



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2024 – 12:05 PM EDT

PDB ID : 5W7B  
Title : Rabbit acyloxyacyl hydrolase (AOAH), proteolytically processed, S262A mutant, with LPS  
Authors : Gorelik, A.; Illes, K.; Nagar, B.  
Deposited on : 2017-06-19  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

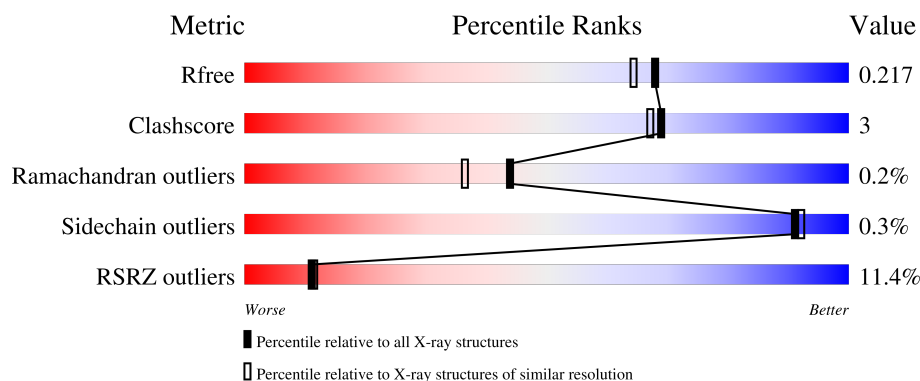
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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.






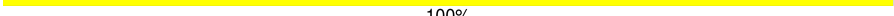
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	141	<div> <div>18%</div> <div>62%</div> <div>33%</div> </div>
1	B	141	<div> <div>26%</div> <div>59%</div> <div>6%</div> <div>34%</div> </div>
2	C	422	<div> <div>6%</div> <div>90%</div> <div>7%</div> </div>
2	D	422	<div> <div>6%</div> <div>90%</div> <div>8%</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	I	2	 100%
4	F	3	 100%
4	J	3	 33%  67%
5	G	3	 100%
5	K	3	 100%
6	H	2	 50%  50%
6	L	2	 100%

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 18101 atoms, of which 8794 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 Acyloxyacyl hydrolase small subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	94	Total	C	H	N	O	S	0	0	0
			1465	476	724	120	135	10			
1	B	93	Total	C	H	N	O	S	0	0	0
			1443	470	711	118	134	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASP	-	expression tag	UNP O18823
A	14	ARG	-	expression tag	UNP O18823
A	15	HIS	-	expression tag	UNP O18823
A	16	HIS	-	expression tag	UNP O18823
A	17	HIS	-	expression tag	UNP O18823
A	18	HIS	-	expression tag	UNP O18823
A	19	HIS	-	expression tag	UNP O18823
A	20	HIS	-	expression tag	UNP O18823
A	21	LYS	-	expression tag	UNP O18823
A	22	LEU	-	expression tag	UNP O18823
B	13	ASP	-	expression tag	UNP O18823
B	14	ARG	-	expression tag	UNP O18823
B	15	HIS	-	expression tag	UNP O18823
B	16	HIS	-	expression tag	UNP O18823
B	17	HIS	-	expression tag	UNP O18823
B	18	HIS	-	expression tag	UNP O18823
B	19	HIS	-	expression tag	UNP O18823
B	20	HIS	-	expression tag	UNP O18823
B	21	LYS	-	expression tag	UNP O18823
B	22	LEU	-	expression tag	UNP O18823

- Molecule 2 is a protein called Acyloxyacyl hydrolase large subunit.



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	413	Total	C	H	N	O	S	0	6	0
			6564	2114	3235	586	613	16			
2	D	412	Total	C	H	N	O	S	0	7	0
			6564	2118	3235	585	610	16			

There are 2 discrepancies between the modelled and reference sequences:

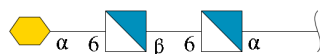
Chain	Residue	Modelled	Actual	Comment	Reference
C	262	ALA	SER	engineered mutation	UNP O18823
D	262	ALA	SER	engineered mutation	UNP O18823

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



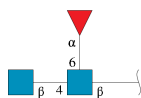
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	2	Total	C	H	N	O		0	0	0
			48	14	24	1	9				
3	I	2	Total	C	H	N	O		0	0	0
			48	14	24	1	9				

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	3	Total	C	H	N	O		0	0	0
			67	20	30	2	15				
4	J	3	Total	C	H	N	O		0	0	0
			67	20	30	2	15				

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



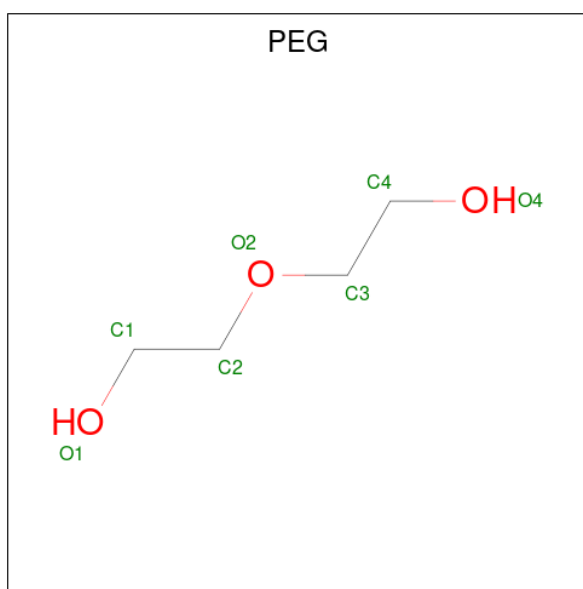
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			
5	K	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
6	L	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



