wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2023 – 04:05 pm GMT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

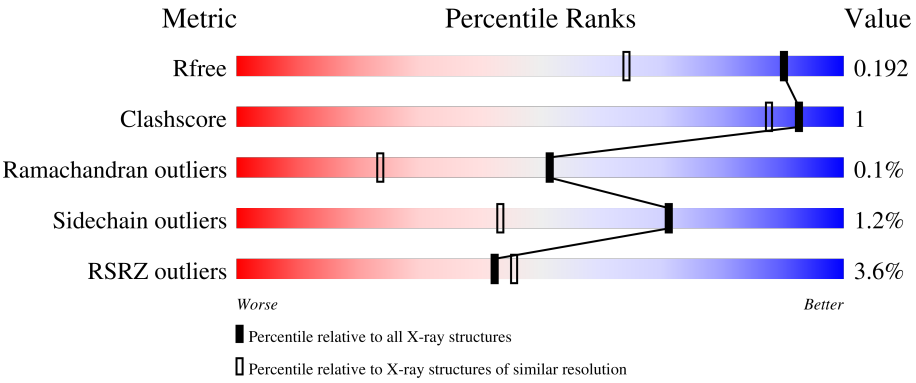
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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 >=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 <=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	4% 97% .
1	B	342	4% 95% 5%
1	C	342	2% 96% .
1	D	342	6% 96% .
1	E	342	4% 97% .

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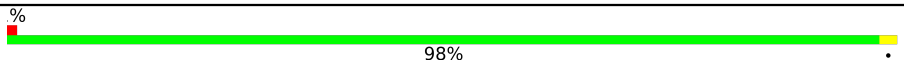
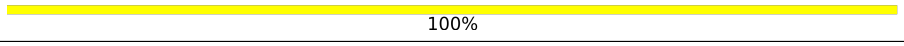
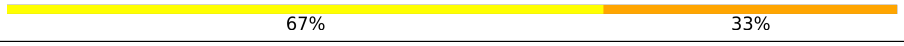
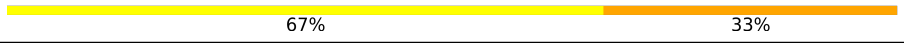
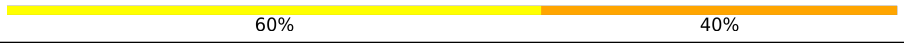
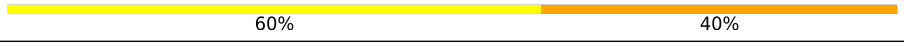
Mol	Chain	Length	Quality of chain
1	F	342	
2	G	3	
2	K	3	
2	L	3	
2	M	3	
3	H	5	
3	I	5	
3	N	5	
4	J	4	
4	O	4	

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

2 Entry composition (i)

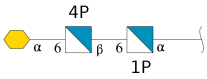
There are 13 unique types of molecules in this entry. The entry contains 19668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called OMPC PORIN.

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

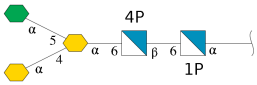
- Molecule 2 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.



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

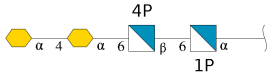
- Molecule 3 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyran

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.



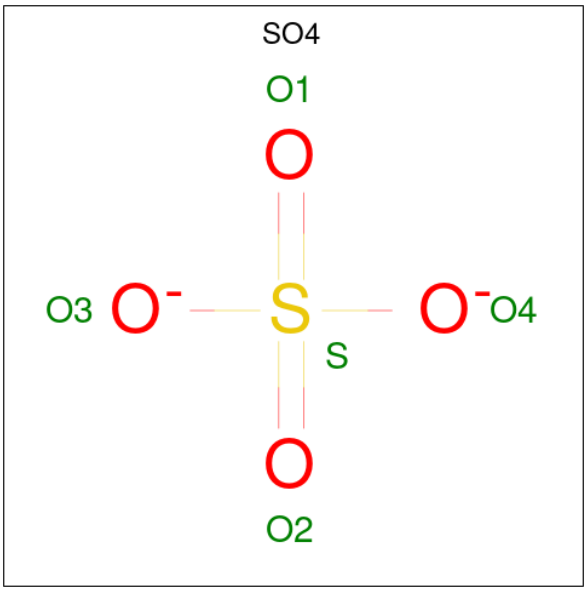
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	5	Total	C	N	O	P	0	0	0
			74	35	2	35	2			
3	I	5	Total	C	N	O	P	0	0	0
			74	35	2	35	2			
3	N	5	Total	C	N	O	P	0	0	0
			74	35	2	35	2			

- 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.



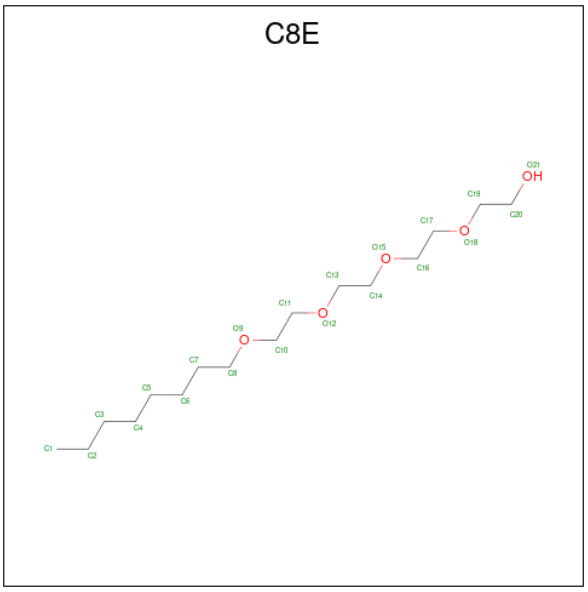
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	P	0	0	0
			61	28	2	29	2			
4	O	4	Total	C	N	O	P	0	0	0
			61	28	2	29	2			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



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

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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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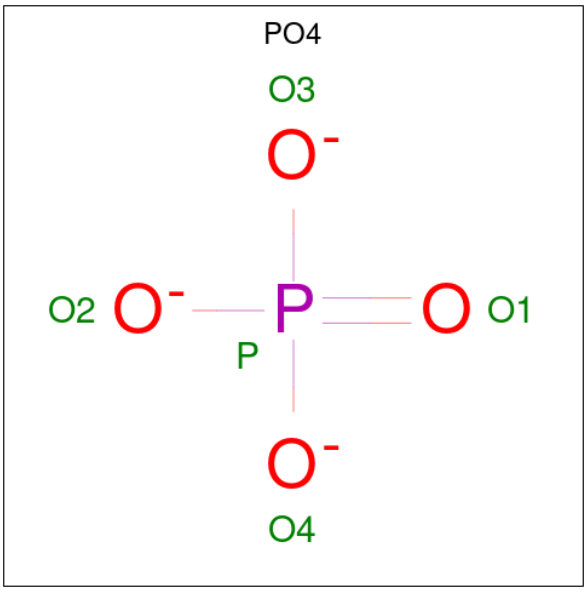
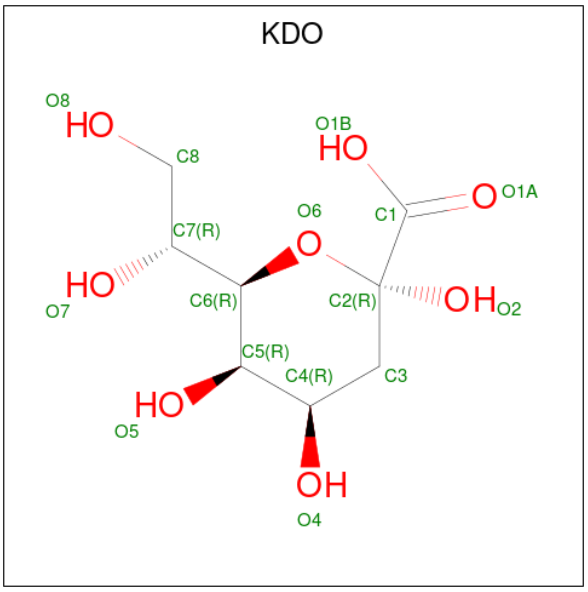
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 10 9 1	0	0
6	C	1	Total C 7 7	0	0
6	D	1	Total C 4 4	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 6 6	0	0
6	D	1	Total C 8 8	0	0
6	D	1	Total C 8 8	0	0
6	D	1	Total C O 11 10 1	0	0
6	D	1	Total C O 4 3 1	0	0
6	D	1	Total C 6 6	0	0
6	E	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_4P).



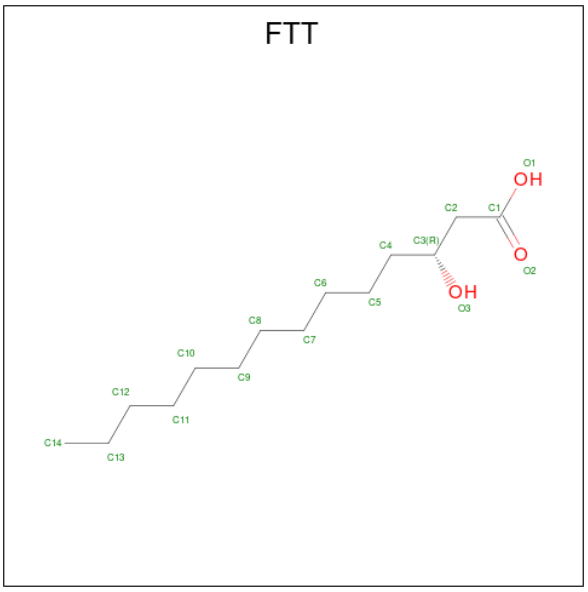
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0
7	C	1	Total O P 5 4 1	0	0
7	D	1	Total O P 5 4 1	0	0
7	E	1	Total O P 5 4 1	0	0
7	F	1	Total O P 5 4 1	0	0

- Molecule 8 is 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid (three-letter code: KDO) (formula: $C_8H_{14}O_8$).



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

- 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 15 13 2	0	0
9	A	1	Total C O 13 11 2	0	0
9	A	1	Total C O 16 14 2	0	0
9	A	1	Total C O 14 12 2	0	0
9	B	1	Total C O 14 12 2	0	0
9	B	1	Total C O 15 13 2	0	0
9	B	1	Total C O 13 11 2	0	0
9	B	1	Total C O 16 14 2	0	0
9	C	1	Total C O 14 12 2	0	0
9	C	1	Total C O 16 14 2	0	0
9	C	1	Total C O 11 9 2	0	0
9	C	1	Total C O 16 14 2	0	0
9	C	1	Total C O 13 11 2	0	0
9	C	1	Total C O 16 14 2	0	0
9	C	1	Total C O 13 11 2	0	0
9	C	1	Total C O 16 14 2	0	0
9	D	1	Total C O 14 12 2	0	0
9	D	1	Total C O 11 9 2	0	0
9	D	1	Total C O 13 11 2	0	0
9	D	1	Total C O 11 9 2	0	0
9	D	1	Total C O 16 14 2	0	0
9	D	1	Total C O 13 11 2	0	0

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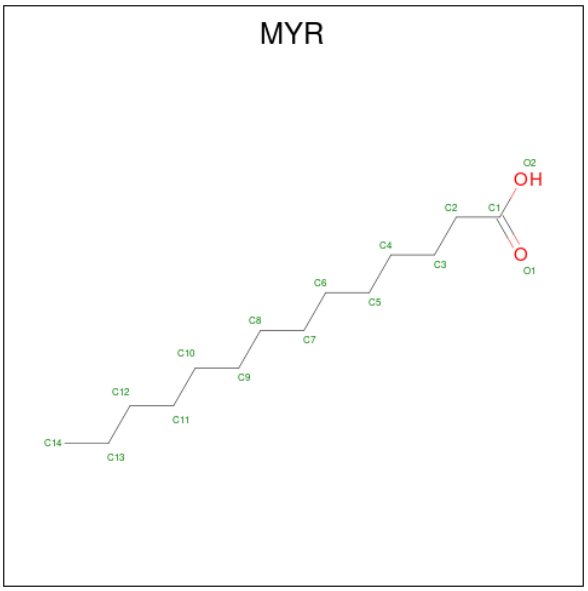
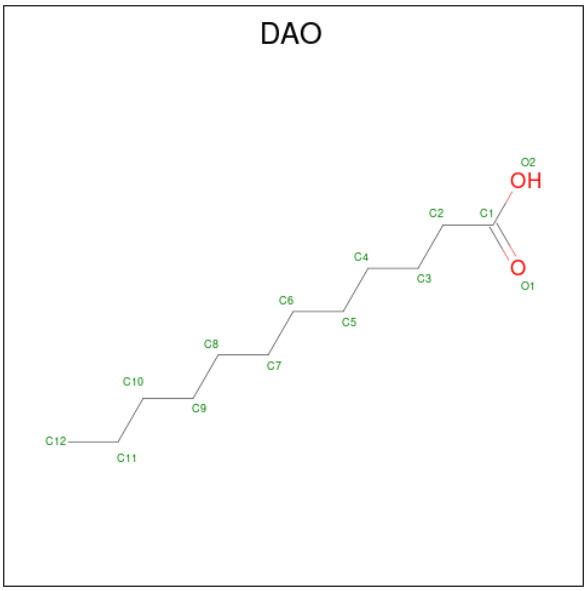
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 16 14 2	0	0
9	D	1	Total C O 14 12 2	0	0
9	E	1	Total C O 14 12 2	0	0
9	E	1	Total C O 14 12 2	0	0
9	E	1	Total C O 12 10 2	0	0
9	E	1	Total C O 15 13 2	0	0
9	F	1	Total C O 14 12 2	0	0
9	F	1	Total C O 12 10 2	0	0
9	F	1	Total C O 13 11 2	0	0
9	F	1	Total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

- Molecule 10 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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: $C_{12}H_{24}O_2$).



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

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

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

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

- Molecule 13 is water.

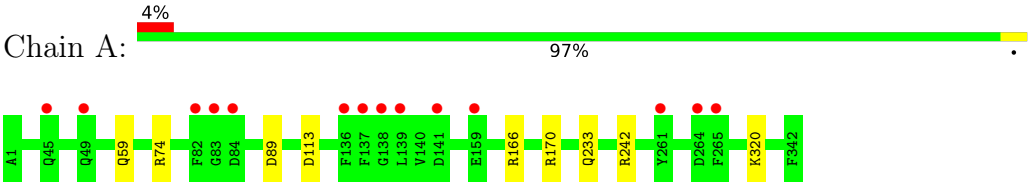
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	321	Total O 321 321	0	0
13	B	316	Total O 316 316	0	0
13	C	324	Total O 324 324	0	0
13	D	296	Total O 296 296	0	0
13	E	303	Total O 303 303	0	0
13	F	350	Total O 350 350	0	0

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.

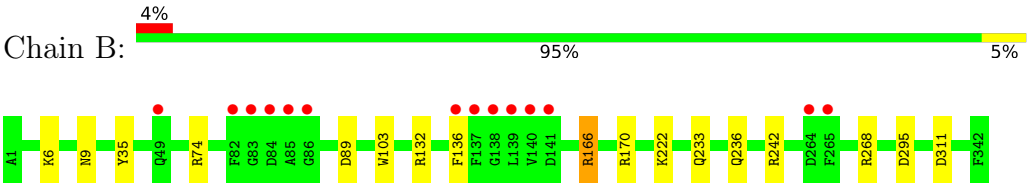
• Molecule 1: OMPC PORIN

Chain A:



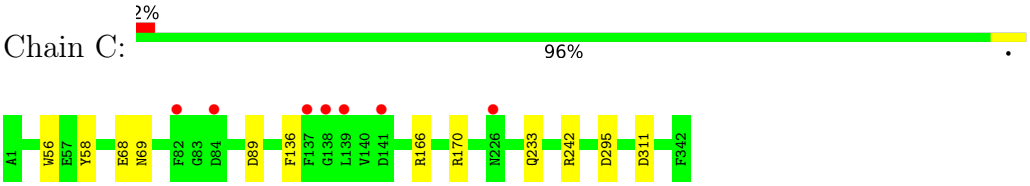
• Molecule 1: OMPC PORIN

Chain B:



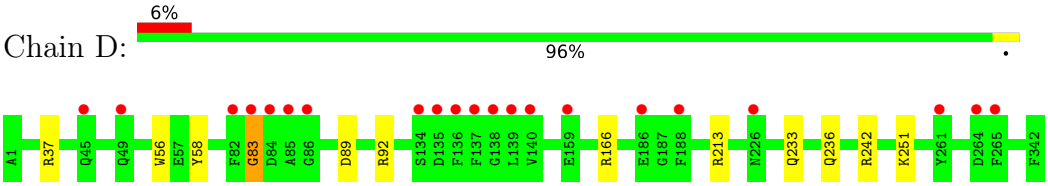
• Molecule 1: OMPC PORIN

Chain C:



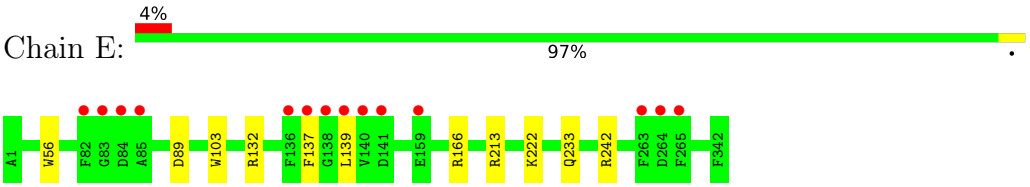
• Molecule 1: OMPC PORIN

Chain D:



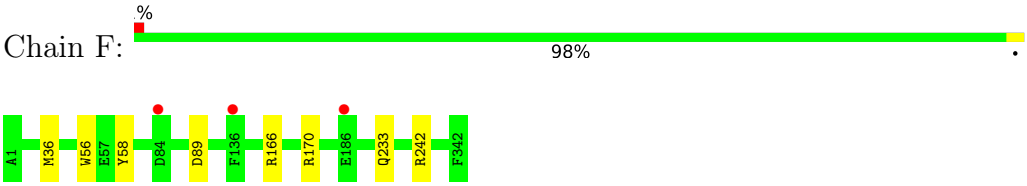
• Molecule 1: OMPC PORIN

Chain E:



• Molecule 1: OMPC PORIN

Chain F:

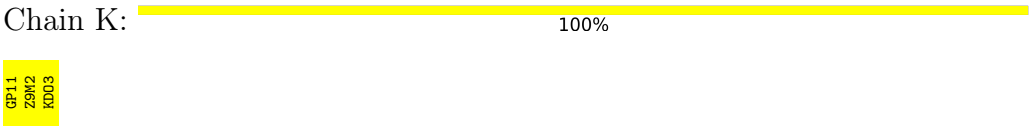


• Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain G:

• 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:

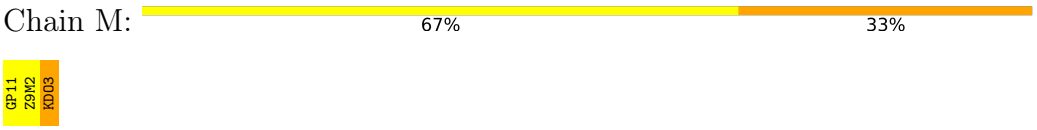


• Molecule 2: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain L:

• 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:



• 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

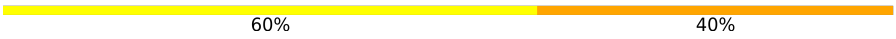
Chain H:

• 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:

• 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:



• 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:

• 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:

4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [1]	1.73 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.155 , 0.183 0.167 , 0.192	Depositor DCC
R_{free} test set	13912 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)	0.38 , 60.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, DAO, GP1, GMH, C8E, Z9M, KDO, SO4, FTT, MYR, PO4

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.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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	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

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

The worst 5 of 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

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%)	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/275 (103%)	279 (99%)	4 (1%)	67	37
1	B	279/275 (102%)	276 (99%)	3 (1%)	73	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	166	ARG
1	F	166	ARG
1	F	233	GLN
1	F	89	ASP
1	C	166	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	2,9	15,16,16	1.51	1 (6%)	23,24,24	1.03	1 (4%)
2	Z9M	G	2	2,9	15,15,16	1.34	1 (6%)	18,22,24	1.09	0
2	KDO	G	3	2	15,15,16	0.82	0	19,21,24	1.37	3 (15%)
3	GP1	H	1	3,9	15,16,16	1.52	1 (6%)	23,24,24	1.50	3 (13%)
3	Z9M	H	2	3,9	15,15,16	1.14	1 (6%)	18,22,24	0.91	0
3	KDO	H	3	3	15,15,16	1.19	1 (6%)	19,21,24	1.30	3 (15%)
3	KDO	H	4	3	15,15,16	0.76	0	19,21,24	1.52	3 (15%)
3	GMH	H	5	3	13,13,14	0.63	0	17,18,20	1.23	2 (11%)
3	GP1	I	1	3,9	15,16,16	1.66	1 (6%)	23,24,24	1.07	2 (8%)
3	Z9M	I	2	3,9	15,15,16	1.53	1 (6%)	18,22,24	1.15	1 (5%)
3	KDO	I	3	3	15,15,16	1.23	1 (6%)	19,21,24	1.56	4 (21%)
3	KDO	I	4	3,12	15,15,16	0.68	0	19,21,24	1.52	2 (10%)
3	GMH	I	5	3	13,13,14	0.99	1 (7%)	17,18,20	1.52	4 (23%)
4	GP1	J	1	4,9	15,16,16	1.40	1 (6%)	23,24,24	1.30	3 (13%)
4	Z9M	J	2	4,9	15,15,16	1.24	1 (6%)	18,22,24	0.70	0
4	KDO	J	3	4	15,15,16	1.13	1 (6%)	19,21,24	1.34	2 (10%)
4	KDO	J	4	4	15,15,16	0.81	0	19,21,24	1.64	5 (26%)
2	GP1	K	1	2,9	15,16,16	1.47	1 (6%)	23,24,24	1.67	5 (21%)
2	Z9M	K	2	2,9	15,15,16	1.36	1 (6%)	18,22,24	1.00	1 (5%)
2	KDO	K	3	2	14,14,16	0.76	0	16,19,24	2.19	2 (12%)
2	GP1	L	1	2,9	15,16,16	1.41	1 (6%)	23,24,24	0.94	1 (4%)
2	Z9M	L	2	2,9	15,15,16	1.29	1 (6%)	18,22,24	0.90	0
2	KDO	L	3	2	15,15,16	0.76	0	19,21,24	1.53	6 (31%)
2	GP1	M	1	2,9	15,16,16	1.53	1 (6%)	23,24,24	0.94	1 (4%)
2	Z9M	M	2	2,9	15,15,16	1.46	1 (6%)	18,22,24	0.81	0
2	KDO	M	3	2	15,15,16	0.74	0	19,21,24	1.39	3 (15%)
3	GP1	N	1	3,9	15,16,16	1.78	1 (6%)	23,24,24	0.93	1 (4%)
3	Z9M	N	2	3,9	15,15,16	1.52	1 (6%)	18,22,24	1.05	1 (5%)
3	KDO	N	3	3	15,15,16	1.18	1 (6%)	19,21,24	1.59	5 (26%)
3	KDO	N	4	3,12	15,15,16	0.63	0	19,21,24	1.54	3 (15%)
3	GMH	N	5	3	13,13,14	0.73	0	17,18,20	1.64	3 (17%)
4	GP1	O	1	4,9	15,16,16	1.45	1 (6%)	23,24,24	1.39	2 (8%)
4	Z9M	O	2	4,9	15,15,16	1.31	1 (6%)	18,22,24	0.68	0
4	KDO	O	3	4	15,15,16	1.05	2 (13%)	19,21,24	1.44	4 (21%)
4	KDO	O	4	4	15,15,16	0.74	0	19,21,24	1.53	3 (15%)

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	2,9	-	2/6/27/27	0/1/1/1
2	Z9M	G	2	2,9	-	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	3,9	-	1/6/27/27	0/1/1/1
3	Z9M	H	2	3,9	-	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	3,9	-	0/6/27/27	0/1/1/1
3	Z9M	I	2	3,9	-	2/7/24/27	0/1/1/1
3	KDO	I	3	3	-	1/10/26/30	0/1/1/1
3	KDO	I	4	3,12	-	1/10/26/30	0/1/1/1
3	GMH	I	5	3	-	4/6/23/26	0/1/1/1
4	GP1	J	1	4,9	-	1/6/27/27	0/1/1/1
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	2,9	-	0/6/27/27	0/1/1/1
2	Z9M	K	2	2,9	-	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	2,9	-	1/6/27/27	0/1/1/1
2	Z9M	L	2	2,9	-	0/7/24/27	0/1/1/1
2	KDO	L	3	2	-	1/10/26/30	0/1/1/1
2	GP1	M	1	2,9	-	1/6/27/27	0/1/1/1
2	Z9M	M	2	2,9	-	0/7/24/27	0/1/1/1
2	KDO	M	3	2	-	2/10/26/30	0/1/1/1
3	GP1	N	1	3,9	-	0/6/27/27	0/1/1/1
3	Z9M	N	2	3,9	-	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	3,12	-	4/10/26/30	0/1/1/1
3	GMH	N	5	3	-	3/6/23/26	0/1/1/1
4	GP1	O	1	4,9	-	1/6/27/27	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	-	2/10/26/30	0/1/1/1

The worst 5 of 25 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

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 30 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

There are no ring outliers.

