



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 08:48 AM BST

PDB ID : 3KK6
Title : Crystal Structure of Cyclooxygenase-1 in complex with celecoxib
Authors : Sidhu, R.S.
Deposited on : 2009-11-04
Resolution : 2.75 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)
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

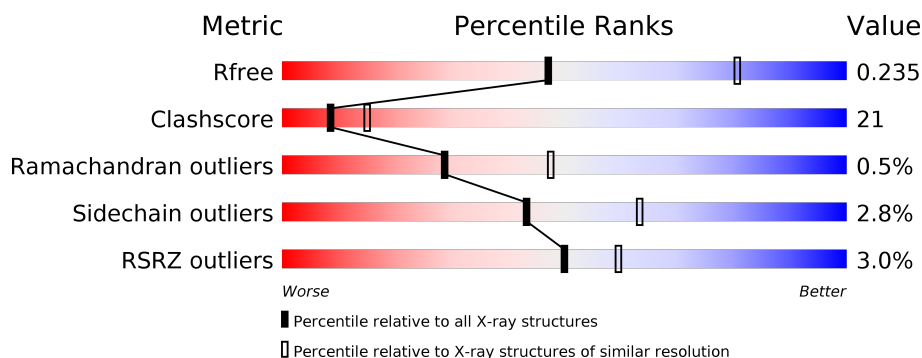
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 $\leq 5\%$. 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>2%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div></div> </div> </div>
1	B	553	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div></div> </div> </div>
2	C	5	<div> <div></div> <div>100%</div> </div>
3	D	2	<div> <div></div> <div>100%</div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
3	G	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	4	 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
2	NAG	C	1	-	-	X	-
2	MAN	C	3	-	-	X	-
2	BMA	C	4	-	-	X	-
2	MAN	C	5	-	-	X	-
3	NAG	G	1	-	-	X	-
6	CEL	A	701	-	-	X	-
7	BOG	B	1751	-	-	X	-
7	BOG	B	1752	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 18050 atoms, of which 8678 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	H	N	O	S	4120	1	0
			8497	2840	4120	731	778	28			
1	B	553	Total	C	H	N	O	S	4219	12	0
			8670	2899	4206	742	795	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	SEE REMARK 999	UNP P05979
B	92	LEU	MET	SEE REMARK 999	UNP P05979

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	H	N	O	33	0	0
			94	34	33	2	25			

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



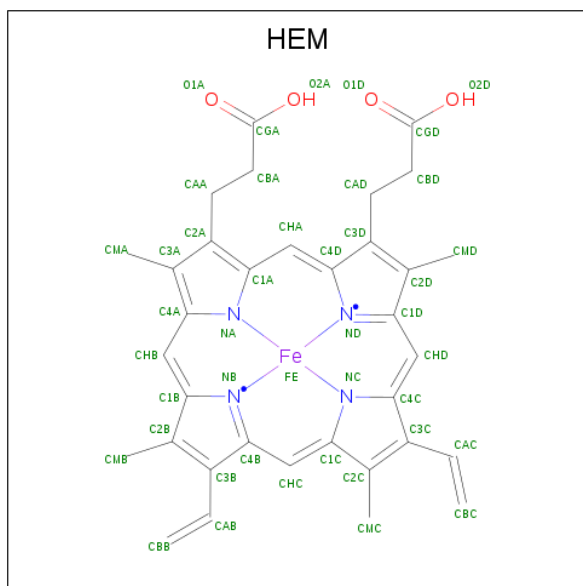
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
3	E	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
3	G	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			

- Molecule 4 is an oligosaccharide called beta-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	F	4	Total	C	H	N	O	40	0	0
			90	28	40	2	20			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	30	0
5	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	30	0

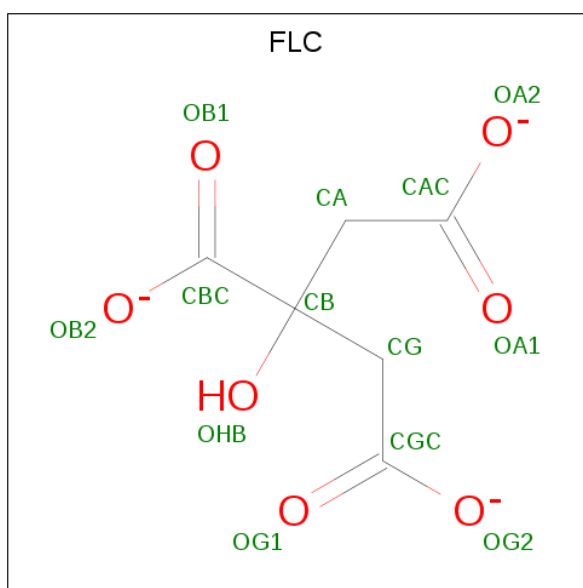
- # CEL
-
- ORTEP diagram of the chemical structure of CEL (C₁₂H₁₀F₃N₂O₂S). The structure features a central pyrazole ring (C1-C5, N1, N2) substituted with a trifluoromethyl group (C4, F1-F3) at C1, a 4-sulfamoylphenyl group (C12-C17, S1, O1, O2, N3) at C2, and a 3-(trifluoromethyl)phenyl group (C5-C11, F1-F3) at C3. The pyrazole ring is in a chair conformation. The sulfamoyl group is in a planar conformation. The trifluoromethyl group is in a planar conformation. The 3-(trifluoromethyl)phenyl group is in a planar conformation. The structure is shown with thermal ellipsoids at the 50% probability level. The title 'CEL' is centered above the structure.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	A	1	Total 40	C 17	F 3	H 14	N 3	O 2	S 1	14	0
6	B	1	Total 40	C 17	F 3	H 14	N 3	O 2	S 1	14	0

-
- Chemical structure of BOG (beta-D-glucopyranosyl-beta-D-glucopyranoside). The structure shows a pyranose ring with substituents labeled C1' through C8'. The ring carbons are labeled C1(R), C2(R), C3(S), C4(S), C5(R), and C6. The substituents are: C1' (O1), C2' (OH, 02), C3' (OH, 03), C4' (OH, 04), C5' (OH, 05), and C6' (C6, 06). The side chain is branched, with C1' connected to C2', C3', and C4'. The side chain carbons are labeled C1', C2', C3', C4', C5', C6', C7', and C8'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	30	0
			47	14	27	6		
7	A	1	Total	C	H	O	28	0
			48	14	28	6		
7	B	1	Total	C	H	O	28	0
			48	14	28	6		
7	B	1	Total	C	H	O	28	0
			48	14	28	6		

- Molecule 8 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	5	0
			18	6	5	7		

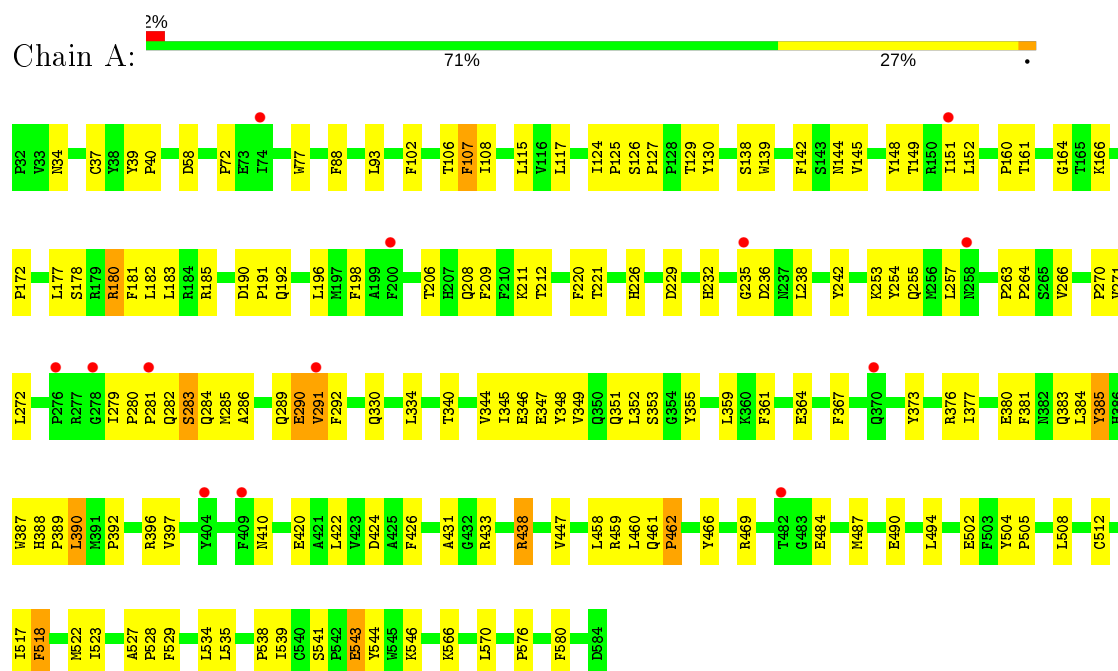
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	55	Total	O	0	0
			55	55		
9	B	50	Total	O	0	0
			50	50		

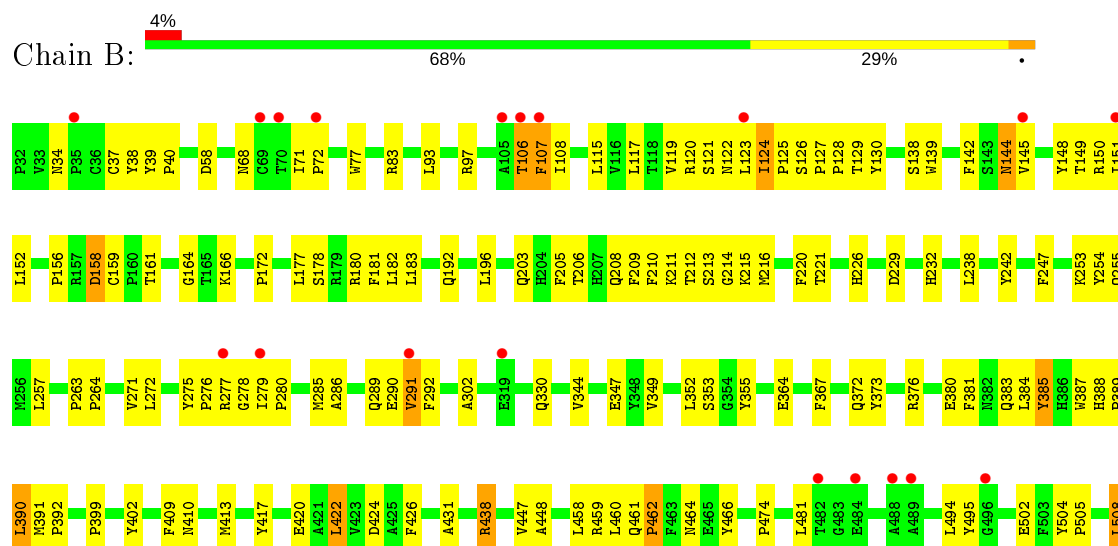
3 Residue-property plots [i](#)

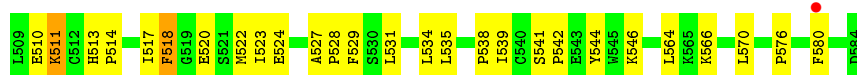
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%



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

Chain D: 100%



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

Chain E: 100%



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

Chain G: 100%



- Molecule 4: beta-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 F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	181.03Å 181.03Å 102.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.41 – 2.75 46.58 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.4 (41.41-2.75) 97.4 (46.58-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.242 0.203 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.489 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.501 for h,-h-k,-l	Depositor
Outliers	0 of 49651 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18050	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CEL, NDG, HEM, FLC, 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	0.45	2/4517 (0.0%)	0.55	6/6155 (0.1%)
1	B	0.44	0/4610	0.56	7/6287 (0.1%)
All	All	0.44	2/9127 (0.0%)	0.55	13/12442 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543[A]	GLU	N-CA	5.09	1.56	1.46
1	A	543[B]	GLU	N-CA	5.09	1.56	1.46

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	A	459	ARG	NE-CZ-NH1	-12.53	114.03	120.30
1	B	459	ARG	NE-CZ-NH1	12.42	126.51	120.30
1	A	459	ARG	NE-CZ-NH2	12.25	126.43	120.30
1	B	180	ARG	NE-CZ-NH2	-12.16	114.22	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	124[B]	ILE	Peptide

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	4377	4120	4173	144	0
1	B	4464	4206	4244	200	1
2	C	61	33	52	28	0
3	D	28	25	24	2	1
3	E	28	25	24	8	0
3	G	28	25	24	10	0
4	F	50	40	43	13	0
5	A	43	30	30	7	0
5	B	43	30	30	10	0
6	A	26	14	14	9	0
6	B	26	14	14	8	0
7	A	40	55	56	4	0
7	B	40	56	55	13	0
8	A	13	5	4	0	0
9	A	55	0	0	3	0
9	B	50	0	0	3	0
All	All	9372	8678	8787	372	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 21.