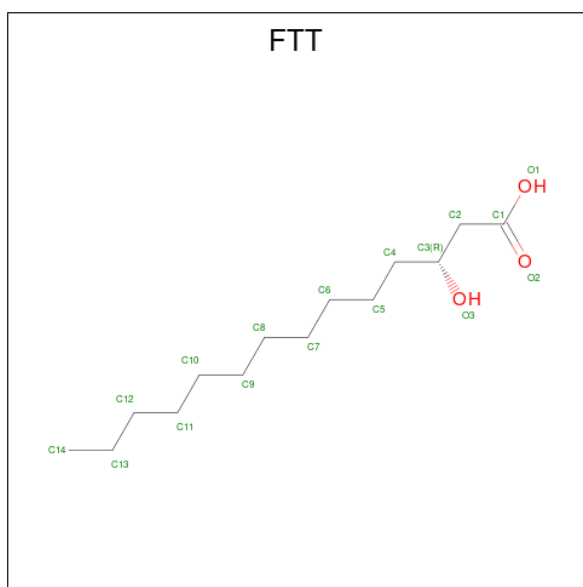
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			17	4	10	3		
7	A	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	D	1	Total	C	H	O	0	0
			17	4	10	3		
7	D	1	Total	C	H	O	0	0
			17	4	10	3		
7	D	1	Total	C	H	O	0	0
			17	4	10	3		
7	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



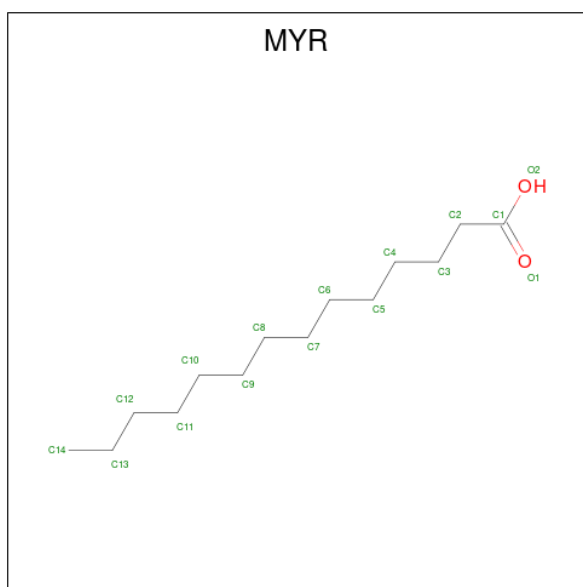
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			24	6	14	4		
8	C	1	Total	C	H	O	0	0
			24	6	14	4		
8	C	1	Total	C	H	O	0	0
			24	6	14	4		
8	C	1	Total	C	H	O	0	0
			24	6	14	4		
8	D	1	Total	C	H	O	0	0
			24	6	14	4		
8	D	1	Total	C	H	O	0	0
			24	6	14	4		
8	D	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 9 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula:  $C_{14}H_{28}O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			42	14	26	2		
9	C	1	Total	C	H	O	0	0
			43	14	27	2		
9	C	1	Total	C	H	O	0	0
			43	14	27	2		
9	B	1	Total	C	H	O	0	0
			42	14	26	2		
9	D	1	Total	C	H	O	0	0
			43	14	27	2		
9	D	1	Total	C	H	O	0	0
			43	14	27	2		

- Molecule 10 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			43	14	27	2		
10	C	1	Total	C	H	O	0	0
			42	14	27	1		
10	B	1	Total	C	H	O	0	0
			43	14	27	2		
10	D	1	Total	C	H	O	0	0
			42	14	27	1		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

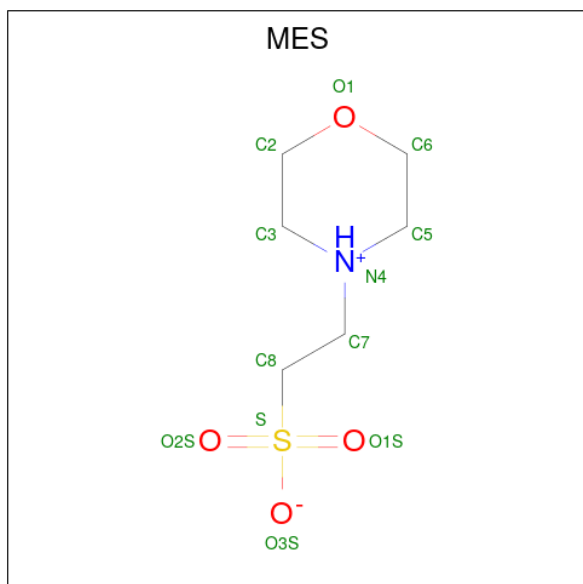
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	3	Total	Ca	0	0
			3	3		
11	D	3	Total	Ca	0	0
			3	3		

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 13 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ) (labeled as "Ligand of Interest" by depositor).



