



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:57 AM UTC

PDB ID : 5FVN / pdb_00005fvn
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

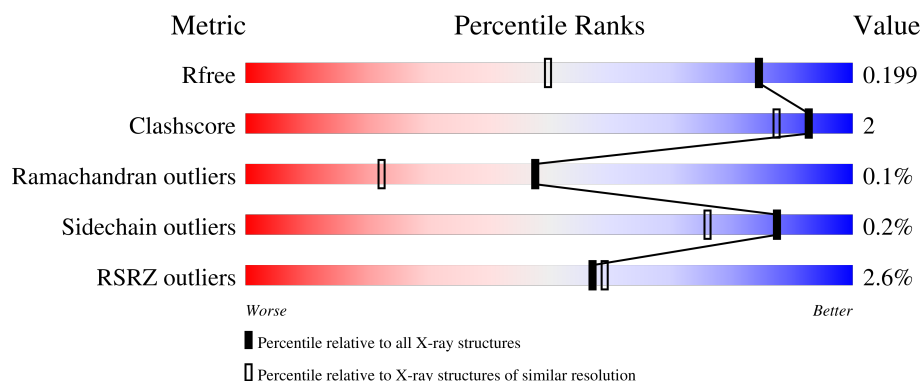
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



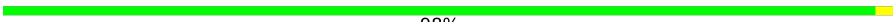
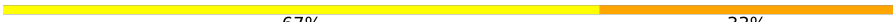
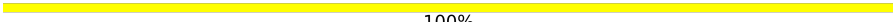
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 ≥ 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	2% 99%
1	B	342	3% 97%
1	C	342	3% 98%
1	D	342	5% 98%
1	E	342	3% 98%

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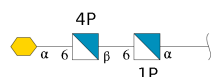
Mol	Chain	Length	Quality of chain
1	F	342	 98%
2	G	3	 67% 33%
2	K	3	 100%
2	L	3	 67% 33%
2	M	3	 67% 33%
3	H	5	 60% 40%
3	I	5	 40% 60%
3	N	5	 60% 40%
4	J	4	 50% 50%
4	O	4	 50% 50%

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

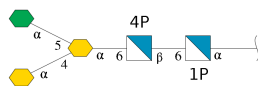
- Molecule 2 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.



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

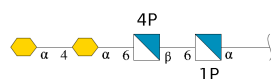
- Molecule 3 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyran

osonic 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.



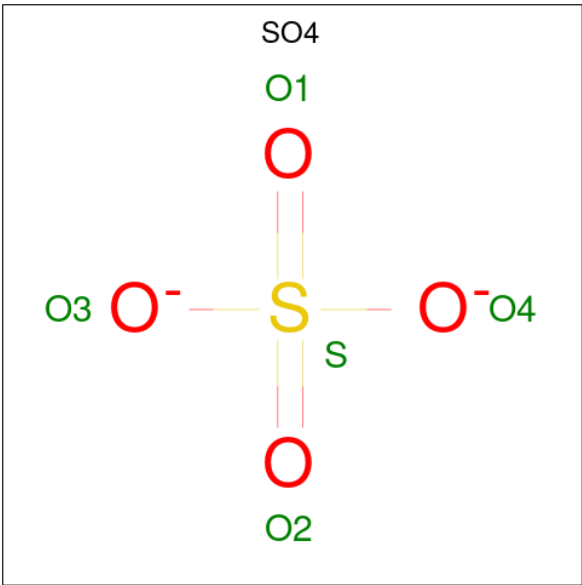
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	5	Total	C	N	O	P	0	0	0
			74	35	2	35	2			
3	I	5	Total	C	N	O	P	0	0	0
			74	35	2	35	2			
3	N	5	Total	C	N	O	P	0	0	0
			74	35	2	35	2			

- 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.



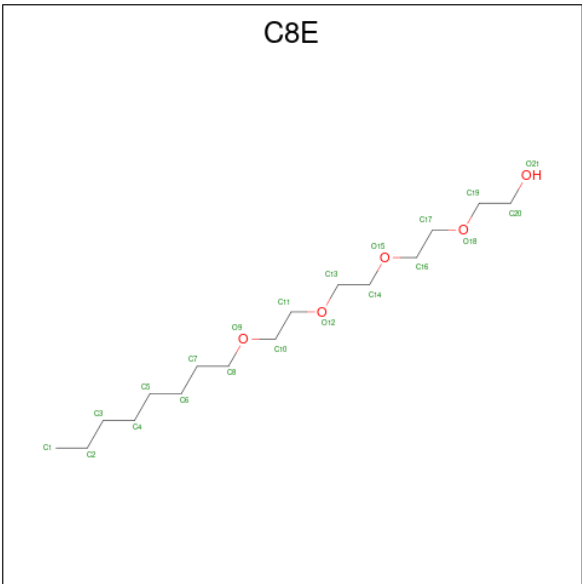
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	P	0	0	0
			61	28	2	29	2			
4	O	4	Total	C	N	O	P	0	0	0
			61	28	2	29	2			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



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

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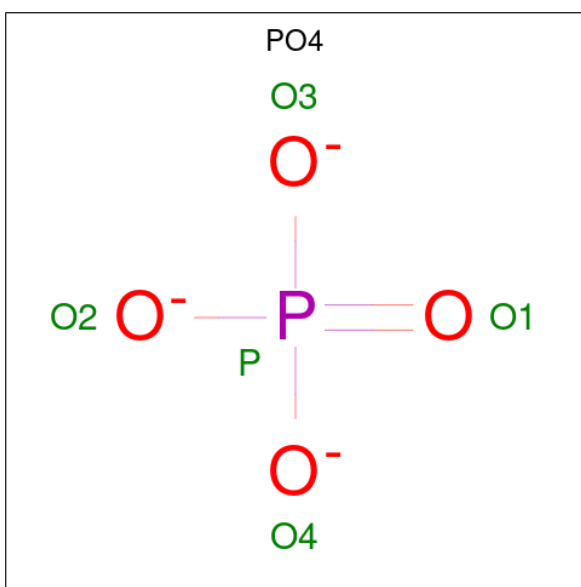
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 4 4	0	0
6	A	1	Total C 6 6	0	0
6	A	1	Total C 4 4	0	0
6	A	1	Total C 5 5	0	0
6	A	1	Total C O 5 4 1	0	0
6	A	1	Total C O 8 5 3	0	0
6	A	1	Total C 8 8	0	0
6	A	1	Total C 7 7	0	0
6	B	1	Total C O 9 8 1	0	0
6	B	1	Total C 3 3	0	0
6	B	1	Total C O 5 3 2	0	0
6	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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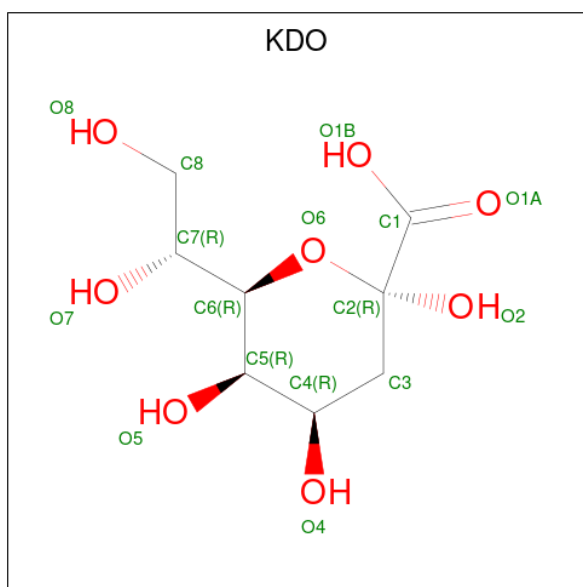
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 10 9 1	0	0
6	C	1	Total C 7 7	0	0
6	D	1	Total C 4 4	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 8 8	0	0
6	D	1	Total C 8 8	0	0
6	D	1	Total C O 11 10 1	0	0
6	D	1	Total C O 4 3 1	0	0
6	D	1	Total C 6 6	0	0
6	E	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 (CCD ID: PO4) (formula: O₄P).



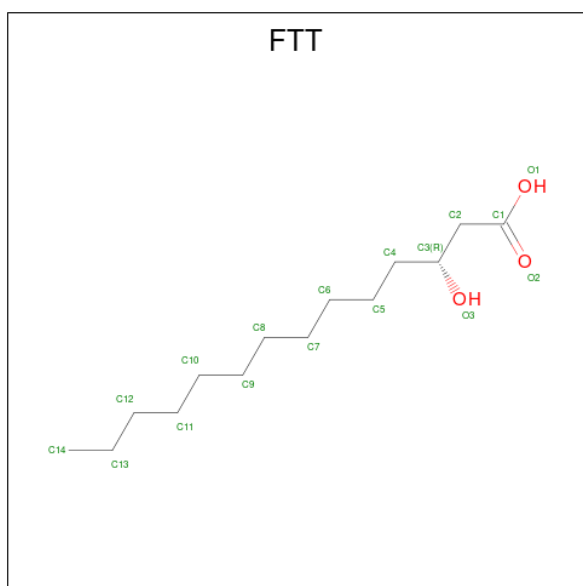
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid (CCD ID: KDO) (formula: C₈H₁₄O₈).



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 (CCD ID: FTT) (formula: $C_{14}H_{28}O_3$).



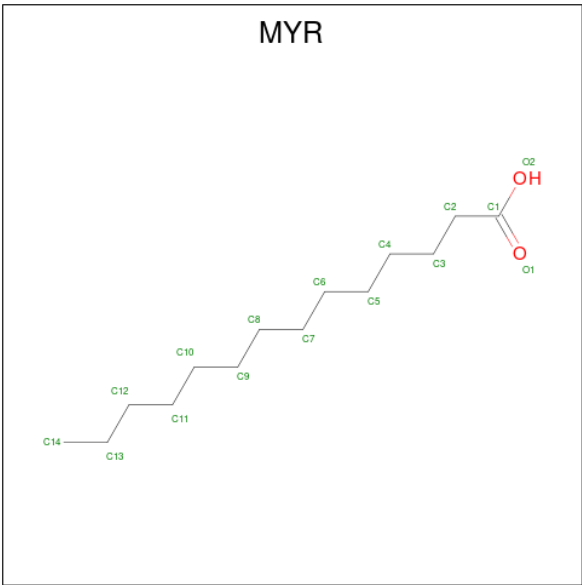
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			15	13	2		
9	A	1	Total	C	O	0	0
			13	11	2		
9	A	1	Total	C	O	0	0
			16	14	2		
9	A	1	Total	C	O	0	0
			14	12	2		
9	B	1	Total	C	O	0	0
			14	12	2		
9	B	1	Total	C	O	0	0
			15	13	2		
9	B	1	Total	C	O	0	0
			13	11	2		
9	B	1	Total	C	O	0	0
			16	14	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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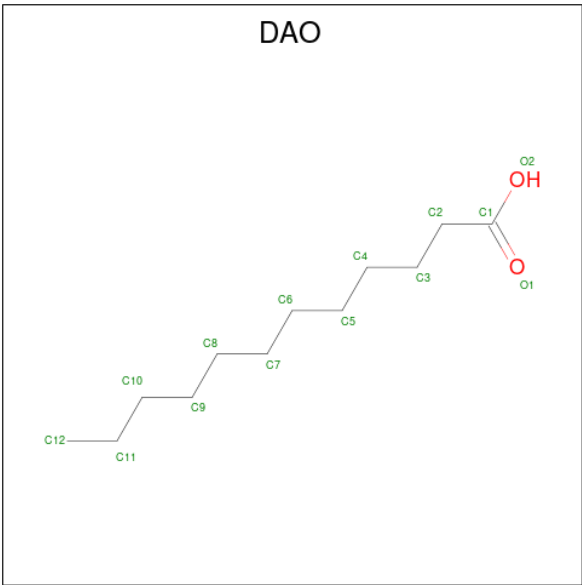
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			16	14	2		
9	D	1	Total	C	O	0	0
			14	12	2		
9	E	1	Total	C	O	0	0
			14	12	2		
9	E	1	Total	C	O	0	0
			14	12	2		
9	E	1	Total	C	O	0	0
			12	10	2		
9	E	1	Total	C	O	0	0
			15	13	2		
9	F	1	Total	C	O	0	0
			14	12	2		
9	F	1	Total	C	O	0	0
			12	10	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 (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



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 (CCD ID: DAO) (formula: C₁₂H₂₄O₂).



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 (CCD ID: 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		

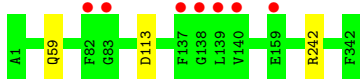
- Molecule 13 is water.

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		

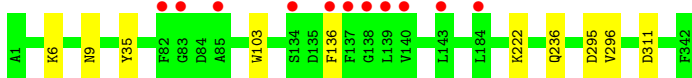
3 Residue-property plots [i](#)

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.

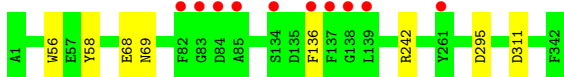
- Molecule 1: OMPC PORIN



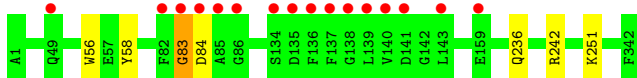
- Molecule 1: OMPC PORIN



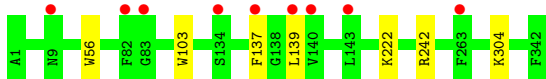
- Molecule 1: OMPC PORIN



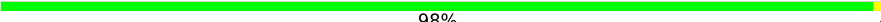
- Molecule 1: OMPC PORIN



- Molecule 1: OMPC PORIN

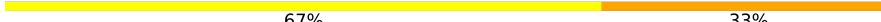


- Molecule 1: OMPC PORIN

Chain F:  98%

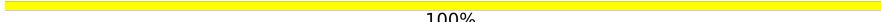


- Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain G:  67% 33%



- 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

Chain K:  100%

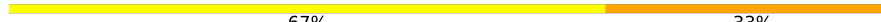


- Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain L:  67% 33%

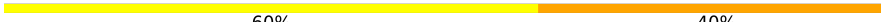


- Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain M:  67% 33%



- 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 H:  60% 40%

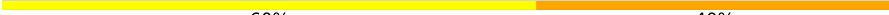


- Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

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, α , β , γ	109.75Å 123.26Å 116.01Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	115.99 – 1.45 115.99 – 1.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (115.99-1.45) 99.9 (115.99-1.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.155 , 0.183 (Not available) , 0.199	Depositor DCC
R_{free} test set	13914 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GMH, Z9M, C8E, SO4, MYR, KDO, GP1, FTT, PO4, CA, DAO

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	0.64	0/2799	0.80	2/3785 (0.1%)
1	B	0.63	0/2768	0.80	0/3743
1	C	0.63	0/2775	0.77	1/3753 (0.0%)
1	D	0.65	1/2784 (0.0%)	0.83	4/3765 (0.1%)
1	E	0.64	0/2782	0.80	1/3763 (0.0%)
1	F	0.61	0/2769	0.76	1/3745 (0.0%)
All	All	0.63	1/16677 (0.0%)	0.79	9/22554 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	84	ASP	CA-C	-6.86	1.44	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	ARG	NE-CZ-NH1	-8.33	113.17	121.50
1	D	242	ARG	NE-CZ-NH2	7.04	125.54	119.20
1	A	242	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	D	84	ASP	N-CA-C	6.94	121.42	112.26
1	F	242	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	C	242	ARG	NE-CZ-NH2	6.47	125.03	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	242	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	A	242	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	D	84	ASP	N-CA-CB	5.11	119.55	111.17

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2722	0	2520	2	0
1	B	2700	0	2475	8	0
1	C	2704	0	2491	6	0
1	D	2710	0	2492	4	0
1	E	2708	0	2498	3	0
1	F	2701	0	2488	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	47	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 2.

All (47) 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
4:O:3:KDO:HO4	4:O:4:KDO:C2	1.98	0.75
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
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
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:F:36:MET:HE1	1:F:38:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/342 (102%)	332 (95%)	16 (5%)	0	100	100
1	B	344/342 (101%)	329 (96%)	14 (4%)	1 (0%)	36	16
1	C	345/342 (101%)	330 (96%)	14 (4%)	1 (0%)	36	16
1	D	346/342 (101%)	329 (95%)	16 (5%)	1 (0%)	36	16
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%)	48	22

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%)	283 (100%)	0	100	100
1	B	279/275 (102%)	277 (99%)	2 (1%)	76	54
1	C	280/275 (102%)	280 (100%)	0	100	100
1	D	281/275 (102%)	281 (100%)	0	100	100
1	E	281/275 (102%)	280 (100%)	1 (0%)	84	70
1	F	279/275 (102%)	277 (99%)	2 (1%)	76	54
All	All	1683/1650 (102%)	1678 (100%)	5 (0%)	87	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	296[A]	VAL
1	B	296[B]	VAL
1	E	304	LYS
1	F	296[A]	VAL
1	F	296[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	B	226	ASN
1	B	236	GLN
1	B	239	ASN
1	C	122	GLN
1	D	226	ASN
1	D	236	GLN
1	D	275	GLN
1	E	239	ASN
1	F	226	ASN
1	F	275	GLN
1	F	341	GLN

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	1.65	1 (6%)	24,24,24	1.08	2 (8%)
2	Z9M	G	2	9,2	15,15,16	1.46	1 (6%)	20,22,24	1.24	3 (15%)
2	KDO	G	3	2	15,15,16	0.79	0	17,21,24	1.41	2 (11%)
3	GP1	H	1	9,3	15,16,16	1.66	1 (6%)	24,24,24	1.60	3 (12%)
3	Z9M	H	2	9,3	15,15,16	1.24	1 (6%)	20,22,24	1.15	1 (5%)
3	KDO	H	3	3	15,15,16	1.10	1 (6%)	17,21,24	1.29	2 (11%)
3	KDO	H	4	3	15,15,16	0.70	0	17,21,24	1.40	2 (11%)
3	GMH	H	5	3	13,13,14	0.64	0	16,18,20	1.20	2 (12%)
3	GP1	I	1	9,3	15,16,16	1.79	1 (6%)	24,24,24	1.10	2 (8%)
3	Z9M	I	2	9,3	15,15,16	1.66	1 (6%)	20,22,24	1.58	3 (15%)
3	KDO	I	3	3	15,15,16	1.13	1 (6%)	17,21,24	1.68	4 (23%)
3	KDO	I	4	12,3	15,15,16	0.66	0	17,21,24	1.56	3 (17%)
3	GMH	I	5	3	13,13,14	0.99	1 (7%)	16,18,20	1.34	3 (18%)
4	GP1	J	1	4,9	15,16,16	1.53	1 (6%)	24,24,24	1.33	3 (12%)
4	Z9M	J	2	4,9	15,15,16	1.35	1 (6%)	20,22,24	0.96	1 (5%)
4	KDO	J	3	4	15,15,16	0.96	1 (6%)	17,21,24	1.32	2 (11%)
4	KDO	J	4	4	15,15,16	0.82	0	17,21,24	1.57	4 (23%)
2	GP1	K	1	9,2	15,16,16	1.60	1 (6%)	24,24,24	2.44	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Z9M	K	2	9,2	15,15,16	1.49	1 (6%)	20,22,24	1.00	1 (5%)
2	KDO	K	3	2	14,14,16	0.77	0	16,19,24	2.14	2 (12%)
2	GP1	L	1	9,2	15,16,16	1.53	1 (6%)	24,24,24	0.98	2 (8%)
2	Z9M	L	2	9,2	15,15,16	1.40	1 (6%)	20,22,24	1.13	2 (10%)
2	KDO	L	3	2	15,15,16	0.69	0	17,21,24	1.61	6 (35%)
2	GP1	M	1	9,2	15,16,16	1.66	1 (6%)	24,24,24	0.95	2 (8%)
2	Z9M	M	2	9,2	15,15,16	1.59	1 (6%)	20,22,24	1.04	1 (5%)
2	KDO	M	3	2	15,15,16	0.69	0	17,21,24	1.40	3 (17%)
3	GP1	N	1	9,3	15,16,16	1.87	1 (6%)	24,24,24	0.93	1 (4%)
3	Z9M	N	2	9,3	15,15,16	1.65	1 (6%)	20,22,24	1.57	2 (10%)
3	KDO	N	3	3	15,15,16	1.05	1 (6%)	17,21,24	1.52	5 (29%)
3	KDO	N	4	12,3	15,15,16	0.62	0	17,21,24	1.61	3 (17%)
3	GMH	N	5	3	13,13,14	0.72	0	16,18,20	1.61	3 (18%)
4	GP1	O	1	4,9	15,16,16	1.57	1 (6%)	24,24,24	1.44	3 (12%)
4	Z9M	O	2	4,9	15,15,16	1.43	1 (6%)	20,22,24	0.90	1 (5%)
4	KDO	O	3	4	15,15,16	0.95	1 (6%)	17,21,24	1.44	3 (17%)
4	KDO	O	4	4	15,15,16	0.66	0	17,21,24	1.50	3 (17%)