The worst 5 of 372 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:A:144:ASN:HD21	2:C:1:NAG:C1	0.96	1.55
1:A:144:ASN:ND2	2:C:1:NAG:C1	1.80	1.36
2:C:4:BMA:O4	2:C:5:MAN:C2	1.81	1.28
2:C:4:BMA:O4	2:C:5:MAN:H2	1.22	1.26
1:B:349:VAL:O	1:B:353:SER:OG	1.53	1.26

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:B:279:ILE:O	3:D:1:NAG:H83[4_565]	1.56	0.04

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	552/553 (100%)	508 (92%)	41 (7%)	3 (0%)	29	47
1	B	563/553 (102%)	507 (90%)	54 (10%)	2 (0%)	34	53
All	All	1115/1106 (101%)	1015 (91%)	95 (8%)	5 (0%)	29	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	A	462	PRO
1	B	462	PRO
1	B	399	PRO
1	A	160	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	462/488 (95%)	451 (98%)	11 (2%)	49	68
1	B	472/488 (97%)	457 (97%)	15 (3%)	39	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	934/976 (96%)	908 (97%)	26 (3%)	43 63

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	106	THR
1	B	158	ASP
1	B	511	LYS
1	B	107	PHE
1	B	144	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	GLN
1	B	370	GLN
1	B	192	GLN
1	A	370	GLN
1	B	68	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

15 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	14,14,15	1.00	1 (7%)	17,19,21	1.92	5 (29%)
2	NAG	C	2	2	14,14,15	1.20	1 (7%)	17,19,21	2.85	7 (41%)
2	MAN	C	3	2	11,11,12	0.86	0	15,15,17	2.51	6 (40%)
2	BMA	C	4	2	11,11,12	0.88	0	15,15,17	2.17	6 (40%)
2	MAN	C	5	2	11,11,12	0.64	0	15,15,17	0.90	1 (6%)
3	NAG	D	1	3	14,14,15	1.15	1 (7%)	17,19,21	1.65	3 (17%)
3	NDG	D	2	3	14,14,15	1.72	4 (28%)	17,19,21	2.31	6 (35%)
3	NAG	E	1	3	14,14,15	1.17	2 (14%)	17,19,21	2.41	4 (23%)
3	NDG	E	2	3	14,14,15	0.86	0	17,19,21	2.38	8 (47%)
4	NAG	F	1	4	14,14,15	1.24	1 (7%)	17,19,21	2.18	5 (29%)
4	NAG	F	2	4	14,14,15	0.82	1 (7%)	17,19,21	2.49	5 (29%)
4	MAN	F	3	4	11,11,12	0.72	0	15,15,17	1.75	4 (26%)
4	BMA	F	4	4	11,11,12	1.08	1 (9%)	15,15,17	1.73	4 (26%)
3	NAG	G	1	3	14,14,15	0.87	0	17,19,21	2.07	5 (29%)
3	NDG	G	2	3	14,14,15	1.55	2 (14%)	17,19,21	2.63	5 (29%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	-3.17	1.38	1.43
3	D	2	NDG	O5-C1	-2.98	1.39	1.43
3	G	2	NDG	O5-C1	-2.73	1.39	1.43
4	F	1	NAG	O5-C1	-2.70	1.39	1.43
4	F	4	BMA	O5-C1	-2.58	1.39	1.43

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C4-C3-C2	-6.43	101.60	111.02
3	G	2	NDG	O5-C1-C2	6.33	121.28	111.29
2	C	2	NAG	O5-C1-C2	-6.26	101.40	111.29
3	G	2	NDG	C4-C3-C2	-6.07	102.12	111.02
4	F	2	NAG	O5-C1-C2	-5.82	102.10	111.29

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NDG	C3-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7
3	E	2	NDG	C4-C5-C6-O6
4	F	3	MAN	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	MAN	C1-C2-C3-C4-C5-O5
4	F	3	MAN	C1-C2-C3-C4-C5-O5
4	F	4	BMA	C1-C2-C3-C4-C5-O5
2	C	4	BMA	C1-C2-C3-C4-C5-O5
2	C	3	MAN	C1-C2-C3-C4-C5-O5

15 monomers are involved in 62 short contacts:

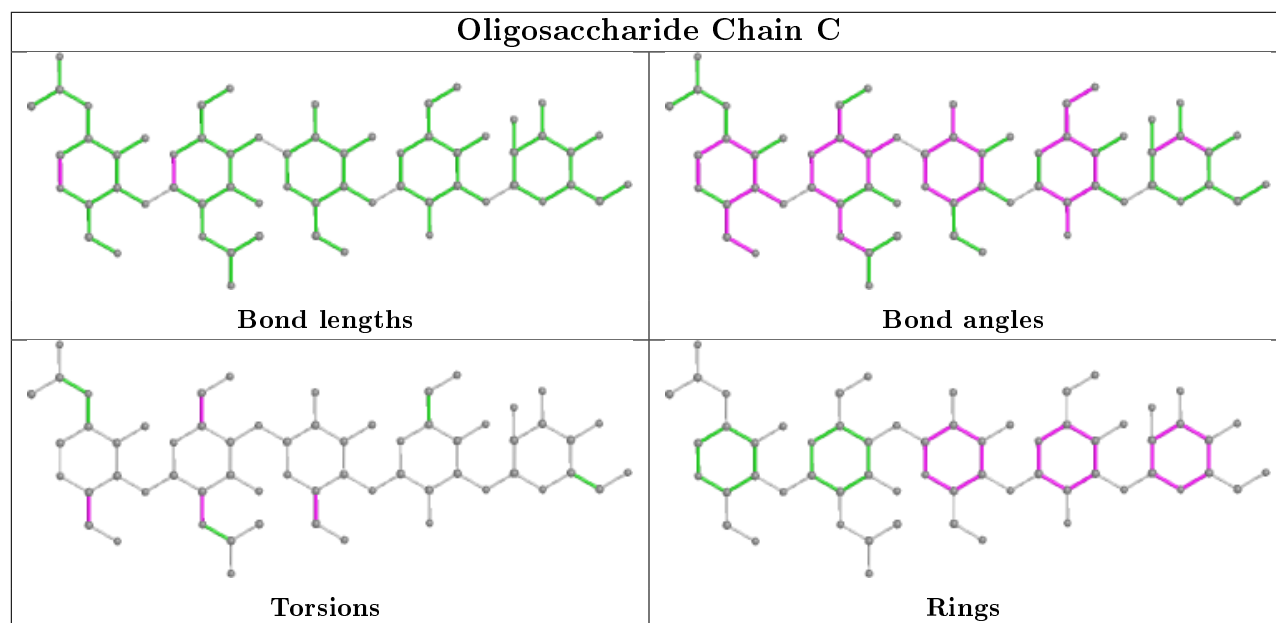
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	5	0
2	C	3	MAN	8	0
4	F	4	BMA	2	0
3	E	2	NDG	5	0