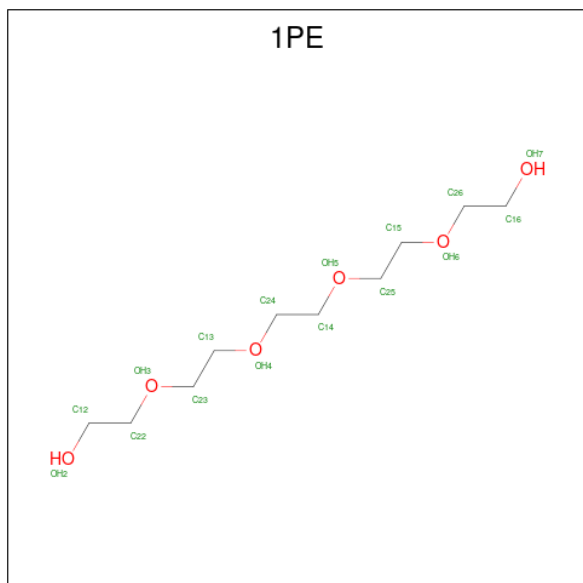
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	C	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
13	D	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

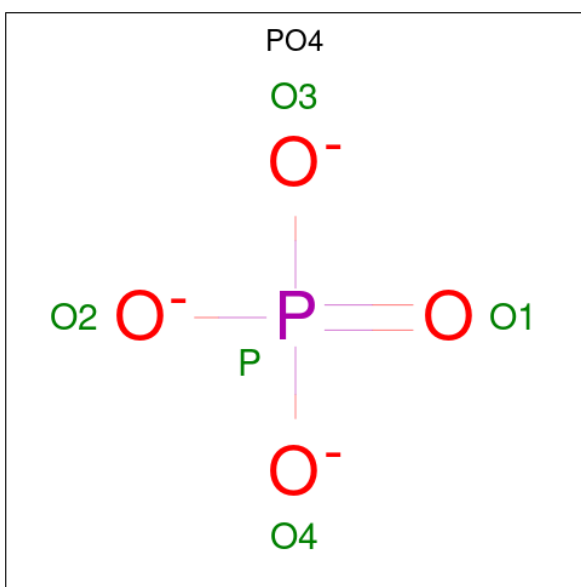
- Molecule 14 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	H	O	0	0
			38	10	22	6		
14	C	1	Total	C	H	O	0	0
			38	10	22	6		
14	D	1	Total	C	H	O	0	0
			38	10	22	6		
14	D	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 15 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



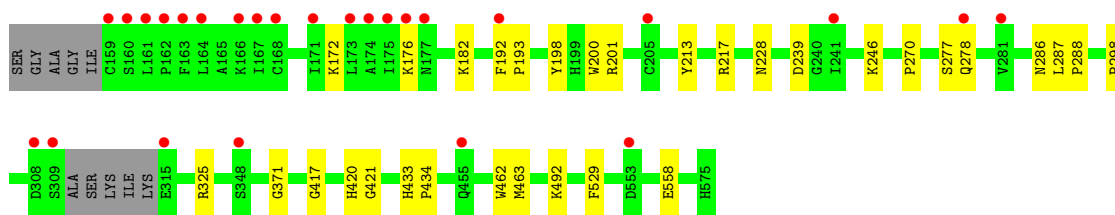


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	O	P	0	0
			5	4	1		
15	C	1	Total	O	P	0	0
			4	3	1		
15	D	1	Total	O	P	0	0
			5	4	1		
15	D	1	Total	O	P	0	0
			4	3	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	24	Total	O	0	0
			24	24		
16	C	236	Total	O	0	0
			236	236		
16	B	17	Total	O	0	0
			17	17		
16	D	171	Total	O	0	0
			171	171		





- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



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

Chain F: 100%



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

Chain J: 33% 67%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%




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

Chain H:  50% 50%

MAG1  
MAG2

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

Chain L:  100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.52Å 138.81Å 89.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 – 1.90 44.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	64.4 (44.77-1.90) 81.1 (44.77-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.185 , 0.213 0.186 , 0.217	Depositor DCC
$R_{free}$ test set	1912 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3851e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FTT, KDO, CA, MYR, SO4, PGE, MES, NAG, PO4, 1PE, PA1, PEG, GCS, FUC

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	0.31	0/759	0.48	0/1034
1	B	0.29	0/750	0.48	0/1023
2	C	0.31	0/3435	0.53	0/4663
2	D	0.30	0/3439	0.52	0/4669
All	All	0.30	0/8383	0.52	0/11389

