



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 01:36 pm BST

PDB ID : 5FVN  
Title : X-ray crystal structure of Enterobacter cloacae OmpE36 porin  
Authors : Arunmanee, W.; Pathania, M.; Soloyova, A.; Brun, A.; Ridley, H.; Basle, A.;  
van den Berg, B.; Lakey, J.H.  
Deposited on : 2016-02-09  
Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

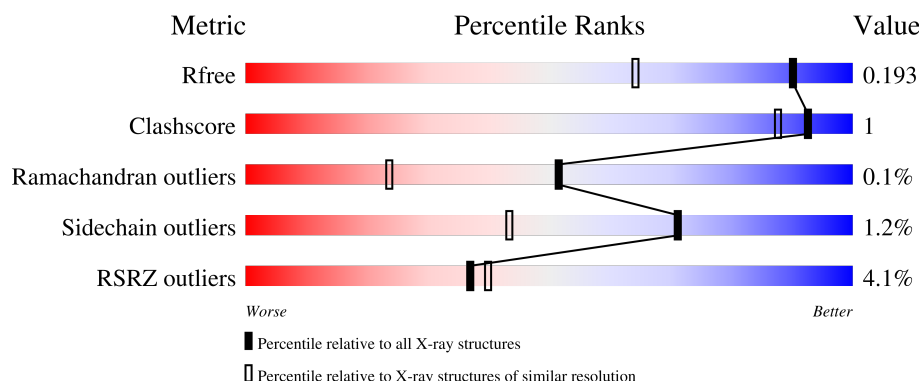
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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.



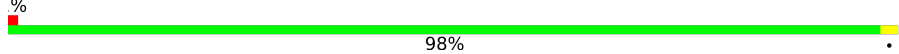
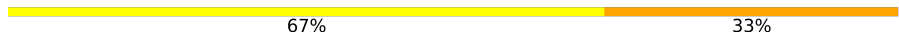
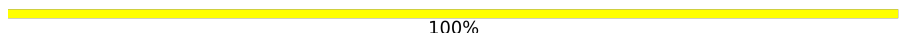

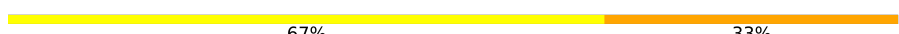
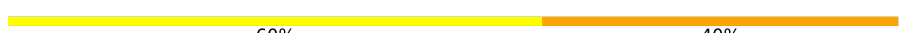




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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  $\leq 5\%$ . 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	342	<div> <div>5%</div> <div>97%</div> <div>.</div> </div>
1	B	342	<div> <div>5%</div> <div>95%</div> <div>5%</div> <div>.</div> </div>
1	C	342	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
1	D	342	<div> <div>6%</div> <div>96%</div> <div>.</div> </div>
1	E	342	<div> <div>4%</div> <div>97%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	342	 98%
2	G	3	 67% 33%
2	K	3	 100%
2	L	3	 67% 33%
2	M	3	 67% 33%
3	H	5	 60% 40%
3	I	5	 40% 60%
3	N	5	 60% 40%
4	J	4	 50% 50%
4	O	4	 50% 50%

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
11	DAO	B	412	-	-	-	X
11	DAO	D	418	-	-	-	X
11	DAO	D	424	-	-	-	X

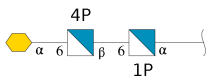


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called OMPC PORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total 2722	C 1704	N 455	O 560	S 3	4	8	0
1	B	342	Total 2700	C 1685	N 451	O 561	S 3	0	4	0
1	C	342	Total 2704	C 1691	N 451	O 559	S 3	0	5	0
1	D	342	Total 2710	C 1693	N 452	O 562	S 3	0	6	0
1	E	342	Total 2708	C 1694	N 451	O 560	S 3	0	6	0
1	F	342	Total 2701	C 1689	N 452	O 557	S 3	0	4	0

- Molecule 2 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.

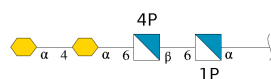


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	3	Total 46	C 20	N 2	O 22	P 2	0	0	0
2	K	3	Total 45	C 20	N 2	O 21	P 2	0	0	0
2	L	3	Total 46	C 20	N 2	O 22	P 2	0	0	0
2	M	3	Total 46	C 20	N 2	O 22	P 2	0	0	0

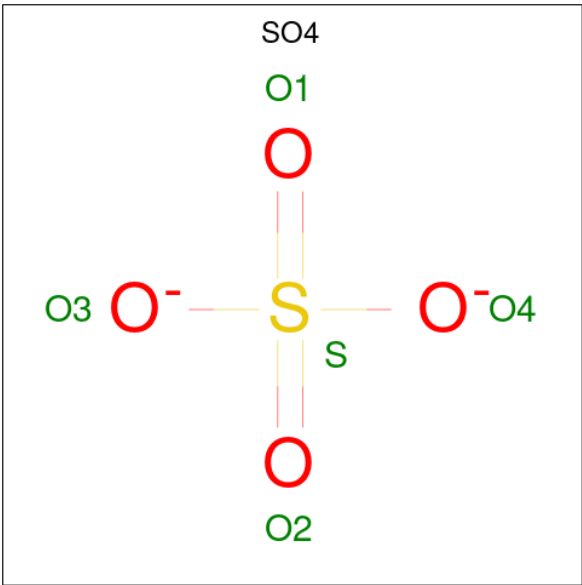
- Molecule 3 is an oligosaccharide called 3-deoxy- $\alpha$ -D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero- $\alpha$ -D-manno-heptopyranose-(1-5)]3-deoxy- $\alpha$ -D-manno-oct-2-ulopyran



- Molecule 4 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.

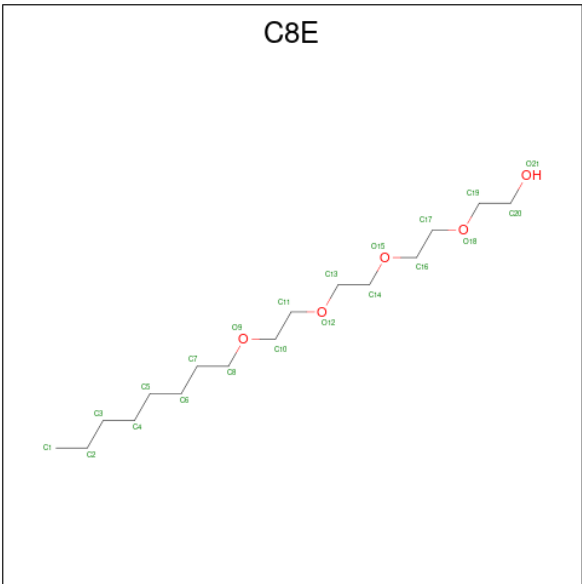


- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 4 4	0	0
6	A	1	Total C 6 6	0	0
6	A	1	Total C 4 4	0	0
6	A	1	Total C 5 5	0	0
6	A	1	Total C O 5 4 1	0	0
6	A	1	Total C O 8 5 3	0	0
6	A	1	Total C 8 8	0	0
6	A	1	Total C 7 7	0	0
6	B	1	Total C O 9 8 1	0	0
6	B	1	Total C 3 3	0	0
6	B	1	Total C O 5 3 2	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C 8 8	0	0
6	C	1	Total C 3 3	0	0
6	C	1	Total C 7 7	0	0
6	C	1	Total C 3 3	0	0
6	C	1	Total C 6 6	0	0
6	C	1	Total C 3 3	0	0
6	C	1	Total C 8 8	0	0
6	C	1	Total C O 11 10 1	0	0
6	C	1	Total C O 11 10 1	0	0

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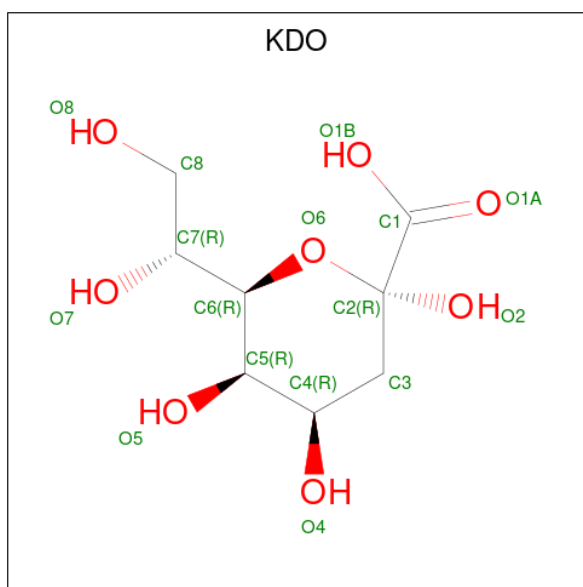
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 10 9 1	0	0
6	C	1	Total C 7 7	0	0
6	D	1	Total C 4 4	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 8 8	0	0
6	D	1	Total C 8 8	0	0
6	D	1	Total C O 11 10 1	0	0
6	D	1	Total C O 4 3 1	0	0
6	D	1	Total C 6 6	0	0
6	E	1	Total C 6 6	0	0
6	F	1	Total C 3 3	0	0
6	F	1	Total C 4 4	0	0
6	F	1	Total C 8 8	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



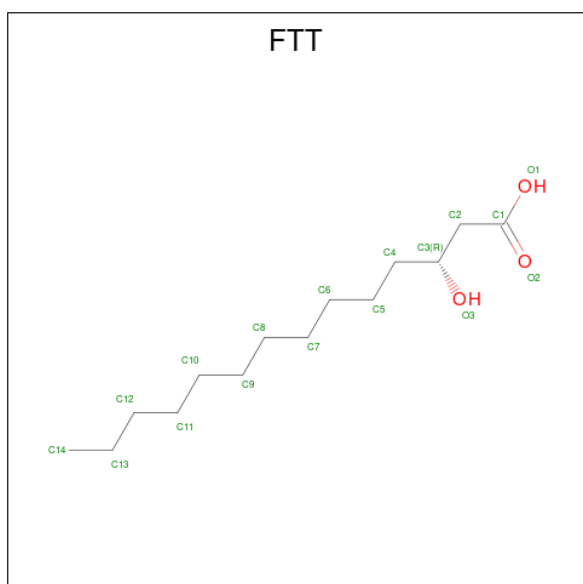
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid (three-letter code: KDO) (formula: C<sub>8</sub>H<sub>14</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			15	8	7		
8	D	1	Total	C	O	0	0
			15	8	7		
8	E	1	Total	C	O	0	0
			15	8	7		

- Molecule 9 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula:  $C_{14}H_{28}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			15	13	2		
9	A	1	Total	C	O	0	0
			13	11	2		
9	A	1	Total	C	O	0	0
			16	14	2		
9	A	1	Total	C	O	0	0
			14	12	2		
9	B	1	Total	C	O	0	0
			14	12	2		
9	B	1	Total	C	O	0	0
			15	13	2		
9	B	1	Total	C	O	0	0
			13	11	2		
9	B	1	Total	C	O	0	0
			16	14	2		
9	C	1	Total	C	O	0	0
			14	12	2		
9	C	1	Total	C	O	0	0
			16	14	2		
9	C	1	Total	C	O	0	0
			11	9	2		
9	C	1	Total	C	O	0	0
			16	14	2		
9	C	1	Total	C	O	0	0
			13	11	2		
9	C	1	Total	C	O	0	0
			16	14	2		
9	C	1	Total	C	O	0	0
			13	11	2		
9	C	1	Total	C	O	0	0
			16	14	2		
9	D	1	Total	C	O	0	0
			14	12	2		
9	D	1	Total	C	O	0	0
			11	9	2		
9	D	1	Total	C	O	0	0
			13	11	2		
9	D	1	Total	C	O	0	0
			11	9	2		
9	D	1	Total	C	O	0	0
			16	14	2		
9	D	1	Total	C	O	0	0
			13	11	2		

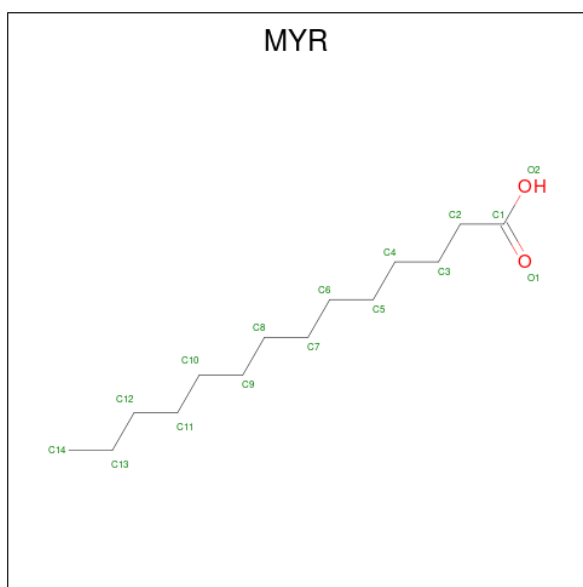
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			16	14	2		
9	D	1	Total	C	O	0	0
			14	12	2		
9	E	1	Total	C	O	0	0
			14	12	2		
9	E	1	Total	C	O	0	0
			14	12	2		
9	E	1	Total	C	O	0	0
			12	10	2		
9	E	1	Total	C	O	0	0
			15	13	2		
9	F	1	Total	C	O	0	0
			14	12	2		
9	F	1	Total	C	O	0	0
			12	10	2		
9	F	1	Total	C	O	0	0
			13	11	2		
9	F	1	Total	C	O	0	0
			12	10	2		
9	F	1	Total	C	O	0	0
			16	14	2		
9	F	1	Total	C	O	0	0
			14	12	2		
9	F	1	Total	C	O	0	0
			11	9	2		
9	F	1	Total	C	O	0	0
			16	14	2		

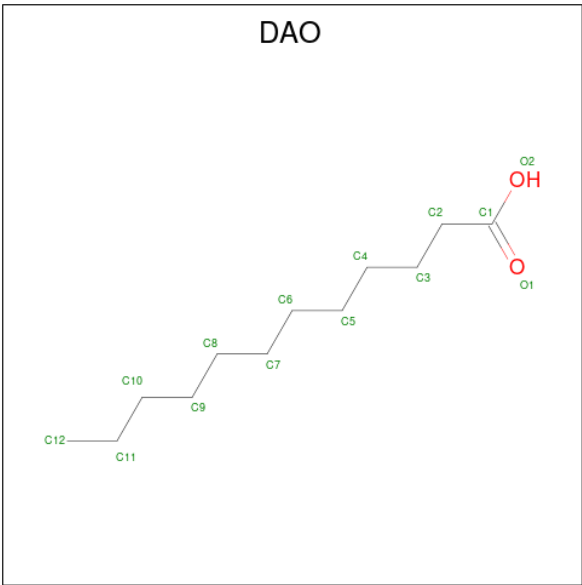
- Molecule 10 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	5	1		
10	B	1	Total	C	O	0	0
			6	5	1		
10	C	1	Total	C	O	0	0
			8	7	1		
10	C	1	Total	C	O	0	0
			9	8	1		
10	D	1	Total	C	O	0	0
			5	4	1		
10	D	1	Total	C	O	0	0
			6	5	1		
10	E	1	Total	C	O	0	0
			6	5	1		
10	F	1	Total	C	O	0	0
			11	10	1		
10	F	1	Total	C	O	0	0
			12	11	1		

- Molecule 11 is LAURIC ACID (three-letter code: DAO) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			5	4	1		
11	A	1	Total	C	O	0	0
			8	7	1		
11	B	1	Total	C	O	0	0
			5	4	1		
11	C	1	Total	C	O	0	0
			5	4	1		
11	C	1	Total	C	O	0	0
			13	12	1		
11	C	1	Total	C	O	0	0
			10	9	1		
11	C	1	Total	C	O	0	0
			8	7	1		
11	D	1	Total	C	O	0	0
			6	5	1		
11	D	1	Total	C	O	0	0
			3	2	1		
11	D	1	Total	C	O	0	0
			5	4	1		
11	E	1	Total	C	O	0	0
			5	4	1		
11	E	1	Total	C	O	0	0
			5	4	1		
11	F	1	Total	C	O	0	0
			5	4	1		
11	F	1	Total	C	O	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	F	1	Total	C	O	0	0
			8	7	1		

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	Ca	0	0
			1	1		
12	F	1	Total	Ca	0	0
			1	1		

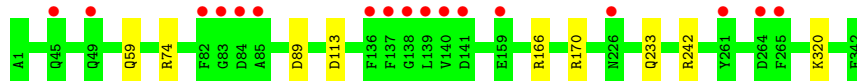
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	321	Total	O	0	0
			321	321		
13	B	316	Total	O	0	0
			316	316		
13	C	324	Total	O	0	0
			324	324		
13	D	296	Total	O	0	0
			296	296		
13	E	303	Total	O	0	0
			303	303		
13	F	350	Total	O	0	0
			350	350		

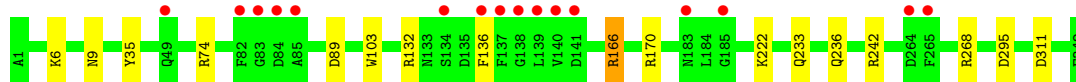
### 3 Residue-property plots [i](#)

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.

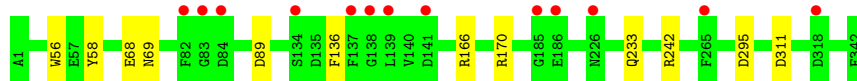
- Molecule 1: OMPC PORIN



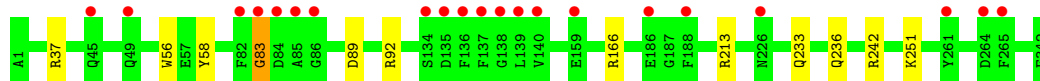
- Molecule 1: OMPC PORIN



- Molecule 1: OMPC PORIN



- Molecule 1: OMPC PORIN



- Molecule 1: OMPC PORIN



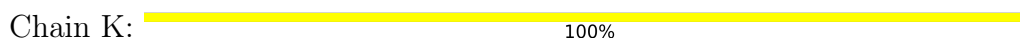
- Molecule 1: OMPC PORIN



- Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose



- Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose



- Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose



- Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose



- Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose



- Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain I:  40% 60%

GP11  
Z9M2  
KD03  
KD04  
GMH5

- Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain N:  60% 40%

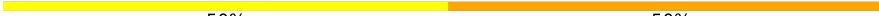
GP11  
Z9M2  
KD03  
KD04  
GMH5

- Molecule 4: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain J:  50% 50%

GP11  
Z9M2  
KD03  
KD04

- Molecule 4: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain O:  50% 50%

GP11  
Z9M2  
KD03  
KD04

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.75Å 123.26Å 116.01Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	115.99 – 1.45 48.60 – 1.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (115.99-1.45) 99.9 (48.60-1.45)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.155 , 0.183 0.167 , 0.193	Depositor DCC
$R_{free}$ test set	13912 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	19668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.10% 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: PO4, C8E, GP1, CA, GMH, FTT, DAO, KDO, MYR, SO4, Z9M

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	0.54	0/2799	0.83	4/3785 (0.1%)
1	B	0.52	0/2768	0.82	8/3743 (0.2%)
1	C	0.51	0/2775	0.81	4/3753 (0.1%)
1	D	0.52	0/2784	0.86	5/3765 (0.1%)
1	E	0.53	0/2782	0.82	4/3763 (0.1%)
1	F	0.49	0/2769	0.77	4/3745 (0.1%)
All	All	0.52	0/16677	0.82	29/22554 (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	D	1	1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	ARG	NE-CZ-NH1	-14.26	113.17	120.30
1	D	242	ARG	NE-CZ-NH2	10.48	125.54	120.30
1	A	242	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	F	242	ARG	NE-CZ-NH2	9.71	125.15	120.30
1	C	242	ARG	NE-CZ-NH2	9.45	125.03	120.30
1	A	242	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	E	242	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	B	242	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	170	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	F	242	ARG	NE-CZ-NH1	-7.45	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	242	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	C	242	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	B	132	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	74	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	F	170	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	E	132	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	B	268	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	170	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	213	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	242	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	74	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	170	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	170	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	92	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	F	170	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	170	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	37	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	E	213	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	B	166	ARG	NE-CZ-NH2	-5.07	117.77	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	84	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	83	GLY	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	2722	0	2520	2	0
1	B	2700	0	2475	8	0
1	C	2704	0	2491	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2710	0	2492	4	0
1	E	2708	0	2498	3	0
1	F	2701	0	2488	2	0
2	G	46	0	17	2	0
2	K	45	0	15	0	0
2	L	46	0	17	2	0
2	M	46	0	17	3	0
3	H	74	0	40	1	0
3	I	74	0	38	4	0
3	N	74	0	37	1	0
4	J	61	0	28	2	0
4	O	61	0	29	2	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
6	A	50	0	76	3	0
6	B	33	0	56	2	0
6	C	69	0	122	4	0
6	D	59	0	102	1	0
6	E	6	0	11	0	0
6	F	15	0	27	2	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
7	F	5	0	0	0	0
8	A	15	0	12	2	0
8	D	15	0	12	2	0
8	E	15	0	12	3	0
9	A	58	0	84	0	0
9	B	58	0	85	0	0
9	C	115	0	172	0	0
9	D	108	0	154	0	0
9	E	55	0	75	0	0
9	F	108	0	153	2	0
10	A	6	0	6	0	0
10	B	6	0	6	0	0
10	C	17	0	22	0	0
10	D	11	0	10	0	0
10	E	6	0	6	0	0
10	F	23	0	34	0	0
11	A	13	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	5	0	4	0	0
11	C	36	0	51	0	0
11	D	14	0	10	0	0
11	E	10	0	8	0	0
11	F	18	0	18	0	0
12	C	1	0	0	0	0
12	F	1	0	0	0	0
13	A	321	0	0	1	0
13	B	316	0	0	5	0
13	C	324	0	0	1	0
13	D	296	0	0	4	0
13	E	303	0	0	0	0
13	F	350	0	0	0	0
All	All	19668	0	16544	46	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 1.