14 monomers are involved in 17 short contacts:

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

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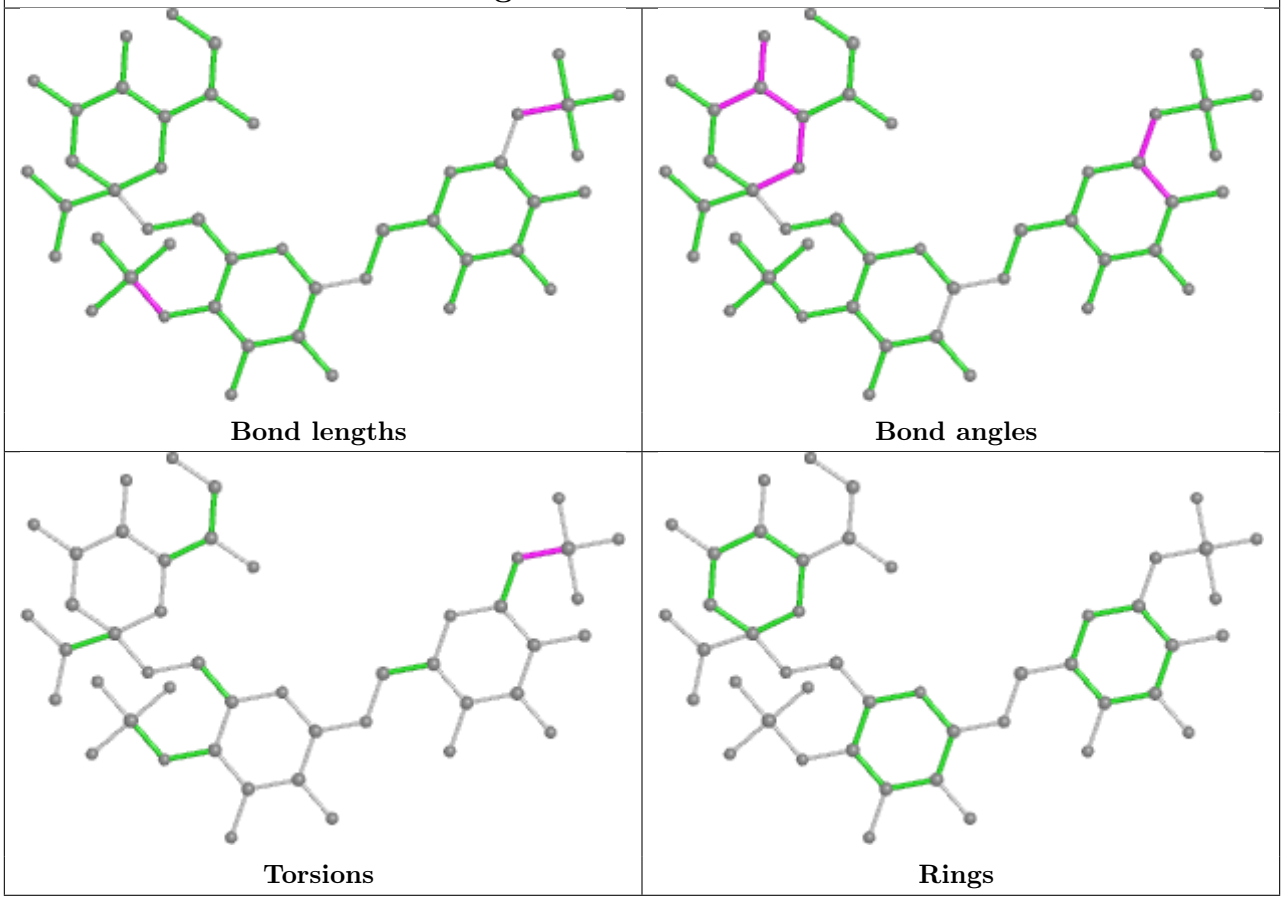
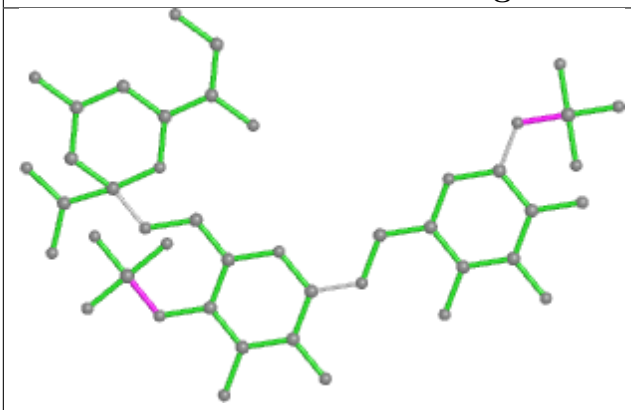
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	3	KDO	1	0

