



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 04:54 PM BST

PDB ID : 2AYL  
Title : 2.0 Angstrom Crystal Structure of Manganese Protoporphyrin IX-reconstituted Ovine Prostaglandin H2 Synthase-1 Complexed With Flurbiprofen  
Authors : Gupta, K.; Selinsky, B.S.; Loll, P.J.  
Deposited on : 2005-09-07  
Resolution : 2.00 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) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

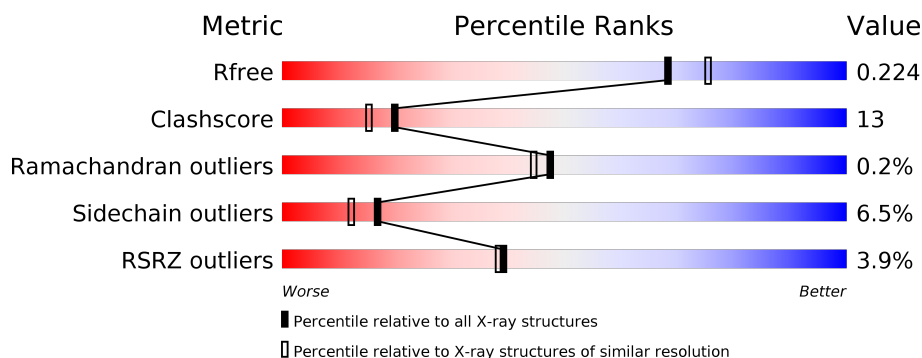
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.




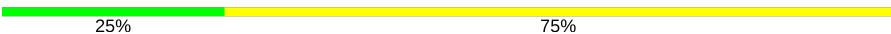
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div></div> </div> </div>
1	B	553	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div></div> </div> </div>
2	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>
3	D	5	<div> <div></div> <div> <div>20%</div> <div>80%</div> </div> </div>
3	G	5	<div> <div></div> <div> <div>20%</div> <div>20%</div> <div>60%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	4	 75%25%
4	H	4	 25%75%

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	2	X	-	-	X
2	NAG	F	2	X	-	-	X
3	NAG	D	2	X	-	X	-
3	MAN	D	3	X	-	X	X
3	MAN	D	4	-	-	-	X
3	MAN	D	5	X	-	-	X
3	NAG	G	2	X	-	-	-
3	MAN	G	3	X	-	-	X
3	MAN	G	4	X	-	-	X
3	MAN	G	5	X	-	-	X
4	MAN	E	3	X	-	-	X
4	MAN	E	4	X	-	-	X
4	MAN	H	4	X	-	-	X
5	BOG	A	752	-	-	-	X
5	BOG	A	754	-	-	-	X
5	BOG	B	1753	-	-	-	X
8	GOL	A	758	-	X	-	-
8	GOL	A	759	-	X	-	-
8	GOL	A	760	-	X	-	-
8	GOL	B	1759	-	X	-	-
8	GOL	B	1760	-	X	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10505 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 G/H synthase 1.

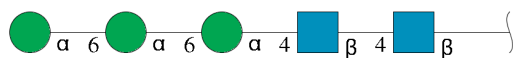
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	2	0
			4504	2918	762	795	29			
1	B	553	Total	C	N	O	S	0	2	0
			4504	2918	762	795	29			

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



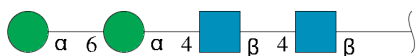
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



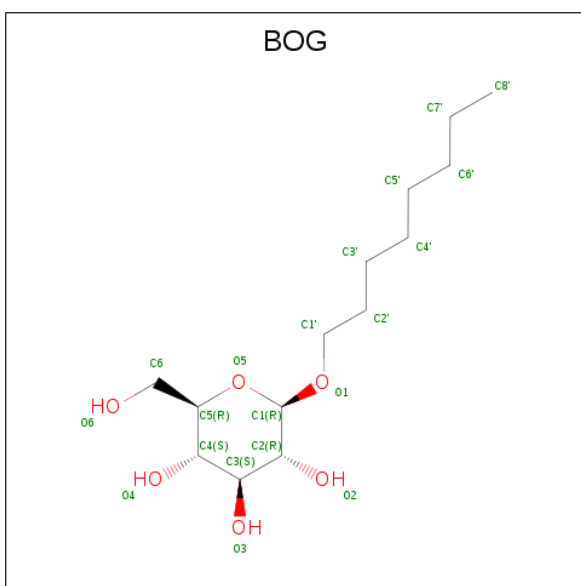
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
			50	28	2	20			
4	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



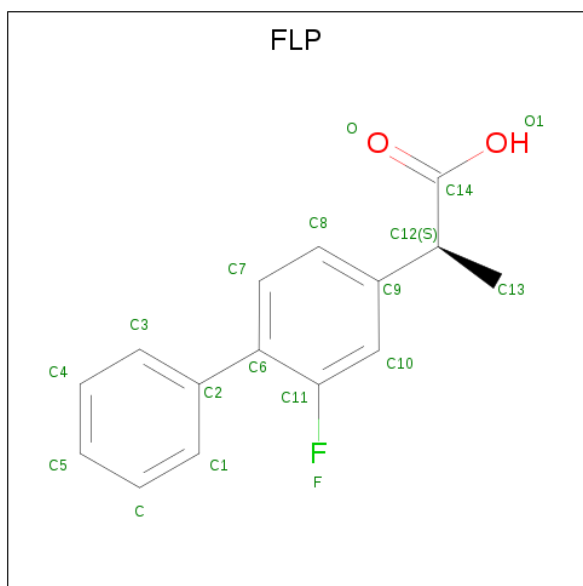
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		
5	A	1	Total	C	O	0	0
			20	14	6		
5	B	1	Total	C	O	0	0
			20	14	6		
5	B	1	Total	C	O	0	0
			20	14	6		

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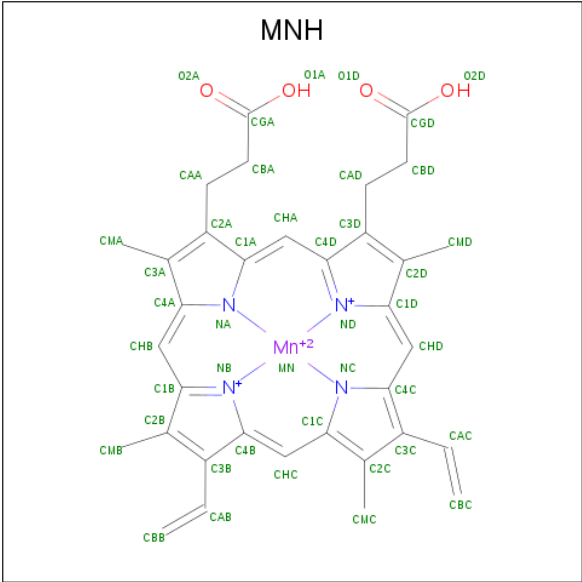
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 6 is FLURBIPROFEN (three-letter code: FLP) (formula:  $C_{15}H_{13}FO_2$ ).



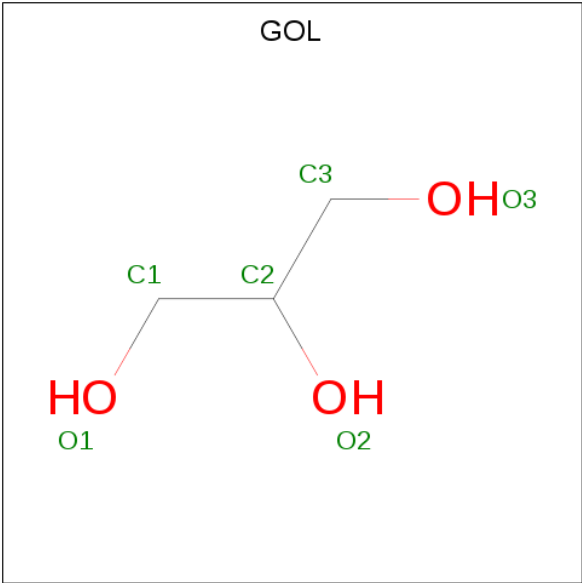
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	F	O	0	1
			36	30	2	4		
6	B	1	Total	C	F	O	0	1
			36	30	2	4		

- Molecule 7 is MANGANESE PROTOPORPHYRIN IX (three-letter code: MNH) (formula:  $C_{34}H_{32}MnN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	Mn	N	O	0	0
			43	34	1	4	4		
7	B	1	Total	C	Mn	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 9 is water.

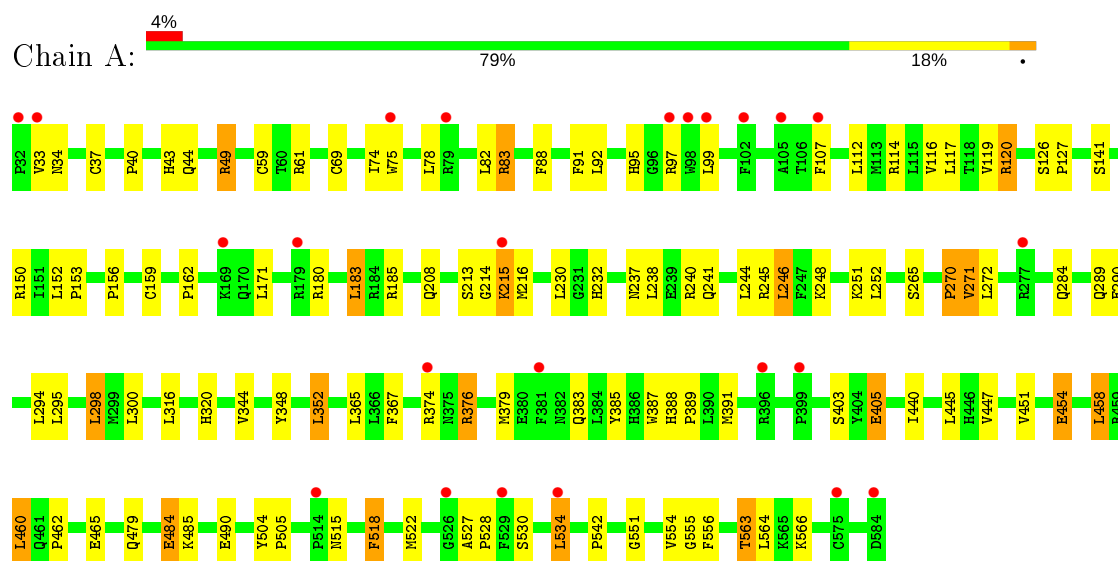
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	434	Total	O	0	0
			434	434		
9	B	457	Total	O	0	0
			457	457		



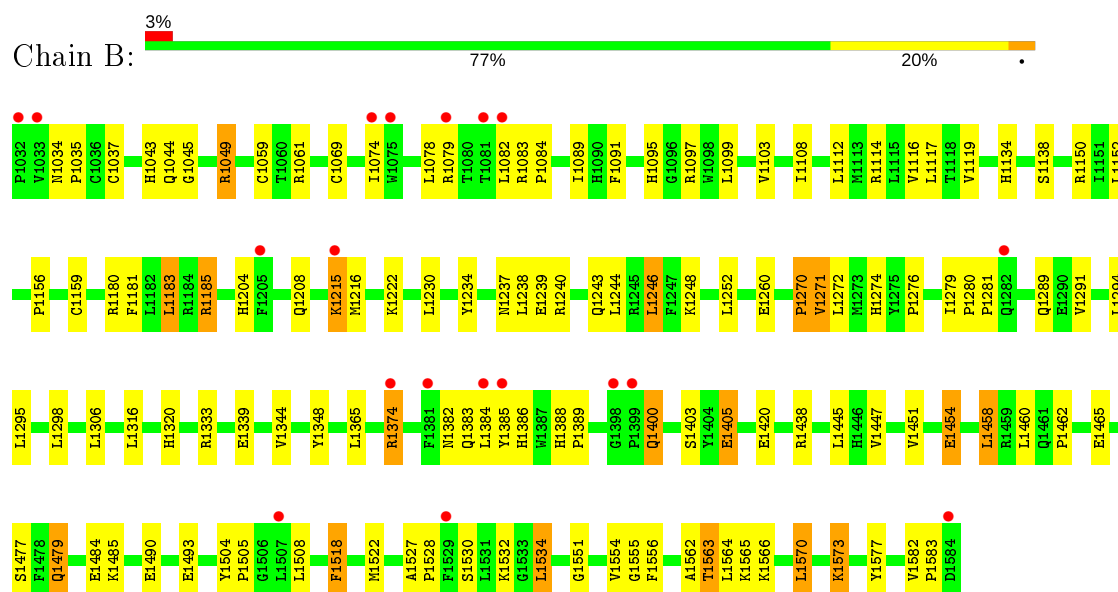
### 3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