All (46) 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)
8:E:403:KDO:C2	2:M:3:KDO:O4	1.81	1.29
8:D:413:KDO:C2	2:L:3:KDO:O4	1.84	1.24
8:A:412:KDO:C2	2:G:3:KDO:O4	1.85	1.24
6:A:408:C8E:H112	13:A:755:HOH:O	1.73	0.88
1:D:251:LYS:HG3	13:D:719:HOH:O	1.73	0.86
3:I:3:KDO:HO4	3:I:4:KDO:C2	1.90	0.81
6:F:401:C8E:H11	9:F:407:FTT:C10	2.11	0.80
1:D:236:GLN:HG3	13:D:719:HOH:O	1.87	0.74
1:C:69:ASN:H	6:C:405:C8E:H13	1.55	0.72
4:O:3:KDO:HO4	4:O:4:KDO:C2	2.09	0.65
3:N:3:KDO:C4	3:N:4:KDO:C2	2.75	0.62
1:D:236:GLN:CG	13:D:719:HOH:O	2.45	0.60
4:J:3:KDO:C4	4:J:4:KDO:C2	2.76	0.59
8:E:403:KDO:C2	2:M:3:KDO:C4	2.79	0.58
6:D:409:C8E:H81	13:D:587:HOH:O	2.04	0.58
3:I:3:KDO:C4	3:I:4:KDO:C2	2.79	0.57
1:B:236:GLN:HG3	13:B:727:HOH:O	2.06	0.56
1:B:236:GLN:CG	13:B:727:HOH:O	2.53	0.56
1:C:68:GLU:HB2	6:C:405:C8E:C1	2.37	0.55
1:C:68:GLU:HA	6:C:405:C8E:H22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:3:KDO:C4	3:H:4:KDO:C2	2.83	0.54
8:D:413:KDO:C2	2:L:3:KDO:C4	2.86	0.52
1:A:59:GLN:HE22	6:A:408:C8E:H132	1.76	0.51
4:O:3:KDO:C4	4:O:4:KDO:C2	2.82	0.51
6:B:403:C8E:H101	13:B:737:HOH:O	2.11	0.51
3:I:3:KDO:O4	3:I:4:KDO:C1	2.55	0.49
1:C:68:GLU:HB2	6:C:405:C8E:H11	1.94	0.48
1:B:103:TRP:CE2	1:B:222:LYS:HE2	2.48	0.48
1:E:137:PHE:HB2	1:E:139:LEU:HD13	1.97	0.47
3:I:3:KDO:H5	3:I:5:GMH:O2	2.16	0.45
1:B:35:TYR:CD1	6:B:403:C8E:H102	2.53	0.44
1:B:236:GLN:HG2	13:B:727:HOH:O	2.17	0.43
1:B:9:ASN:HB3	13:C:610:HOH:O	2.18	0.43
8:A:412:KDO:C2	2:G:3:KDO:C4	2.89	0.43
6:F:403:C8E:H13	9:F:406:FTT:H22	2.01	0.43
1:E:103:TRP:CE2	1:E:222:LYS:HE2	2.54	0.43
1:B:295:ASP:OD1	1:B:311:ASP:OD1	2.37	0.42
4:J:3:KDO:O4	4:J:4:KDO:C1	2.55	0.42
8:E:403:KDO:C3	2:M:3:KDO:O4	2.63	0.42
1:D:56:TRP:CZ2	1:D:58:TYR:HB2	2.55	0.42
1:F:56:TRP:CZ2	1:F:58:TYR:HB2	2.56	0.41
1:B:6:LYS:HE2	13:B:660:HOH:O	2.20	0.41
1:C:56:TRP:CZ2	1:C:58:TYR:HB2	2.55	0.41
1:A:113:ASP:OD2	6:A:407:C8E:H102	2.21	0.41
1:C:295:ASP:OD1	1:C:311:ASP:OD1	2.40	0.40
1:E:56:TRP:CD1	1:F:36:MET:HG2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	348/342 (102%)	332 (95%)	16 (5%)	0	100	100
1	B	344/342 (101%)	329 (96%)	14 (4%)	1 (0%)	41	18
1	C	345/342 (101%)	330 (96%)	14 (4%)	1 (0%)	41	18
1	D	346/342 (101%)	329 (95%)	16 (5%)	1 (0%)	41	18
1	E	346/342 (101%)	330 (95%)	16 (5%)	0	100	100
1	F	344/342 (101%)	332 (96%)	12 (4%)	0	100	100
All	All	2073/2052 (101%)	1982 (96%)	88 (4%)	3 (0%)	51	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	PHE
1	C	136	PHE
1	D	83	GLY

### 5.3.2 Protein sidechains ⓘ

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	283/275 (103%)	279 (99%)	4 (1%)	67	37
1	B	279/275 (102%)	276 (99%)	3 (1%)	73	48
1	C	280/275 (102%)	277 (99%)	3 (1%)	73	48
1	D	281/275 (102%)	278 (99%)	3 (1%)	73	48
1	E	281/275 (102%)	278 (99%)	3 (1%)	73	48
1	F	279/275 (102%)	276 (99%)	3 (1%)	73	48
All	All	1683/1650 (102%)	1664 (99%)	19 (1%)	71	48

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	166	ARG

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	320	LYS
1	B	89	ASP
1	B	166	ARG
1	B	233	GLN
1	C	89	ASP
1	C	166	ARG
1	C	233	GLN
1	D	89	ASP
1	D	166	ARG
1	D	233	GLN
1	E	89	ASP
1	E	166	ARG
1	E	233	GLN
1	F	89	ASP
1	F	166	ARG
1	F	233	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

35 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	GP1	G	1	9,2	15,16,16	1.51	1 (6%)	23,24,24	1.03	1 (4%)
2	Z9M	G	2	9,2	15,15,16	1.34	1 (6%)	18,22,24	1.09	0
2	KDO	G	3	2	12,15,16	0.55	0	16,21,24	1.48	4 (25%)
3	GP1	H	1	9,3	15,16,16	1.52	1 (6%)	23,24,24	1.50	3 (13%)
3	Z9M	H	2	9,3	15,15,16	1.14	1 (6%)	18,22,24	0.91	0
3	KDO	H	3	3	12,15,16	1.06	1 (8%)	16,21,24	1.42	4 (25%)
3	KDO	H	4	3	12,15,16	0.34	0	16,21,24	1.44	2 (12%)
3	GMH	H	5	3	13,13,14	0.63	0	17,18,20	1.23	2 (11%)
3	GP1	I	1	9,3	15,16,16	1.66	1 (6%)	23,24,24	1.07	2 (8%)
3	Z9M	I	2	9,3	15,15,16	1.53	1 (6%)	18,22,24	1.15	1 (5%)
3	KDO	I	3	3	12,15,16	1.14	1 (8%)	16,21,24	1.62	5 (31%)
3	KDO	I	4	3,12	12,15,16	0.34	0	16,21,24	1.45	2 (12%)
3	GMH	I	5	3	13,13,14	0.99	1 (7%)	17,18,20	1.52	4 (23%)
4	GP1	J	1	9,4	15,16,16	1.40	1 (6%)	23,24,24	1.30	3 (13%)
4	Z9M	J	2	9,4	15,15,16	1.24	1 (6%)	18,22,24	0.70	0
4	KDO	J	3	4	12,15,16	0.58	0	16,21,24	1.35	2 (12%)
4	KDO	J	4	4	12,15,16	0.67	0	16,21,24	1.65	4 (25%)
2	GP1	K	1	9,2	15,16,16	1.47	1 (6%)	23,24,24	1.67	5 (21%)
2	Z9M	K	2	9,2	15,15,16	1.36	1 (6%)	18,22,24	1.00	1 (5%)
2	KDO	K	3	2	11,14,16	0.60	0	13,19,24	2.21	1 (7%)
2	GP1	L	1	9,2	15,16,16	1.41	1 (6%)	23,24,24	0.94	1 (4%)
2	Z9M	L	2	9,2	15,15,16	1.29	1 (6%)	18,22,24	0.90	0
2	KDO	L	3	2	12,15,16	0.38	0	16,21,24	1.50	4 (25%)
2	GP1	M	1	9,2	15,16,16	1.53	1 (6%)	23,24,24	0.94	1 (4%)
2	Z9M	M	2	9,2	15,15,16	1.46	1 (6%)	18,22,24	0.81	0
2	KDO	M	3	2	12,15,16	0.37	0	16,21,24	1.38	3 (18%)
3	GP1	N	1	9,3	15,16,16	1.78	1 (6%)	23,24,24	0.93	1 (4%)
3	Z9M	N	2	9,3	15,15,16	1.52	1 (6%)	18,22,24	1.05	1 (5%)
3	KDO	N	3	3	12,15,16	1.00	1 (8%)	16,21,24	1.61	4 (25%)
3	KDO	N	4	3,12	12,15,16	0.36	0	16,21,24	1.31	1 (6%)
3	GMH	N	5	3	13,13,14	0.73	0	17,18,20	1.64	3 (17%)
4	GP1	O	1	9,4	15,16,16	1.45	1 (6%)	23,24,24	1.39	2 (8%)
4	Z9M	O	2	9,4	15,15,16	1.31	1 (6%)	18,22,24	0.68	0
4	KDO	O	3	4	12,15,16	0.50	0	16,21,24	1.33	2 (12%)
4	KDO	O	4	4	12,15,16	0.34	0	16,21,24	1.42	2 (12%)

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	GP1	G	1	9,2	-	2/6/27/27	0/1/1/1
2	Z9M	G	2	9,2	-	0/7/24/27	0/1/1/1
2	KDO	G	3	2	-	0/6/26/30	0/1/1/1
3	GP1	H	1	9,3	-	1/6/27/27	0/1/1/1
3	Z9M	H	2	9,3	-	0/7/24/27	0/1/1/1
3	KDO	H	3	3	-	0/6/26/30	0/1/1/1
3	KDO	H	4	3	-	0/6/26/30	0/1/1/1
3	GMH	H	5	3	-	0/6/23/26	0/1/1/1
3	GP1	I	1	9,3	-	0/6/27/27	0/1/1/1
3	Z9M	I	2	9,3	-	2/7/24/27	0/1/1/1
3	KDO	I	3	3	-	0/6/26/30	0/1/1/1
3	KDO	I	4	3,12	-	1/6/26/30	0/1/1/1
3	GMH	I	5	3	-	4/6/23/26	0/1/1/1
4	GP1	J	1	9,4	-	1/6/27/27	0/1/1/1
4	Z9M	J	2	9,4	-	0/7/24/27	0/1/1/1
4	KDO	J	3	4	-	0/6/26/30	0/1/1/1
4	KDO	J	4	4	-	0/6/26/30	0/1/1/1
2	GP1	K	1	9,2	-	0/6/27/27	0/1/1/1
2	Z9M	K	2	9,2	-	0/7/24/27	0/1/1/1
2	KDO	K	3	2	-	2/6/22/30	0/1/1/1
2	GP1	L	1	9,2	-	1/6/27/27	0/1/1/1
2	Z9M	L	2	9,2	-	0/7/24/27	0/1/1/1
2	KDO	L	3	2	-	0/6/26/30	0/1/1/1
2	GP1	M	1	9,2	-	1/6/27/27	0/1/1/1
2	Z9M	M	2	9,2	-	0/7/24/27	0/1/1/1
2	KDO	M	3	2	-	0/6/26/30	0/1/1/1
3	GP1	N	1	9,3	-	0/6/27/27	0/1/1/1
3	Z9M	N	2	9,3	-	0/7/24/27	0/1/1/1
3	KDO	N	3	3	-	0/6/26/30	0/1/1/1
3	KDO	N	4	3,12	-	2/6/26/30	0/1/1/1
3	GMH	N	5	3	-	3/6/23/26	0/1/1/1
4	GP1	O	1	9,4	-	1/6/27/27	0/1/1/1
4	Z9M	O	2	9,4	-	0/7/24/27	0/1/1/1
4	KDO	O	3	4	-	0/6/26/30	0/1/1/1
4	KDO	O	4	4	-	0/6/26/30	0/1/1/1

All (22) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	GP1	P4B-O1	6.46	1.71	1.59
3	I	1	GP1	P4B-O1	-5.77	1.48	1.59
3	H	1	GP1	P4B-O1	-5.54	1.48	1.59
3	N	2	Z9M	P1-O4	-5.48	1.49	1.59
2	G	1	GP1	P4B-O1	-5.42	1.49	1.59
2	M	1	GP1	P4B-O1	-5.39	1.49	1.59
3	I	2	Z9M	P1-O4	-5.38	1.49	1.59
2	M	2	Z9M	P1-O4	-5.30	1.49	1.59
2	K	1	GP1	P4B-O1	-5.26	1.49	1.59
4	O	1	GP1	P4B-O1	-5.23	1.49	1.59
4	J	1	GP1	P4B-O1	-5.08	1.49	1.59
2	K	2	Z9M	P1-O4	-5.07	1.49	1.59
2	L	1	GP1	P4B-O1	-5.03	1.49	1.59
2	G	2	Z9M	P1-O4	-4.81	1.50	1.59
4	O	2	Z9M	P1-O4	-4.68	1.50	1.59
2	L	2	Z9M	P1-O4	-4.44	1.50	1.59
4	J	2	Z9M	P1-O4	-4.29	1.51	1.59
3	H	2	Z9M	P1-O4	-3.89	1.52	1.59
3	I	3	KDO	O5-C5	-3.84	1.33	1.43
3	H	3	KDO	O5-C5	-3.53	1.34	1.43
3	N	3	KDO	O5-C5	-3.13	1.35	1.43
3	I	5	GMH	O5-C5	2.22	1.45	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	KDO	O6-C6-C5	7.59	117.80	109.94
2	K	1	GP1	O1-P4B-O8B	-5.39	88.58	109.39
3	H	1	GP1	O1-P4B-O8B	4.91	128.34	109.39
3	N	5	GMH	C1-O5-C5	4.77	119.30	111.48
4	O	1	GP1	O1-C1-C2	4.54	116.62	108.40
3	H	4	KDO	O6-C2-C3	3.82	116.58	109.87
3	I	4	KDO	O6-C2-C3	3.82	116.57	109.87
4	O	4	KDO	O6-C2-C3	3.81	116.56	109.87
3	I	5	GMH	O5-C1-C2	-3.58	105.25	110.77
3	H	4	KDO	C6-O6-C2	3.50	118.83	111.34
3	H	5	GMH	C1-O5-C5	3.47	117.17	111.48
3	N	2	Z9M	C1-O5-C5	3.45	116.87	112.19
4	J	1	GP1	O1-C1-C2	3.37	114.50	108.40
4	J	4	KDO	O4-C4-C3	-3.22	101.96	109.94
2	K	1	GP1	O9B-P4B-O1	3.13	120.00	105.99
4	J	4	KDO	O6-C2-C3	3.11	115.32	109.87
4	J	4	KDO	C6-O6-C2	3.09	117.94	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	KDO	C6-O6-C2	3.09	117.94	111.34
4	J	3	KDO	C4-C5-C6	-3.08	104.22	110.41
4	O	4	KDO	C6-O6-C2	3.05	117.87	111.34
2	G	3	KDO	C4-C5-C6	-3.02	104.35	110.41
3	I	3	KDO	O5-C5-C4	-3.00	104.25	109.99
4	J	1	GP1	O9B-P4B-O1	2.92	119.06	105.99
3	I	3	KDO	C3-C4-C5	2.89	114.88	110.69
3	H	1	GP1	O9B-P4B-O1	-2.88	93.07	105.99
2	K	1	GP1	O1-C1-C2	2.87	113.60	108.40
3	I	2	Z9M	C1-O5-C5	2.83	116.03	112.19
4	O	3	KDO	C6-O6-C2	2.81	117.36	111.34
4	O	3	KDO	C4-C5-C6	-2.79	104.81	110.41
2	L	3	KDO	C4-C5-C6	-2.74	104.91	110.41
3	I	3	KDO	C4-C5-C6	-2.73	104.91	110.41
3	N	4	KDO	O6-C2-C3	2.72	114.65	109.87
3	N	1	GP1	O3-C3-C2	-2.71	105.34	110.22
2	M	3	KDO	C6-O6-C2	2.70	117.12	111.34
3	H	3	KDO	C4-C5-C6	-2.69	104.99	110.41
2	K	2	Z9M	C1-O5-C5	2.67	115.81	112.19
3	H	5	GMH	C1-C2-C3	2.66	112.94	109.67
3	N	3	KDO	C4-C5-C6	-2.65	105.09	110.41
2	L	1	GP1	O1-C1-C2	2.55	113.02	108.40
2	M	1	GP1	O1-C1-C2	2.49	112.91	108.40
2	M	3	KDO	C4-C5-C6	-2.49	105.41	110.41
4	J	3	KDO	C6-O6-C2	2.44	116.56	111.34
3	I	5	GMH	O2-C2-C1	2.42	114.10	109.15
3	I	1	GP1	O1-C1-C2	2.42	112.78	108.40
3	I	5	GMH	C1-O5-C5	2.38	115.37	111.48
2	K	1	GP1	O7B-P4B-O1	2.36	116.57	105.99
4	J	1	GP1	O3-C3-C4	-2.36	104.89	110.35
3	H	3	KDO	C6-O6-C2	2.34	116.34	111.34
2	M	3	KDO	C3-C4-C5	2.33	114.07	110.69
3	N	3	KDO	O5-C5-C4	-2.32	105.56	109.99
3	N	3	KDO	C3-C4-C5	2.26	113.97	110.69
3	I	1	GP1	O7B-P4B-O1	2.25	116.09	105.99
2	G	3	KDO	C3-C2-C1	-2.22	107.07	111.93
3	H	3	KDO	C3-C2-C1	-2.22	107.07	111.93
3	I	5	GMH	C1-C2-C3	-2.22	106.93	109.67
4	J	4	KDO	O4-C4-C5	2.21	114.56	110.14
3	N	5	GMH	O5-C1-C2	2.18	114.13	110.77
2	L	3	KDO	O4-C4-C5	-2.18	105.78	110.14
2	K	1	GP1	O5-C1-O1	-2.16	108.55	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	5	GMH	O2-C2-C3	2.14	114.43	110.14
2	L	3	KDO	C6-O6-C2	2.14	115.92	111.34
2	L	3	KDO	C3-C4-C5	2.12	113.76	110.69
3	I	3	KDO	C3-C2-C1	-2.10	107.34	111.93
2	G	3	KDO	C6-O6-C2	2.09	115.81	111.34
4	O	1	GP1	O3-C3-C4	-2.08	105.53	110.35
3	I	4	KDO	O8-C8-C7	-2.07	106.57	111.07
3	H	1	GP1	O1-C1-C2	2.04	112.10	108.40
3	H	3	KDO	C3-C4-C5	2.03	113.64	110.69
2	G	1	GP1	O1-C1-C2	2.02	112.06	108.40
2	G	3	KDO	O5-C5-C6	2.01	115.26	109.94
3	I	3	KDO	C6-O6-C2	2.00	115.63	111.34

There are no chirality outliers.

All (21) torsion outliers are listed below:

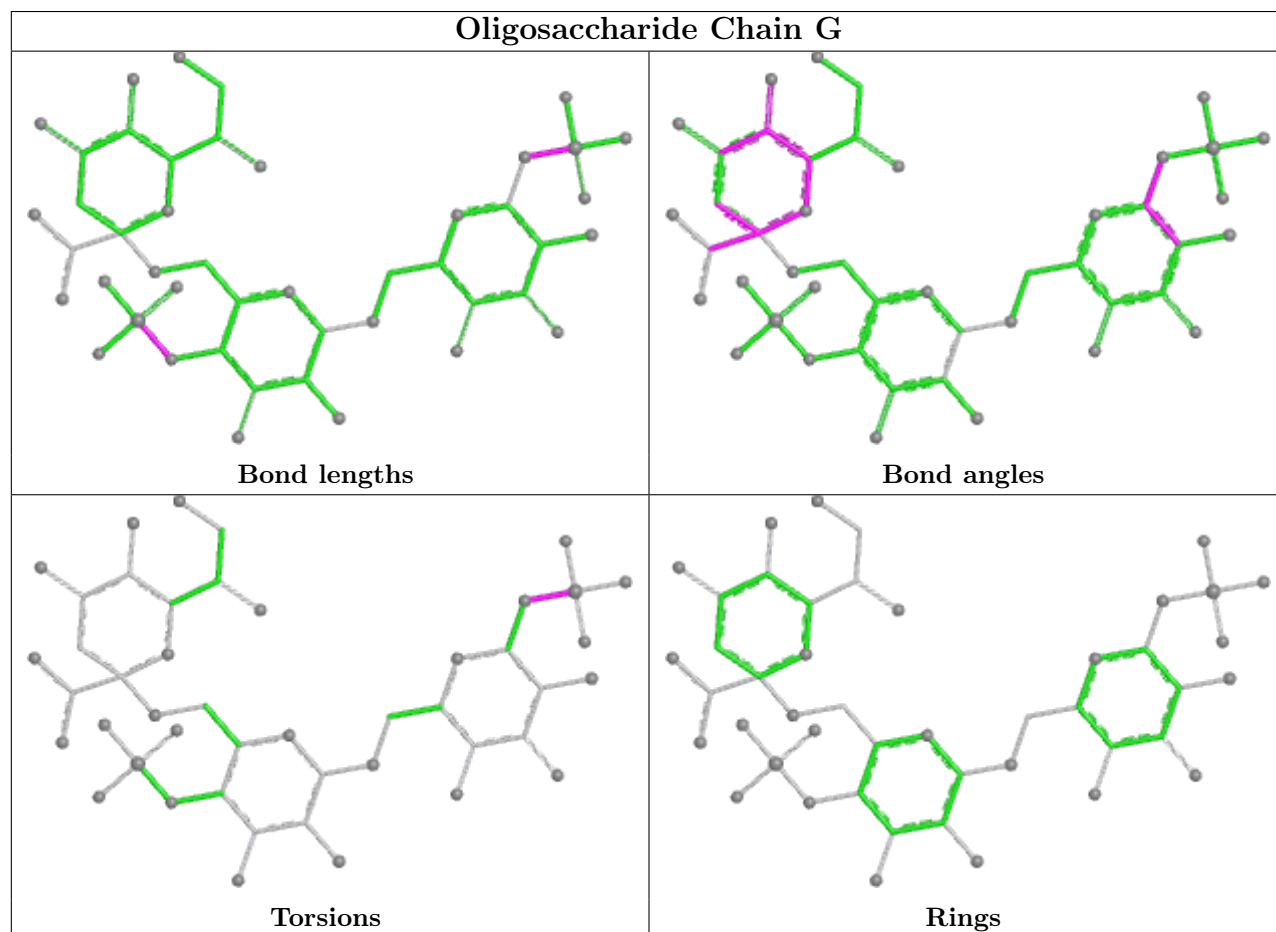
Mol	Chain	Res	Type	Atoms
3	I	5	GMH	C5-C6-C7-O7
3	I	5	GMH	O6-C6-C7-O7
3	N	4	KDO	C5-C6-C7-C8
3	N	4	KDO	O6-C6-C7-O7
3	N	5	GMH	O5-C5-C6-O6
2	G	1	GP1	C1-O1-P4B-O8B
2	K	3	KDO	C6-C7-C8-O8
3	I	5	GMH	O5-C5-C6-C7
3	I	2	Z9M	C4-O4-P1-O9
3	I	4	KDO	C5-C6-C7-C8
3	I	5	GMH	O5-C5-C6-O6
2	G	1	GP1	C1-O1-P4B-O9B
2	L	1	GP1	C1-O1-P4B-O7B
2	M	1	GP1	C1-O1-P4B-O7B
3	H	1	GP1	C1-O1-P4B-O9B
3	I	2	Z9M	C4-O4-P1-O7
3	N	5	GMH	C4-C5-C6-O6
4	J	1	GP1	C1-O1-P4B-O9B
4	O	1	GP1	C1-O1-P4B-O7B
2	K	3	KDO	O7-C7-C8-O8
3	N	5	GMH	C4-C5-C6-C7

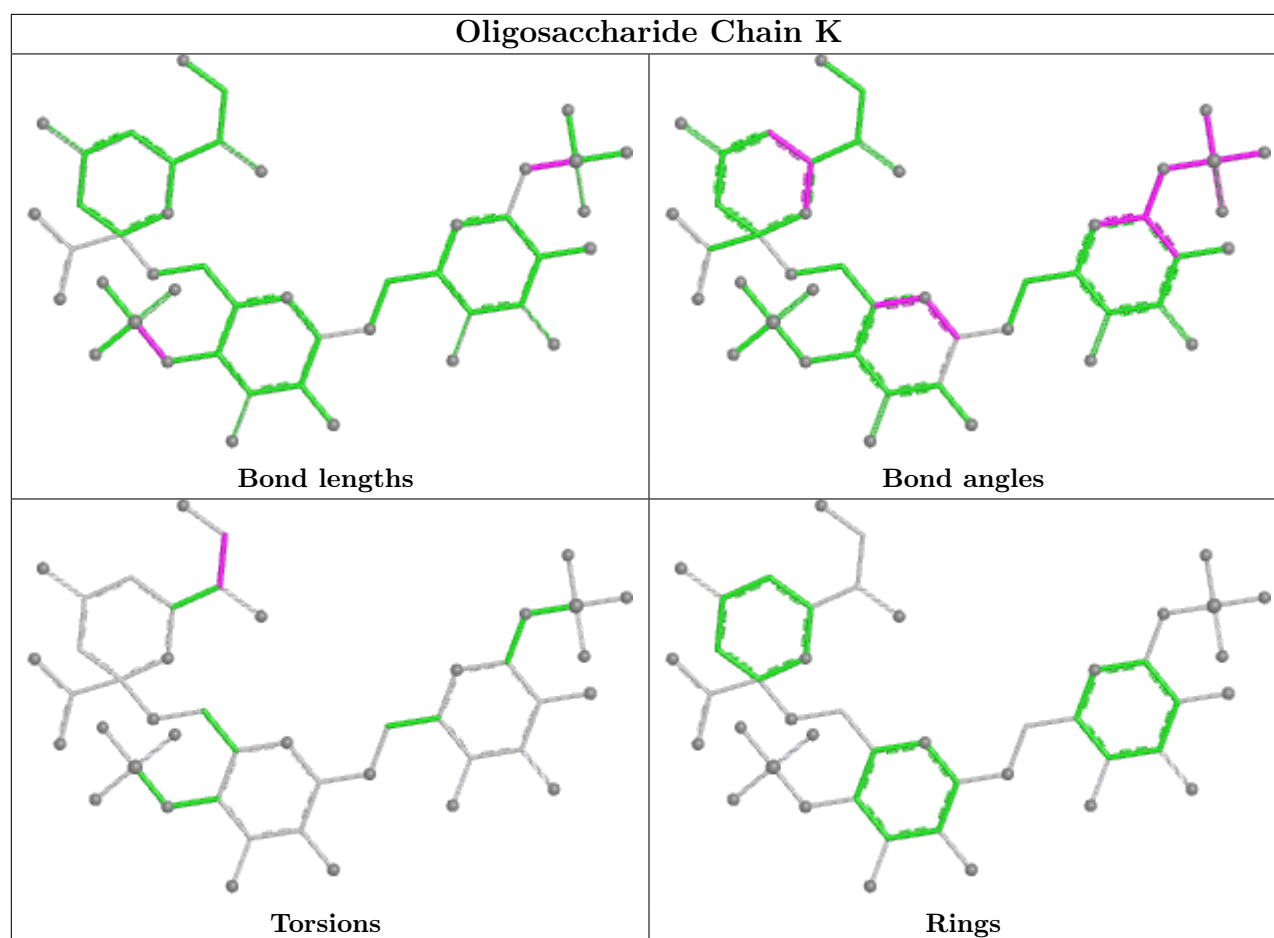
There are no ring outliers.