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

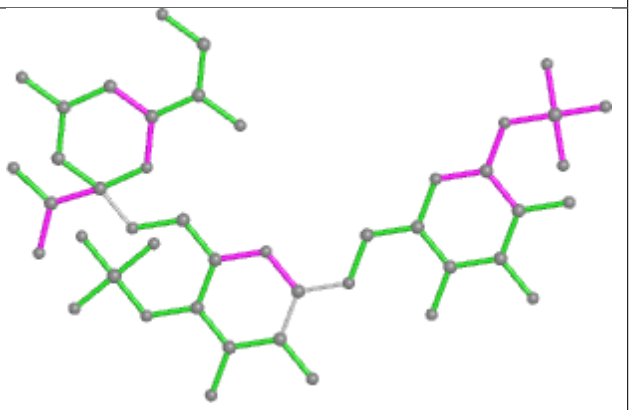
Oligosaccharide Chain G



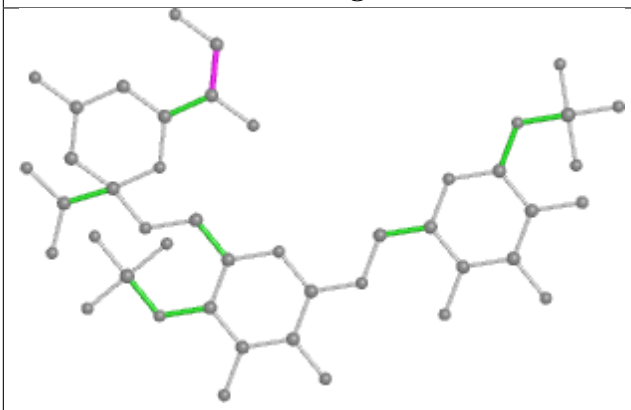
Oligosaccharide Chain K



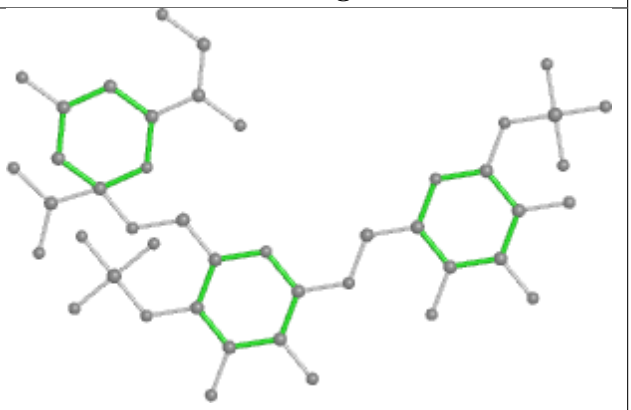
Bond lengths



Bond angles

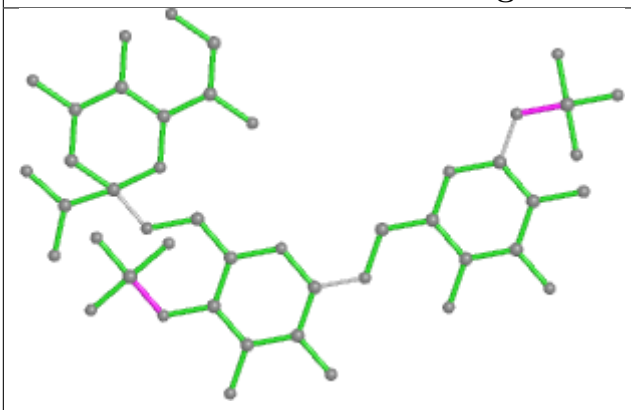


Torsions

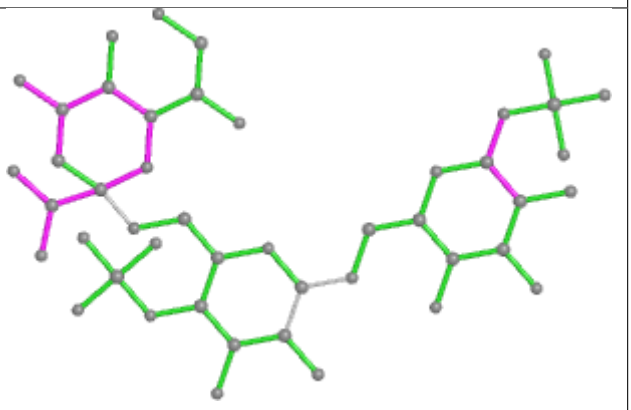


Rings

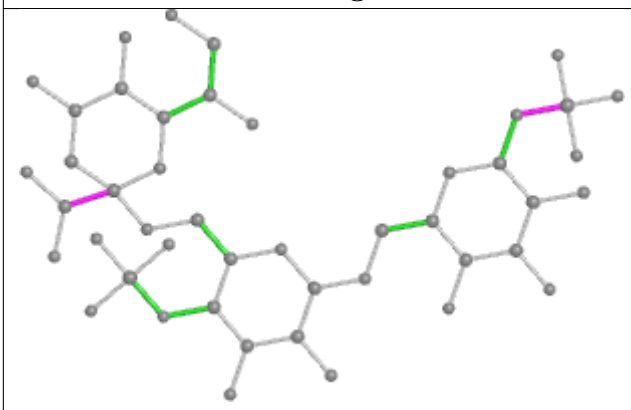
Oligosaccharide Chain L



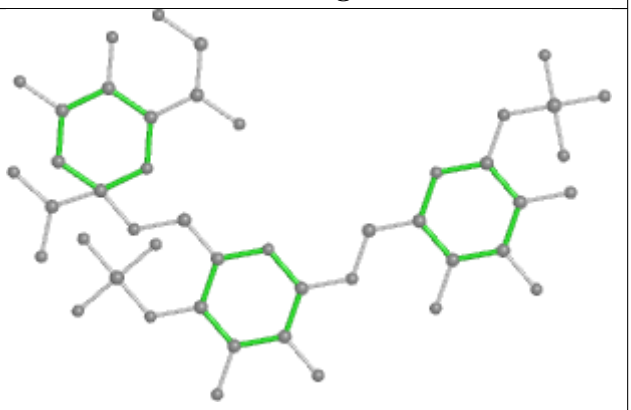
Bond lengths



Bond angles

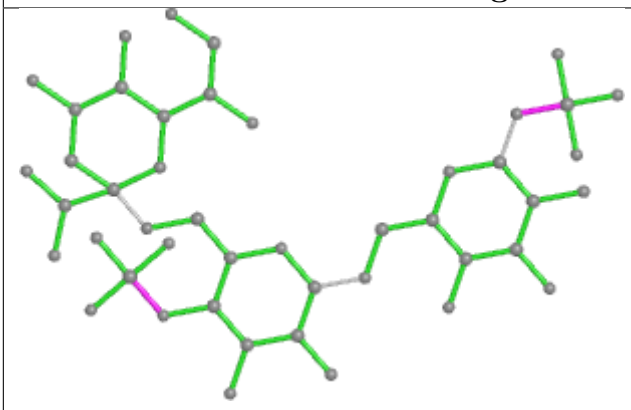


Torsions

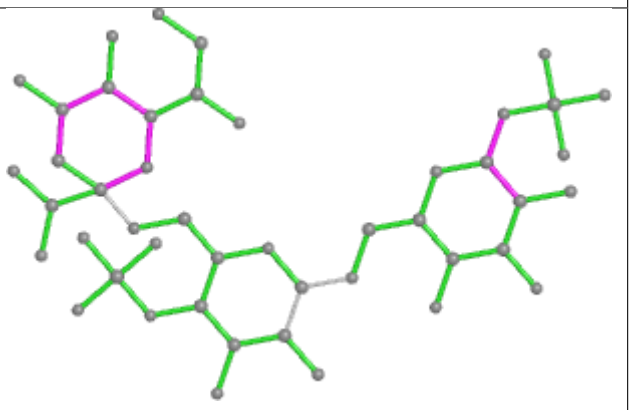


Rings

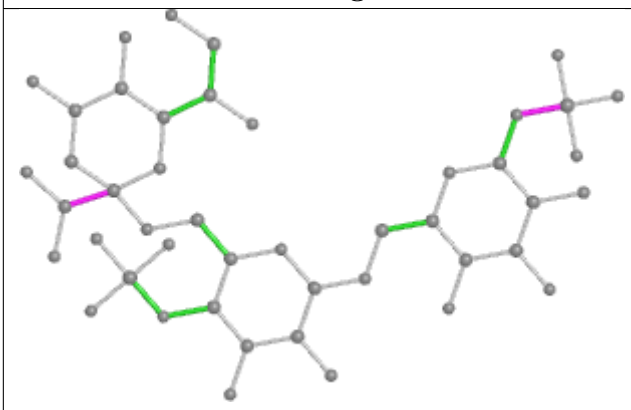
Oligosaccharide Chain M



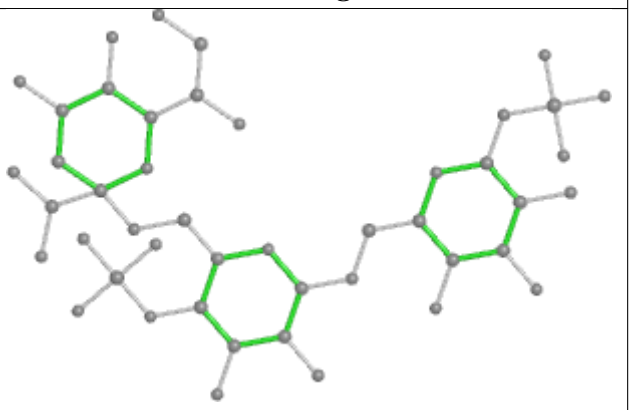
Bond lengths



Bond angles

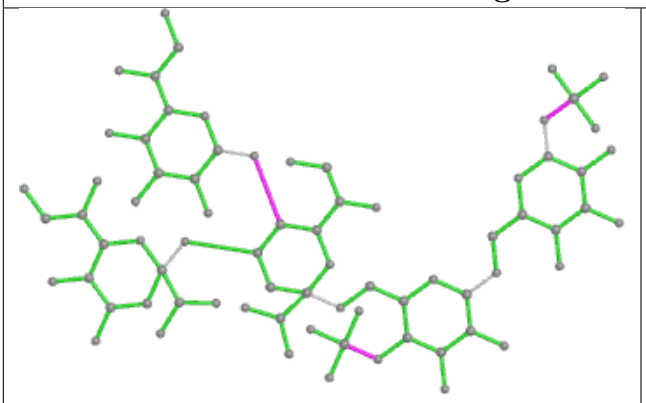


Torsions

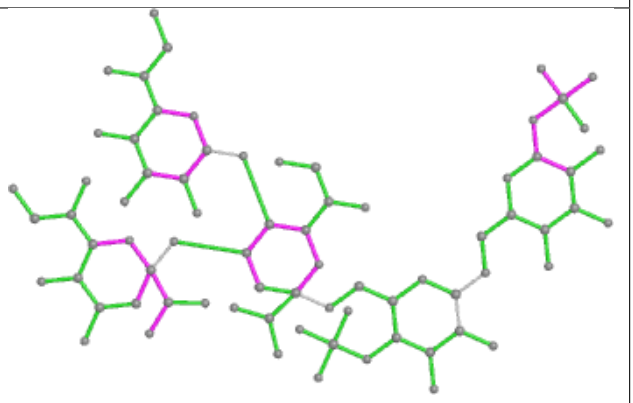


Rings

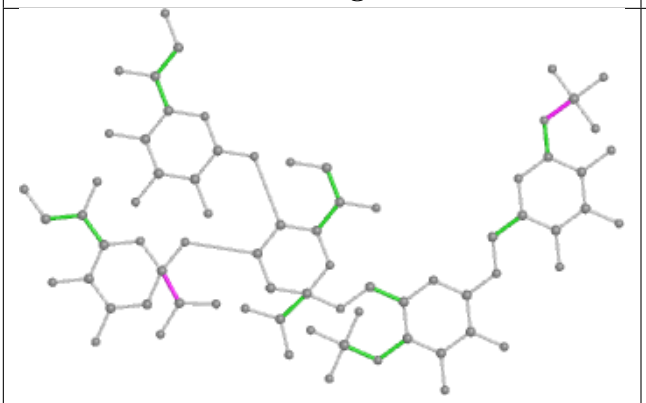
Oligosaccharide Chain H



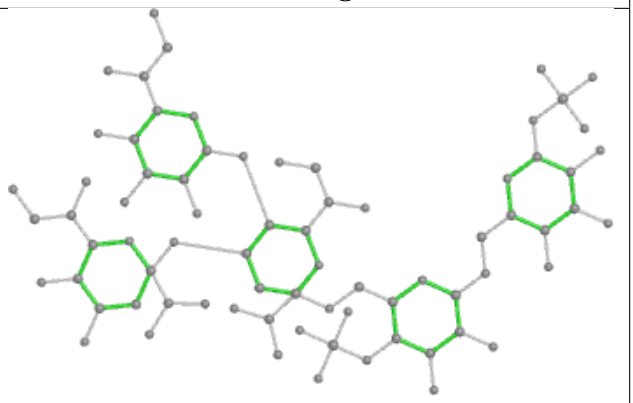
Bond lengths



Bond angles

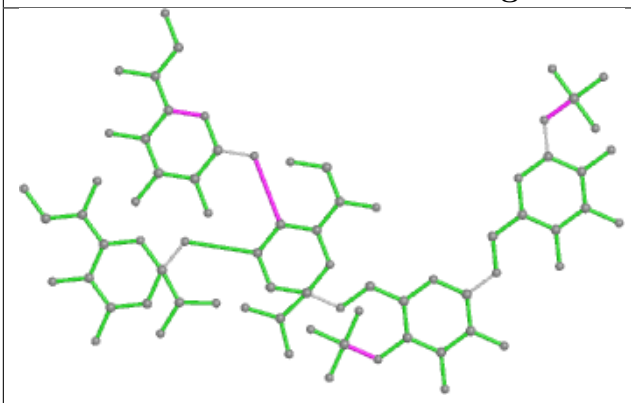


Torsions

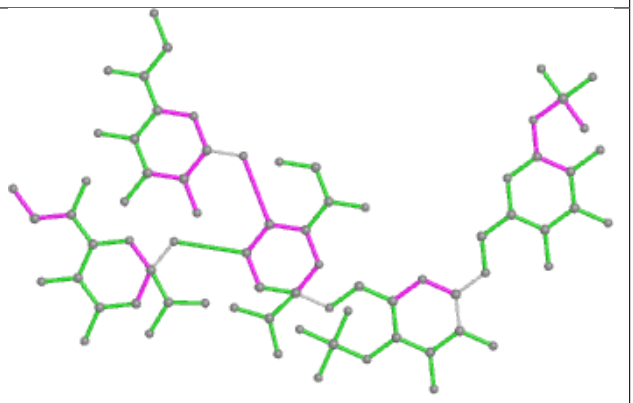


Rings

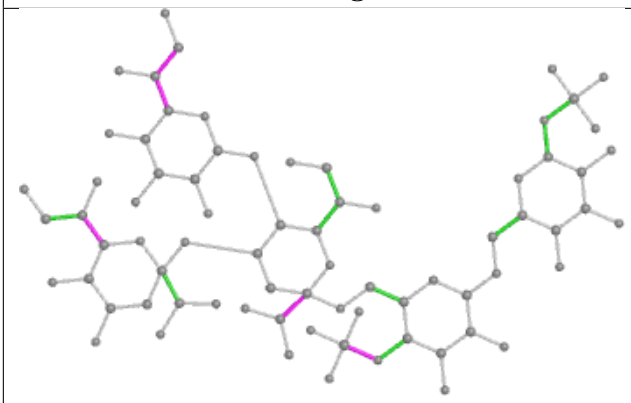
Oligosaccharide Chain I



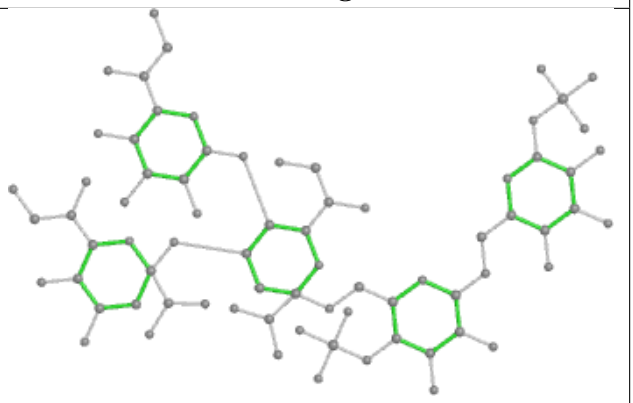
Bond lengths



Bond angles

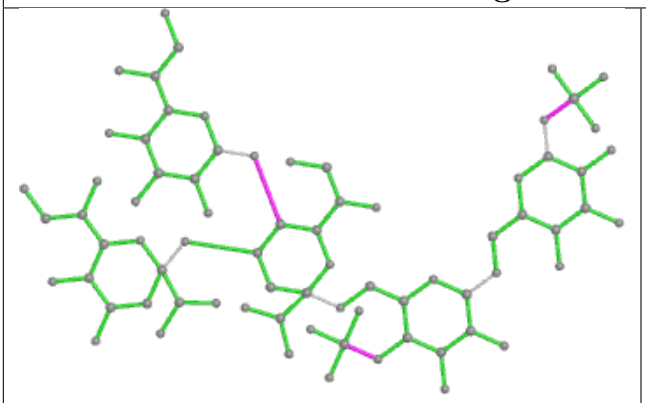


Torsions

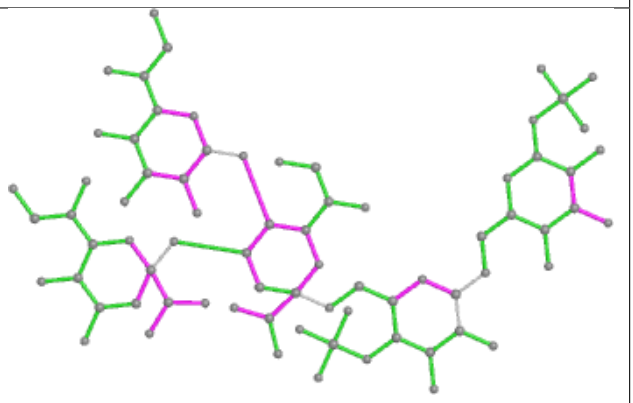


Rings

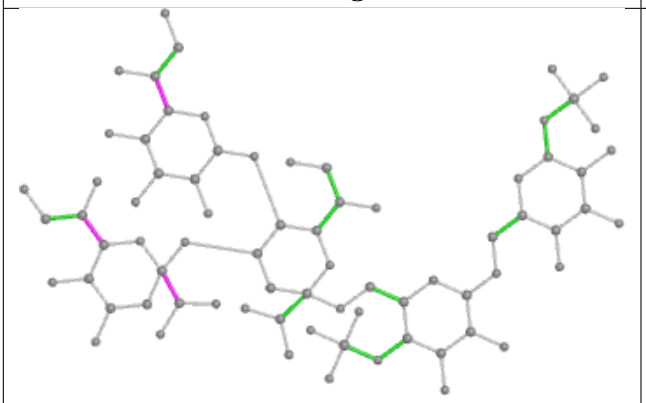
Oligosaccharide Chain N



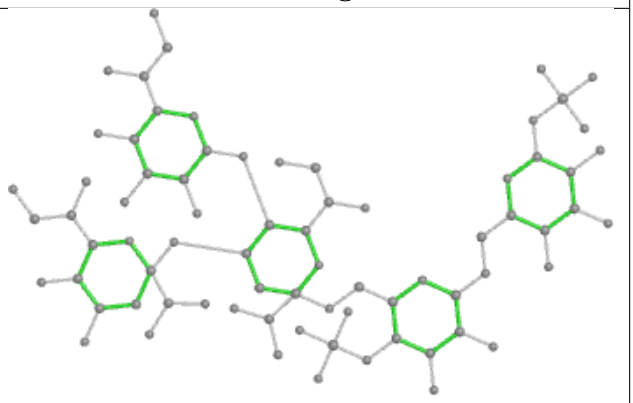
Bond lengths



Bond angles

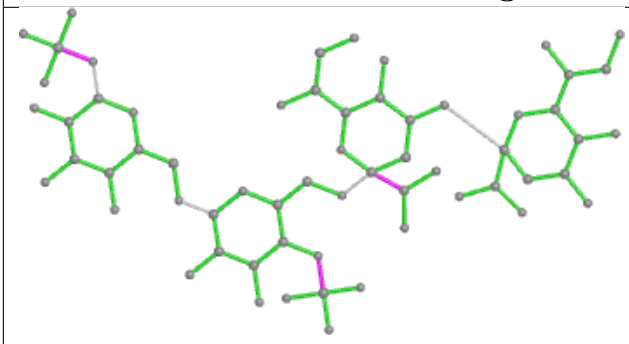


Torsions

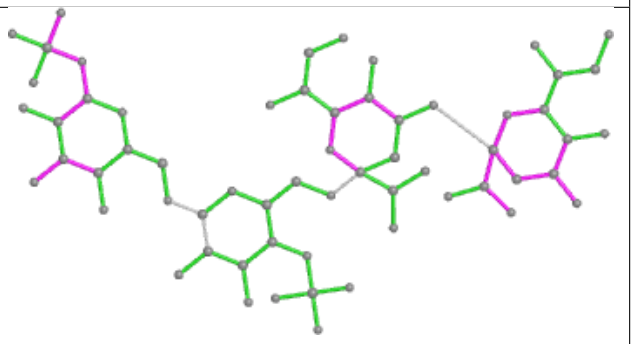


Rings

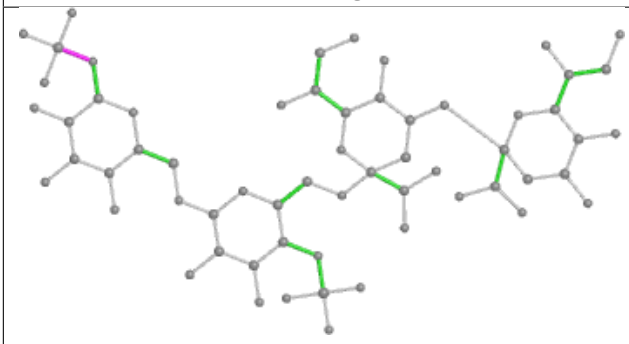
Oligosaccharide Chain J



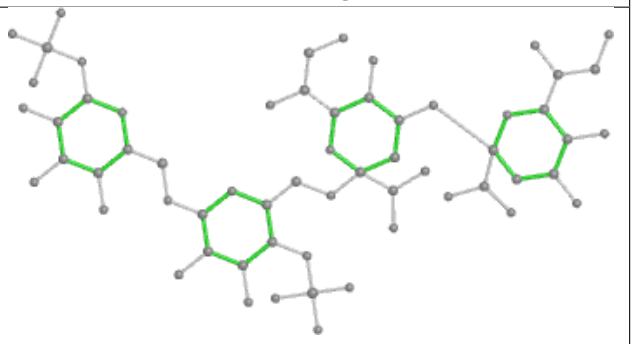
Bond lengths



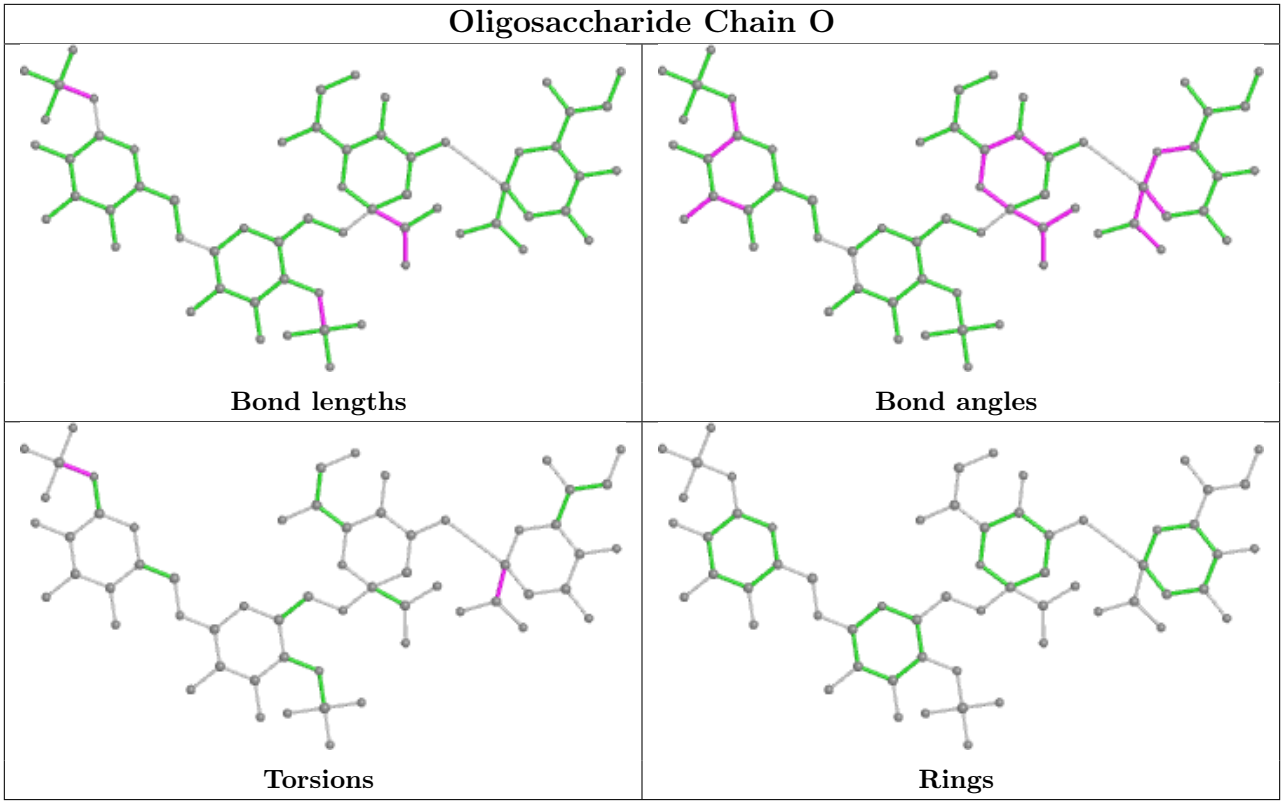
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
11	DAO	D	418	9	1,2,13	1.37	0	1,1,13	0.76	0
5	SO4	D	401	-	4,4,4	0.21	0	6,6,6	0.46	0
9	FTT	A	418	4,11	13,13,16	0.55	0	13,13,17	1.47	1 (7%)
9	FTT	D	425	4	13,13,16	0.54	0	13,13,17	1.55	2 (15%)
6	C8E	D	409	-	3,3,20	0.55	0	2,2,19	0.34	0
9	FTT	B	407	2	13,13,16	0.51	0	13,13,17	1.08	1 (7%)
9	FTT	D	414	2	13,13,16	0.57	0	13,13,17	0.69	1 (7%)
9	FTT	B	409	11,3	12,12,16	0.59	0	12,12,17	1.11	2 (16%)
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	$\#\|Z\|>2$
8	KDO	E	403	-	15,15,16	0.68	0	19,21,24	1.70	3 (15%)
10	MYR	C	419	9	7,7,15	0.60	0	6,6,15	0.56	0
9	FTT	A	415	2,10	15,15,16	0.43	0	15,15,17	0.92	1 (6%)
10	MYR	F	411	9	10,10,15	0.43	0	9,9,15	0.63	0
6	C8E	B	401	-	8,8,20	0.38	0	7,7,19	0.58	0
6	C8E	A	404	-	5,5,20	0.30	0	4,4,19	0.26	0
6	C8E	D	406	-	7,7,20	0.33	0	6,6,19	0.46	0
7	PO4	E	402	-	4,4,4	0.63	0	6,6,6	0.81	0
6	C8E	C	403	-	2,2,20	0.25	0	0,1,19	-	-
6	C8E	A	408	-	7,7,20	0.48	0	6,6,19	0.44	0
9	FTT	C	422	4	15,15,16	0.28	0	15,15,17	1.40	3 (20%)
9	FTT	B	410	10,3	15,15,16	0.44	0	15,15,17	0.85	0
6	C8E	C	409	-	9,9,20	0.35	0	8,8,19	0.43	0
11	DAO	F	413	9	4,4,13	0.65	0	3,3,13	0.54	0
6	C8E	C	402	-	6,6,20	0.53	0	5,5,19	0.82	0
9	FTT	F	416	4,10	15,15,16	0.29	0	15,15,17	0.81	0
7	PO4	F	404	-	4,4,4	0.54	0	6,6,6	0.80	0
8	KDO	A	412	-	15,15,16	0.87	1 (6%)	19,21,24	1.44	3 (15%)
6	C8E	A	407	-	4,4,20	0.50	0	3,3,19	0.25	0
9	FTT	C	416	10,3	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
9	FTT	A	413	2	14,14,16	0.38	0	14,14,17	0.76	0
9	FTT	B	408	3	14,14,16	0.40	0	14,14,17	0.72	0
11	DAO	C	420	9	12,12,13	0.44	0	11,11,13	0.58	0
6	C8E	A	405	-	3,3,20	0.38	0	2,2,19	0.64	0
9	FTT	C	423	4,11	12,12,16	0.63	0	12,12,17	1.19	1 (8%)
6	C8E	A	402	-	2,2,20	0.45	0	1,1,19	0.11	0
6	C8E	C	408	-	10,10,20	0.35	0	9,9,19	0.39	0
9	FTT	E	406	2	13,13,16	0.35	0	13,13,17	0.89	0
10	MYR	A	416	9	5,5,15	0.64	0	4,4,15	0.72	0
6	C8E	D	403	-	5,5,20	0.32	0	4,4,19	0.32	0
9	FTT	F	410	3	15,15,16	0.38	0	15,15,17	1.29	3 (20%)
9	FTT	D	422	2,10	15,15,16	0.37	0	15,15,17	0.80	0
9	FTT	E	404	11,2	13,13,16	0.61	0	13,13,17	1.31	1 (7%)
6	C8E	D	402	-	3,3,20	0.35	0	2,2,19	0.67	0
6	C8E	B	404	-	7,7,20	0.29	0	6,6,19	0.34	0
11	DAO	F	418	9	7,7,13	0.57	0	6,6,13	0.58	0
10	MYR	B	411	9	5,5,15	0.61	0	4,4,15	0.78	0
5	SO4	A	401	-	4,4,4	0.19	0	6,6,6	0.57	0
9	FTT	D	421	11,2	12,12,16	0.57	0	12,12,17	1.11	1 (8%)
11	DAO	F	412	9	4,4,13	0.63	0	3,3,13	0.64	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%)
6	C8E	B	402	-	2,2,20	0.45	0	0,1,19	-	-
6	C8E	C	405	-	2,2,20	0.18	0	0,1,19	-	-
11	DAO	C	414	9	4,4,13	0.63	0	3,3,13	0.58	0
6	C8E	C	410	-	6,6,20	0.32	0	5,5,19	0.47	0
8	KDO	D	413	-	15,15,16	0.90	1 (6%)	19,21,24	1.68	3 (15%)
11	DAO	A	417	9	4,4,13	0.64	0	3,3,13	1.00	0
6	C8E	E	401	-	5,5,20	0.29	0	4,4,19	0.35	0
10	MYR	E	409	9	5,5,15	0.62	0	4,4,15	0.65	0
11	DAO	E	405	9	4,4,13	0.67	0	3,3,13	1.03	0
9	FTT	D	417	2	10,10,16	0.62	0	10,10,17	1.12	1 (10%)
9	FTT	C	424	4,10	15,15,16	0.32	0	15,15,17	0.87	0
9	FTT	F	408	11,3	12,12,16	0.70	0	12,12,17	1.00	1 (8%)
11	DAO	C	421	9	9,9,13	0.58	0	8,8,13	0.44	0
6	C8E	F	403	-	7,7,20	0.35	0	6,6,19	0.47	0
9	FTT	D	415	11,2	10,10,16	0.56	0	10,10,17	1.47	1 (10%)
9	FTT	F	407	11,3	11,11,16	0.74	0	11,11,17	1.24	1 (9%)
9	FTT	F	409	10,3	11,11,16	0.64	0	11,11,17	0.97	1 (9%)
9	FTT	C	413	11,3	13,13,16	0.72	0	13,13,17	1.36	1 (7%)
7	PO4	C	411	-	4,4,4	0.84	0	6,6,6	0.97	0
9	FTT	C	417	11,3	15,15,16	0.44	0	15,15,17	0.81	0
11	DAO	D	424	9	4,4,13	0.63	0	3,3,13	0.67	0
6	C8E	C	406	-	7,7,20	0.30	0	6,6,19	0.41	0
6	C8E	F	401	-	2,2,20	0.24	0	0,1,19	-	-
6	C8E	D	410	-	5,5,20	0.26	0	4,4,19	0.35	0
6	C8E	A	406	-	4,4,20	0.34	0	3,3,19	0.32	0
6	C8E	B	403	-	4,4,20	0.29	0	3,3,19	0.31	0
11	DAO	A	419	9	7,7,13	0.50	0	6,6,13	0.83	0
9	FTT	F	415	4,11	10,10,16	0.57	0	10,10,17	1.46	1 (10%)
6	C8E	C	407	-	10,10,20	0.34	0	9,9,19	0.44	0
6	C8E	A	409	-	7,7,20	0.28	0	6,6,19	0.50	0
9	FTT	A	414	11,2	12,12,16	0.53	0	12,12,17	1.45	2 (16%)
9	FTT	D	420	2	15,15,16	0.34	0	15,15,17	0.83	0
11	DAO	C	426	9	7,7,13	0.55	0	6,6,13	0.69	0
6	C8E	D	408	-	10,10,20	0.39	0	9,9,19	0.26	0
10	MYR	D	419	9	4,4,15	0.69	0	3,3,15	0.90	0
9	FTT	F	414	4	13,13,16	0.41	0	13,13,17	0.60	0
11	DAO	E	410	9	4,4,13	0.63	0	3,3,13	0.78	0
9	FTT	E	407	11,2	11,11,16	0.53	0	11,11,17	1.33	2 (18%)
7	PO4	B	406	-	4,4,4	1.10	0	6,6,6	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	C8E	D	407	-	7,7,20	0.30	0	6,6,19	0.29	0
11	DAO	D	412	-	5,5,13	0.54	0	4,4,13	0.84	0
9	FTT	E	408	2,10	14,14,16	0.55	0	14,14,17	0.97	1 (7%)
7	PO4	D	411	-	4,4,4	0.60	0	6,6,6	1.15	0
6	C8E	B	405	-	7,7,20	0.30	0	6,6,19	0.67	0
9	FTT	C	415	3	15,15,16	0.56	0	15,15,17	1.06	1 (6%)
9	FTT	C	418	11,3	12,12,16	0.61	0	12,12,17	1.01	1 (8%)
6	C8E	C	404	-	5,5,20	0.24	0	4,4,19	0.33	0
9	FTT	D	416	2,10	12,12,16	0.57	0	12,12,17	0.86	0
6	C8E	A	410	-	6,6,20	0.25	0	5,5,19	0.48	0
10	MYR	D	423	9	5,5,15	0.60	0	4,4,15	0.74	0
6	C8E	A	403	-	3,3,20	0.40	0	2,2,19	0.62	0
10	MYR	F	417	9	11,11,15	0.44	0	10,10,15	0.63	0
6	C8E	C	401	-	2,2,20	0.28	0	0,1,19	-	-
7	PO4	A	411	-	4,4,4	0.97	0	6,6,6	0.78	0
6	C8E	D	405	-	5,5,20	0.28	0	4,4,19	0.34	0
10	MYR	C	425	9	8,8,15	0.46	0	7,7,15	0.64	0
6	C8E	D	404	-	5,5,20	0.28	0	4,4,19	0.34	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
9	FTT	A	418	4,11	-	5/12/12/15	-
9	FTT	D	425	4	-	4/12/12/15	-
6	C8E	D	409	-	-	0/0/1/18	-
9	FTT	B	407	2	-	1/12/12/15	-
9	FTT	D	414	2	-	7/12/12/15	-
9	FTT	B	409	11,3	-	3/11/11/15	-
11	DAO	B	412	9	-	1/1/2/11	-
8	KDO	E	403	-	-	1/10/26/30	0/1/1/1
10	MYR	C	419	9	-	0/4/5/13	-
9	FTT	A	415	2,10	-	7/14/14/15	-
10	MYR	F	411	9	-	0/7/8/13	-
6	C8E	B	401	-	-	3/6/6/18	-
6	C8E	A	404	-	-	1/3/3/18	-
6	C8E	D	406	-	-	4/5/5/18	-
6	C8E	A	408	-	-	3/5/5/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FTT	C	422	4	-	4/14/14/15	-
9	FTT	B	410	10,3	-	5/14/14/15	-
6	C8E	C	409	-	-	2/7/7/18	-
11	DAO	F	413	9	-	0/1/2/11	-
6	C8E	C	402	-	-	2/4/4/18	-
9	FTT	F	416	4,10	-	6/14/14/15	-
8	KDO	A	412	-	-	1/10/26/30	0/1/1/1
6	C8E	A	407	-	-	2/2/2/18	-
9	FTT	C	416	10,3	-	1/9/9/15	-
6	C8E	F	402	-	-	0/1/1/18	-
9	FTT	A	413	2	-	3/13/13/15	-
9	FTT	B	408	3	-	1/13/13/15	-
11	DAO	C	420	9	-	0/9/10/11	-
6	C8E	A	405	-	-	0/1/1/18	-
9	FTT	C	423	4,11	-	1/11/11/15	-
6	C8E	C	408	-	-	3/8/8/18	-
9	FTT	E	406	2	-	2/12/12/15	-
10	MYR	A	416	9	-	0/2/3/13	-
6	C8E	D	403	-	-	0/3/3/18	-
9	FTT	F	410	3	-	5/14/14/15	-
9	FTT	D	422	2,10	-	5/14/14/15	-
9	FTT	E	404	11,2	-	6/12/12/15	-
6	C8E	D	402	-	-	1/1/1/18	-
6	C8E	B	404	-	-	2/5/5/18	-
11	DAO	F	418	9	-	2/4/5/11	-
10	MYR	B	411	9	-	1/2/3/13	-
9	FTT	D	421	11,2	-	0/11/11/15	-
11	DAO	F	412	9	-	0/1/2/11	-
9	FTT	F	406	2	-	1/12/12/15	-
11	DAO	C	414	9	-	1/1/2/11	-
6	C8E	C	410	-	-	2/4/4/18	-
8	KDO	D	413	-	-	2/10/26/30	0/1/1/1
11	DAO	A	417	9	-	1/1/2/11	-
6	C8E	E	401	-	-	3/3/3/18	-
10	MYR	E	409	9	-	1/2/3/13	-
11	DAO	E	405	9	-	0/1/2/11	-
9	FTT	D	417	2	-	3/9/9/15	-
9	FTT	C	424	4,10	-	3/14/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FTT	F	408	11,3	-	5/11/11/15	-
11	DAO	C	421	9	-	1/6/7/11	-
6	C8E	F	403	-	-	2/5/5/18	-
9	FTT	D	415	11,2	-	1/9/9/15	-
9	FTT	F	407	11,3	-	3/10/10/15	-
9	FTT	F	409	10,3	-	2/10/10/15	-
9	FTT	C	413	11,3	-	2/12/12/15	-
9	FTT	C	417	11,3	-	2/14/14/15	-
11	DAO	D	424	9	-	1/1/2/11	-
6	C8E	C	406	-	-	0/5/5/18	-
6	C8E	D	410	-	-	0/3/3/18	-
6	C8E	A	406	-	-	0/2/2/18	-
6	C8E	B	403	-	-	1/2/2/18	-
11	DAO	A	419	9	-	0/4/5/11	-
9	FTT	F	415	4,11	-	1/9/9/15	-
6	C8E	C	407	-	-	1/8/8/18	-
6	C8E	A	409	-	-	0/5/5/18	-
9	FTT	A	414	11,2	-	0/11/11/15	-
9	FTT	D	420	2	-	3/14/14/15	-
11	DAO	C	426	9	-	3/4/5/11	-
6	C8E	D	408	-	-	1/8/8/18	-
10	MYR	D	419	9	-	1/1/2/13	-
9	FTT	F	414	4	-	2/12/12/15	-
11	DAO	E	410	9	-	1/1/2/11	-
9	FTT	E	407	11,2	-	1/10/10/15	-
6	C8E	D	407	-	-	2/5/5/18	-
11	DAO	D	412	-	-	2/2/3/11	-
9	FTT	E	408	2,10	-	7/13/13/15	-
6	C8E	B	405	-	-	1/5/5/18	-
9	FTT	C	415	3	-	2/14/14/15	-
9	FTT	C	418	11,3	-	4/11/11/15	-
6	C8E	C	404	-	-	1/3/3/18	-
9	FTT	D	416	2,10	-	6/11/11/15	-
6	C8E	A	410	-	-	0/4/4/18	-
10	MYR	D	423	9	-	1/2/3/13	-
6	C8E	A	403	-	-	0/1/1/18	-
10	MYR	F	417	9	-	3/8/9/13	-
6	C8E	D	405	-	-	0/3/3/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MYR	C	425	9	-	2/5/6/13	-
6	C8E	D	404	-	-	0/3/3/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	413	KDO	C2-C1	-2.78	1.50	1.52
8	A	412	KDO	C2-C1	-2.54	1.50	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	403	KDO	O6-C2-C3	5.14	117.53	110.46
8	D	413	KDO	O6-C2-C3	4.84	117.12	110.46
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

There are no chirality outliers.

5 of 177 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

There are no ring outliers.

12 monomers are involved in 19 short contacts:

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

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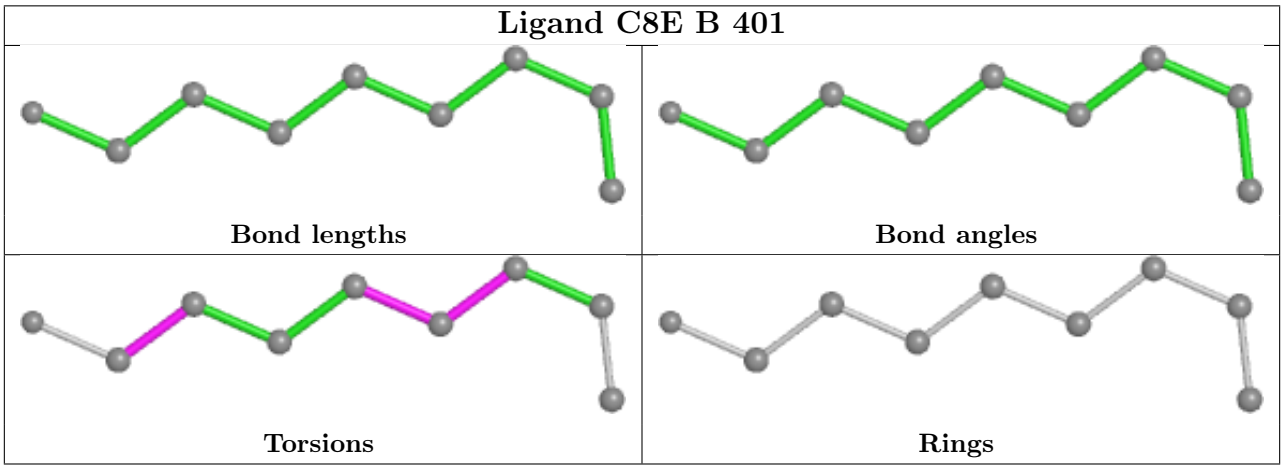
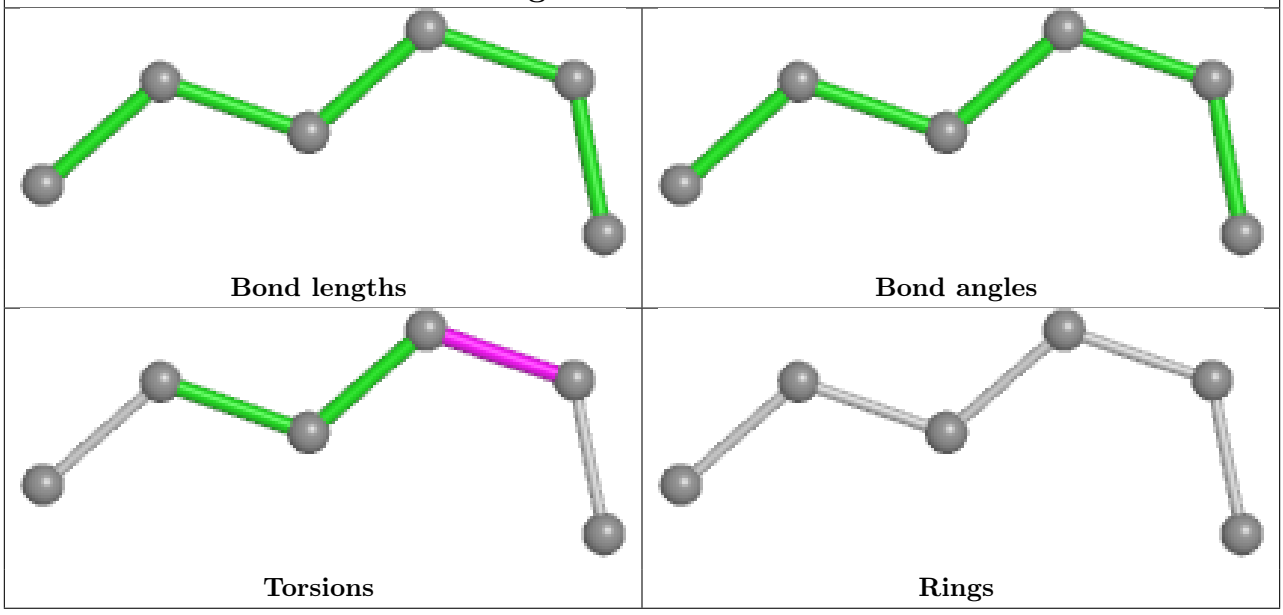
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	407	FTT	1	0
6	F	401	C8E	1	0
6	B	403	C8E	2	0

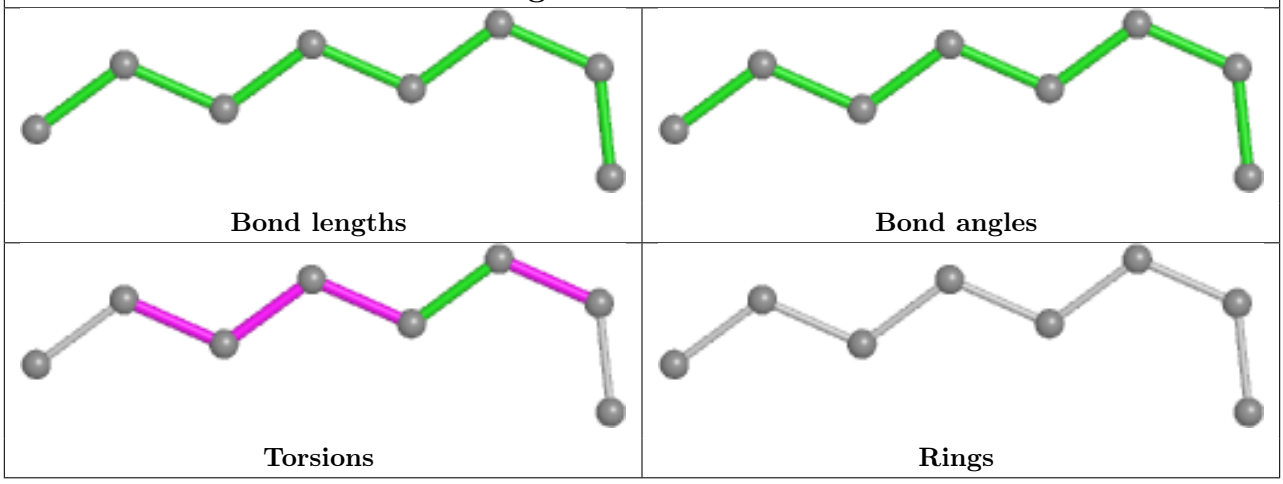
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