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	741	724	724	3	0
1	B	732	711	711	8	0
2	C	3329	3235	3247	25	0
2	D	3329	3235	3249	23	0
3	E	24	24	22	0	0
3	I	24	24	22	0	0
4	F	37	30	26	0	0
4	J	37	30	26	2	0
5	G	38	37	34	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	38	37	34	0	0
6	H	28	27	25	0	0
6	L	28	27	25	0	0
7	A	14	20	20	0	0
7	C	70	100	100	5	0
7	D	28	40	40	6	0
8	A	10	14	14	0	0
8	C	30	42	42	0	0
8	D	30	42	42	1	0
9	A	16	26	26	0	0
9	B	16	26	26	0	0
9	C	32	54	54	0	0
9	D	32	54	54	0	0
10	A	16	27	27	0	0
10	B	16	27	27	0	0
10	C	15	27	27	0	0
10	D	15	27	27	0	0
11	C	3	0	0	0	0
11	D	3	0	0	0	0
12	C	5	0	0	0	0
12	D	5	0	0	0	0
13	B	12	13	12	0	0
13	C	12	13	12	0	0
13	D	12	13	12	1	0
14	C	32	44	44	1	0
14	D	32	44	44	1	0
15	C	9	0	0	0	0
15	D	9	0	0	1	0
16	A	24	0	0	0	1
16	B	17	0	0	1	0
16	C	236	0	0	3	1
16	D	171	0	0	3	0
All	All	9307	8794	8795	60	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 60 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)
2:C:281:VAL:O	16:C:701:HOH:O	1.98	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:LYS:NZ	16:D:701:HOH:O	2.22	0.72
2:C:172:LYS:O	2:C:176:LYS:HG3	1.98	0.63
1:B:77:VAL:HG12	1:B:77:VAL:O	2.01	0.59
1:A:77:VAL:HG12	1:A:77:VAL:O	2.05	0.56

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:306:HOH:O	16:C:828:HOH:O[4_454]	2.02	0.18

## 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	92/141 (65%)	88 (96%)	4 (4%)	0	100	100
1	B	91/141 (64%)	89 (98%)	2 (2%)	0	100	100
2	C	415/422 (98%)	402 (97%)	12 (3%)	1 (0%)	44	36
2	D	415/422 (98%)	396 (95%)	18 (4%)	1 (0%)	44	36
All	All	1013/1126 (90%)	975 (96%)	36 (4%)	2 (0%)	44	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	371	GLY
2	C	371	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	86/130 (66%)	85 (99%)	1 (1%)	67	68
1	B	85/130 (65%)	84 (99%)	1 (1%)	67	68
2	C	366/366 (100%)	365 (100%)	1 (0%)	91	92
2	D	366/366 (100%)	366 (100%)	0	100	100
All	All	903/992 (91%)	900 (100%)	3 (0%)	91	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
2	C	224	HIS
1	B	70	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
2	C	224	HIS

### 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](#)

20 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
3	NAG	E	1	3,1	14,14,15	0.99	1 (7%)	17,19,21	0.81	1 (5%)
3	FUC	E	2	3	10,10,11	0.84	0	14,14,16	0.81	0
4	PA1	F	1	4,15,9	11,11,12	1.62	3 (27%)	13,15,17	1.14	0
4	GCS	F	2	4,9,15	11,11,12	1.74	2 (18%)	13,15,17	0.91	0
4	KDO	F	3	4	15,15,16	1.62	3 (20%)	17,21,24	2.36	4 (23%)
5	NAG	G	1	2,5	14,14,15	0.81	1 (7%)	17,19,21	0.53	0
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	1.20	3 (17%)
5	FUC	G	3	5	10,10,11	0.91	1 (10%)	14,14,16	0.66	0
6	NAG	H	1	2,6	14,14,15	0.44	0	17,19,21	0.51	0
6	NAG	H	2	6	14,14,15	1.11	1 (7%)	17,19,21	1.37	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.31	0	17,19,21	0.40	0
3	FUC	I	2	3	10,10,11	0.72	0	14,14,16	0.77	0
4	PA1	J	1	4,15,9	11,11,12	1.69	3 (27%)	13,15,17	1.18	1 (7%)
4	GCS	J	2	4,9,15	11,11,12	1.77	3 (27%)	13,15,17	1.75	4 (30%)
4	KDO	J	3	4	15,15,16	1.32	2 (13%)	17,21,24	2.18	5 (29%)
5	NAG	K	1	2,5	14,14,15	0.53	0	17,19,21	0.45	0
5	NAG	K	2	5	14,14,15	0.20	0	17,19,21	0.61	0
5	FUC	K	3	5	10,10,11	0.61	0	14,14,16	0.89	0
6	NAG	L	1	2,6	14,14,15	0.23	0	17,19,21	0.85	1 (5%)
6	NAG	L	2	6	14,14,15	0.48	0	17,19,21	1.27	1 (5%)

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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
4	PA1	F	1	4,15,9	-	0/2/19/22	0/1/1/1
4	GCS	F	2	4,9,15	-	0/2/19/22	0/1/1/1
4	KDO	F	3	4	-	0/10/26/30	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
6	NAG	H	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	I	2	3	-	-	0/1/1/1
4	PA1	J	1	4,15,9	-	0/2/19/22	0/1/1/1
4	GCS	J	2	4,9,15	-	0/2/19/22	0/1/1/1
4	KDO	J	3	4	-	3/10/26/30	0/1/1/1
5	NAG	K	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	FUC	K	3	5	-	-	0/1/1/1
6	NAG	L	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	GCS	O5-C1	4.29	1.50	1.43
4	J	1	PA1	O5-C1	4.19	1.50	1.43
4	J	2	GCS	O5-C1	4.05	1.50	1.43
4	F	1	PA1	O5-C1	3.96	1.50	1.43
6	H	2	NAG	O5-C1	-3.93	1.37	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	KDO	O6-C6-C5	7.23	118.16	107.94
4	J	3	KDO	O6-C2-C1	5.04	117.24	107.72
6	H	2	NAG	C3-C4-C5	4.10	117.66	110.23
4	F	3	KDO	O6-C2-C3	4.00	115.93	110.56
6	L	2	NAG	C1-O5-C5	3.82	117.30	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