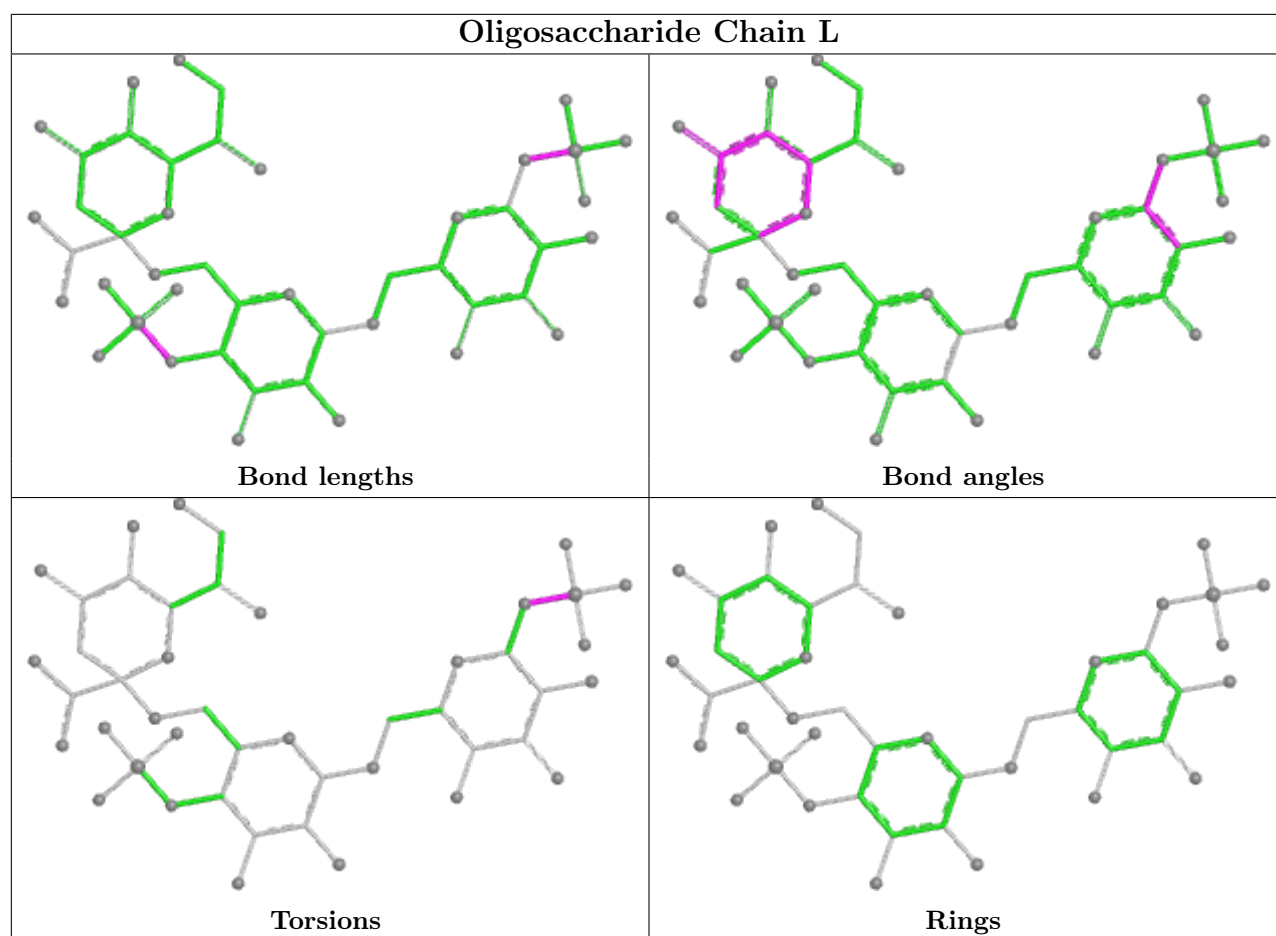
14 monomers are involved in 17 short contacts:

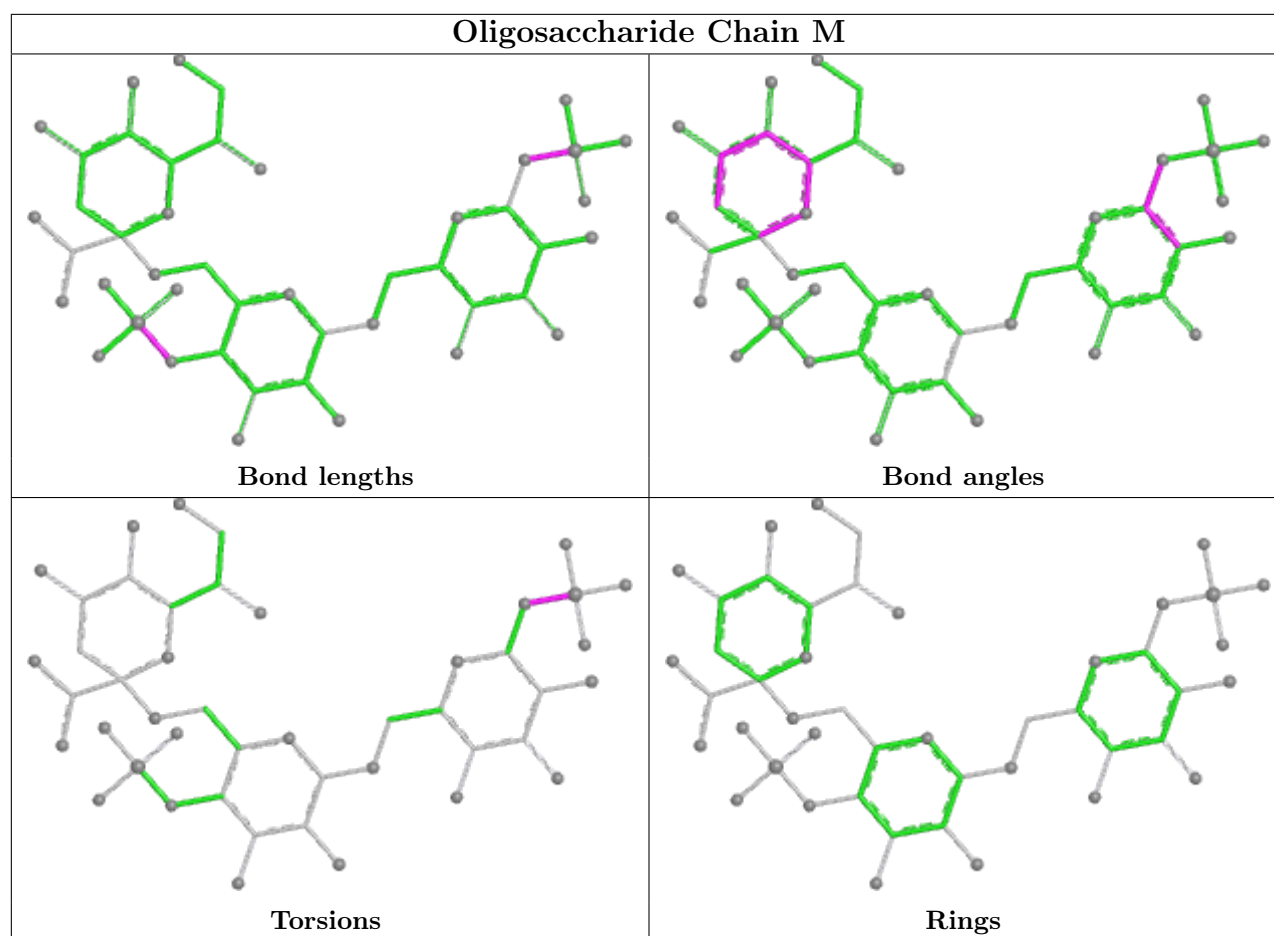
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	3	KDO	3	0
4	O	3	KDO	2	0
4	O	4	KDO	2	0
3	N	4	KDO	1	0
3	H	3	KDO	1	0
4	J	3	KDO	2	0
2	L	3	KDO	2	0
4	J	4	KDO	2	0
3	N	3	KDO	1	0
3	I	4	KDO	3	0
3	H	4	KDO	1	0
3	I	5	GMH	1	0
3	I	3	KDO	4	0
2	G	3	KDO	2	0

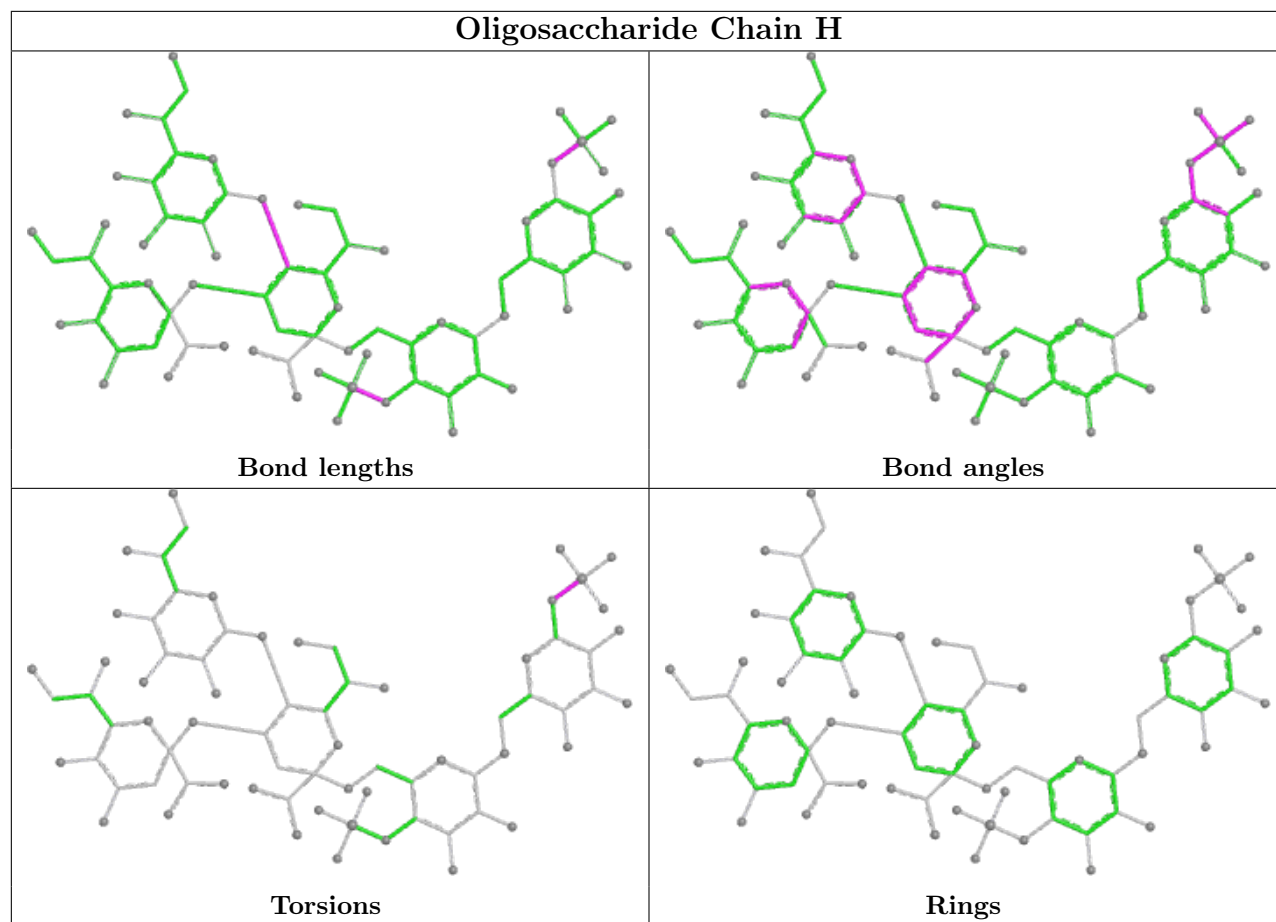
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