#### • Molecule 1: Prostaglandin G/H synthase 1



#### • Molecule 1: Prostaglandin G/H synthase 1



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

Chain C:  50% 50%

MAG1  
MAG2

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

Chain F:  100%

MAG1  
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  20% 80%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5

- Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  20% 20% 60%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5

- Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  75% 25%

MAG1  
MAG2  
MAN3  
MAN4

- Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  25% 75%

MAG1  
MAG2  
MAN3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.93Å   206.55Å   221.55Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	43.33 – 2.00 43.32 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.33-2.00) 99.4 (43.32-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218   ,   0.237 0.204   ,   0.224	Depositor DCC
$R_{free}$ test set	11371 reflections (6.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, FLP, MNH, BOG, 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	0.34	0/4643	0.60	0/6302
1	B	0.35	0/4643	0.60	0/6302
All	All	0.34	0/9286	0.60	0/12604

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4504	0	4407	103	0
1	B	4504	0	4405	114	0
2	C	28	0	25	1	0
2	F	28	0	25	1	0
3	D	61	0	52	13	0
3	G	61	0	52	8	0
4	E	50	0	43	3	0
4	H	50	0	43	2	0
5	A	80	0	112	7	0
5	B	60	0	84	5	0
6	A	36	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	36	0	24	0	0
7	A	43	0	30	3	0
7	B	43	0	30	0	0
8	A	18	0	12	2	0
8	B	12	0	8	0	0
9	A	434	0	0	8	0
9	B	457	0	0	13	0
All	All	10505	0	9376	236	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 13.

The worst 5 of 236 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:1215:LYS:H	1:B:1215:LYS:HD3	1.28	0.98
1:B:1215:LYS:NZ	1:B:1222:LYS:HD2	1.84	0.93
1:A:83:ARG:HH12	5:A:751:BOG:H3	1.32	0.93
1:A:127:PRO:HD3	1:A:374:ARG:HH22	1.37	0.89
1:A:352:LEU:HD21	1:A:518:PHE:CZ	2.08	0.87

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	553/553 (100%)	538 (97%)	14 (2%)	1 (0%)	47	44
1	B	553/553 (100%)	538 (97%)	14 (2%)	1 (0%)	47	44
All	All	1106/1106 (100%)	1076 (97%)	28 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PRO
1	B	1270	PRO

### 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	490/488 (100%)	458 (94%)	32 (6%)	17	12
1	B	490/488 (100%)	459 (94%)	31 (6%)	18	13
All	All	980/976 (100%)	917 (94%)	63 (6%)	17	13

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	LEU
1	B	1180	ARG
1	B	1556	PHE
1	A	556	PHE
1	A	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1056	GLN
1	B	1203	GLN
1	B	1442	HIS
1	B	1095	HIS
1	B	1204	HIS

### 5.3.3 RNA [i](#)

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 ⓘ

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	1,2	14,14,15	0.61	0	17,19,21	0.70	1 (5%)
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	0.83	0
3	NAG	D	1	1,3	14,14,15	0.68	0	17,19,21	0.85	0
3	NAG	D	2	3	14,14,15	0.77	0	17,19,21	1.79	3 (17%)
3	MAN	D	3	3	11,11,12	0.81	0	15,15,17	1.61	3 (20%)
3	MAN	D	4	3	11,11,12	0.63	0	15,15,17	1.15	1 (6%)
3	MAN	D	5	3	11,11,12	0.58	0	15,15,17	0.75	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.50	0	17,19,21	0.71	1 (5%)
4	NAG	E	2	4	14,14,15	0.65	0	17,19,21	0.70	0
4	MAN	E	3	4	11,11,12	0.72	0	15,15,17	0.97	1 (6%)
4	MAN	E	4	4	11,11,12	0.61	0	15,15,17	0.88	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.86	0	17,19,21	0.86	1 (5%)
2	NAG	F	2	2	14,14,15	0.65	0	17,19,21	0.82	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.66	0	17,19,21	0.80	0
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	1.51	2 (11%)
3	MAN	G	3	3	11,11,12	0.50	0	15,15,17	0.64	0
3	MAN	G	4	3	11,11,12	0.64	0	15,15,17	1.17	1 (6%)
3	MAN	G	5	3	11,11,12	0.66	0	15,15,17	0.86	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.46	0	17,19,21	0.63	0
4	NAG	H	2	4	14,14,15	0.52	0	17,19,21	0.82	0
4	MAN	H	3	4	11,11,12	0.50	0	15,15,17	0.74	0
4	MAN	H	4	4	11,11,12	0.54	0	15,15,17	0.87	1 (6%)

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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	1/1/5/7	1/6/23/26	0/1/1/1
3	MAN	D	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	1/1/1/1
3	MAN	D	5	3	1/1/4/5	1/2/19/22	1/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	MAN	E	3	4	1/1/4/5	1/2/19/22	1/1/1/1
4	MAN	E	4	4	1/1/4/5	2/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	1/1/5/7	1/6/23/26	0/1/1/1
3	MAN	G	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	G	4	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	G	5	3	1/1/4/5	1/2/19/22	1/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	MAN	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	1/1/4/5	2/2/19/22	1/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	MAN	C1-O5-C5	4.69	118.54	112.19
3	D	2	NAG	C1-O5-C5	4.42	118.18	112.19
3	D	2	NAG	C4-C3-C2	-4.24	104.80	111.02
3	G	2	NAG	C1-O5-C5	4.14	117.81	112.19
3	D	4	MAN	C1-O5-C5	3.51	116.95	112.19

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	2	NAG	C1

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Mol	Chain	Res	Type	Atom
2	C	2	NAG	C1
3	G	4	MAN	C1
4	H	4	MAN	C1
4	E	4	MAN	C1

5 of 27 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	D	2	NAG	C3-C2-N2-C7
3	D	4	MAN	C4-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6

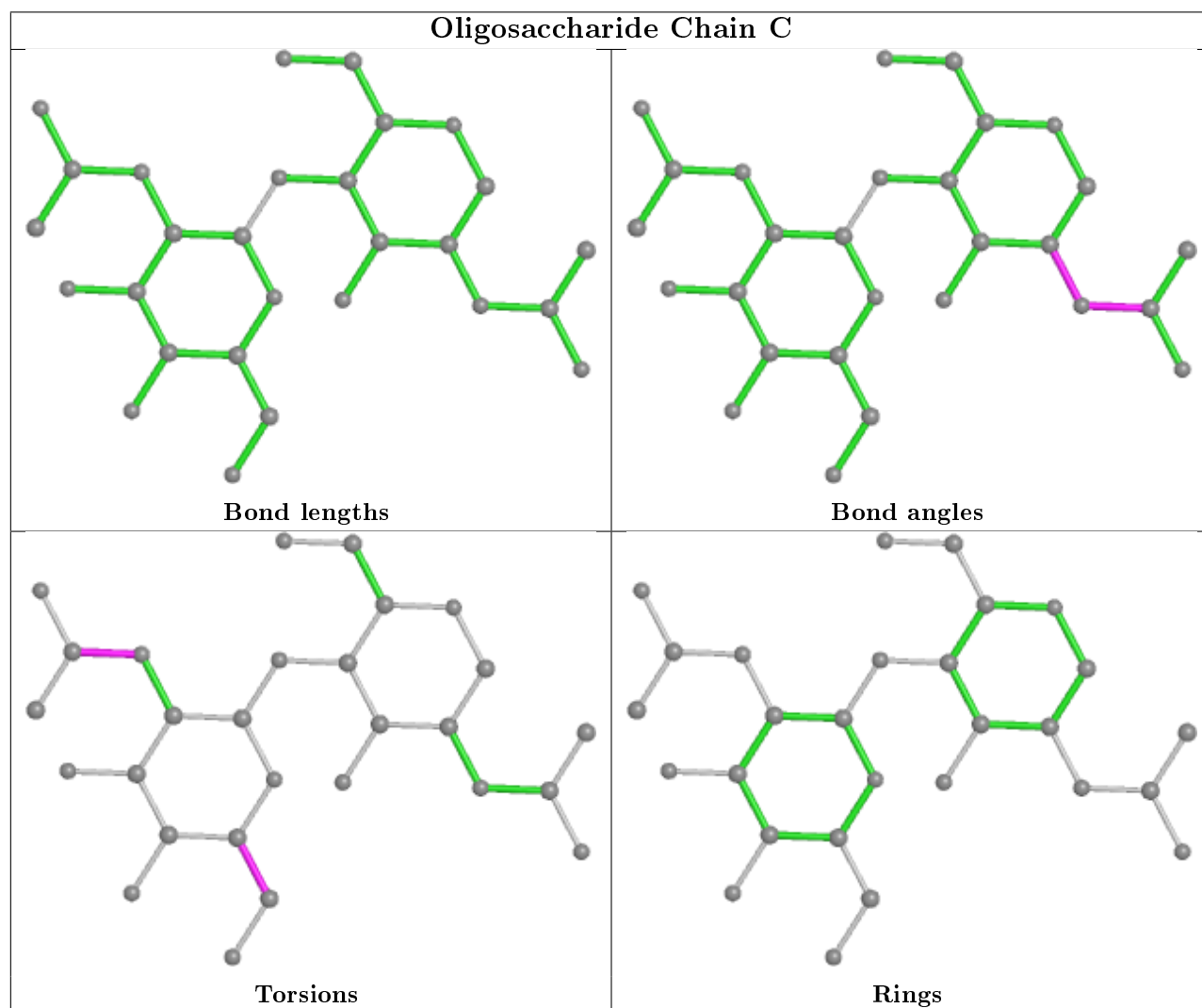
5 of 6 ring outliers are listed below:

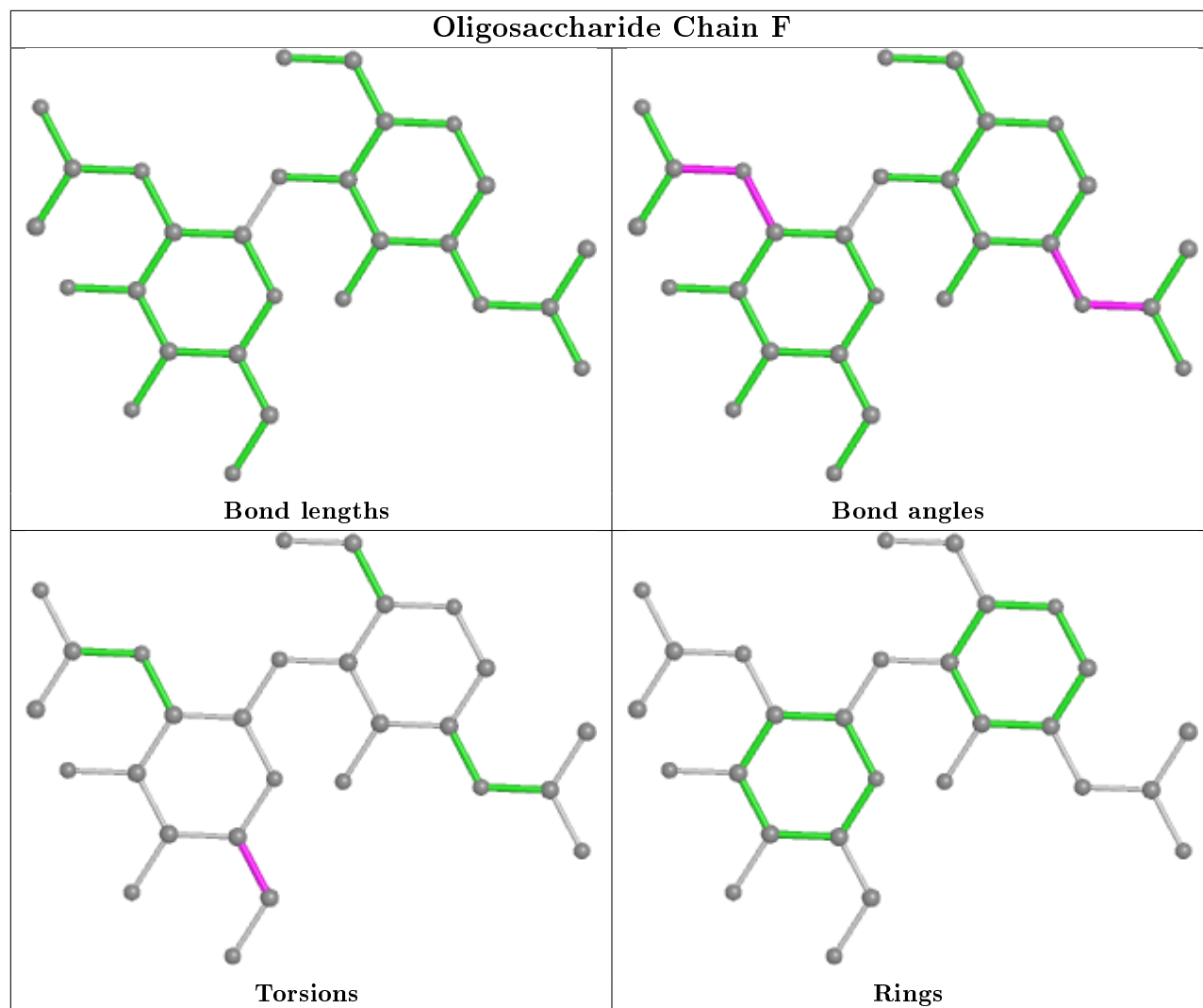
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	C1-C2-C3-C4-C5-O5
3	G	5	MAN	C1-C2-C3-C4-C5-O5
3	D	5	MAN	C1-C2-C3-C4-C5-O5
4	E	4	MAN	C1-C2-C3-C4-C5-O5
4	E	3	MAN	C1-C2-C3-C4-C5-O5

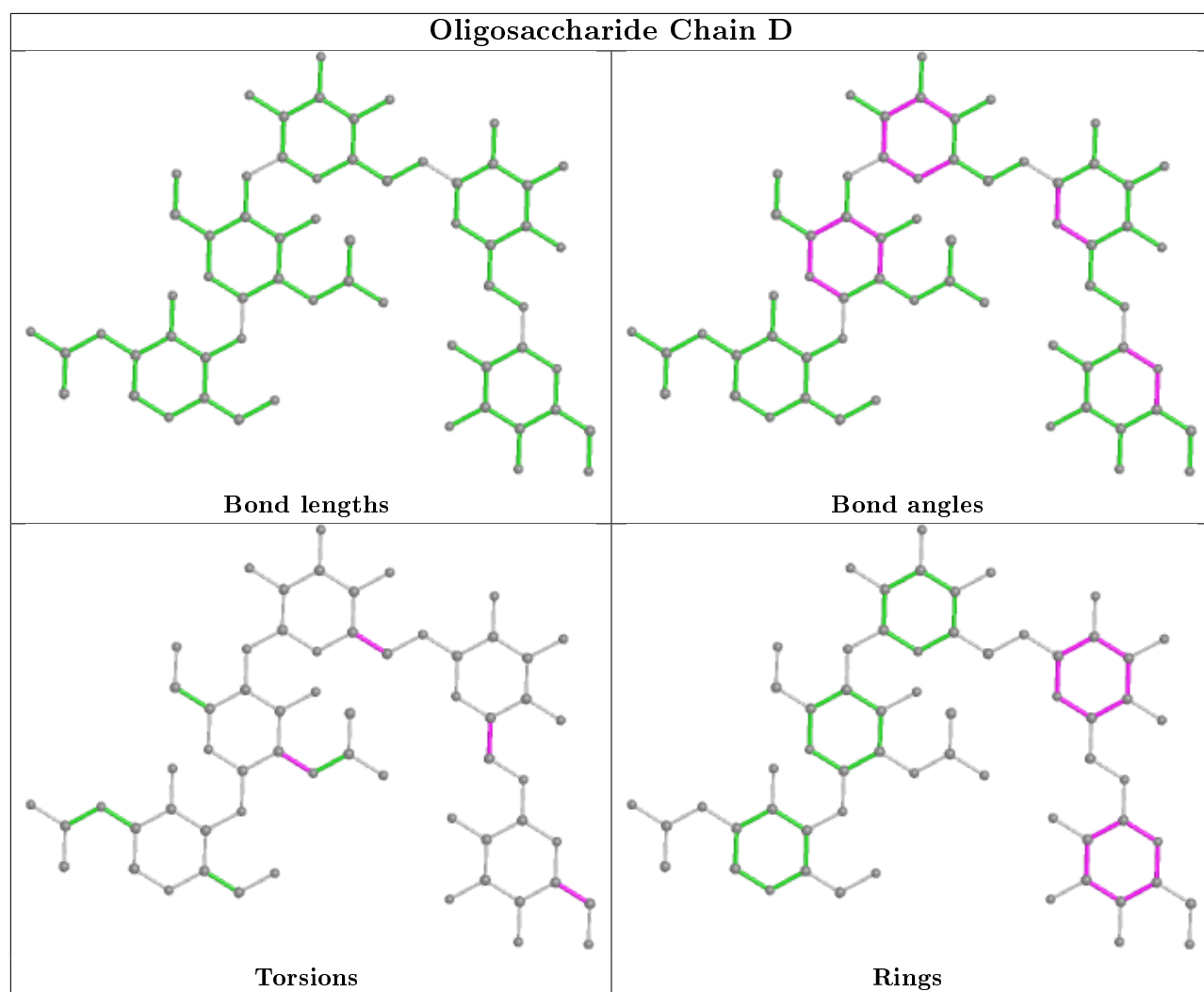
15 monomers are involved in 28 short contacts:

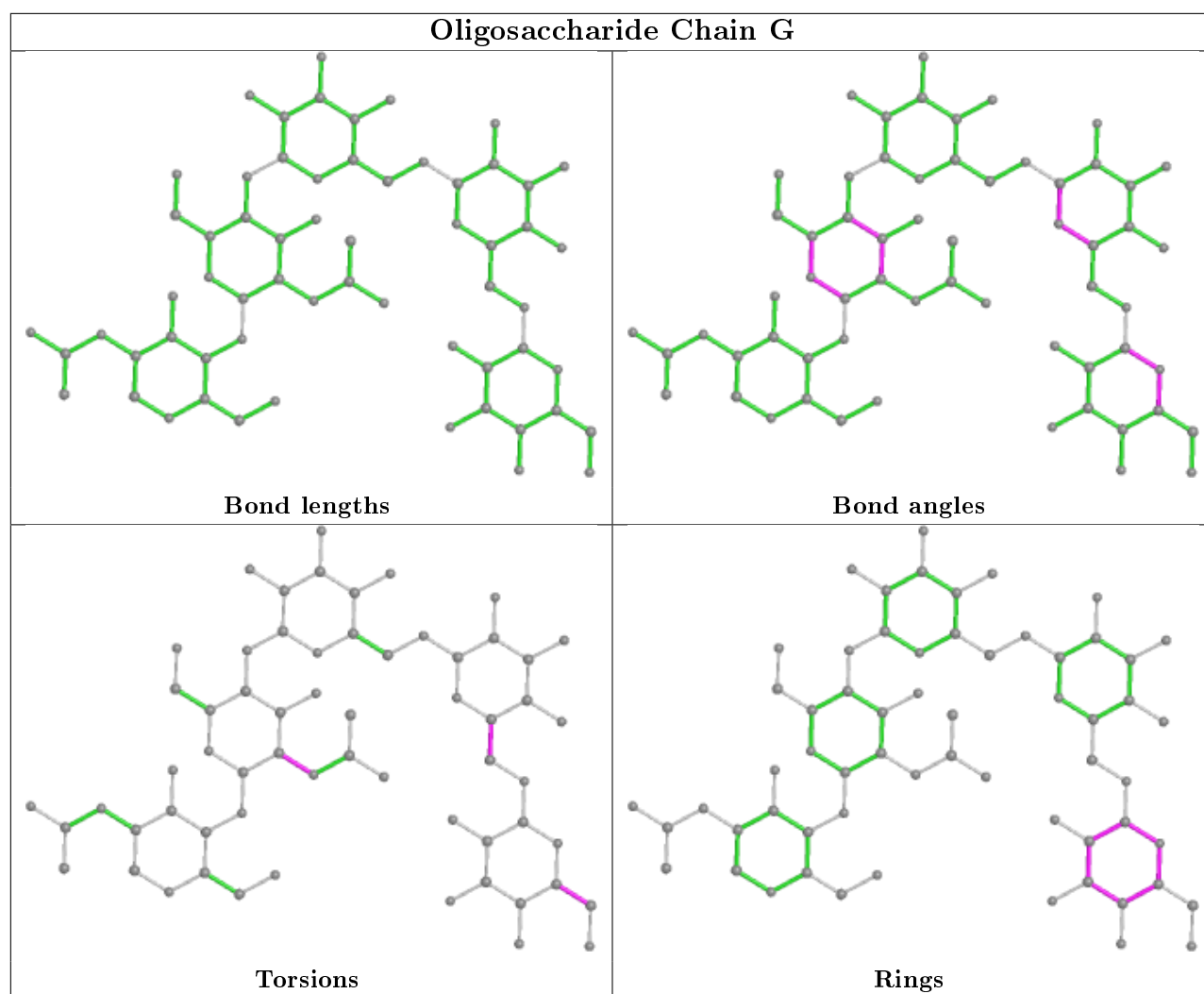
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	1	0
4	H	3	MAN	2	0
3	D	4	MAN	3	0
4	H	2	NAG	1	0
3	G	4	MAN	3	0
2	F	1	NAG	1	0
3	G	5	MAN	3	0
3	G	2	NAG	4	0
2	C	1	NAG	1	0
3	D	2	NAG	8	0
3	D	5	MAN	4	0
4	E	3	MAN	3	0
3	G	3	MAN	1	0
3	D	3	MAN	6	0
4	E	2	NAG	3	0