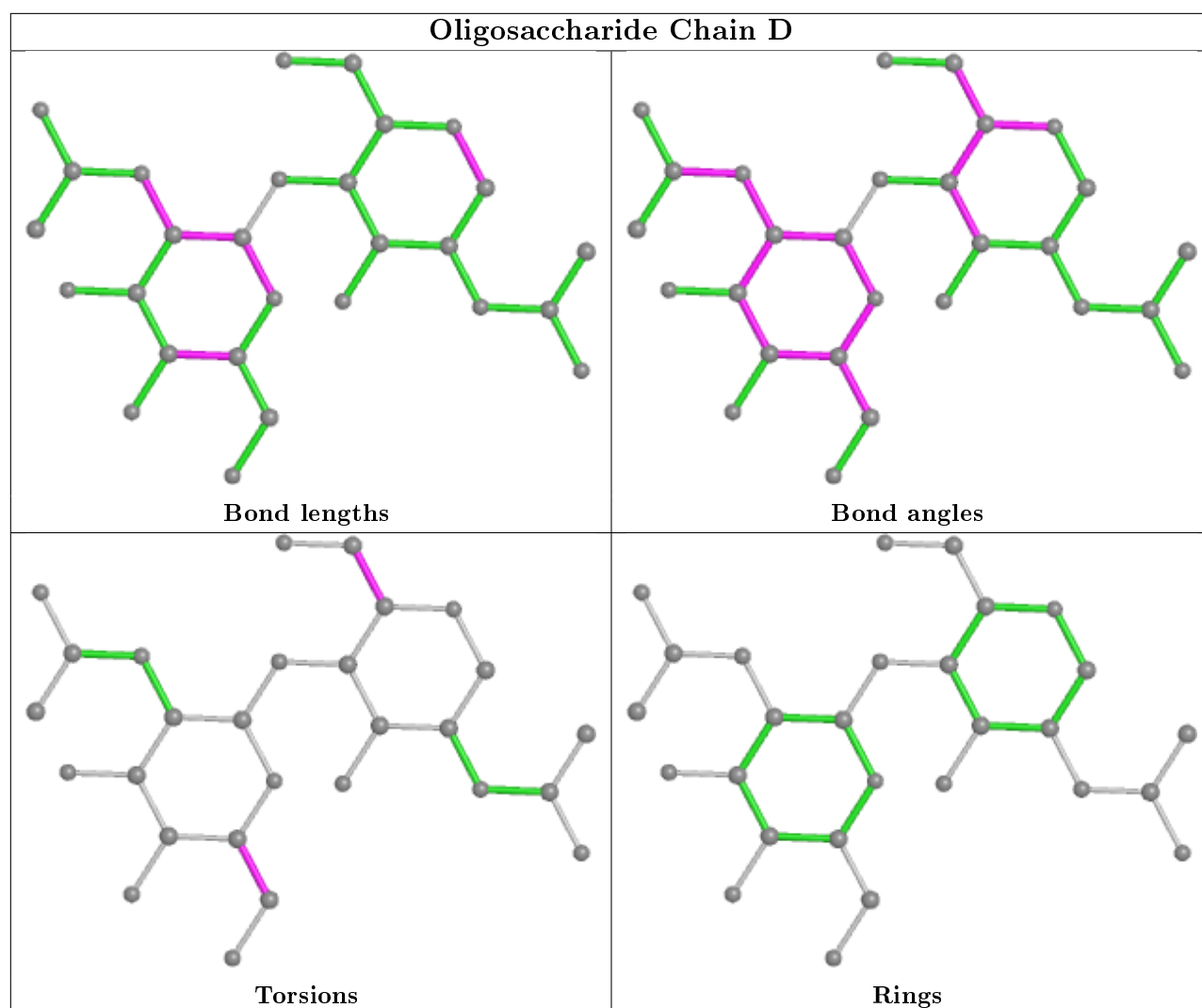
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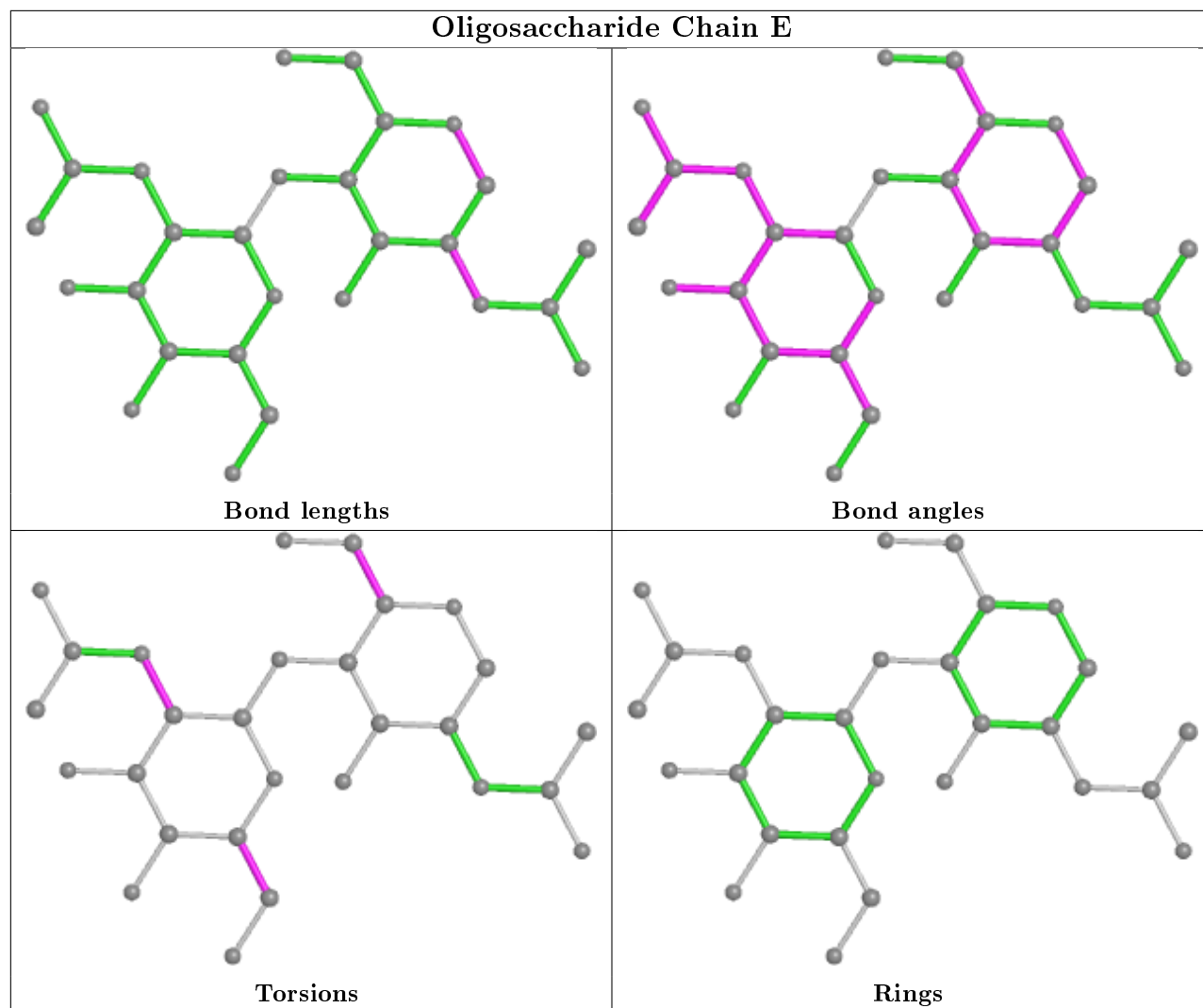
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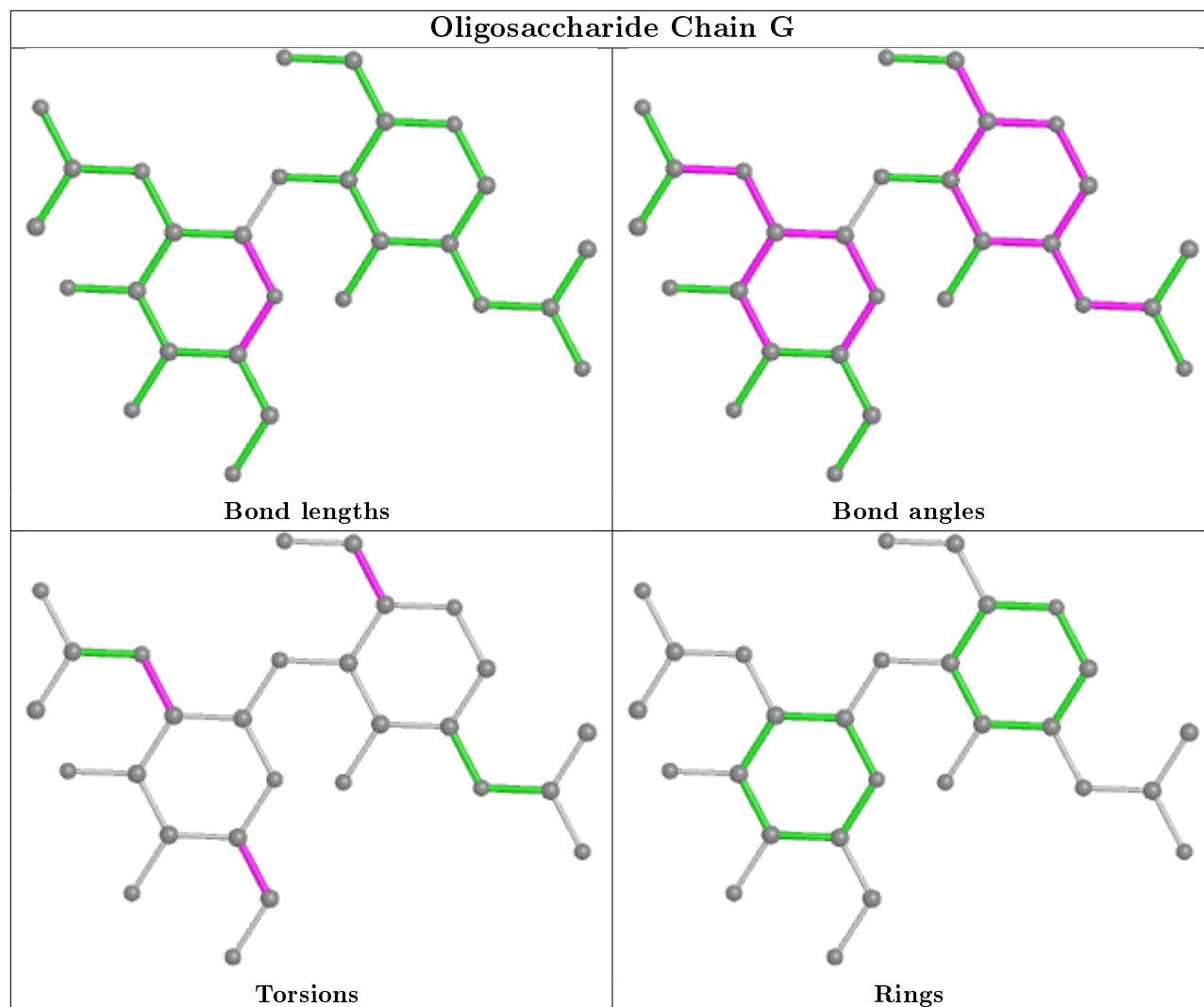
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NDG	3	0
4	F	3	MAN	2	0
2	C	5	MAN	12	0
3	E	1	NAG	5	0
2	C	4	BMA	20	0
3	G	1	NAG	9	0
3	D	1	NAG	2	1
2	C	1	NAG	7	0
2	C	2	NAG	3	0
4	F	2	NAG	6	0
3	D	2	NDG	1	0

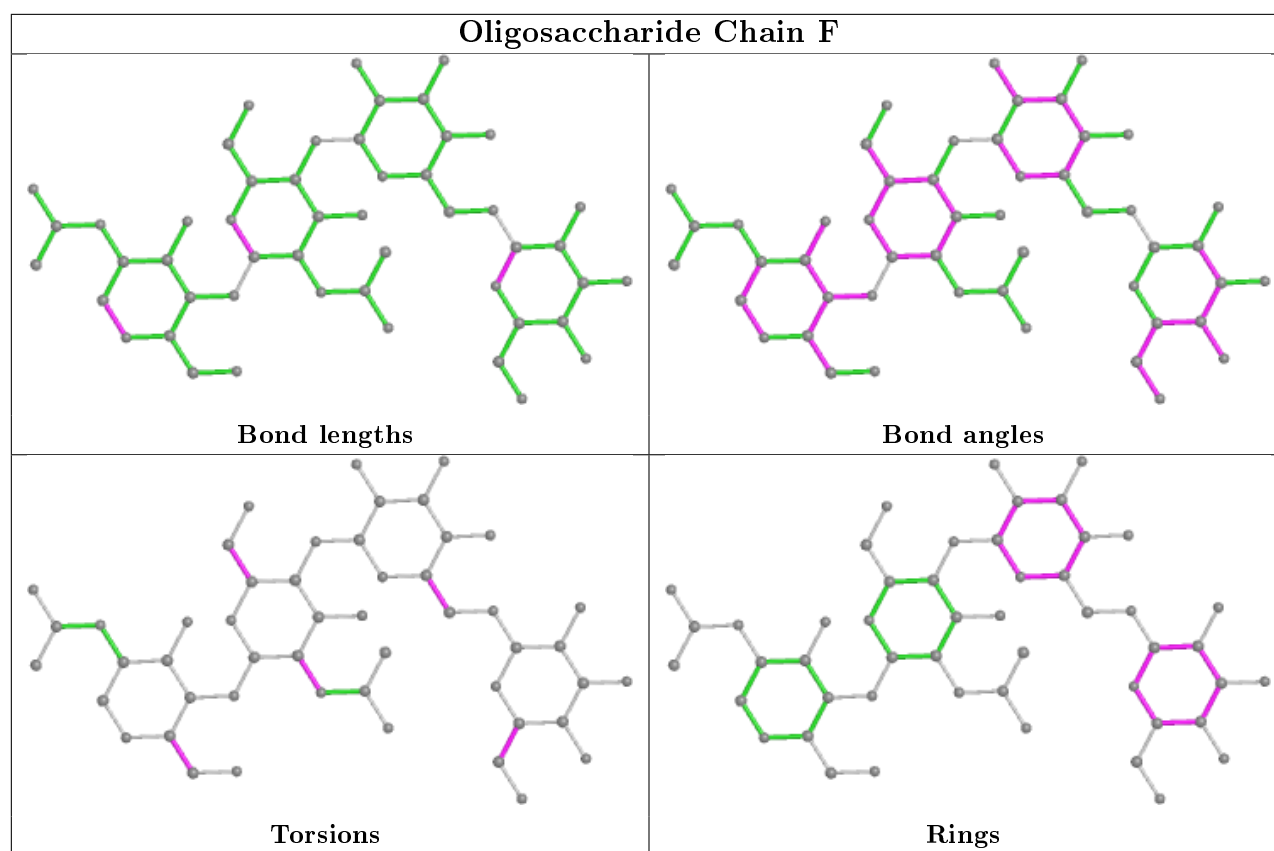
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