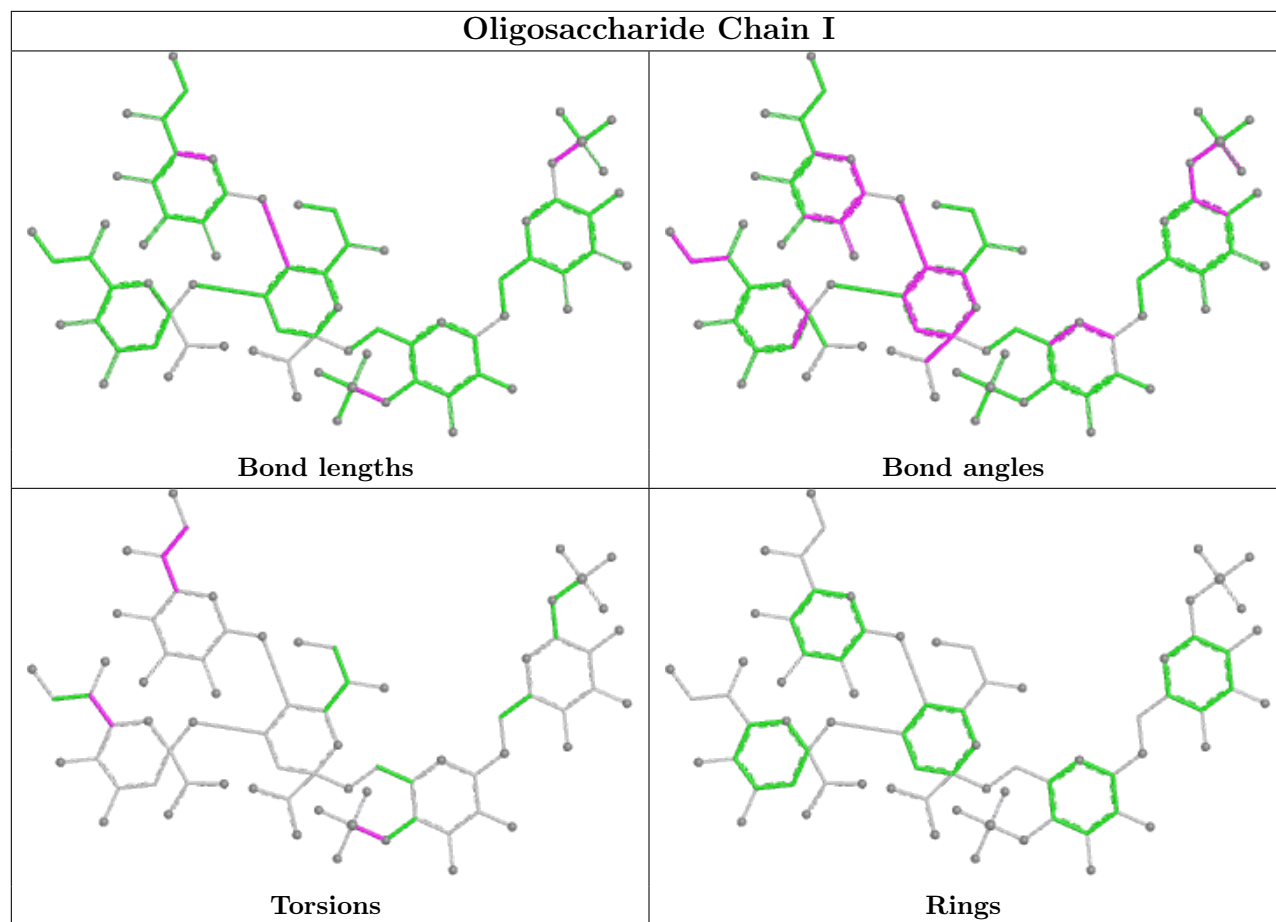


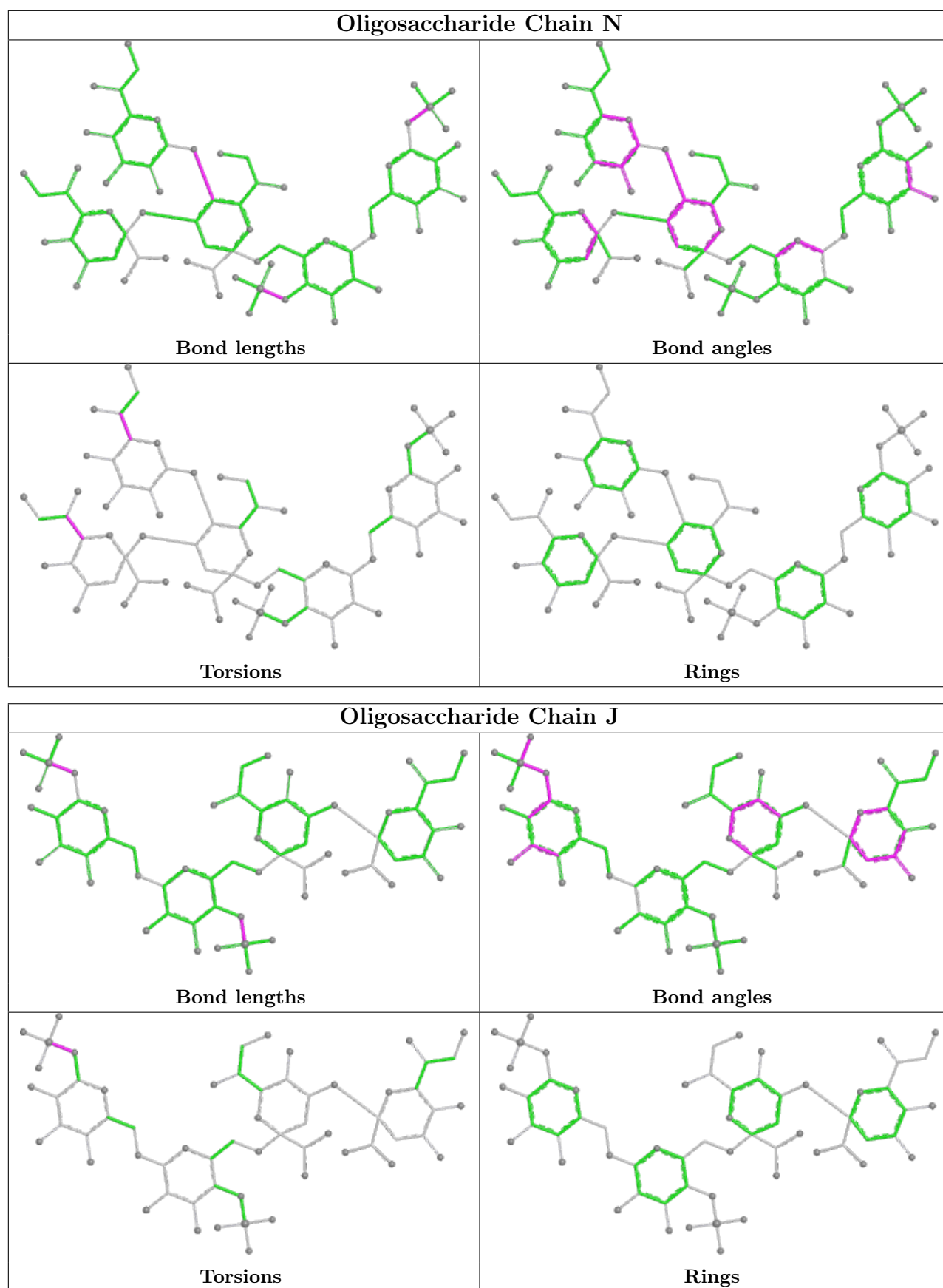


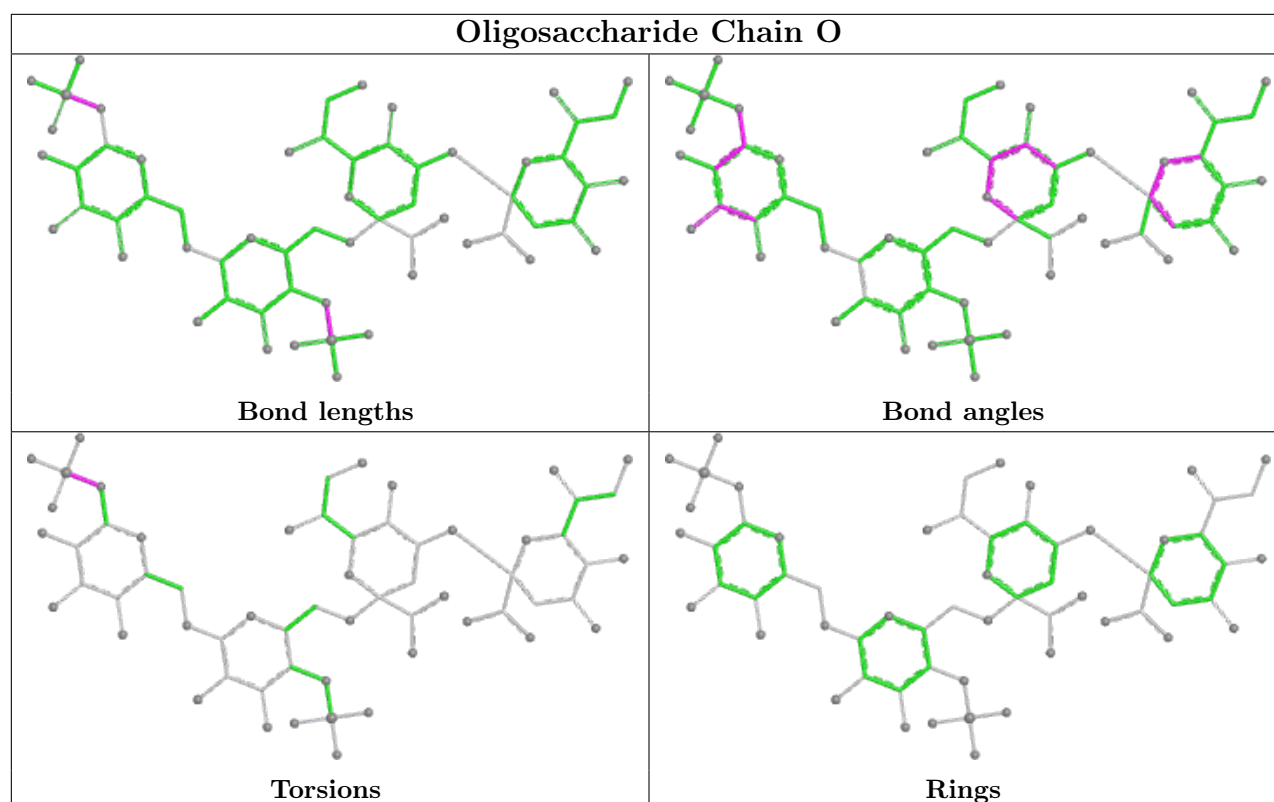












## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 2 are monoatomic - leaving 108 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	C8E	F	401	-	2,2,20	0.24	0	0,1,19	-	-
6	C8E	A	402	-	2,2,20	0.45	0	1,1,19	0.11	0
6	C8E	B	404	-	7,7,20	0.29	0	6,6,19	0.34	0
9	FTT	B	407	2	13,13,16	0.51	0	13,13,17	1.08	1 (7%)
6	C8E	E	401	-	5,5,20	0.29	0	4,4,19	0.35	0
11	DAO	C	426	9	7,7,13	0.55	0	6,6,13	0.69	0
11	DAO	C	421	9	9,9,13	0.58	0	8,8,13	0.44	0
6	C8E	D	410	-	5,5,20	0.26	0	4,4,19	0.35	0
9	FTT	D	425	4	13,13,16	0.54	0	13,13,17	1.55	2 (15%)
6	C8E	D	404	-	5,5,20	0.28	0	4,4,19	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	FTT	F	406	2	13,13,16	0.53	0	13,13,17	1.03	1 (7%)
11	DAO	E	405	9	4,4,13	0.67	0	3,3,13	1.03	0
6	C8E	B	405	-	7,7,20	0.30	0	6,6,19	0.67	0
9	FTT	A	415	2,10	15,15,16	0.43	0	15,15,17	0.92	1 (6%)
9	FTT	E	407	11,2	11,11,16	0.53	0	11,11,17	1.33	2 (18%)
6	C8E	C	407	-	10,10,20	0.34	0	9,9,19	0.44	0
6	C8E	A	410	-	6,6,20	0.25	0	5,5,19	0.48	0
11	DAO	F	412	9	4,4,13	0.63	0	3,3,13	0.64	0
10	MYR	C	419	9	7,7,15	0.60	0	6,6,15	0.56	0
10	MYR	F	411	9	10,10,15	0.43	0	9,9,15	0.63	0
6	C8E	D	407	-	7,7,20	0.30	0	6,6,19	0.29	0
6	C8E	C	409	-	9,9,20	0.35	0	8,8,19	0.43	0
9	FTT	A	414	11,2	12,12,16	0.53	0	12,12,17	1.45	2 (16%)
6	C8E	D	409	-	3,3,20	0.55	0	2,2,19	0.34	0
6	C8E	D	408	-	10,10,20	0.39	0	9,9,19	0.26	0
11	DAO	E	410	9	4,4,13	0.63	0	3,3,13	0.78	0
6	C8E	A	407	-	4,4,20	0.50	0	3,3,19	0.25	0
9	FTT	C	416	3,10	10,10,16	0.69	0	10,10,17	1.20	1 (10%)
6	C8E	F	402	-	3,3,20	0.35	0	2,2,19	0.62	0
10	MYR	B	411	9	5,5,15	0.61	0	4,4,15	0.78	0
7	PO4	C	411	-	4,4,4	0.84	0	6,6,6	0.97	0
9	FTT	D	415	11,2	10,10,16	0.56	0	10,10,17	1.47	1 (10%)
6	C8E	B	402	-	2,2,20	0.45	0	0,1,19	-	-
11	DAO	A	417	9	4,4,13	0.64	0	3,3,13	1.00	0
9	FTT	E	404	11,2	13,13,16	0.61	0	13,13,17	1.31	1 (7%)
6	C8E	C	402	-	6,6,20	0.53	0	5,5,19	0.82	0
9	FTT	D	422	2,10	15,15,16	0.37	0	15,15,17	0.80	0
5	SO4	A	401	-	4,4,4	0.19	0	6,6,6	0.57	0
6	C8E	D	406	-	7,7,20	0.33	0	6,6,19	0.46	0
6	C8E	D	402	-	3,3,20	0.35	0	2,2,19	0.67	0
10	MYR	A	416	9	5,5,15	0.64	0	4,4,15	0.72	0
9	FTT	A	413	2	14,14,16	0.38	0	14,14,17	0.76	0
9	FTT	F	407	3,11	11,11,16	0.74	0	11,11,17	1.24	1 (9%)
7	PO4	E	402	-	4,4,4	0.63	0	6,6,6	0.81	0
10	MYR	C	425	9	8,8,15	0.46	0	7,7,15	0.64	0
11	DAO	D	418	9	1,2,13	1.37	0	1,1,13	0.76	0
9	FTT	C	423	11,4	12,12,16	0.63	0	12,12,17	1.19	1 (8%)
9	FTT	C	415	3	15,15,16	0.56	0	15,15,17	1.06	1 (6%)
6	C8E	D	405	-	5,5,20	0.28	0	4,4,19	0.34	0
6	C8E	D	403	-	5,5,20	0.32	0	4,4,19	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	FTT	D	421	11,2	12,12,16	0.57	0	12,12,17	1.11	1 (8%)
9	FTT	C	424	4,10	15,15,16	0.32	0	15,15,17	0.87	0
9	FTT	D	416	2,10	12,12,16	0.57	0	12,12,17	0.86	0
9	FTT	A	418	11,4	13,13,16	0.55	0	13,13,17	1.47	1 (7%)
6	C8E	C	410	-	6,6,20	0.32	0	5,5,19	0.47	0
7	PO4	D	411	-	4,4,4	0.60	0	6,6,6	1.15	0
9	FTT	F	414	4	13,13,16	0.41	0	13,13,17	0.60	0
6	C8E	A	409	-	7,7,20	0.28	0	6,6,19	0.50	0
8	KDO	D	413	-	12,15,16	0.32	0	16,21,24	1.47	2 (12%)
9	FTT	C	418	3,11	12,12,16	0.61	0	12,12,17	1.01	1 (8%)
9	FTT	D	417	2	10,10,16	0.62	0	10,10,17	1.12	1 (10%)
6	C8E	C	405	-	2,2,20	0.18	0	0,1,19	-	-
9	FTT	C	422	4	15,15,16	0.28	0	15,15,17	1.40	3 (20%)
8	KDO	A	412	-	12,15,16	0.29	0	16,21,24	1.36	2 (12%)
6	C8E	C	406	-	7,7,20	0.30	0	6,6,19	0.41	0
10	MYR	D	423	9	5,5,15	0.60	0	4,4,15	0.74	0
5	SO4	D	401	-	4,4,4	0.21	0	6,6,6	0.46	0
9	FTT	C	417	3,11	15,15,16	0.44	0	15,15,17	0.81	0
9	FTT	B	408	3	14,14,16	0.40	0	14,14,17	0.72	0
6	C8E	A	408	-	7,7,20	0.48	0	6,6,19	0.44	0
7	PO4	F	404	-	4,4,4	0.54	0	6,6,6	0.80	0
6	C8E	A	406	-	4,4,20	0.34	0	3,3,19	0.32	0
6	C8E	F	403	-	7,7,20	0.35	0	6,6,19	0.47	0
11	DAO	A	419	9	7,7,13	0.50	0	6,6,13	0.83	0
10	MYR	D	419	9	4,4,15	0.69	0	3,3,15	0.90	0
7	PO4	B	406	-	4,4,4	1.10	0	6,6,6	0.66	0
6	C8E	B	403	-	4,4,20	0.29	0	3,3,19	0.31	0
9	FTT	F	408	3,11	12,12,16	0.70	0	12,12,17	1.00	1 (8%)
10	MYR	F	417	9	11,11,15	0.44	0	10,10,15	0.63	0
6	C8E	C	403	-	2,2,20	0.25	0	0,1,19	-	-
6	C8E	C	408	-	10,10,20	0.35	0	9,9,19	0.39	0
11	DAO	C	414	9	4,4,13	0.63	0	3,3,13	0.58	0
6	C8E	C	401	-	2,2,20	0.28	0	0,1,19	-	-
9	FTT	F	415	11,4	10,10,16	0.57	0	10,10,17	1.46	1 (10%)
6	C8E	A	404	-	5,5,20	0.30	0	4,4,19	0.26	0
9	FTT	F	410	3	15,15,16	0.38	0	15,15,17	1.29	3 (20%)
9	FTT	C	413	3,11	13,13,16	0.72	0	13,13,17	1.36	1 (7%)
9	FTT	D	414	2	13,13,16	0.57	0	13,13,17	0.69	1 (7%)
11	DAO	F	418	9	7,7,13	0.57	0	6,6,13	0.58	0
11	DAO	B	412	9	4,4,13	0.62	0	3,3,13	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	FTT	E	406	2	13,13,16	0.35	0	13,13,17	0.89	0
9	FTT	F	416	4,10	15,15,16	0.29	0	15,15,17	0.81	0
10	MYR	E	409	9	5,5,15	0.62	0	4,4,15	0.65	0
6	C8E	A	403	-	3,3,20	0.40	0	2,2,19	0.62	0
11	DAO	F	413	9	4,4,13	0.65	0	3,3,13	0.54	0
11	DAO	D	424	9	4,4,13	0.63	0	3,3,13	0.67	0
11	DAO	D	412	-	5,5,13	0.54	0	4,4,13	0.84	0
6	C8E	A	405	-	3,3,20	0.38	0	2,2,19	0.64	0
9	FTT	B	409	3,11	12,12,16	0.59	0	12,12,17	1.11	2 (16%)
11	DAO	C	420	9	12,12,13	0.44	0	11,11,13	0.58	0
9	FTT	B	410	3,10	15,15,16	0.44	0	15,15,17	0.85	0
9	FTT	D	420	2	15,15,16	0.34	0	15,15,17	0.83	0
9	FTT	F	409	3,10	11,11,16	0.64	0	11,11,17	0.97	1 (9%)
6	C8E	C	404	-	5,5,20	0.24	0	4,4,19	0.33	0
8	KDO	E	403	-	12,15,16	0.36	0	16,21,24	1.53	2 (12%)
7	PO4	A	411	-	4,4,4	0.97	0	6,6,6	0.78	0
6	C8E	B	401	-	8,8,20	0.38	0	7,7,19	0.58	0
9	FTT	E	408	2,10	14,14,16	0.55	0	14,14,17	0.97	1 (7%)

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	C8E	B	404	-	-	2/5/5/18	-
9	FTT	B	407	2	-	1/12/12/15	-
6	C8E	E	401	-	-	3/3/3/18	-
11	DAO	C	426	9	-	3/4/5/11	-
11	DAO	C	421	9	-	1/6/7/11	-
6	C8E	D	410	-	-	0/3/3/18	-
9	FTT	D	425	4	-	4/12/12/15	-
6	C8E	D	404	-	-	0/3/3/18	-
9	FTT	F	406	2	-	1/12/12/15	-
11	DAO	E	405	9	-	0/1/2/11	-
6	C8E	B	405	-	-	1/5/5/18	-
9	FTT	A	415	2,10	-	7/14/14/15	-
9	FTT	E	407	11,2	-	1/10/10/15	-
6	C8E	C	407	-	-	1/8/8/18	-
6	C8E	A	410	-	-	0/4/4/18	-
11	DAO	F	412	9	-	0/1/2/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MYR	C	419	9	-	0/4/5/13	-
10	MYR	F	411	9	-	0/7/8/13	-
6	C8E	D	407	-	-	2/5/5/18	-
6	C8E	C	409	-	-	2/7/7/18	-
9	FTT	A	414	11,2	-	0/11/11/15	-
6	C8E	D	409	-	-	0/0/1/18	-
6	C8E	D	408	-	-	1/8/8/18	-
11	DAO	E	410	9	-	1/1/2/11	-
6	C8E	A	407	-	-	2/2/2/18	-
9	FTT	C	416	3,10	-	1/9/9/15	-
6	C8E	F	402	-	-	0/1/1/18	-
10	MYR	B	411	9	-	1/2/3/13	-
9	FTT	D	415	11,2	-	1/9/9/15	-
11	DAO	A	417	9	-	1/1/2/11	-
9	FTT	E	404	11,2	-	6/12/12/15	-
6	C8E	C	402	-	-	2/4/4/18	-
9	FTT	D	422	2,10	-	5/14/14/15	-
6	C8E	D	406	-	-	4/5/5/18	-
6	C8E	D	402	-	-	1/1/1/18	-
10	MYR	A	416	9	-	0/2/3/13	-
9	FTT	A	413	2	-	3/13/13/15	-
9	FTT	F	407	3,11	-	3/10/10/15	-
10	MYR	C	425	9	-	2/5/6/13	-
9	FTT	C	423	11,4	-	1/11/11/15	-
9	FTT	C	415	3	-	2/14/14/15	-
6	C8E	D	405	-	-	0/3/3/18	-
6	C8E	D	403	-	-	0/3/3/18	-
9	FTT	D	421	11,2	-	0/11/11/15	-
9	FTT	C	424	4,10	-	3/14/14/15	-
9	FTT	D	416	2,10	-	6/11/11/15	-
9	FTT	A	418	11,4	-	5/12/12/15	-
6	C8E	C	410	-	-	2/4/4/18	-
9	FTT	F	414	4	-	2/12/12/15	-
6	C8E	A	409	-	-	0/5/5/18	-
8	KDO	D	413	-	-	0/6/26/30	0/1/1/1
9	FTT	C	418	3,11	-	4/11/11/15	-
9	FTT	D	417	2	-	3/9/9/15	-
9	FTT	C	422	4	-	4/14/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	KDO	A	412	-	-	0/6/26/30	0/1/1/1
6	C8E	C	406	-	-	0/5/5/18	-
10	MYR	D	423	9	-	1/2/3/13	-
9	FTT	C	417	3,11	-	2/14/14/15	-
9	FTT	B	408	3	-	1/13/13/15	-
6	C8E	A	408	-	-	3/5/5/18	-
6	C8E	A	406	-	-	0/2/2/18	-
6	C8E	F	403	-	-	2/5/5/18	-
11	DAO	A	419	9	-	0/4/5/11	-
10	MYR	D	419	9	-	1/1/2/13	-
6	C8E	B	403	-	-	1/2/2/18	-
9	FTT	F	408	3,11	-	5/11/11/15	-
10	MYR	F	417	9	-	3/8/9/13	-
6	C8E	C	408	-	-	3/8/8/18	-
11	DAO	C	414	9	-	1/1/2/11	-
9	FTT	F	415	11,4	-	1/9/9/15	-
6	C8E	A	404	-	-	1/3/3/18	-
9	FTT	F	410	3	-	5/14/14/15	-
9	FTT	C	413	3,11	-	2/12/12/15	-
9	FTT	D	414	2	-	7/12/12/15	-
11	DAO	F	418	9	-	2/4/5/11	-
11	DAO	B	412	9	-	1/1/2/11	-
9	FTT	E	406	2	-	2/12/12/15	-
9	FTT	F	416	4,10	-	6/14/14/15	-
10	MYR	E	409	9	-	1/2/3/13	-
6	C8E	A	403	-	-	0/1/1/18	-
11	DAO	F	413	9	-	0/1/2/11	-
11	DAO	D	424	9	-	1/1/2/11	-
11	DAO	D	412	-	-	2/2/3/11	-
6	C8E	A	405	-	-	0/1/1/18	-
9	FTT	B	409	3,11	-	3/11/11/15	-
11	DAO	C	420	9	-	0/9/10/11	-
9	FTT	B	410	3,10	-	5/14/14/15	-
9	FTT	D	420	2	-	3/14/14/15	-
9	FTT	F	409	3,10	-	2/10/10/15	-
6	C8E	C	404	-	-	1/3/3/18	-
8	KDO	E	403	-	-	0/6/26/30	0/1/1/1
6	C8E	B	401	-	-	3/6/6/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FTT	E	408	2,10	-	7/13/13/15	-

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	418	FTT	O2-C1-C2	-4.80	111.43	125.43
9	D	425	FTT	O2-C1-C2	-4.38	112.67	125.43
9	C	413	FTT	O2-C1-C2	-4.38	112.68	125.43
8	E	403	KDO	O6-C2-C3	4.36	117.53	109.87
9	F	415	FTT	O2-C1-C2	-4.20	113.19	125.43
8	D	413	KDO	O6-C2-C3	4.13	117.12	109.87
9	D	415	FTT	O2-C1-C2	-3.91	114.03	125.43
9	C	423	FTT	O2-C1-C2	-3.63	114.84	125.43
9	A	414	FTT	O2-C1-C2	-3.59	114.97	125.43
8	A	412	KDO	C6-O6-C2	3.51	118.85	111.34
8	A	412	KDO	O6-C2-C3	3.49	115.99	109.87
8	D	413	KDO	C6-O6-C2	3.48	118.78	111.34
8	E	403	KDO	C6-O6-C2	3.48	118.77	111.34
9	B	407	FTT	O2-C1-C2	-3.44	115.39	125.43
9	E	404	FTT	O2-C1-C2	-3.32	115.76	125.43
9	F	406	FTT	O2-C1-C2	-3.29	115.83	125.43
9	C	418	FTT	O2-C1-C2	-3.02	116.64	125.43
9	D	417	FTT	O2-C1-C2	-2.96	116.79	125.43
9	C	416	FTT	O2-C1-C2	-2.88	117.02	125.43
9	F	407	FTT	O2-C1-C2	-2.87	117.07	125.43
9	E	407	FTT	O2-C1-C2	-2.77	117.34	125.43
9	D	421	FTT	O2-C1-C2	-2.73	117.47	125.43
9	F	408	FTT	O2-C1-C2	-2.71	117.54	125.43
9	B	409	FTT	O2-C1-C2	-2.38	118.50	125.43
9	F	410	FTT	C5-C4-C3	-2.31	108.20	114.85
9	E	407	FTT	C3-C2-C1	2.27	116.74	112.75
9	F	410	FTT	O2-C1-C2	-2.27	118.81	125.43
9	A	415	FTT	C5-C4-C3	-2.23	108.44	114.85
9	A	414	FTT	C4-C3-C2	-2.22	105.33	112.91
9	F	409	FTT	O2-C1-C2	-2.19	119.04	125.43
9	C	422	FTT	C11-C10-C9	-2.19	103.31	114.42
9	D	425	FTT	C3-C2-C1	-2.19	108.90	112.75
9	E	408	FTT	C10-C9-C8	-2.14	103.57	114.42
9	D	414	FTT	O2-C1-C2	-2.10	119.30	125.43
9	F	410	FTT	C4-C3-C2	-2.10	105.73	112.91
9	C	422	FTT	C7-C6-C5	-2.09	103.80	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	415	FTT	C4-C3-C2	-2.08	105.80	112.91
9	C	422	FTT	C5-C4-C3	-2.03	109.00	114.85
9	B	409	FTT	C3-C2-C1	2.01	116.28	112.75

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	418	FTT	O2-C1-C2-C3
9	A	418	FTT	C2-C3-C4-C5
9	A	418	FTT	O3-C3-C4-C5
9	C	417	FTT	C1-C2-C3-C4
9	C	417	FTT	C1-C2-C3-O3
9	D	414	FTT	C1-C2-C3-O3
9	E	404	FTT	C1-C2-C3-C4
9	E	404	FTT	C1-C2-C3-O3
9	F	407	FTT	O2-C1-C2-C3
9	F	410	FTT	C1-C2-C3-O3
10	B	411	MYR	C1-C2-C3-C4
10	D	423	MYR	C1-C2-C3-C4
6	A	408	C8E	O12-C13-C14-O15
6	C	409	C8E	C6-C7-C8-O9
6	A	408	C8E	O9-C10-C11-O12
6	D	407	C8E	C2-C3-C4-C5
9	A	418	FTT	C4-C5-C6-C7
9	D	425	FTT	C11-C10-C9-C8
6	C	407	C8E	C11-C10-O9-C8
9	A	415	FTT	C10-C11-C12-C13
9	D	422	FTT	C9-C10-C11-C12
6	C	408	C8E	C2-C3-C4-C5
6	D	408	C8E	C2-C3-C4-C5
9	A	415	FTT	C11-C10-C9-C8
9	D	417	FTT	C5-C6-C7-C8
9	B	408	FTT	C9-C10-C11-C12
11	C	414	DAO	C1-C2-C3-C4
9	F	410	FTT	C6-C7-C8-C9
9	A	413	FTT	C9-C10-C11-C12
9	D	422	FTT	C6-C7-C8-C9
6	B	403	C8E	O9-C10-C11-O12
9	B	410	FTT	C9-C10-C11-C12
9	E	408	FTT	C7-C8-C9-C10
9	B	410	FTT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
9	F	410	FTT	C7-C8-C9-C10
11	F	418	DAO	C3-C4-C5-C6
9	E	408	FTT	C4-C5-C6-C7
9	C	422	FTT	C6-C7-C8-C9
9	D	422	FTT	C10-C11-C12-C13
9	D	416	FTT	O3-C3-C4-C5
9	E	404	FTT	O3-C3-C4-C5
9	F	408	FTT	O3-C3-C4-C5
9	E	408	FTT	C6-C7-C8-C9
9	F	416	FTT	C7-C8-C9-C10
6	C	409	C8E	C7-C8-O9-C10
6	B	401	C8E	C2-C3-C4-C5
6	C	408	C8E	C4-C5-C6-C7
9	C	413	FTT	C4-C5-C6-C7
9	F	416	FTT	C10-C11-C12-C13
9	B	410	FTT	C10-C11-C12-C13
9	A	418	FTT	C6-C7-C8-C9
6	E	401	C8E	C2-C3-C4-C5
9	D	420	FTT	C10-C11-C12-C13
9	A	413	FTT	C10-C11-C12-C13
9	F	407	FTT	C6-C7-C8-C9
9	C	415	FTT	C10-C11-C12-C13
6	F	403	C8E	C2-C3-C4-C5
9	C	418	FTT	C6-C7-C8-C9
9	D	422	FTT	C1-C2-C3-O3
9	E	408	FTT	C1-C2-C3-O3
9	F	409	FTT	C1-C2-C3-O3
9	F	416	FTT	C1-C2-C3-O3
6	B	404	C8E	C5-C6-C7-C8
6	C	402	C8E	C4-C5-C6-C7
9	F	407	FTT	C7-C8-C9-C10
9	D	414	FTT	C5-C6-C7-C8
9	C	422	FTT	C10-C11-C12-C13
9	E	406	FTT	C9-C10-C11-C12
6	D	406	C8E	C1-C2-C3-C4
9	B	410	FTT	C11-C12-C13-C14
6	D	407	C8E	C4-C5-C6-C7
10	C	425	MYR	C3-C4-C5-C6
10	F	417	MYR	C7-C8-C9-C10
9	C	413	FTT	O2-C1-C2-C3
9	D	415	FTT	O2-C1-C2-C3
9	D	422	FTT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	A	417	DAO	C1-C2-C3-C4
11	D	424	DAO	C1-C2-C3-C4
9	D	416	FTT	C2-C3-C4-C5
9	E	404	FTT	C2-C3-C4-C5
9	F	408	FTT	C2-C3-C4-C5
6	E	401	C8E	C1-C2-C3-C4
6	B	401	C8E	C3-C4-C5-C6
9	D	414	FTT	C9-C10-C11-C12
6	B	405	C8E	C2-C3-C4-C5
9	C	418	FTT	C4-C5-C6-C7
9	D	416	FTT	C6-C7-C8-C9
9	D	414	FTT	C11-C10-C9-C8
9	D	425	FTT	C9-C10-C11-C12
6	B	401	C8E	C6-C7-C8-O9
9	C	424	FTT	C5-C6-C7-C8
9	D	420	FTT	C9-C10-C11-C12
9	F	414	FTT	C9-C10-C11-C12
6	E	401	C8E	C3-C4-C5-C6
9	E	408	FTT	C9-C10-C11-C12
6	C	404	C8E	C3-C4-C5-C6
9	C	422	FTT	C4-C5-C6-C7
11	F	418	DAO	C4-C5-C6-C7
6	D	406	C8E	C5-C6-C7-C8
9	C	424	FTT	C11-C10-C9-C8
9	B	409	FTT	C5-C6-C7-C8
6	C	410	C8E	C1-C2-C3-C4
10	F	417	MYR	C11-C10-C9-C8
9	F	414	FTT	C4-C5-C6-C7
9	D	414	FTT	C1-C2-C3-C4
9	F	409	FTT	C1-C2-C3-C4
9	F	410	FTT	C1-C2-C3-C4
9	F	416	FTT	C1-C2-C3-C4
9	D	414	FTT	C7-C8-C9-C10
6	C	408	C8E	C11-C10-O9-C8
9	B	410	FTT	C1-C2-C3-O3
6	D	402	C8E	C1-C2-C3-C4
10	E	409	MYR	C1-C2-C3-C4
11	C	421	DAO	C1-C2-C3-C4
11	C	426	DAO	C1-C2-C3-C4
11	D	412	DAO	C1-C2-C3-C4
9	D	417	FTT	C6-C7-C8-C9
6	B	404	C8E	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
11	C	426	DAO	C4-C5-C6-C7
9	D	420	FTT	C4-C5-C6-C7
9	D	425	FTT	C7-C8-C9-C10
11	D	412	DAO	C2-C3-C4-C5
6	C	402	C8E	C3-C4-C5-C6
9	C	416	FTT	O2-C1-C2-C3
9	C	418	FTT	O2-C1-C2-C3
9	C	423	FTT	O2-C1-C2-C3
9	D	416	FTT	O2-C1-C2-C3
9	D	425	FTT	O2-C1-C2-C3
9	E	404	FTT	O2-C1-C2-C3
9	F	408	FTT	O2-C1-C2-C3
9	F	415	FTT	O2-C1-C2-C3
9	C	422	FTT	C5-C6-C7-C8
11	C	426	DAO	C2-C3-C4-C5
10	D	419	MYR	C1-C2-C3-C4
11	B	412	DAO	C1-C2-C3-C4
11	E	410	DAO	C1-C2-C3-C4
9	D	414	FTT	C4-C5-C6-C7
9	D	416	FTT	C3-C4-C5-C6
9	E	406	FTT	C4-C5-C6-C7
9	A	413	FTT	C4-C5-C6-C7
9	A	415	FTT	C5-C6-C7-C8
9	C	415	FTT	C7-C8-C9-C10
6	A	404	C8E	C1-C2-C3-C4
9	F	410	FTT	C11-C12-C13-C14
9	A	415	FTT	C11-C12-C13-C14
9	F	416	FTT	C11-C10-C9-C8
6	A	408	C8E	C14-C13-O12-C11
6	D	406	C8E	C3-C4-C5-C6
9	A	415	FTT	C1-C2-C3-O3
9	A	415	FTT	C7-C8-C9-C10
9	B	409	FTT	C11-C10-C9-C8
9	F	416	FTT	C4-C5-C6-C7
9	E	407	FTT	C2-C3-C4-C5
9	F	408	FTT	C6-C7-C8-C9
10	C	425	MYR	C2-C3-C4-C5
6	A	407	C8E	C11-C10-O9-C8
10	F	417	MYR	C6-C7-C8-C9
9	B	407	FTT	C5-C6-C7-C8
6	D	406	C8E	C4-C5-C6-C7
6	F	403	C8E	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
9	F	406	FTT	O2-C1-C2-C3
9	D	416	FTT	C5-C6-C7-C8
9	C	424	FTT	C11-C12-C13-C14
9	F	408	FTT	C3-C4-C5-C6
6	A	407	C8E	C7-C8-O9-C10
9	E	408	FTT	C1-C2-C3-C4
9	C	418	FTT	C3-C4-C5-C6
9	E	408	FTT	C3-C4-C5-C6
6	C	410	C8E	C4-C5-C6-C7
9	B	409	FTT	C6-C7-C8-C9
9	E	404	FTT	C4-C5-C6-C7
9	D	417	FTT	O3-C3-C4-C5
9	A	415	FTT	C9-C10-C11-C12