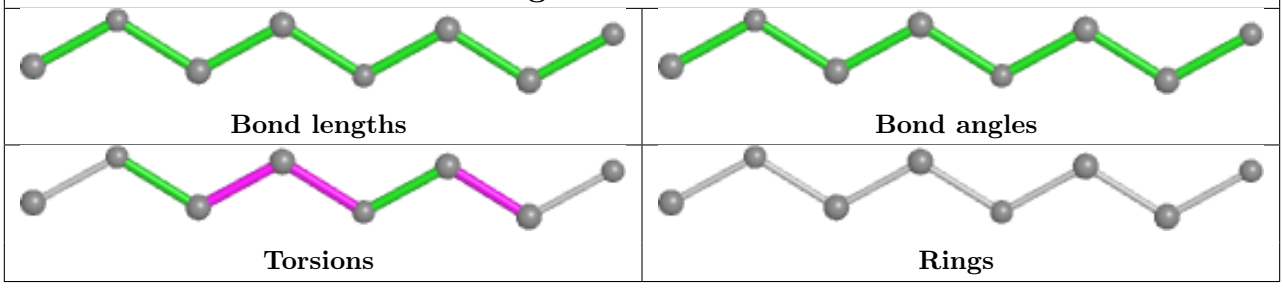
Ligand C8E A 404



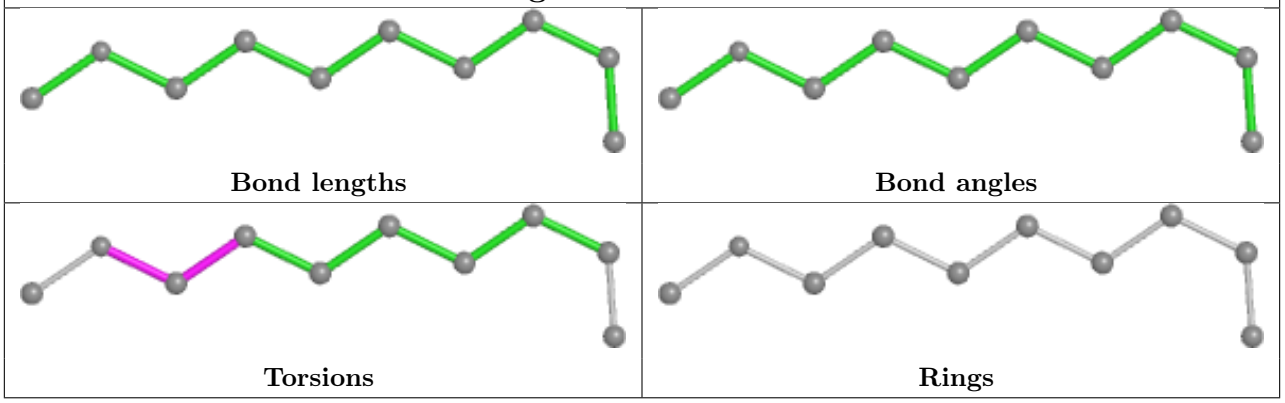
Ligand C8E D 406



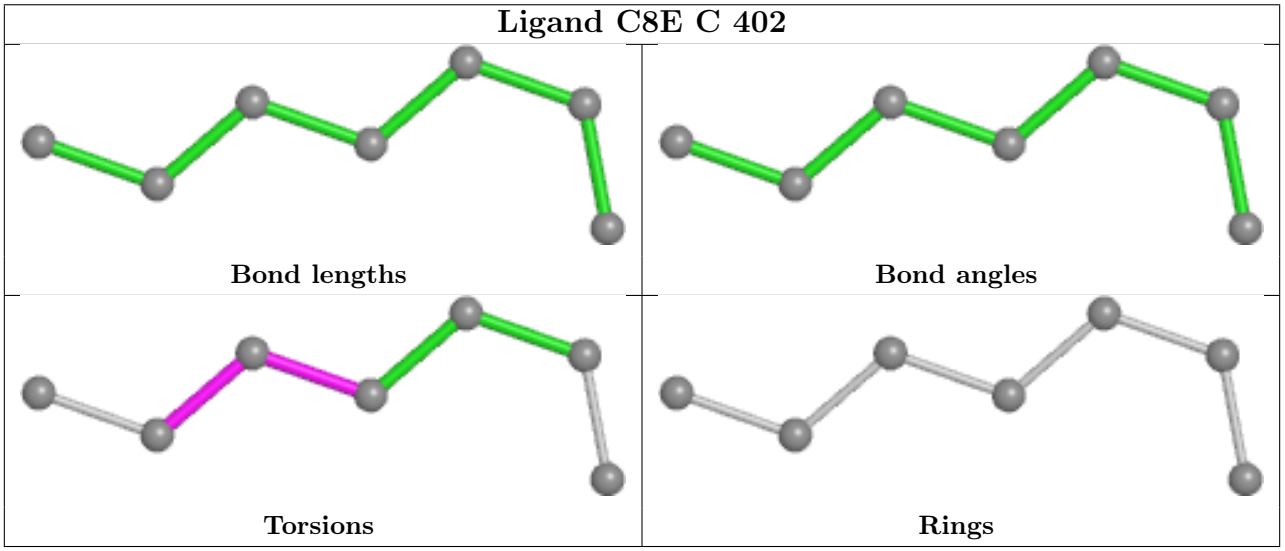
Ligand C8E A 408



Ligand C8E C 409



Ligand C8E C 402



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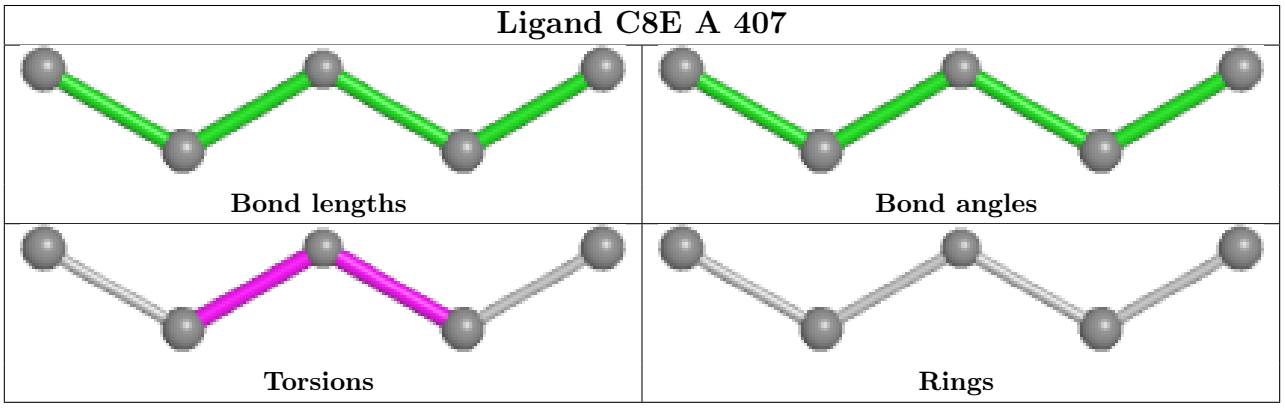
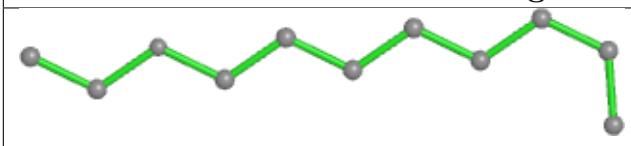
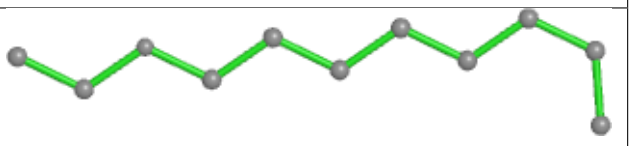


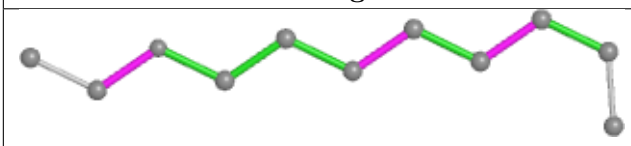
Ligand C8E C 408



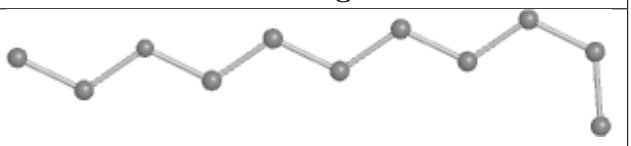
Bond lengths



Bond angles

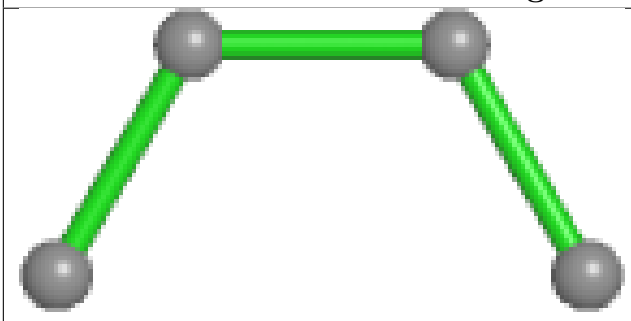


Torsions

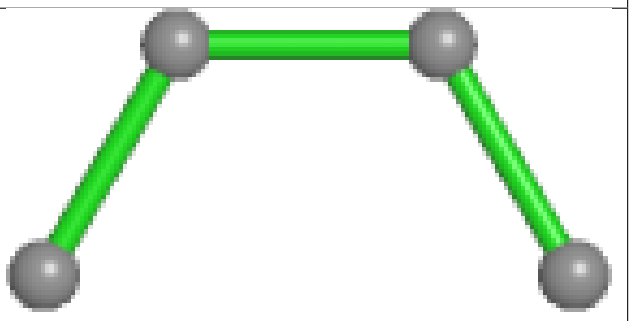


Rings

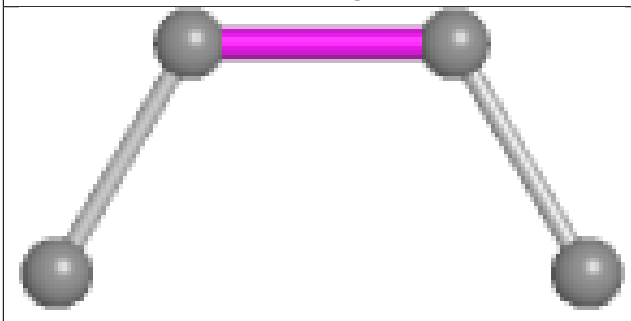
Ligand C8E D 402



Bond lengths



Bond angles



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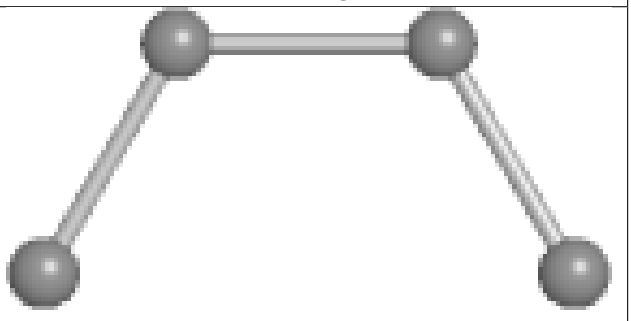
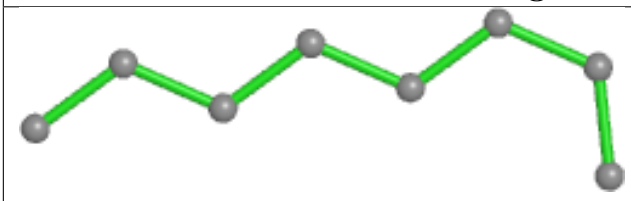
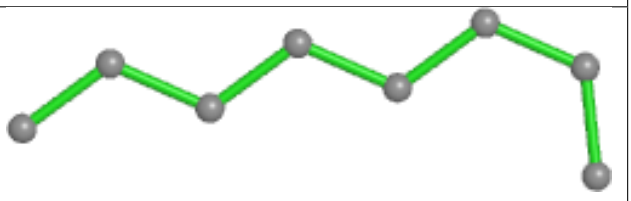


Rings

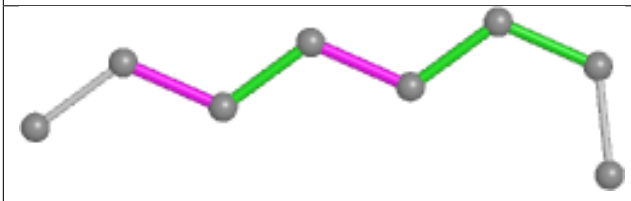
Ligand C8E B 404



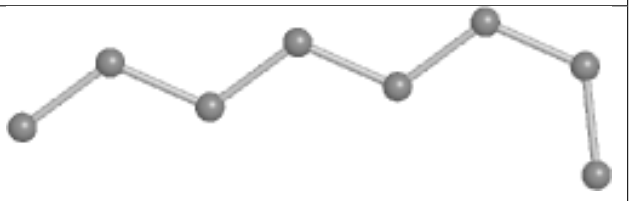
Bond lengths



Bond angles

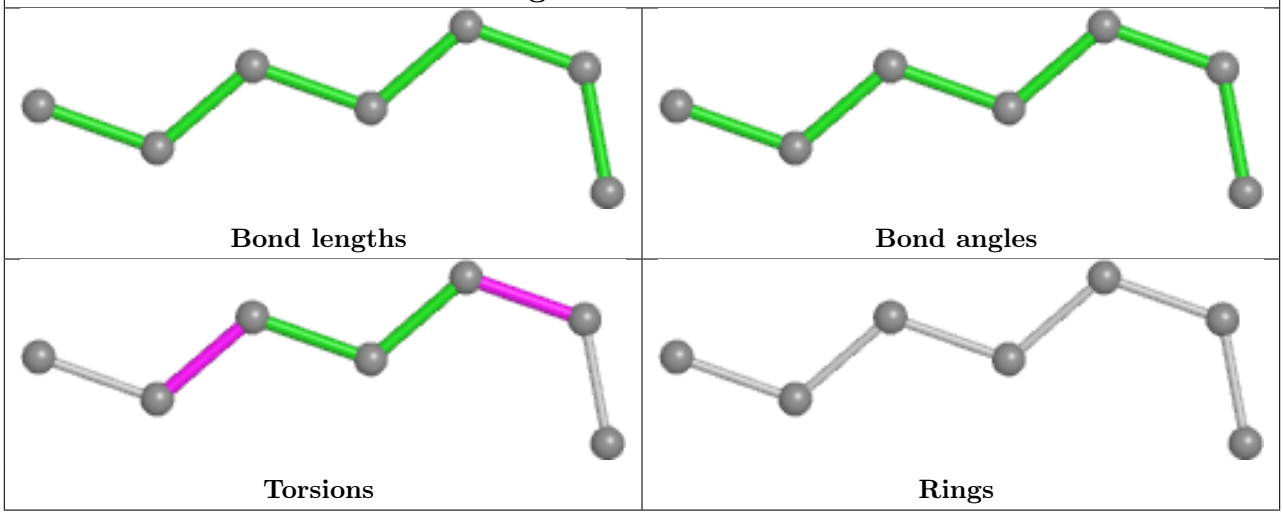


Torsions

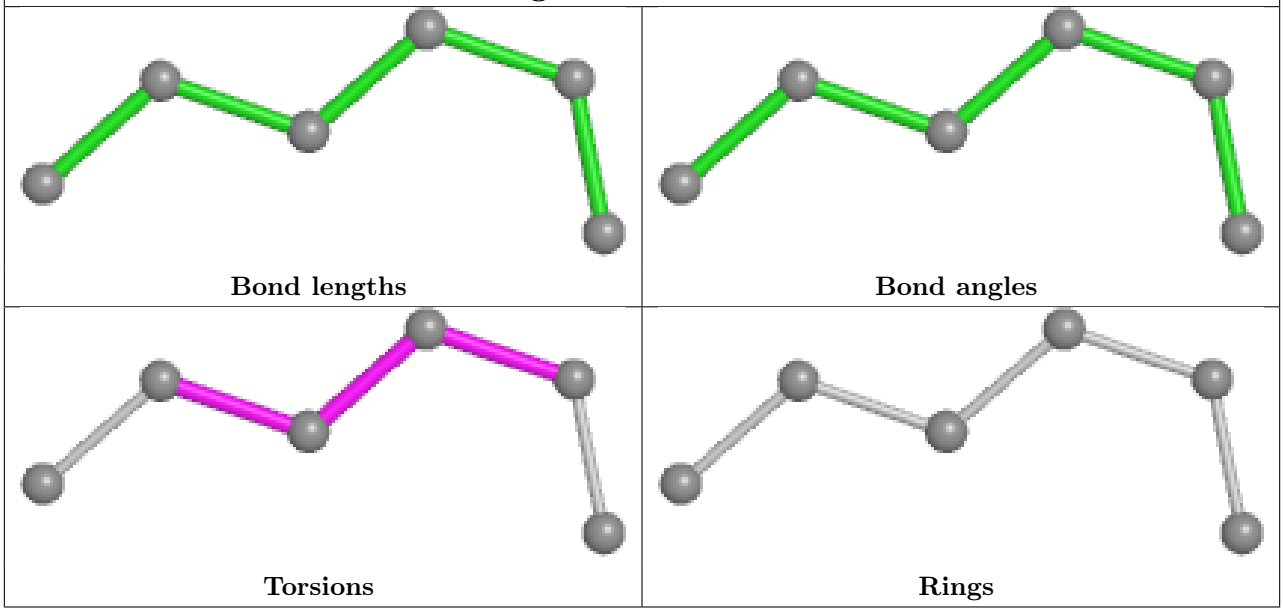


Rings

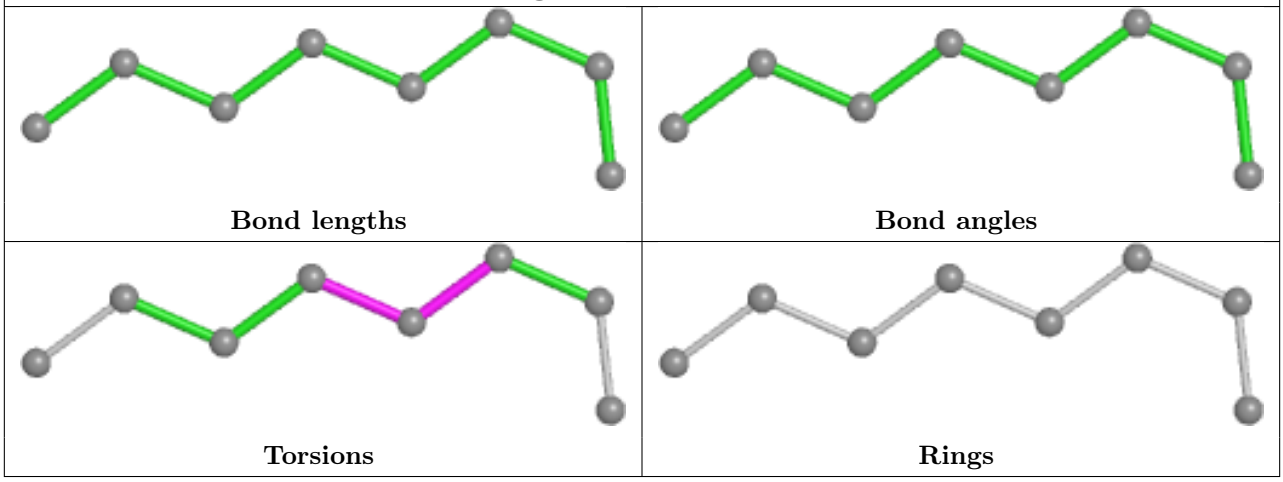
Ligand C8E C 410



Ligand C8E E 401



Ligand C8E F 403



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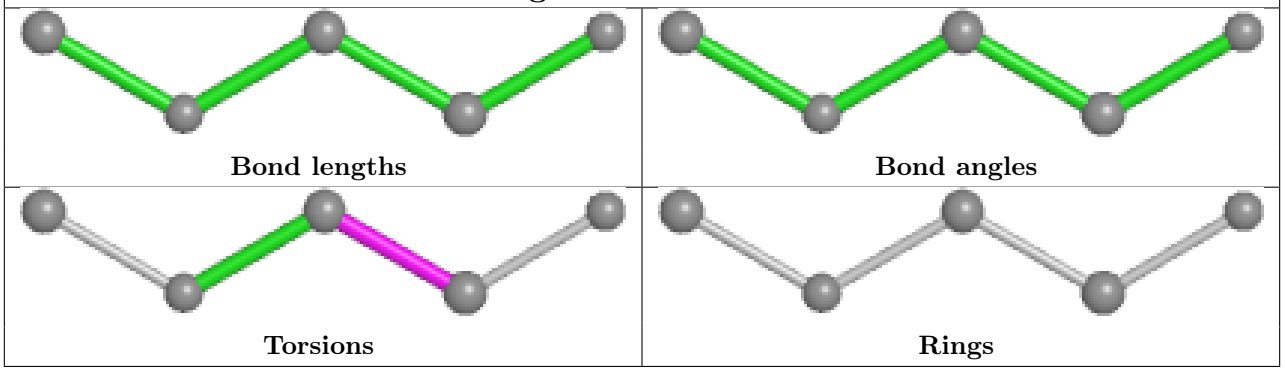

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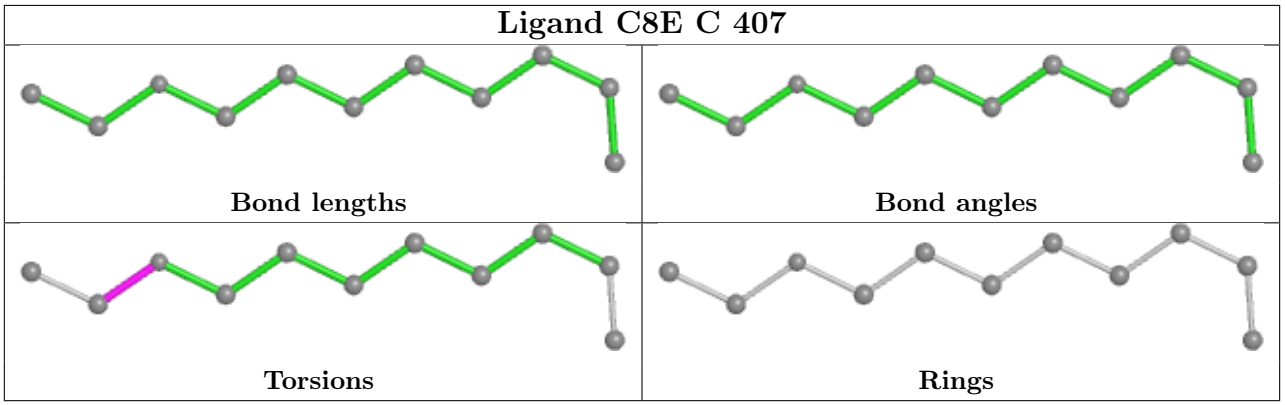
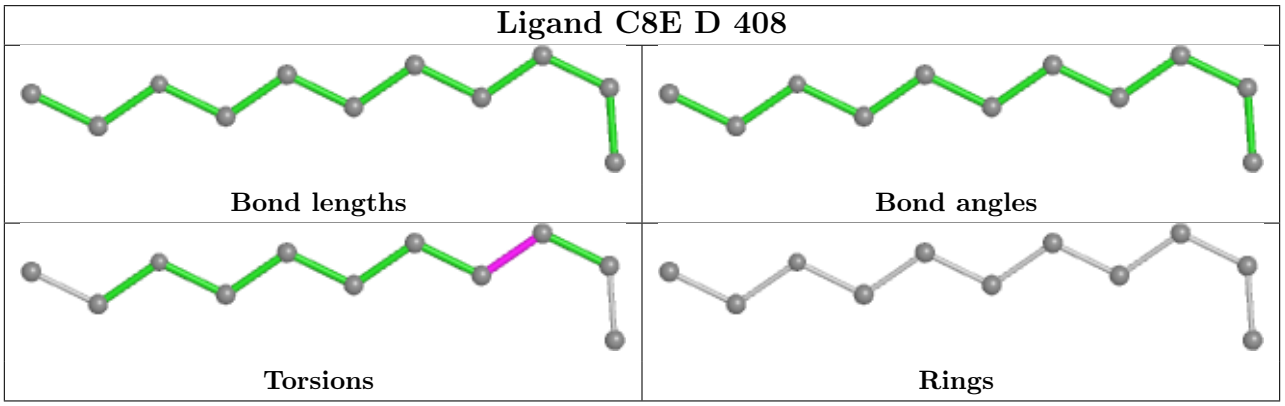
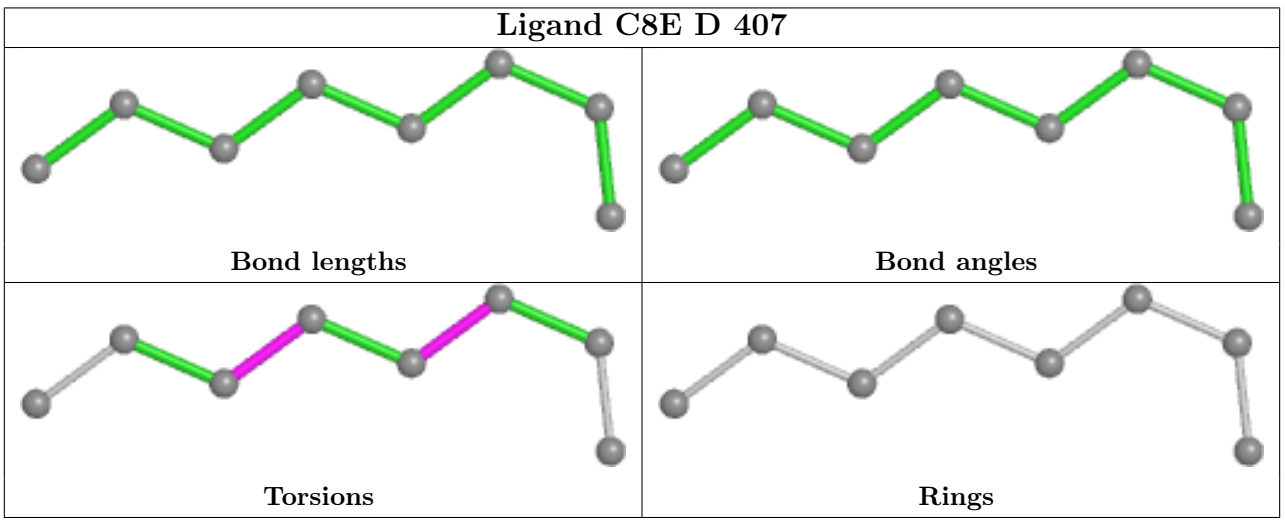