9 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
6	CEL	A	701	-	27,28,28	3.42	10 (37%)	37,43,43	1.86	8 (21%)
7	BOG	B	1751	-	20,20,20	1.35	4 (20%)	25,25,25	1.99	6 (24%)
8	FLC	A	900	-	3,12,12	3.07	2 (66%)	3,17,17	3.12	2 (66%)
7	BOG	A	751	-	20,20,20	0.89	1 (5%)	25,25,25	1.86	5 (20%)
7	BOG	B	1752	-	20,20,20	0.85	1 (5%)	25,25,25	2.51	4 (16%)
5	HEM	A	601	-	27,50,50	2.14	5 (18%)	17,82,82	1.49	2 (11%)
7	BOG	A	754	-	20,20,20	0.93	1 (5%)	25,25,25	1.76	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CEL	B	1701	-	27,28,28	3.74	11 (40%)	37,43,43	2.32	11 (29%)
5	HEM	B	601	-	27,50,50	2.18	6 (22%)	17,82,82	1.56	5 (29%)

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
6	CEL	A	701	-	-	10/20/20/20	0/3/3/3
7	BOG	B	1751	-	-	6/11/31/31	0/1/1/1
8	FLC	A	900	-	-	3/6/16/16	-
7	BOG	A	751	-	-	8/11/31/31	0/1/1/1
7	BOG	B	1752	-	1/1/5/5	3/11/31/31	0/1/1/1
5	HEM	A	601	-	-	5/6/54/54	-
7	BOG	A	754	-	-	8/11/31/31	0/1/1/1
6	CEL	B	1701	-	-	7/20/20/20	0/3/3/3
5	HEM	B	601	-	-	2/6/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	CEL	O1-S1	9.99	1.62	1.43
6	B	1701	CEL	O1-S1	9.88	1.62	1.43
6	A	701	CEL	O2-S1	9.67	1.61	1.43
6	B	1701	CEL	O2-S1	9.05	1.60	1.43
6	B	1701	CEL	C15-S1	8.92	1.91	1.77

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1701	CEL	O2-S1-C15	8.54	116.88	107.35
7	B	1752	BOG	O1-C1-C2	7.94	120.70	108.30
7	B	1752	BOG	O5-C1-O1	6.27	124.82	109.97
7	B	1751	BOG	O5-C1-C2	-5.61	98.47	110.35
6	A	701	CEL	O2-S1-N3	5.31	115.23	107.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1752	BOG	C1

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1751	BOG	C2-C1-O1-C1'
7	B	1751	BOG	O5-C1-O1-C1'
8	A	900	FLC	CAC-CA-CB-CBC
8	A	900	FLC	CAC-CA-CB-CG
8	A	900	FLC	CAC-CA-CB-OHB

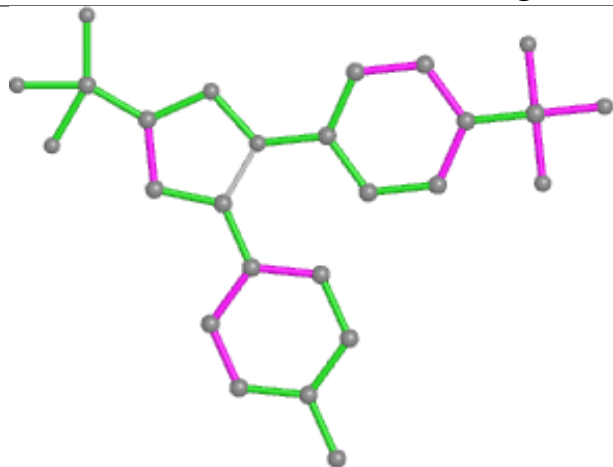
There are no ring outliers.

8 monomers are involved in 51 short contacts:

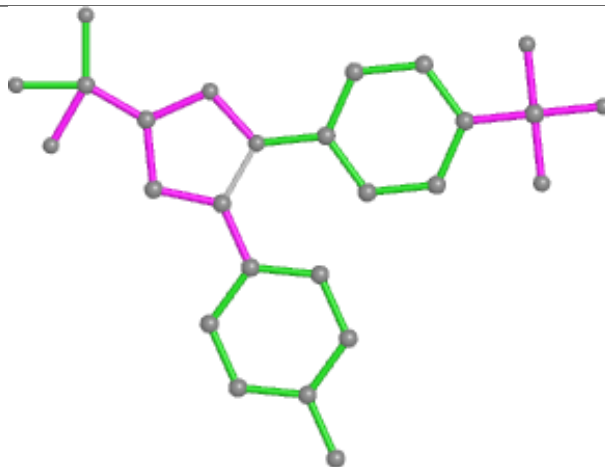
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	CEL	9	0
7	B	1751	BOG	12	0
7	A	751	BOG	1	0
7	B	1752	BOG	1	0
5	A	601	HEM	7	0
7	A	754	BOG	3	0
6	B	1701	CEL	8	0
5	B	601	HEM	10	0

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

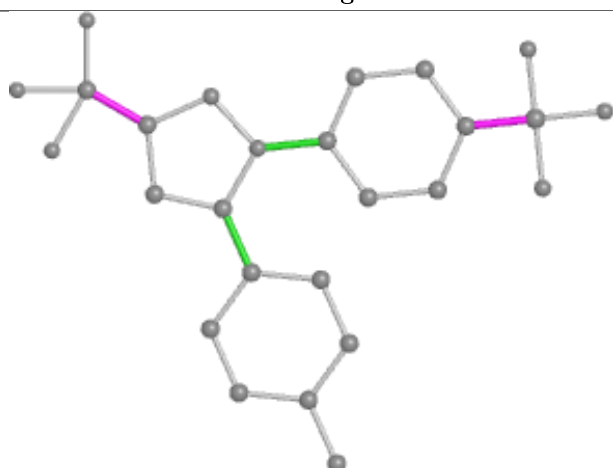
Ligand CEL A 701



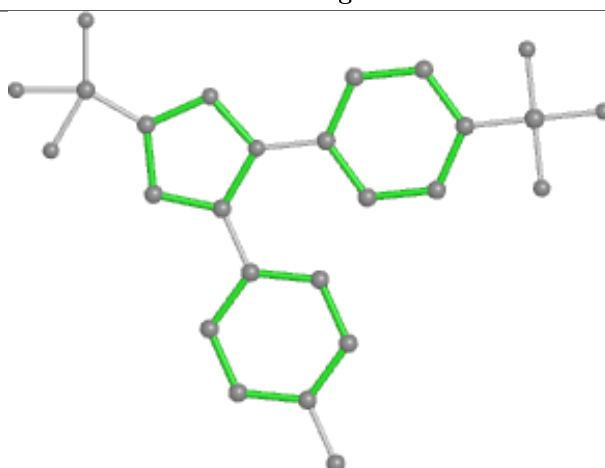
Bond lengths



Bond angles

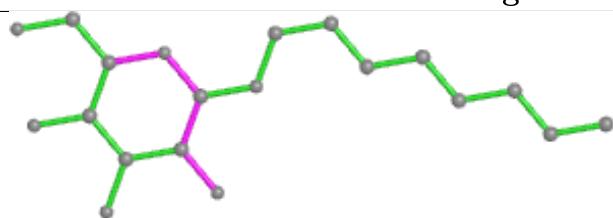


Torsions

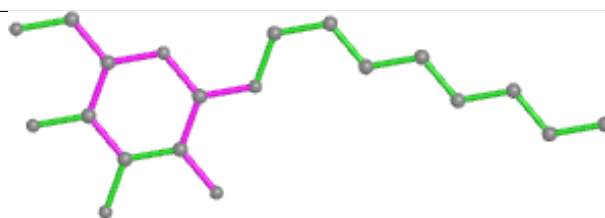


Rings

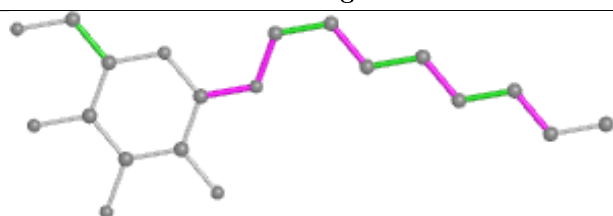
Ligand BOG B 1751



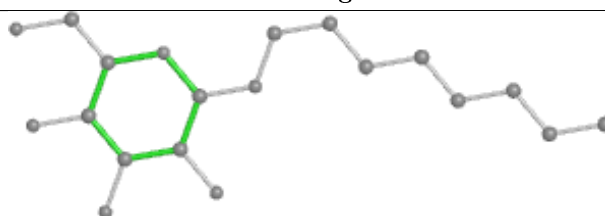
Bond lengths



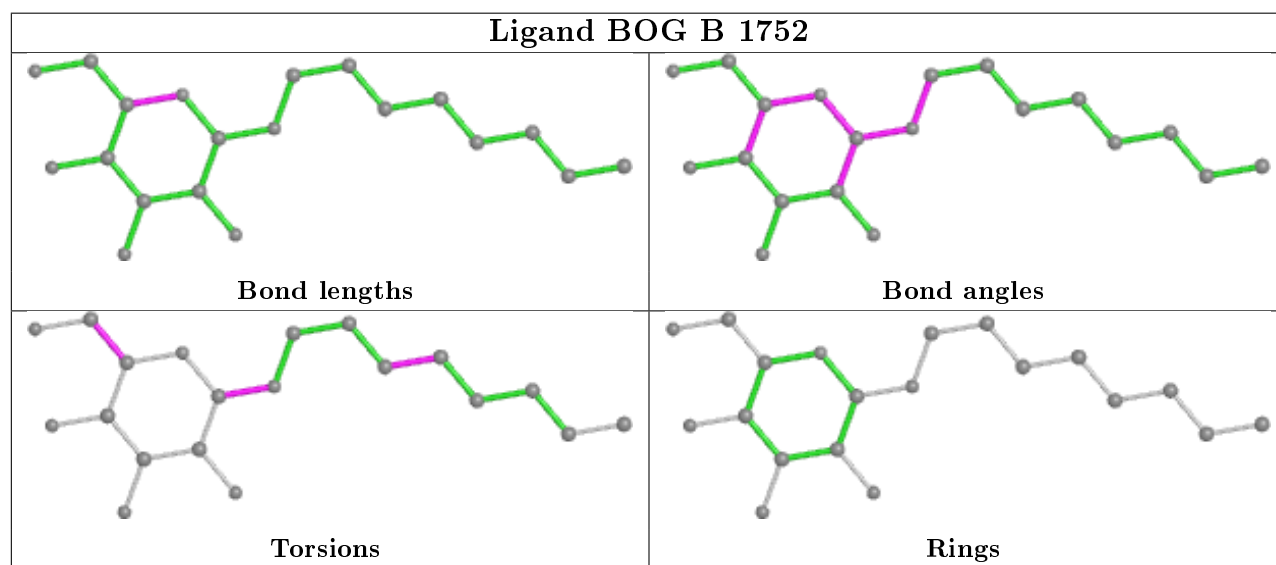
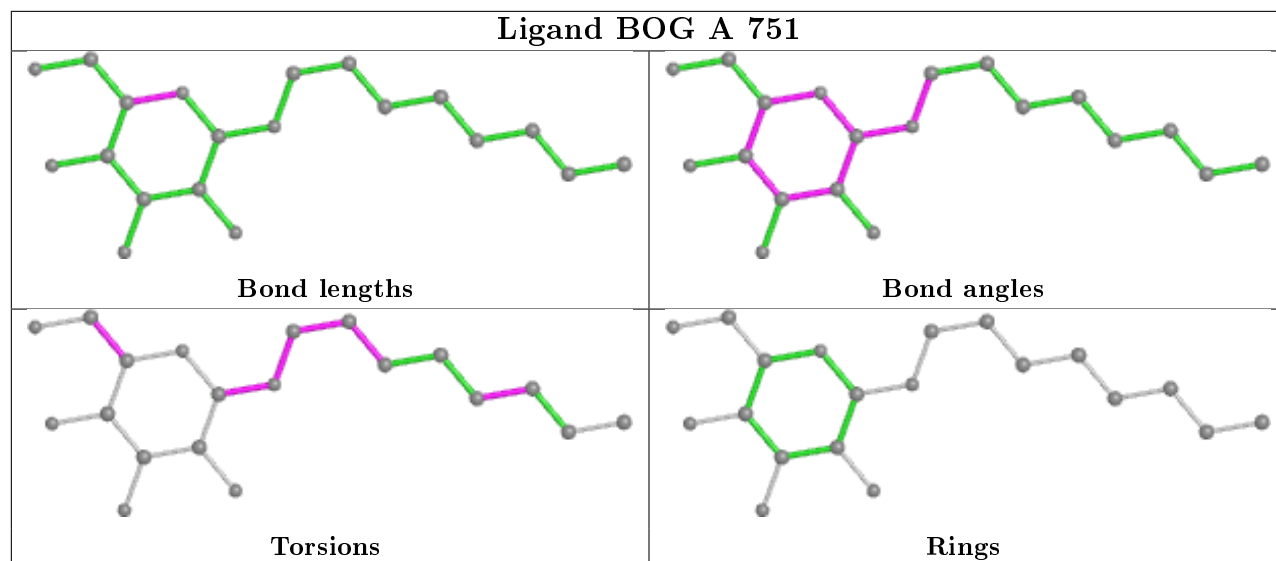
Bond angles