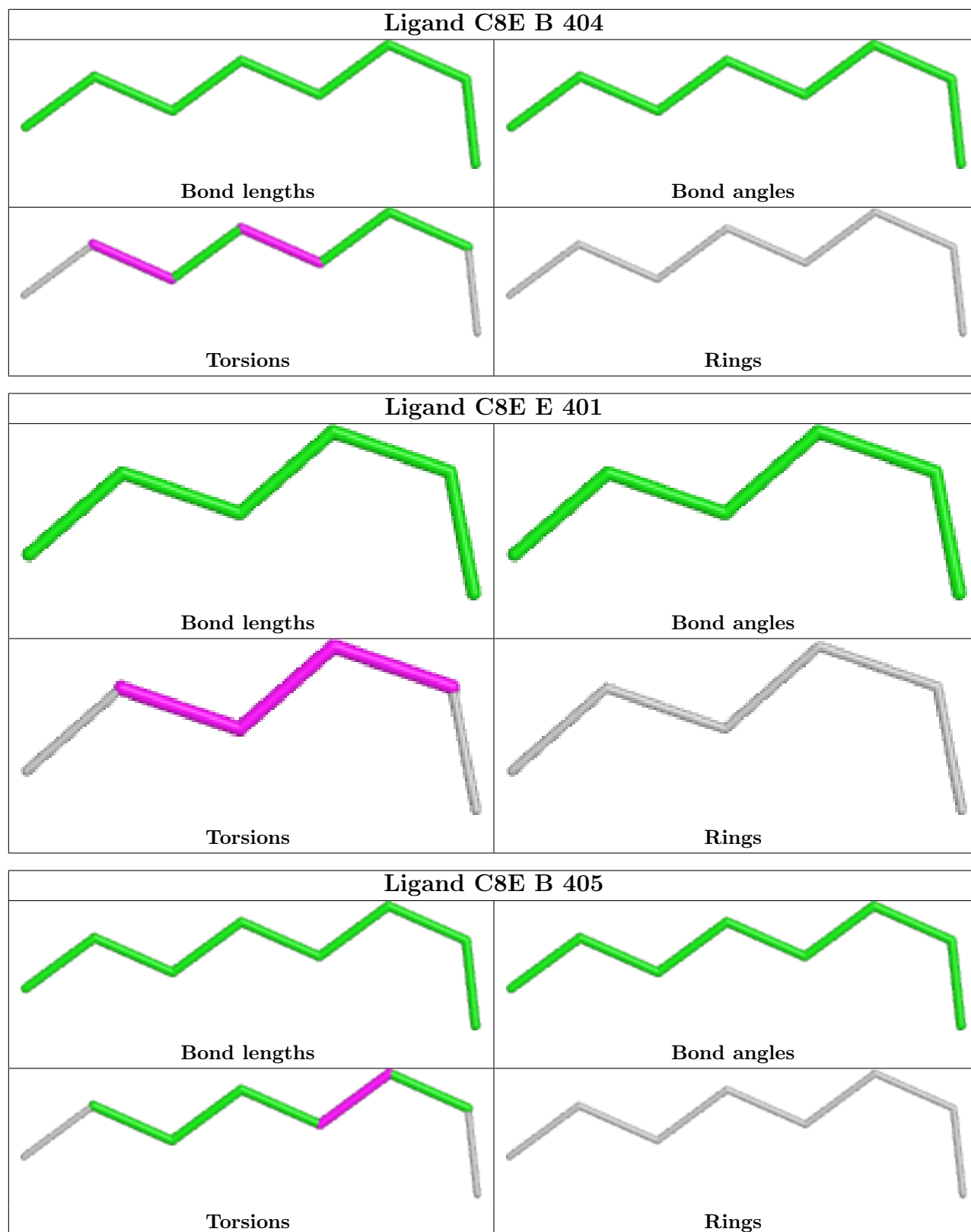
There are no ring outliers.

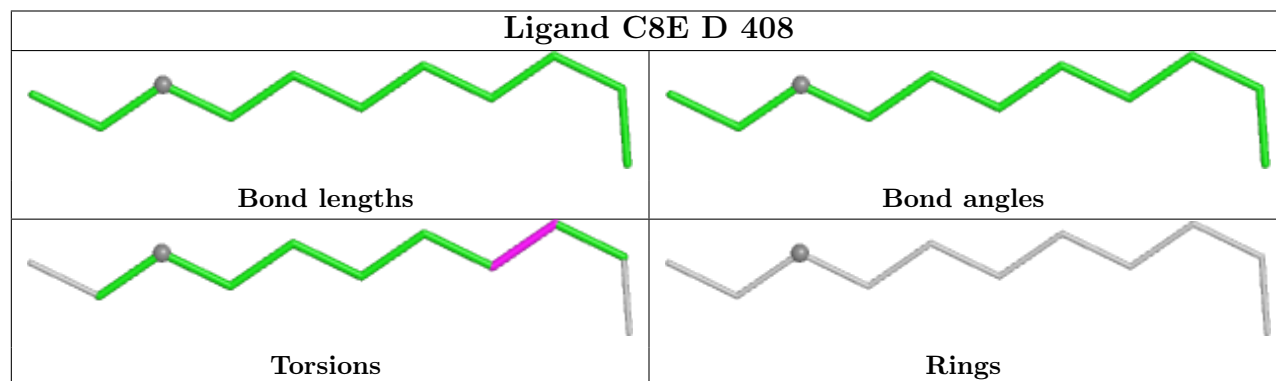
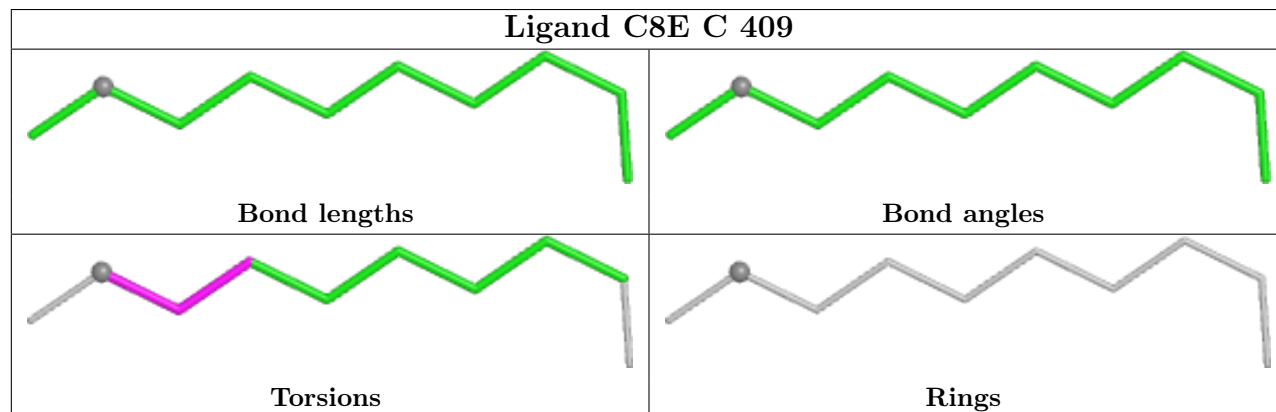
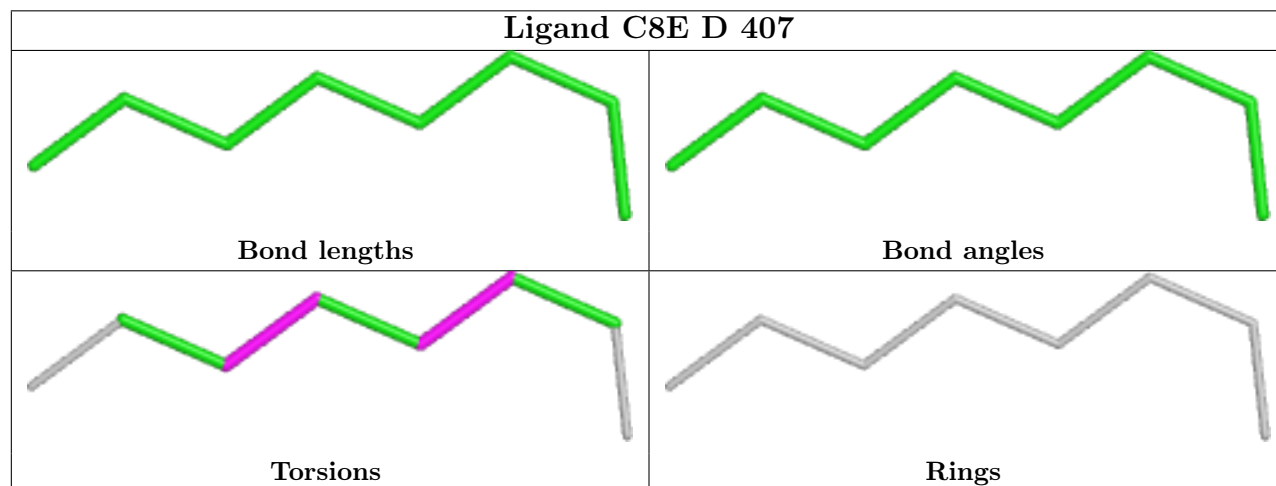
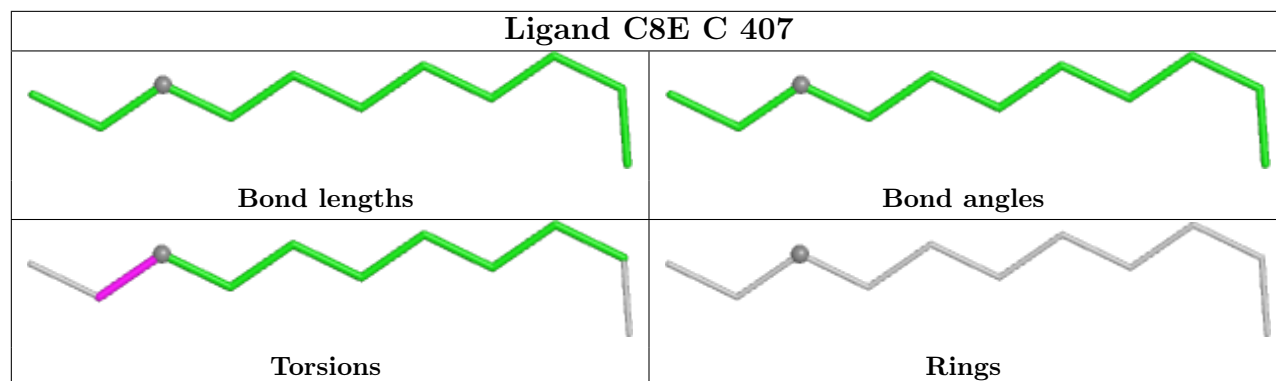
12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	401	C8E	1	0
9	F	406	FTT	1	0
6	D	409	C8E	1	0
6	A	407	C8E	1	0
9	F	407	FTT	1	0
8	D	413	KDO	2	0
6	C	405	C8E	4	0
8	A	412	KDO	2	0
6	A	408	C8E	2	0
6	F	403	C8E	1	0
6	B	403	C8E	2	0
8	E	403	KDO	3	0

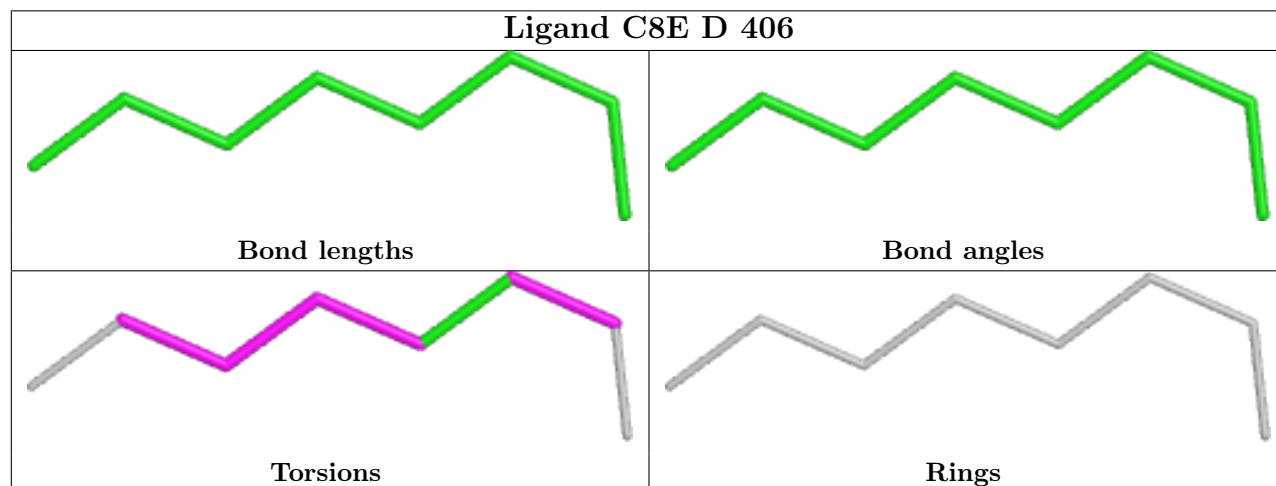
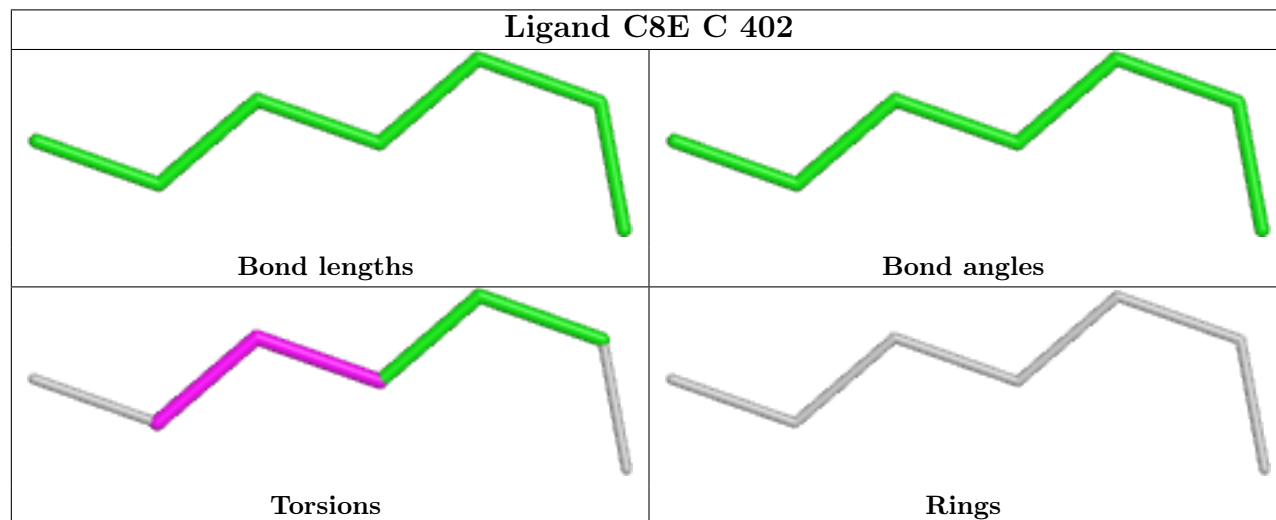
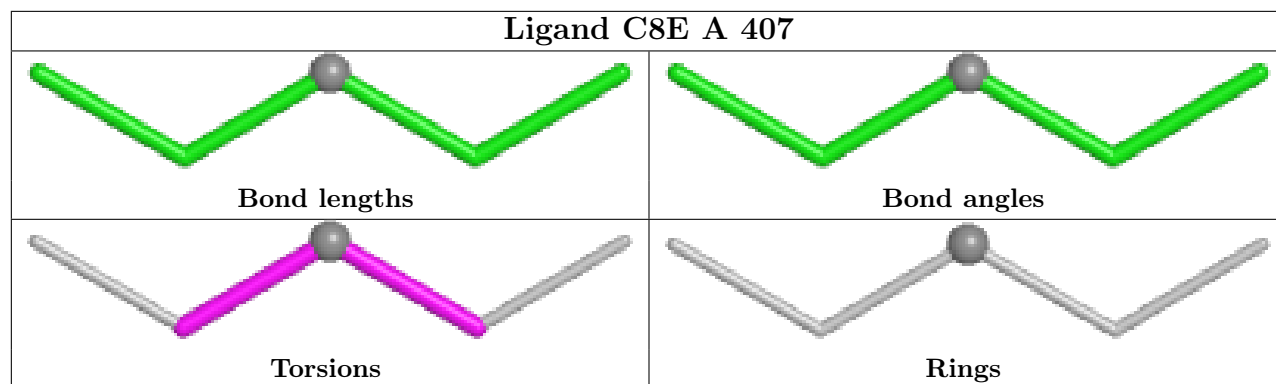
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

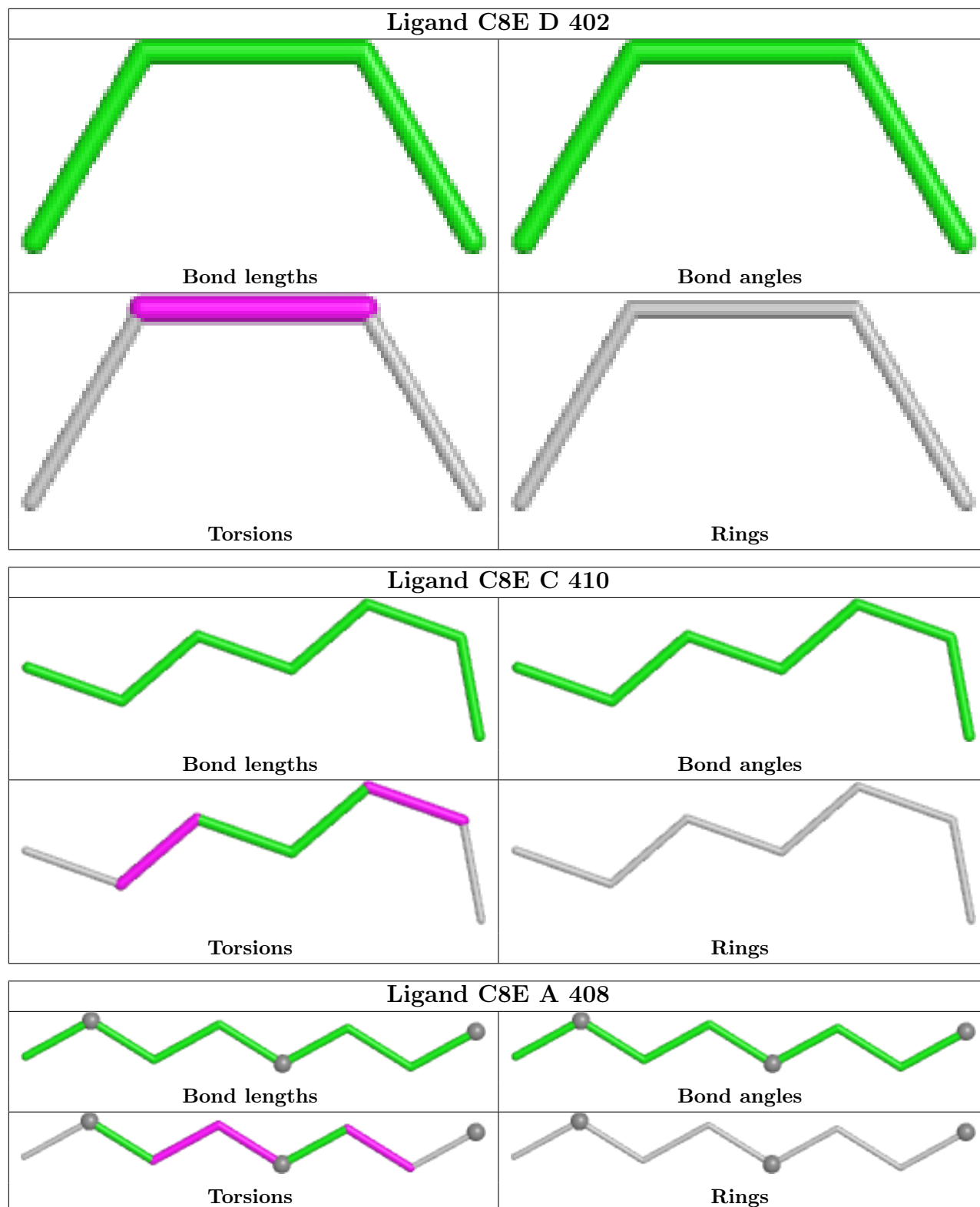
equivalents in the CSD to analyse the geometry.