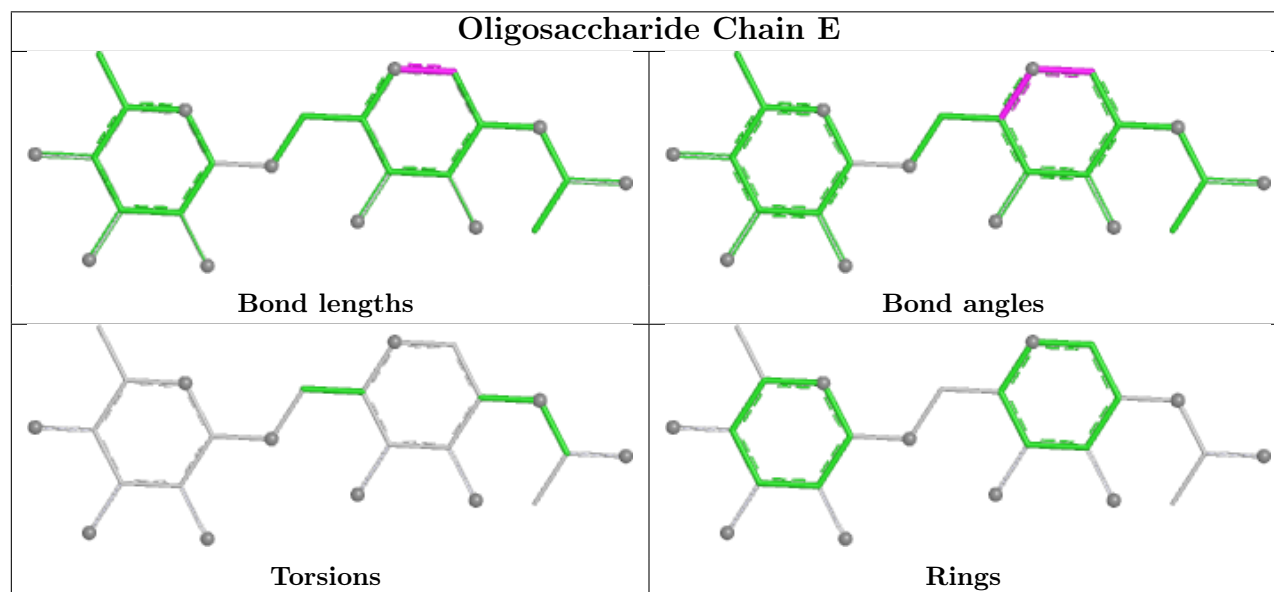
Mol	Chain	Res	Type	Atoms
6	L	1	NAG	O5-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
4	J	3	KDO	C5-C6-C7-C8

