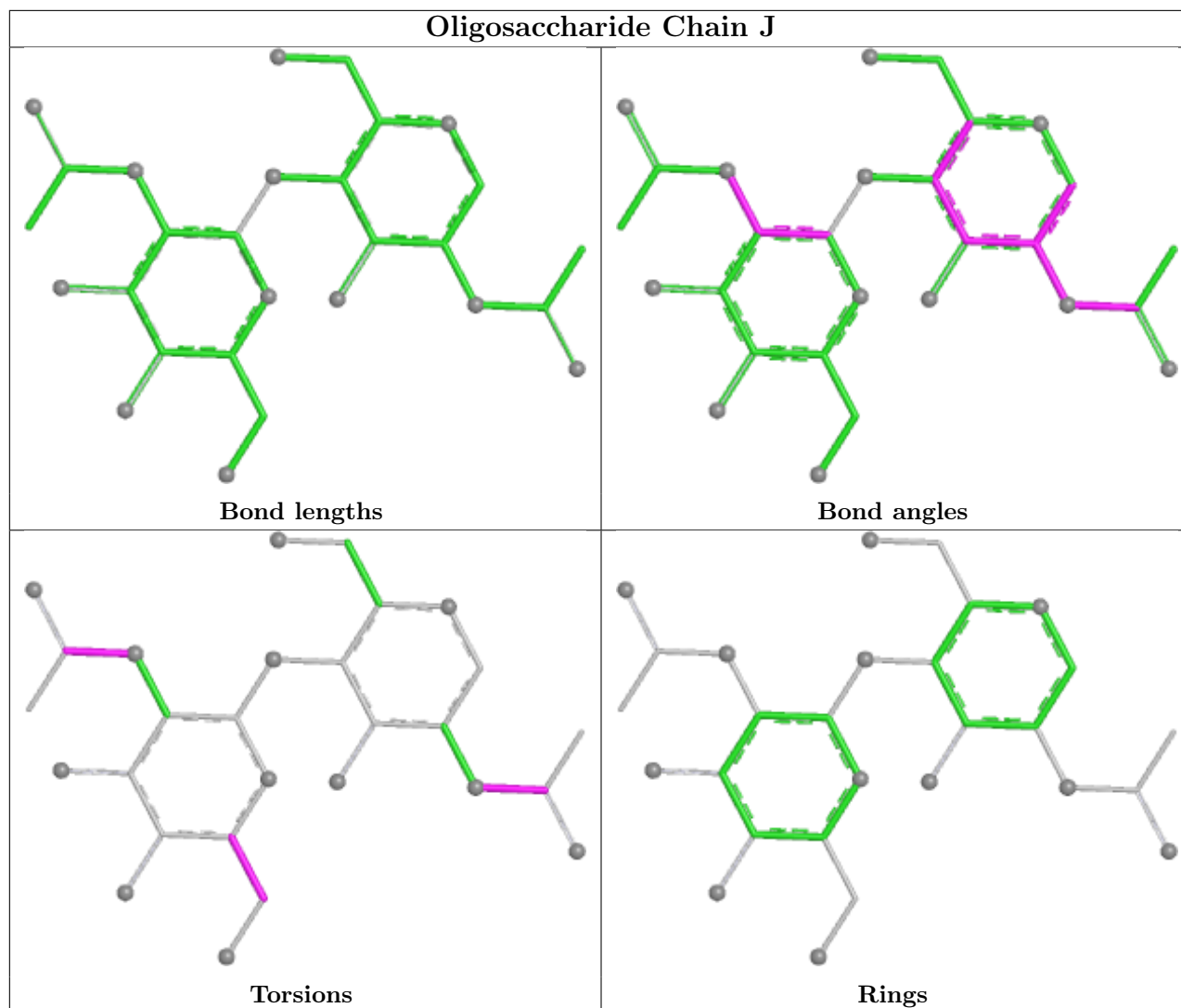
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
6	CO3	B	1002	-	3,3,3	3.01	1 (33%)	2,3,3	0.61	0
7	SCN	A	3002	-	1,2,2	2.76	1 (100%)	0,1,1	-	-
9	FMT	A	2002	-	2,2,2	3.27	2 (100%)	1,1,1	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CO3	A	1001	-	3,3,3	3.00	1 (33%)	2,3,3	0.73	0
9	FMT	B	2004	-	2,2,2	3.25	2 (100%)	1,1,1	0.70	0
9	FMT	A	2001	-	2,2,2	3.47	2 (100%)	1,1,1	0.58	0
8	HEM	A	3003	1	50,50,50	2.21	10 (20%)	67,82,82	1.28	8 (11%)
8	HEM	B	1003	1	50,50,50	2.91	22 (44%)	67,82,82	1.66	11 (16%)
9	FMT	B	2003	-	2,2,2	3.37	2 (100%)	1,1,1	0.69	0
10	OSM	B	3021	-	1,3,3	0.24	0	0,2,2	-	-