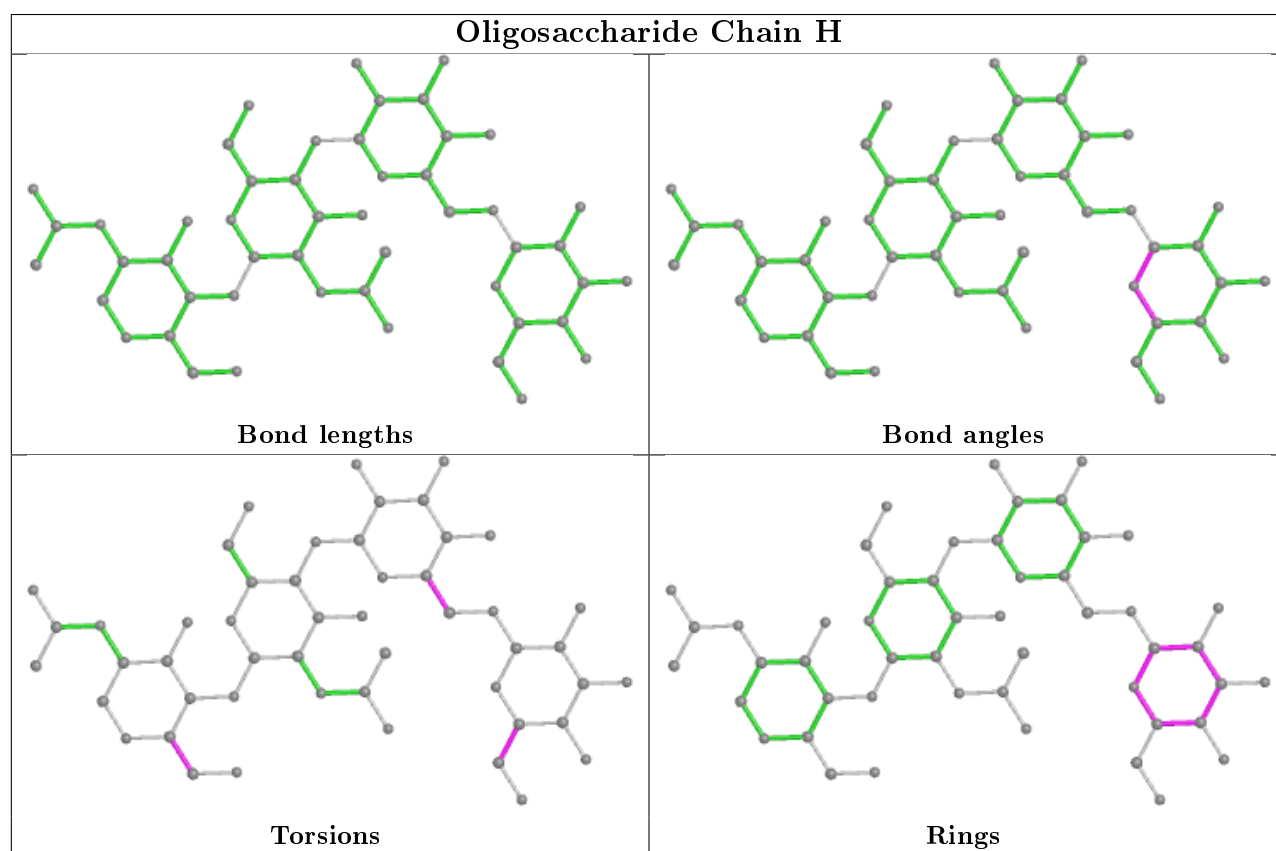
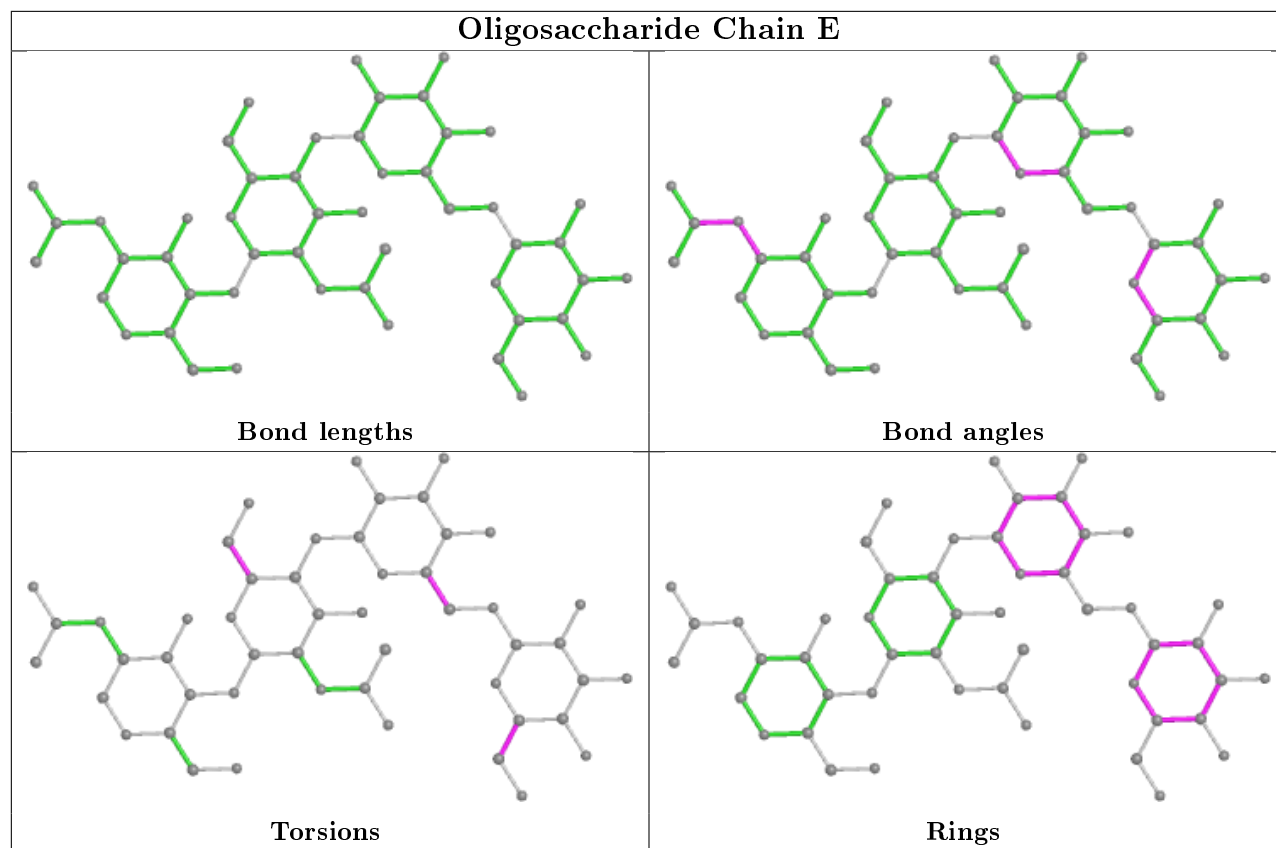
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry

18 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$
7	MNH	A	601	-	32,50,50	6.00	21 (65%)	19,82,82	7.11	15 (78%)
5	BOG	B	1750	-	20,20,20	1.71	5 (25%)	25,25,25	0.90	2 (8%)
6	FLP	A	1701[B]	-	16,19,19	2.27	7 (43%)	22,26,26	0.90	1 (4%)
5	BOG	A	754	-	20,20,20	1.71	5 (25%)	25,25,25	0.90	2 (8%)
8	GOL	A	760	-	5,5,5	4.54	5 (100%)	5,5,5	5.81	3 (60%)
8	GOL	A	758	-	5,5,5	4.46	5 (100%)	5,5,5	5.71	3 (60%)
7	MNH	B	1601	-	32,50,50	5.97	21 (65%)	19,82,82	7.38	12 (63%)
5	BOG	A	751	-	20,20,20	1.71	6 (30%)	25,25,25	0.81	1 (4%)
6	FLP	B	2701[A]	-	16,19,19	2.36	9 (56%)	22,26,26	0.88	0
8	GOL	B	1760	-	5,5,5	4.52	5 (100%)	5,5,5	5.70	3 (60%)
6	FLP	B	2701[B]	-	16,19,19	2.29	7 (43%)	22,26,26	0.91	1 (4%)
8	GOL	B	1759	-	5,5,5	4.52	5 (100%)	5,5,5	5.79	3 (60%)
8	GOL	A	759	-	5,5,5	4.52	5 (100%)	5,5,5	5.71	3 (60%)
5	BOG	A	752	-	20,20,20	1.79	5 (25%)	25,25,25	0.88	2 (8%)
6	FLP	A	1701[A]	-	16,19,19	2.34	9 (56%)	22,26,26	0.88	0
5	BOG	B	1751	-	20,20,20	1.72	6 (30%)	25,25,25	0.85	2 (8%)
5	BOG	B	1753	-	20,20,20	1.70	5 (25%)	25,25,25	0.88	2 (8%)
5	BOG	A	753	-	20,20,20	1.71	5 (25%)	25,25,25	0.88	2 (8%)

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
7	MNH	A	601	-	-	1/10/114/114	-
5	BOG	B	1750	-	-	4/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FLP	A	1701[B]	-	-	0/8/12/12	0/2/2/2
5	BOG	A	754	-	-	8/11/31/31	0/1/1/1
8	GOL	A	760	-	-	2/4/4/4	-
8	GOL	A	758	-	-	2/4/4/4	-
7	MNH	B	1601	-	-	1/10/114/114	-
5	BOG	A	751	-	-	6/11/31/31	0/1/1/1
6	FLP	B	2701[A]	-	-	0/8/12/12	0/2/2/2
8	GOL	B	1760	-	-	2/4/4/4	-
6	FLP	B	2701[B]	-	-	0/8/12/12	0/2/2/2
8	GOL	B	1759	-	-	3/4/4/4	-
8	GOL	A	759	-	-	2/4/4/4	-
5	BOG	A	752	-	-	7/11/31/31	0/1/1/1
6	FLP	A	1701[A]	-	-	0/8/12/12	0/2/2/2
5	BOG	B	1751	-	-	5/11/31/31	0/1/1/1
5	BOG	B	1753	-	-	8/11/31/31	0/1/1/1
5	BOG	A	753	-	-	4/11/31/31	0/1/1/1

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1601	MNH	C3C-C2C	-17.03	1.34	1.55
7	A	601	MNH	C3C-C2C	-17.02	1.34	1.55
7	A	601	MNH	CHD-C1D	-9.68	1.37	1.53
7	B	1601	MNH	CHD-C4C	-9.61	1.38	1.53
7	A	601	MNH	CHD-C4C	-9.57	1.38	1.53

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	MNH	C4C-CHD-C1D	18.58	151.96	112.37
7	B	1601	MNH	C4C-CHD-C1D	17.80	150.31	112.37
7	B	1601	MNH	C1C-CHC-C4B	15.87	146.18	112.37
7	A	601	MNH	C1C-CHC-C4B	15.31	144.99	112.37
7	B	1601	MNH	CAA-C2A-C1A	-15.23	116.60	127.30

There are no chirality outliers.

5 of 55 torsion outliers are listed below:



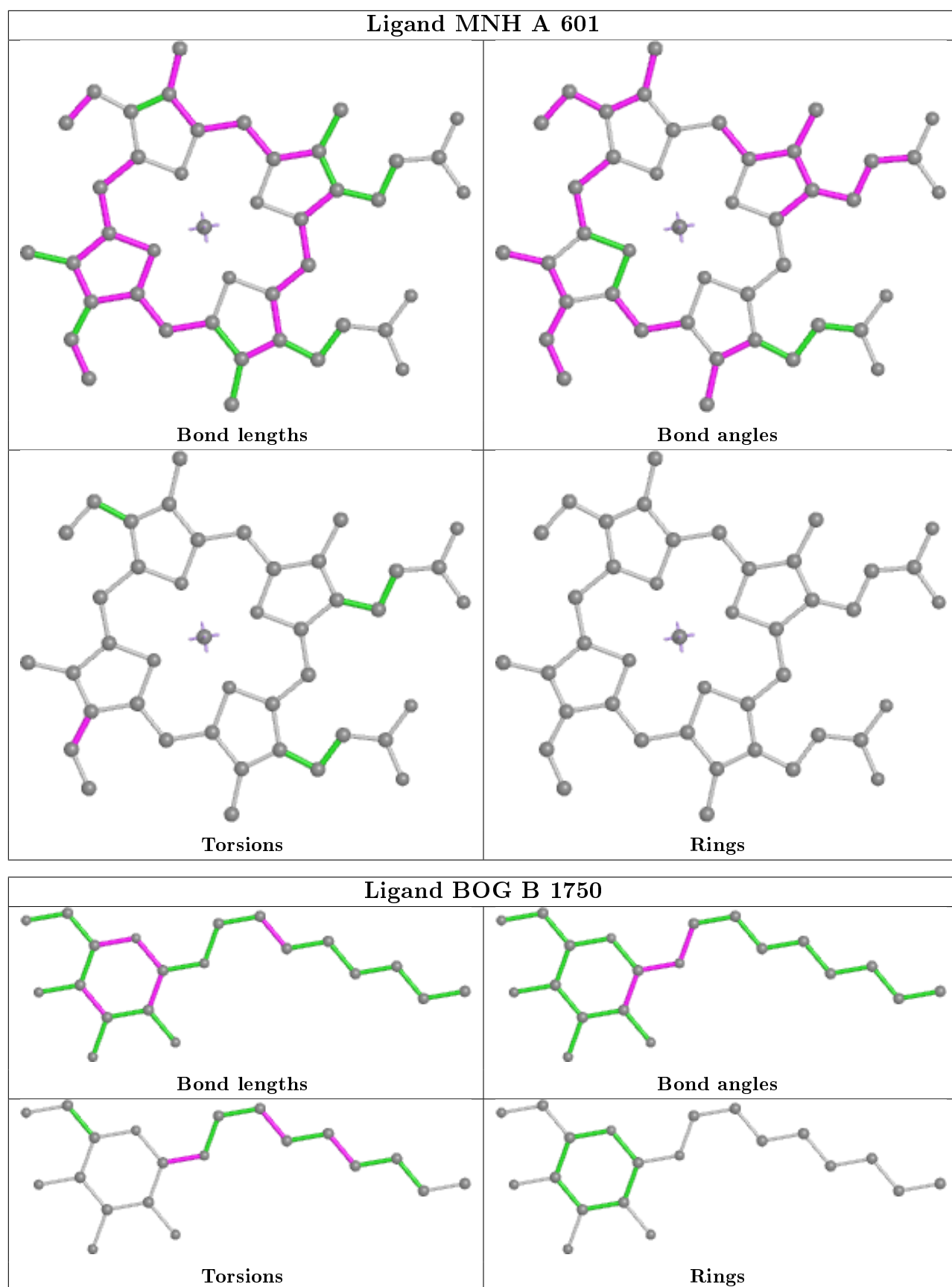
Mol	Chain	Res	Type	Atoms
7	A	601	MNH	C4C-C3C-CAC-CBC
8	A	759	GOL	O1-C1-C2-O2
8	A	759	GOL	C1-C2-C3-O3
8	A	758	GOL	C1-C2-C3-O3
8	B	1760	GOL	O1-C1-C2-O2