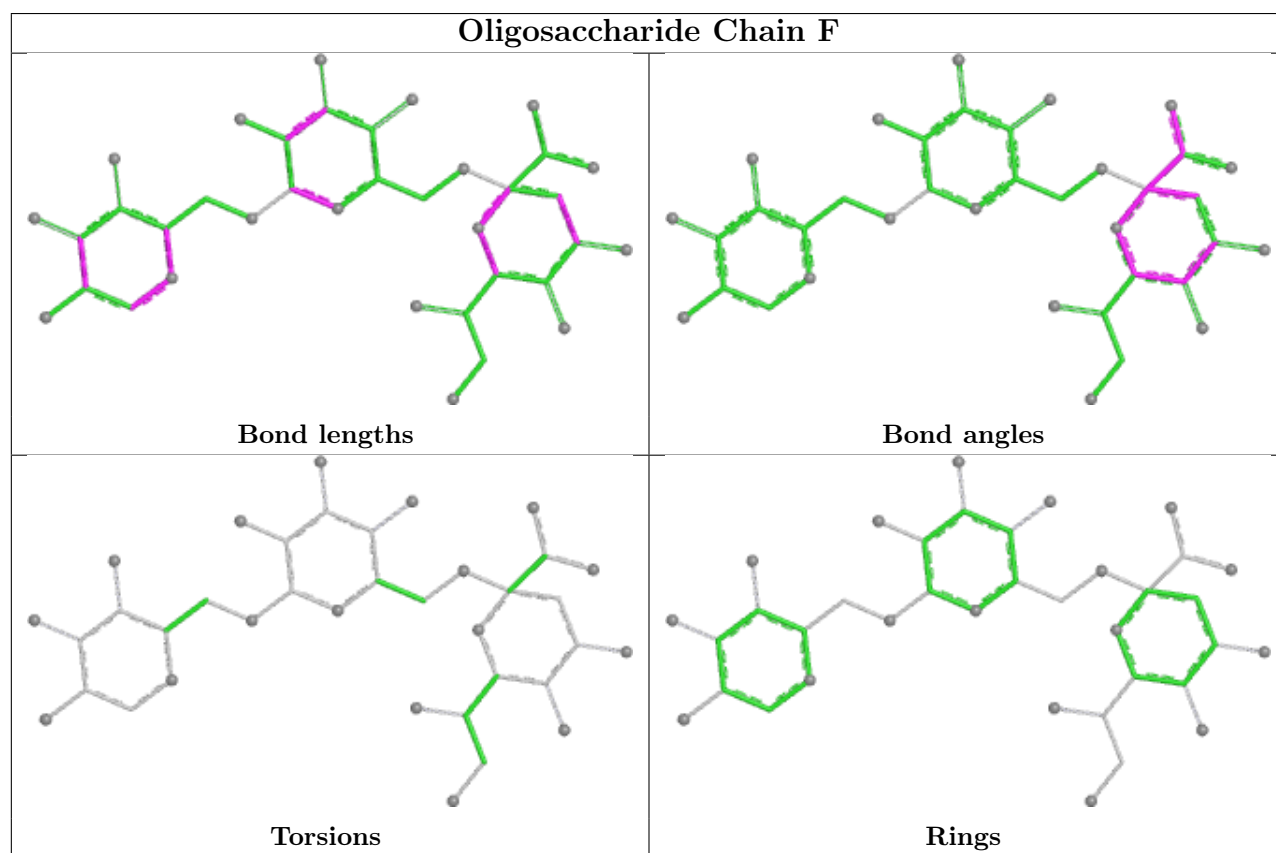
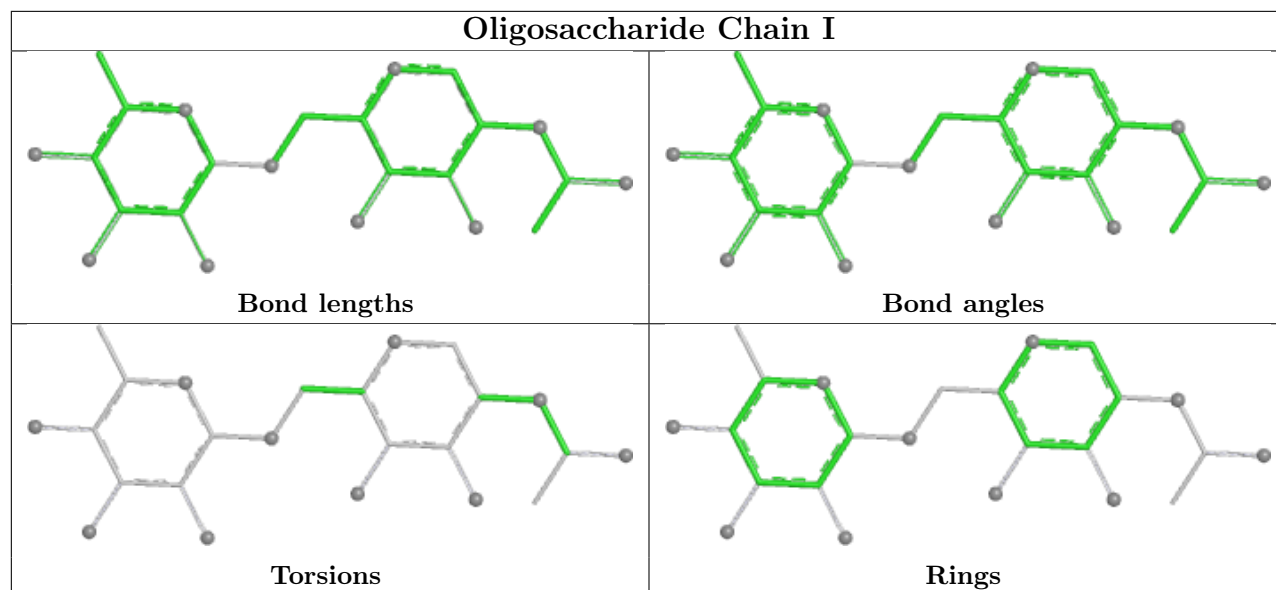
There are no ring outliers.