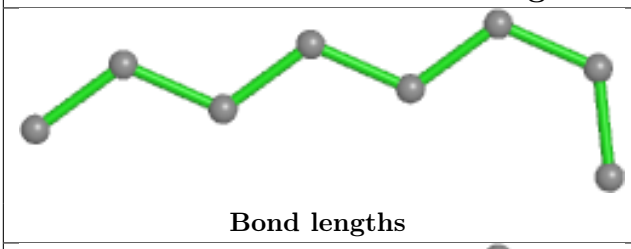
Ligand C8E D 408



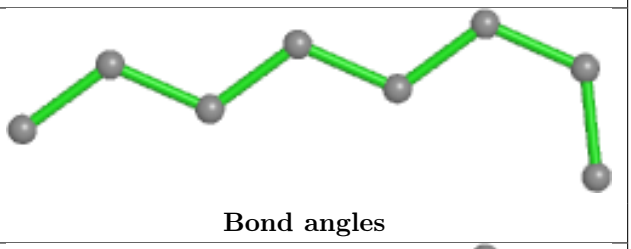
Ligand C8E D 407



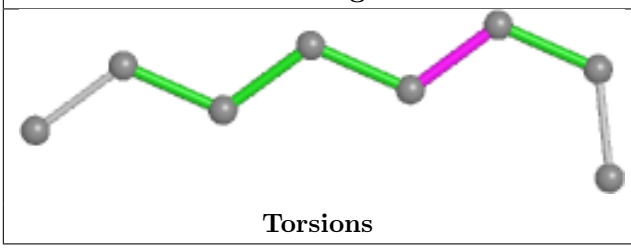
Ligand C8E B 405



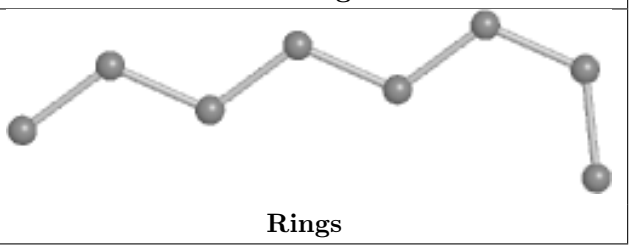
Bond lengths



Bond angles

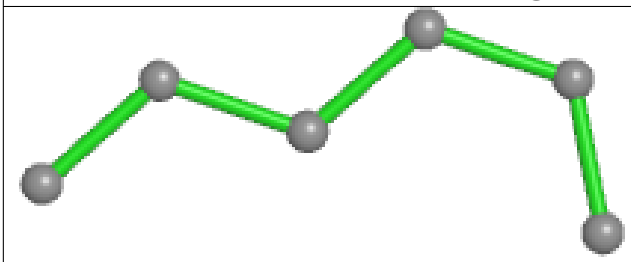


Torsions

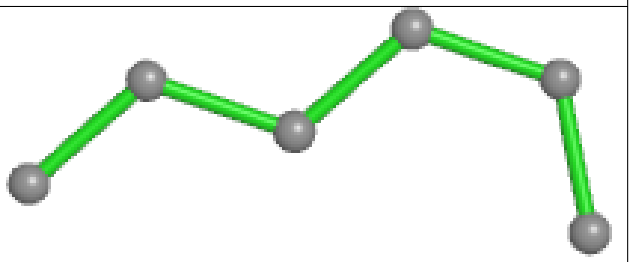


Rings

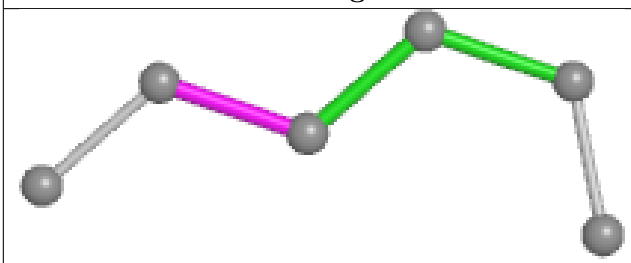
Ligand C8E C 404



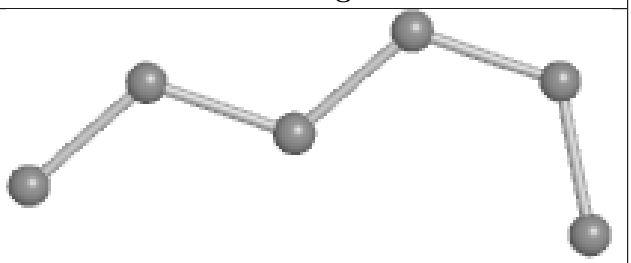
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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%)	0.17	14 (4%)	37	40	9, 15, 28, 59	1 (0%)
1	B	342/342 (100%)	0.17	14 (4%)	37	40	9, 15, 31, 77	0
1	C	342/342 (100%)	0.09	7 (2%)	65	67	9, 14, 30, 54	0
1	D	342/342 (100%)	0.25	21 (6%)	21	23	10, 16, 31, 96	0
1	E	342/342 (100%)	0.16	14 (4%)	37	40	10, 15, 32, 58	0
1	F	342/342 (100%)	0.00	3 (0%)	84	86	9, 14, 25, 40	0
All	All	2052/2052 (100%)	0.14	73 (3%)	42	46	9, 15, 30, 96	1 (0%)

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	LEU	8.7
1	D	83	GLY	8.0
1	A	139	LEU	7.1
1	E	139	LEU	6.9
1	D	137	PHE	6.5

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

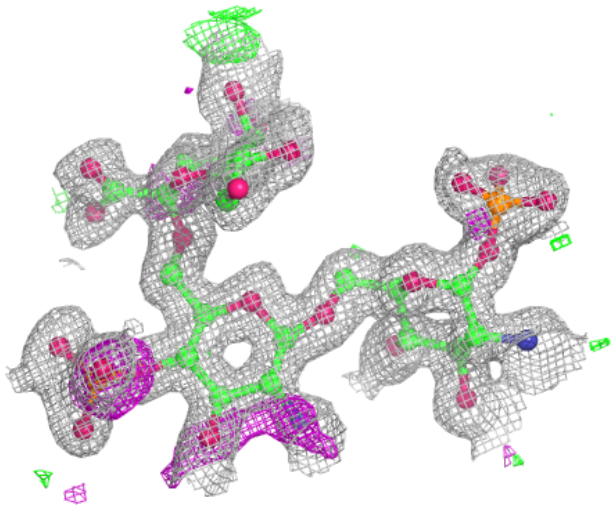
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

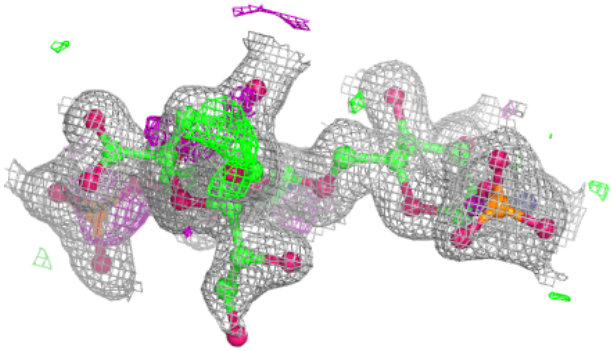
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KDO	K	3	14/16	0.62	0.29	42,49,65,65	0
3	GMH	I	5	13/14	0.77	0.21	36,45,58,69	0
3	GMH	H	5	13/14	0.80	0.28	32,36,40,48	0
2	GP1	K	1	16/16	0.85	0.31	34,37,66,67	0
3	GMH	N	5	13/14	0.86	0.21	31,36,54,59	0
2	KDO	M	3	15/16	0.88	0.21	23,27,35,38	0
2	KDO	G	3	15/16	0.89	0.28	24,29,40,48	0
2	KDO	L	3	15/16	0.89	0.25	25,28,40,44	0
3	KDO	H	3	15/16	0.90	0.21	22,26,33,41	0
3	KDO	H	4	15/16	0.92	0.14	18,20,25,27	0
2	Z9M	K	2	15/16	0.92	0.21	25,29,34,40	0
4	KDO	J	4	15/16	0.92	0.12	12,19,22,23	0
4	KDO	O	3	15/16	0.92	0.14	13,21,31,35	0
2	GP1	L	1	16/16	0.93	0.19	24,26,44,49	0
2	GP1	G	1	16/16	0.93	0.21	22,27,48,52	0
4	KDO	O	4	15/16	0.93	0.12	17,18,21,24	0
3	KDO	N	3	15/16	0.94	0.14	18,25,33,37	0
3	KDO	N	4	15/16	0.94	0.12	15,16,20,29	0
2	Z9M	G	2	15/16	0.94	0.22	22,24,31,34	0
4	KDO	J	3	15/16	0.94	0.12	16,21,30,34	0
3	GP1	H	1	16/16	0.94	0.13	22,24,50,51	0
3	KDO	I	3	15/16	0.94	0.10	18,23,31,31	0
2	GP1	M	1	16/16	0.94	0.15	23,26,47,49	0
3	Z9M	H	2	15/16	0.95	0.16	20,21,26,26	0
3	KDO	I	4	15/16	0.95	0.09	14,15,19,24	0
4	GP1	O	1	16/16	0.95	0.09	18,20,41,43	0
2	Z9M	L	2	15/16	0.95	0.17	23,24,30,30	0
4	GP1	J	1	16/16	0.95	0.08	17,19,44,44	0
2	Z9M	M	2	15/16	0.96	0.20	21,21,26,27	0
3	GP1	N	1	16/16	0.97	0.07	16,19,34,34	0
3	Z9M	I	2	15/16	0.97	0.06	18,21,41,41	0
4	Z9M	O	2	15/16	0.97	0.06	17,18,24,27	0
4	Z9M	J	2	15/16	0.97	0.07	16,17,26,26	0
3	GP1	I	1	16/16	0.97	0.07	17,19,33,35	0
3	Z9M	N	2	15/16	0.98	0.07	18,21,29,32	0

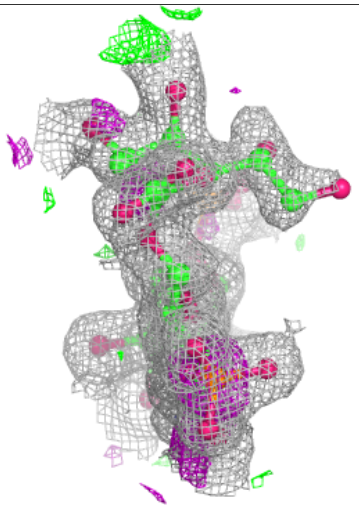
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

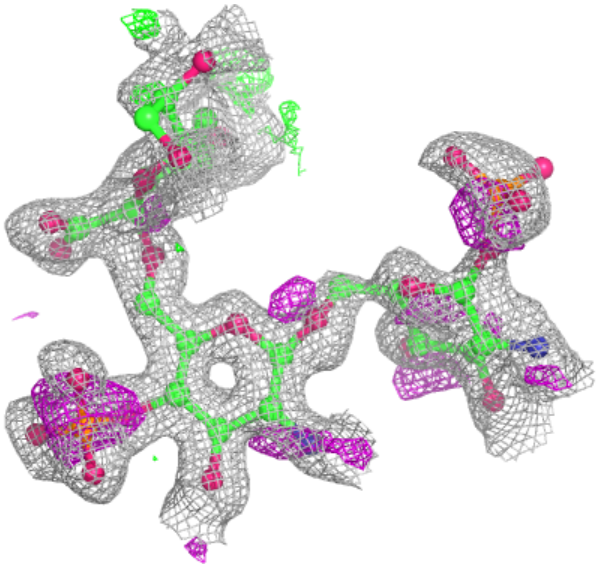


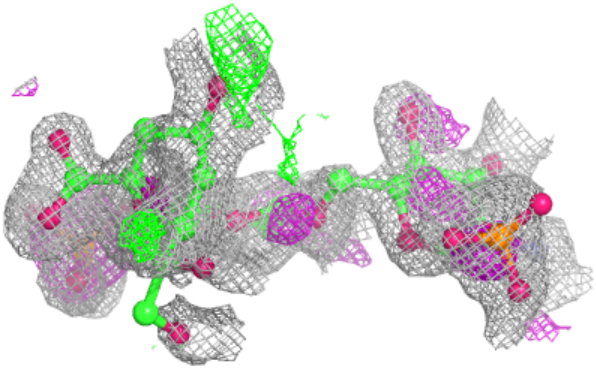


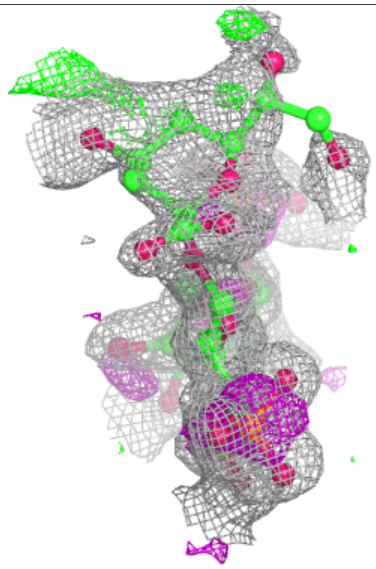


Electron density around Chain K:

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

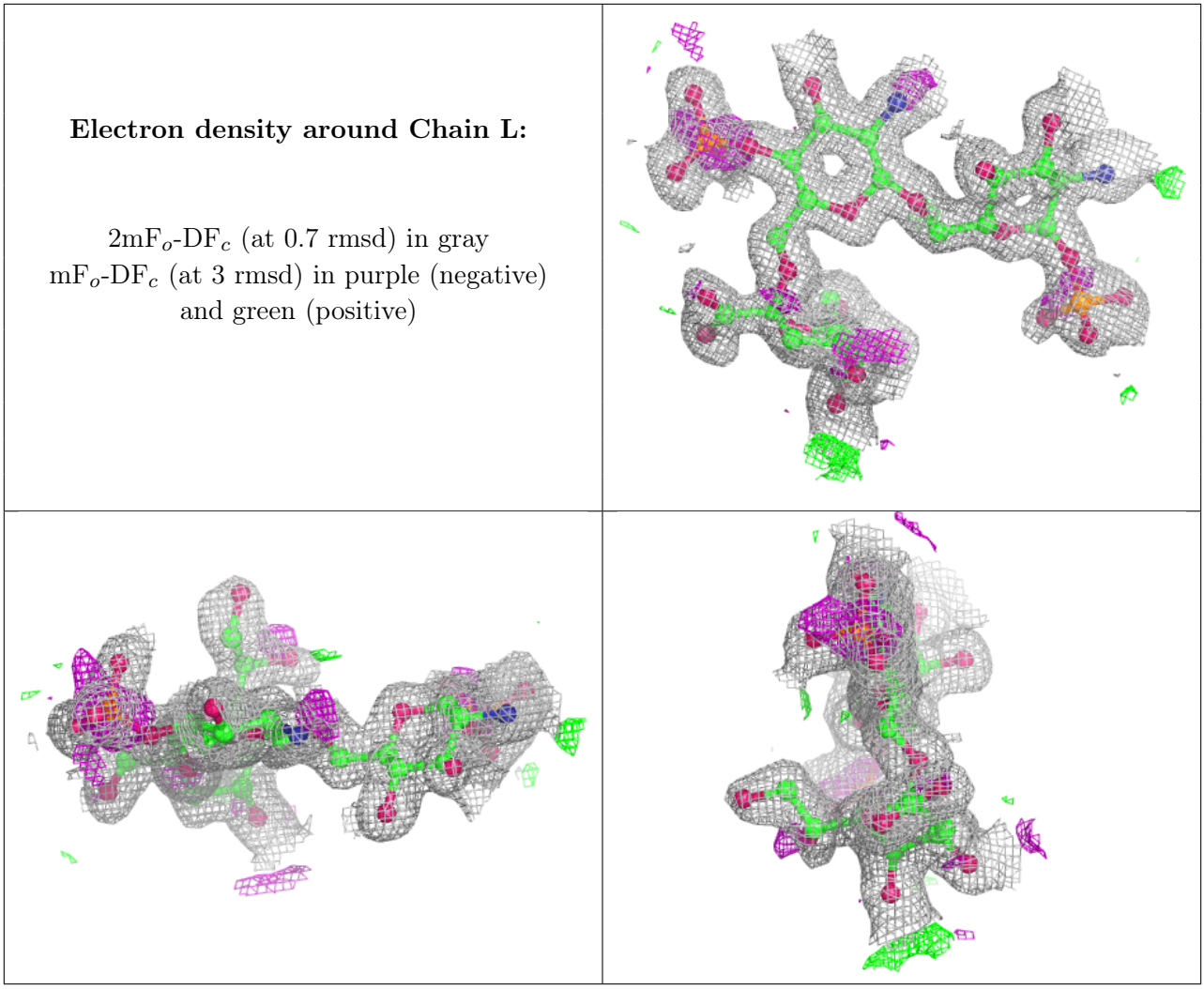






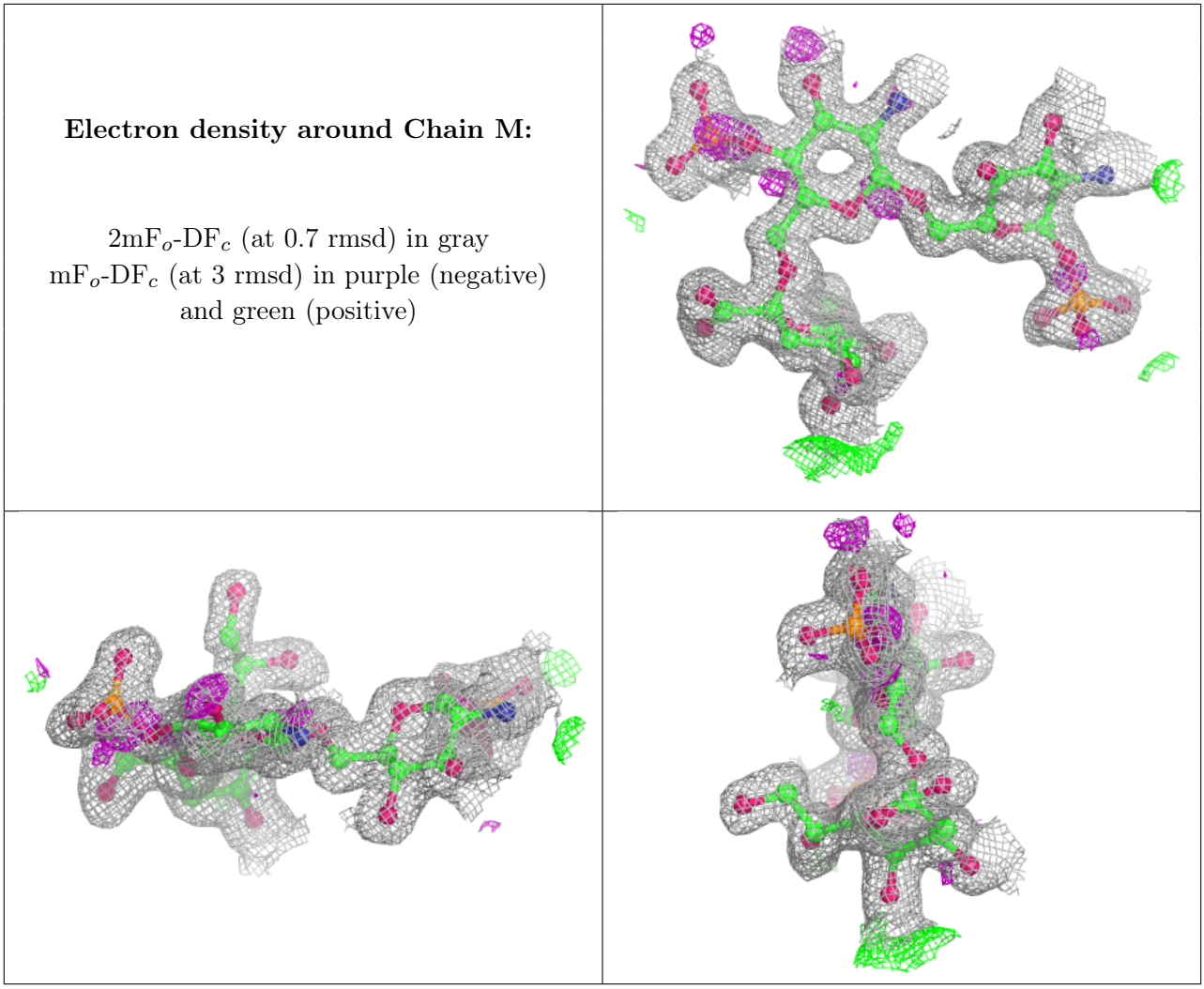
Electron density around Chain L:

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



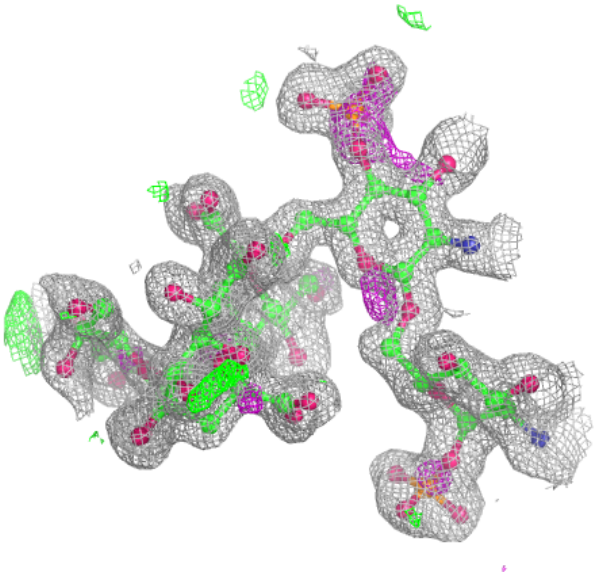
Electron density around Chain M:

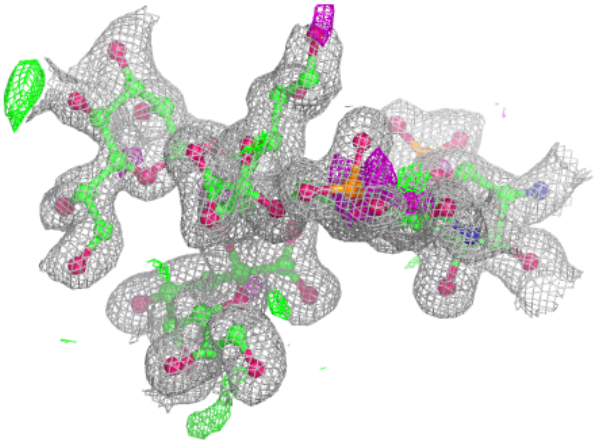
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

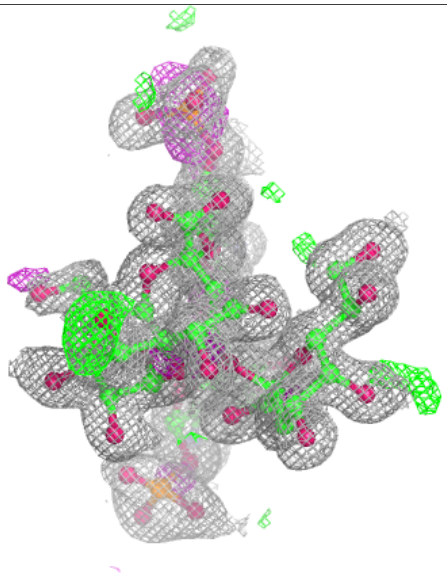


Electron density around Chain H:

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

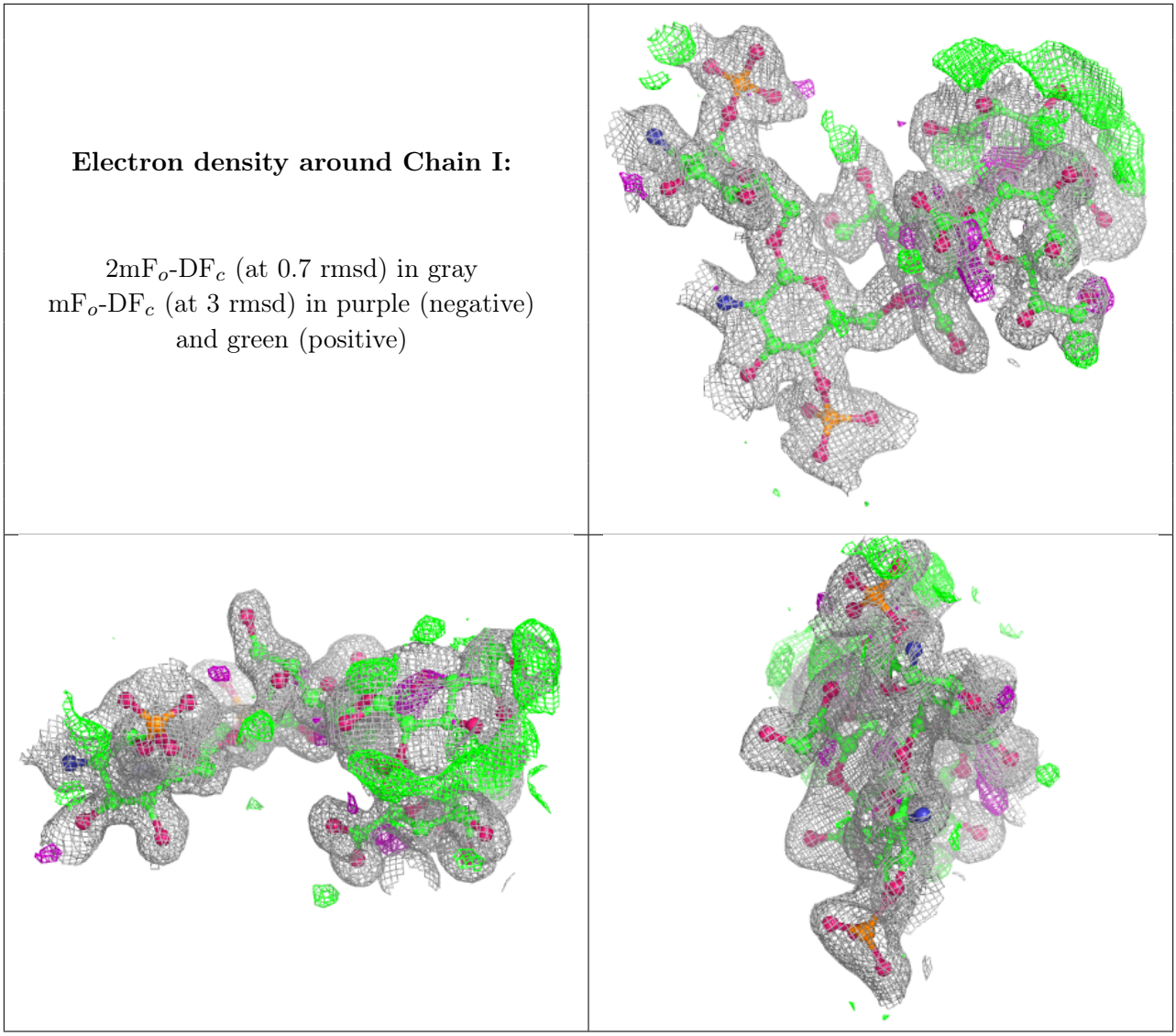






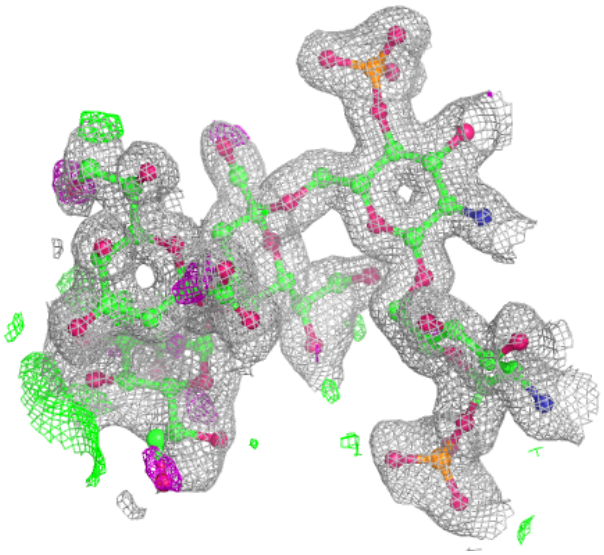
Electron density around Chain I:

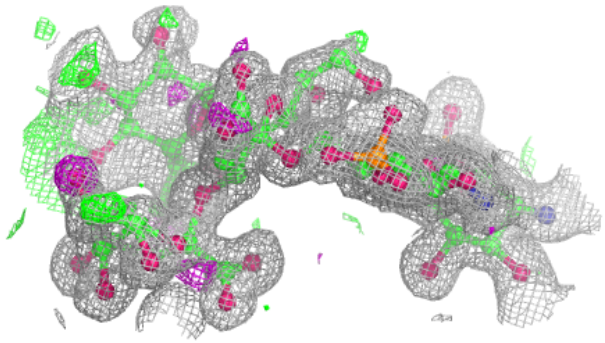
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