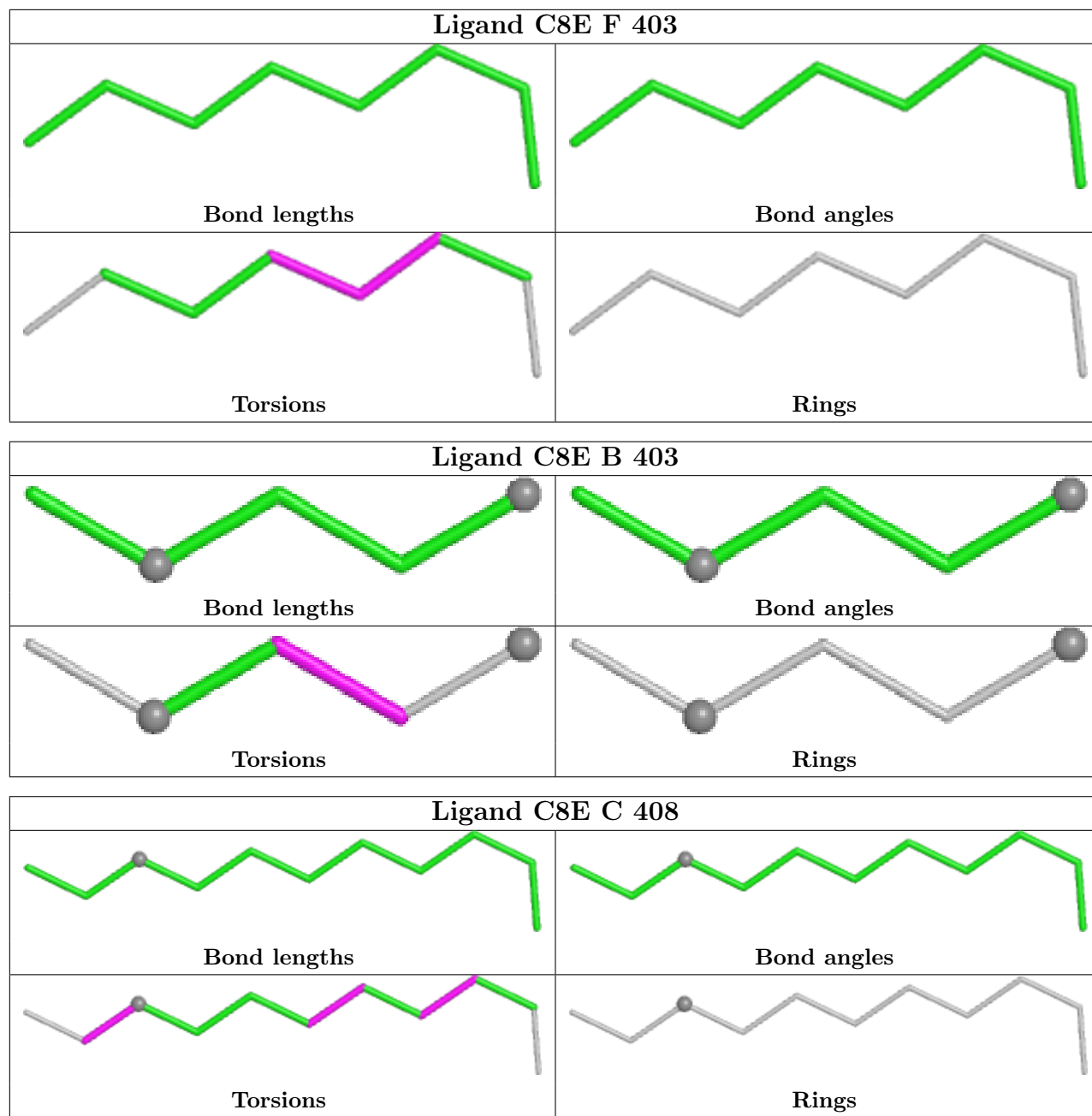


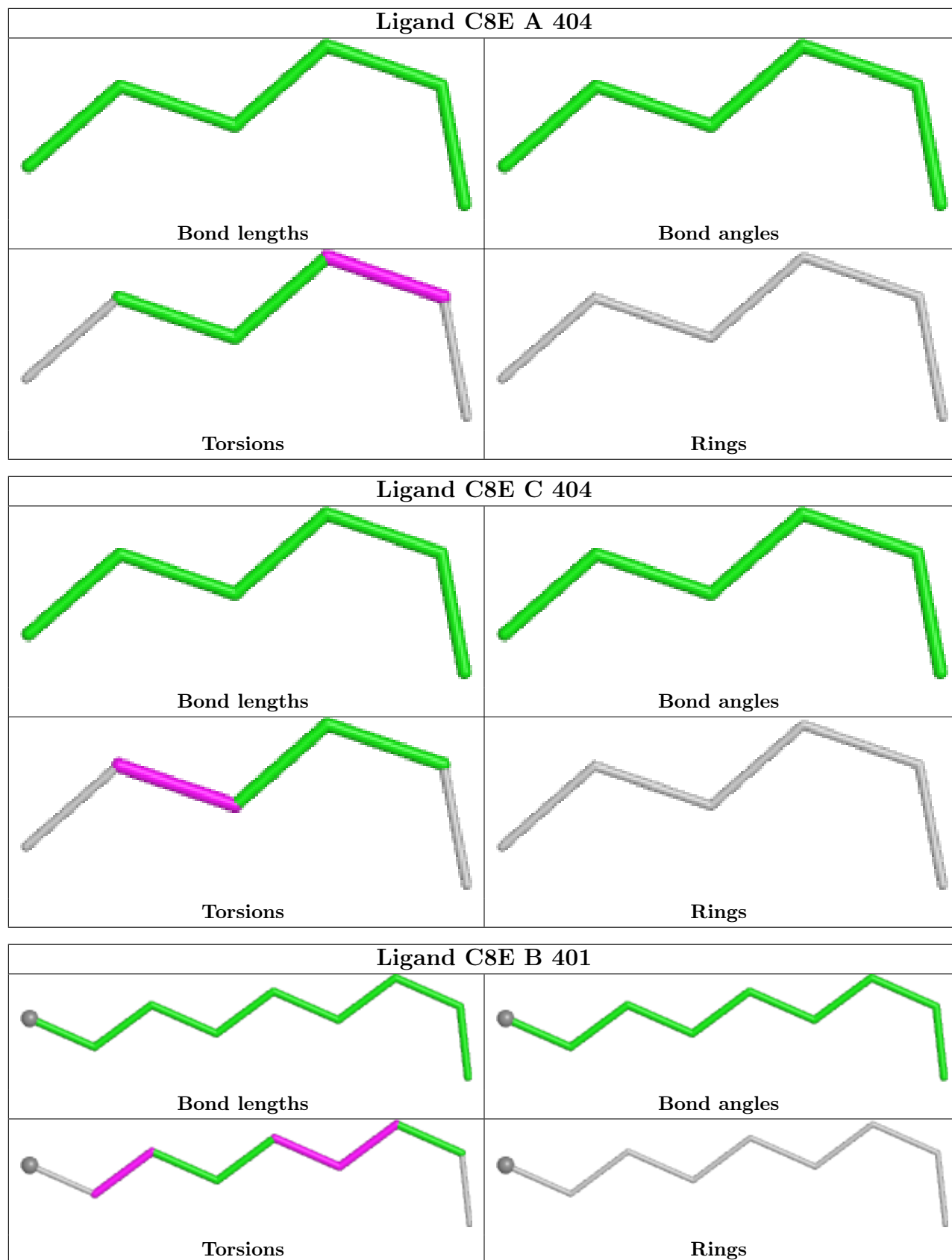












## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	342/342 (100%)	0.31	17 (4%)	28 31	9, 15, 28, 59	1 (0%)
1	B	342/342 (100%)	0.31	16 (4%)	31 34	9, 15, 31, 77	0
1	C	342/342 (100%)	0.23	13 (3%)	40 43	9, 14, 30, 54	0
1	D	342/342 (100%)	0.40	21 (6%)	21 23	10, 16, 31, 96	0
1	E	342/342 (100%)	0.30	15 (4%)	34 37	10, 15, 32, 58	0
1	F	342/342 (100%)	0.15	3 (0%)	84 86	9, 14, 25, 40	0
All	All	2052/2052 (100%)	0.28	85 (4%)	37 40	9, 15, 30, 96	1 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	LEU	9.3
1	D	83	GLY	8.3
1	A	139	LEU	7.7
1	E	139	LEU	7.2
1	D	84	ASP	6.6
1	B	137	PHE	6.5
1	D	137	PHE	6.5
1	A	138	GLY	6.2
1	D	138	GLY	6.2
1	A	82	PHE	5.9
1	B	136	PHE	5.7
1	C	138	GLY	5.7
1	D	265	PHE	5.6
1	A	137	PHE	5.6
1	D	136	PHE	5.5
1	D	139	LEU	5.4
1	B	84	ASP	5.2
1	B	138	GLY	5.1
1	D	134	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	82	PHE	5.0
1	E	265	PHE	4.8
1	E	137	PHE	4.5
1	E	138	GLY	4.5
1	E	82	PHE	4.5
1	B	140	VAL	4.4
1	D	85	ALA	4.1
1	B	83	GLY	4.0
1	D	82	PHE	3.9
1	A	159	GLU	3.9
1	D	49	GLN	3.9
1	D	159	GLU	3.8
1	E	85	ALA	3.7
1	E	141	ASP	3.6
1	E	84	ASP	3.5
1	C	226	ASN	3.3
1	E	264	ASP	3.3
1	A	83	GLY	3.2
1	B	265	PHE	3.1
1	C	137	PHE	3.1
1	A	84	ASP	3.1
1	B	85	ALA	3.1
1	F	186	GLU	2.9
1	D	135	ASP	2.9
1	C	82	PHE	2.9
1	C	139	LEU	2.9
1	D	140	VAL	2.9
1	A	136	PHE	2.8
1	E	140	VAL	2.8
1	C	84	ASP	2.8
1	F	136	PHE	2.8
1	A	264	ASP	2.8
1	F	84	ASP	2.8
1	B	264[A]	ASP	2.7
1	B	49	GLN	2.7
1	E	136	PHE	2.7
1	E	83	GLY	2.7
1	D	261	TYR	2.6
1	C	141	ASP	2.6
1	D	186	GLU	2.6
1	E	159	GLU	2.6
1	B	185	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	265	PHE	2.6
1	A	261	TYR	2.5
1	A	141	ASP	2.5
1	D	264[A]	ASP	2.5
1	A	49	GLN	2.5
1	D	188	PHE	2.4
1	D	86	GLY	2.3
1	D	45	GLN	2.3
1	E	263	PHE	2.3
1	A	140	VAL	2.3
1	A	45	GLN	2.3
1	A	226	ASN	2.3
1	B	183	ASN	2.3
1	B	141	ASP	2.3
1	B	134	SER	2.2
1	C	134	SER	2.1
1	C	265	PHE	2.1
1	E	49	GLN	2.1
1	D	226	ASN	2.1
1	C	185	GLY	2.1
1	C	186	GLU	2.1
1	C	318	ASP	2.1
1	A	85	ALA	2.1
1	C	83	GLY	2.0

## 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
2	KDO	K	3	14/16	0.60	0.30	42,49,65,65	0
3	GMH	I	5	13/14	0.76	0.22	36,45,58,69	0
3	GMH	H	5	13/14	0.79	0.28	32,36,40,48	0
2	GP1	K	1	16/16	0.83	0.34	34,37,66,67	0

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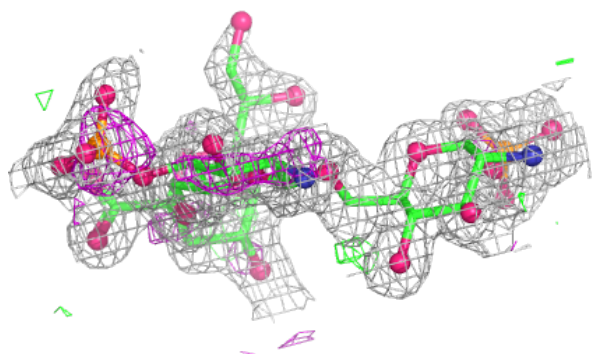
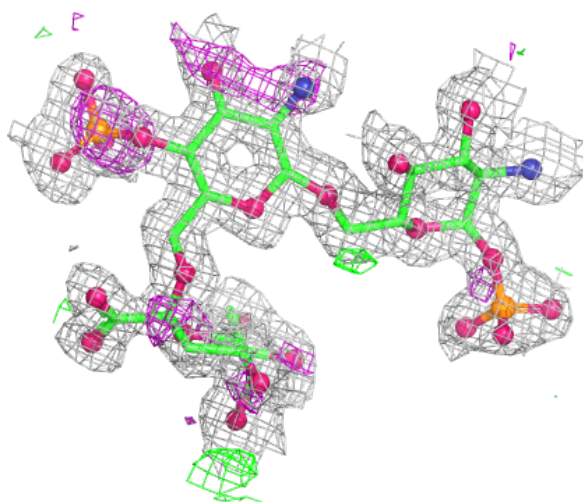
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GMH	N	5	13/14	0.84	0.23	31,36,54,59	0
2	KDO	G	3	15/16	0.87	0.30	24,29,40,48	0
2	KDO	L	3	15/16	0.87	0.26	25,28,40,44	0
2	KDO	M	3	15/16	0.87	0.23	23,27,35,38	0
3	KDO	H	3	15/16	0.89	0.22	22,26,33,41	0
3	KDO	H	4	15/16	0.90	0.15	18,20,25,27	0
2	Z9M	K	2	15/16	0.90	0.23	25,29,34,40	0
2	GP1	G	1	16/16	0.91	0.22	22,27,48,52	0
4	KDO	J	4	15/16	0.91	0.13	12,19,22,23	0
2	Z9M	G	2	15/16	0.92	0.22	22,24,31,34	0
2	GP1	M	1	16/16	0.92	0.16	23,26,47,49	0
2	GP1	L	1	16/16	0.92	0.20	24,26,44,49	0
4	KDO	O	3	15/16	0.92	0.15	13,21,31,35	0
4	KDO	O	4	15/16	0.92	0.13	17,18,21,24	0
3	GP1	H	1	16/16	0.93	0.14	22,24,50,51	0
3	KDO	N	3	15/16	0.93	0.15	18,25,33,37	0
3	KDO	I	3	15/16	0.93	0.12	18,23,31,31	0
4	GP1	J	1	16/16	0.94	0.09	17,19,44,44	0
4	KDO	J	3	15/16	0.94	0.13	16,21,30,34	0
3	KDO	I	4	15/16	0.94	0.10	14,15,19,24	0
3	KDO	N	4	15/16	0.94	0.12	15,16,20,29	0
3	Z9M	H	2	15/16	0.94	0.17	20,21,26,26	0
2	Z9M	L	2	15/16	0.95	0.18	23,24,30,30	0
4	GP1	O	1	16/16	0.95	0.09	18,20,41,43	0
4	Z9M	J	2	15/16	0.96	0.07	16,17,26,26	0
4	Z9M	O	2	15/16	0.96	0.07	17,18,24,27	0
2	Z9M	M	2	15/16	0.96	0.21	21,21,26,27	0
3	GP1	N	1	16/16	0.96	0.07	16,19,34,34	0
3	Z9M	N	2	15/16	0.97	0.08	18,21,29,32	0
3	GP1	I	1	16/16	0.97	0.08	17,19,33,35	0
3	Z9M	I	2	15/16	0.97	0.06	18,21,41,41	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.

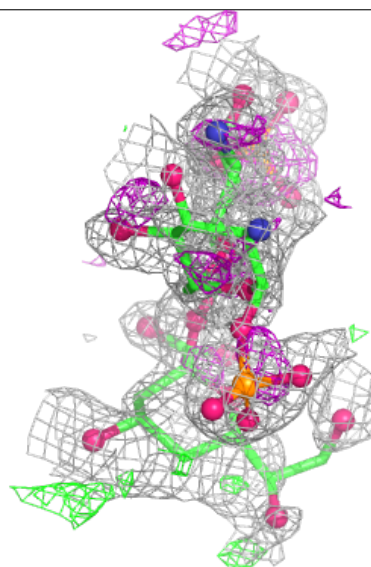
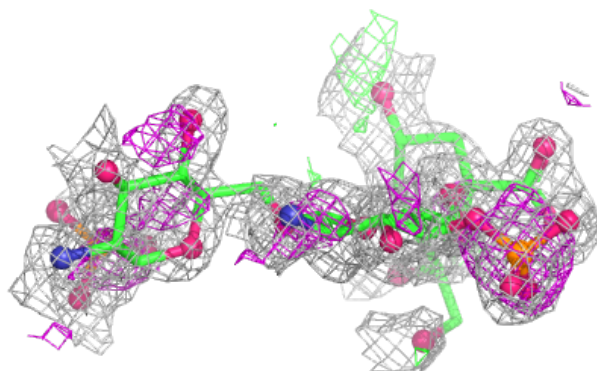
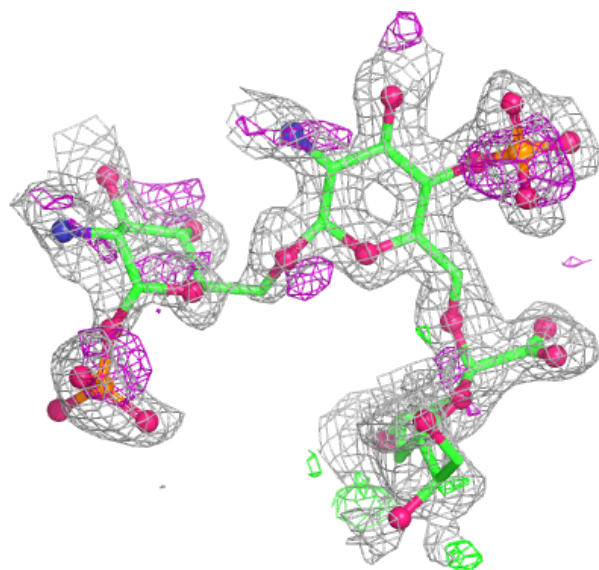
**Electron density around Chain G:**

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



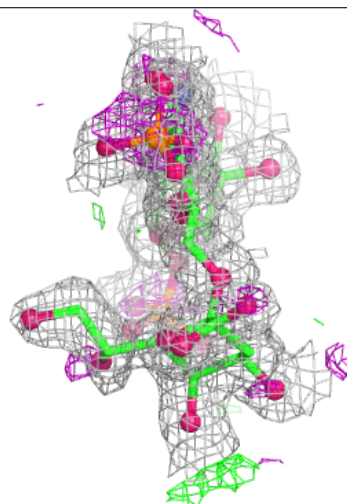
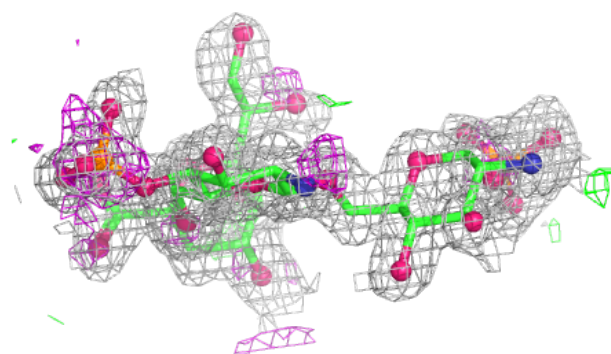
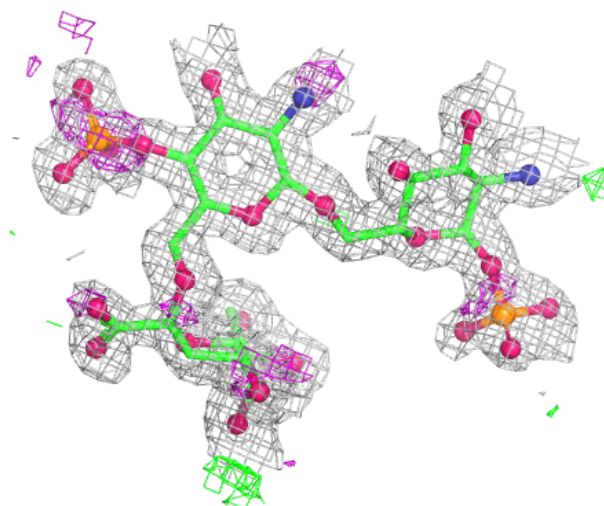
**Electron density around Chain K:**

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



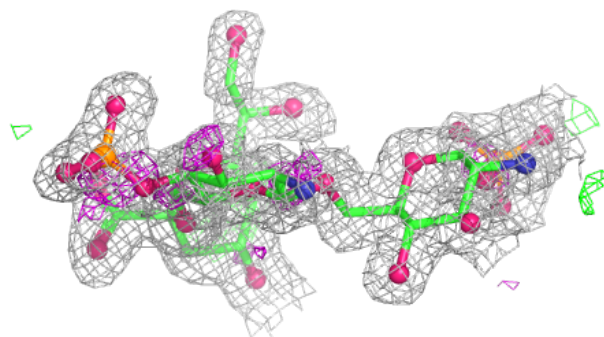
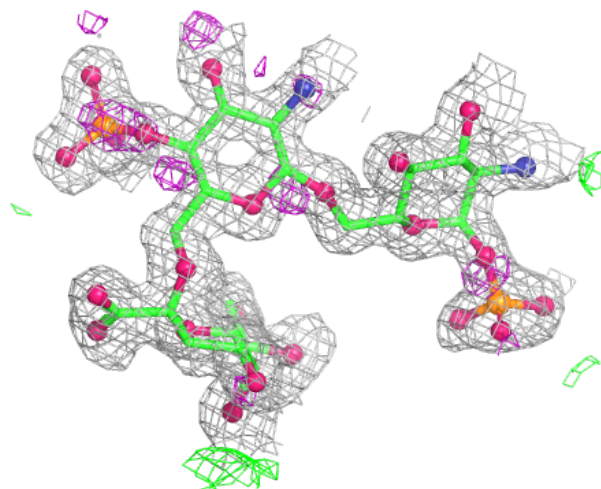
**Electron density around Chain L:**

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



**Electron density around Chain M:**

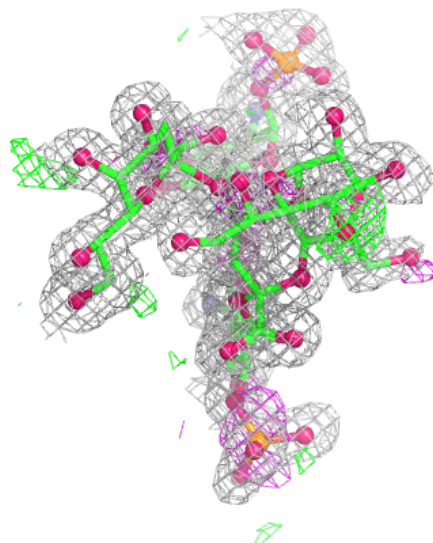
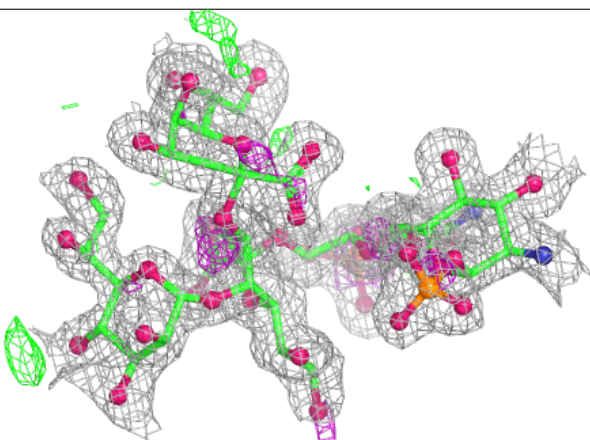
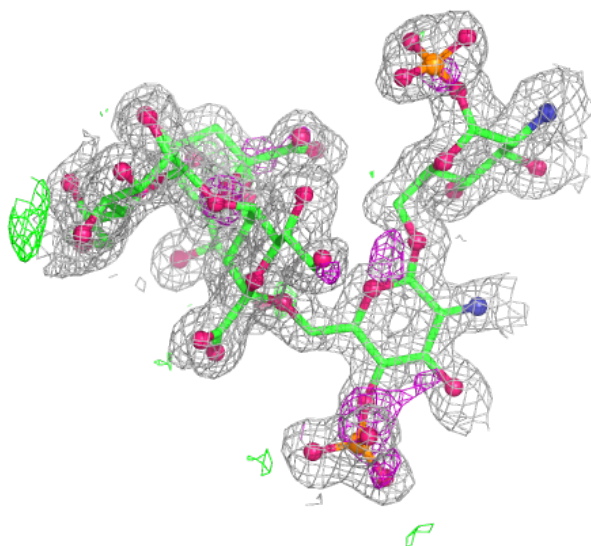
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





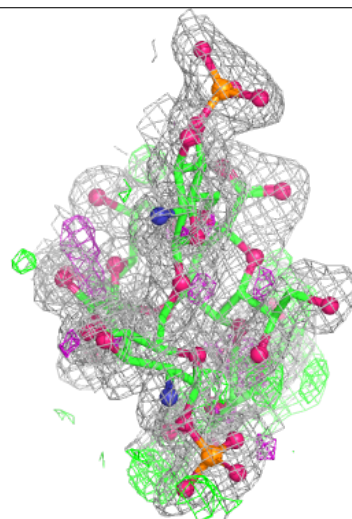
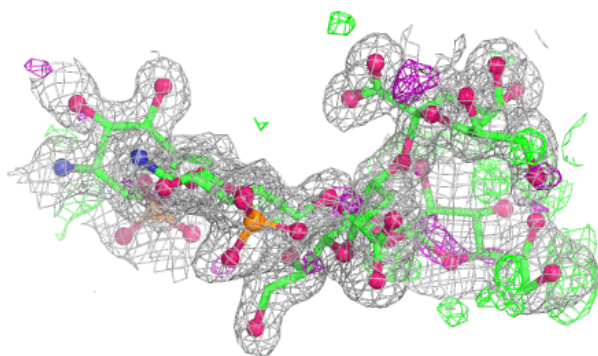
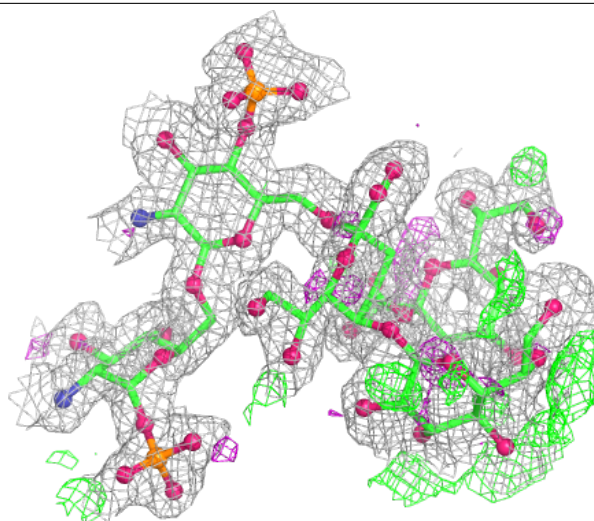
**Electron density around Chain H:**

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



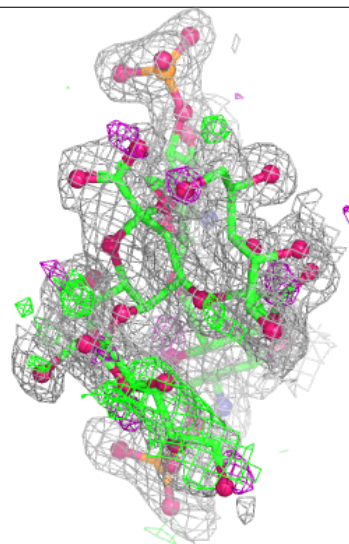
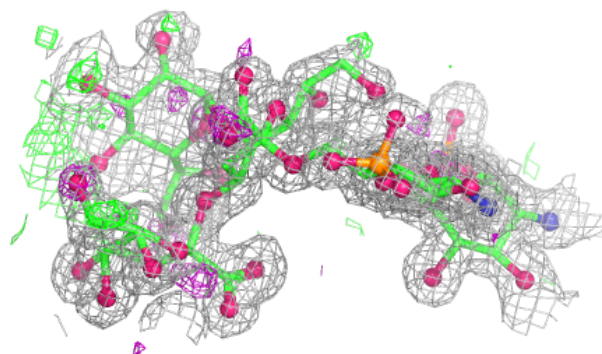
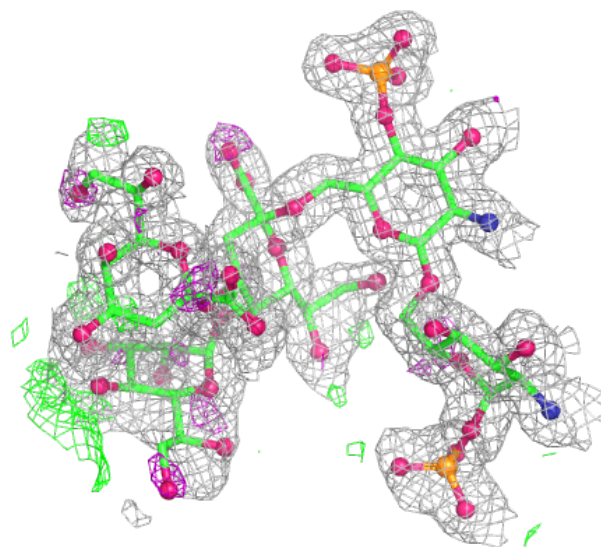
**Electron density around Chain I:**