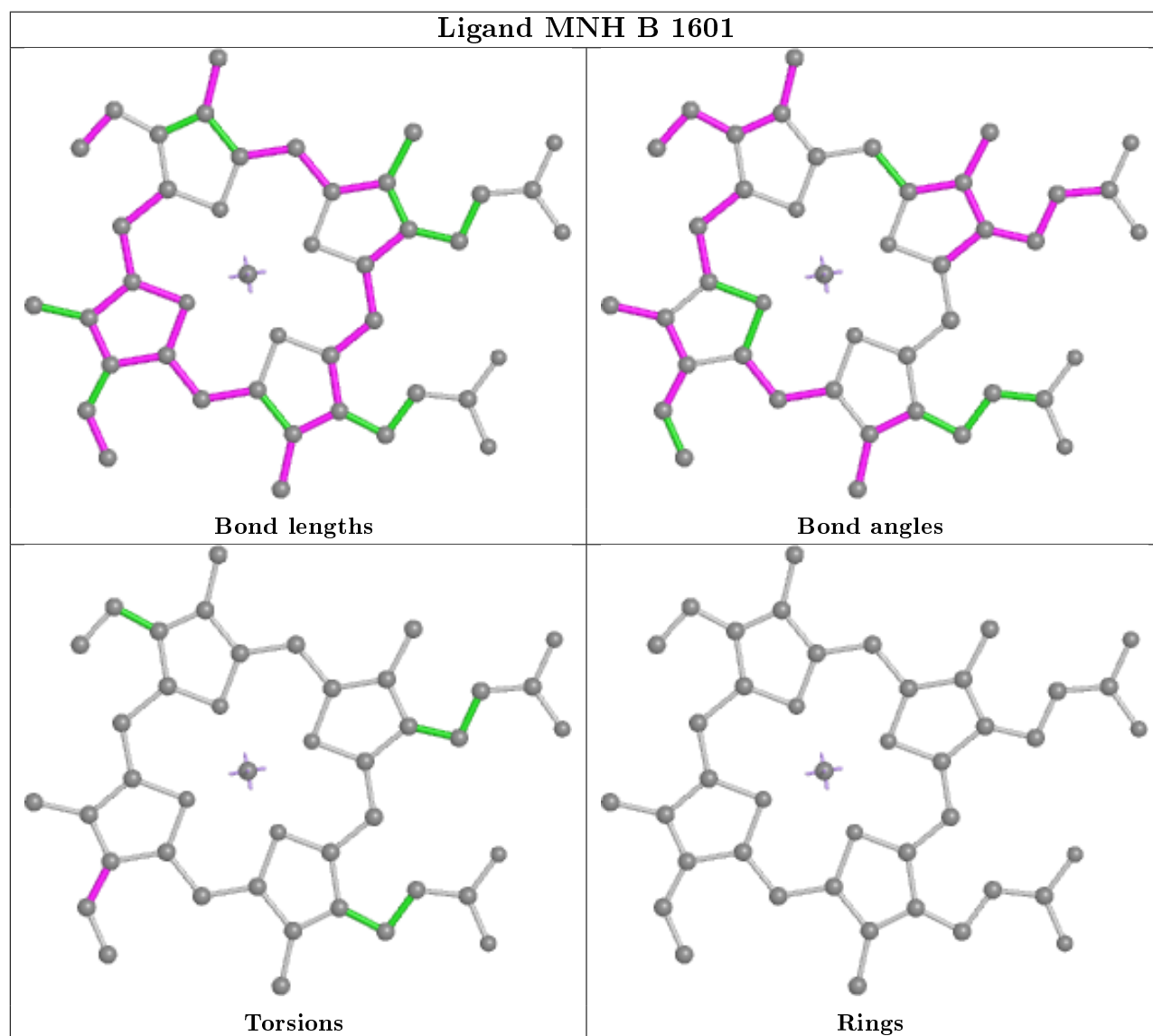
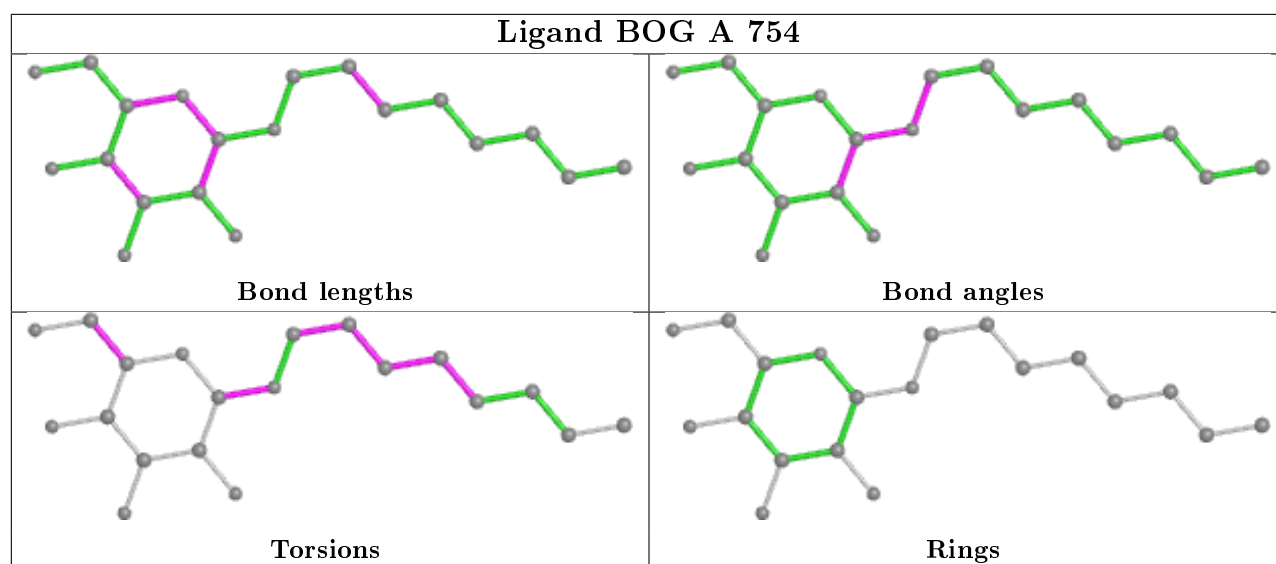
There are no ring outliers.

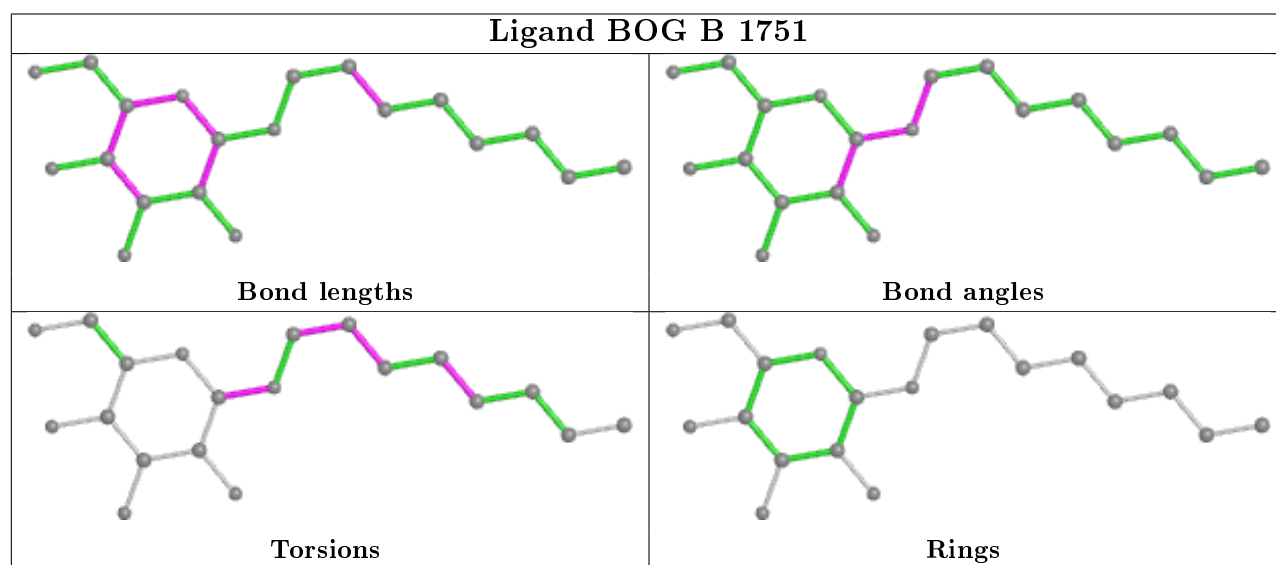
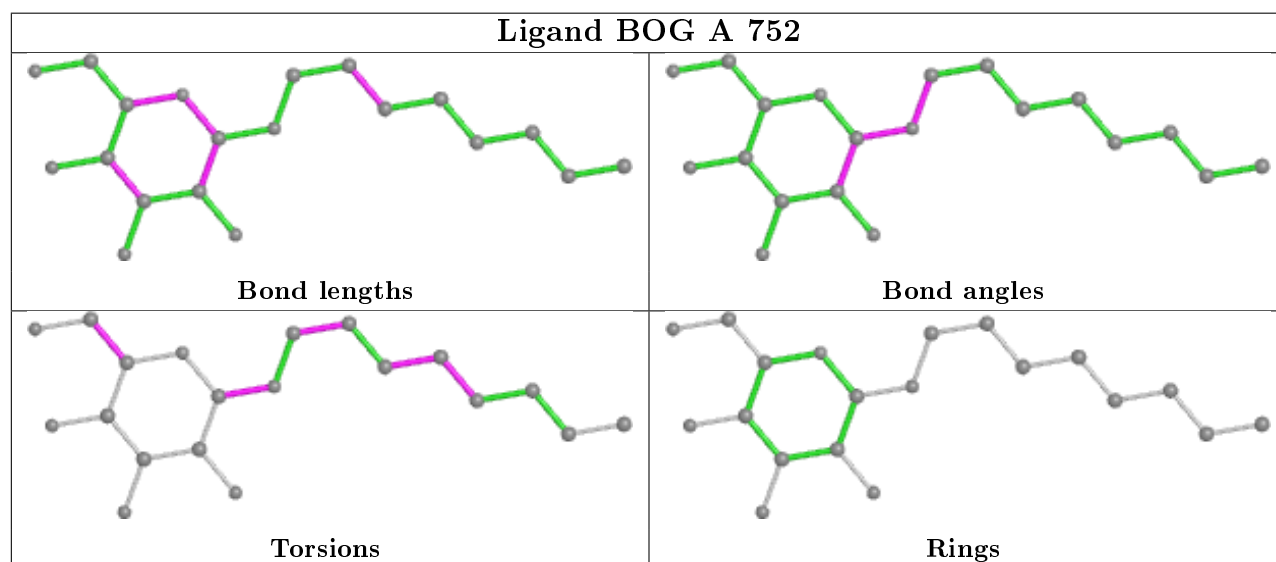
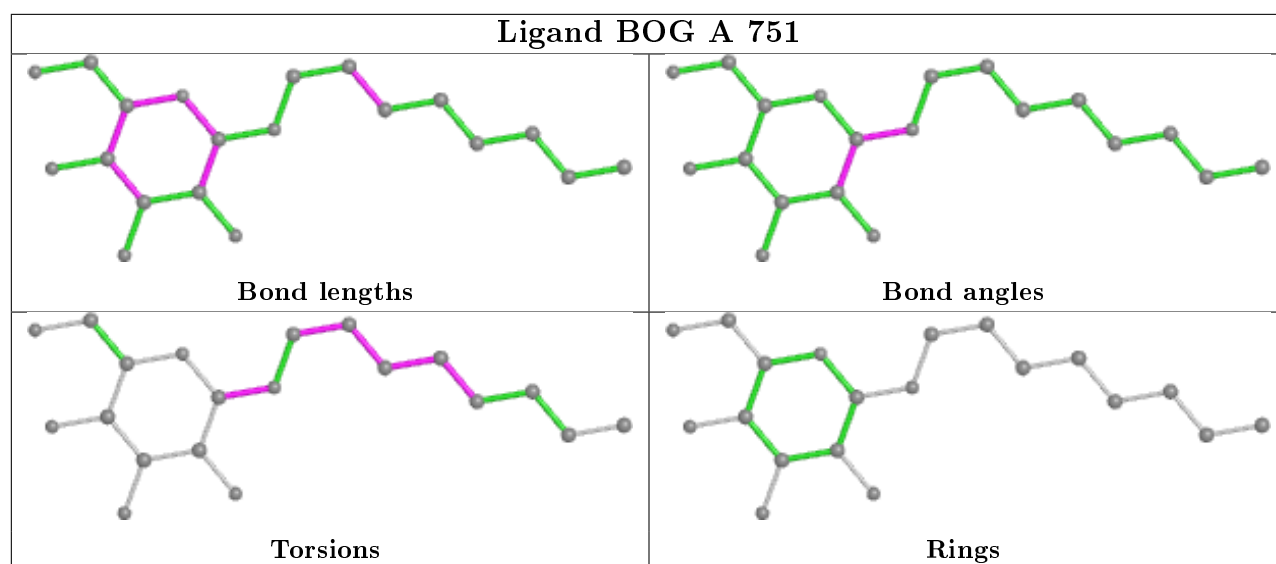
6 monomers are involved in 17 short contacts:

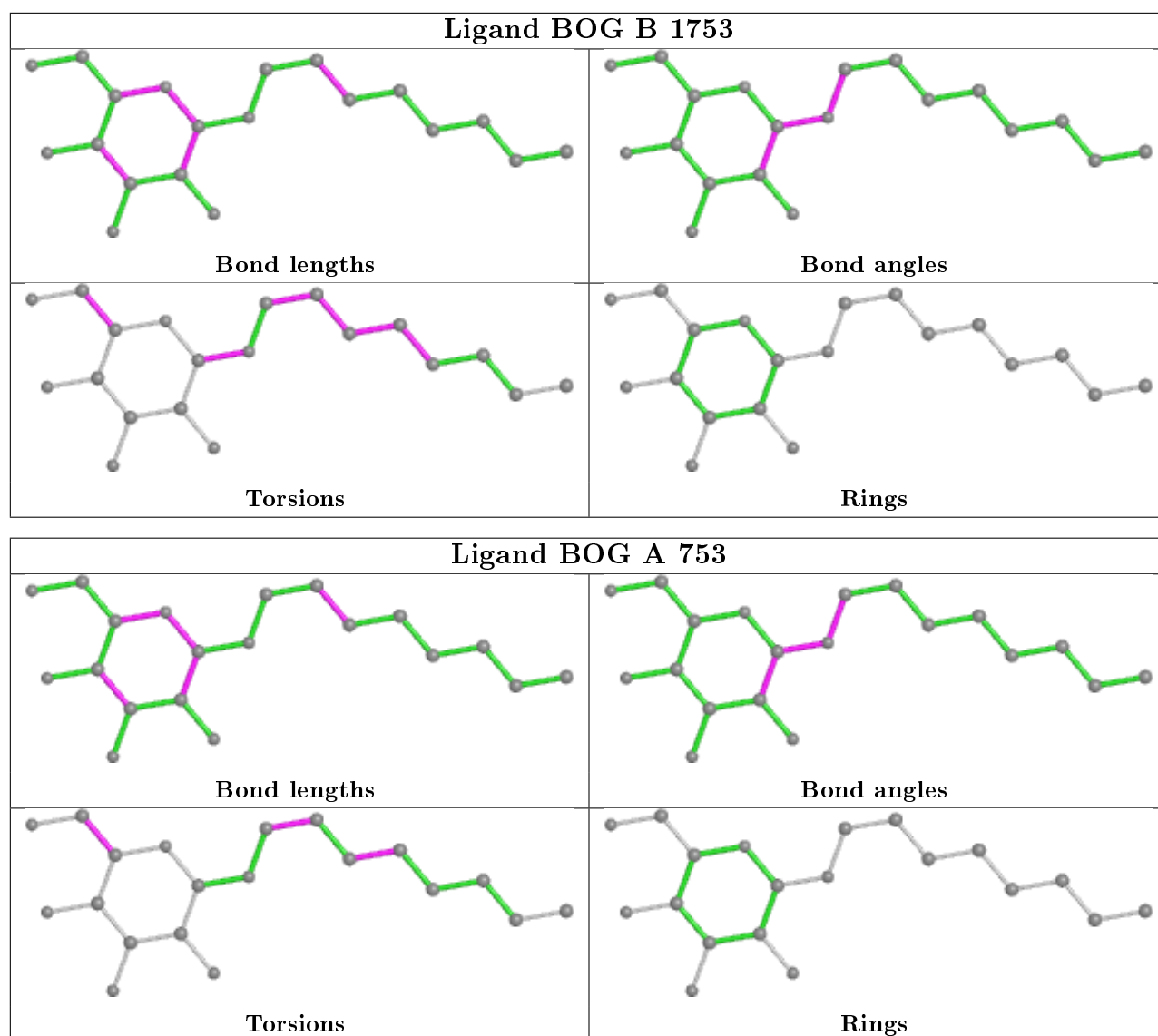
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	MNH	3	0
5	A	754	BOG	1	0
5	A	751	BOG	6	0
8	A	759	GOL	2	0
5	B	1751	BOG	4	0
5	B	1753	BOG	1	0

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	553/553 (100%)	0.09	24 (4%) 35 34	20, 30, 43, 53	0
1	B	553/553 (100%)	0.08	19 (3%) 45 44	20, 29, 42, 55	0
All	All	1106/1106 (100%)	0.09	43 (3%) 39 38	20, 29, 42, 55	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TRP	5.8
1	B	1584	ASP	5.5
1	A	107	PHE	5.4
1	A	584	ASP	5.4
1	B	1075	TRP	5.0

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	G	4	11/12	0.31	0.57	73,75,77,79	0
4	MAN	E	4	11/12	0.38	0.52	80,81,81,81	0
3	MAN	D	4	11/12	0.47	0.51	75,77,78,79	0
2	NAG	C	2	14/15	0.51	0.59	63,65,66,67	0

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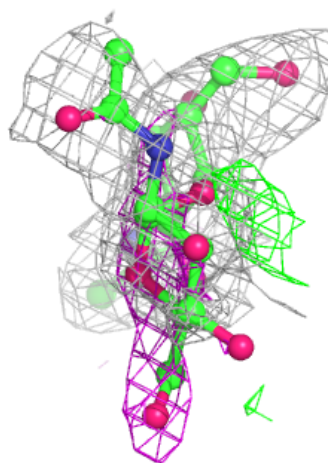
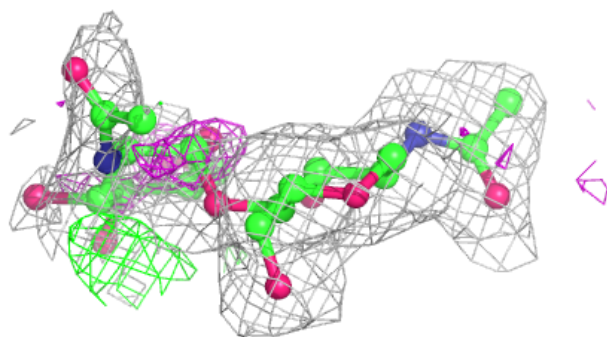
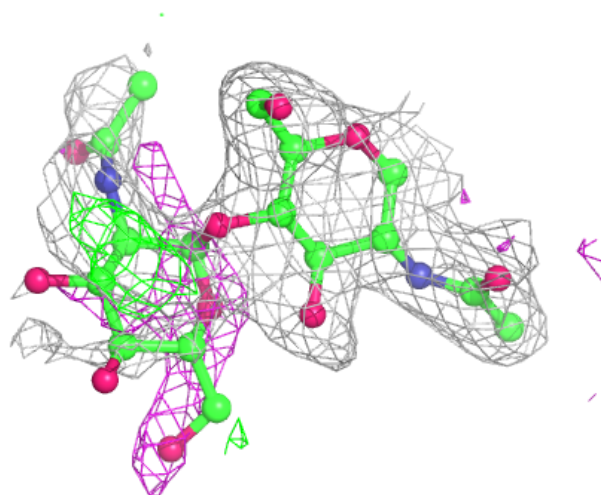
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MAN	G	5	11/12	0.51	0.47	80,80,81,81	0
4	MAN	H	4	11/12	0.53	0.57	75,77,77,78	0
3	MAN	D	3	11/12	0.59	0.45	62,66,70,73	0
4	MAN	H	3	11/12	0.63	0.39	62,66,69,73	0
3	NAG	D	2	14/15	0.67	0.25	45,48,52,57	0
4	MAN	E	3	11/12	0.69	0.57	69,72,75,78	0
3	MAN	G	3	11/12	0.70	0.40	59,62,66,70	0
2	NAG	F	2	14/15	0.75	0.41	59,61,62,62	0
4	NAG	E	2	14/15	0.75	0.22	53,56,60,65	0
3	MAN	D	5	11/12	0.78	0.44	79,79,79,80	0
3	NAG	G	2	14/15	0.79	0.23	42,45,48,54	0
2	NAG	C	1	14/15	0.81	0.17	47,51,54,59	0
2	NAG	F	1	14/15	0.84	0.23	48,51,53,57	0
4	NAG	H	2	14/15	0.88	0.15	44,46,51,57	0
4	NAG	E	1	14/15	0.90	0.10	40,42,45,50	0
3	NAG	D	1	14/15	0.93	0.10	28,29,33,39	0
4	NAG	H	1	14/15	0.94	0.07	33,35,38,41	0
3	NAG	G	1	14/15	0.94	0.10	25,26,30,35	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

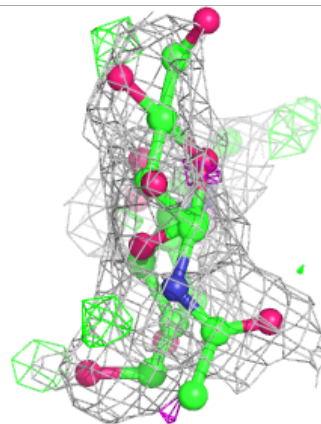
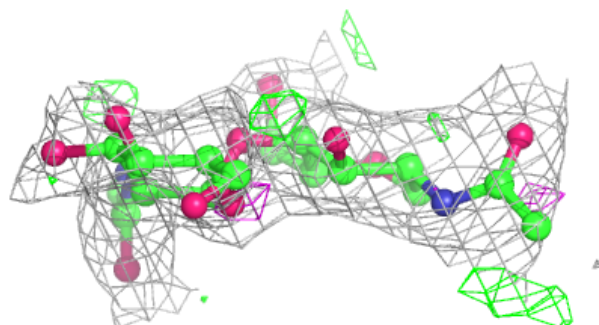
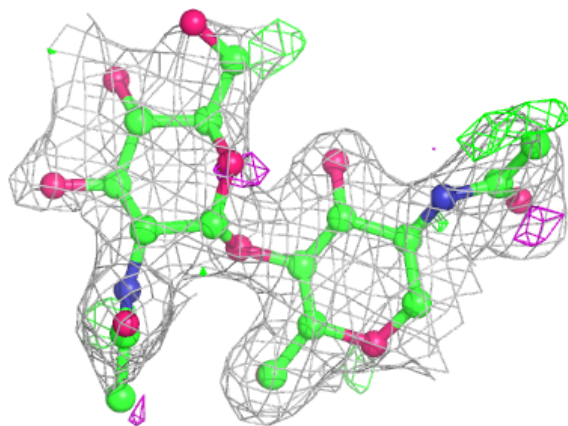
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