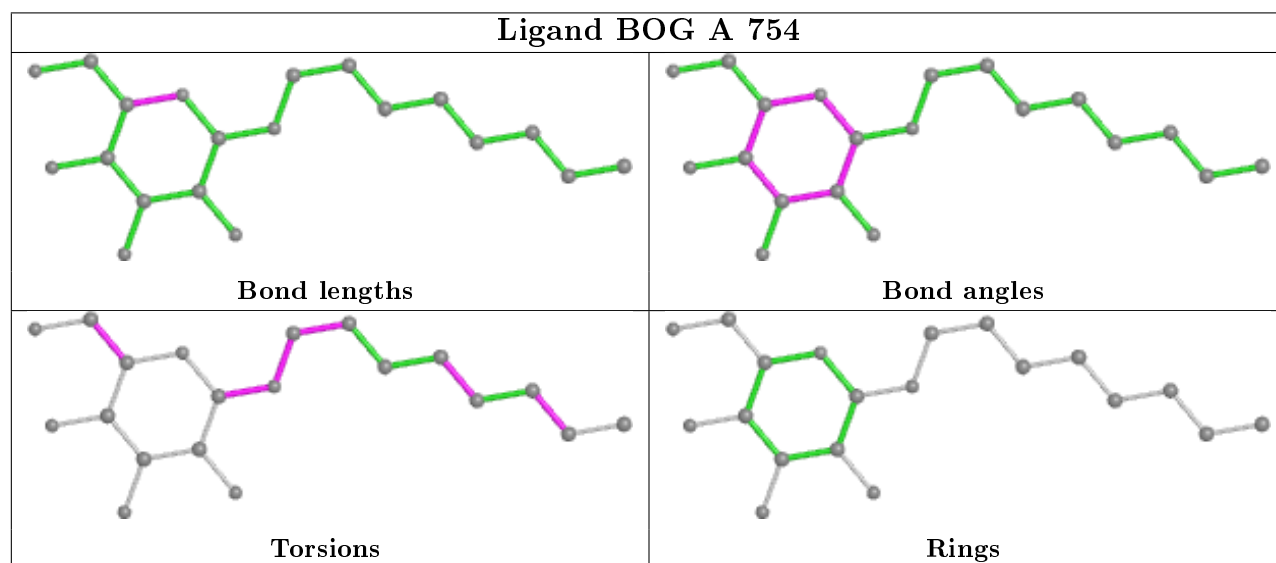
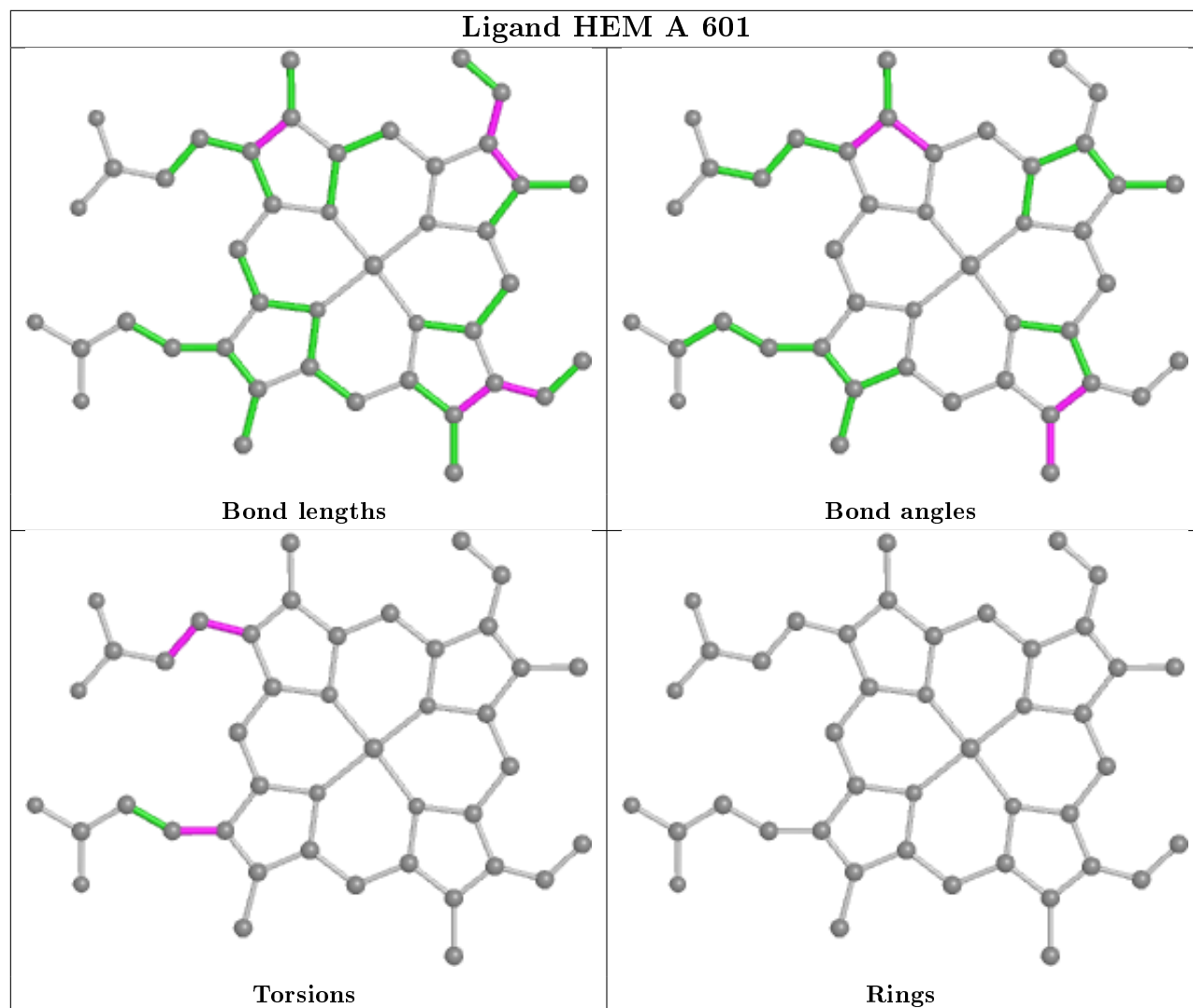