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



**Electron density around Chain N:**

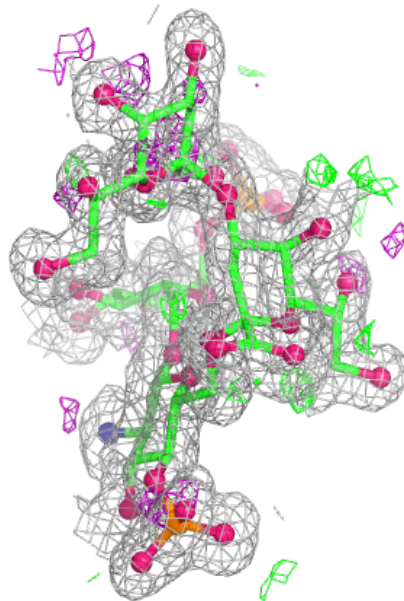
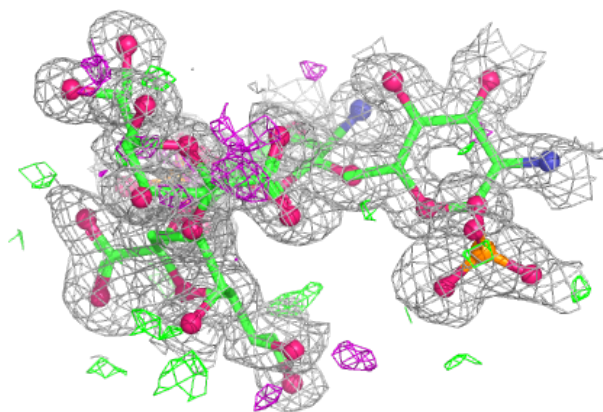
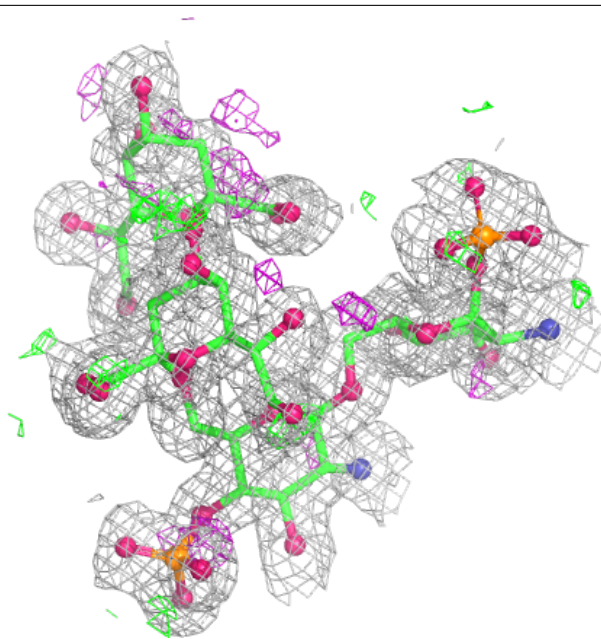
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

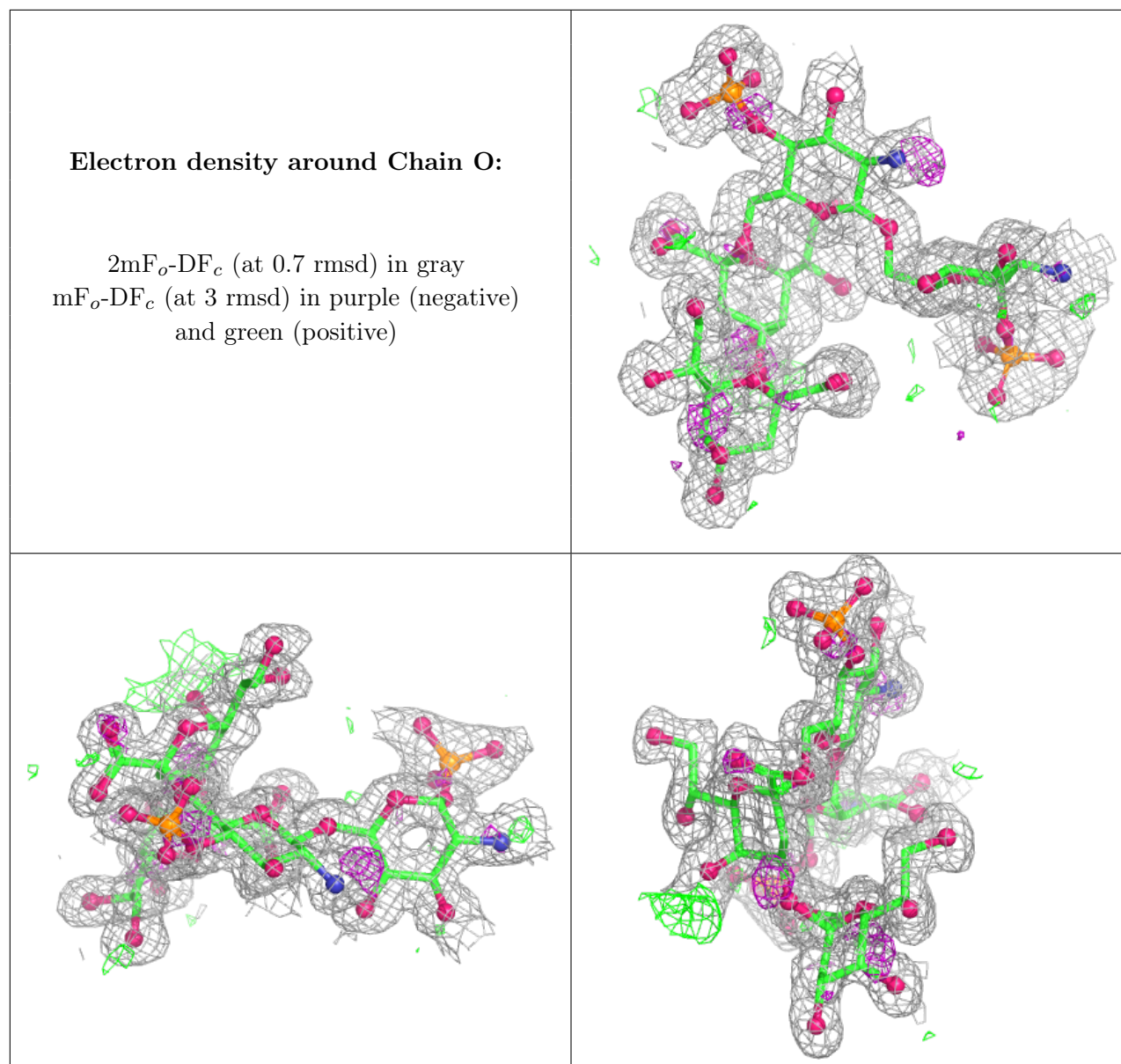




**Electron density around Chain J:**

$2mF_o-DF_c$  (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
11	DAO	E	405	5/14	0.37	0.29	52,54,57,63	0
9	FTT	E	404	14/17	0.52	0.26	38,46,48,57	0
9	FTT	C	413	14/17	0.52	0.27	33,47,58,61	0
11	DAO	A	417	5/14	0.54	0.39	55,57,59,63	0
10	MYR	A	416	6/16	0.55	0.30	47,52,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	FTT	B	407	14/17	0.57	0.19	35,40,55,61	0
9	FTT	D	417	11/17	0.60	0.26	46,51,67,67	0
9	FTT	D	425	14/17	0.62	0.25	33,45,53,62	0
11	DAO	D	424	5/14	0.63	0.50	47,58,58,73	0
11	DAO	C	414	5/14	0.63	0.19	49,50,63,63	0
9	FTT	F	406	14/17	0.65	0.18	38,42,47,48	0
11	DAO	B	412	5/14	0.66	0.64	39,48,59,60	0
6	C8E	A	407	5/21	0.66	0.25	18,20,26,28	0
10	MYR	E	409	6/16	0.67	0.33	41,44,51,54	0
11	DAO	E	410	5/14	0.67	0.37	49,54,55,56	0
11	DAO	D	418	3/14	0.68	0.44	51,51,52,53	0
9	FTT	D	414	14/17	0.69	0.19	36,47,53,54	0
9	FTT	A	415	16/17	0.69	0.25	27,39,59,66	0
11	DAO	A	419	8/14	0.70	0.17	40,41,44,57	0
10	MYR	D	423	6/16	0.73	0.18	43,47,49,50	0
10	MYR	B	411	6/16	0.73	0.23	43,60,68,68	0
6	C8E	A	402	3/21	0.74	0.27	33,33,41,41	0
6	C8E	D	405	6/21	0.74	0.15	30,37,41,42	0
9	FTT	D	421	13/17	0.75	0.15	27,30,46,71	0
9	FTT	A	414	13/17	0.76	0.19	29,33,39,41	0
6	C8E	B	404	8/21	0.76	0.14	41,46,47,47	0
9	FTT	D	415	11/17	0.76	0.18	33,36,41,41	0
6	C8E	E	401	6/21	0.76	0.19	44,52,63,65	0
6	C8E	C	406	8/21	0.77	0.20	30,33,33,35	0
6	C8E	D	406	8/21	0.77	0.16	48,52,54,58	0
6	C8E	A	409	8/21	0.78	0.19	29,34,38,38	0
6	C8E	D	407	8/21	0.79	0.20	25,41,44,48	0
11	DAO	C	426	8/14	0.79	0.21	37,62,72,73	0
9	FTT	A	418	14/17	0.80	0.19	39,44,66,68	0
6	C8E	B	405	8/21	0.80	0.11	38,39,41,41	0
10	MYR	F	411	11/16	0.80	0.12	26,31,36,36	0
6	C8E	A	410	7/21	0.80	0.20	38,39,40,41	0
6	C8E	C	409	10/21	0.80	0.14	35,38,50,54	0
10	MYR	D	419	5/16	0.80	0.29	16,25,37,38	0
6	C8E	C	410	7/21	0.81	0.26	23,24,39,43	0
6	C8E	D	404	6/21	0.81	0.12	32,41,41,43	0
6	C8E	D	408	11/21	0.81	0.23	27,41,43,43	0
9	FTT	E	407	12/17	0.81	0.16	26,29,36,39	0
6	C8E	B	402	3/21	0.81	0.10	46,46,50,55	0
6	C8E	C	404	6/21	0.82	0.16	28,41,49,51	0
6	C8E	C	403	3/21	0.82	0.13	45,45,46,50	0
6	C8E	C	408	11/21	0.82	0.21	36,39,45,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	FTT	B	409	13/17	0.82	0.18	21,26,42,44	0
6	C8E	C	402	7/21	0.83	0.29	25,32,38,43	0
6	C8E	A	404	6/21	0.83	0.14	39,46,50,51	0
6	C8E	D	402	4/21	0.83	0.18	32,33,34,39	0
6	C8E	B	403	5/21	0.83	0.20	30,32,33,41	0
6	C8E	A	403	4/21	0.83	0.13	62,71,76,79	0
9	FTT	F	415	11/17	0.83	0.12	22,23,28,34	0
6	C8E	B	401	9/21	0.83	0.16	31,43,63,64	0
9	FTT	B	410	16/17	0.84	0.22	23,30,36,39	0
9	FTT	A	413	15/17	0.84	0.13	15,22,26,38	0
9	FTT	F	416	16/17	0.84	0.17	21,32,42,45	0
6	C8E	D	410	6/21	0.84	0.22	40,43,45,45	0
6	C8E	D	403	6/21	0.84	0.21	39,44,51,56	0
9	FTT	D	416	13/17	0.84	0.17	29,43,53,54	0
10	MYR	F	417	12/16	0.85	0.13	29,32,44,50	0
9	FTT	D	420	16/17	0.85	0.14	17,23,28,30	0
9	FTT	E	408	15/17	0.85	0.23	25,31,40,41	0
8	KDO	D	413	15/16	0.85	0.21	14,22,27,27	0
9	FTT	F	410	16/17	0.85	0.13	28,33,39,41	0
11	DAO	D	412	6/14	0.86	0.10	44,48,51,57	0
6	C8E	D	409	4/21	0.86	0.31	21,23,30,39	0
6	C8E	F	402	4/21	0.86	0.16	41,44,47,47	0
7	PO4	D	411	5/5	0.86	0.26	32,37,40,47	0
9	FTT	D	422	16/17	0.86	0.18	28,36,41,43	0
11	DAO	F	418	8/14	0.86	0.19	34,49,64,66	0
7	PO4	E	402	5/5	0.87	0.25	34,35,41,44	0
6	C8E	A	405	4/21	0.87	0.13	77,80,84,87	0
6	C8E	A	408	8/21	0.87	0.23	19,29,52,66	0
10	MYR	C	425	9/16	0.87	0.15	33,55,63,71	0
9	FTT	C	423	13/17	0.88	0.11	20,22,34,39	0
6	C8E	C	407	11/21	0.88	0.18	33,35,43,47	0
6	C8E	A	406	5/21	0.88	0.11	57,64,67,74	0
8	KDO	A	412	15/16	0.88	0.24	18,23,30,30	0
6	C8E	C	401	3/21	0.88	0.21	45,45,50,51	0
9	FTT	E	406	14/17	0.89	0.11	18,21,25,26	0
9	FTT	C	415	16/17	0.89	0.14	23,32,37,38	0
7	PO4	A	411	5/5	0.90	0.21	36,36,41,47	0
9	FTT	F	407	12/17	0.90	0.13	19,24,43,48	0
11	DAO	C	421	10/14	0.90	0.12	25,30,32,33	0
9	FTT	F	409	12/17	0.90	0.11	21,26,34,38	0
8	KDO	E	403	15/16	0.90	0.17	19,21,26,27	0
6	C8E	F	403	8/21	0.91	0.17	40,43,47,47	0

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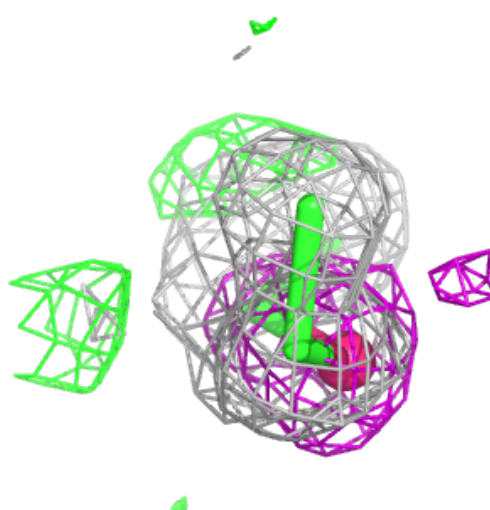
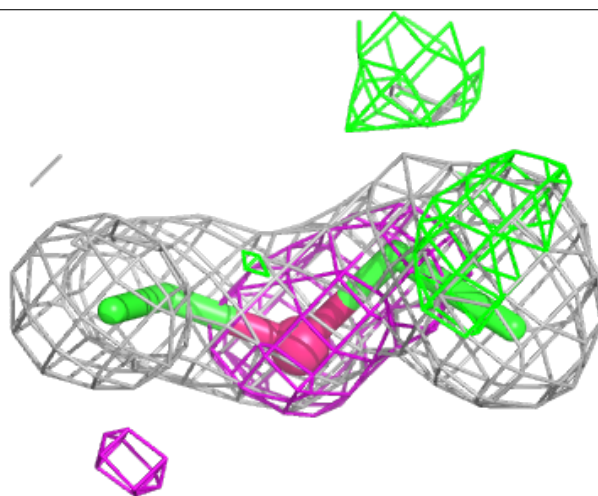
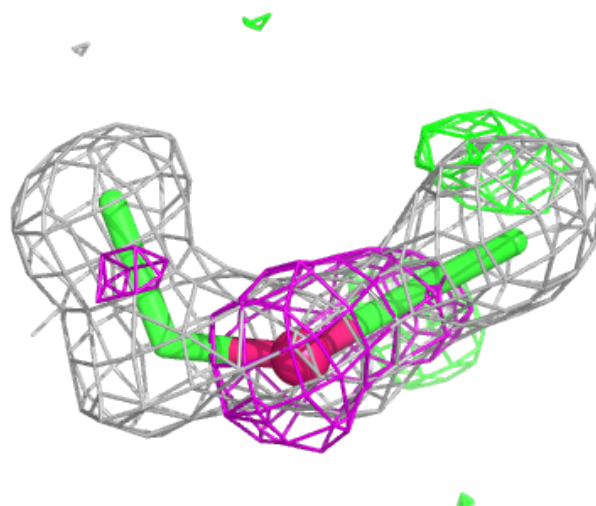
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MYR	C	419	8/16	0.91	0.15	22,30,32,32	0
7	PO4	B	406	5/5	0.91	0.19	31,33,40,44	0
7	PO4	F	404	5/5	0.91	0.21	31,36,45,45	0
9	FTT	C	416	11/17	0.91	0.11	18,20,24,30	0
11	DAO	C	420	13/14	0.92	0.10	22,27,31,33	0
9	FTT	B	408	15/17	0.92	0.10	19,21,36,37	0
11	DAO	F	412	5/14	0.92	0.11	26,27,35,40	0
9	FTT	C	422	16/17	0.92	0.11	15,20,27,31	0
7	PO4	C	411	5/5	0.93	0.24	32,35,44,44	0
6	C8E	C	405	3/21	0.93	0.16	26,26,28,35	0
9	FTT	C	424	16/17	0.93	0.10	18,30,41,41	0
6	C8E	F	401	3/21	0.93	0.10	21,21,30,37	0
9	FTT	F	408	13/17	0.94	0.12	19,31,46,46	0
9	FTT	F	414	14/17	0.94	0.09	16,18,24,27	0
11	DAO	F	413	5/14	0.94	0.16	33,34,49,62	0
9	FTT	C	418	13/17	0.94	0.14	19,26,52,55	0
9	FTT	C	417	16/17	0.96	0.09	18,20,30,34	0
5	SO4	A	401	5/5	0.98	0.09	17,19,22,27	0
5	SO4	D	401	5/5	0.99	0.11	18,21,25,29	0
12	CA	C	412	1/1	1.00	0.08	12,12,12,12	0
12	CA	F	405	1/1	1.00	0.09	13,13,13,13	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.



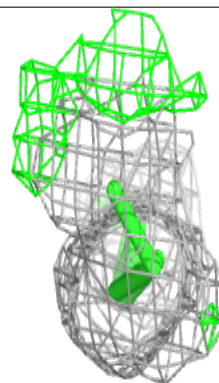
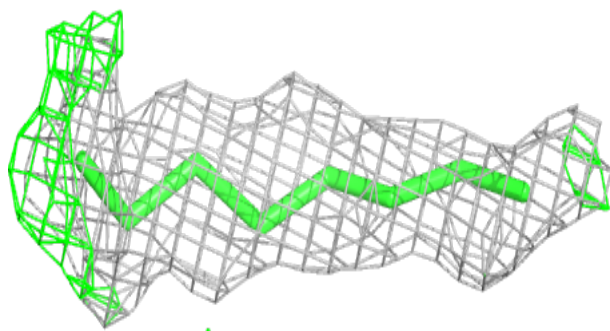
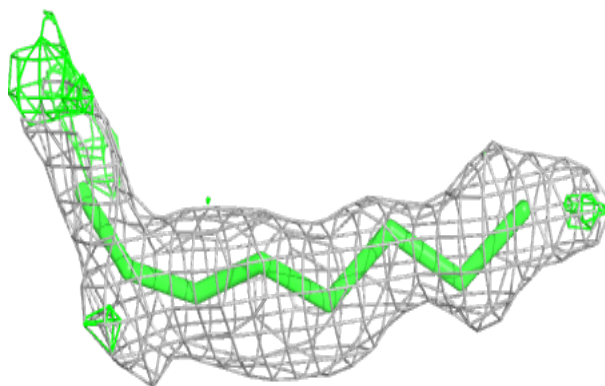
**Electron density around C8E A 407:**

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

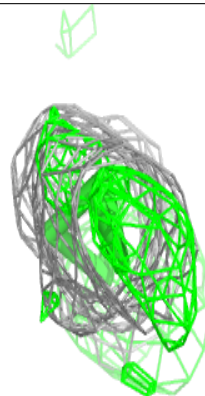
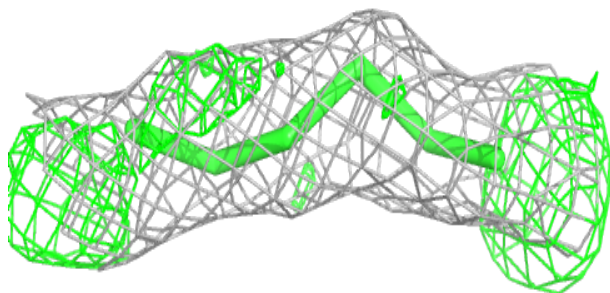
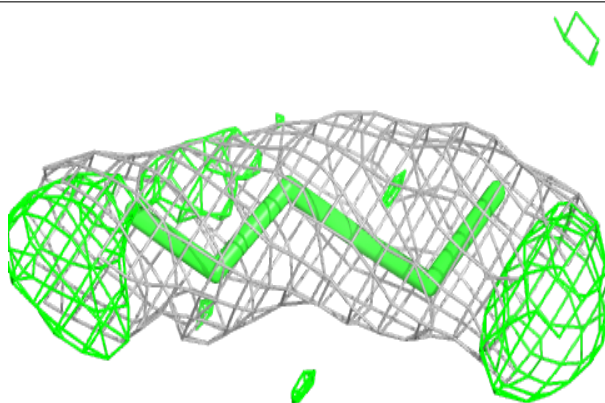


**Electron density around C8E B 404:**

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

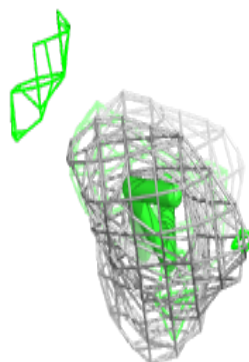
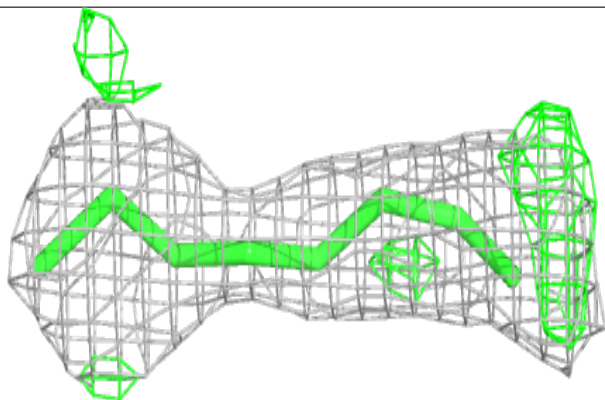
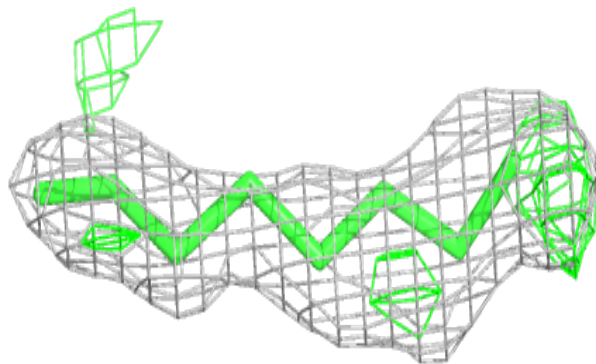
**Electron density around C8E E 401:**

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

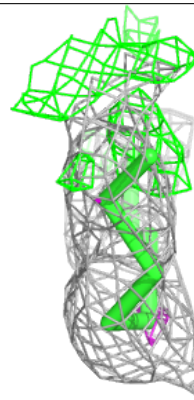
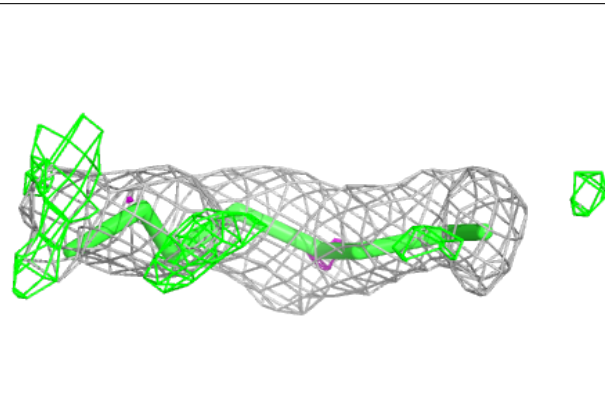
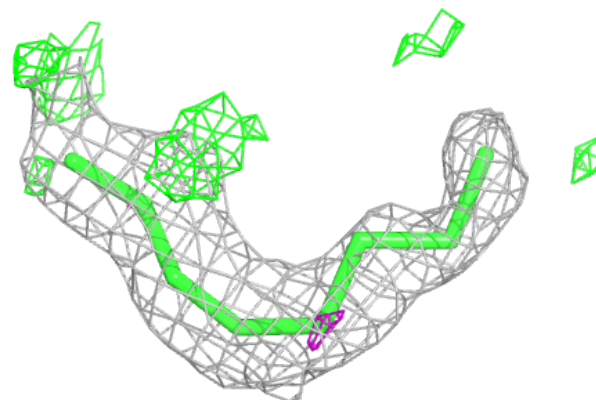