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	-	0/10/26/30	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	-	0/10/26/30	0/1/1/1
3	KDO	H	4	3	-	1/10/26/30	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	-	1/7/24/27	0/1/1/1
3	KDO	I	3	3	-	0/10/26/30	0/1/1/1
3	KDO	I	4	12,3	-	2/10/26/30	0/1/1/1
3	GMH	I	5	3	-	5/6/23/26	0/1/1/1
4	GP1	J	1	4,9	-	0/6/27/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Z9M	J	2	4,9	-	0/7/24/27	0/1/1/1
4	KDO	J	3	4	-	0/10/26/30	0/1/1/1
4	KDO	J	4	4	-	0/10/26/30	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	-	2/10/22/30	0/1/1/1
2	GP1	L	1	9,2	-	0/6/27/27	0/1/1/1
2	Z9M	L	2	9,2	-	0/7/24/27	0/1/1/1
2	KDO	L	3	2	-	0/10/26/30	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	-	0/10/26/30	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	-	0/10/26/30	0/1/1/1
3	KDO	N	4	12,3	-	5/10/26/30	0/1/1/1
3	GMH	N	5	3	-	3/6/23/26	0/1/1/1
4	GP1	O	1	4,9	-	0/6/27/27	0/1/1/1
4	Z9M	O	2	4,9	-	0/7/24/27	0/1/1/1
4	KDO	O	3	4	-	0/10/26/30	0/1/1/1
4	KDO	O	4	4	-	1/10/26/30	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	GP1	P4B-O1	6.83	1.71	1.59
3	I	1	GP1	P4B-O1	-6.34	1.48	1.59
3	H	1	GP1	P4B-O1	-6.09	1.48	1.59
3	N	2	Z9M	P1-O4	-6.03	1.49	1.59
2	G	1	GP1	P4B-O1	-5.97	1.49	1.59
2	M	1	GP1	P4B-O1	-5.93	1.49	1.59
3	I	2	Z9M	P1-O4	-5.92	1.49	1.59
2	M	2	Z9M	P1-O4	-5.84	1.49	1.59
2	K	1	GP1	P4B-O1	-5.79	1.49	1.59
4	O	1	GP1	P4B-O1	-5.76	1.49	1.59
4	J	1	GP1	P4B-O1	-5.60	1.49	1.59
2	K	2	Z9M	P1-O4	-5.59	1.49	1.59
2	L	1	GP1	P4B-O1	-5.55	1.49	1.59
2	G	2	Z9M	P1-O4	-5.31	1.50	1.59
4	O	2	Z9M	P1-O4	-5.16	1.50	1.59
2	L	2	Z9M	P1-O4	-4.91	1.50	1.59
4	J	2	Z9M	P1-O4	-4.75	1.51	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	Z9M	P1-O4	-4.31	1.52	1.59
3	I	3	KDO	O5-C5	-3.64	1.33	1.43
3	H	3	KDO	O5-C5	-3.35	1.34	1.43
3	N	3	KDO	O5-C5	-2.96	1.35	1.43
4	O	3	KDO	O1B-C1	-2.65	1.22	1.30
3	I	5	GMH	O5-C5	2.21	1.45	1.43
4	J	3	KDO	C2-C1	-2.14	1.49	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	GP1	P4B-O1-C1	8.30	145.78	123.54
2	K	3	KDO	O6-C6-C5	7.09	117.80	109.78
2	K	1	GP1	O1-P4B-O8B	-5.82	88.58	109.33
3	H	1	GP1	O1-P4B-O8B	5.33	128.34	109.33
3	N	2	Z9M	P1-O4-C4	5.16	137.22	123.43
3	I	2	Z9M	P1-O4-C4	4.81	136.28	123.43
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	4.48	116.58	110.56
3	I	4	KDO	O6-C2-C3	4.47	116.57	110.56
4	O	4	KDO	O6-C2-C3	4.46	116.56	110.56
2	K	1	GP1	O9B-P4B-O1	3.63	120.00	105.85
3	N	4	KDO	O1A-C1-C2	-3.63	115.01	122.85
4	J	4	KDO	O6-C2-C3	3.55	115.32	110.56
3	N	2	Z9M	C1-O5-C5	3.50	116.87	112.19
3	H	5	GMH	C1-O5-C5	3.47	117.17	111.48
4	J	1	GP1	O9B-P4B-O1	3.39	119.06	105.85
4	J	1	GP1	O1-C1-C2	3.37	114.50	108.40
3	H	1	GP1	O9B-P4B-O1	-3.28	93.07	105.85
4	J	4	KDO	O4-C4-C3	-3.17	101.96	109.86
4	J	3	KDO	C4-C5-C6	-3.11	104.22	110.51
2	K	3	KDO	O1B-C1-C2	3.10	120.77	112.71
2	G	3	KDO	C4-C5-C6	-3.05	104.35	110.51
3	N	4	KDO	O6-C2-C3	3.04	114.65	110.56
3	I	3	KDO	C3-C4-C5	2.93	114.88	110.67
4	O	4	KDO	O1A-C1-C2	-2.91	116.56	122.85
2	L	2	Z9M	P1-O4-C4	2.90	131.18	123.43
2	K	1	GP1	O1-C1-C2	2.87	113.60	108.40
3	I	2	Z9M	C1-O5-C5	2.87	116.03	112.19
3	I	3	KDO	O5-C5-C4	-2.84	104.25	110.05
3	N	4	KDO	O1B-C1-C2	2.83	120.07	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	3	KDO	O1A-C1-C2	-2.82	116.75	122.85
4	O	3	KDO	C4-C5-C6	-2.82	104.81	110.51
2	L	3	KDO	C4-C5-C6	-2.77	104.91	110.51
3	I	3	KDO	C4-C5-C6	-2.77	104.91	110.51
2	K	1	GP1	O7B-P4B-O1	2.75	116.57	105.85
3	H	3	KDO	C4-C5-C6	-2.73	104.99	110.51
4	J	2	Z9M	P1-O4-C4	2.72	130.69	123.43
3	N	1	GP1	O3-C3-C2	-2.71	105.34	110.22
2	G	2	Z9M	P1-O4-C4	2.71	130.67	123.43
3	H	2	Z9M	P1-O4-C4	2.71	130.67	123.43
2	K	2	Z9M	C1-O5-C5	2.71	115.81	112.19
3	N	3	KDO	C4-C5-C6	-2.68	105.09	110.51
3	I	1	GP1	O7B-P4B-O1	2.63	116.09	105.85
3	H	4	KDO	O1A-C1-C2	-2.57	117.30	122.85
2	L	1	GP1	O1-C1-C2	2.55	113.02	108.40
2	M	3	KDO	C4-C5-C6	-2.52	105.41	110.51
3	N	3	KDO	O1A-C1-C2	-2.50	117.46	122.85
2	M	1	GP1	O1-C1-C2	2.49	112.91	108.40
2	L	3	KDO	O1B-C1-C2	2.48	119.16	112.71
4	O	2	Z9M	P1-O4-C4	2.46	129.99	123.43
2	M	2	Z9M	C1-C2-N2	-2.45	107.17	111.38
3	I	1	GP1	O1-C1-C2	2.42	112.78	108.40
4	J	4	KDO	O1A-C1-C2	-2.40	117.66	122.85
2	L	3	KDO	O1A-C1-C2	-2.39	117.69	122.85
3	I	5	GMH	C1-O5-C5	2.38	115.37	111.48
4	O	3	KDO	O1B-C1-C2	2.37	118.87	112.71
2	M	3	KDO	C3-C4-C5	2.36	114.07	110.67
4	J	1	GP1	O3-C3-C4	-2.33	104.89	110.38
3	I	5	GMH	O5-C1-C2	-2.32	105.25	110.79
2	G	2	Z9M	O7-P1-O4	2.31	114.84	105.85
4	J	3	KDO	O1A-C1-C2	-2.30	117.87	122.85
3	N	3	KDO	C3-C4-C5	2.29	113.97	110.67
3	H	5	GMH	C1-C2-C3	2.26	112.94	109.64
3	N	3	KDO	O1B-C1-C2	2.22	118.48	112.71
3	I	3	KDO	O6-C6-C7	2.21	110.89	106.60
3	N	3	KDO	O5-C5-C4	-2.20	105.56	110.05
4	O	1	GP1	O9B-P4B-O1	2.20	114.41	105.85
2	L	1	GP1	O7B-P4B-O1	2.19	114.40	105.85
3	I	4	KDO	O8-C8-C7	-2.18	106.57	111.16
2	L	2	Z9M	O4-C4-C5	2.17	113.36	108.76
2	K	1	GP1	O5-C1-O1	-2.16	108.55	111.36
2	L	3	KDO	C3-C4-C5	2.15	113.76	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	GP1	O1-P4B-O8B	2.13	116.94	109.33
3	I	5	GMH	O2-C2-C1	2.13	114.10	109.22
4	J	4	KDO	O4-C4-C5	2.13	114.56	110.15
2	L	3	KDO	O4-C4-C5	-2.11	105.78	110.15
2	L	3	KDO	O6-C2-C3	-2.09	107.74	110.56
2	G	1	GP1	O1-P4B-O8B	-2.08	101.91	109.33
2	G	3	KDO	O5-C5-C6	2.08	115.26	109.94
2	G	2	Z9M	O4-C4-C5	2.07	113.14	108.76
3	N	5	GMH	O2-C2-C3	2.06	114.43	110.15
2	M	3	KDO	O1B-C1-C2	2.06	118.08	112.71
3	H	3	KDO	C3-C4-C5	2.06	113.64	110.67
4	O	1	GP1	O3-C3-C4	-2.05	105.53	110.38
3	I	2	Z9M	O8-P1-O4	2.05	113.82	105.85
4	O	4	KDO	O1B-C1-C2	2.04	118.02	112.71
3	H	1	GP1	O1-C1-C2	2.04	112.10	108.40
2	G	1	GP1	O1-C1-C2	2.02	112.06	108.40
3	I	4	KDO	O6-C6-C5	-2.01	105.09	107.94
3	N	5	GMH	O7-C7-C6	-2.01	106.93	111.16

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	5	GMH	O5-C5-C6-C7
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	K	3	KDO	C6-C7-C8-O8
3	I	4	KDO	C5-C6-C7-C8
3	N	5	GMH	C4-C5-C6-C7
3	I	5	GMH	O5-C5-C6-O6
3	I	2	Z9M	C4-O4-P1-O9
3	N	4	KDO	O1A-C1-C2-O6
4	O	4	KDO	O1A-C1-C2-O6
3	H	4	KDO	O1A-C1-C2-O6
3	I	5	GMH	C4-C5-C6-C7
3	I	4	KDO	O6-C6-C7-O7
3	N	4	KDO	C5-C6-C7-O7
3	N	5	GMH	C4-C5-C6-O6
3	N	4	KDO	O1A-C1-C2-C3

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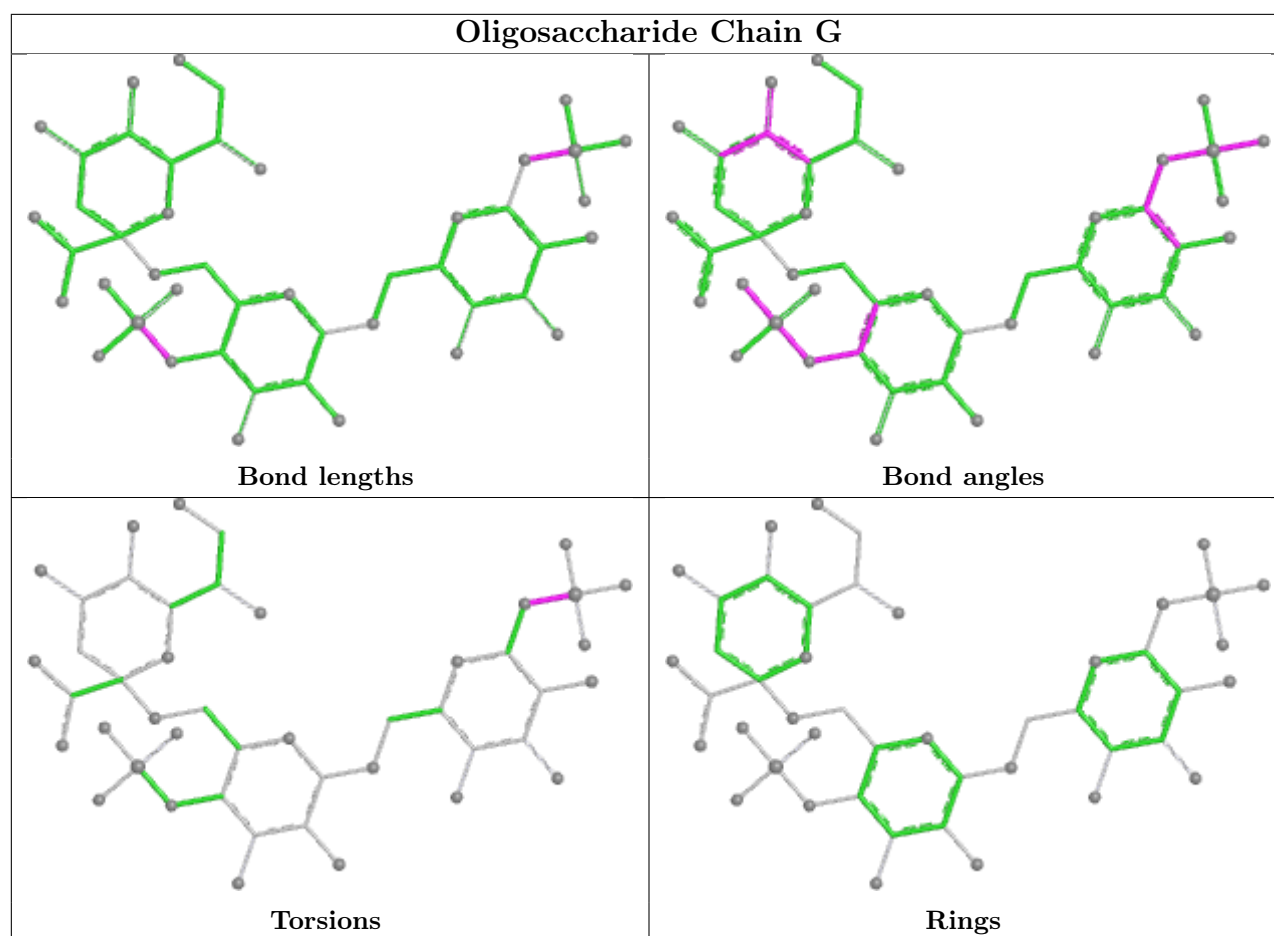
Mol	Chain	Res	Type	Atoms
2	K	3	KDO	O7-C7-C8-O8
2	G	1	GP1	C1-O1-P4B-O9B
2	M	1	GP1	C1-O1-P4B-O9B
2	G	1	GP1	C1-O1-P4B-O8B
3	H	1	GP1	C1-O1-P4B-O8B

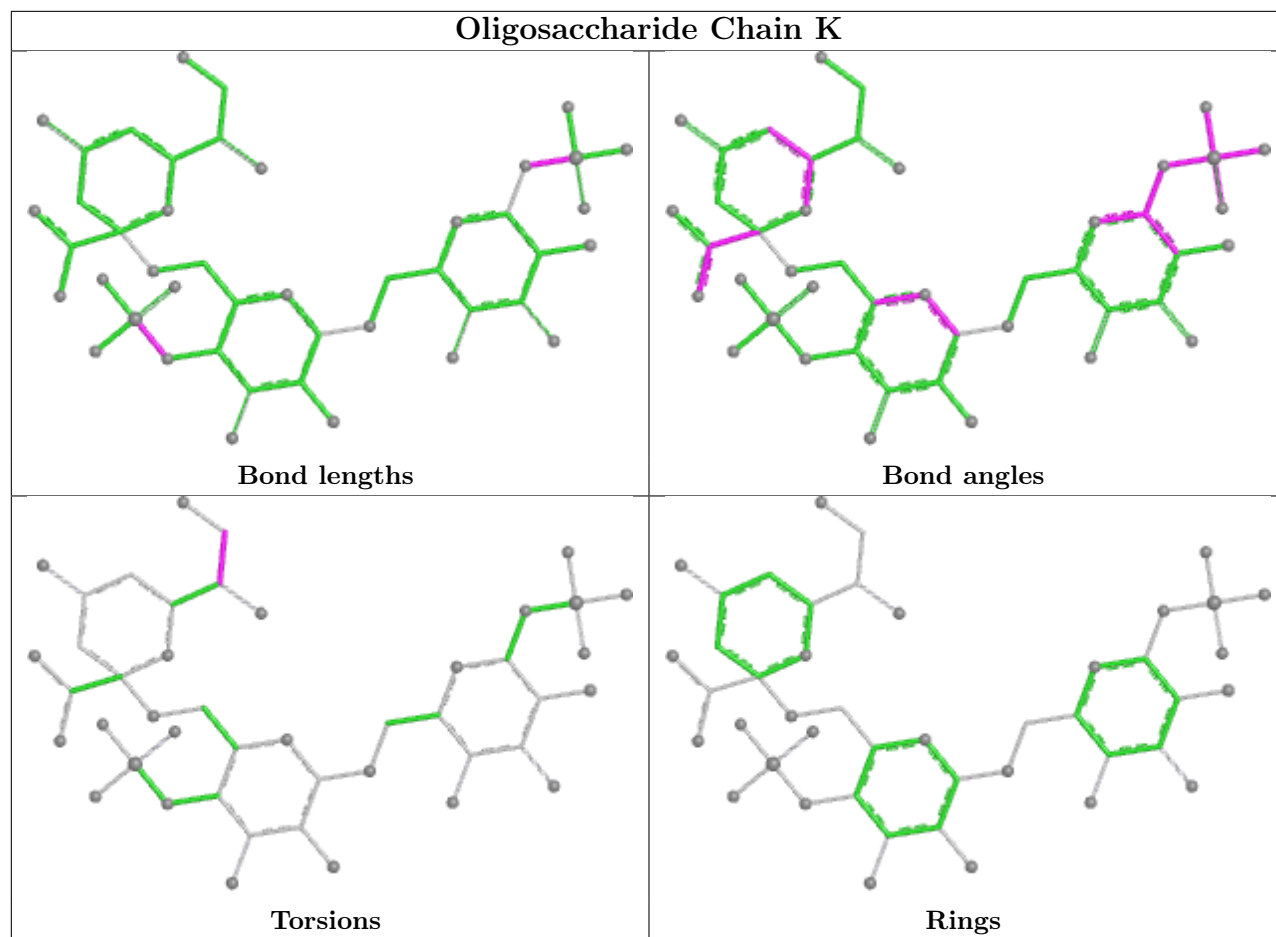
There are no ring outliers.

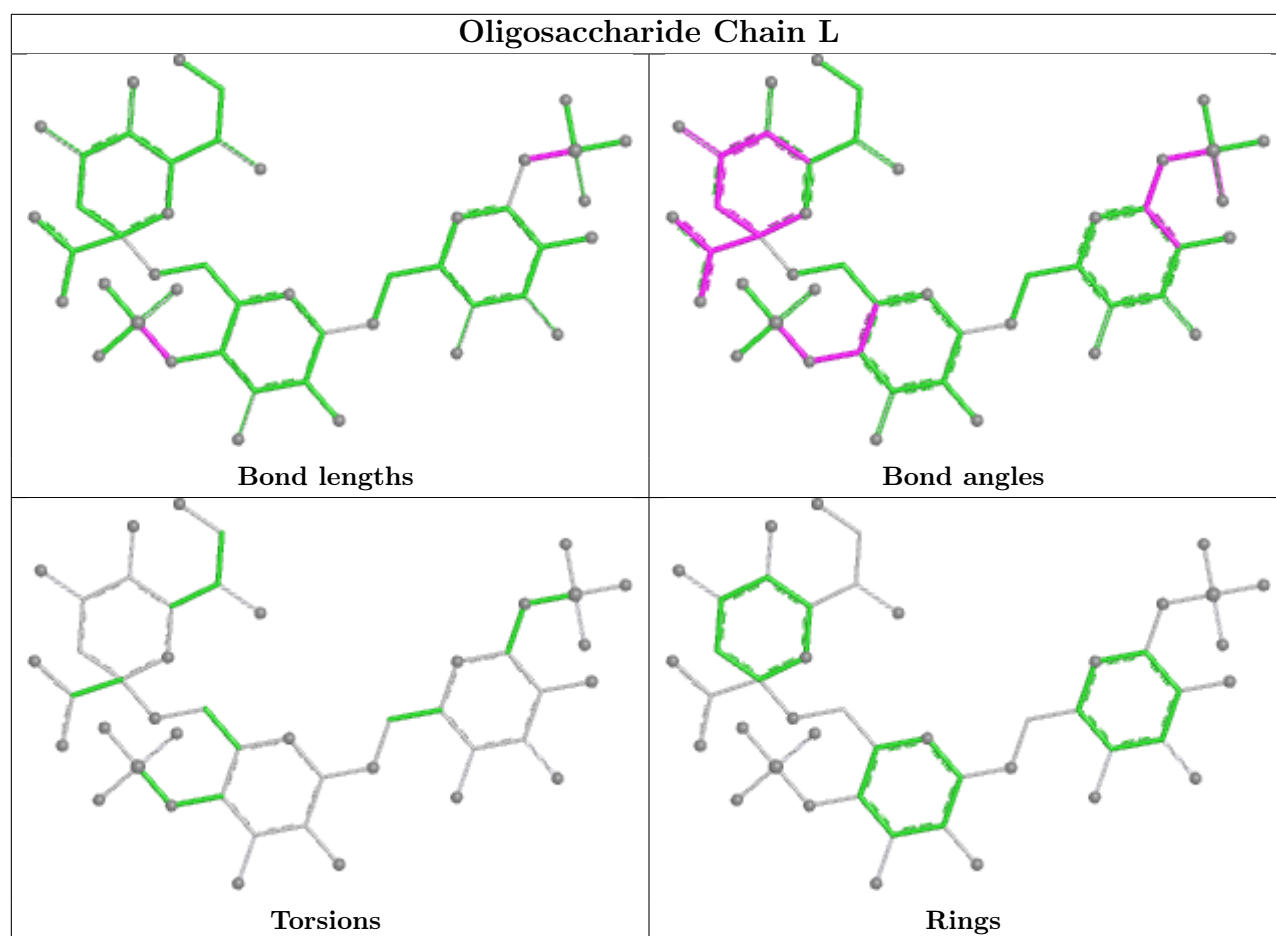
14 monomers are involved in 17 short contacts:

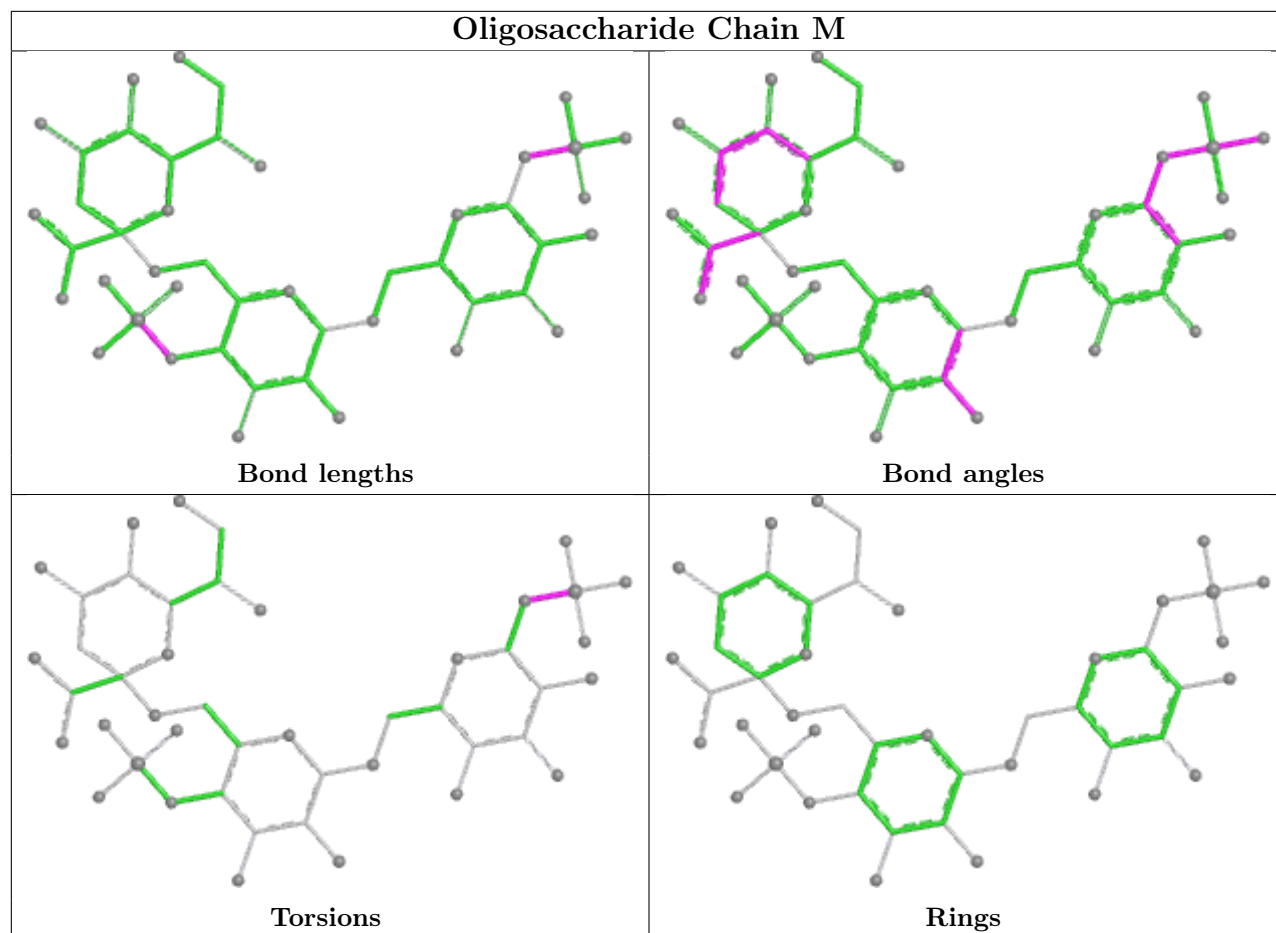
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	4	KDO	1	0
4	O	4	KDO	2	0
3	H	3	KDO	1	0
3	I	4	KDO	3	0
2	L	3	KDO	2	0
3	I	3	KDO	4	0
4	J	4	KDO	2	0
2	G	3	KDO	2	0
3	H	4	KDO	1	0
4	J	3	KDO	2	0
3	N	3	KDO	1	0
2	M	3	KDO	3	0
4	O	3	KDO	2	0
3	I	5	GMH	1	0