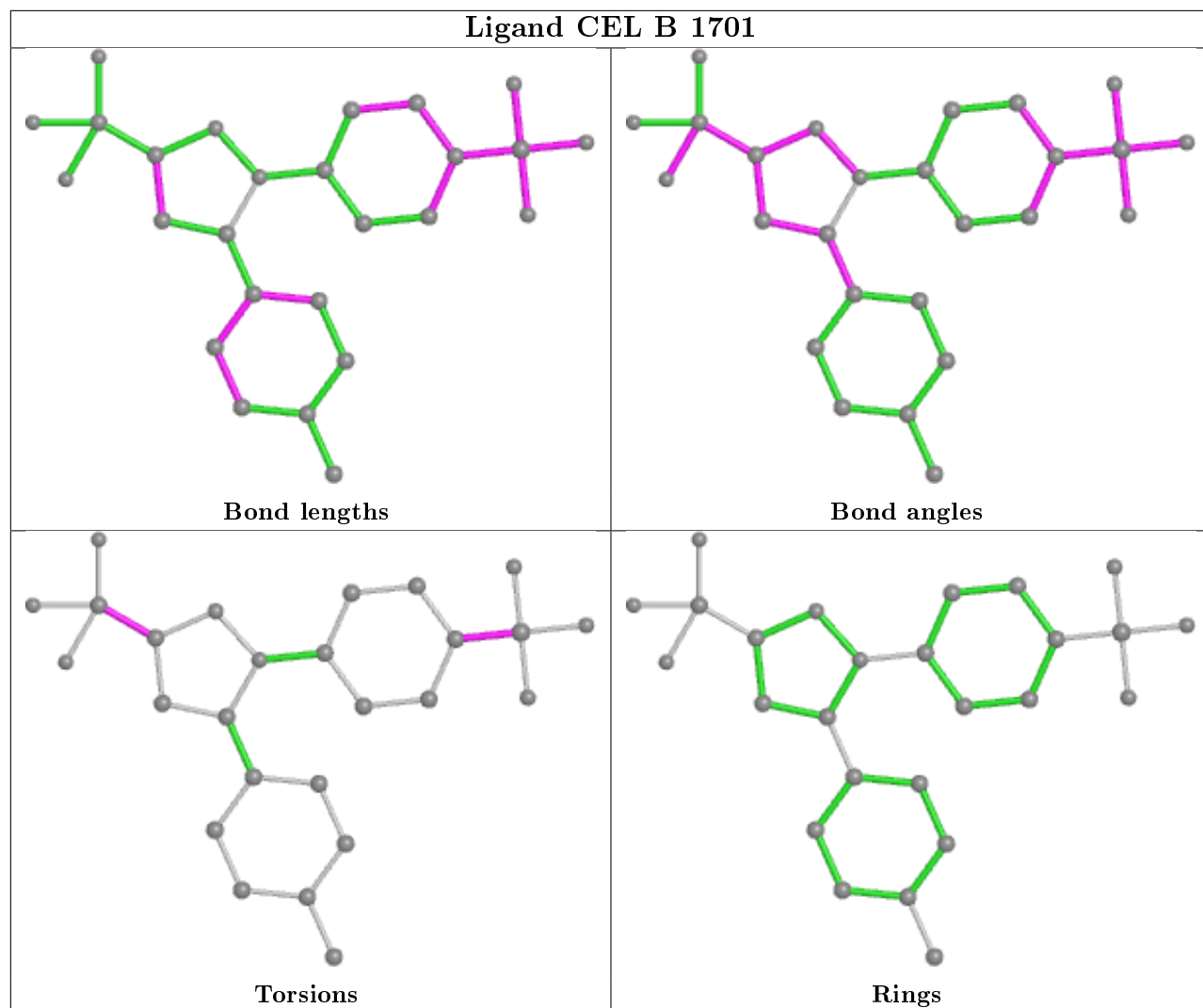
Torsions

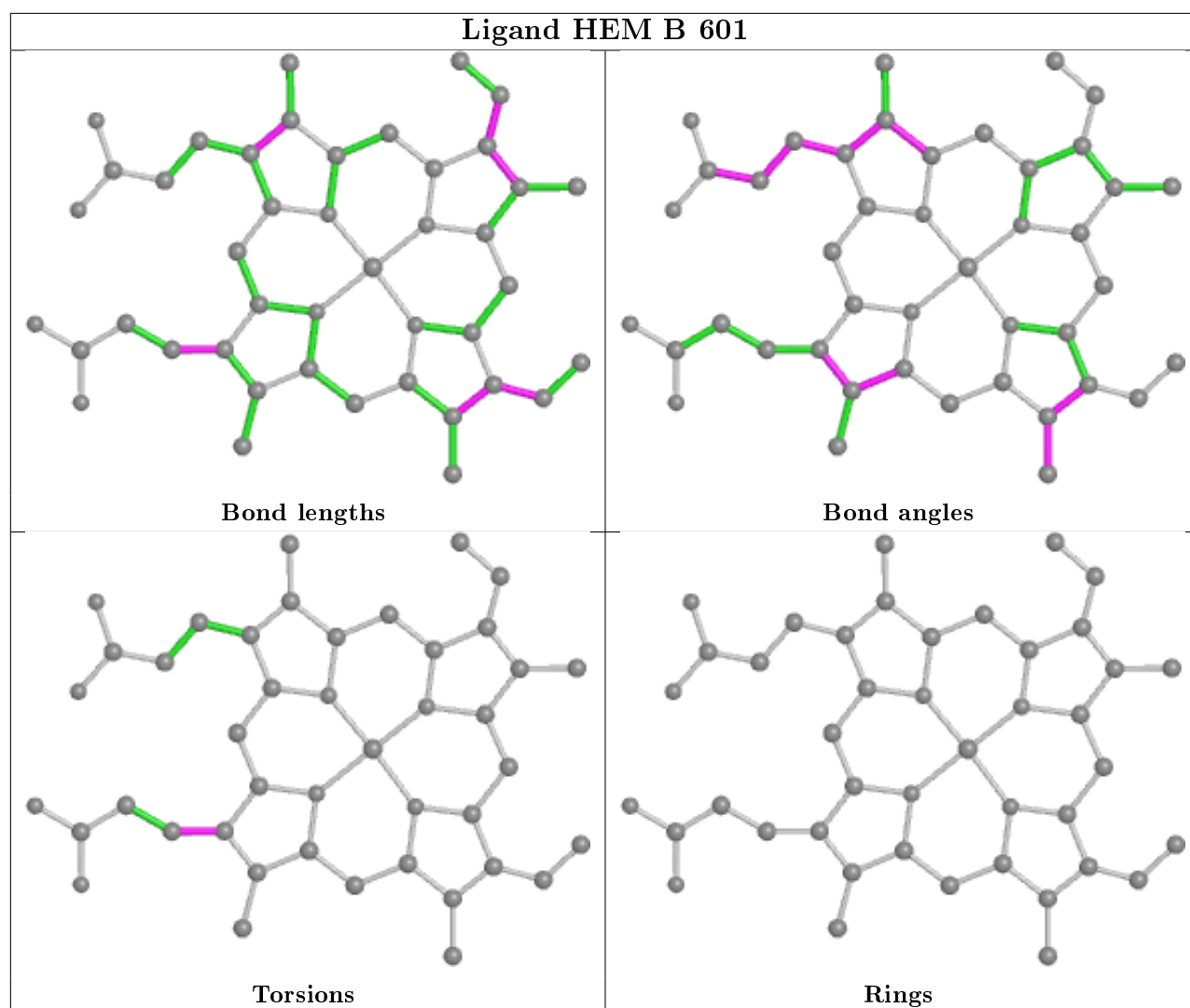


Rings









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, 95th 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 ²)	Q<0.9
1	A	553/553 (100%)	0.31	13 (2%) 59 68	52, 87, 130, 213	0
1	B	553/553 (100%)	0.31	20 (3%) 42 51	54, 86, 129, 195	3 (0%)
All	All	1106/1106 (100%)	0.31	33 (2%) 50 59	52, 86, 130, 213	3 (0%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	GLY	3.6
1	B	69	CYS	3.1
1	B	277	ARG	3.1
1	A	409	PHE	3.0
1	B	291	VAL	3.0

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, 95th 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.

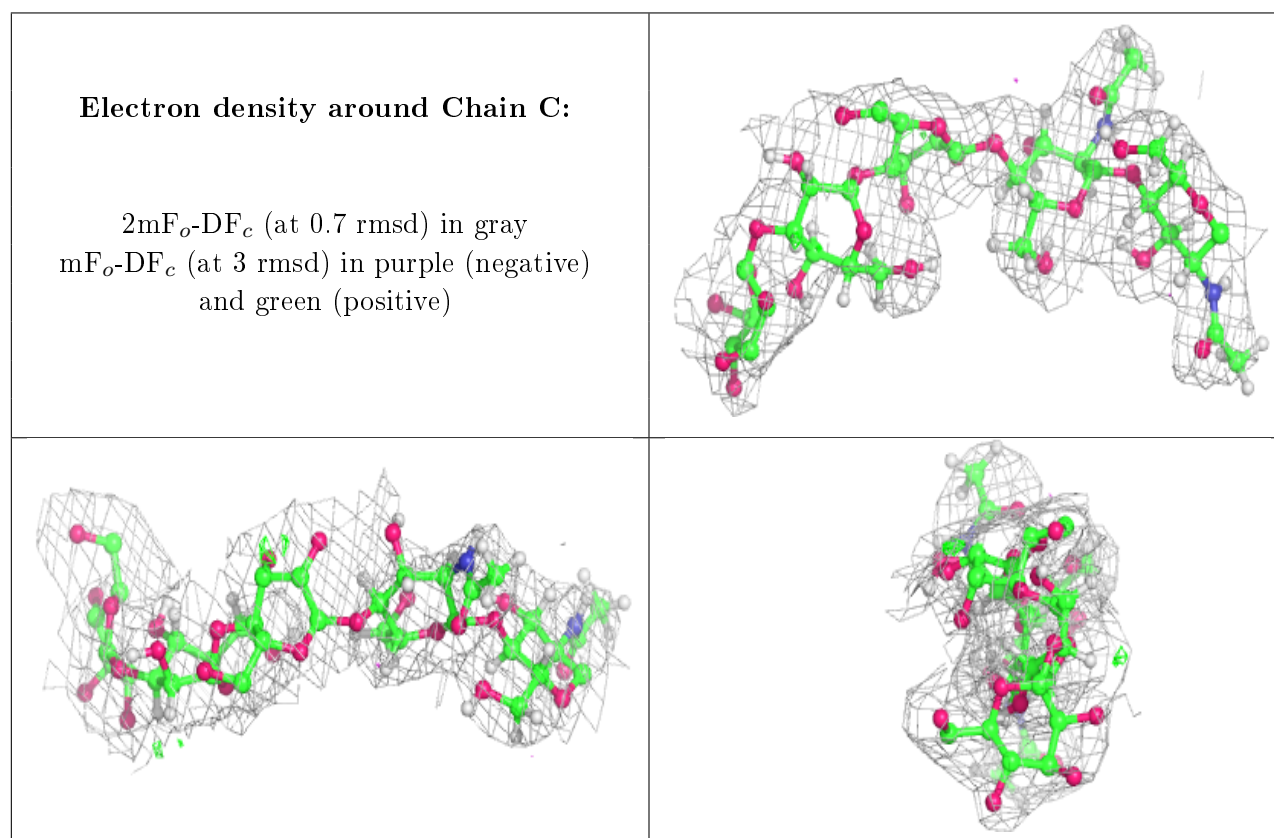
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	C	4	11/12	0.83	0.12	74,88,182,186	9
4	MAN	F	3	11/12	0.88	0.10	78,164,171,176	6
3	NDG	G	2	14/15	0.89	0.24	70,70,181,190	13
2	MAN	C	3	11/12	0.90	0.14	168,175,190,195	0
2	MAN	C	5	11/12	0.91	0.13	100,141,159,165	0

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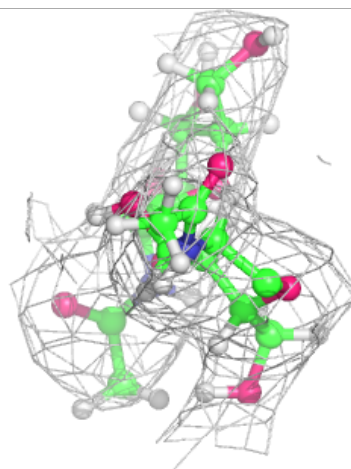
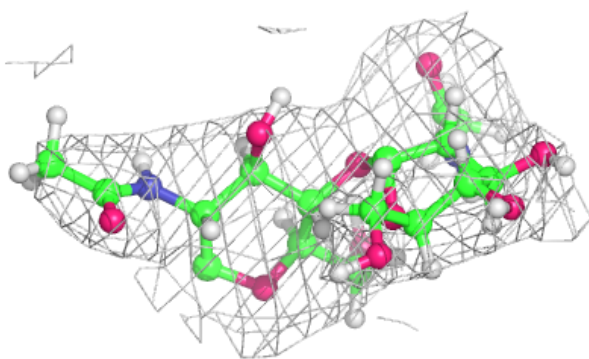
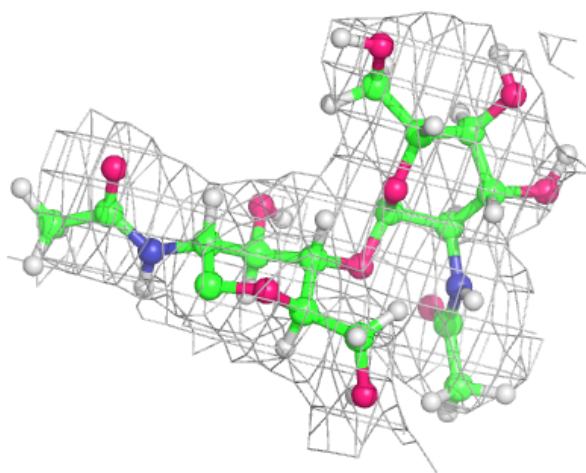
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NDG	E	2	14/15	0.92	0.17	97,97,134,141	13
4	BMA	F	4	11/12	0.92	0.15	72,72,163,167	10
3	NAG	D	1	14/15	0.92	0.15	74,77,135,153	12
3	NAG	G	1	14/15	0.93	0.16	57,106,129,135	12
4	NAG	F	2	14/15	0.93	0.14	75,101,137,158	12
2	NAG	C	2	14/15	0.94	0.15	59,83,131,146	12
3	NDG	D	2	14/15	0.95	0.15	79,79,140,146	13
3	NAG	E	1	14/15	0.96	0.18	75,78,108,120	12
4	NAG	F	1	14/15	0.97	0.15	46,77,96,110	12
2	NAG	C	1	14/15	0.97	0.15	34,53,80,93	12

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.