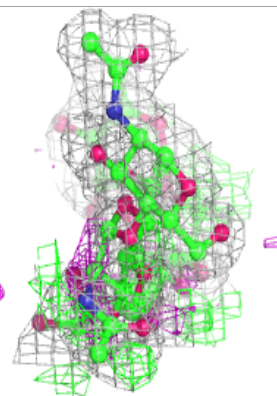
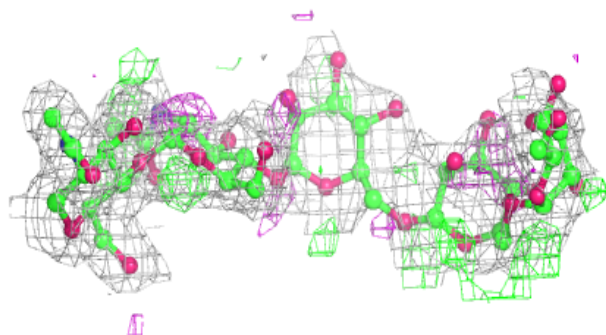
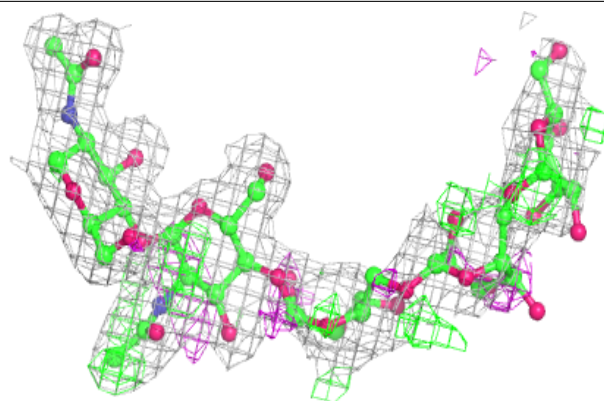
**Electron density around Chain F:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

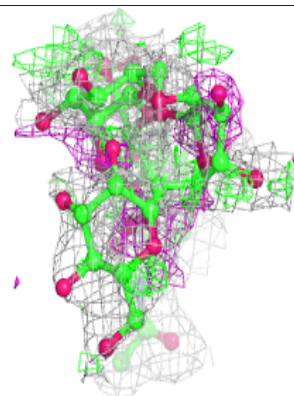
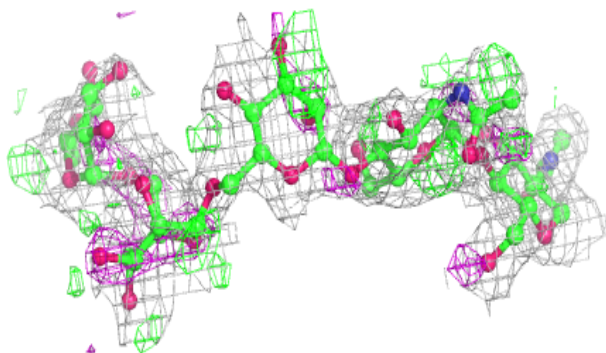
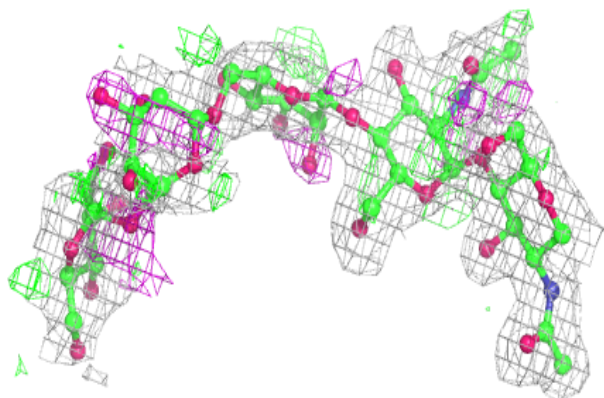


**Electron density around Chain D:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

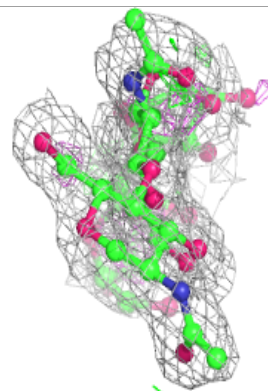
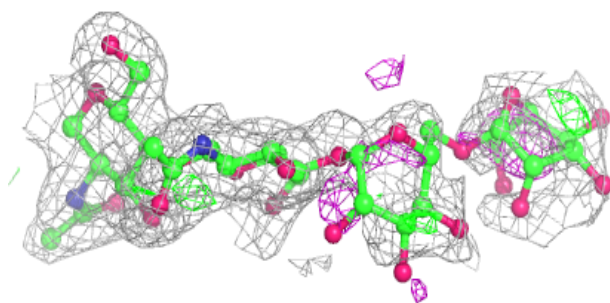
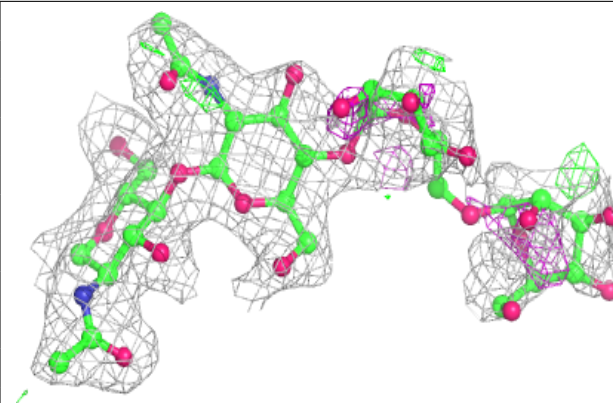
**Electron density around Chain G:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

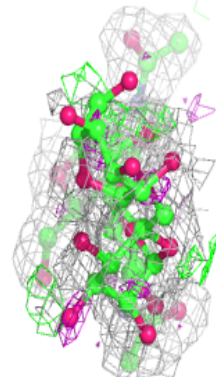
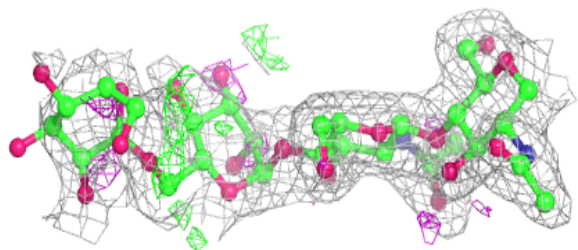
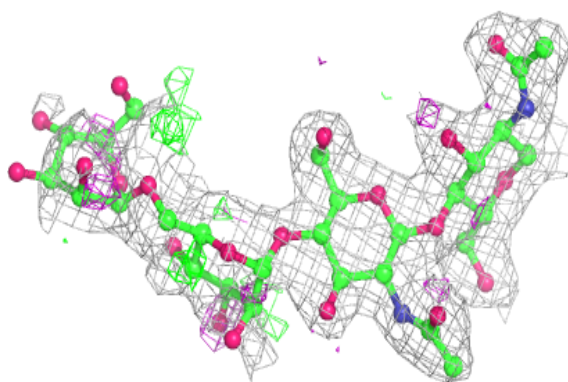


**Electron density around Chain E:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain H:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.4 Ligands ⓘ

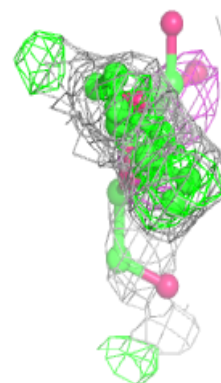
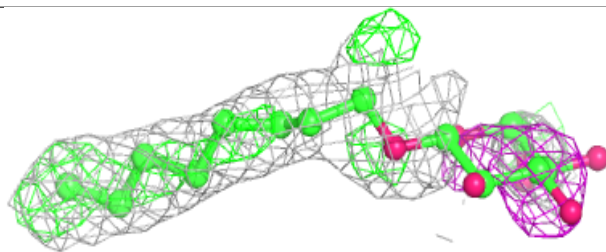
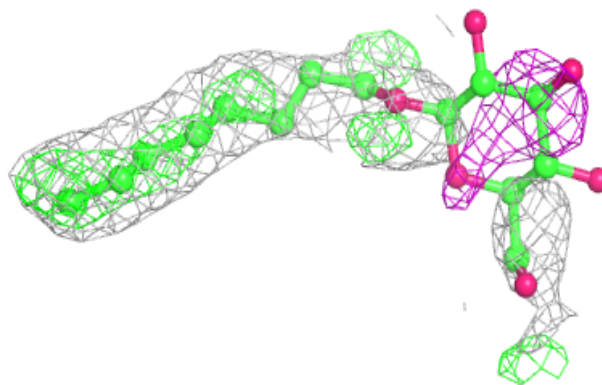
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BOG	A	752	20/20	0.04	0.52	94,101,102,102	0
5	BOG	A	754	20/20	0.32	0.54	96,99,99,100	0
5	BOG	B	1753	20/20	0.44	0.49	90,94,95,95	0
8	GOL	B	1760	6/6	0.55	0.36	66,67,67,68	0
5	BOG	B	1751	20/20	0.57	0.32	77,80,81,81	0
5	BOG	A	753	20/20	0.70	0.25	63,67,68,69	0
5	BOG	B	1750	20/20	0.72	0.40	84,84,89,89	0
5	BOG	A	751	20/20	0.73	0.26	69,70,71,71	0
8	GOL	A	760	6/6	0.76	0.20	61,62,62,63	0
8	GOL	A	758	6/6	0.78	0.28	38,44,45,45	0
8	GOL	B	1759	6/6	0.80	0.21	36,39,41,46	0
8	GOL	A	759	6/6	0.80	0.22	43,45,47,47	0
7	MNH	A	601	43/43	0.88	0.17	32,37,42,44	0
6	FLP	A	1701[B]	18/18	0.89	0.17	35,36,37,37	18
6	FLP	B	2701[B]	18/18	0.89	0.18	37,38,38,38	18
6	FLP	A	1701[A]	18/18	0.89	0.17	29,29,30,31	18
6	FLP	B	2701[A]	18/18	0.89	0.18	25,26,27,27	18
7	MNH	B	1601	43/43	0.90	0.16	32,36,42,44	0

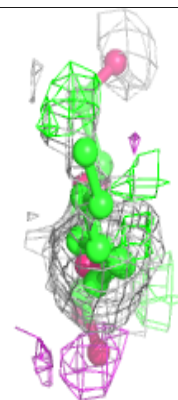
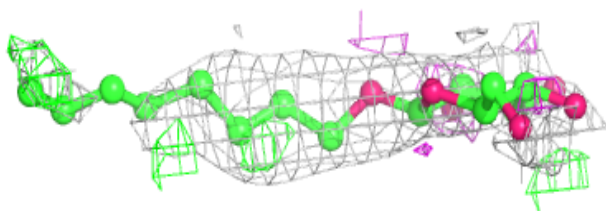
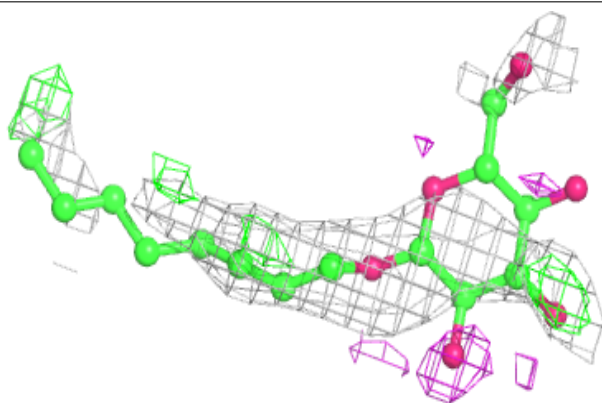
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around BOG A 752:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BOG A 754:**