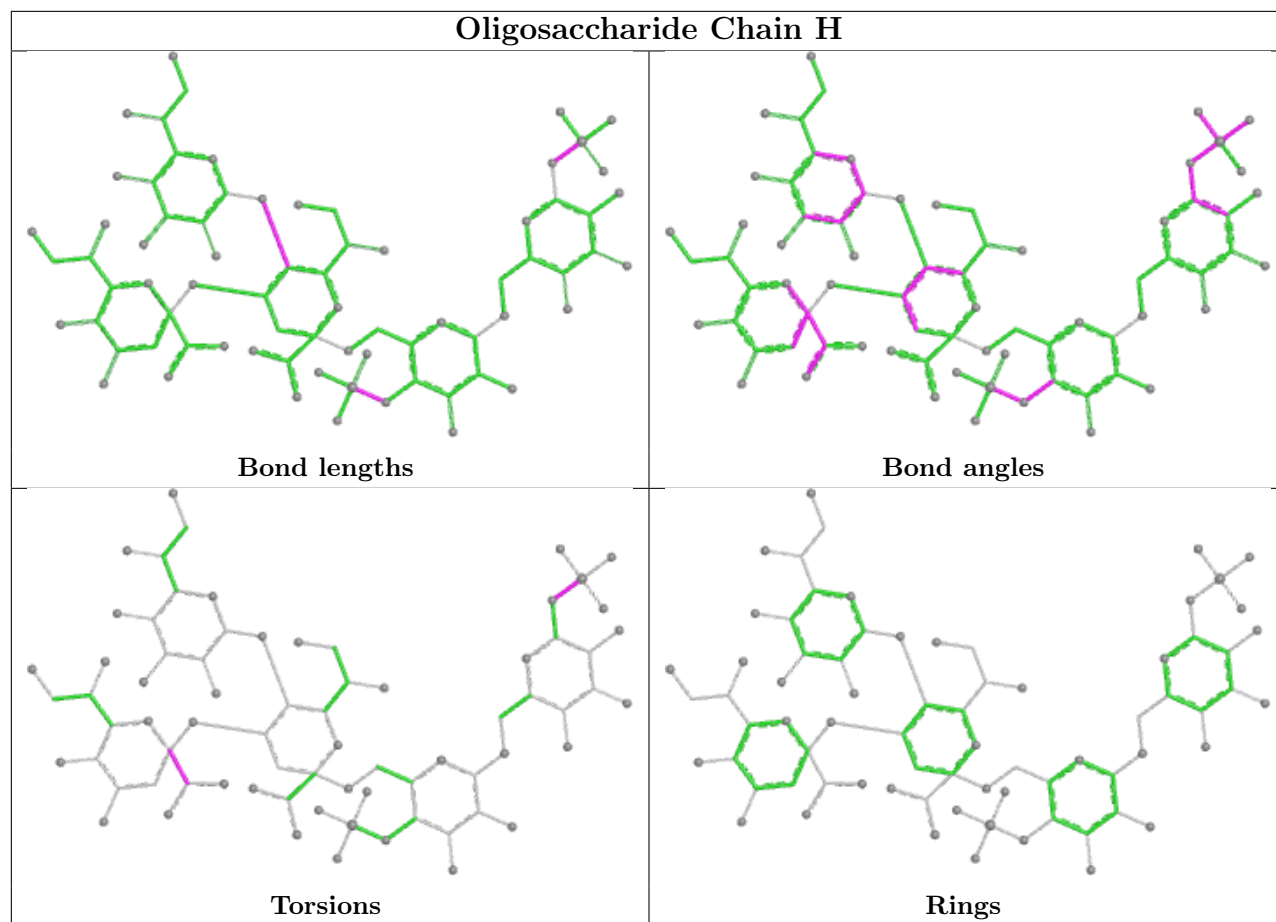
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

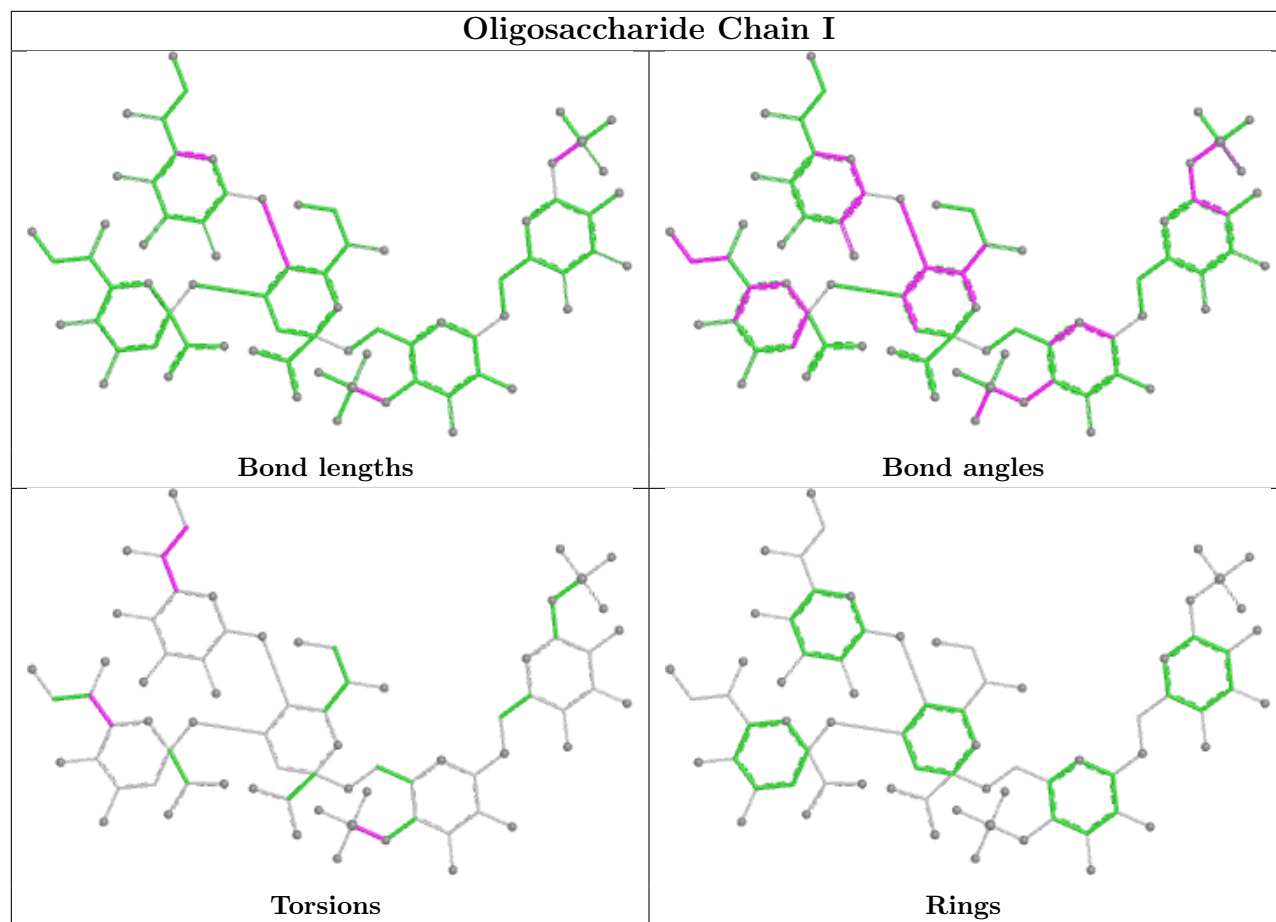


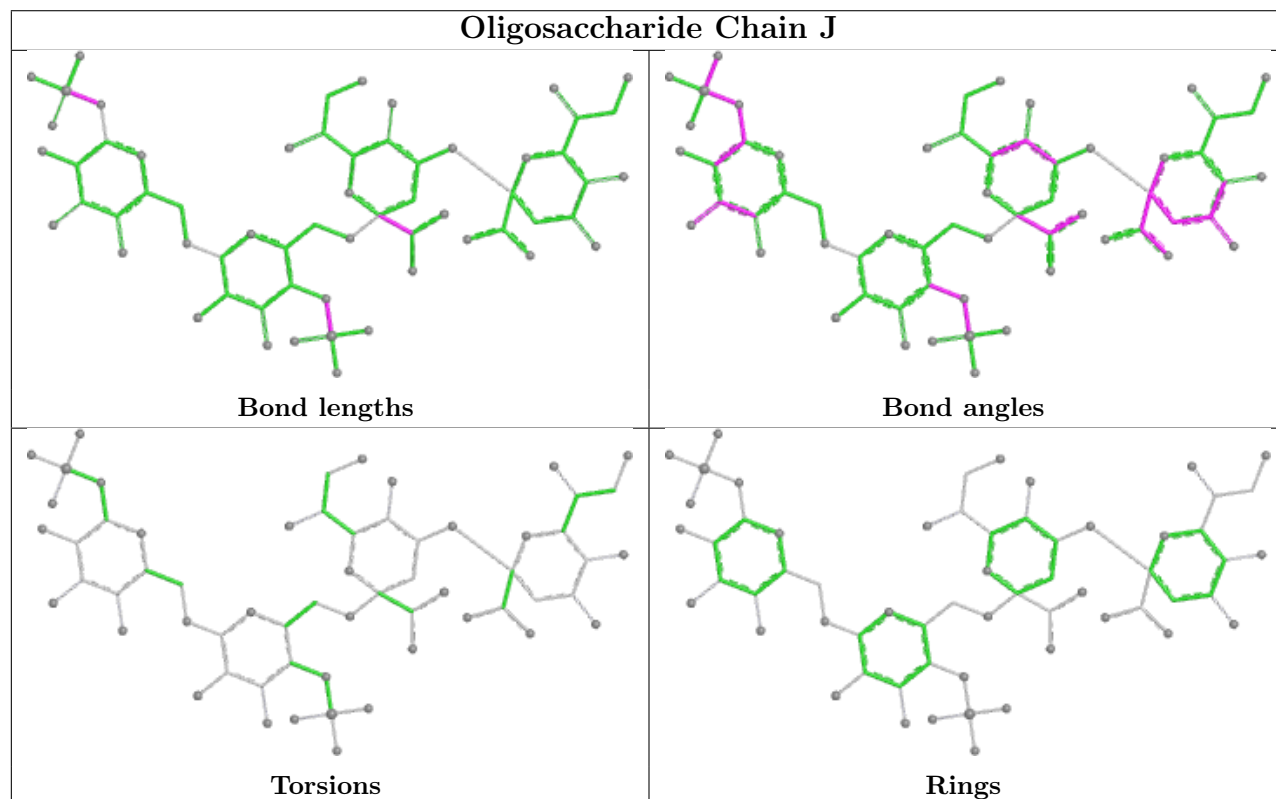
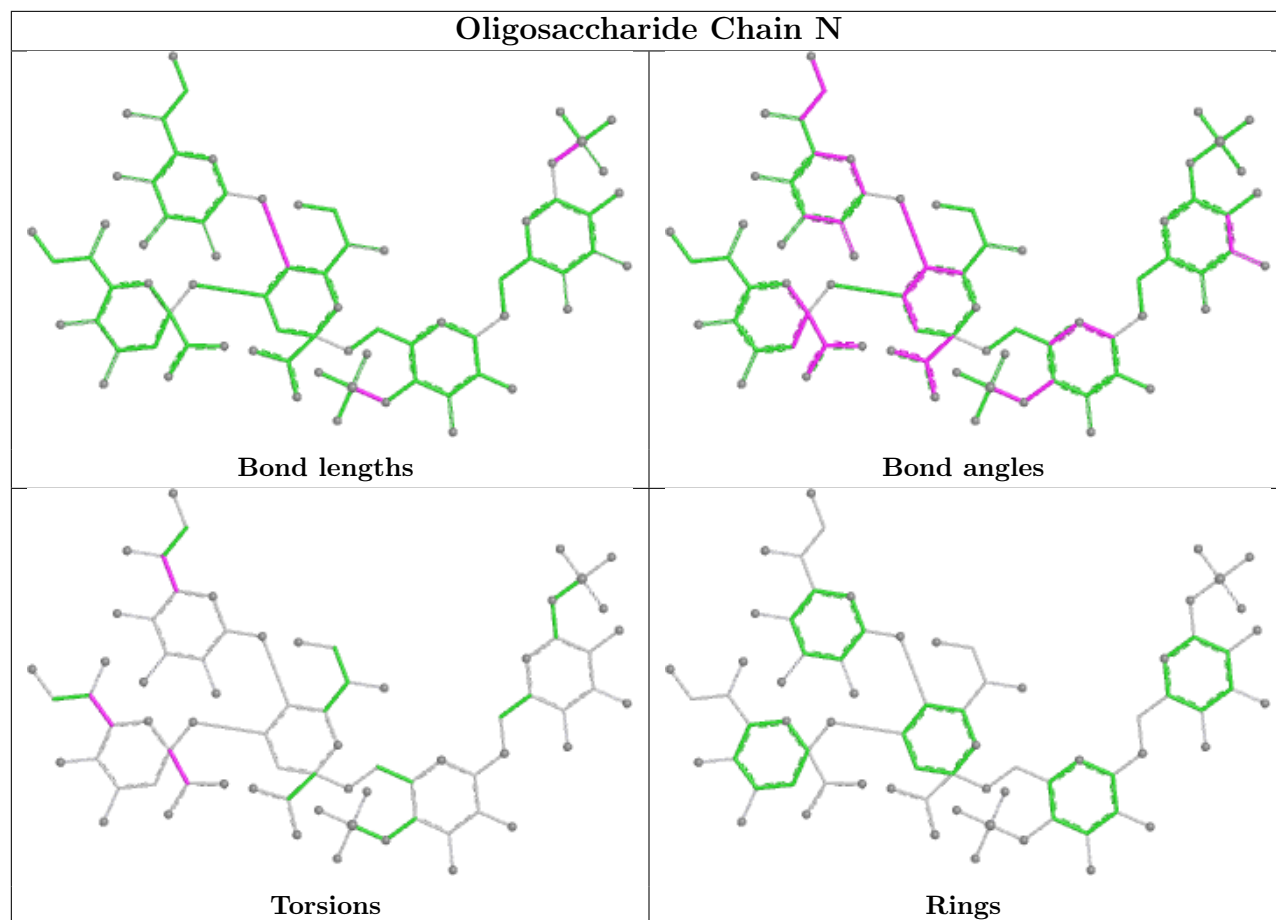