**Electron density around C8E D 406:**

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

**Electron density around C8E D 407:**

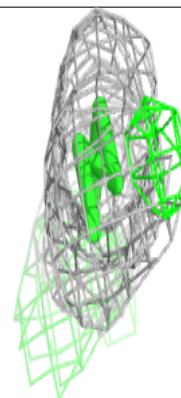
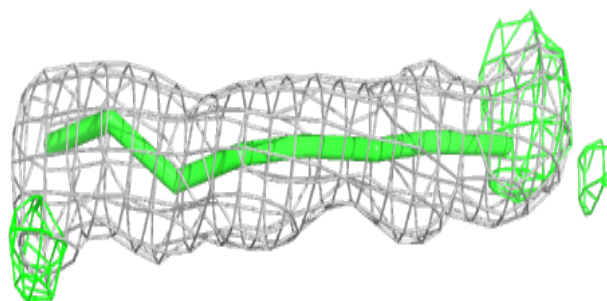
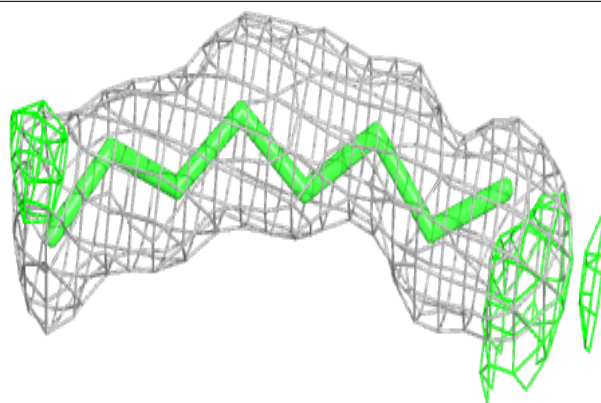
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



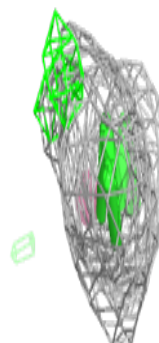
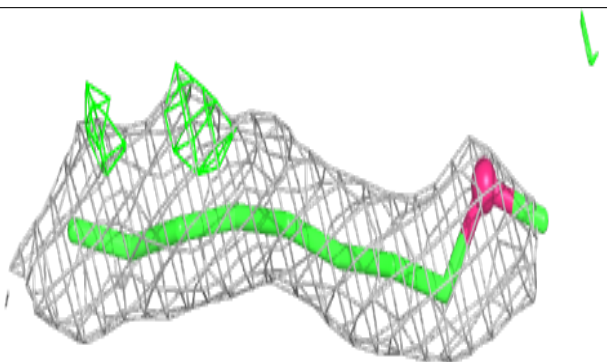
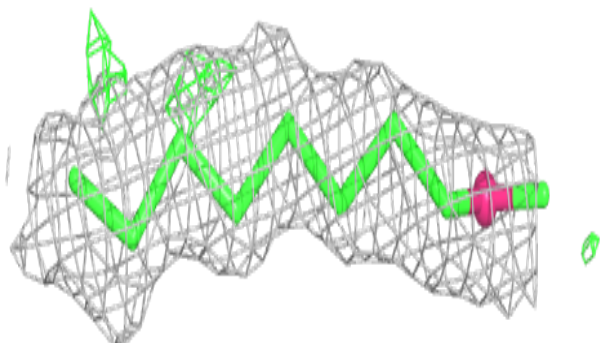


**Electron density around C8E B 405:**

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

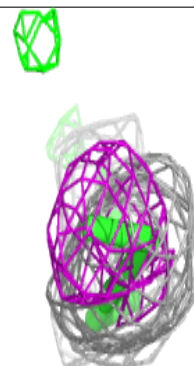
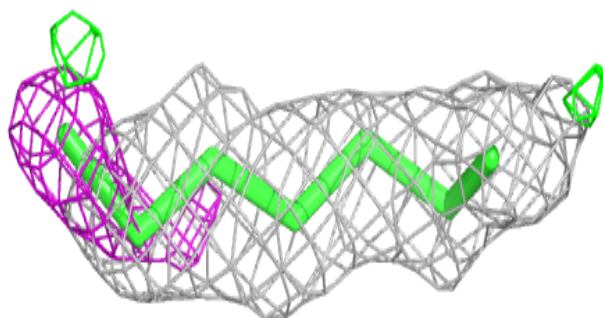
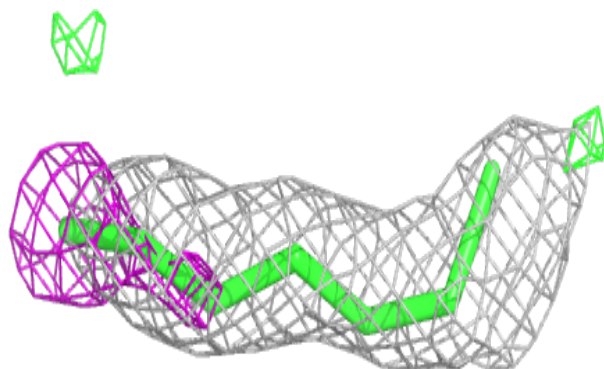
**Electron density around C8E C 409:**

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

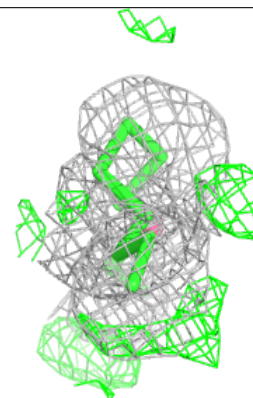
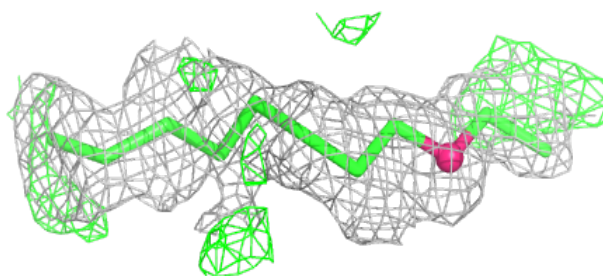
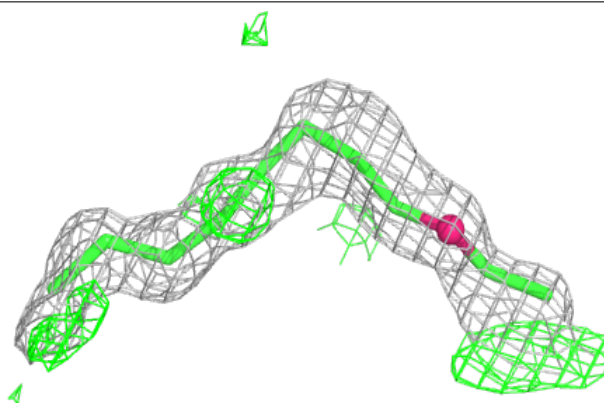


**Electron density around C8E C 410:**

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

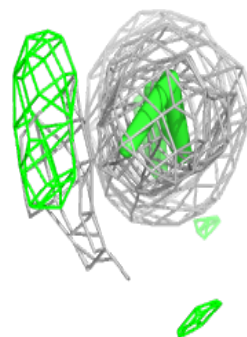
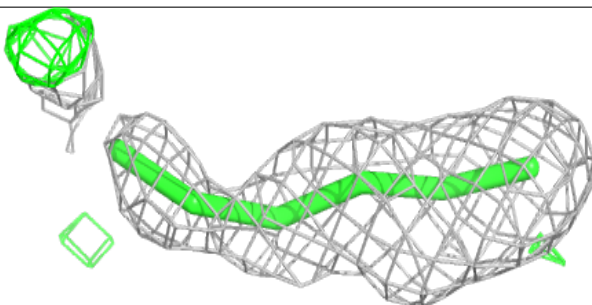
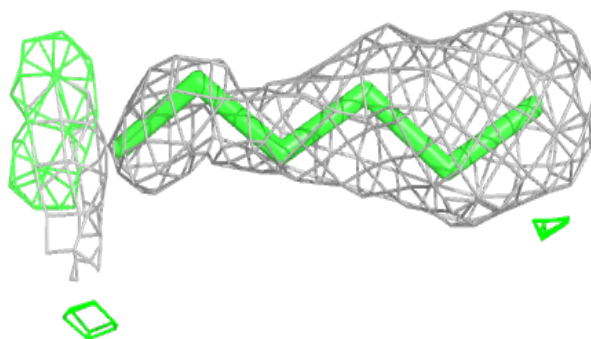
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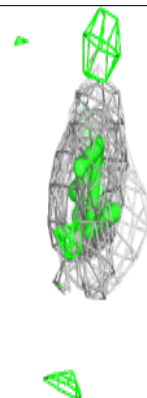
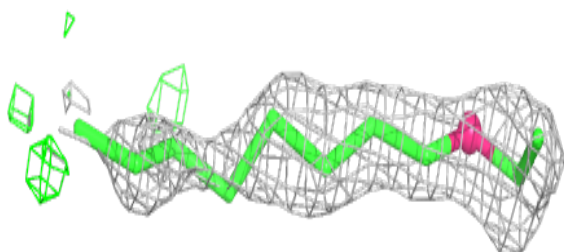
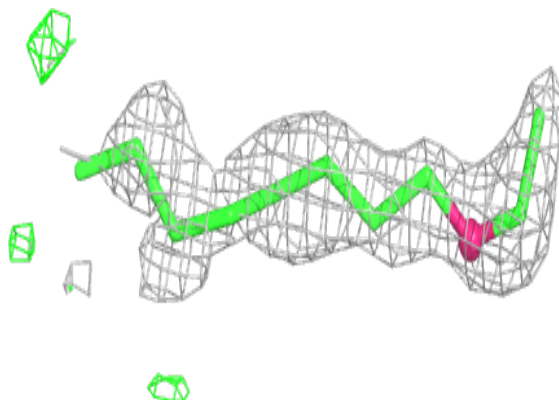


**Electron density around C8E C 404:**

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

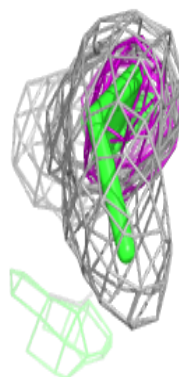
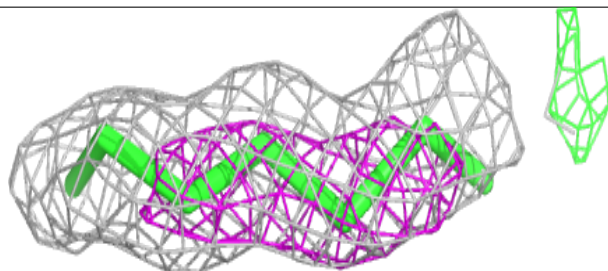
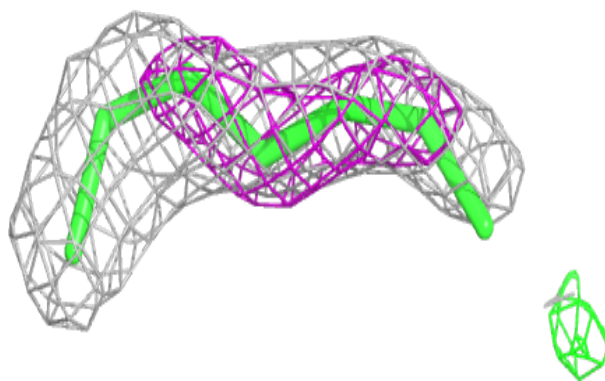
**Electron density around C8E C 408:**

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

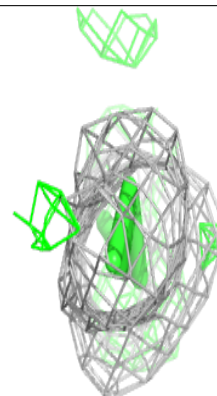
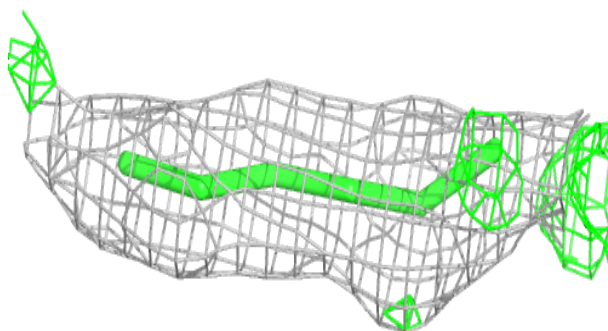
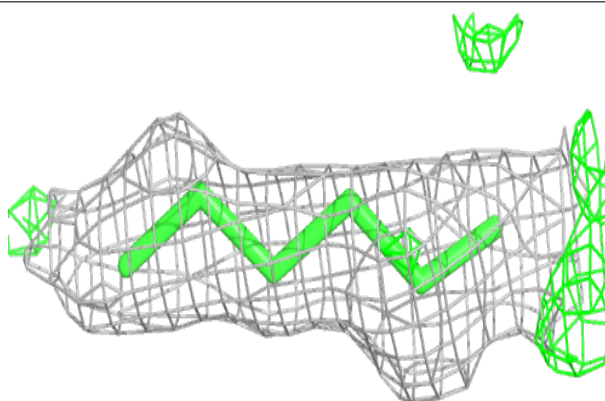


**Electron density around C8E C 402:**

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

**Electron density around C8E A 404:**

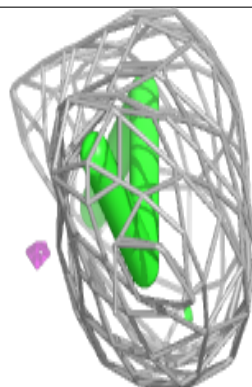
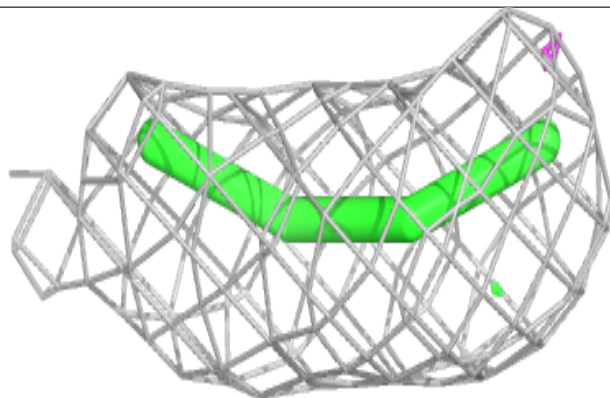
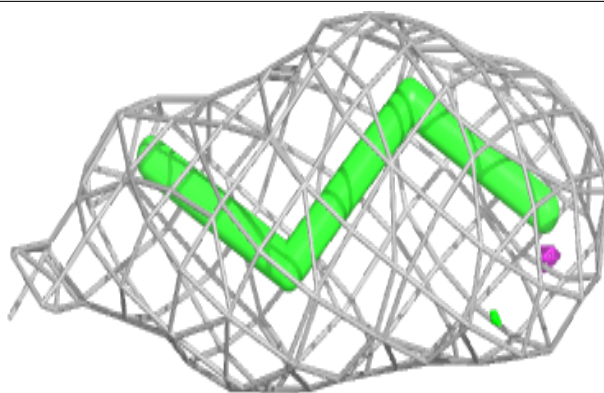
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



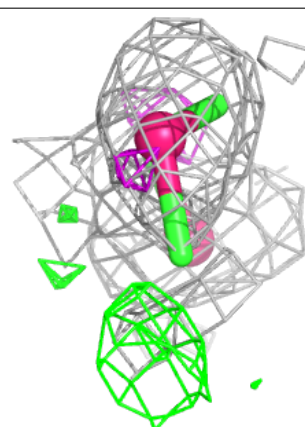
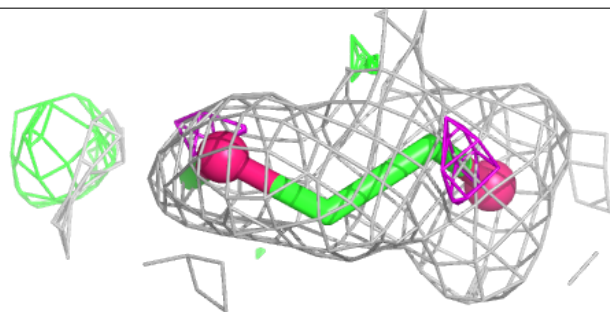
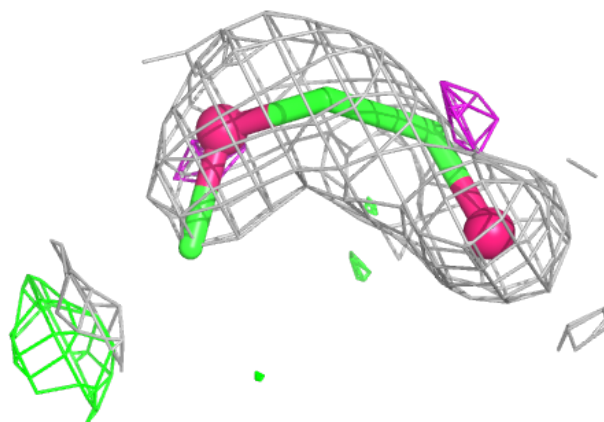


**Electron density around C8E D 402:**

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

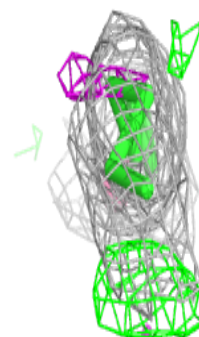
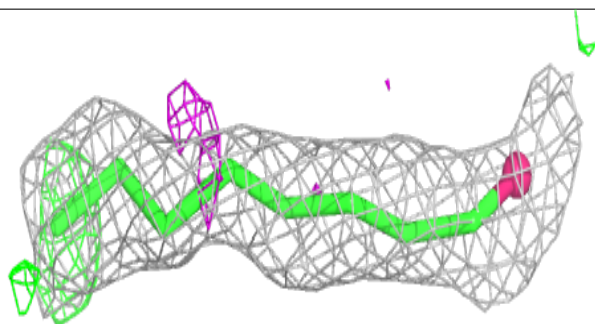
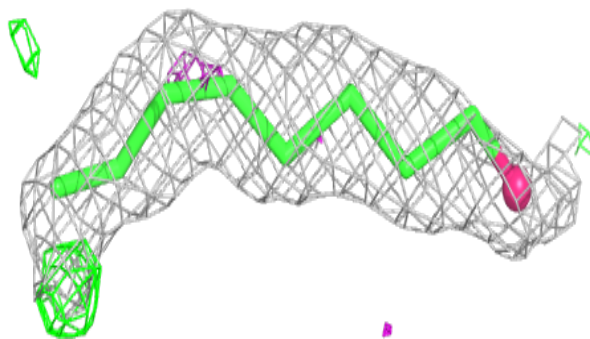
**Electron density around C8E B 403:**

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

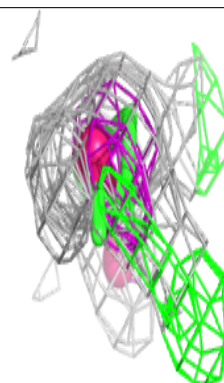
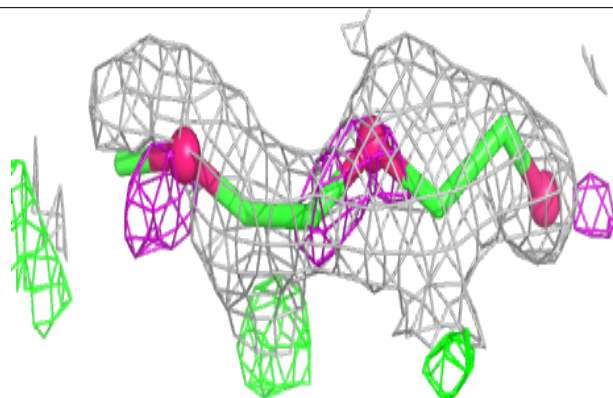
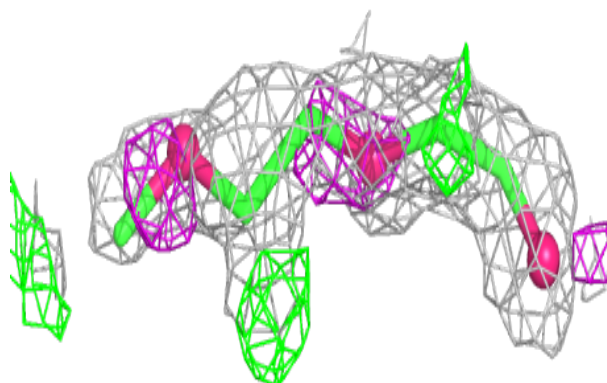


**Electron density around C8E B 401:**

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

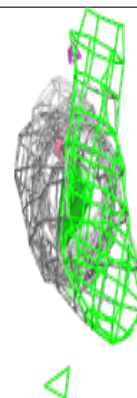
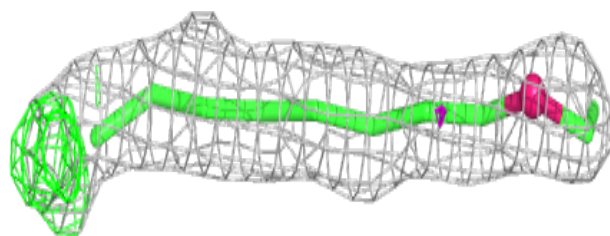
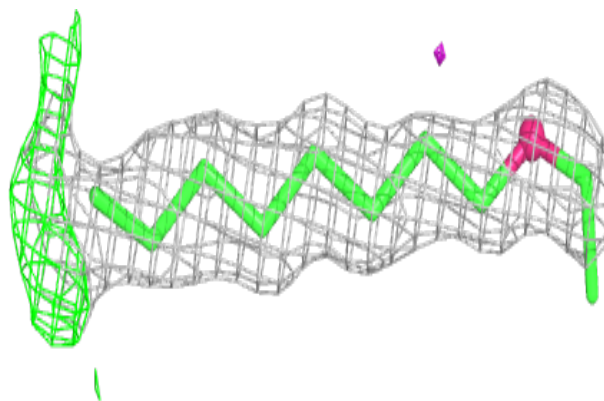
**Electron density around C8E A 408:**

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

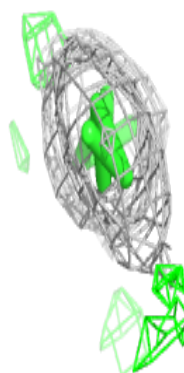
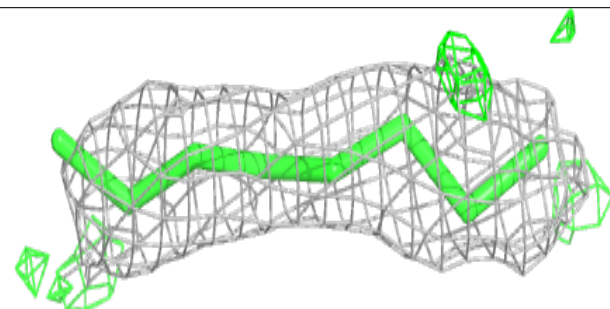
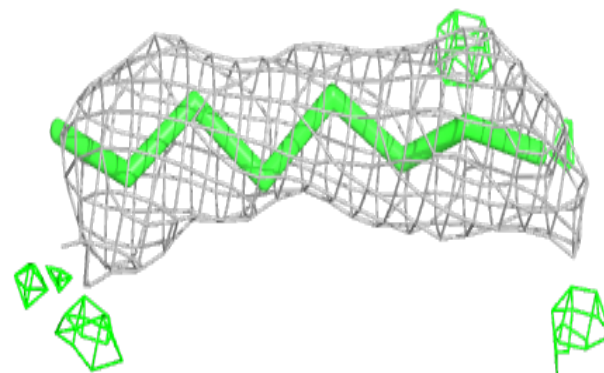


**Electron density around C8E C 407:**

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

**Electron density around C8E F 403:**

$2mF_o-DF_c$  (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.