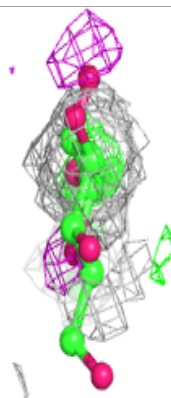
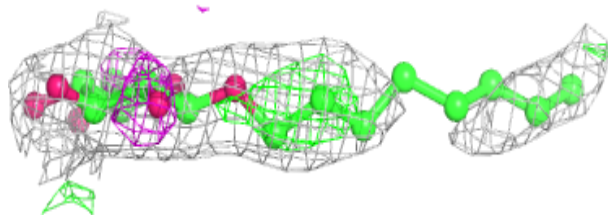
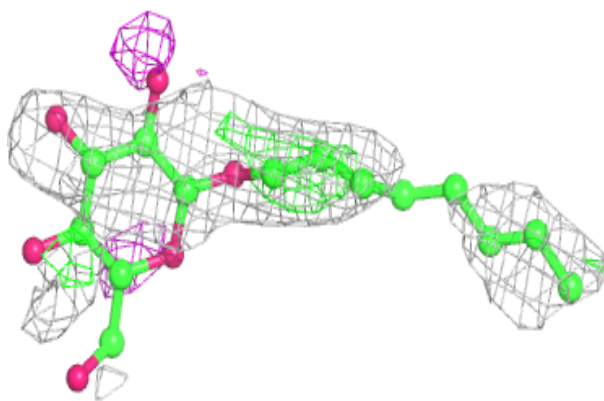
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



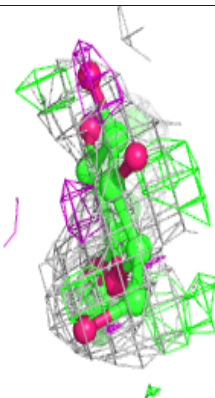
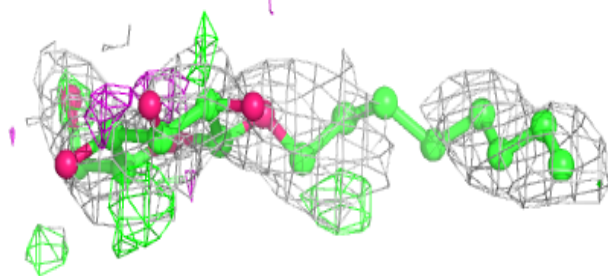
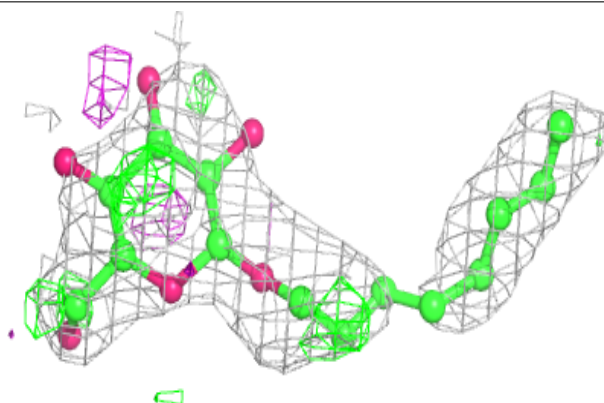


**Electron density around BOG B 1753:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

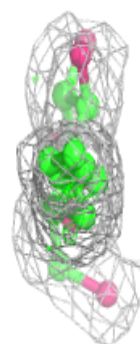
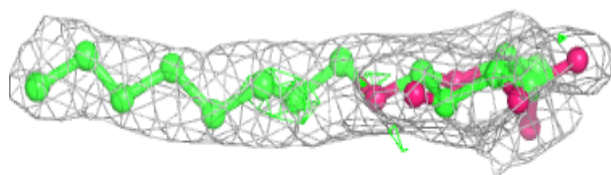
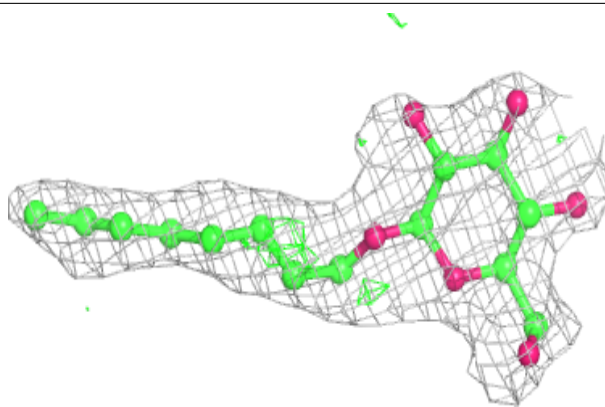
**Electron density around BOG B 1751:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

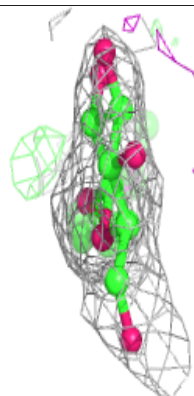
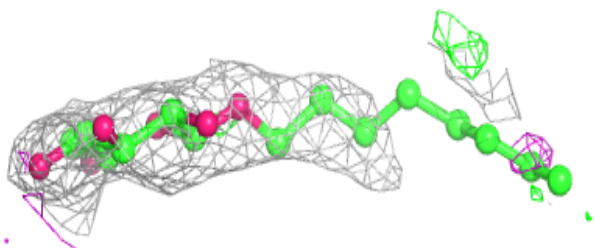
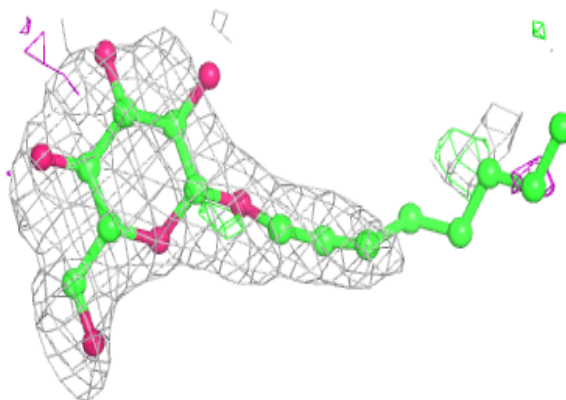


**Electron density around BOG A 753:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

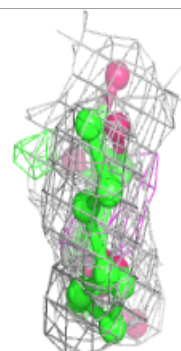
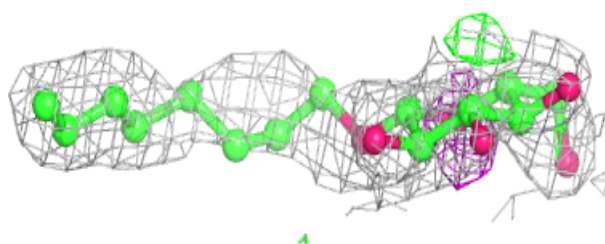
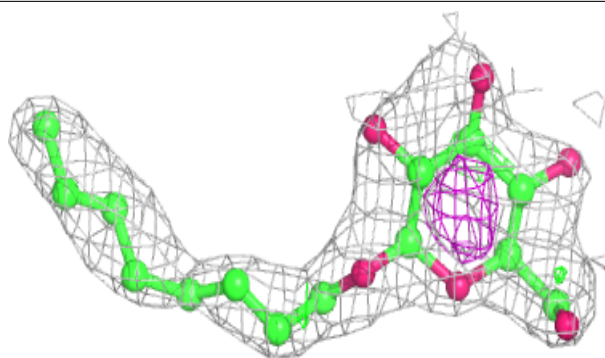
**Electron density around BOG B 1750:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BOG A 751:**

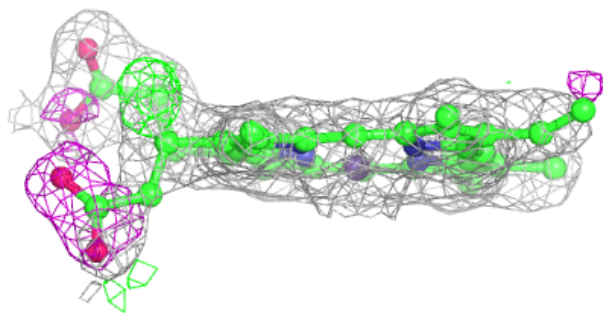
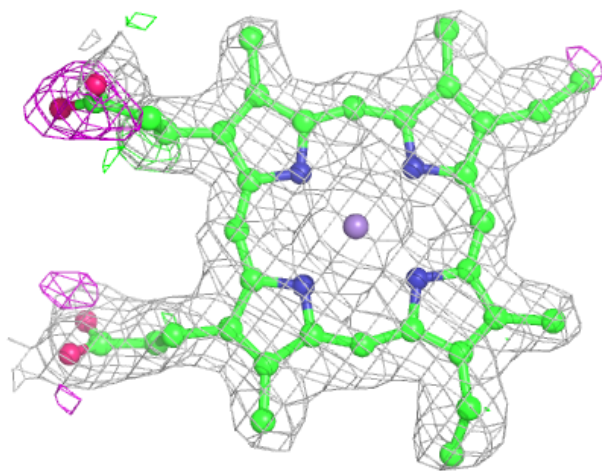
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





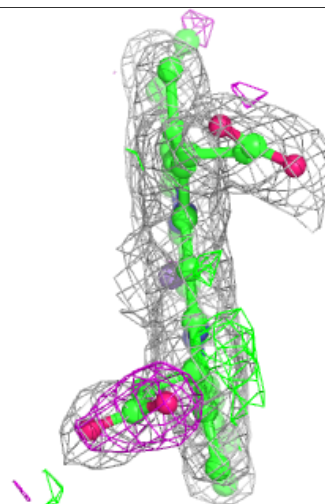
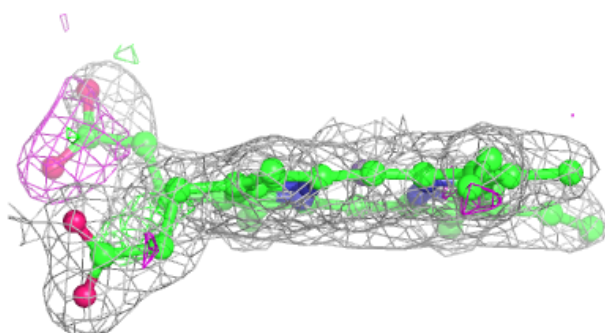
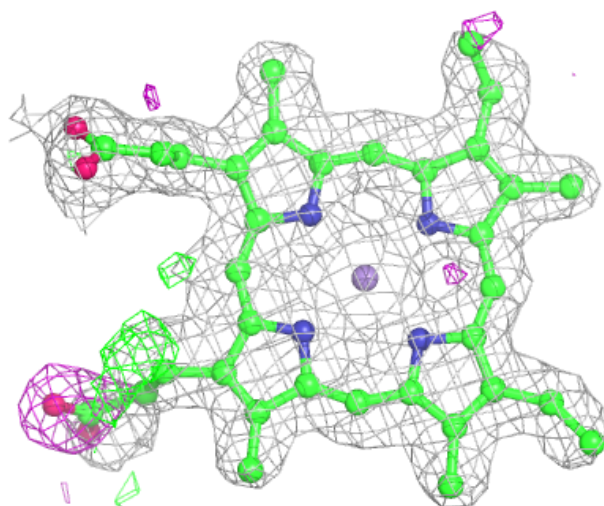
**Electron density around MNH A 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MNH B 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.