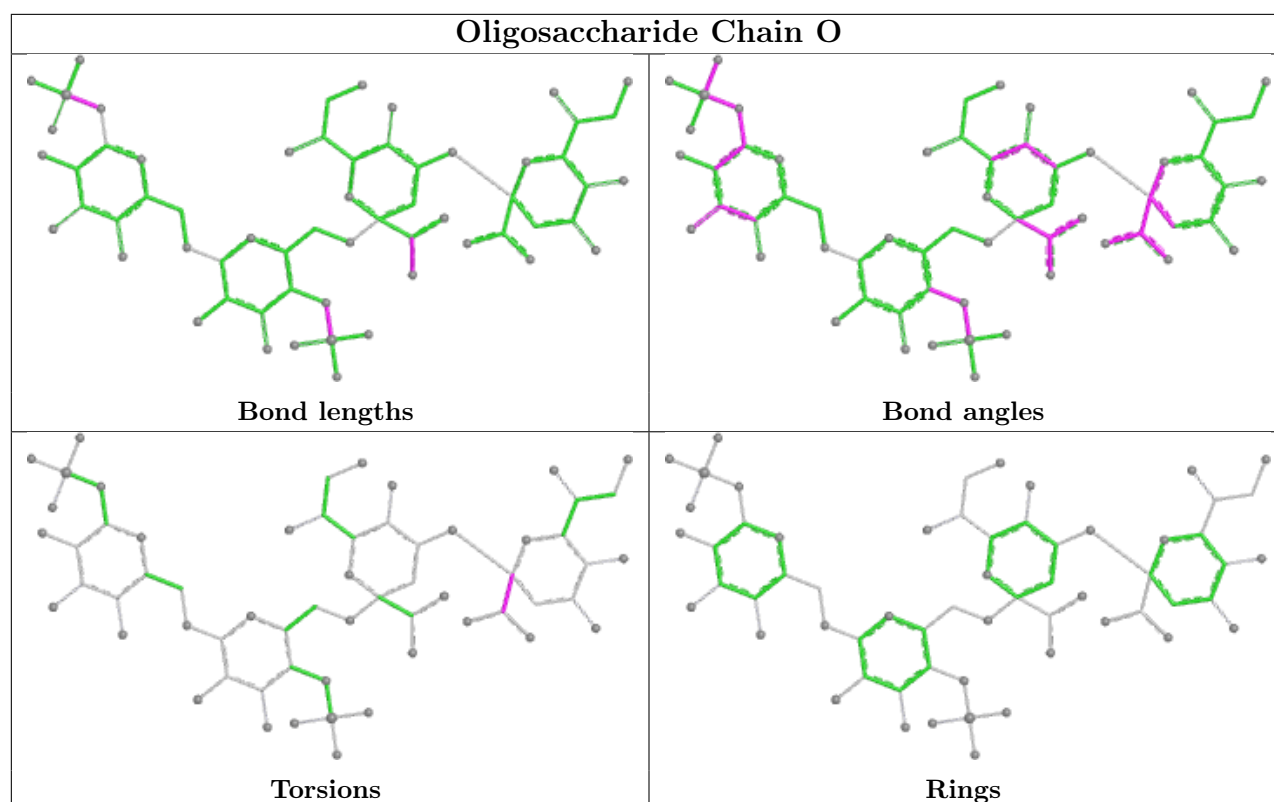












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
10	MYR	C	419	9	6,7,15	0.57	0	5,6,15	0.45	0
6	C8E	A	406	-	4,4,20	0.36	0	3,3,19	0.32	0
5	SO4	A	401	-	4,4,4	0.30	0	6,6,6	0.58	0
9	FTT	A	415	10,2	14,15,16	0.37	0	15,15,17	0.93	1 (6%)
9	FTT	F	415	4,11	9,10,16	0.57	0	10,10,17	1.46	1 (10%)
9	FTT	F	410	3	14,15,16	0.37	0	15,15,17	1.31	4 (26%)
6	C8E	B	402	-	2,2,20	0.41	0	1,1,19	0.04	0
6	C8E	A	410	-	6,6,20	0.25	0	5,5,19	0.49	0
11	DAO	E	405	9	3,4,13	0.67	0	2,3,13	0.94	0
6	C8E	D	402	-	3,3,20	0.34	0	2,2,19	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	FTT	A	413	2	13,14,16	0.39	0	14,14,17	0.77	0
10	MYR	D	423	9	4,5,15	0.58	0	3,4,15	0.57	0
6	C8E	D	403	-	5,5,20	0.33	0	4,4,19	0.34	0
6	C8E	B	401	-	8,8,20	0.40	0	7,7,19	0.58	0
6	C8E	F	402	-	3,3,20	0.34	0	2,2,19	0.63	0
6	C8E	C	407	-	10,10,20	0.33	0	9,9,19	0.44	0
6	C8E	A	407	-	4,4,20	0.49	0	3,3,19	0.24	0
9	FTT	F	407	3,11	10,11,16	0.75	0	11,11,17	1.25	1 (9%)
11	DAO	A	417	9	3,4,13	0.64	0	2,3,13	0.87	0
6	C8E	D	404	-	5,5,20	0.28	0	4,4,19	0.36	0
6	C8E	A	403	-	3,3,20	0.39	0	2,2,19	0.64	0
6	C8E	D	409	-	3,3,20	0.55	0	2,2,19	0.34	0
6	C8E	C	408	-	10,10,20	0.34	0	9,9,19	0.39	0
9	FTT	B	408	3	13,14,16	0.39	0	14,14,17	0.73	0
6	C8E	C	405	-	2,2,20	0.24	0	1,1,19	0.28	0
10	MYR	C	425	9	7,8,15	0.44	0	6,7,15	0.55	0
9	FTT	E	408	10,2	13,14,16	0.55	0	14,14,17	0.97	1 (7%)
6	C8E	E	401	-	5,5,20	0.30	0	4,4,19	0.38	0
9	FTT	A	418	4,11	12,13,16	0.55	0	13,13,17	1.47	1 (7%)
11	DAO	D	412	-	4,5,13	0.54	0	3,4,13	0.60	0
6	C8E	D	407	-	7,7,20	0.30	0	6,6,19	0.29	0
7	PO4	A	411	-	4,4,4	1.02	0	6,6,6	0.81	0
8	KDO	A	412	-	15,15,16	0.75	0	17,21,24	1.29	2 (11%)
9	FTT	D	417	2	9,10,16	0.64	0	10,10,17	1.12	1 (10%)
11	DAO	C	421	9	8,9,13	0.59	0	7,8,13	0.36	0
6	C8E	A	402	-	2,2,20	0.45	0	1,1,19	0.10	0
6	C8E	D	406	-	7,7,20	0.34	0	6,6,19	0.47	0
9	FTT	C	413	3,11	12,13,16	0.67	0	13,13,17	1.37	1 (7%)
9	FTT	D	416	10,2	11,12,16	0.56	0	12,12,17	0.87	0
11	DAO	E	410	9	3,4,13	0.62	0	2,3,13	0.68	0
6	C8E	B	404	-	7,7,20	0.30	0	6,6,19	0.34	0
9	FTT	F	414	4	12,13,16	0.42	0	13,13,17	0.62	0
6	C8E	D	405	-	5,5,20	0.28	0	4,4,19	0.36	0
9	FTT	F	406	2	12,13,16	0.53	0	13,13,17	1.03	1 (7%)
9	FTT	C	423	4,11	11,12,16	0.56	0	12,12,17	1.19	1 (8%)
6	C8E	F	401	-	2,2,20	0.19	0	1,1,19	0.33	0
6	C8E	C	404	-	5,5,20	0.24	0	4,4,19	0.35	0
9	FTT	B	410	3,10	14,15,16	0.43	0	15,15,17	0.86	0
10	MYR	F	411	9	9,10,15	0.40	0	8,9,15	0.63	0
6	C8E	A	408	-	7,7,20	0.49	0	6,6,19	0.44	0
9	FTT	C	422	4	14,15,16	0.30	0	15,15,17	1.42	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	FTT	C	424	4,10	14,15,16	0.22	0	15,15,17	0.88	0
7	PO4	F	404	-	4,4,4	0.55	0	6,6,6	0.84	0
11	DAO	D	418	9	1,2,13	1.43	0	0,1,13	-	-
7	PO4	D	411	-	4,4,4	0.63	0	6,6,6	1.20	0
6	C8E	C	406	-	7,7,20	0.31	0	6,6,19	0.42	0
10	MYR	D	419	9	3,4,15	0.66	0	2,3,15	0.83	0
5	SO4	D	401	-	4,4,4	0.32	0	6,6,6	0.47	0
9	FTT	E	406	2	12,13,16	0.35	0	13,13,17	0.91	0
11	DAO	C	420	9	11,12,13	0.43	0	10,11,13	0.56	0
9	FTT	D	420	2	14,15,16	0.34	0	15,15,17	0.83	0
10	MYR	E	409	9	4,5,15	0.61	0	3,4,15	0.49	0
6	C8E	B	403	-	4,4,20	0.30	0	3,3,19	0.31	0
7	PO4	C	411	-	4,4,4	0.88	0	6,6,6	1.01	0
6	C8E	B	405	-	7,7,20	0.31	0	6,6,19	0.68	0
9	FTT	B	409	3,11	11,12,16	0.59	0	12,12,17	1.14	2 (16%)
11	DAO	A	419	9	6,7,13	0.49	0	5,6,13	0.72	0
9	FTT	E	407	11,2	10,11,16	0.53	0	11,11,17	1.36	2 (18%)
6	C8E	C	402	-	6,6,20	0.57	0	5,5,19	0.83	0
11	DAO	F	412	9	3,4,13	0.65	0	2,3,13	0.47	0
7	PO4	B	406	-	4,4,4	1.16	0	6,6,6	0.70	0
11	DAO	F	413	9	3,4,13	0.64	0	2,3,13	0.39	0
8	KDO	D	413	-	15,15,16	0.73	0	17,21,24	1.62	3 (17%)
6	C8E	C	401	-	2,2,20	0.23	0	1,1,19	0.05	0
9	FTT	D	414	2	12,13,16	0.54	0	13,13,17	0.69	1 (7%)
11	DAO	C	414	9	3,4,13	0.63	0	2,3,13	0.51	0
6	C8E	D	408	-	10,10,20	0.40	0	9,9,19	0.27	0
10	MYR	A	416	9	4,5,15	0.63	0	3,4,15	0.56	0
10	MYR	F	417	9	10,11,15	0.42	0	9,10,15	0.57	0
10	MYR	B	411	9	4,5,15	0.60	0	3,4,15	0.64	0
6	C8E	C	410	-	6,6,20	0.33	0	5,5,19	0.48	0
6	C8E	A	404	-	5,5,20	0.30	0	4,4,19	0.27	0
6	C8E	F	403	-	7,7,20	0.37	0	6,6,19	0.49	0
9	FTT	C	417	3,11	14,15,16	0.38	0	15,15,17	0.82	0
9	FTT	C	416	3,10	9,10,16	0.71	0	10,10,17	1.21	1 (10%)
9	FTT	B	407	2	12,13,16	0.51	0	13,13,17	1.08	1 (7%)
7	PO4	E	402	-	4,4,4	0.64	0	6,6,6	0.85	0
9	FTT	C	415	3	14,15,16	0.50	0	15,15,17	1.07	1 (6%)
11	DAO	B	412	9	3,4,13	0.61	0	2,3,13	0.61	0
11	DAO	C	426	9	6,7,13	0.54	0	5,6,13	0.53	0
9	FTT	C	418	3,11	11,12,16	0.60	0	12,12,17	1.02	1 (8%)
9	FTT	A	414	11,2	11,12,16	0.54	0	12,12,17	1.47	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	KDO	E	403	-	15,15,16	0.62	0	17,21,24	1.65	3 (17%)
9	FTT	F	408	3,11	11,12,16	0.68	0	12,12,17	1.00	1 (8%)
9	FTT	F	416	4,10	14,15,16	0.28	0	15,15,17	0.82	0
11	DAO	F	418	9	6,7,13	0.56	0	5,6,13	0.37	0
6	C8E	A	405	-	3,3,20	0.37	0	2,2,19	0.65	0
11	DAO	D	424	9	3,4,13	0.64	0	2,3,13	0.48	0
9	FTT	D	425	4	12,13,16	0.53	0	13,13,17	1.56	2 (15%)
6	C8E	C	403	-	2,2,20	0.19	0	1,1,19	0.01	0
9	FTT	D	415	11,2	9,10,16	0.55	0	10,10,17	1.48	1 (10%)
9	FTT	F	409	3,10	10,11,16	0.50	0	11,11,17	0.98	1 (9%)
6	C8E	A	409	-	7,7,20	0.28	0	6,6,19	0.51	0
6	C8E	D	410	-	5,5,20	0.26	0	4,4,19	0.37	0
9	FTT	E	404	11,2	12,13,16	0.60	0	13,13,17	1.32	1 (7%)
6	C8E	C	409	-	9,9,20	0.35	0	8,8,19	0.44	0
9	FTT	D	421	11,2	11,12,16	0.57	0	12,12,17	1.13	1 (8%)
9	FTT	D	422	10,2	14,15,16	0.36	0	15,15,17	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MYR	C	419	9	-	0/5/5/13	-
6	C8E	A	406	-	-	0/2/2/18	-
9	FTT	A	415	10,2	-	7/14/14/15	-
9	FTT	F	415	4,11	-	1/9/9/15	-
9	FTT	F	410	3	-	5/14/14/15	-
6	C8E	A	410	-	-	0/4/4/18	-
11	DAO	E	405	9	-	0/2/2/11	-
6	C8E	D	402	-	-	1/1/1/18	-
9	FTT	A	413	2	-	3/13/13/15	-
10	MYR	D	423	9	-	1/3/3/13	-
6	C8E	D	403	-	-	0/3/3/18	-
6	C8E	B	401	-	-	3/6/6/18	-
6	C8E	F	402	-	-	0/1/1/18	-
6	C8E	C	407	-	-	1/8/8/18	-
6	C8E	A	407	-	-	2/2/2/18	-
9	FTT	F	407	3,11	-	3/10/10/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	DAO	A	417	9	-	2/2/2/11	-
6	C8E	D	404	-	-	0/3/3/18	-
6	C8E	A	403	-	-	0/1/1/18	-
6	C8E	D	409	-	-	0/0/1/18	-
6	C8E	C	408	-	-	3/8/8/18	-
9	FTT	B	408	3	-	1/13/13/15	-
10	MYR	C	425	9	-	2/6/6/13	-
9	FTT	E	408	10,2	-	7/13/13/15	-
6	C8E	E	401	-	-	3/3/3/18	-
9	FTT	A	418	4,11	-	5/12/12/15	-
11	DAO	D	412	-	-	2/3/3/11	-
6	C8E	D	407	-	-	2/5/5/18	-
8	KDO	A	412	-	-	1/10/26/30	0/1/1/1
9	FTT	D	417	2	-	2/9/9/15	-
11	DAO	C	421	9	-	2/7/7/11	-
6	C8E	D	406	-	-	4/5/5/18	-
9	FTT	C	413	3,11	-	2/12/12/15	-
9	FTT	D	416	10,2	-	6/11/11/15	-
11	DAO	E	410	9	-	2/2/2/11	-
6	C8E	B	404	-	-	2/5/5/18	-
9	FTT	F	414	4	-	2/12/12/15	-
6	C8E	D	405	-	-	0/3/3/18	-
9	FTT	F	406	2	-	1/12/12/15	-
9	FTT	C	423	4,11	-	1/11/11/15	-
6	C8E	C	404	-	-	1/3/3/18	-
9	FTT	B	410	3,10	-	5/14/14/15	-
10	MYR	F	411	9	-	0/8/8/13	-
6	C8E	A	408	-	-	3/5/5/18	-
9	FTT	C	422	4	-	4/14/14/15	-
9	FTT	C	424	4,10	-	3/14/14/15	-
6	C8E	C	406	-	-	0/5/5/18	-
10	MYR	D	419	9	-	2/2/2/13	-
9	FTT	E	406	2	-	2/12/12/15	-
11	DAO	C	420	9	-	0/10/10/11	-
9	FTT	D	420	2	-	4/14/14/15	-
10	MYR	E	409	9	-	2/3/3/13	-
6	C8E	B	403	-	-	1/2/2/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	C8E	B	405	-	-	1/5/5/18	-
9	FTT	B	409	3,11	-	3/11/11/15	-
11	DAO	A	419	9	-	0/5/5/11	-
9	FTT	E	407	11,2	-	1/10/10/15	-
6	C8E	C	402	-	-	2/4/4/18	-
11	DAO	F	412	9	-	1/2/2/11	-
11	DAO	F	413	9	-	0/2/2/11	-
8	KDO	D	413	-	-	2/10/26/30	0/1/1/1
9	FTT	D	414	2	-	7/12/12/15	-
11	DAO	C	414	9	-	1/2/2/11	-
6	C8E	D	408	-	-	1/8/8/18	-
10	MYR	A	416	9	-	0/3/3/13	-
10	MYR	F	417	9	-	4/9/9/13	-
10	MYR	B	411	9	-	1/3/3/13	-
6	C8E	C	410	-	-	2/4/4/18	-
6	C8E	A	404	-	-	1/3/3/18	-
6	C8E	F	403	-	-	2/5/5/18	-
9	FTT	C	417	3,11	-	2/14/14/15	-
9	FTT	C	416	3,10	-	1/9/9/15	-
9	FTT	B	407	2	-	2/12/12/15	-
9	FTT	C	415	3	-	2/14/14/15	-
11	DAO	B	412	9	-	1/2/2/11	-
11	DAO	C	426	9	-	3/5/5/11	-
9	FTT	C	418	3,11	-	4/11/11/15	-
9	FTT	A	414	11,2	-	0/11/11/15	-
8	KDO	E	403	-	-	1/10/26/30	0/1/1/1
9	FTT	F	408	3,11	-	5/11/11/15	-
9	FTT	F	416	4,10	-	6/14/14/15	-
11	DAO	F	418	9	-	2/5/5/11	-
6	C8E	A	405	-	-	0/1/1/18	-
11	DAO	D	424	9	-	1/2/2/11	-
9	FTT	D	425	4	-	4/12/12/15	-
9	FTT	D	415	11,2	-	1/9/9/15	-
9	FTT	F	409	3,10	-	2/10/10/15	-
6	C8E	A	409	-	-	0/5/5/18	-
6	C8E	D	410	-	-	0/3/3/18	-
9	FTT	E	404	11,2	-	6/12/12/15	-
6	C8E	C	409	-	-	2/7/7/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FTT	D	421	11,2	-	0/11/11/15	-
9	FTT	D	422	10,2	-	5/14/14/15	-

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	403	KDO	O6-C2-C3	5.18	117.53	110.56
8	D	413	KDO	O6-C2-C3	4.88	117.12	110.56
9	A	418	FTT	O2-C1-C2	-4.79	111.43	125.38
9	D	425	FTT	O2-C1-C2	-4.37	112.67	125.38
9	C	413	FTT	O2-C1-C2	-4.36	112.68	125.38
9	F	415	FTT	O2-C1-C2	-4.19	113.19	125.38
8	A	412	KDO	O6-C2-C3	4.04	115.99	110.56
9	D	415	FTT	O2-C1-C2	-3.90	114.03	125.38
9	C	423	FTT	O2-C1-C2	-3.62	114.84	125.38
9	A	414	FTT	O2-C1-C2	-3.58	114.97	125.38
8	D	413	KDO	O1A-C1-C2	-3.47	115.36	122.85
9	B	407	FTT	O2-C1-C2	-3.43	115.39	125.38
9	E	404	FTT	O2-C1-C2	-3.30	115.76	125.38
9	F	406	FTT	O2-C1-C2	-3.28	115.83	125.38
9	C	418	FTT	O2-C1-C2	-3.00	116.64	125.38
8	E	403	KDO	O1A-C1-C2	-2.96	116.46	122.85
9	D	417	FTT	O2-C1-C2	-2.95	116.79	125.38
9	C	416	FTT	O2-C1-C2	-2.87	117.02	125.38
9	F	407	FTT	O2-C1-C2	-2.85	117.07	125.38
9	E	407	FTT	O2-C1-C2	-2.76	117.34	125.38
9	D	421	FTT	O2-C1-C2	-2.72	117.47	125.38
9	F	408	FTT	O2-C1-C2	-2.69	117.54	125.38
8	A	412	KDO	O1A-C1-C2	-2.51	117.43	122.85
9	A	414	FTT	C4-C3-C2	-2.40	105.33	113.05
9	E	407	FTT	C3-C2-C1	2.37	116.74	112.70
9	B	409	FTT	O2-C1-C2	-2.36	118.50	125.38
9	F	410	FTT	C5-C4-C3	-2.35	108.20	114.68
8	E	403	KDO	O1B-C1-C2	2.28	118.65	112.71
9	F	410	FTT	C4-C3-C2	-2.27	105.73	113.05
9	A	415	FTT	C5-C4-C3	-2.27	108.44	114.68
9	F	410	FTT	O2-C1-C2	-2.26	118.81	125.38
9	C	415	FTT	C4-C3-C2	-2.25	105.80	113.05
9	D	425	FTT	C3-C2-C1	-2.23	108.90	112.70
9	C	422	FTT	C11-C10-C9	-2.19	103.31	114.37
9	F	409	FTT	O2-C1-C2	-2.18	119.04	125.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	408	FTT	C10-C9-C8	-2.14	103.57	114.37
9	B	409	FTT	C3-C2-C1	2.10	116.28	112.70
9	C	422	FTT	C7-C6-C5	-2.09	103.80	114.37
9	D	414	FTT	O2-C1-C2	-2.09	119.30	125.38
8	D	413	KDO	O1B-C1-C2	2.08	118.11	112.71
9	C	422	FTT	C5-C4-C3	-2.06	109.00	114.68
9	F	410	FTT	O3-C3-C2	2.00	114.78	109.45

There are no chirality outliers.

All (185) 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	D	419	MYR	O1-C1-C2-C3
10	E	409	MYR	O1-C1-C2-C3
10	F	417	MYR	O1-C1-C2-C3
11	A	417	DAO	O1-C1-C2-C3
11	C	421	DAO	O1-C1-C2-C3
11	E	410	DAO	O1-C1-C2-C3
11	F	412	DAO	O1-C1-C2-C3
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	C	407	C8E	C11-C10-O9-C8
9	A	418	FTT	C4-C5-C6-C7
6	D	407	C8E	C2-C3-C4-C5
9	A	415	FTT	C10-C11-C12-C13
9	D	425	FTT	C11-C10-C9-C8
6	C	409	C8E	C7-C8-O9-C10
6	C	408	C8E	C2-C3-C4-C5
9	D	417	FTT	C5-C6-C7-C8
9	D	422	FTT	C9-C10-C11-C12
6	B	403	C8E	O9-C10-C11-O12

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

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Mol	Chain	Res	Type	Atoms
9	E	406	FTT	C9-C10-C11-C12
6	D	406	C8E	C1-C2-C3-C4
6	B	401	C8E	C6-C7-C8-O9
6	D	407	C8E	C4-C5-C6-C7
9	D	422	FTT	C5-C6-C7-C8
10	C	425	MYR	C3-C4-C5-C6
10	F	417	MYR	C7-C8-C9-C10
9	F	408	FTT	C2-C3-C4-C5
6	E	401	C8E	C1-C2-C3-C4
9	D	414	FTT	C9-C10-C11-C12
6	B	401	C8E	C3-C4-C5-C6
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
9	F	414	FTT	C9-C10-C11-C12
9	D	420	FTT	C9-C10-C11-C12
6	E	401	C8E	C3-C4-C5-C6
9	C	424	FTT	C5-C6-C7-C8
11	A	417	DAO	C1-C2-C3-C4
11	D	424	DAO	C1-C2-C3-C4
9	E	408	FTT	C9-C10-C11-C12
9	C	422	FTT	C4-C5-C6-C7
9	D	416	FTT	C2-C3-C4-C5
6	C	404	C8E	C3-C4-C5-C6
9	C	424	FTT	C11-C10-C9-C8
11	F	418	DAO	C4-C5-C6-C7
6	C	410	C8E	C1-C2-C3-C4
6	D	406	C8E	C5-C6-C7-C8
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	B	409	FTT	C5-C6-C7-C8
10	B	411	MYR	C1-C2-C3-C4
10	D	423	MYR	C1-C2-C3-C4
10	E	409	MYR	C1-C2-C3-C4
11	C	421	DAO	C1-C2-C3-C4
11	D	412	DAO	C1-C2-C3-C4
10	F	417	MYR	C11-C10-C9-C8
9	F	414	FTT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	A	415	FTT	C1-C2-C3-O3
9	B	410	FTT	C1-C2-C3-O3
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
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	D	414	FTT	C7-C8-C9-C10
6	D	402	C8E	C1-C2-C3-C4
10	D	419	MYR	C1-C2-C3-C4
6	C	408	C8E	C11-C10-O9-C8
9	D	417	FTT	C6-C7-C8-C9
8	D	413	KDO	O1A-C1-C2-O6
8	E	403	KDO	O1A-C1-C2-O6
9	D	416	FTT	C3-C4-C5-C6
11	C	426	DAO	C4-C5-C6-C7
6	B	404	C8E	C3-C4-C5-C6
9	D	420	FTT	C4-C5-C6-C7
11	D	412	DAO	C2-C3-C4-C5
9	C	422	FTT	C5-C6-C7-C8
9	D	425	FTT	C7-C8-C9-C10
6	C	402	C8E	C3-C4-C5-C6
11	B	412	DAO	C1-C2-C3-C4
11	E	410	DAO	C1-C2-C3-C4
11	C	426	DAO	C2-C3-C4-C5
9	D	414	FTT	C4-C5-C6-C7
9	E	406	FTT	C4-C5-C6-C7
9	A	415	FTT	C5-C6-C7-C8
9	A	413	FTT	C4-C5-C6-C7
9	C	415	FTT	C7-C8-C9-C10
9	A	415	FTT	C11-C12-C13-C14
6	A	404	C8E	C1-C2-C3-C4
9	F	410	FTT	C11-C12-C13-C14
9	F	416	FTT	C11-C10-C9-C8
9	F	406	FTT	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	408	C8E	C14-C13-O12-C11
9	A	415	FTT	C7-C8-C9-C10
6	D	406	C8E	C3-C4-C5-C6
8	A	412	KDO	O1A-C1-C2-O6
9	B	409	FTT	C11-C10-C9-C8
9	F	416	FTT	C4-C5-C6-C7
9	F	408	FTT	C6-C7-C8-C9
10	C	425	MYR	C2-C3-C4-C5
9	E	408	FTT	C1-C2-C3-C4
9	B	407	FTT	C5-C6-C7-C8
10	F	417	MYR	C6-C7-C8-C9
6	A	407	C8E	C11-C10-O9-C8
8	D	413	KDO	O1B-C1-C2-C3
9	E	407	FTT	C2-C3-C4-C5
9	F	408	FTT	C3-C4-C5-C6
6	A	407	C8E	C7-C8-O9-C10
6	D	406	C8E	C4-C5-C6-C7
6	F	403	C8E	C3-C4-C5-C6
11	C	426	DAO	C1-C2-C3-C4
9	D	416	FTT	C5-C6-C7-C8
9	C	424	FTT	C11-C12-C13-C14
9	C	418	FTT	C3-C4-C5-C6
9	E	408	FTT	C3-C4-C5-C6
9	B	407	FTT	O2-C1-C2-C3
9	D	420	FTT	O2-C1-C2-C3
6	C	410	C8E	C4-C5-C6-C7
9	B	409	FTT	C6-C7-C8-C9
9	A	415	FTT	C9-C10-C11-C12
9	E	404	FTT	C4-C5-C6-C7

There are no ring outliers.

12 monomers are involved in 19 short contacts:

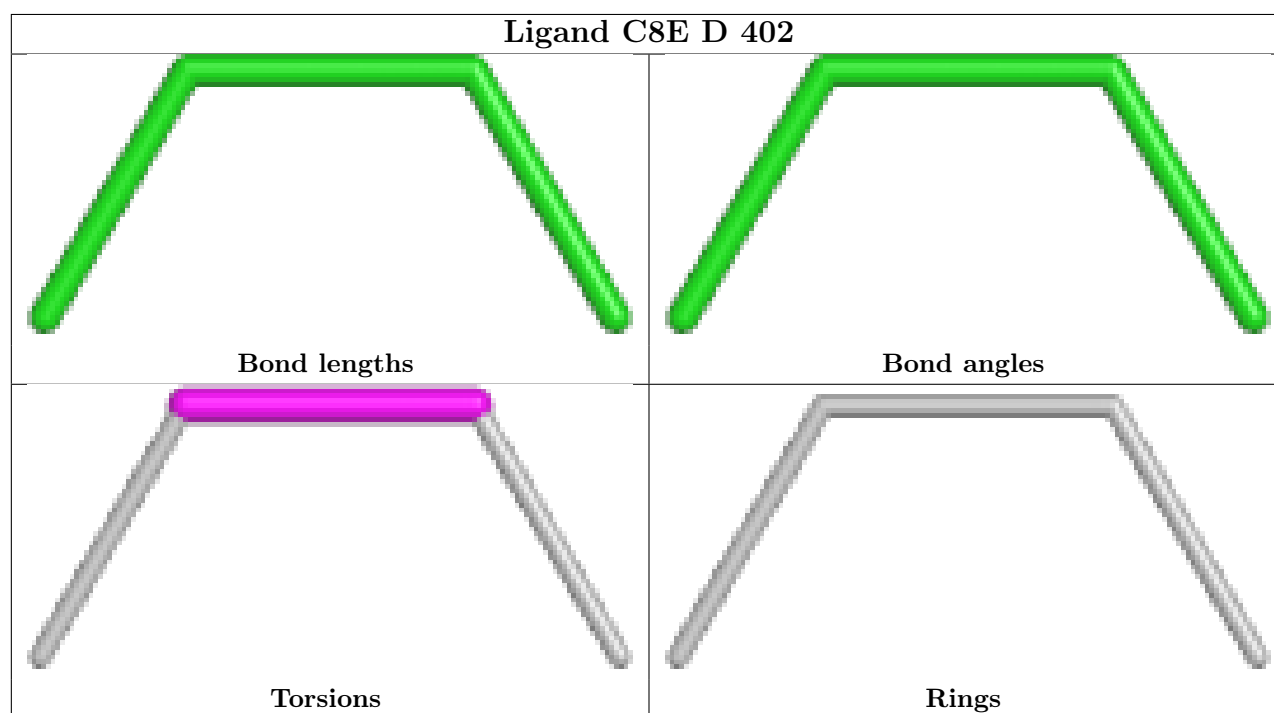
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	407	C8E	1	0
9	F	407	FTT	1	0
6	D	409	C8E	1	0
6	C	405	C8E	4	0
8	A	412	KDO	2	0
9	F	406	FTT	1	0
6	F	401	C8E	1	0
6	A	408	C8E	2	0