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
10	OSM	B	3021	-	-	0/0/1/1	-
8	HEM	A	3003	1	-	2/14/54/54	-
8	HEM	B	1003	1	-	4/14/54/54	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1003	HEM	FE-NC	10.62	2.30	1.95
8	B	1003	HEM	C3D-C2D	7.39	1.52	1.36
8	A	3003	HEM	C3D-C2D	6.96	1.51	1.36
8	A	3003	HEM	FE-NC	6.42	2.16	1.95
8	B	1003	HEM	FE-NB	6.25	2.14	1.94

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1003	HEM	C3B-C2B-C1B	5.60	110.62	106.41
8	A	3003	HEM	C4D-ND-C1D	5.01	111.14	105.21
8	B	1003	HEM	C2B-C1B-NB	-4.91	104.19	109.84
8	B	1003	HEM	C1B-NB-C4B	4.16	110.14	105.21
8	B	1003	HEM	C4D-ND-C1D	4.15	110.12	105.21

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

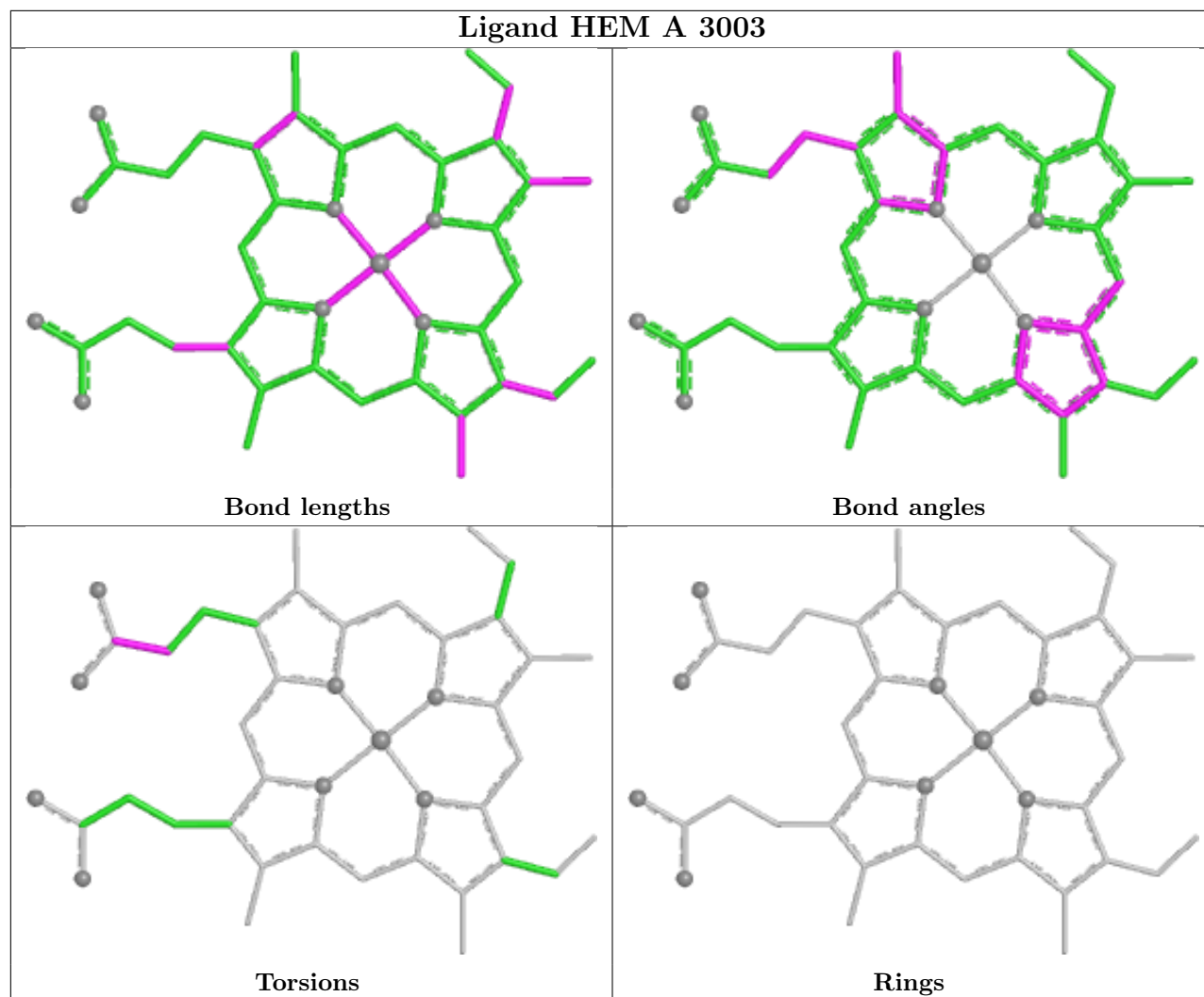
Mol	Chain	Res	Type	Atoms
8	A	3003	HEM	CAD-CBD-CGD-O1D
8	A	3003	HEM	CAD-CBD-CGD-O2D
8	B	1003	HEM	CAA-CBA-CGA-O2A
8	B	1003	HEM	CAD-CBD-CGD-O2D
8	B	1003	HEM	CAA-CBA-CGA-O1A