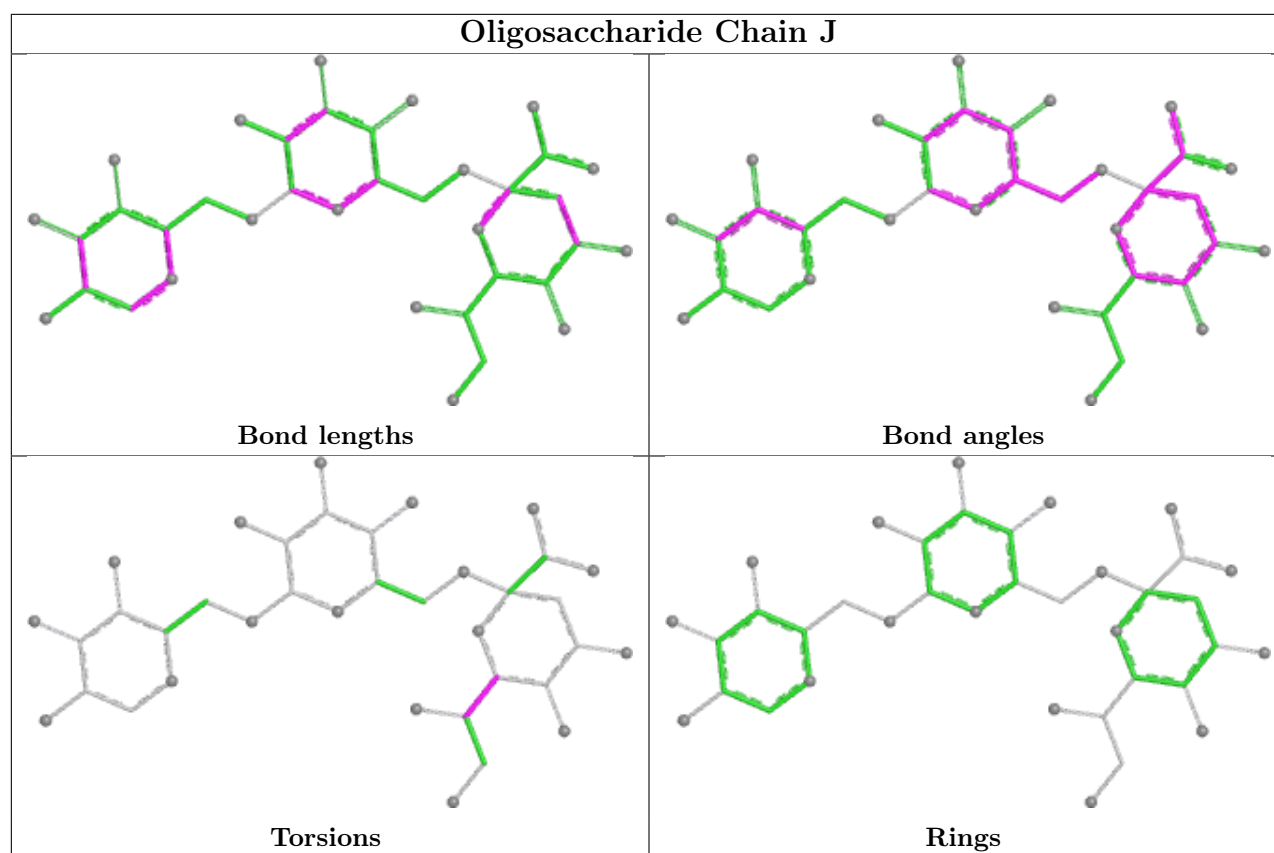
2 monomers are involved in 2 short contacts:

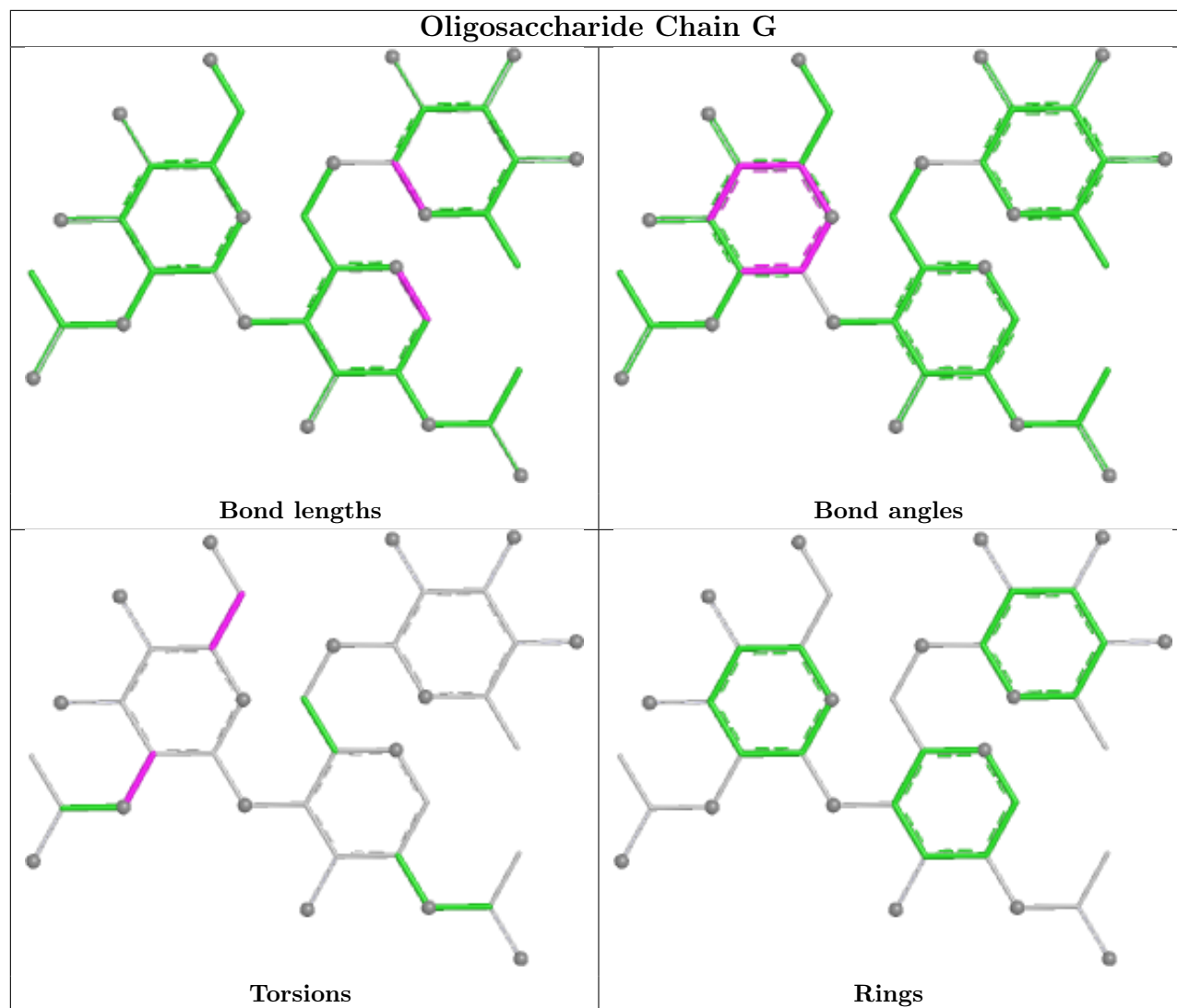
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	3	KDO	1	0
4	J	2	GCS	1	0