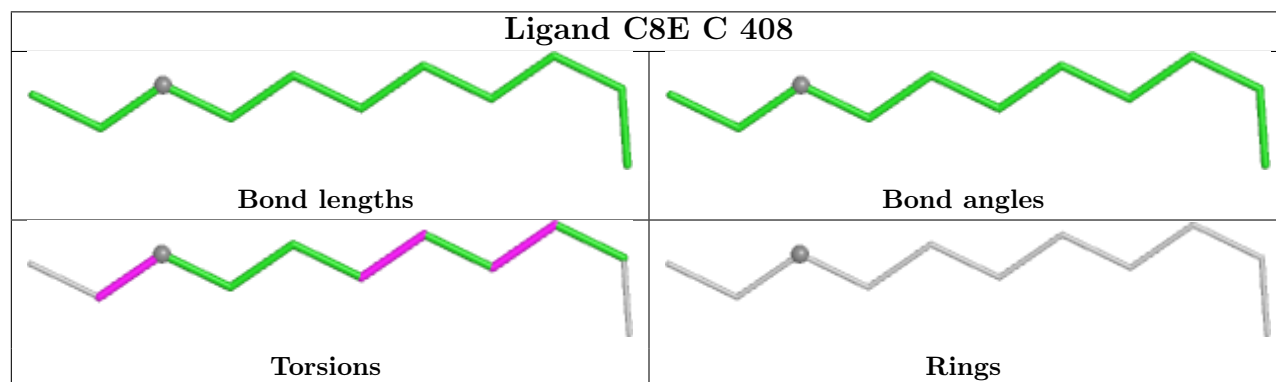
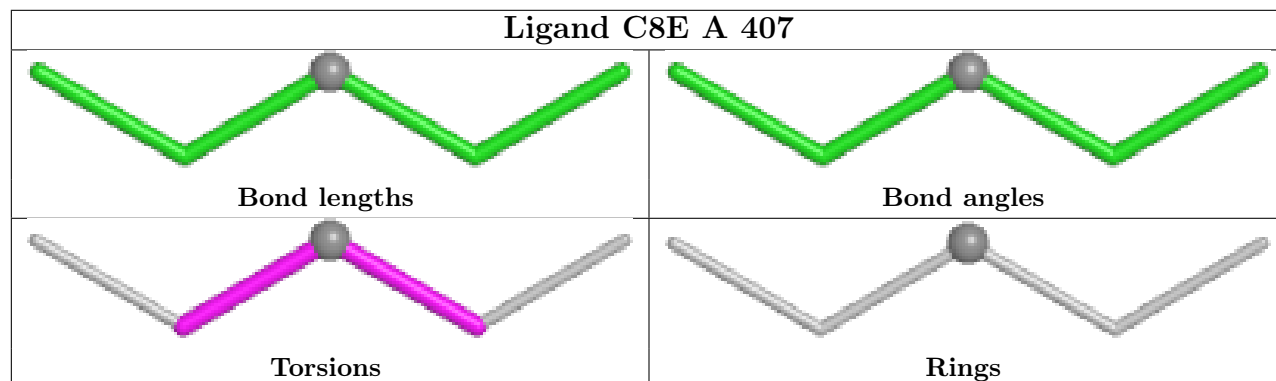
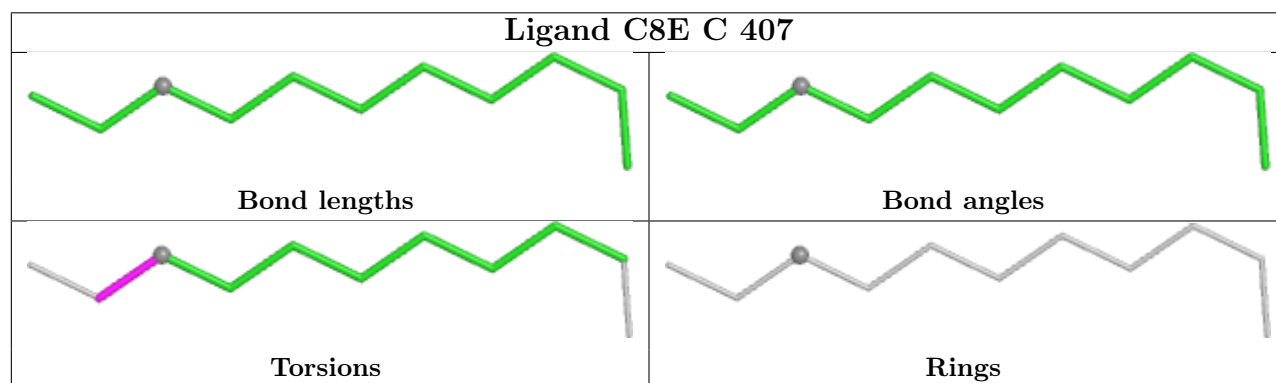
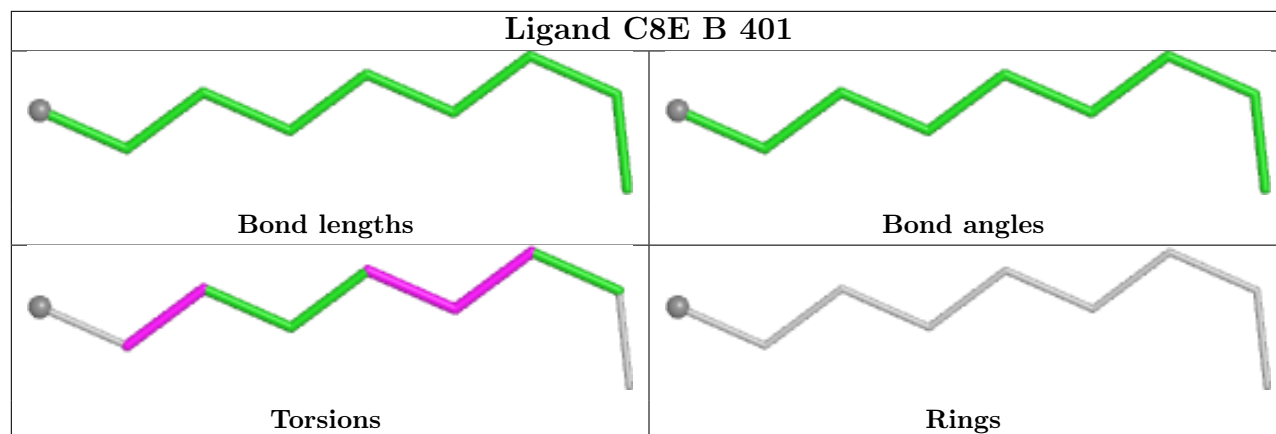
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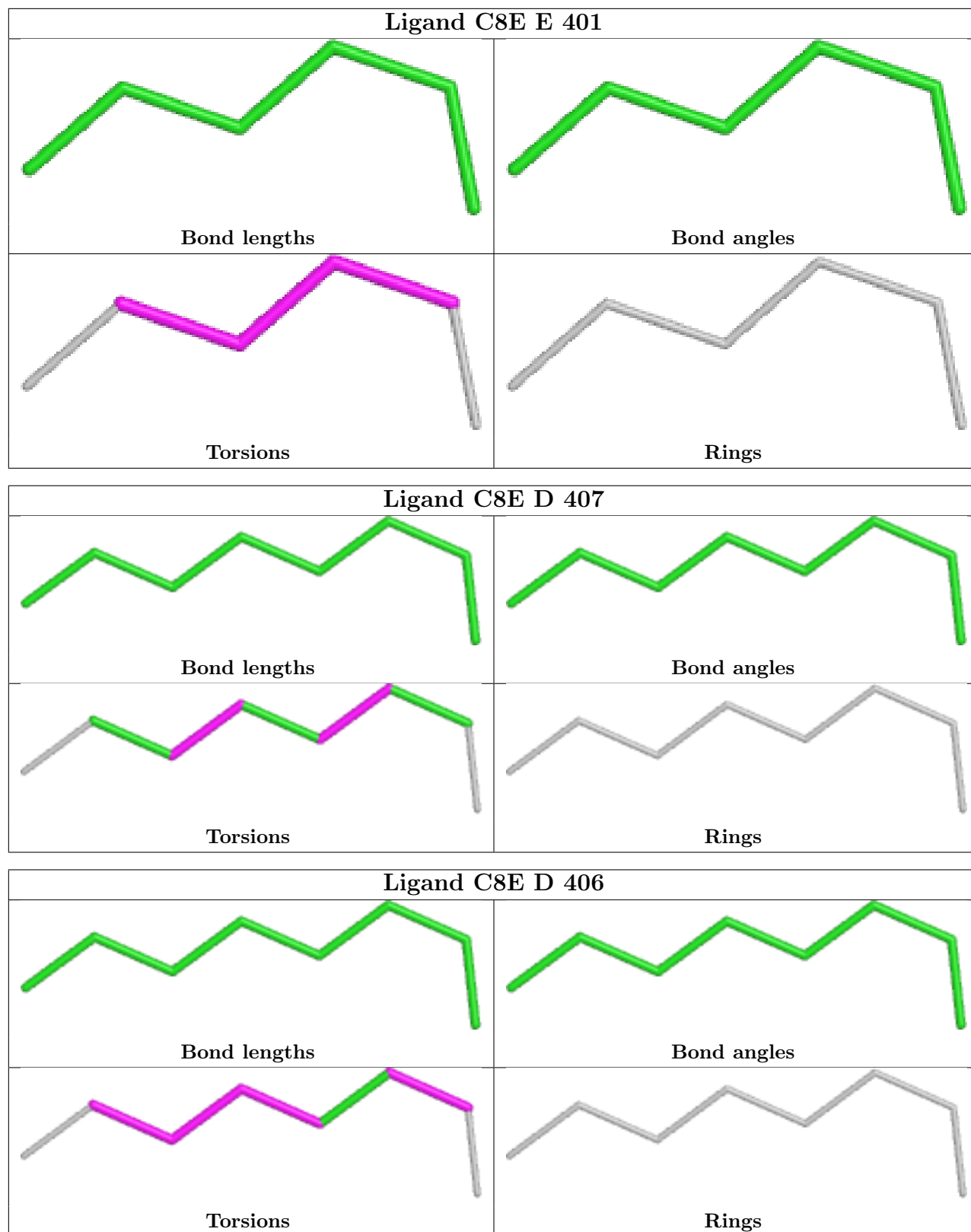
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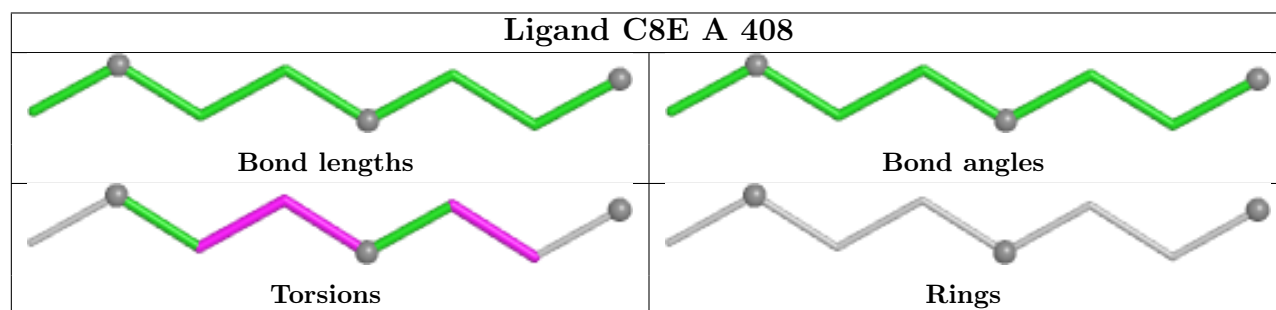
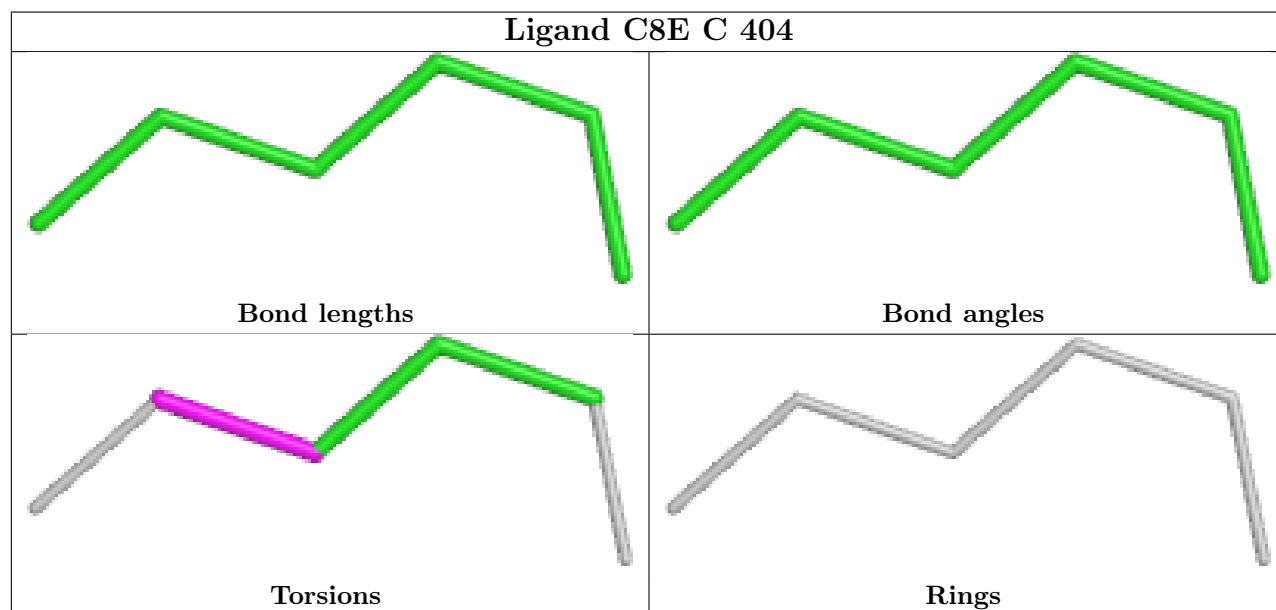
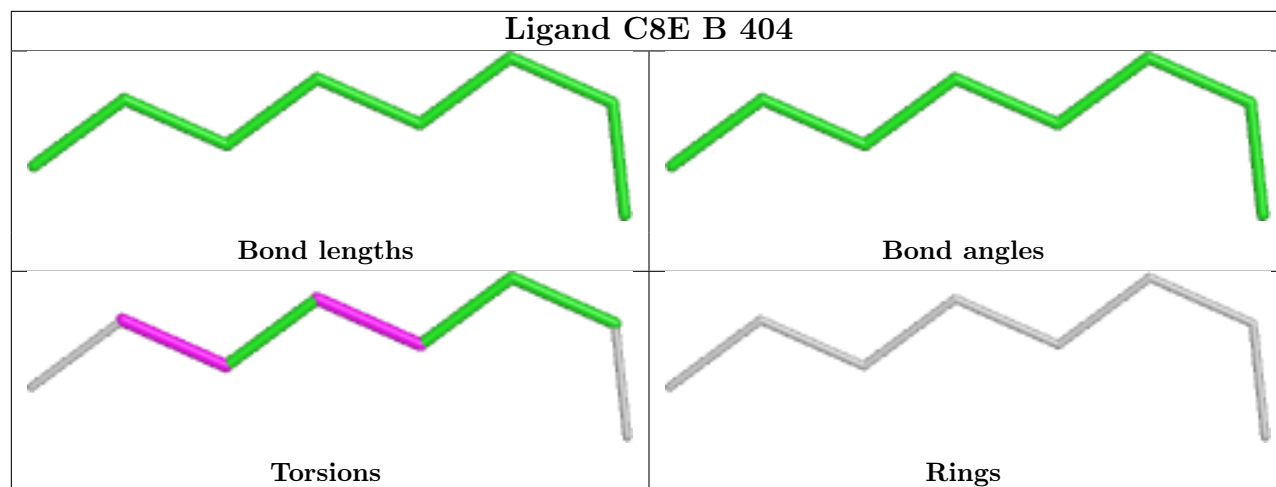
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	403	C8E	2	0
8	D	413	KDO	2	0
6	F	403	C8E	1	0
8	E	403	KDO	3	0

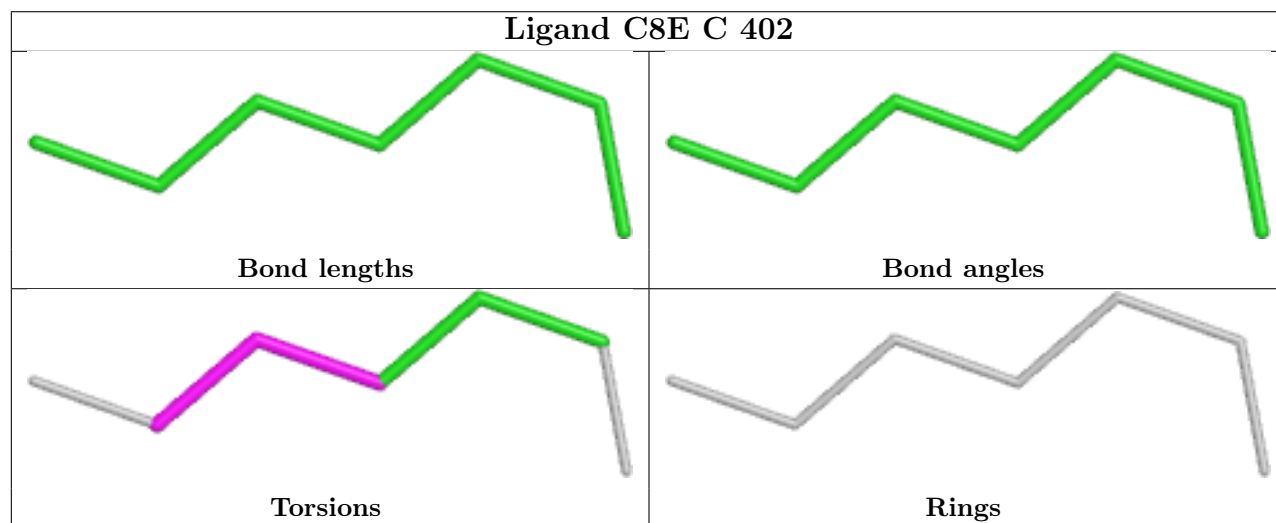
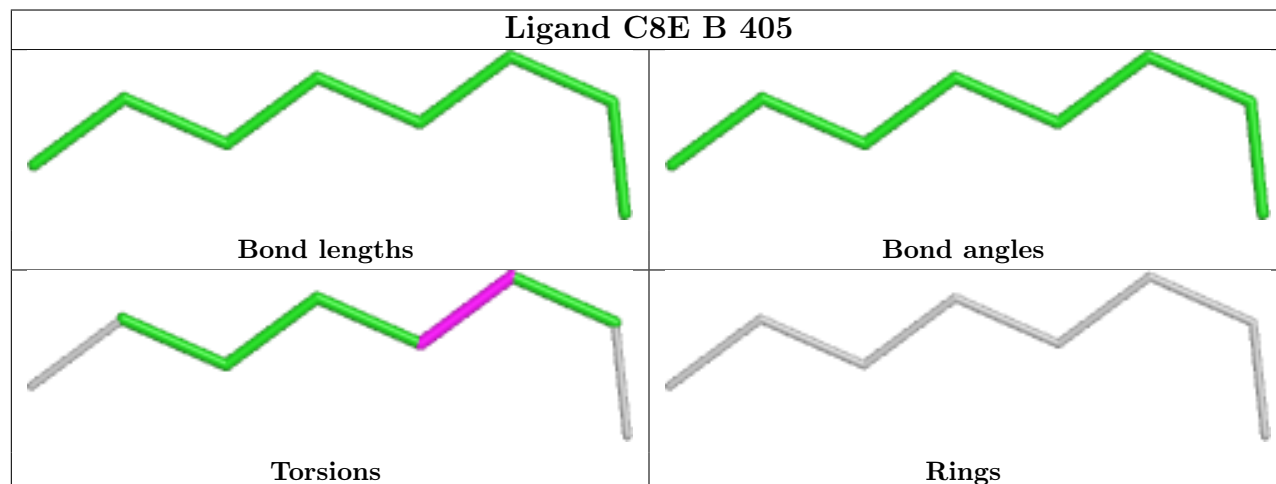
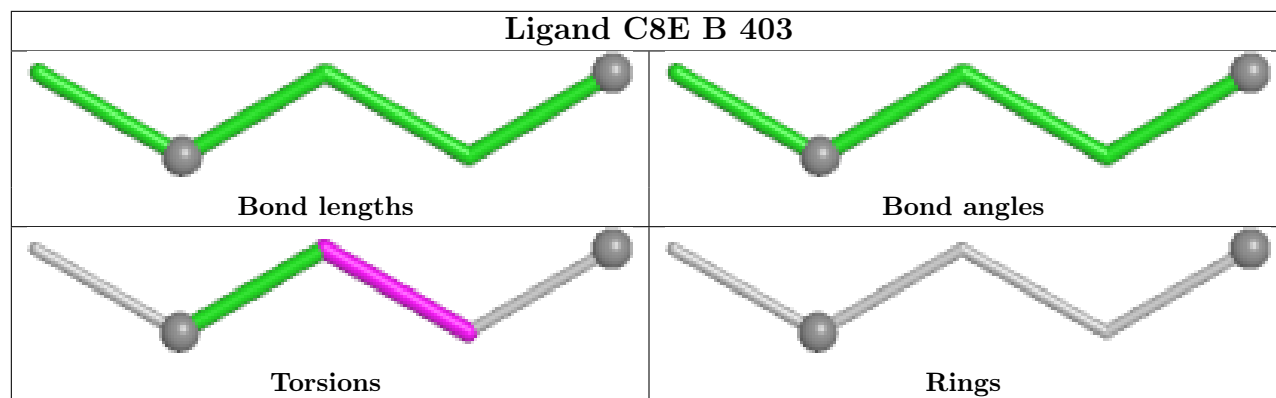
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