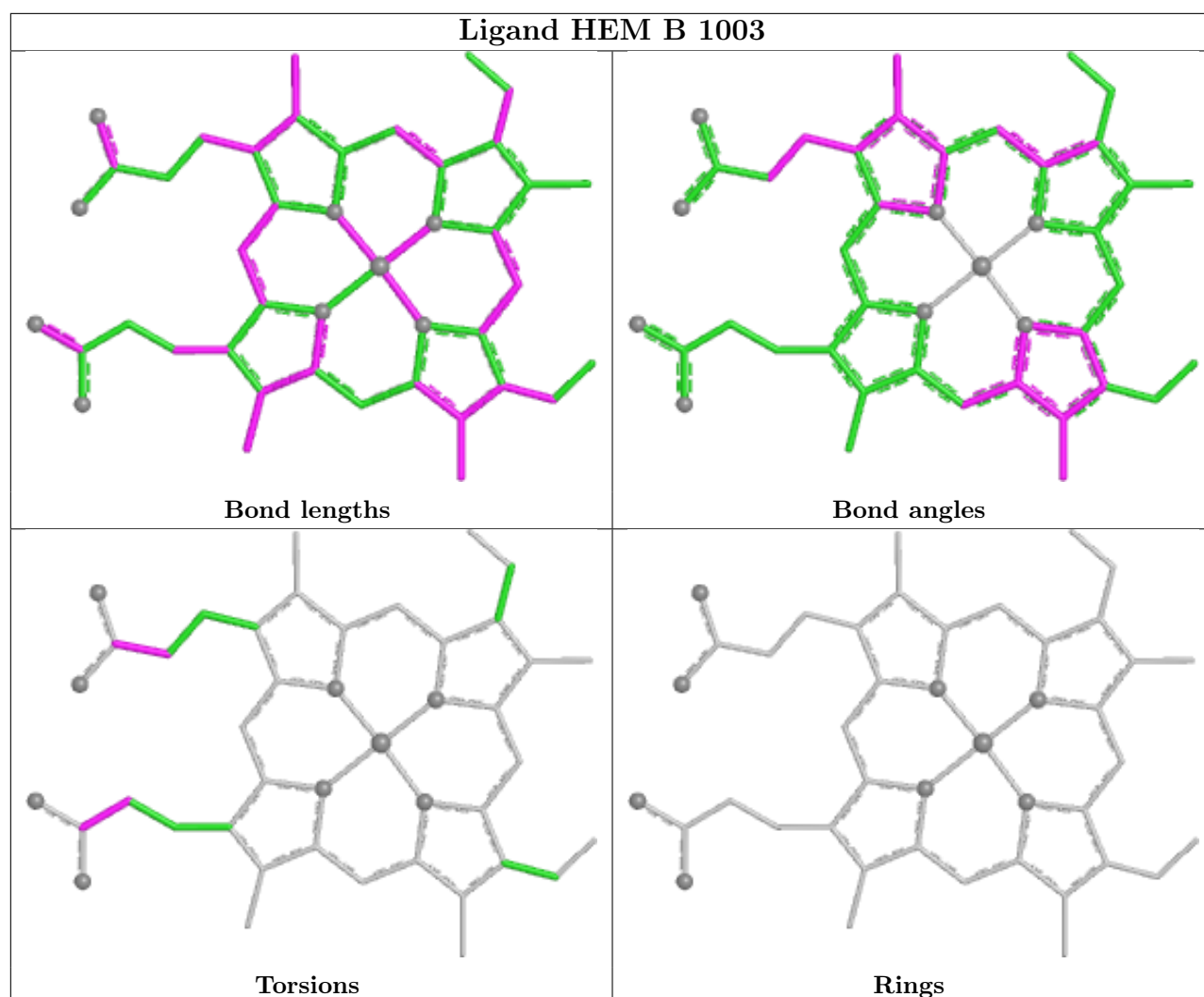
There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3002	SCN	3	0
9	A	2002	FMT	2	0
9	B	2004	FMT	1	0
9	A	2001	FMT	1	0
8	A	3003	HEM	11	0
8	B	1003	HEM	5	0
9	B	2003	FMT	2	0
10	B	3021	OSM	2	0

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





## 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.