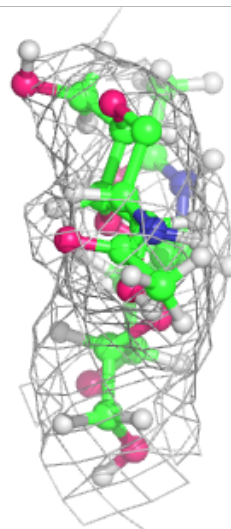
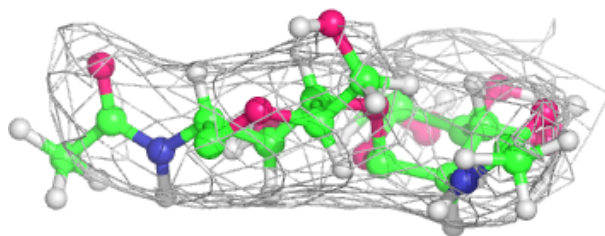
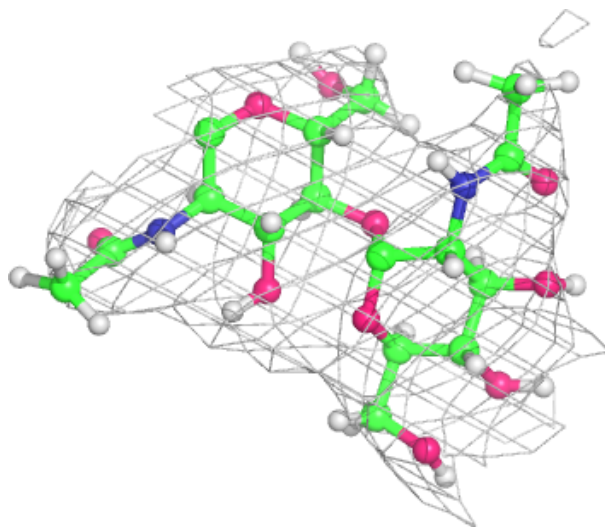
Electron density around Chain D:

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



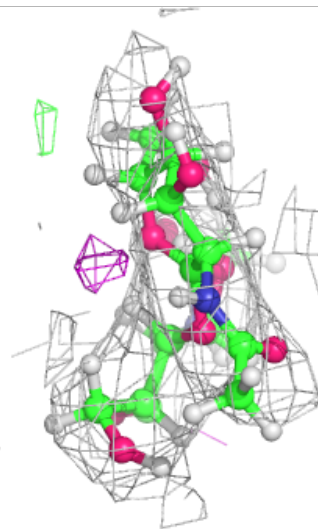
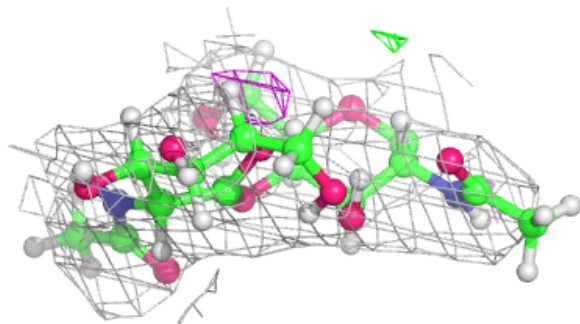
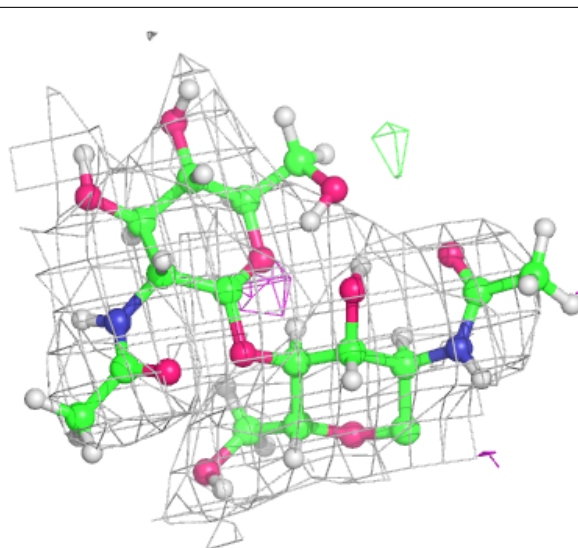
Electron density around Chain E:

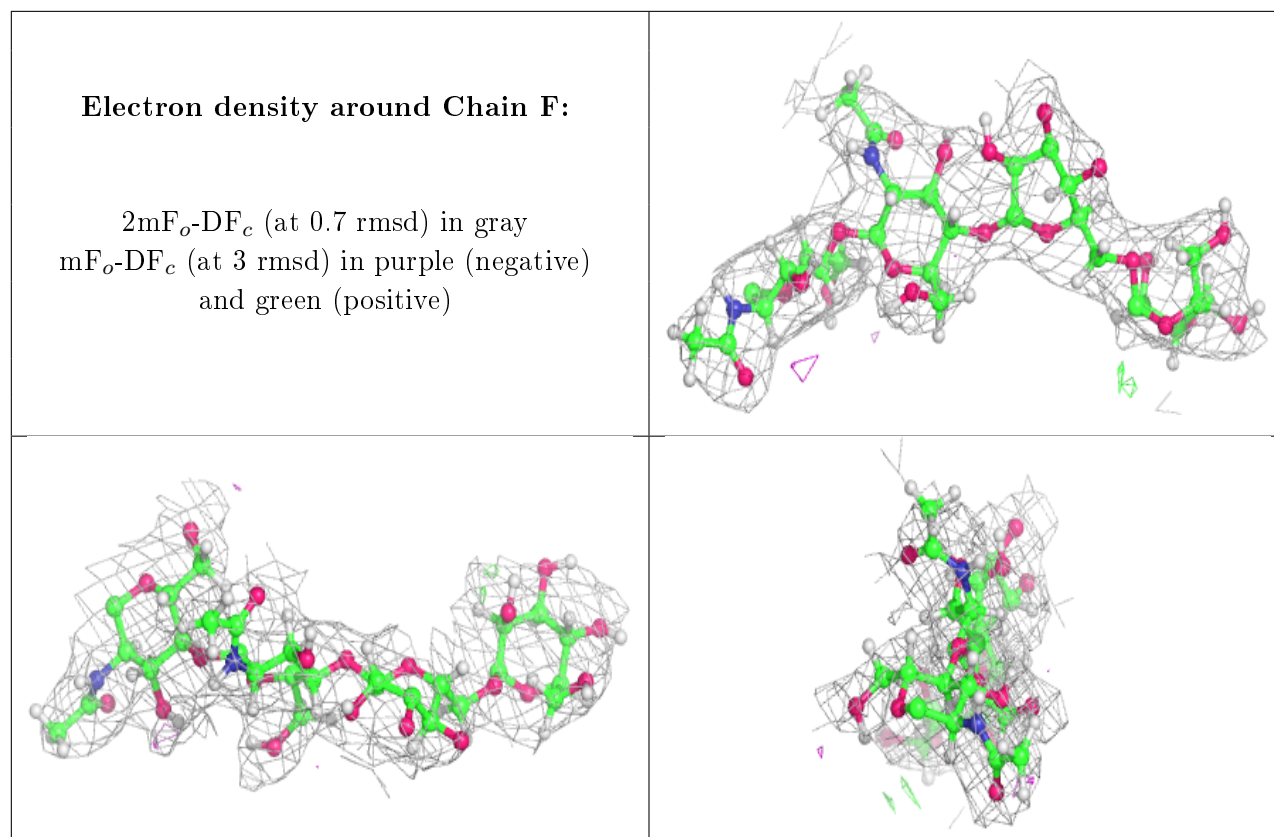
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands [i](#)

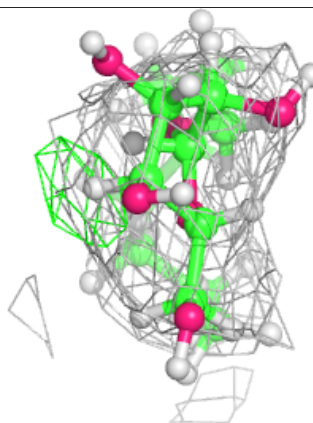
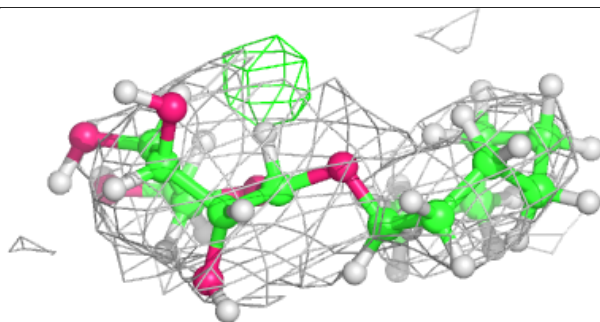
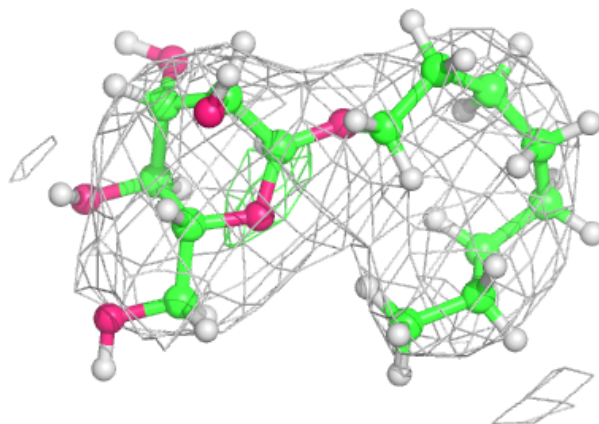
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	FLC	A	900	13/13	0.87	0.18	61,143,174,180	6
7	BOG	B	1752	20/20	0.90	0.17	70,70,156,159	28
7	BOG	A	754	20/20	0.90	0.15	68,80,130,136	28
7	BOG	A	751	20/20	0.92	0.20	67,78,129,150	30
6	CEL	B	1701	26/26	0.95	0.36	22,52,65,66	40
7	BOG	B	1751	20/20	0.96	0.21	37,68,111,134	28
5	HEM	A	601	43/43	0.96	0.18	28,51,126,149	32
5	HEM	B	601	43/43	0.96	0.19	45,78,116,157	30
6	CEL	A	701	26/26	0.97	0.16	49,77,95,121	14

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.

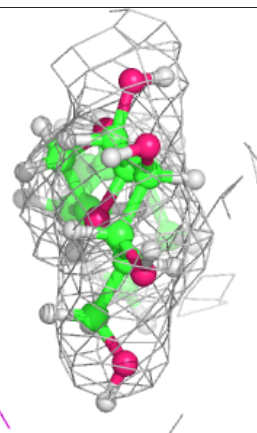
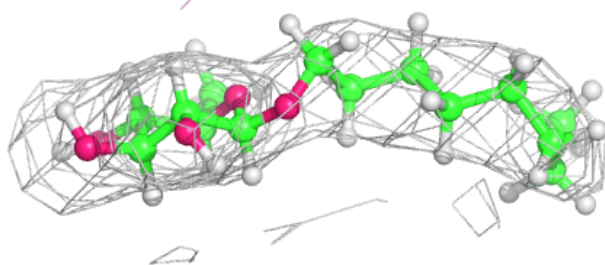
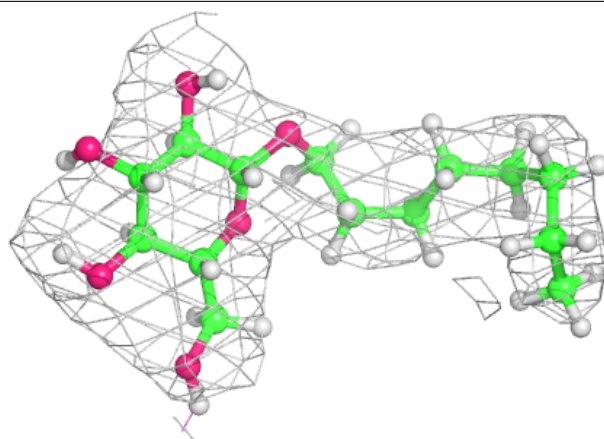
Electron density around BOG B 1752:

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

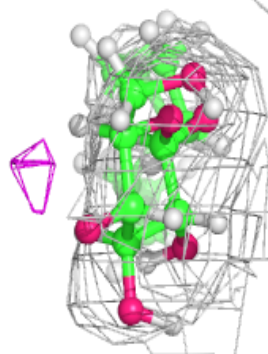
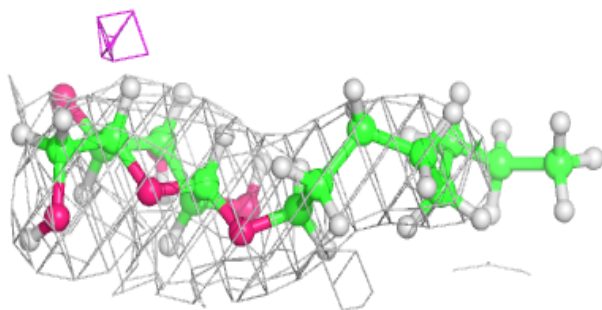
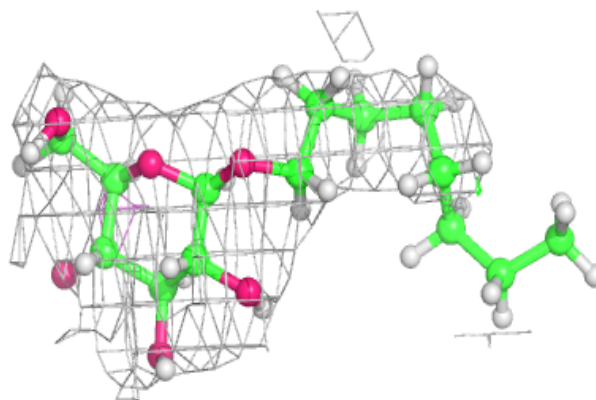


Electron density around BOG A 754:

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and green (positive)

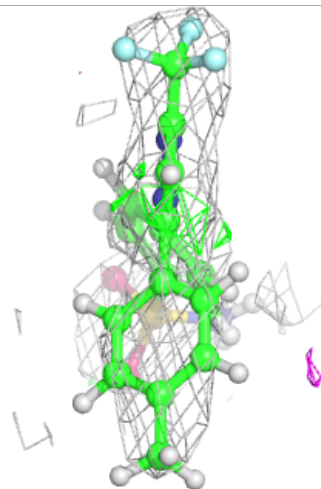
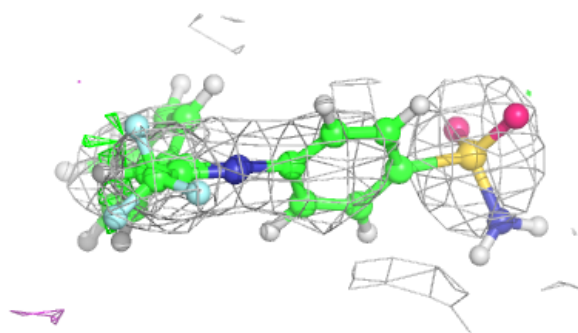
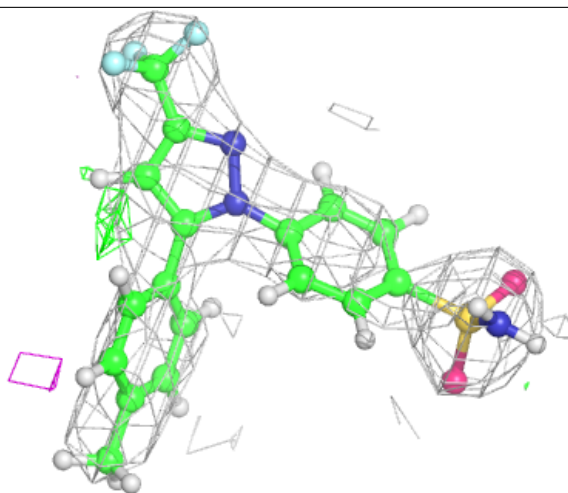
**Electron density around BOG A 751:**

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



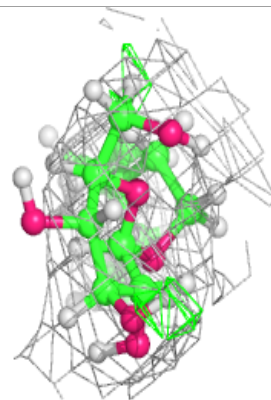
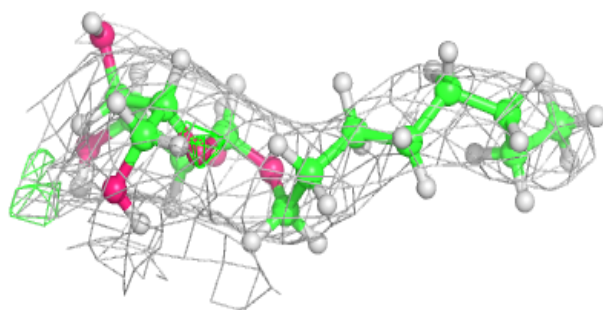
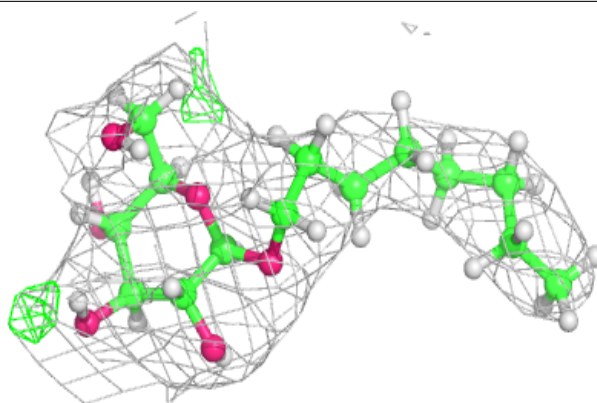
Electron density around CEL B 1701:

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



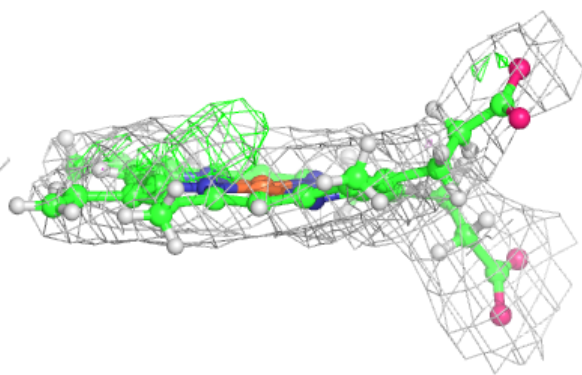
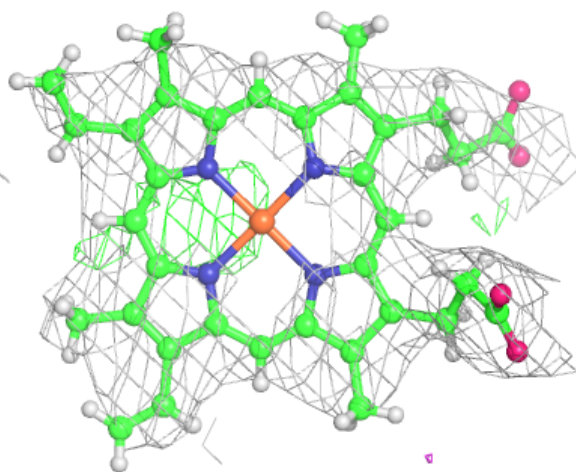
Electron density around BOG B 1751:

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



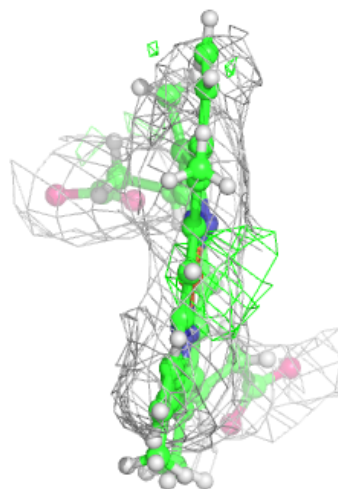
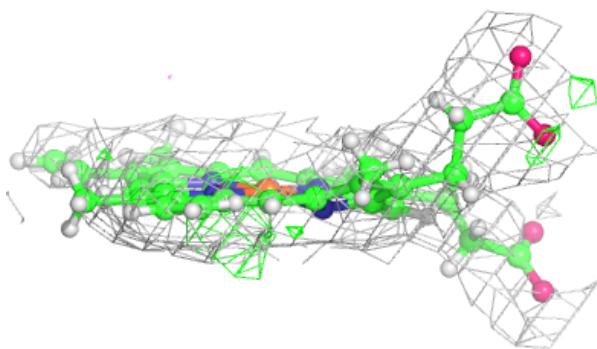
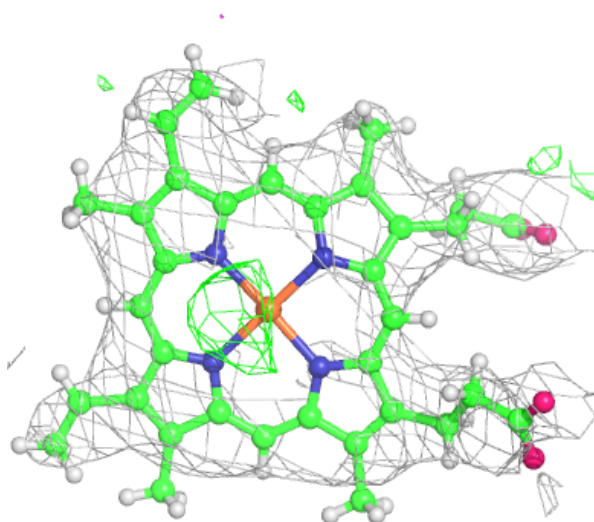
Electron density around HEM A 601:

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



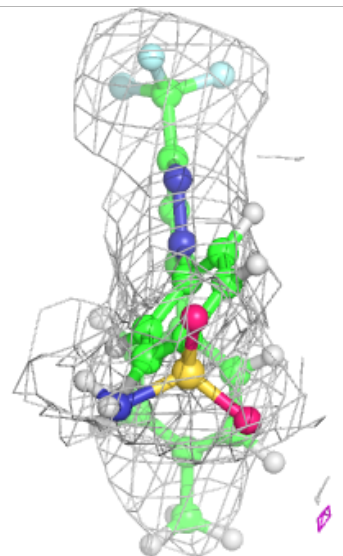
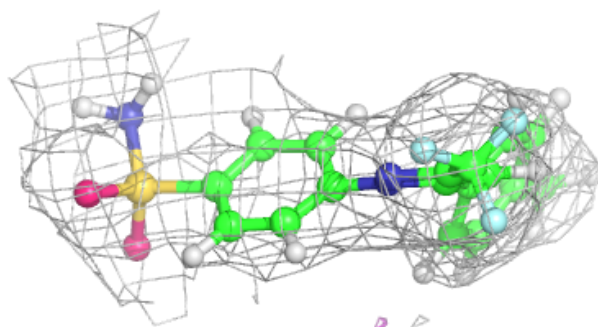
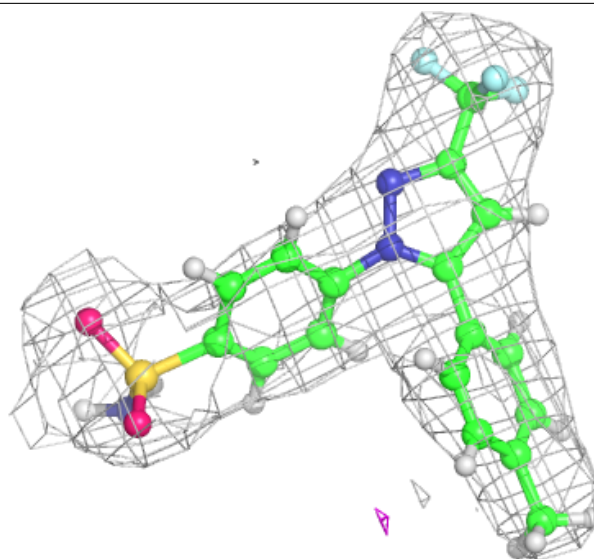
Electron density around HEM B 601:

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



Electron density around CEL A 701:

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 [i](#)

There are no such residues in this entry.