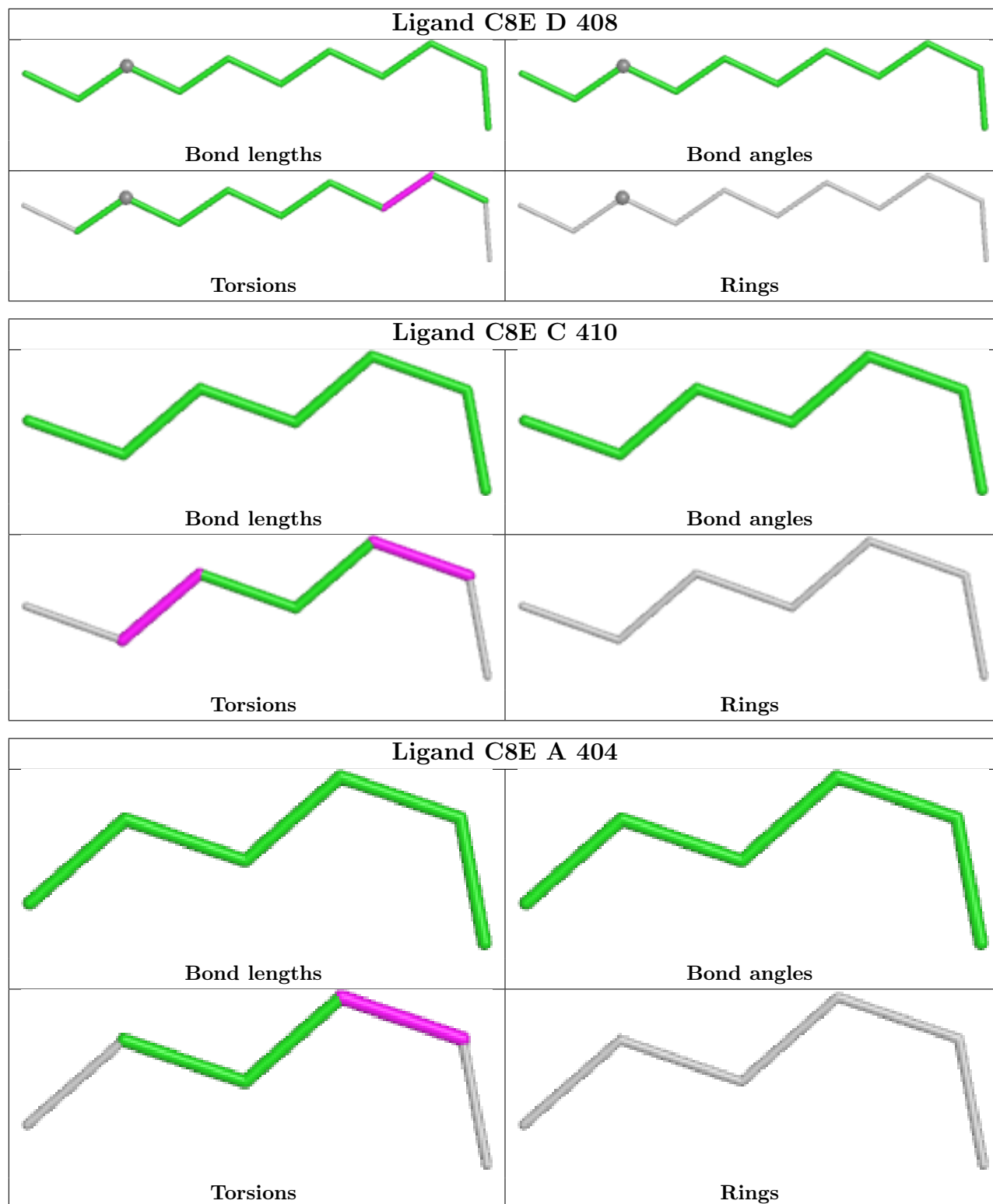


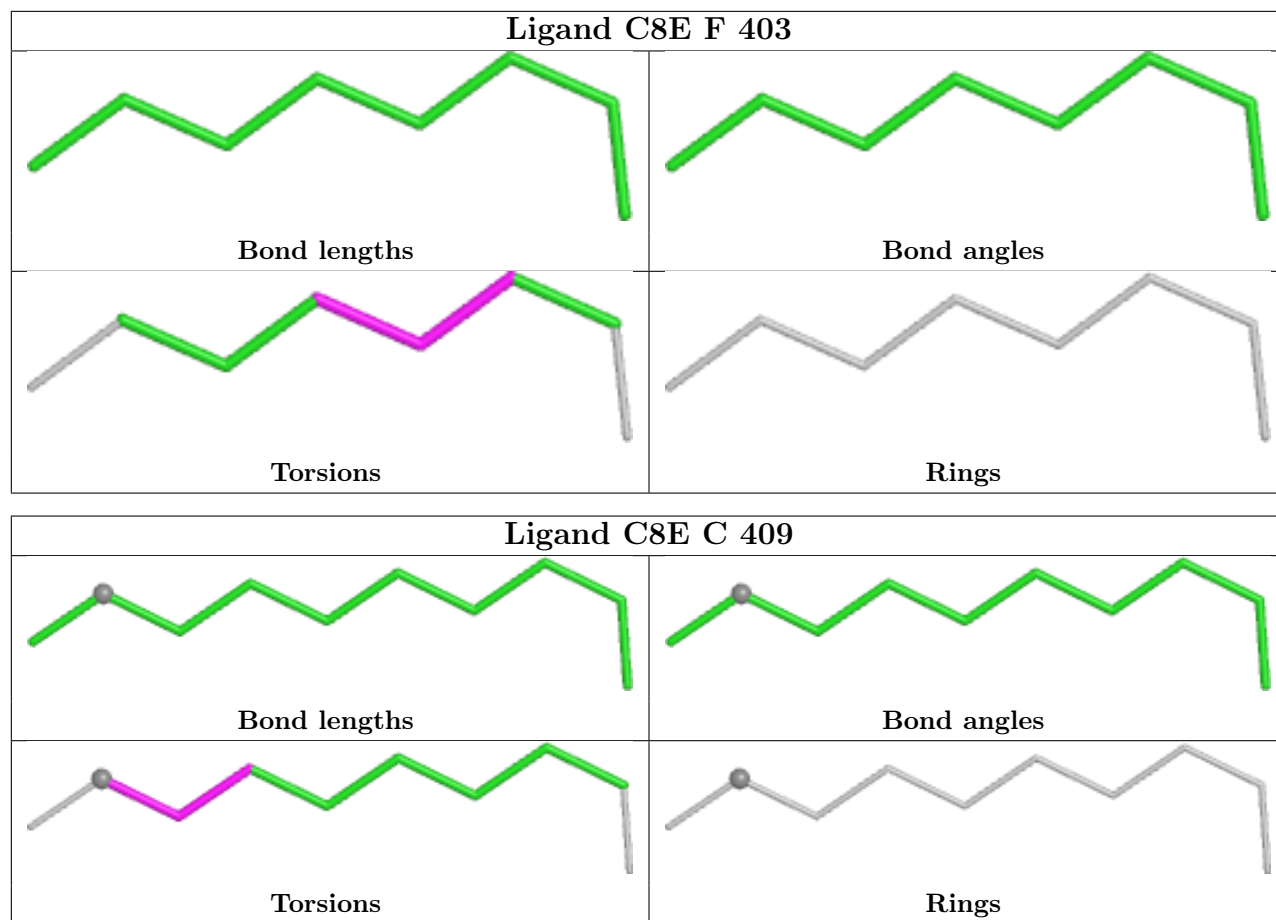












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/342 (100%)	-0.23	7 (2%) 65 67	8, 15, 28, 59	9 (2%)
1	B	342/342 (100%)	-0.27	11 (3%) 50 53	8, 15, 31, 77	4 (1%)
1	C	342/342 (100%)	-0.30	10 (2%) 53 56	7, 14, 30, 54	5 (1%)
1	D	342/342 (100%)	-0.12	16 (4%) 36 38	8, 16, 31, 96	6 (1%)
1	E	342/342 (100%)	-0.25	9 (2%) 57 59	8, 15, 32, 58	6 (1%)
1	F	342/342 (100%)	-0.40	0 100 100	8, 14, 25, 40	4 (1%)
All	All	2052/2052 (100%)	-0.26	53 (2%) 57 59	7, 15, 30, 96	34 (1%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	140	VAL	6.6
1	D	139	LEU	5.8
1	A	139	LEU	5.8
1	D	136	PHE	5.7
1	D	137	PHE	5.7
1	D	83	GLY	5.5
1	B	184	LEU	4.4
1	E	143	LEU	4.3
1	A	140	VAL	4.1
1	A	82	PHE	4.1
1	D	134	SER	4.1
1	D	84	ASP	4.0
1	E	82	PHE	3.9
1	D	138	GLY	3.7
1	B	140	VAL	3.7
1	A	138	GLY	3.7
1	B	139	LEU	3.6
1	E	140	VAL	3.4
1	B	82	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	137	PHE	3.2
1	E	139	LEU	3.0
1	C	82	PHE	3.0
1	B	83	GLY	3.0
1	C	261	TYR	2.9
1	D	159	GLU	2.9
1	D	135	ASP	2.9
1	B	143	LEU	2.9
1	C	84	ASP	2.8
1	D	82	PHE	2.8
1	C	83	GLY	2.8
1	E	134	SER	2.7
1	D	143	LEU	2.7
1	B	85	ALA	2.7
1	C	136	PHE	2.7
1	C	137	PHE	2.6
1	A	159	GLU	2.6
1	B	134	SER	2.5
1	D	85	ALA	2.4
1	A	137	PHE	2.4
1	B	136	PHE	2.4
1	A	83	GLY	2.4
1	B	138	GLY	2.4
1	C	85	ALA	2.3
1	E	137	PHE	2.2
1	D	49	GLN	2.2
1	D	141	ASP	2.2
1	C	139	LEU	2.1
1	C	138	GLY	2.1
1	D	86	GLY	2.1
1	E	263	PHE	2.0
1	C	134	SER	2.0
1	E	83	GLY	2.0
1	E	9	ASN	2.0

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

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

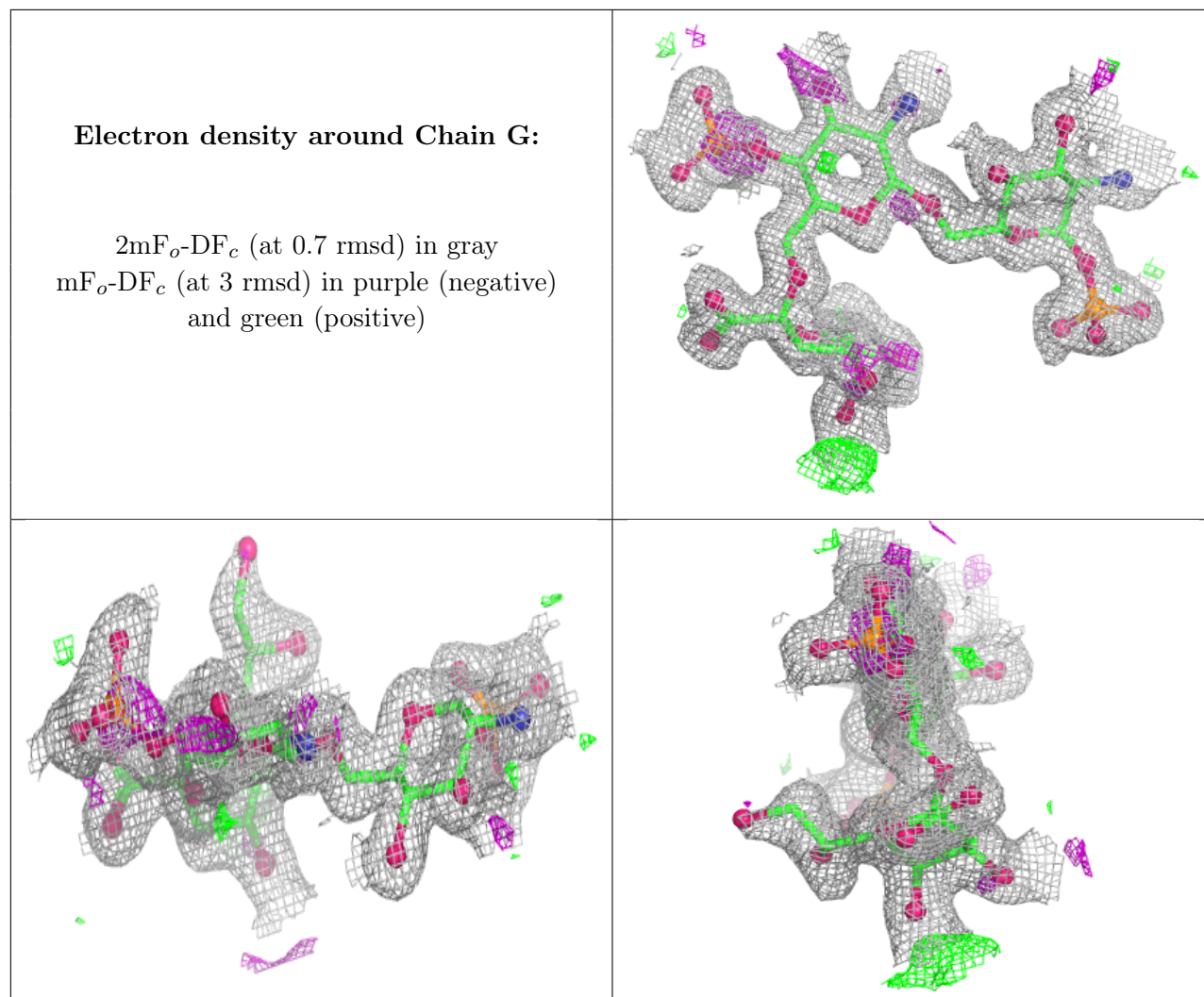
6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KDO	K	3	14/16	0.65	0.20	42,49,65,65	0
3	GMH	I	5	13/14	0.72	0.19	36,45,58,69	0
3	GMH	H	5	13/14	0.85	0.11	32,36,40,48	0
3	GMH	N	5	13/14	0.85	0.16	31,36,54,59	0
2	GP1	K	1	16/16	0.88	0.11	34,37,66,67	0
2	KDO	G	3	15/16	0.91	0.10	24,29,40,48	0
2	KDO	L	3	15/16	0.91	0.09	25,28,40,44	0
3	KDO	H	3	15/16	0.91	0.10	22,26,33,41	0
2	KDO	M	3	15/16	0.93	0.09	23,27,35,38	0
4	KDO	O	3	15/16	0.94	0.08	13,21,31,35	0
2	Z9M	K	2	15/16	0.95	0.09	25,29,34,40	0
3	KDO	N	3	15/16	0.95	0.09	18,25,33,37	0
2	GP1	L	1	16/16	0.95	0.07	24,26,44,49	0
4	KDO	J	3	15/16	0.95	0.08	16,21,30,34	0
3	KDO	I	4	15/16	0.95	0.07	14,15,19,24	0
3	GP1	H	1	16/16	0.96	0.07	22,24,50,51	0
2	Z9M	G	2	15/16	0.96	0.08	22,24,31,34	0
3	KDO	N	4	15/16	0.96	0.07	15,16,20,29	0
3	KDO	H	4	15/16	0.96	0.07	18,20,25,27	0
2	GP1	M	1	16/16	0.96	0.07	23,26,47,49	0
4	KDO	J	4	15/16	0.96	0.07	12,19,22,23	0
2	GP1	G	1	16/16	0.96	0.07	22,27,48,52	0
3	Z9M	H	2	15/16	0.97	0.07	20,21,26,26	0
2	Z9M	L	2	15/16	0.97	0.06	23,24,30,30	0
3	Z9M	I	2	15/16	0.97	0.06	18,21,41,41	0
4	GP1	O	1	16/16	0.97	0.06	18,20,41,43	0
3	KDO	I	3	15/16	0.97	0.07	18,23,31,31	0
4	KDO	O	4	15/16	0.97	0.06	17,18,21,24	0
4	Z9M	J	2	15/16	0.98	0.05	16,17,26,26	0
3	Z9M	N	2	15/16	0.98	0.05	18,21,29,32	0
2	Z9M	M	2	15/16	0.98	0.07	21,21,26,27	0
3	GP1	I	1	16/16	0.98	0.05	17,19,33,35	0
4	Z9M	O	2	15/16	0.98	0.05	17,18,24,27	0
3	GP1	N	1	16/16	0.98	0.05	16,19,34,34	0
4	GP1	J	1	16/16	0.98	0.05	17,19,44,44	0

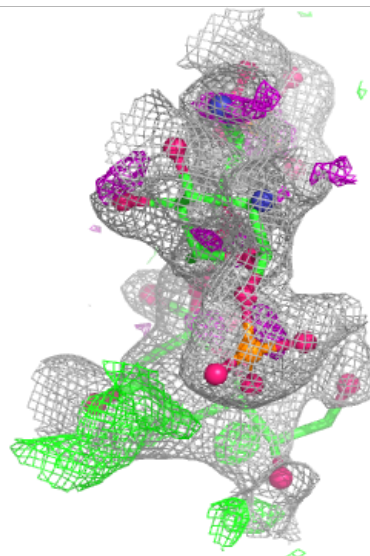
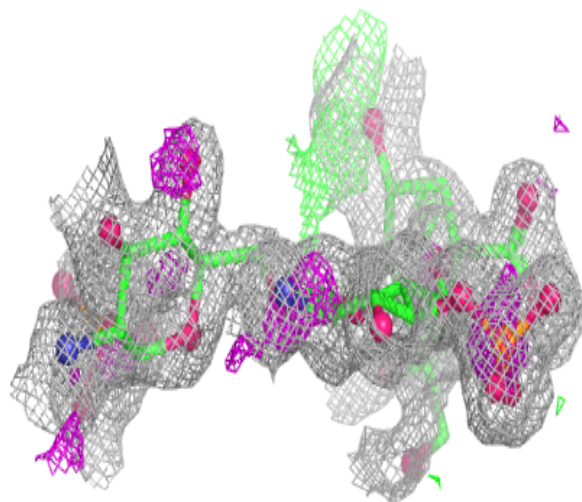
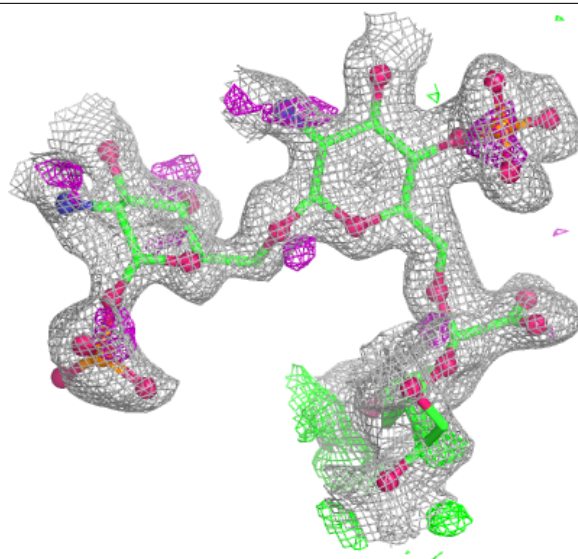
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



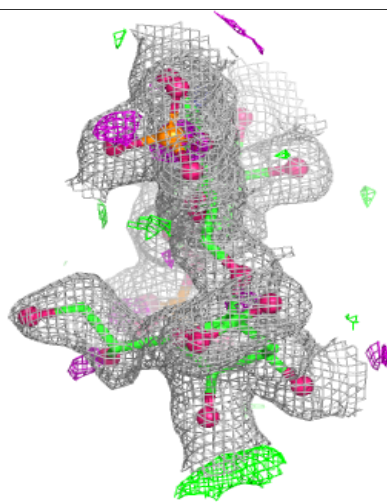
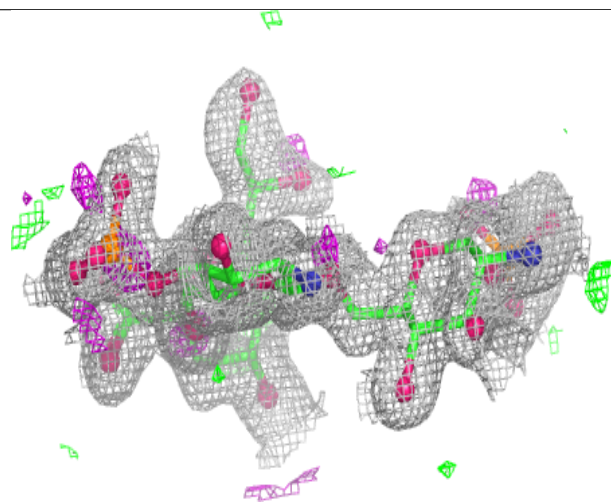
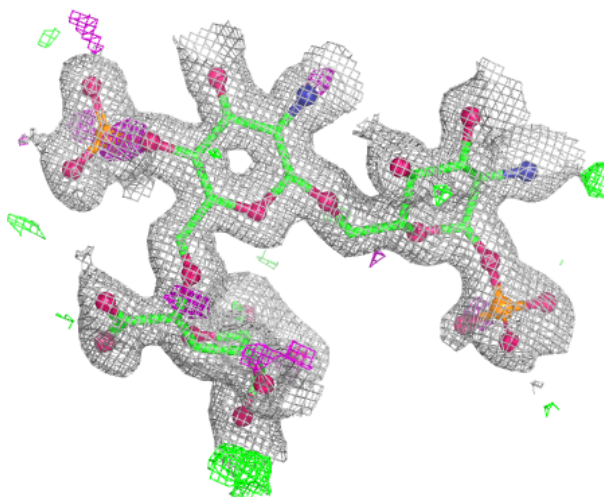
Electron density around Chain K:

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



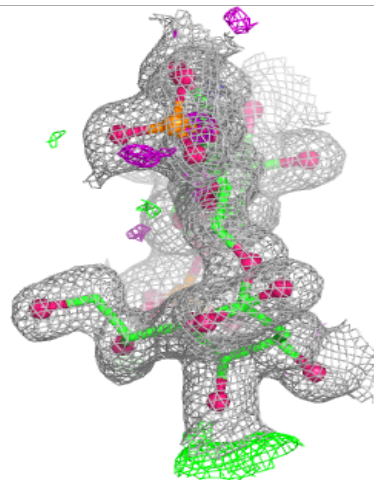
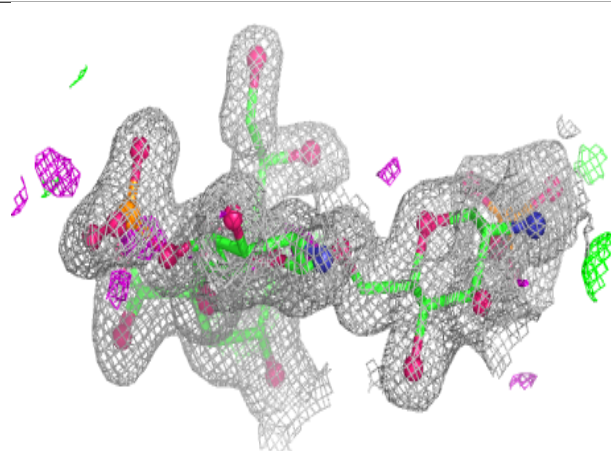
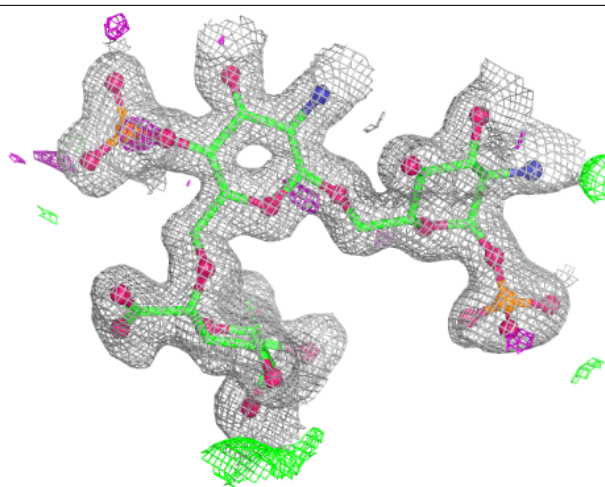
Electron density around Chain L:

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



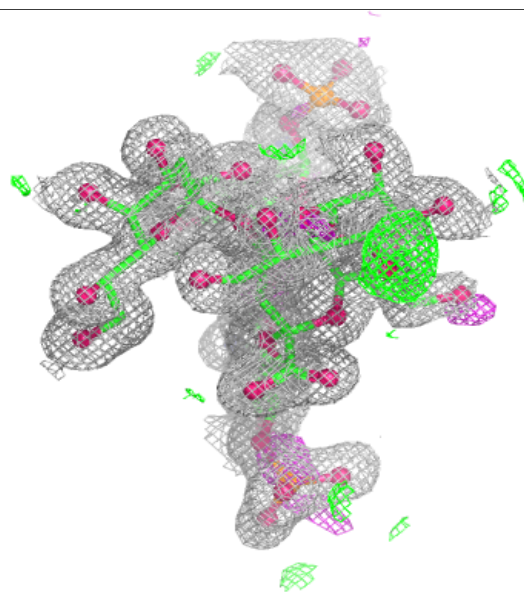
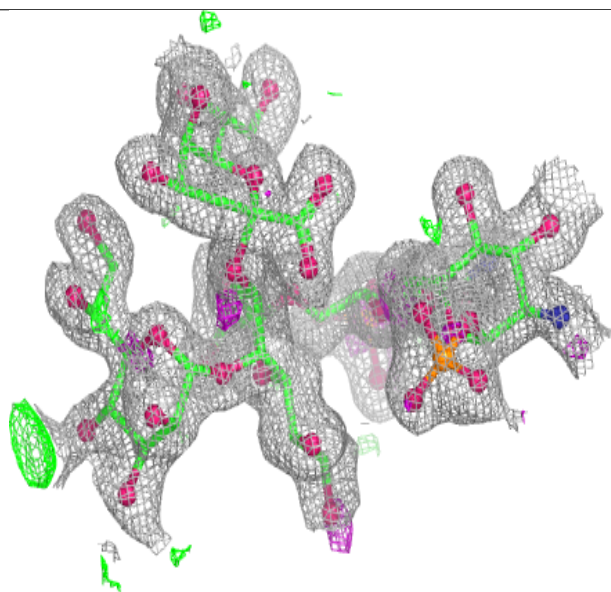
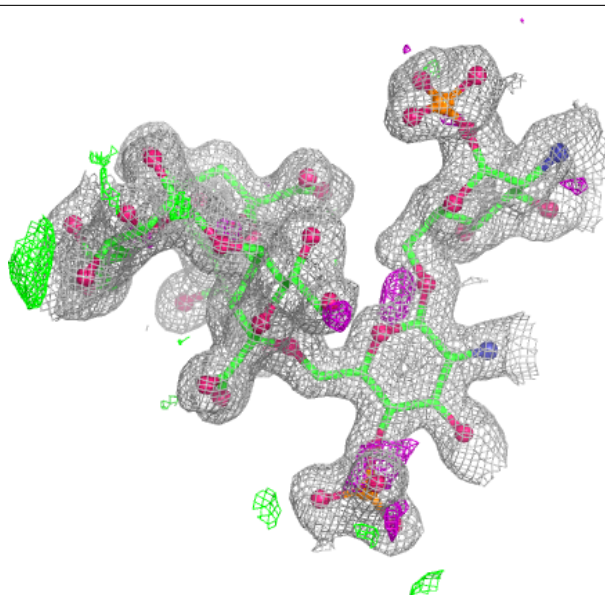
Electron density around Chain M:

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



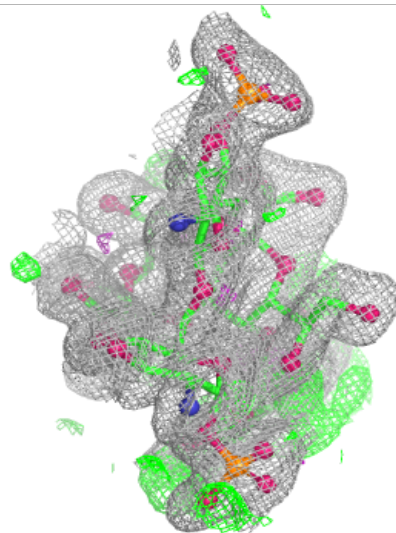
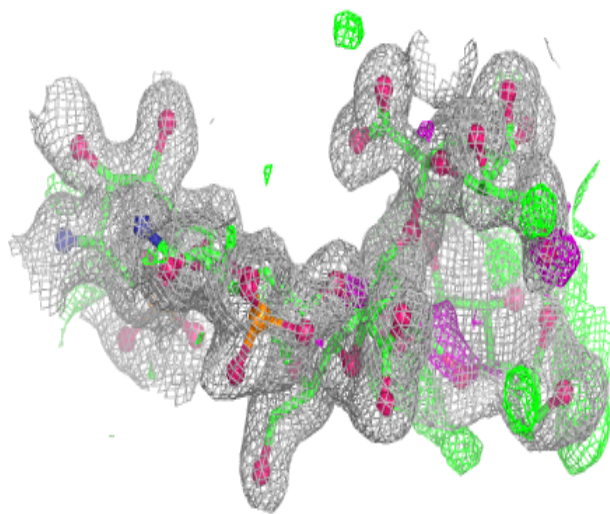
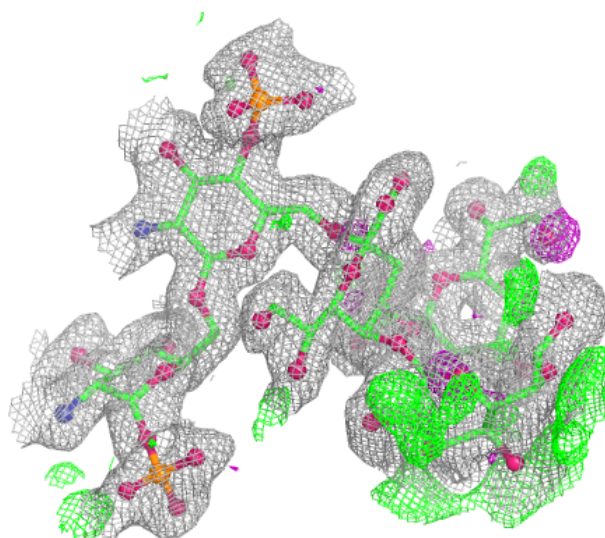
Electron density around Chain H:

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



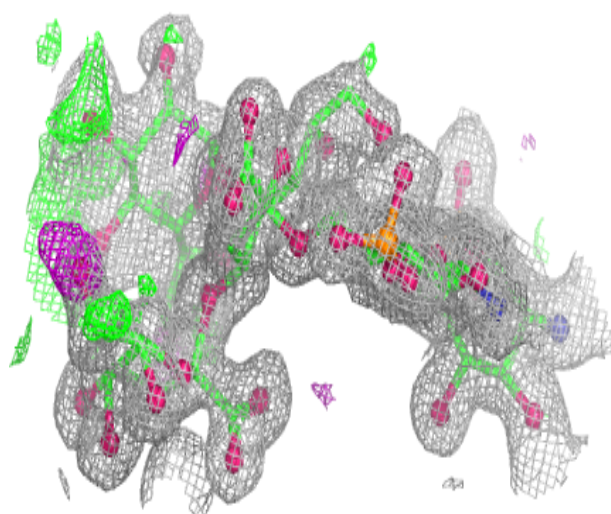
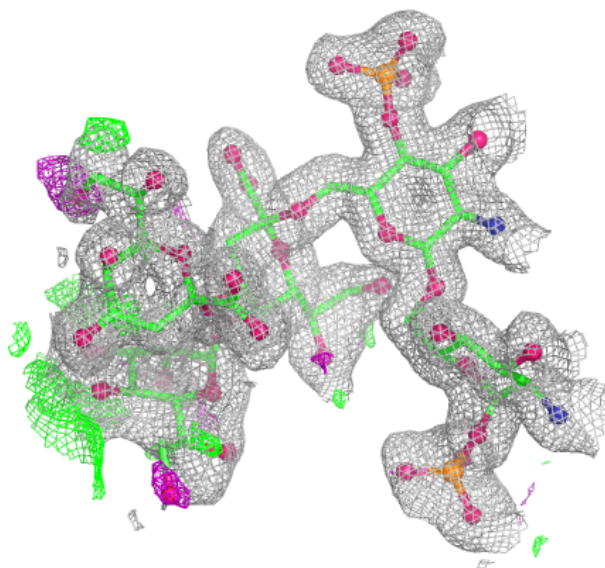
Electron density around Chain I:

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



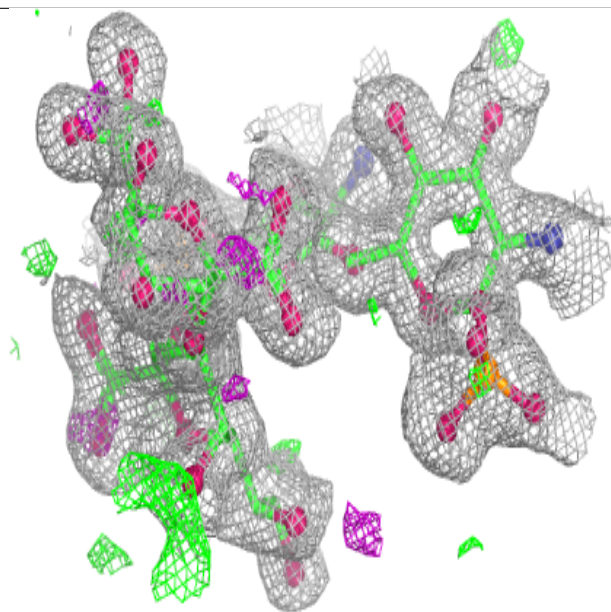
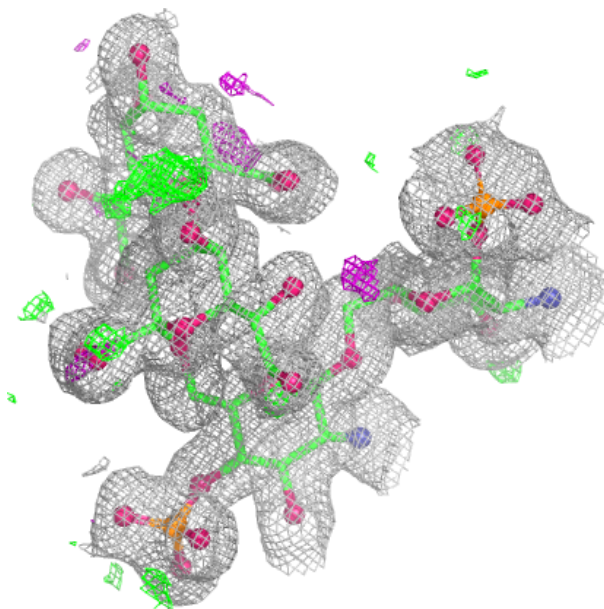
Electron density around Chain N:

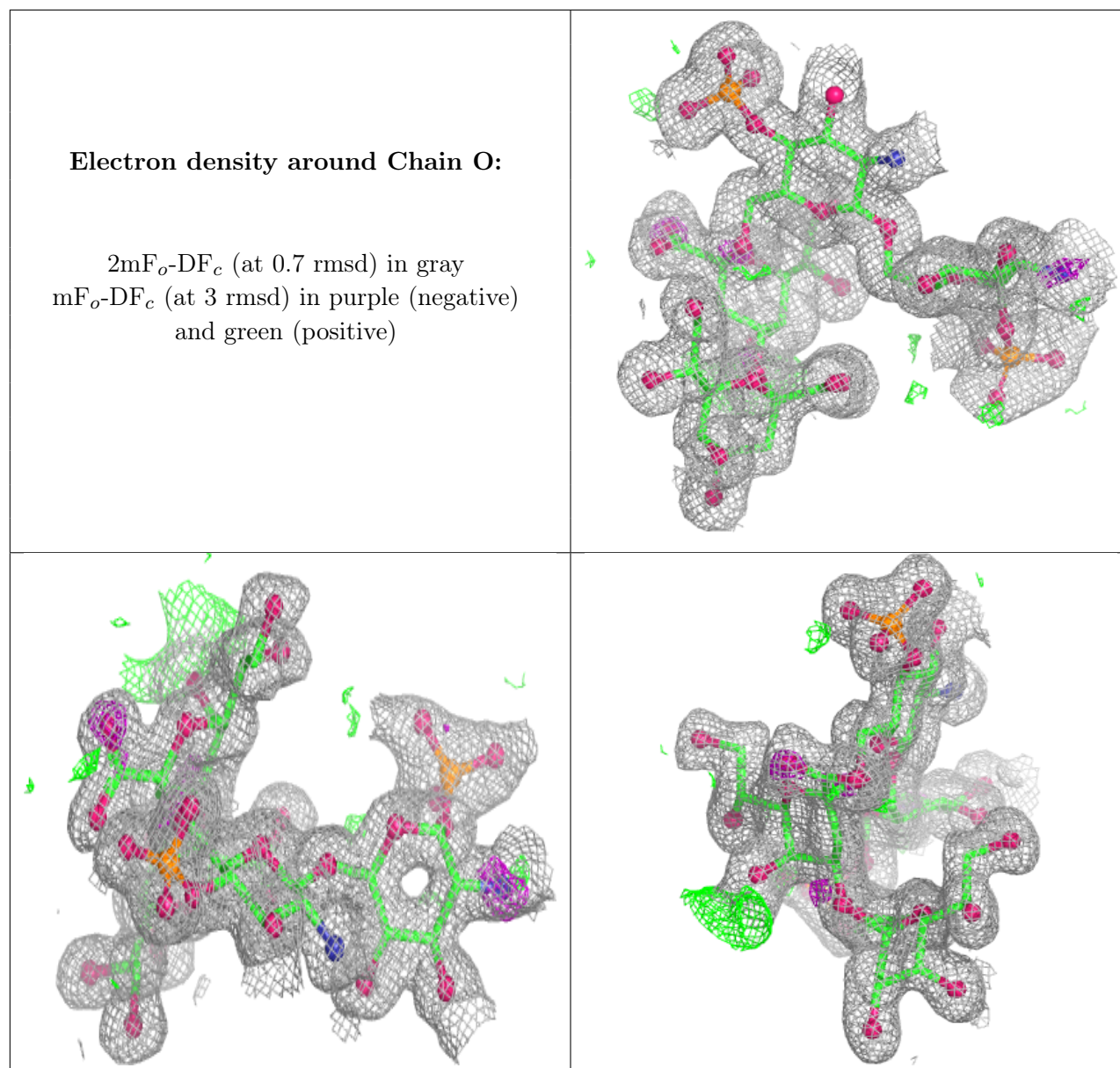
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	DAO	A	417	5/14	0.58	0.26	55,57,59,63	0
11	DAO	D	424	5/14	0.58	0.33	47,58,58,73	0
11	DAO	E	410	5/14	0.58	0.27	49,54,55,56	0
10	MYR	A	416	6/16	0.63	0.28	47,52,55,57	0
11	DAO	C	414	5/14	0.64	0.25	49,50,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	DAO	D	418	3/14	0.64	0.25	51,51,52,53	0
11	DAO	E	405	5/14	0.65	0.22	52,54,57,63	0
11	DAO	B	412	5/14	0.66	0.28	39,48,59,60	0
9	FTT	E	404	14/17	0.70	0.26	38,46,48,57	0
9	FTT	D	425	14/17	0.71	0.24	33,45,53,62	0
6	C8E	A	402	3/21	0.72	0.26	33,33,41,41	0
9	FTT	C	413	14/17	0.72	0.25	33,47,58,61	0
10	MYR	B	411	6/16	0.75	0.26	43,60,68,68	0
9	FTT	A	415	16/17	0.76	0.20	27,39,59,66	0
10	MYR	E	409	6/16	0.77	0.22	41,44,51,54	0
9	FTT	D	414	14/17	0.77	0.20	36,47,53,54	0
11	DAO	C	426	8/14	0.78	0.24	37,62,72,73	0
6	C8E	D	403	6/21	0.78	0.24	39,44,51,56	0
6	C8E	E	401	6/21	0.78	0.27	44,52,63,65	0
6	C8E	A	404	6/21	0.78	0.25	39,46,50,51	0
10	MYR	D	423	6/16	0.78	0.21	43,47,49,50	0
6	C8E	D	404	6/21	0.79	0.20	32,41,41,43	0
9	FTT	B	407	14/17	0.79	0.21	35,40,55,61	0
9	FTT	F	406	14/17	0.79	0.21	38,42,47,48	0
6	C8E	C	408	11/21	0.80	0.19	36,39,45,49	0
6	C8E	A	407	5/21	0.80	0.20	18,20,26,28	0
6	C8E	A	410	7/21	0.80	0.19	38,39,40,41	0
6	C8E	D	406	8/21	0.80	0.24	48,52,54,58	0
6	C8E	D	408	11/21	0.80	0.19	27,41,43,43	0
6	C8E	C	407	11/21	0.81	0.19	33,35,43,47	0
10	MYR	D	419	5/16	0.81	0.15	16,25,37,38	0
9	FTT	D	415	11/17	0.81	0.17	33,36,41,41	0
6	C8E	B	404	8/21	0.81	0.19	41,46,47,47	0
9	FTT	D	417	11/17	0.82	0.19	46,51,67,67	0
11	DAO	D	412	6/14	0.82	0.20	44,48,51,57	0
6	C8E	B	405	8/21	0.82	0.19	38,39,41,41	0
11	DAO	A	419	8/14	0.82	0.18	40,41,44,57	0
6	C8E	D	407	8/21	0.82	0.23	25,41,44,48	0
6	C8E	C	409	10/21	0.82	0.20	35,38,50,54	0
6	C8E	A	406	5/21	0.83	0.27	57,64,67,74	0
6	C8E	D	405	6/21	0.83	0.18	30,37,41,42	0
6	C8E	C	403	3/21	0.83	0.23	45,45,46,50	0
6	C8E	A	409	8/21	0.84	0.17	29,34,38,38	0
6	C8E	C	410	7/21	0.84	0.18	23,24,39,43	0
6	C8E	C	406	8/21	0.84	0.16	30,33,33,35	0
6	C8E	A	408	8/21	0.85	0.19	19,29,52,66	0
9	FTT	D	421	13/17	0.85	0.16	27,30,46,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	C8E	B	403	5/21	0.85	0.17	30,32,33,41	0
6	C8E	C	404	6/21	0.85	0.19	28,41,49,51	0
6	C8E	A	405	4/21	0.85	0.32	77,80,84,87	0
6	C8E	F	403	8/21	0.86	0.18	40,43,47,47	0
6	C8E	D	409	4/21	0.86	0.24	21,23,30,39	0
9	FTT	A	418	14/17	0.86	0.17	39,44,66,68	0
6	C8E	D	410	6/21	0.86	0.16	40,43,45,45	0
10	MYR	C	425	9/16	0.86	0.22	33,55,63,71	0
6	C8E	B	401	9/21	0.86	0.18	31,43,63,64	0
11	DAO	F	418	8/14	0.86	0.21	34,49,64,66	0
6	C8E	D	402	4/21	0.87	0.15	32,33,34,39	0
9	FTT	B	410	16/17	0.87	0.14	23,30,36,39	0
9	FTT	F	410	16/17	0.87	0.15	28,33,39,41	0
9	FTT	F	416	16/17	0.87	0.15	21,32,42,45	0
6	C8E	B	402	3/21	0.87	0.19	46,46,50,55	0
9	FTT	D	422	16/17	0.87	0.14	28,36,41,43	0
6	C8E	F	402	4/21	0.87	0.23	41,44,47,47	0
9	FTT	D	420	16/17	0.88	0.13	17,23,28,30	0
7	PO4	E	402	5/5	0.88	0.13	34,35,41,44	0
9	FTT	A	414	13/17	0.88	0.13	29,33,39,41	0
6	C8E	C	401	3/21	0.88	0.22	45,45,50,51	0
6	C8E	C	402	7/21	0.88	0.20	25,32,38,43	0
6	C8E	A	403	4/21	0.88	0.21	62,71,76,79	0
11	DAO	C	421	10/14	0.88	0.14	25,30,32,33	0
9	FTT	B	409	13/17	0.89	0.14	21,26,42,44	0
10	MYR	F	411	11/16	0.89	0.14	26,31,36,36	0
10	MYR	F	417	12/16	0.89	0.15	29,32,44,50	0
9	FTT	A	413	15/17	0.89	0.12	15,22,26,38	0
10	MYR	C	419	8/16	0.89	0.17	22,30,32,32	0
6	C8E	C	405	3/21	0.90	0.17	26,26,28,35	0
9	FTT	D	416	13/17	0.90	0.16	29,43,53,54	0
9	FTT	E	408	15/17	0.90	0.12	25,31,40,41	0
9	FTT	C	415	16/17	0.91	0.13	23,32,37,38	0
7	PO4	A	411	5/5	0.91	0.12	36,36,41,47	0
7	PO4	C	411	5/5	0.91	0.12	32,35,44,44	0
7	PO4	D	411	5/5	0.91	0.11	32,37,40,47	0
11	DAO	F	412	5/14	0.91	0.15	26,27,35,40	0
11	DAO	F	413	5/14	0.91	0.17	33,34,49,62	0
6	C8E	F	401	3/21	0.91	0.15	21,21,30,37	0
7	PO4	F	404	5/5	0.92	0.11	31,36,45,45	0
9	FTT	E	406	14/17	0.92	0.10	18,21,25,26	0
9	FTT	E	407	12/17	0.92	0.11	26,29,36,39	0

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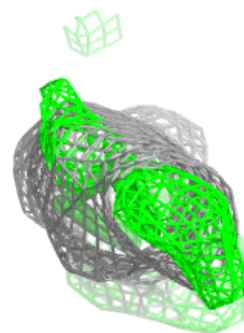
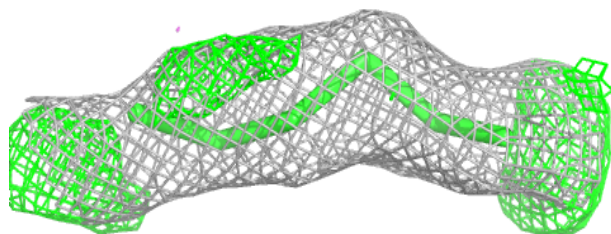
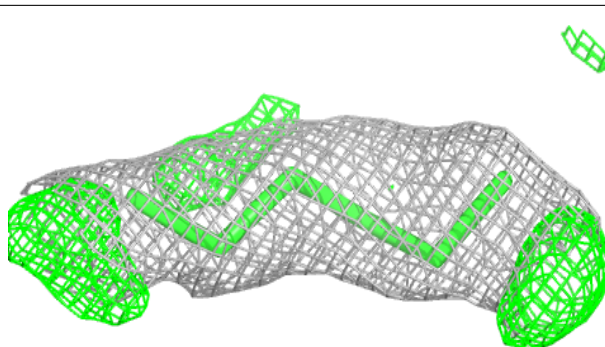
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PO4	B	406	5/5	0.92	0.11	31,33,40,44	0
9	FTT	C	422	16/17	0.92	0.11	15,20,27,31	0
9	FTT	F	408	13/17	0.92	0.15	19,31,46,46	0
9	FTT	C	424	16/17	0.92	0.13	18,30,41,41	0
9	FTT	F	415	11/17	0.92	0.11	22,23,28,34	0
9	FTT	F	409	12/17	0.93	0.11	21,26,34,38	0
9	FTT	F	407	12/17	0.93	0.13	19,24,43,48	0
9	FTT	C	423	13/17	0.93	0.10	20,22,34,39	0
9	FTT	B	408	15/17	0.94	0.11	19,21,36,37	0
11	DAO	C	420	13/14	0.94	0.10	22,27,31,33	0
9	FTT	C	418	13/17	0.94	0.15	19,26,52,55	0
8	KDO	D	413	15/16	0.94	0.08	14,22,27,27	0
8	KDO	E	403	15/16	0.95	0.07	19,21,26,27	0
8	KDO	A	412	15/16	0.95	0.07	18,23,30,30	0
9	FTT	C	416	11/17	0.96	0.08	18,20,24,30	0
9	FTT	F	414	14/17	0.96	0.08	16,18,24,27	0
9	FTT	C	417	16/17	0.97	0.07	18,20,30,34	0
5	SO4	A	401	5/5	0.99	0.09	17,19,22,27	0
5	SO4	D	401	5/5	0.99	0.10	18,21,25,29	0
12	CA	C	412	1/1	1.00	0.01	12,12,12,12	0
12	CA	F	405	1/1	1.00	0.01	13,13,13,13	0

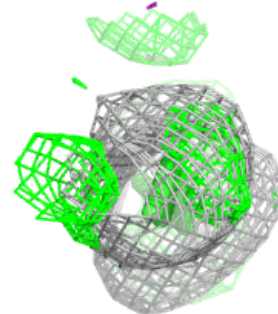
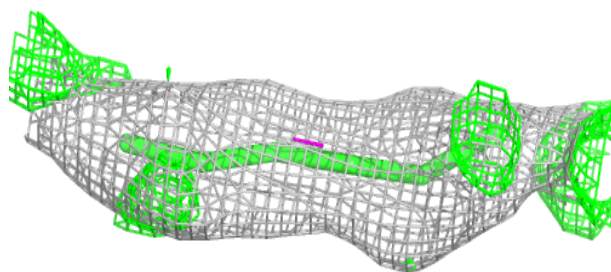
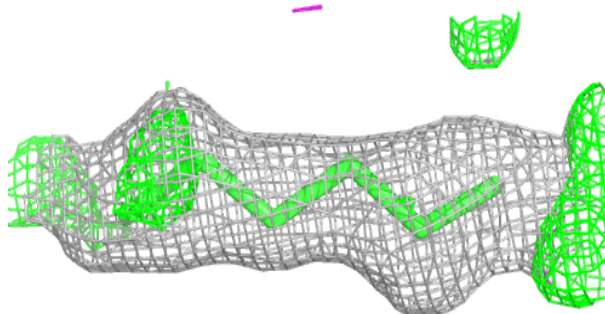
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E 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)