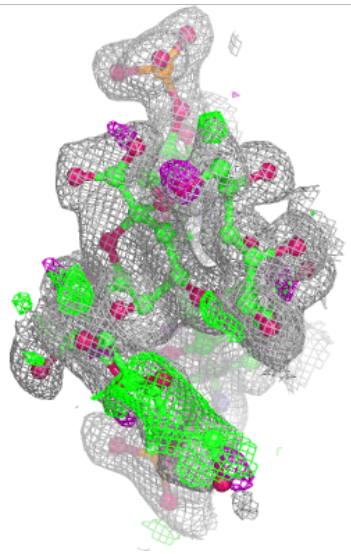


Electron density around Chain N:

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

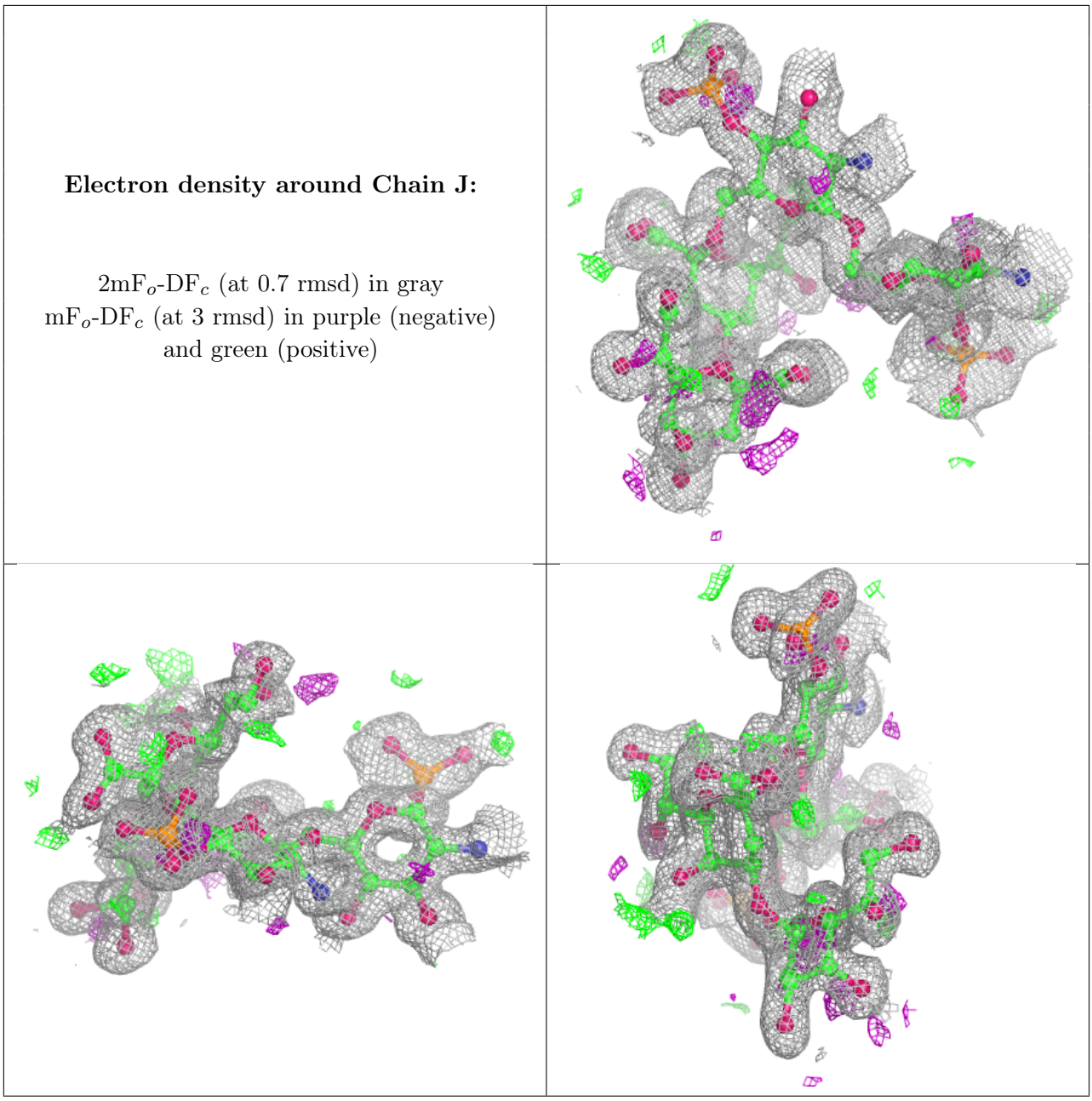






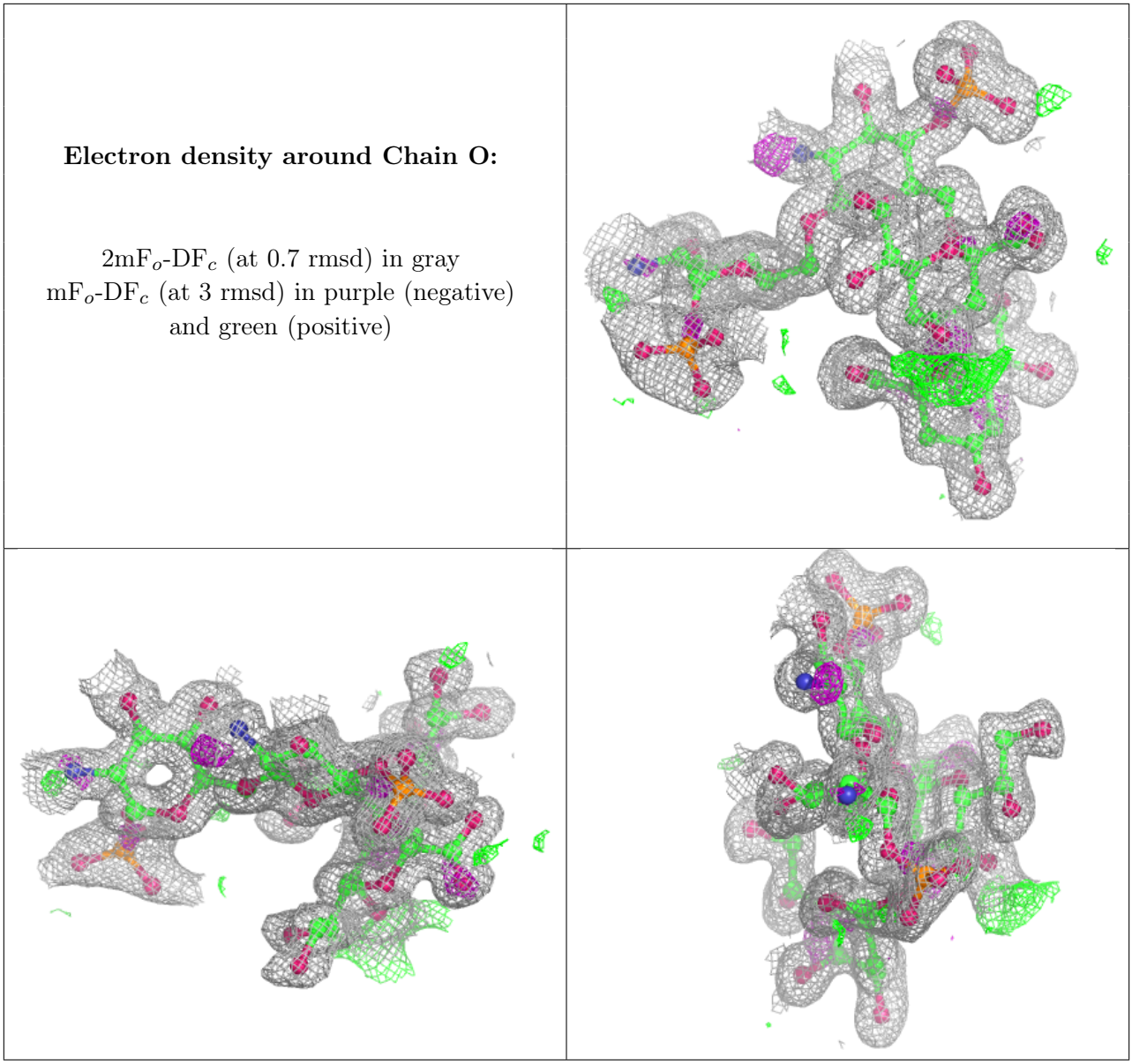
Electron density around Chain J:

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



Electron density around Chain O:

$2mF_o$-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^{th} 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	E	405	5/14	0.40	0.27	52,54,57,63	0
9	FTT	E	404	14/17	0.52	0.25	38,46,48,57	0
9	FTT	C	413	14/17	0.53	0.26	33,47,58,61	0
10	MYR	A	416	6/16	0.56	0.32	47,52,55,57	0
11	DAO	A	417	5/14	0.60	0.39	55,57,59,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	DAO	C	414	5/14	0.62	0.19	49,50,63,63	0
9	FTT	B	407	14/17	0.62	0.18	35,40,55,61	0
11	DAO	D	424	5/14	0.63	0.49	47,58,58,73	0
9	FTT	D	417	11/17	0.63	0.26	46,51,67,67	0
9	FTT	D	425	14/17	0.65	0.23	33,45,53,62	0
9	FTT	F	406	14/17	0.66	0.18	38,42,47,48	0
11	DAO	B	412	5/14	0.68	0.61	39,48,59,60	0
11	DAO	D	418	3/14	0.68	0.42	51,51,52,53	0
9	FTT	A	415	16/17	0.70	0.25	27,39,59,66	0
11	DAO	E	410	5/14	0.70	0.36	49,54,55,56	0
10	MYR	E	409	6/16	0.71	0.30	41,44,51,54	0
6	C8E	A	407	5/21	0.71	0.24	18,20,26,28	0
9	FTT	D	414	14/17	0.72	0.18	36,47,53,54	0
11	DAO	A	419	8/14	0.72	0.17	40,41,44,57	0
6	C8E	A	402	3/21	0.74	0.30	33,33,41,41	0
10	MYR	B	411	6/16	0.75	0.24	43,60,68,68	0
9	FTT	D	415	11/17	0.75	0.18	33,36,41,41	0
10	MYR	D	423	6/16	0.76	0.18	43,47,49,50	0
6	C8E	B	404	8/21	0.76	0.14	41,46,47,47	0
9	FTT	D	421	13/17	0.77	0.14	27,30,46,71	0
6	C8E	D	405	6/21	0.77	0.13	30,37,41,42	0
6	C8E	D	406	8/21	0.77	0.16	48,52,54,58	0
9	FTT	A	414	13/17	0.77	0.18	29,33,39,41	0
6	C8E	E	401	6/21	0.78	0.19	44,52,63,65	0
10	MYR	D	419	5/16	0.79	0.27	16,25,37,38	0
6	C8E	A	409	8/21	0.80	0.18	29,34,38,38	0
6	C8E	C	406	8/21	0.80	0.17	30,33,33,35	0
6	C8E	D	404	6/21	0.80	0.13	32,41,41,43	0
6	C8E	B	405	8/21	0.81	0.11	38,39,41,41	0
6	C8E	C	403	3/21	0.81	0.12	45,45,46,50	0
6	C8E	A	410	7/21	0.81	0.19	38,39,40,41	0
10	MYR	F	411	11/16	0.81	0.12	26,31,36,36	0
9	FTT	A	418	14/17	0.81	0.18	39,44,66,68	0
6	C8E	D	407	8/21	0.81	0.17	25,41,44,48	0
6	C8E	C	409	10/21	0.82	0.13	35,38,50,54	0
6	C8E	C	410	7/21	0.82	0.25	23,24,39,43	0
6	C8E	B	402	3/21	0.82	0.10	46,46,50,55	0
6	C8E	D	408	11/21	0.82	0.23	27,41,43,43	0
9	FTT	E	407	12/17	0.82	0.14	26,29,36,39	0
6	C8E	C	408	11/21	0.83	0.21	36,39,45,49	0
6	C8E	A	404	6/21	0.83	0.13	39,46,50,51	0
6	C8E	B	403	5/21	0.83	0.20	30,32,33,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	C8E	A	403	4/21	0.83	0.12	62,71,76,79	0
6	C8E	D	402	4/21	0.84	0.18	32,33,34,39	0
6	C8E	D	410	6/21	0.84	0.21	40,43,45,45	0
11	DAO	C	426	8/14	0.84	0.19	37,62,72,73	0
6	C8E	D	403	6/21	0.84	0.20	39,44,51,56	0
9	FTT	F	415	11/17	0.84	0.12	22,23,28,34	0
9	FTT	B	410	16/17	0.84	0.20	23,30,36,39	0
6	C8E	C	404	6/21	0.84	0.15	28,41,49,51	0
9	FTT	D	420	16/17	0.85	0.14	17,23,28,30	0
9	FTT	A	413	15/17	0.85	0.13	15,22,26,38	0
9	FTT	F	416	16/17	0.85	0.16	21,32,42,45	0
6	C8E	B	401	9/21	0.85	0.15	31,43,63,64	0
9	FTT	B	409	13/17	0.85	0.16	21,26,42,44	0
6	C8E	F	402	4/21	0.85	0.16	41,44,47,47	0
6	C8E	C	402	7/21	0.86	0.27	25,32,38,43	0
9	FTT	F	410	16/17	0.86	0.13	28,33,39,41	0
9	FTT	E	408	15/17	0.86	0.23	25,31,40,41	0
11	DAO	D	412	6/14	0.86	0.10	44,48,51,57	0
6	C8E	A	406	5/21	0.87	0.11	57,64,67,74	0
10	MYR	F	417	12/16	0.87	0.12	29,32,44,50	0
9	FTT	D	422	16/17	0.87	0.18	28,36,41,43	0
6	C8E	A	405	4/21	0.87	0.12	77,80,84,87	0
11	DAO	F	418	8/14	0.87	0.18	34,49,64,66	0
8	KDO	D	413	15/16	0.88	0.20	14,22,27,27	0
9	FTT	D	416	13/17	0.88	0.16	29,43,53,54	0
6	C8E	D	409	4/21	0.88	0.29	21,23,30,39	0
6	C8E	A	408	8/21	0.88	0.22	19,29,52,66	0
10	MYR	C	425	9/16	0.88	0.15	33,55,63,71	0
7	PO4	D	411	5/5	0.88	0.24	32,37,40,47	0
7	PO4	E	402	5/5	0.88	0.25	34,35,41,44	0
8	KDO	A	412	15/16	0.89	0.24	18,23,30,30	0
9	FTT	C	423	13/17	0.89	0.10	20,22,34,39	0
6	C8E	C	401	3/21	0.89	0.20	45,45,50,51	0
6	C8E	C	407	11/21	0.89	0.17	33,35,43,47	0
9	FTT	E	406	14/17	0.90	0.10	18,21,25,26	0
11	DAO	C	421	10/14	0.90	0.12	25,30,32,33	0
9	FTT	C	415	16/17	0.90	0.13	23,32,37,38	0
9	FTT	F	409	12/17	0.91	0.11	21,26,34,38	0
8	KDO	E	403	15/16	0.91	0.16	19,21,26,27	0
7	PO4	A	411	5/5	0.91	0.20	36,36,41,47	0
9	FTT	F	407	12/17	0.91	0.12	19,24,43,48	0
6	C8E	F	403	8/21	0.92	0.17	40,43,47,47	0

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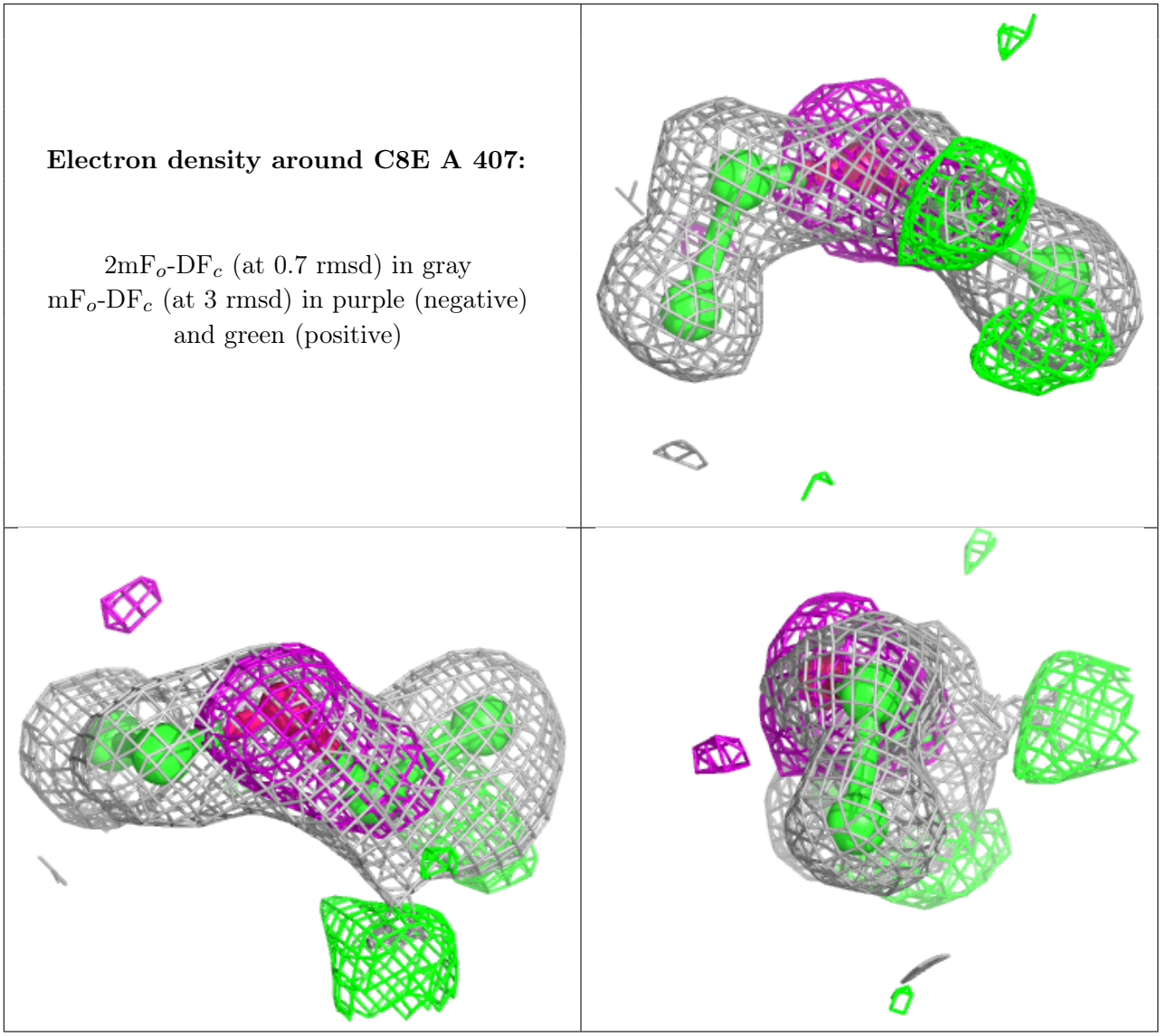
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MYR	C	419	8/16	0.92	0.15	22,30,32,32	0
7	PO4	B	406	5/5	0.92	0.18	31,33,40,44	0
7	PO4	F	404	5/5	0.92	0.19	31,36,45,45	0
9	FTT	C	416	11/17	0.92	0.10	18,20,24,30	0
9	FTT	C	422	16/17	0.93	0.10	15,20,27,31	0
11	DAO	C	420	13/14	0.93	0.09	22,27,31,33	0
9	FTT	B	408	15/17	0.93	0.09	19,21,36,37	0
6	C8E	F	401	3/21	0.93	0.10	21,21,30,37	0
11	DAO	F	412	5/14	0.93	0.10	26,27,35,40	0
6	C8E	C	405	3/21	0.93	0.17	26,26,28,35	0
7	PO4	C	411	5/5	0.94	0.23	32,35,44,44	0
9	FTT	C	424	16/17	0.94	0.10	18,30,41,41	0
9	FTT	F	414	14/17	0.94	0.09	16,18,24,27	0
11	DAO	F	413	5/14	0.94	0.14	33,34,49,62	0
9	FTT	F	408	13/17	0.94	0.12	19,31,46,46	0
9	FTT	C	418	13/17	0.95	0.13	19,26,52,55	0
9	FTT	C	417	16/17	0.96	0.08	18,20,30,34	0
5	SO4	A	401	5/5	0.99	0.08	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	0.08	12,12,12,12	0
12	CA	F	405	1/1	1.00	0.08	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.

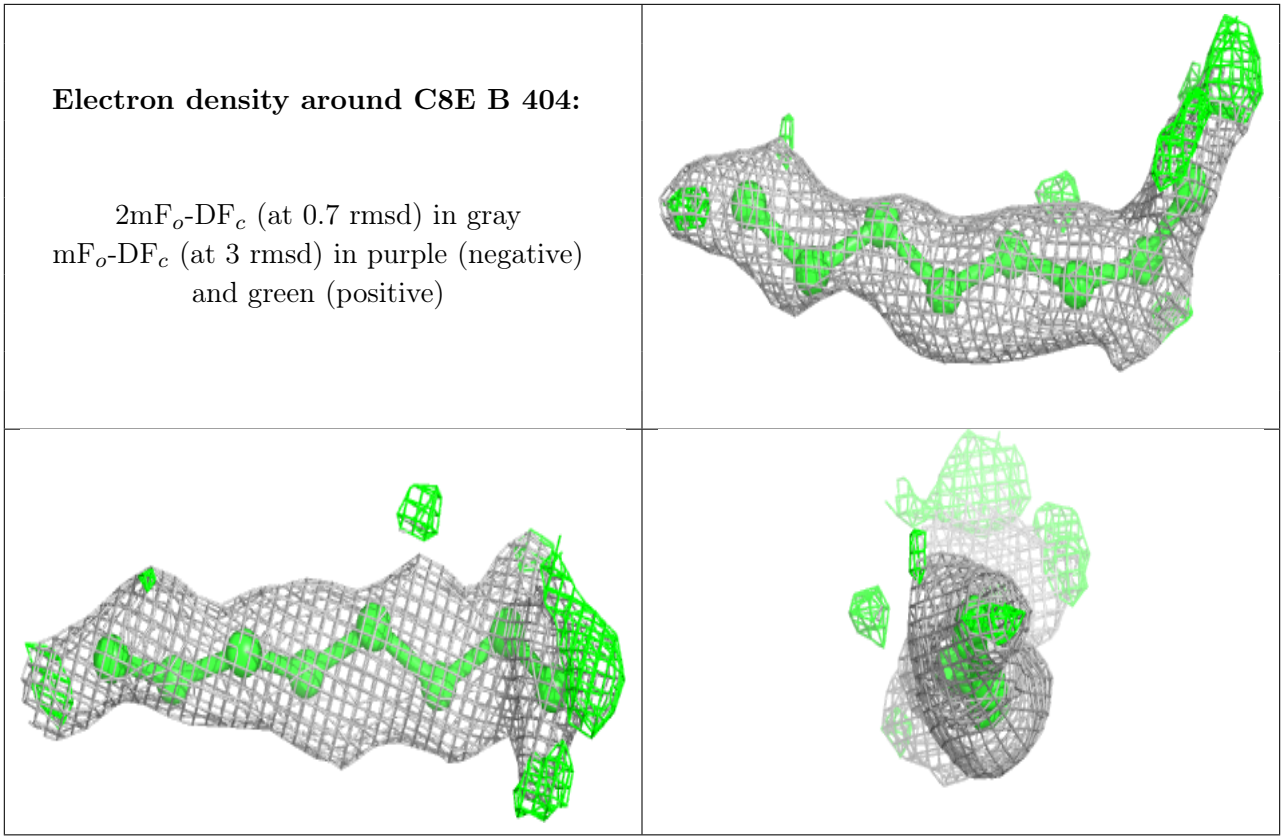
Electron density around C8E A 407:

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



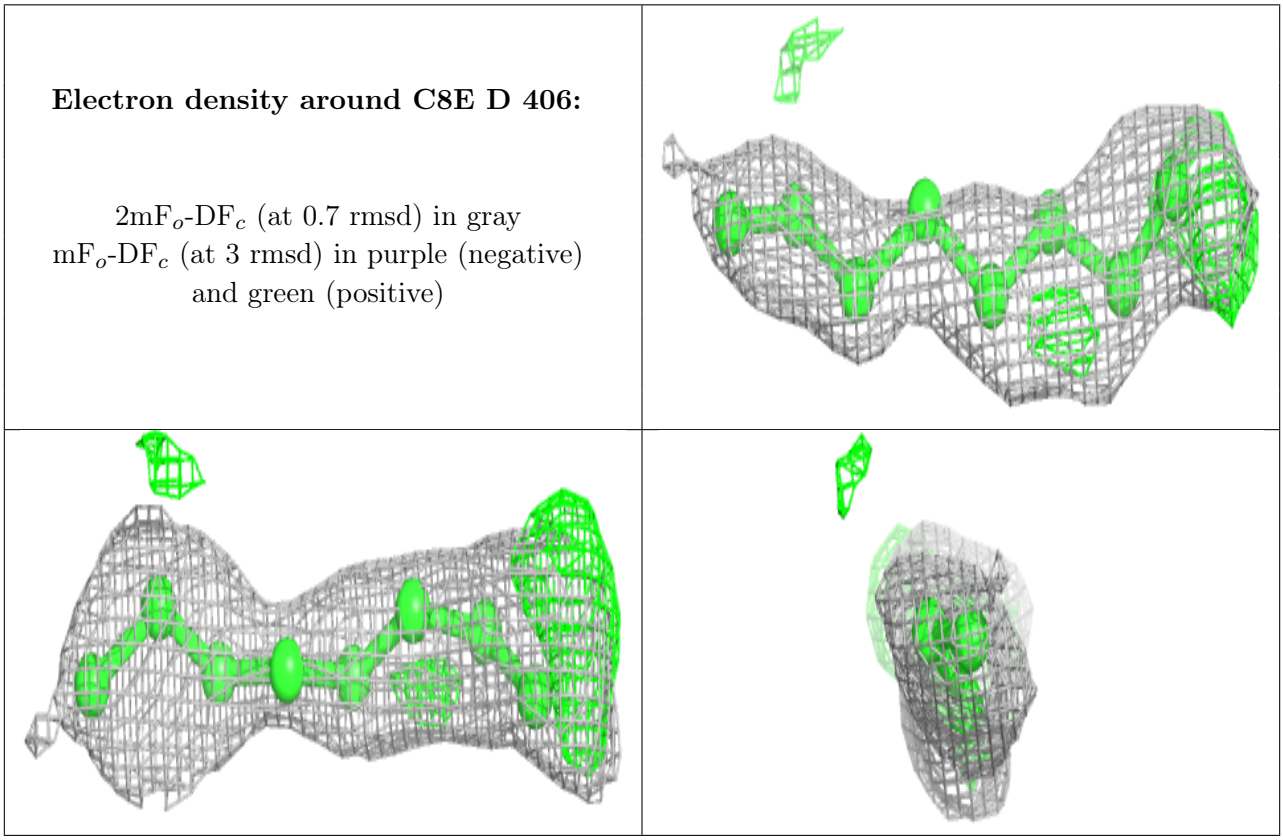
Electron density around C8E B 404:

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



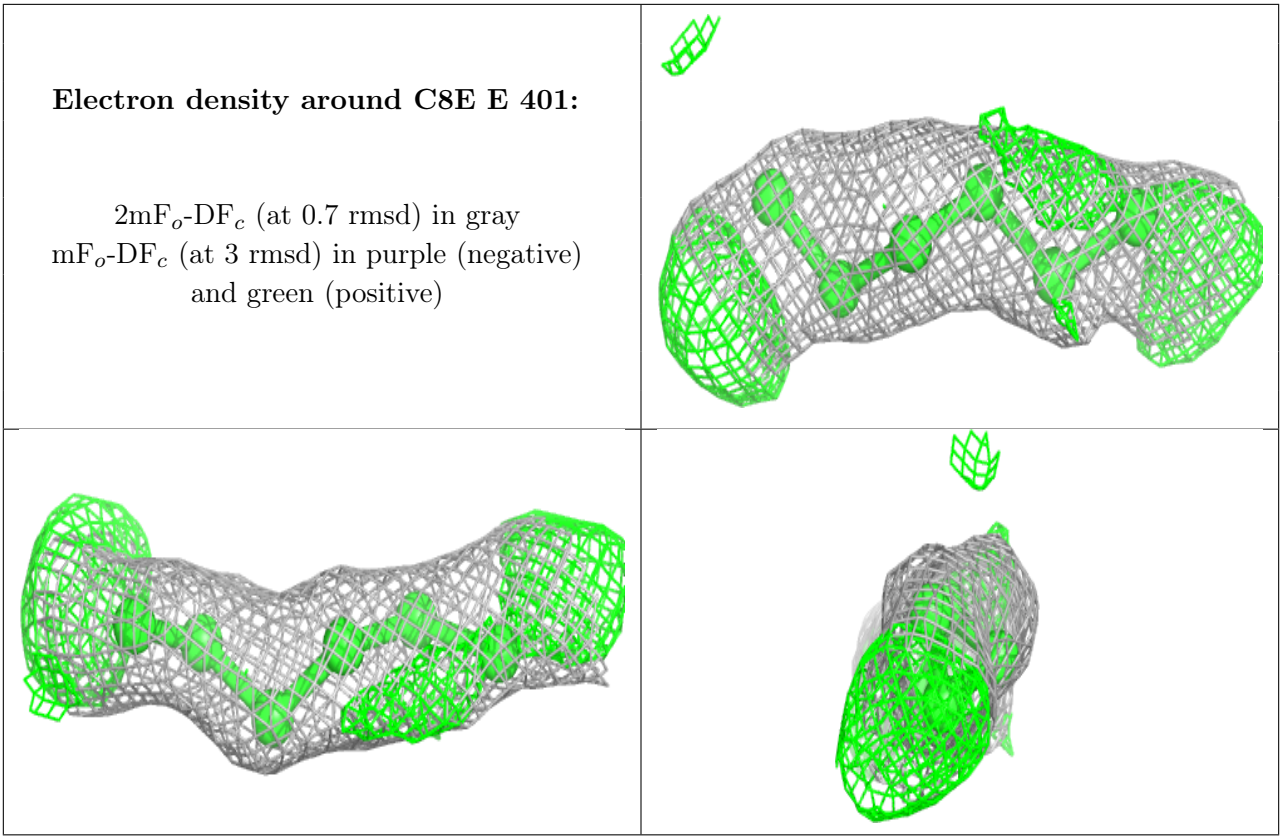
Electron density around C8E D 406:

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



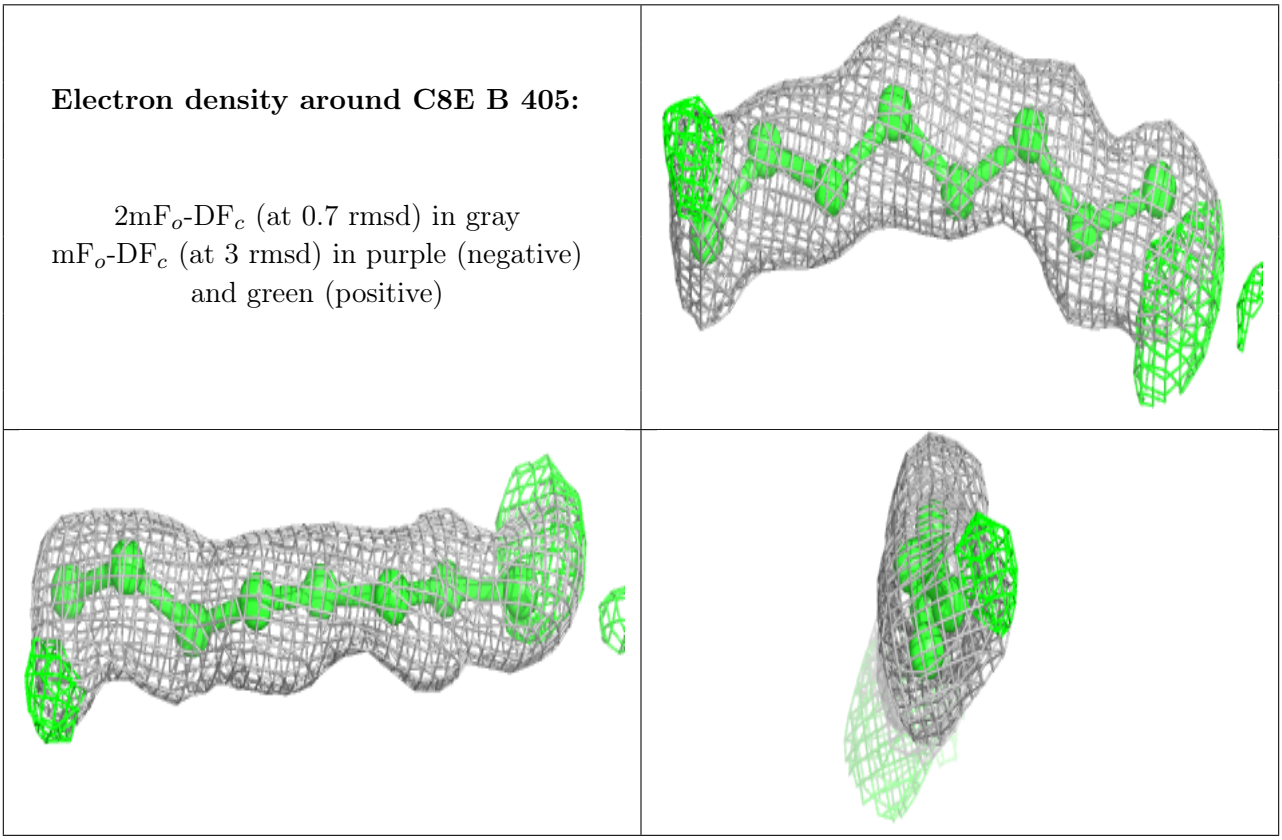
Electron density around C8E E 401:

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



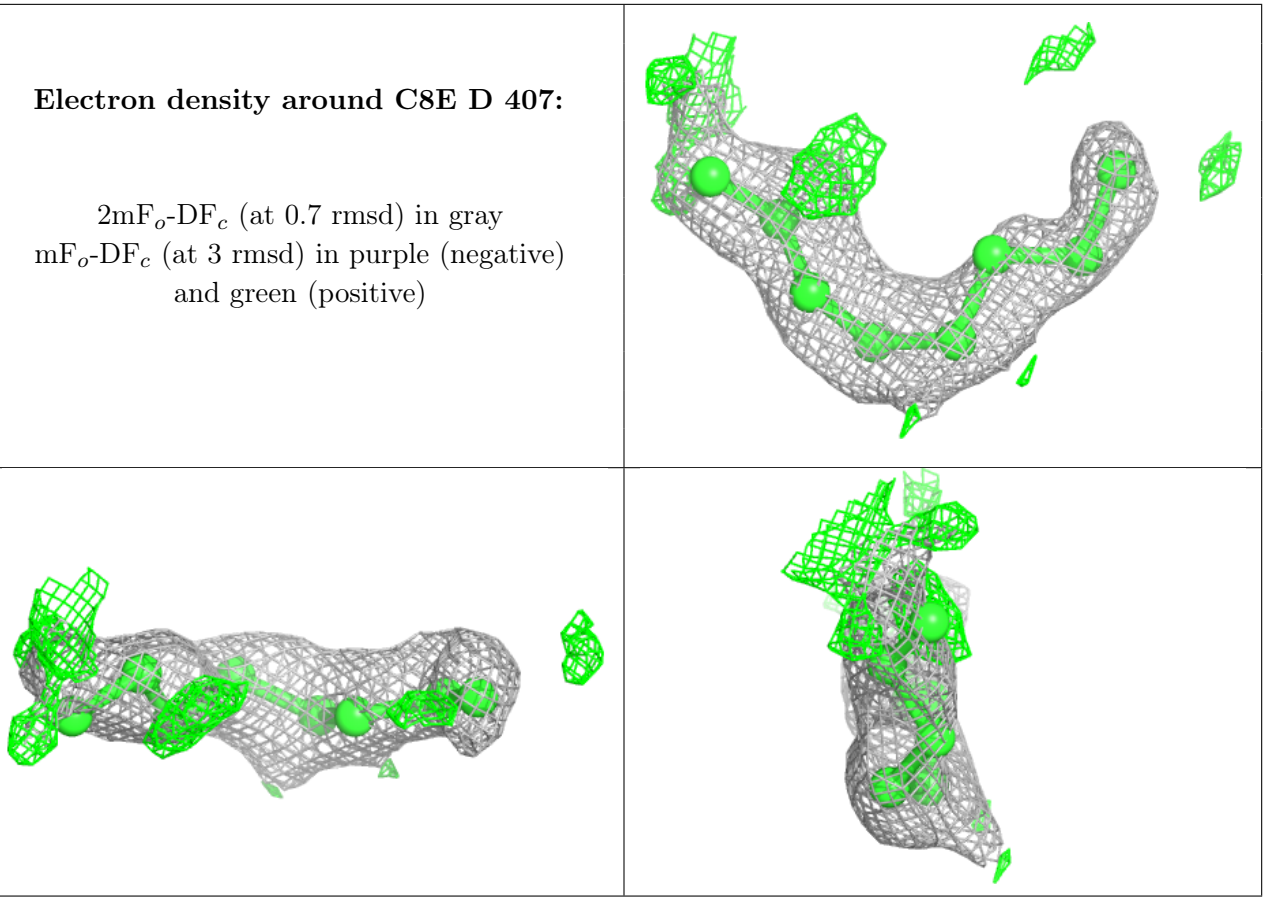
Electron density around C8E B 405:

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



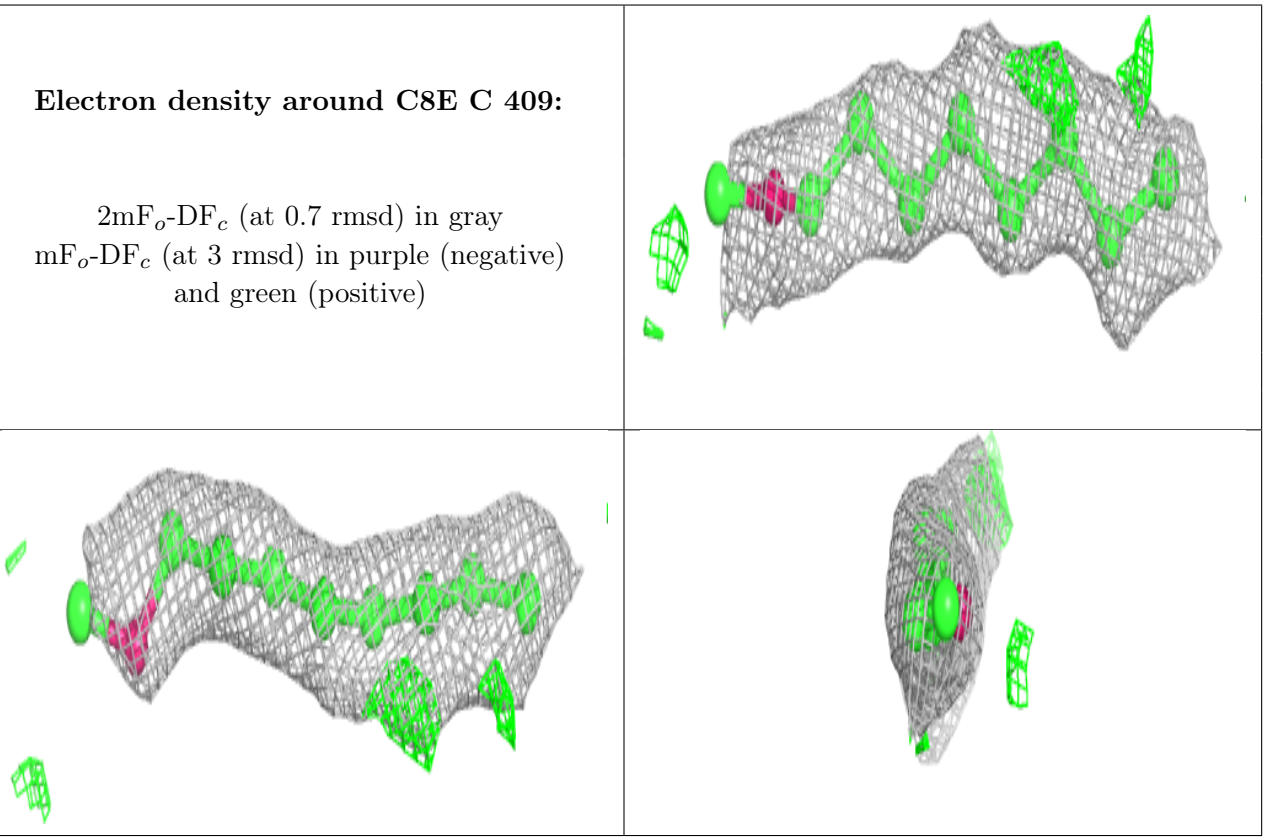
Electron density around C8E D 407:

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



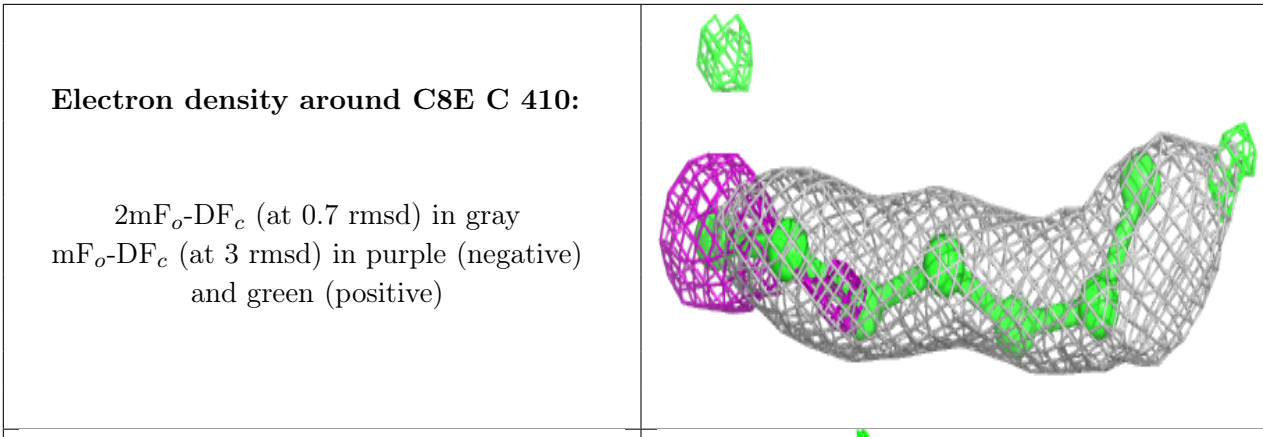
Electron density around C8E C 409:

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



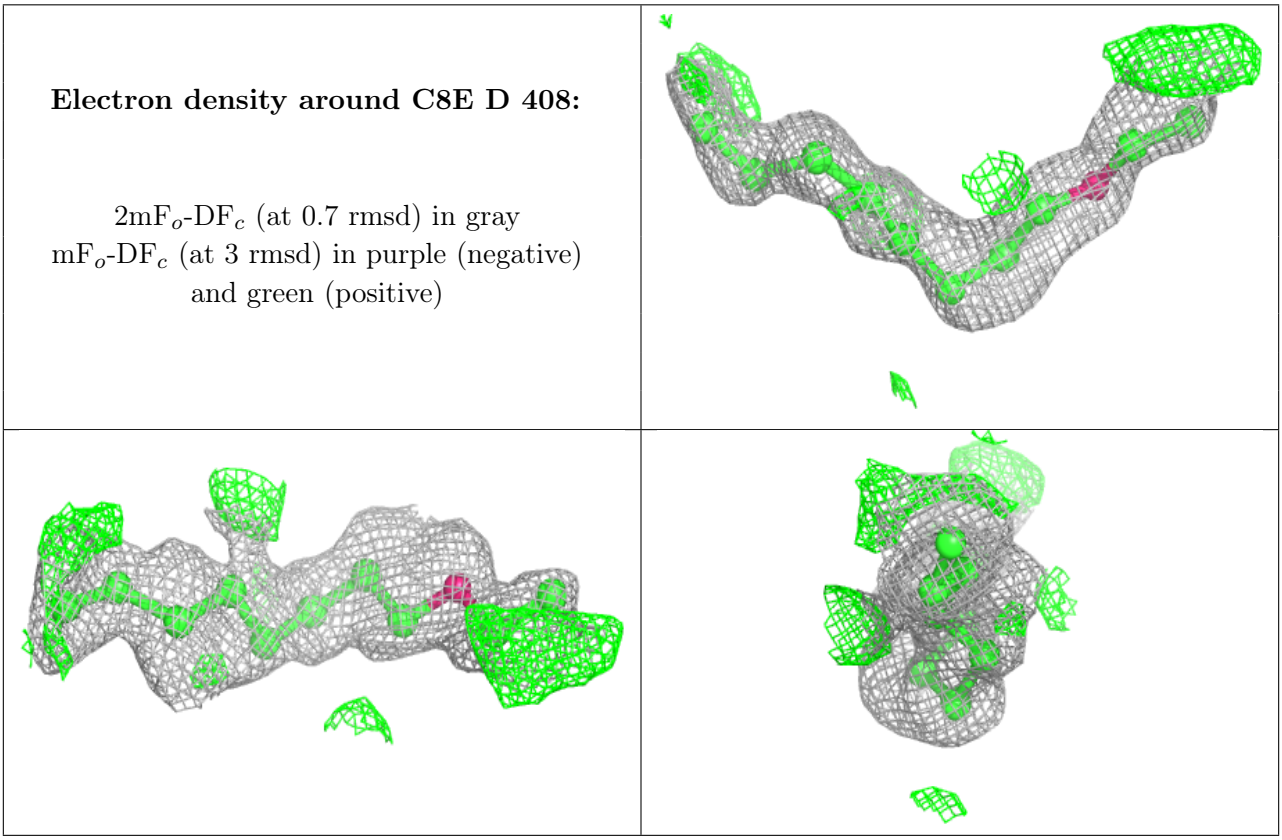
Electron density around C8E C 410:

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



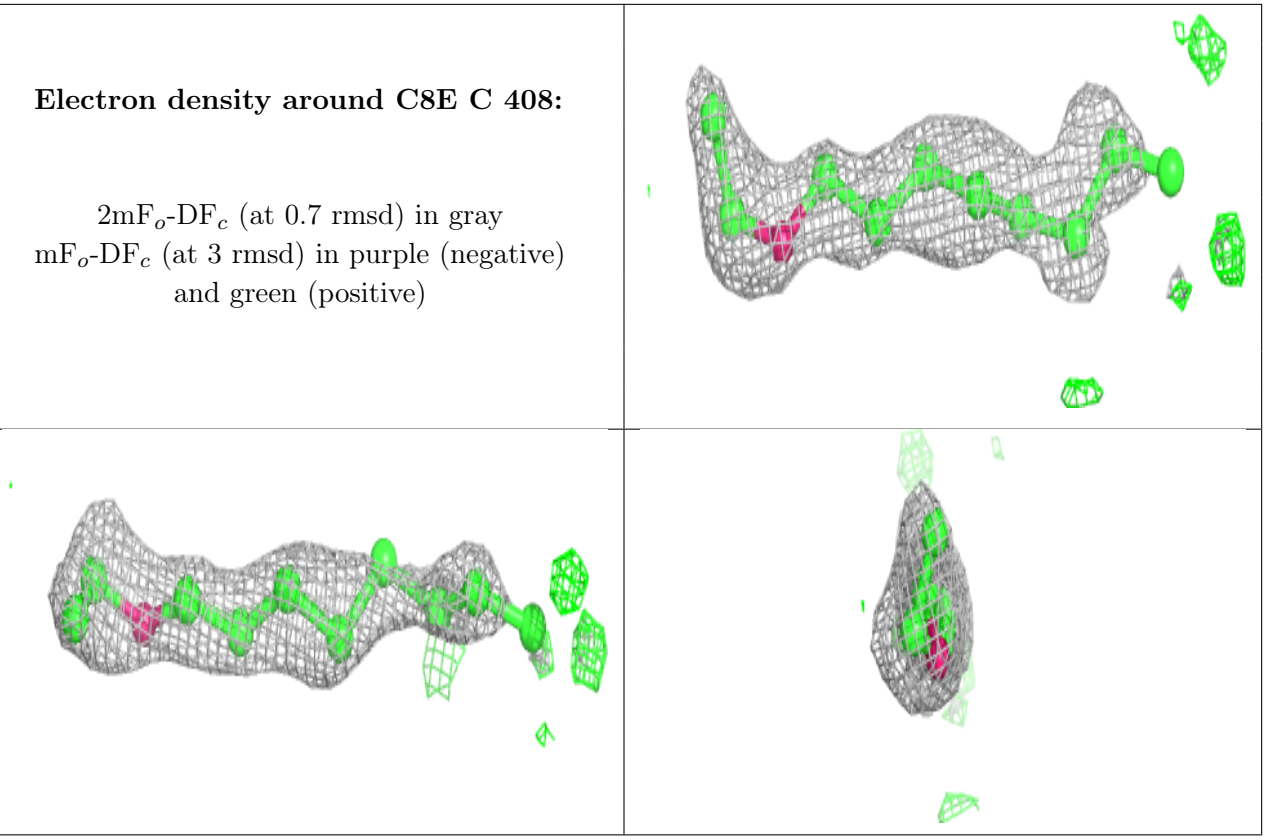
Electron density around C8E D 408:

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



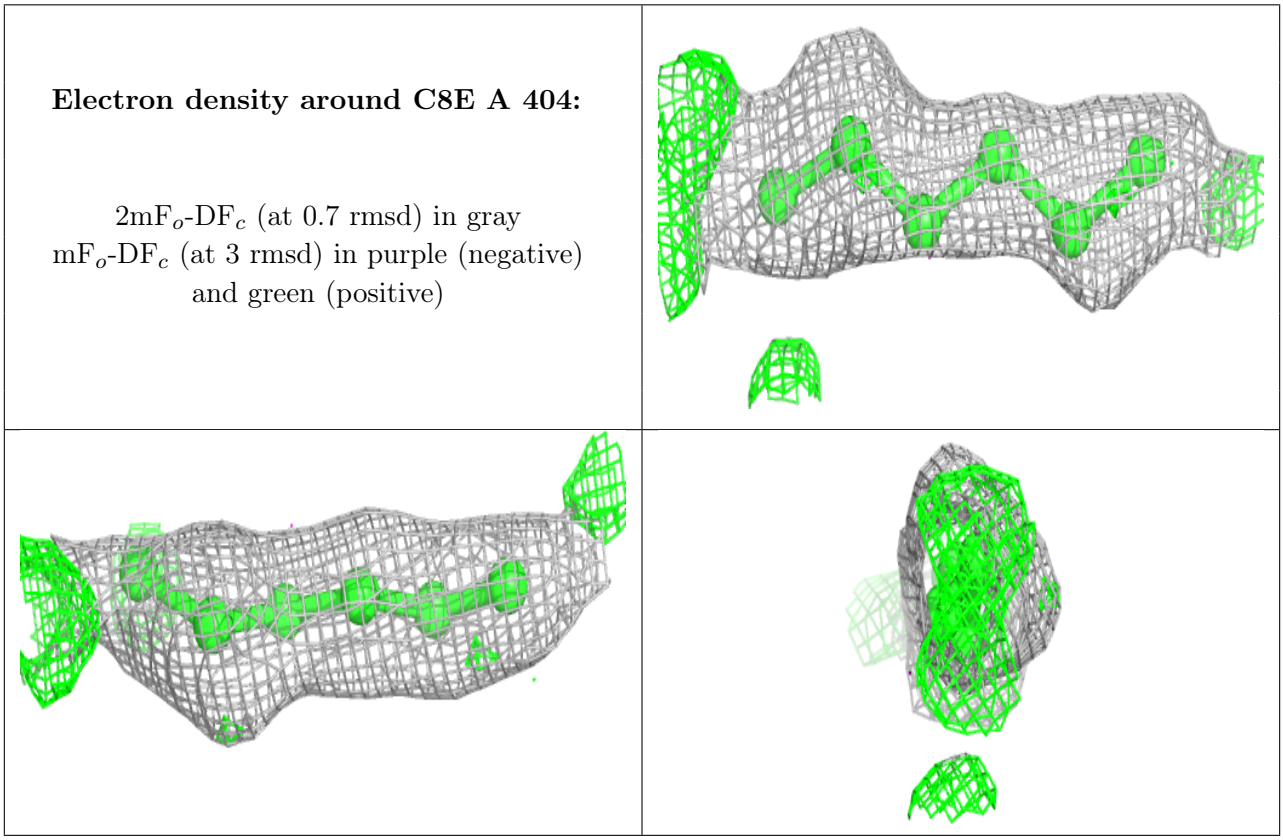
Electron density around C8E C 408:

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



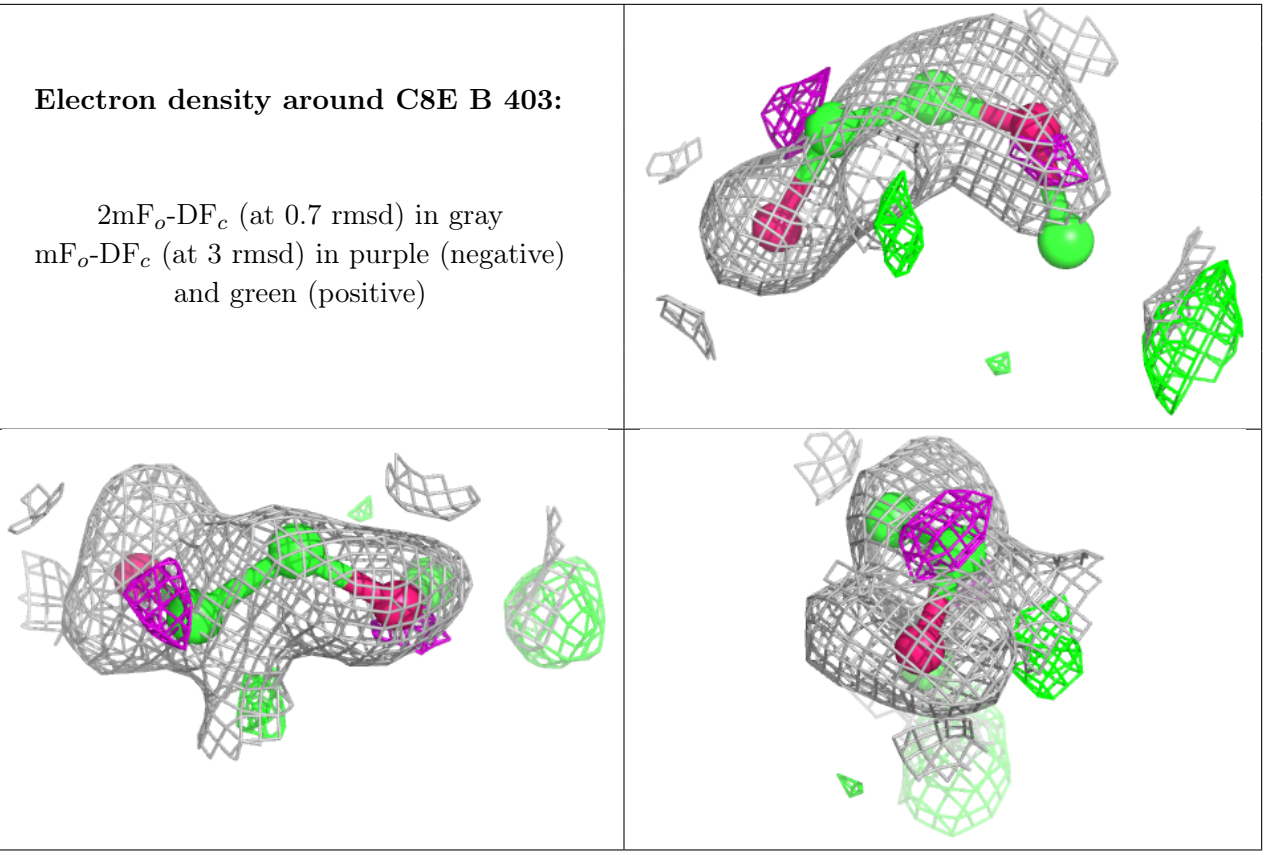
Electron density around C8E A 404:

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



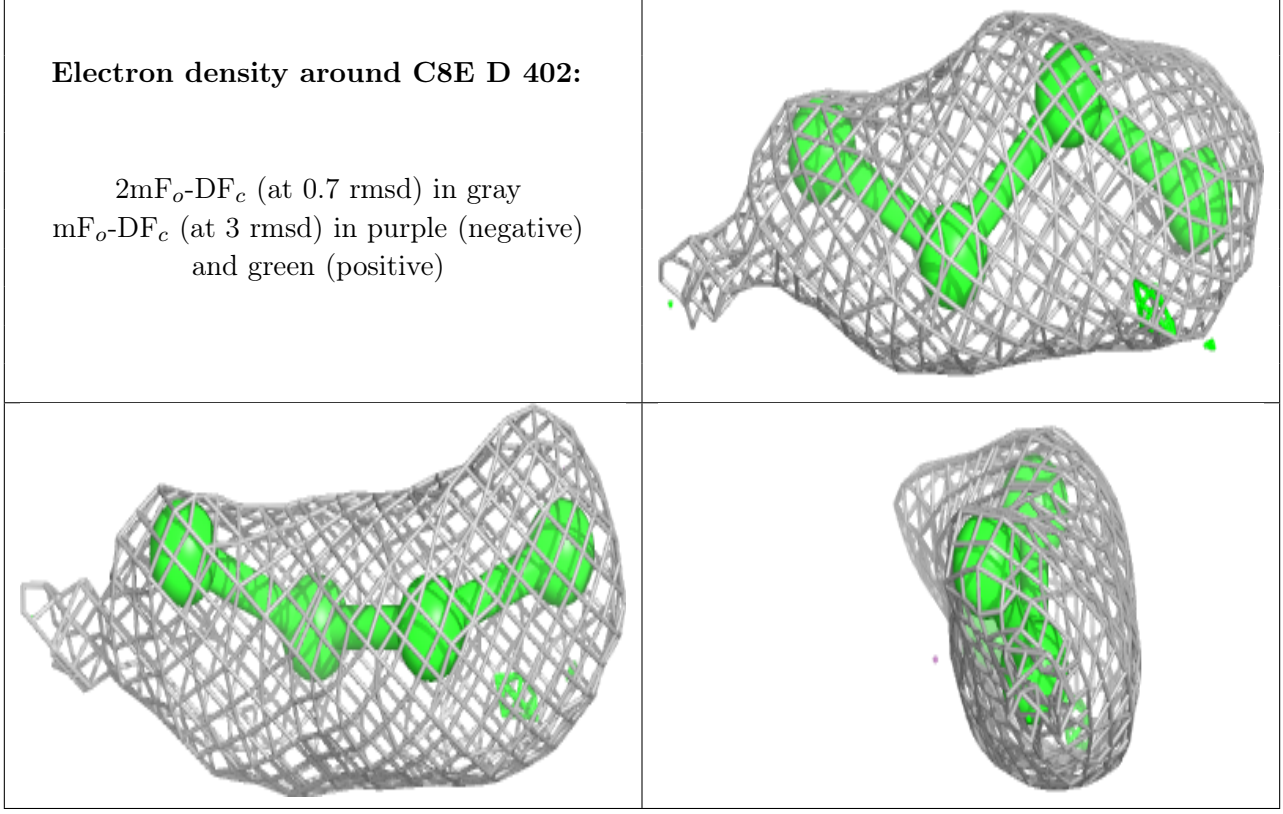
Electron density around C8E B 403:

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



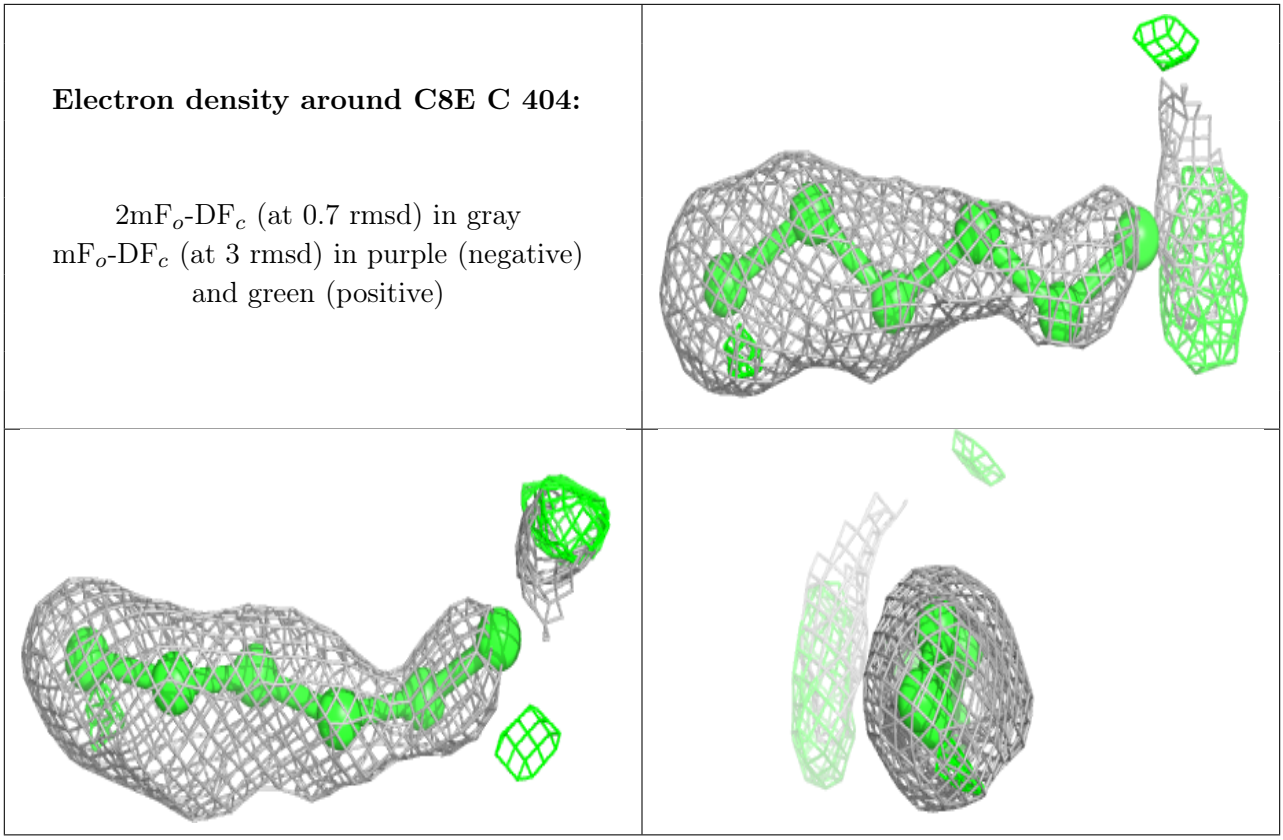
Electron density around C8E D 402:

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



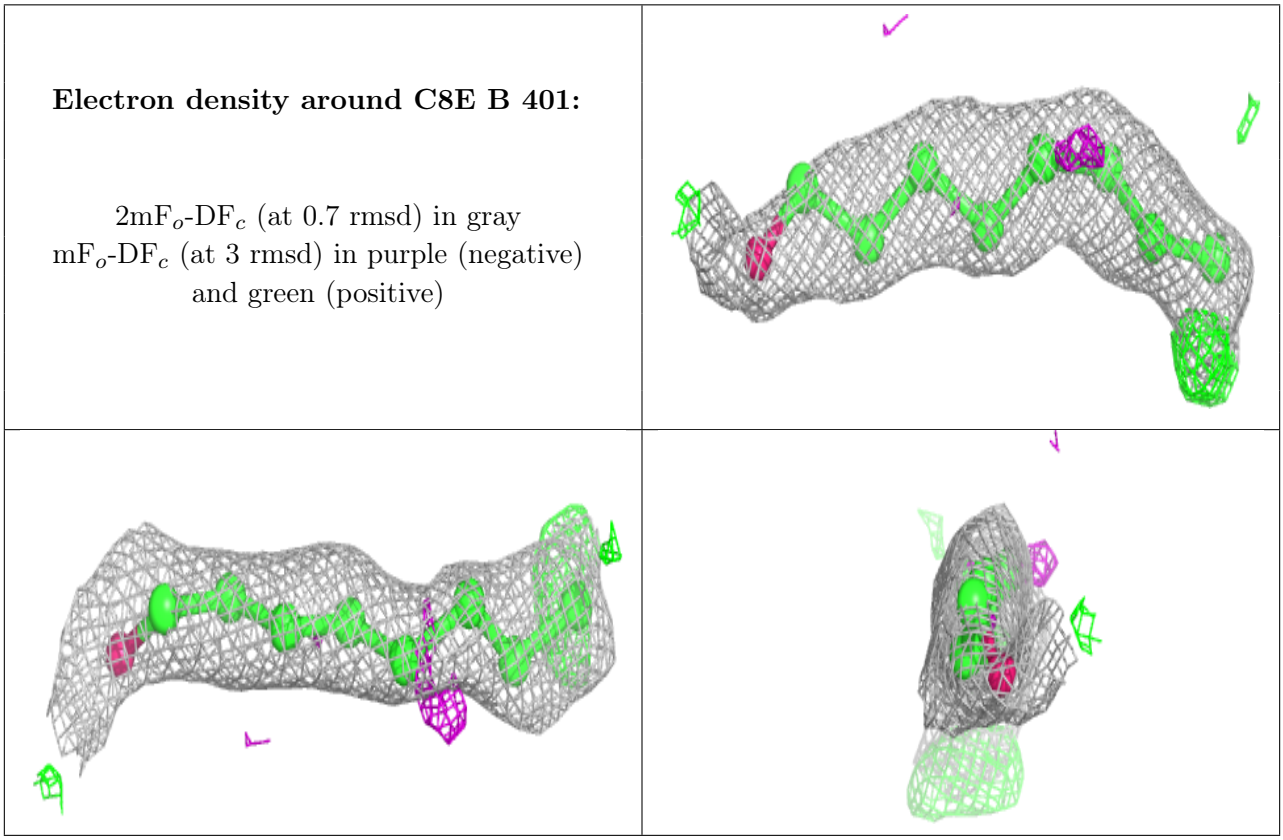
Electron density around C8E C 404:

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



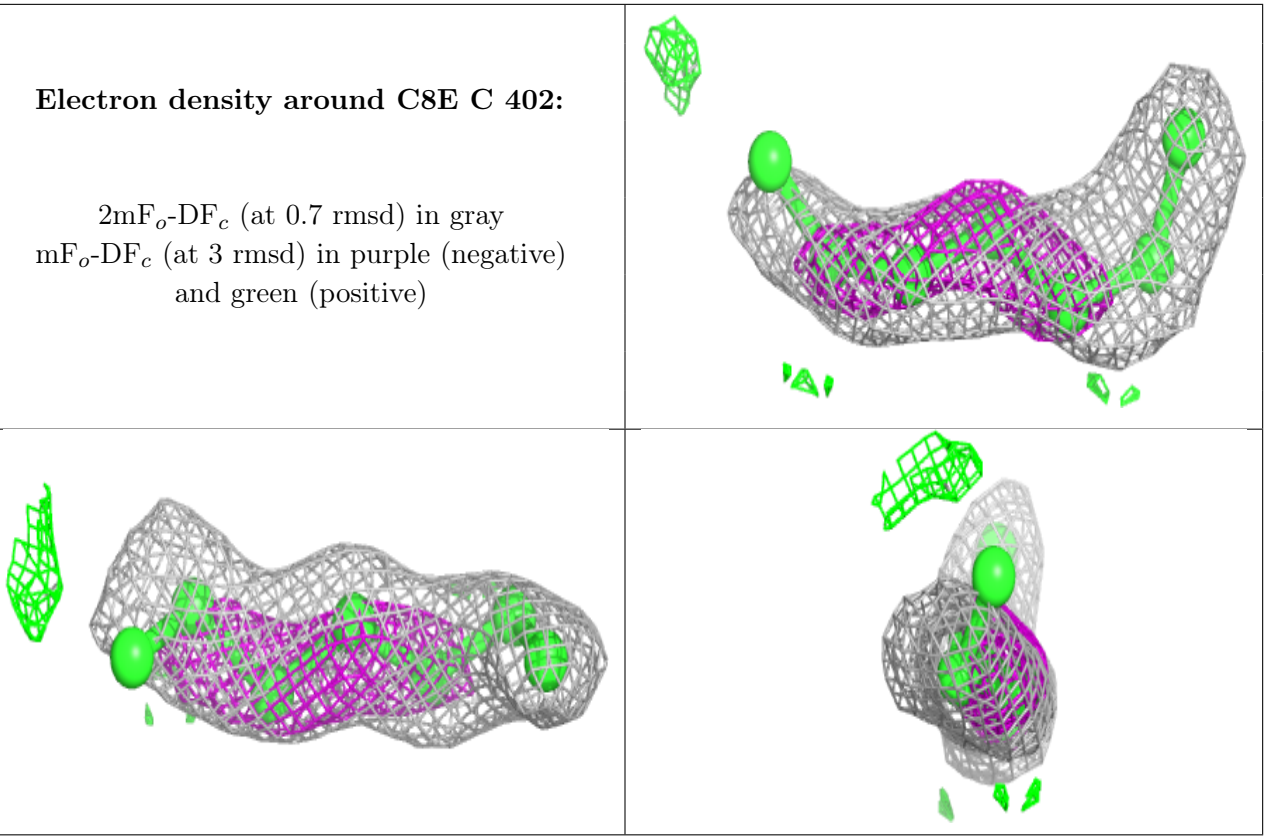
Electron density around C8E B 401:

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



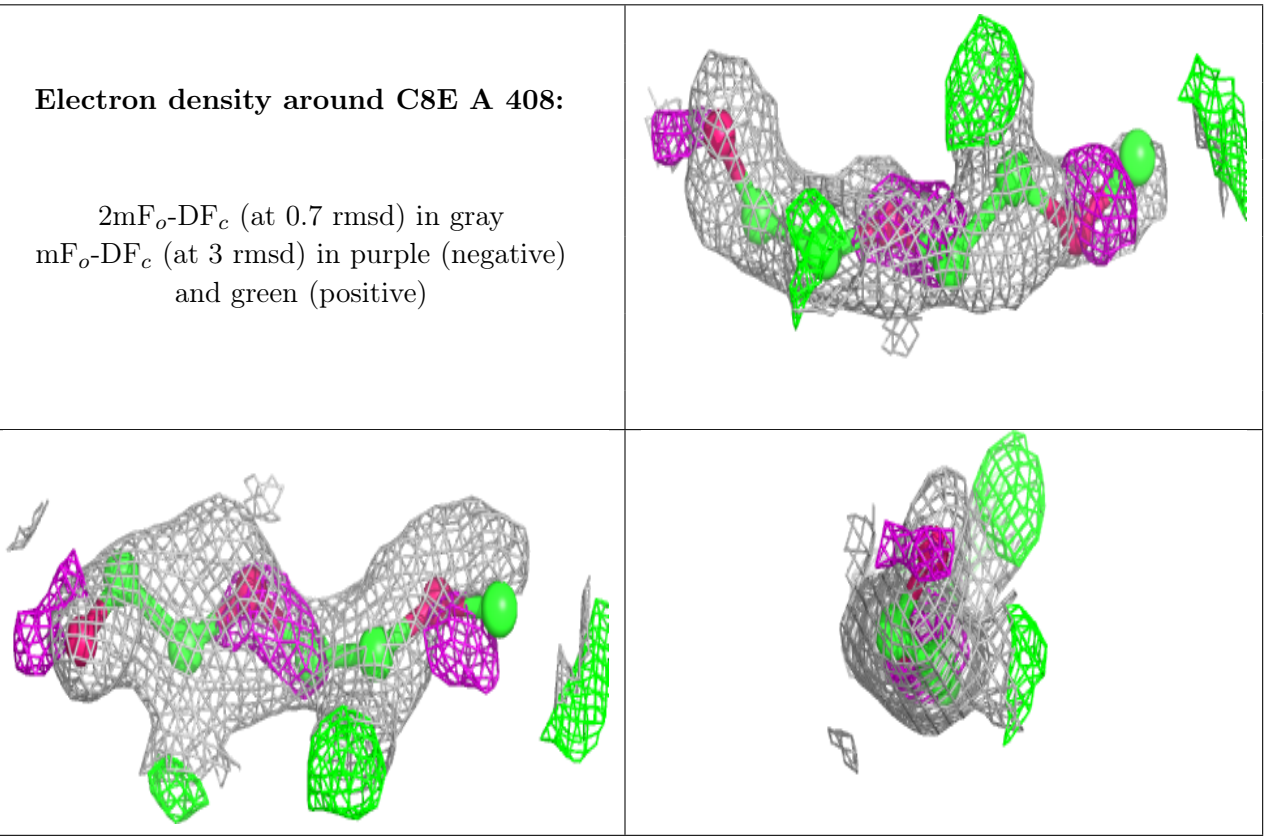
Electron density around C8E C 402:

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



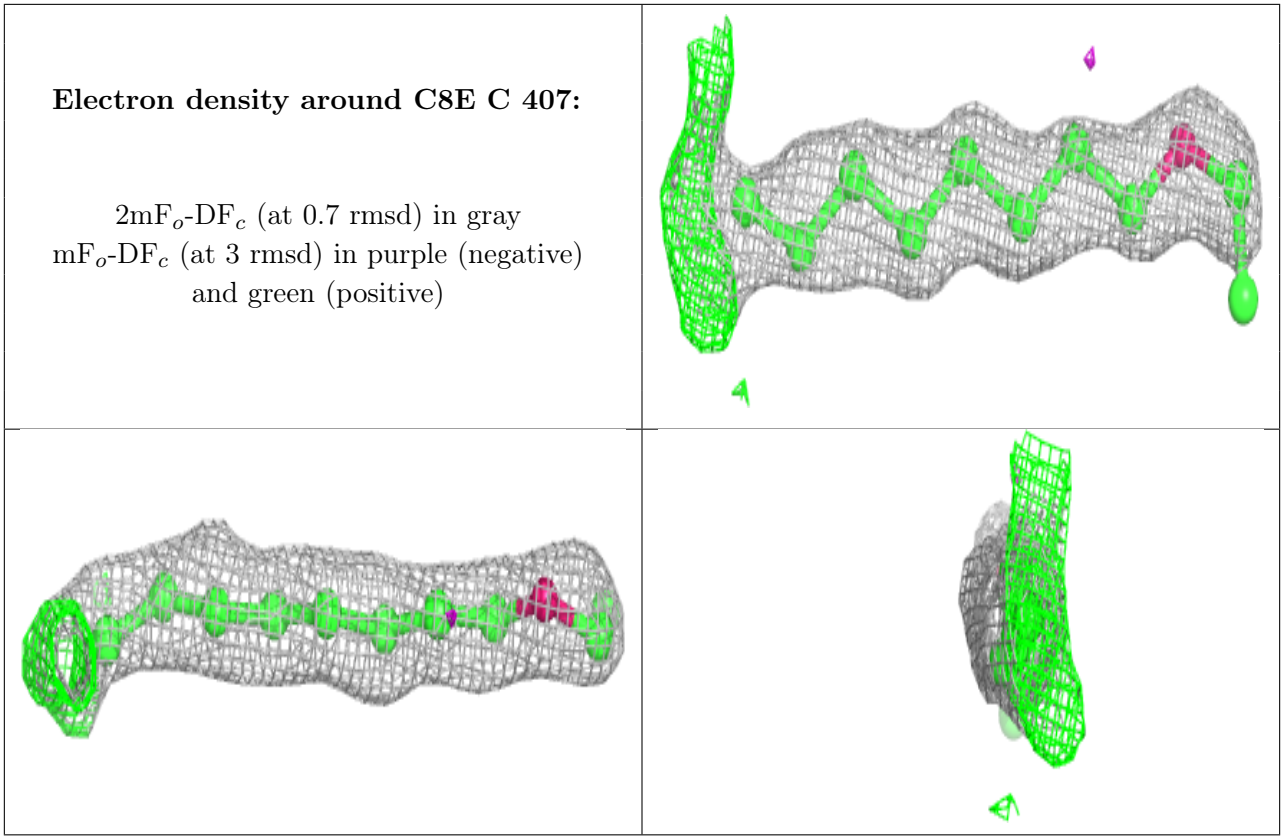
Electron density around C8E A 408:

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



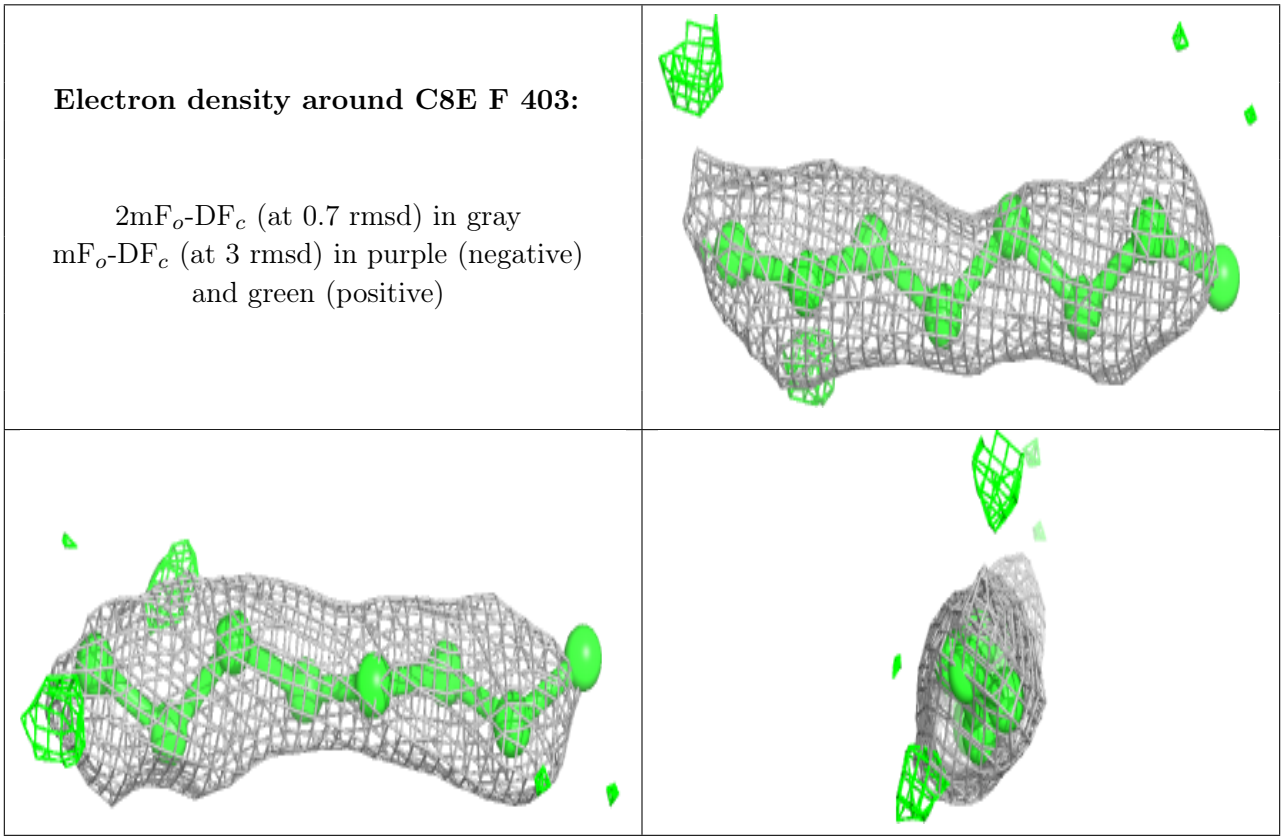
Electron density around C8E C 407:

$2mF_o$-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.