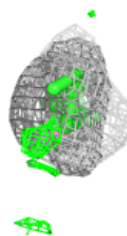
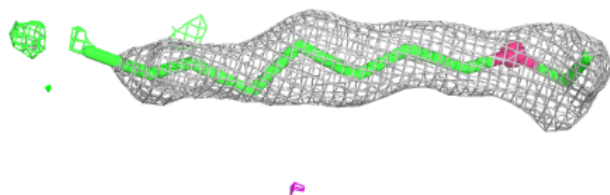
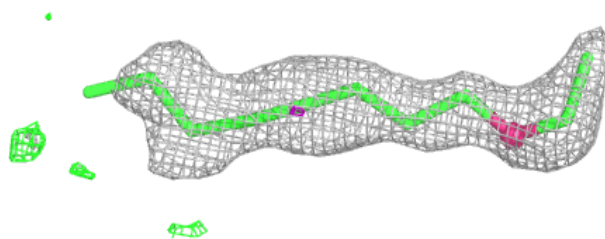
**Electron density around C8E A 404:**

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



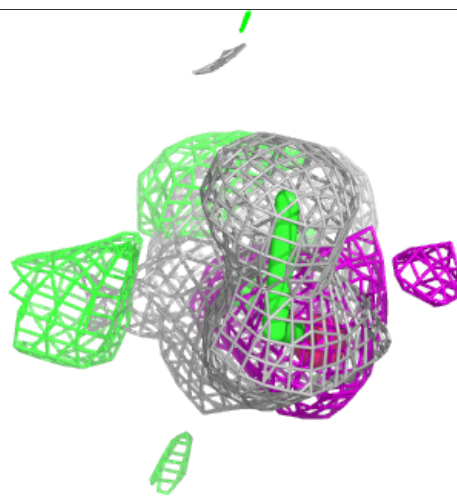
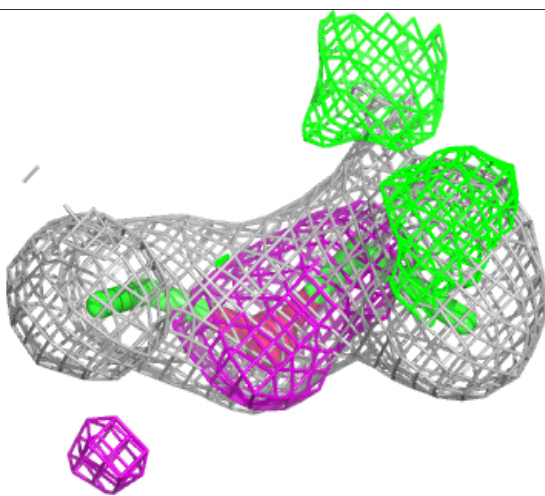
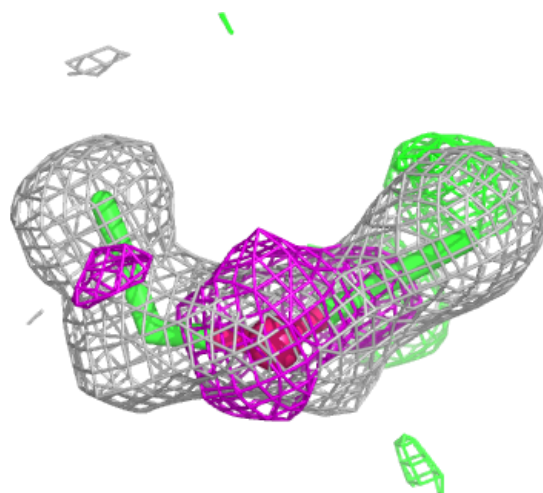
Electron density around C8E C 408:

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



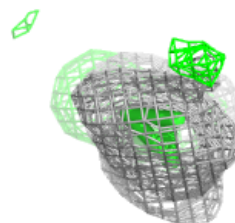
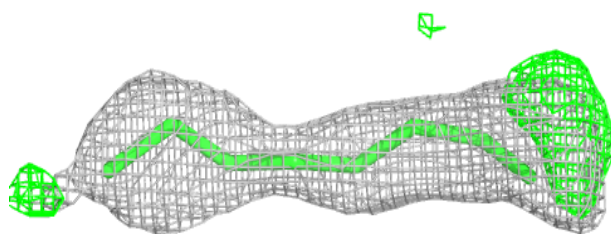
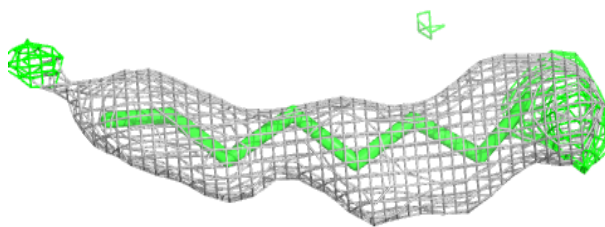
Electron density around C8E A 407:

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

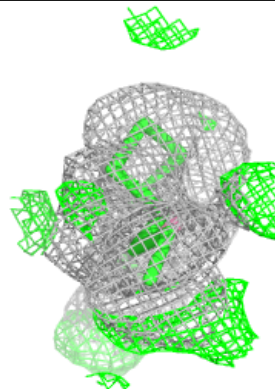
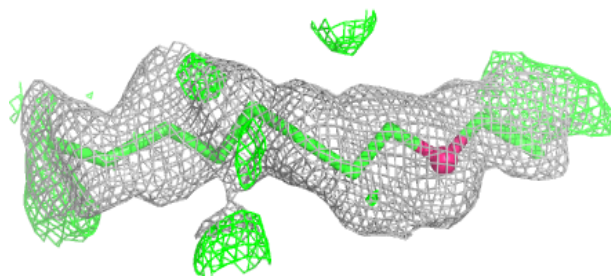
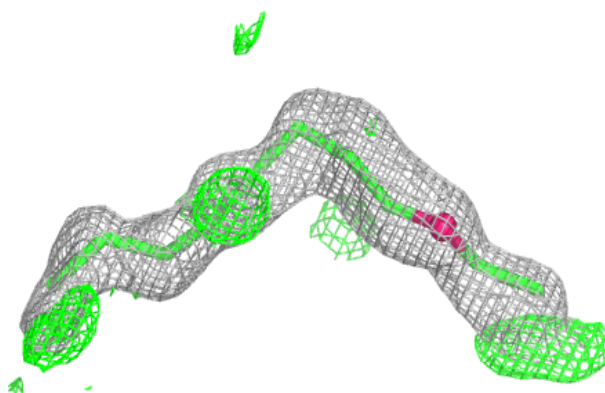


Electron density around C8E D 406:

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

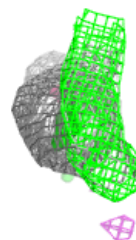
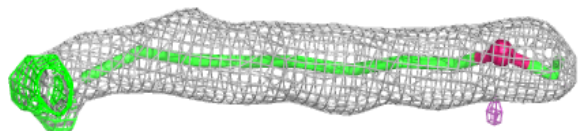
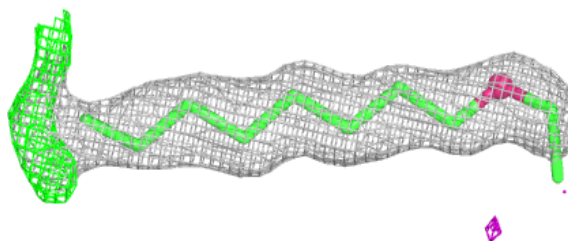
**Electron density around C8E D 408:**

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

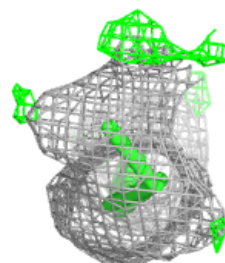
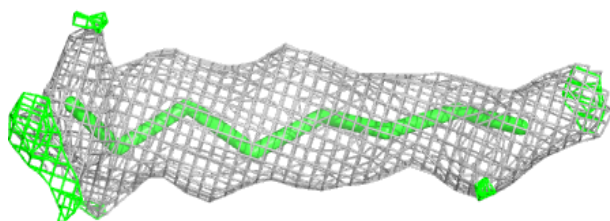
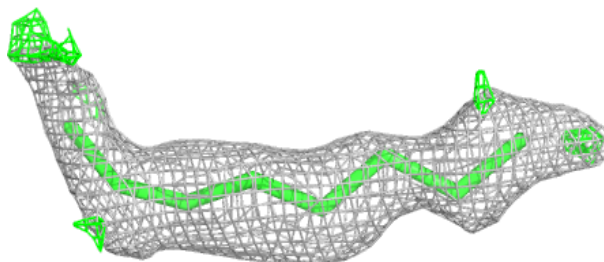


Electron density around C8E C 407:

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

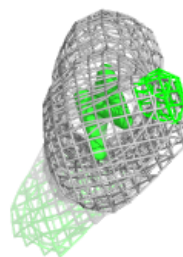
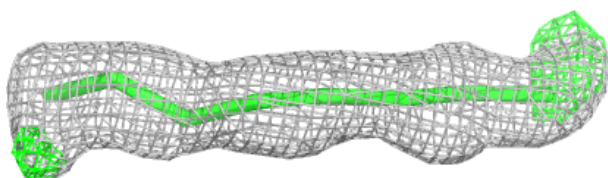
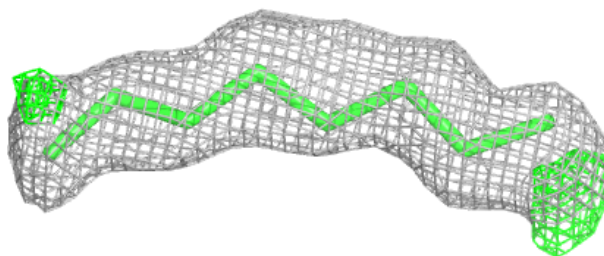
**Electron density around C8E B 404:**

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

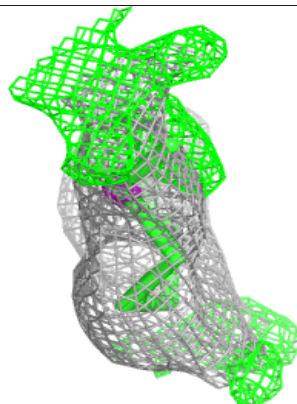
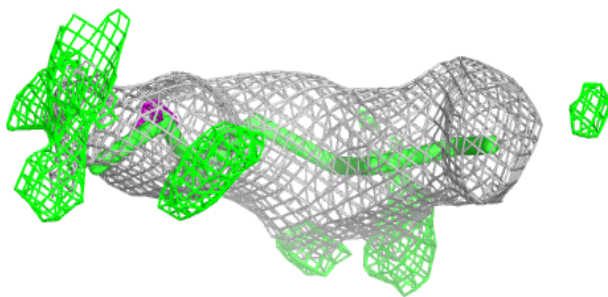
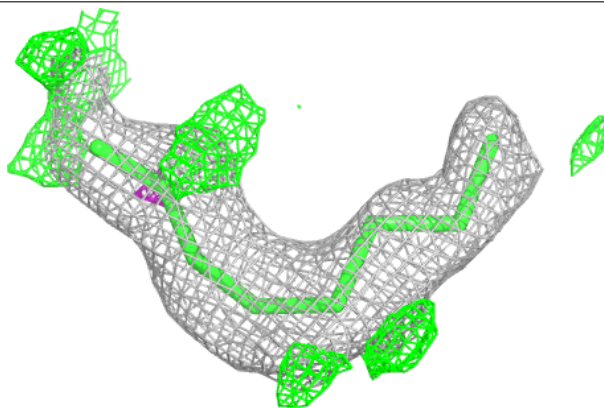


Electron density around C8E B 405:

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

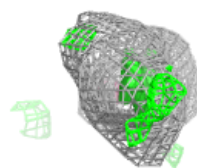
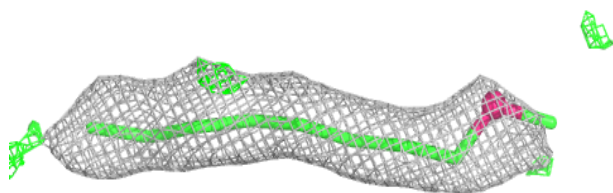
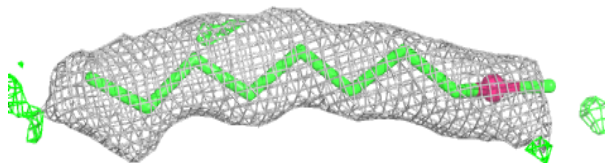
**Electron density around C8E D 407:**

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

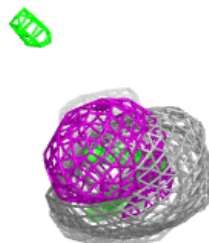
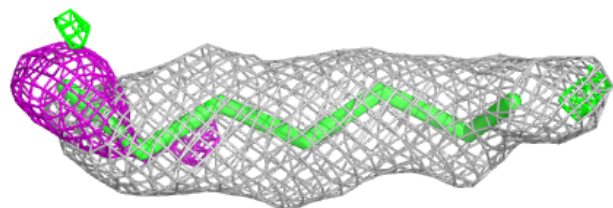
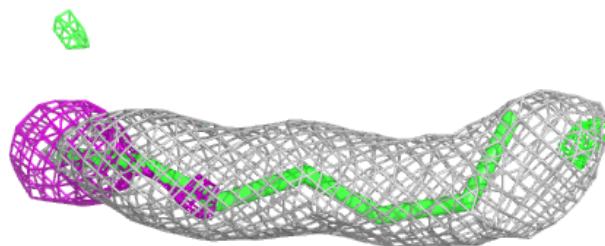


Electron density around C8E C 409:

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

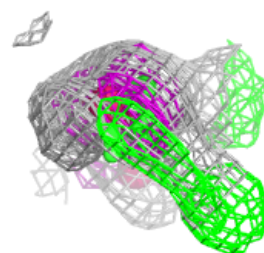
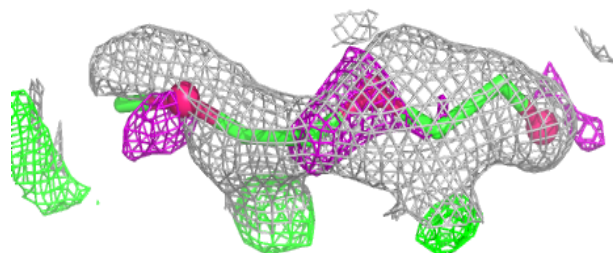
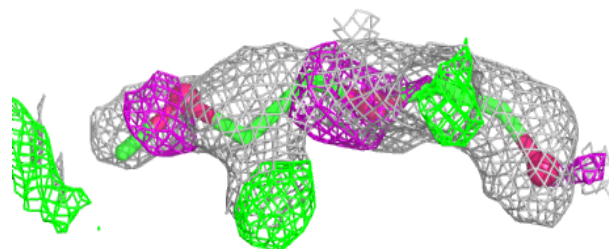
**Electron density around C8E C 410:**

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

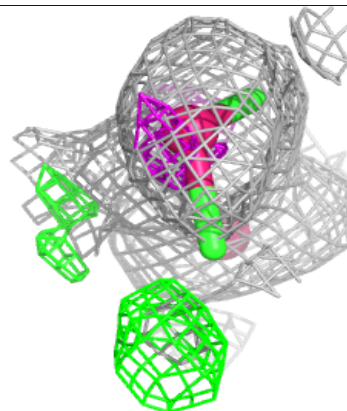
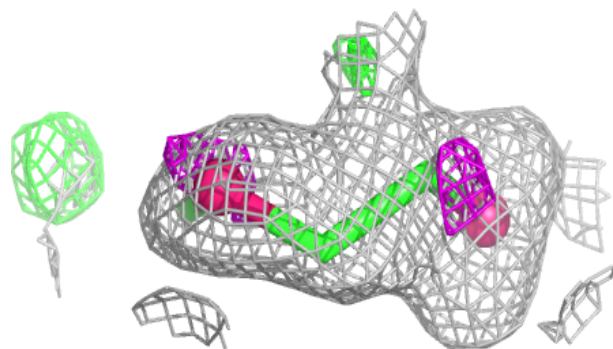
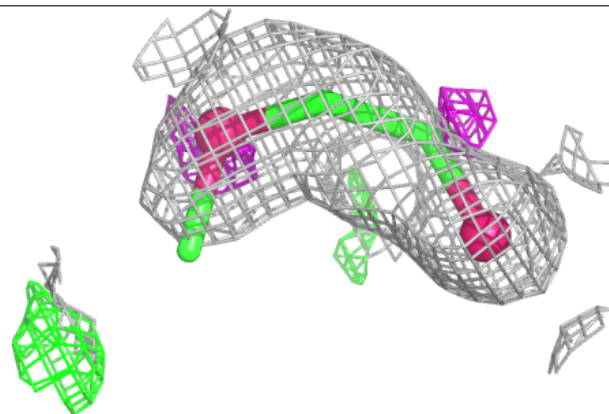


Electron density around C8E A 408:

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

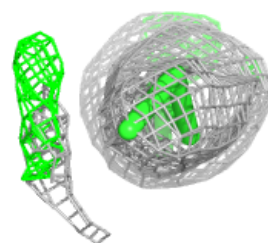
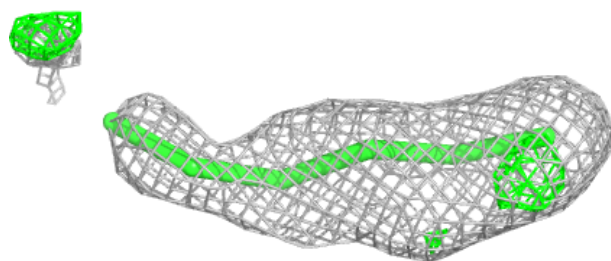
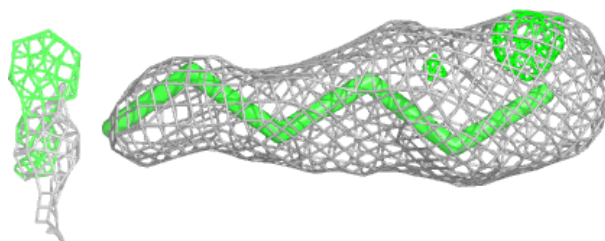
**Electron density around C8E B 403:**

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

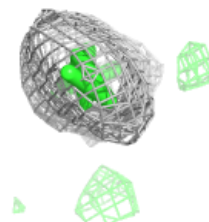
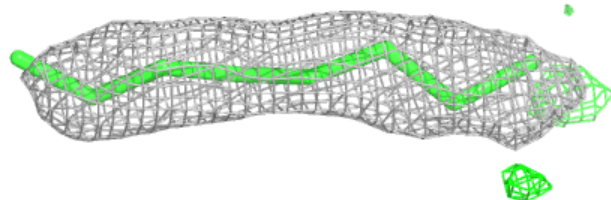
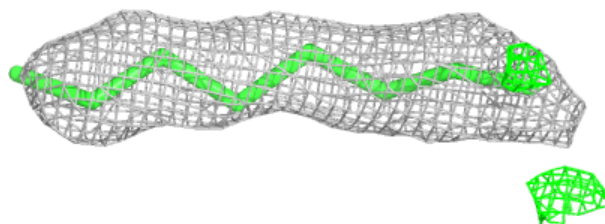


Electron density around C8E C 404:

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

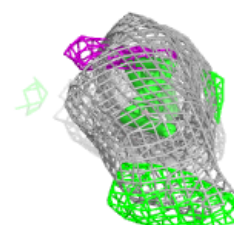
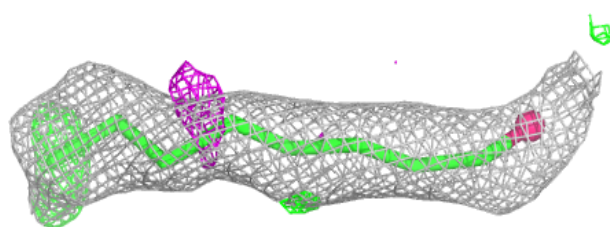
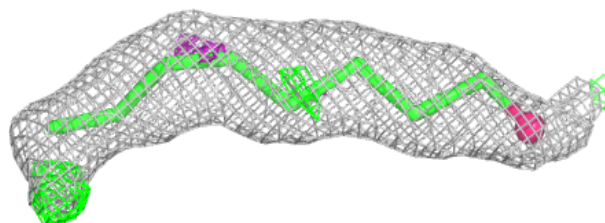
**Electron density around C8E F 403:**

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

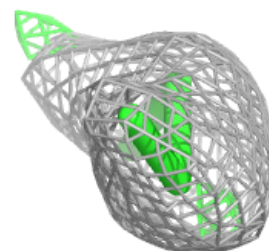
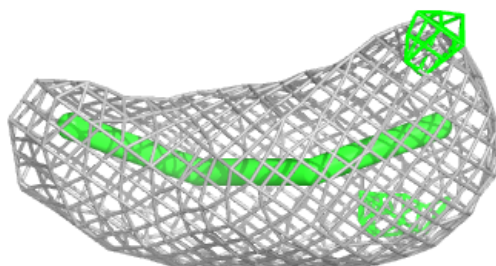
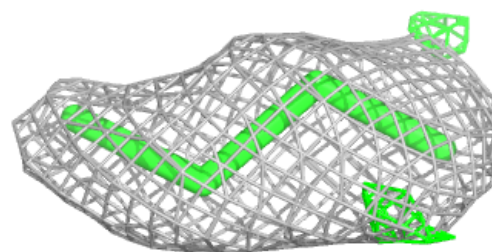


Electron density around C8E B 401:

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

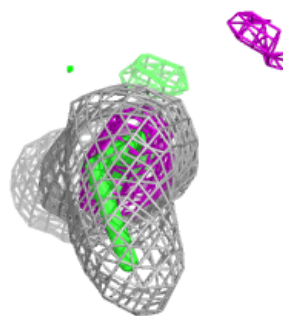
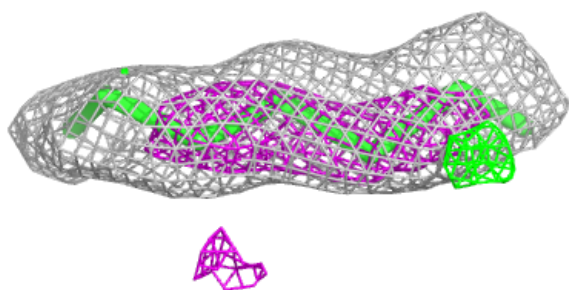
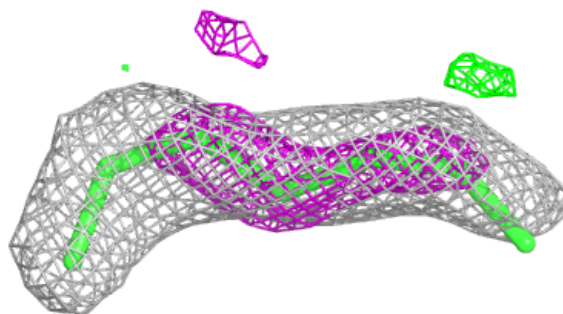
**Electron density around C8E D 402:**

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



Electron density around C8E 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.