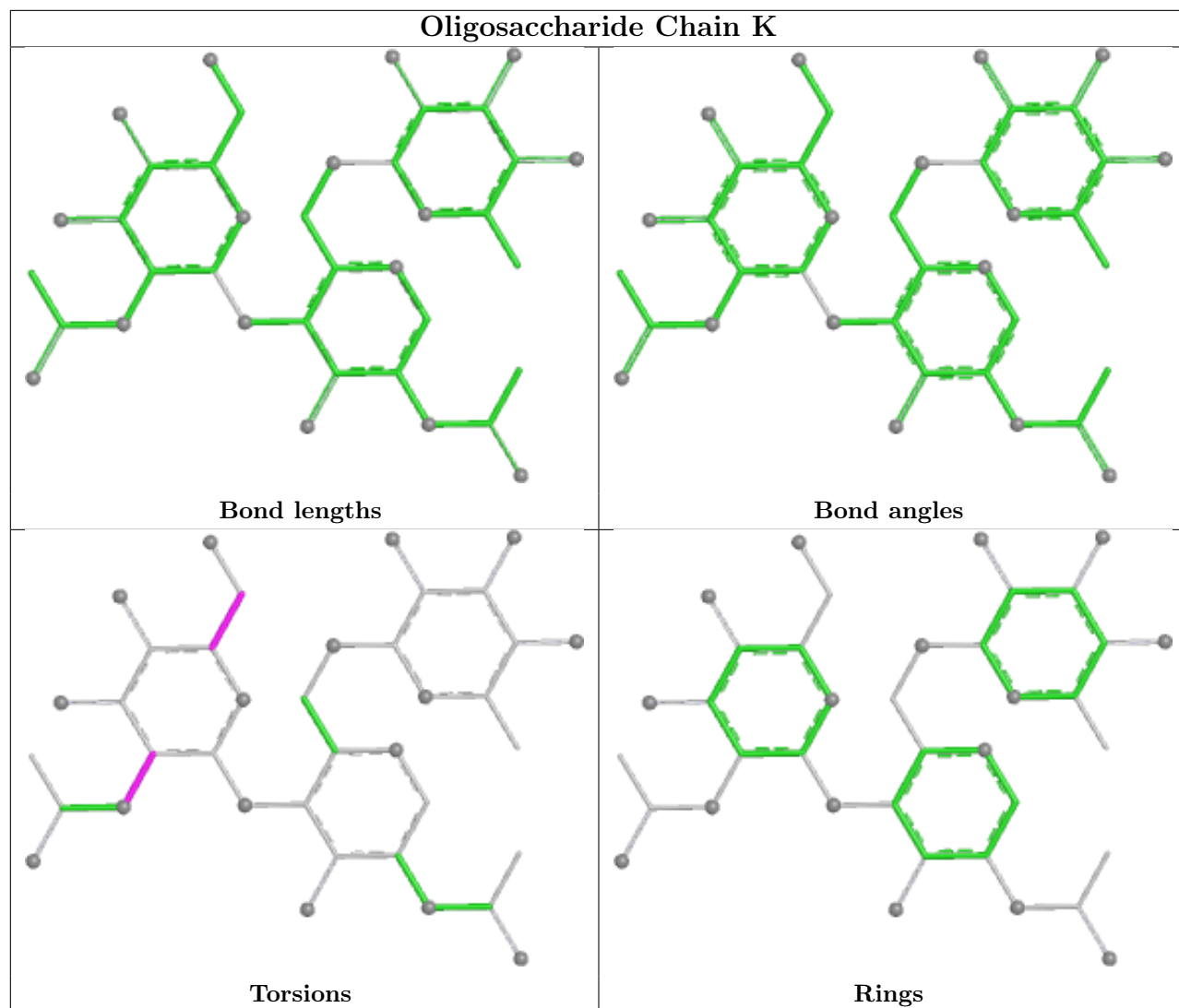
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



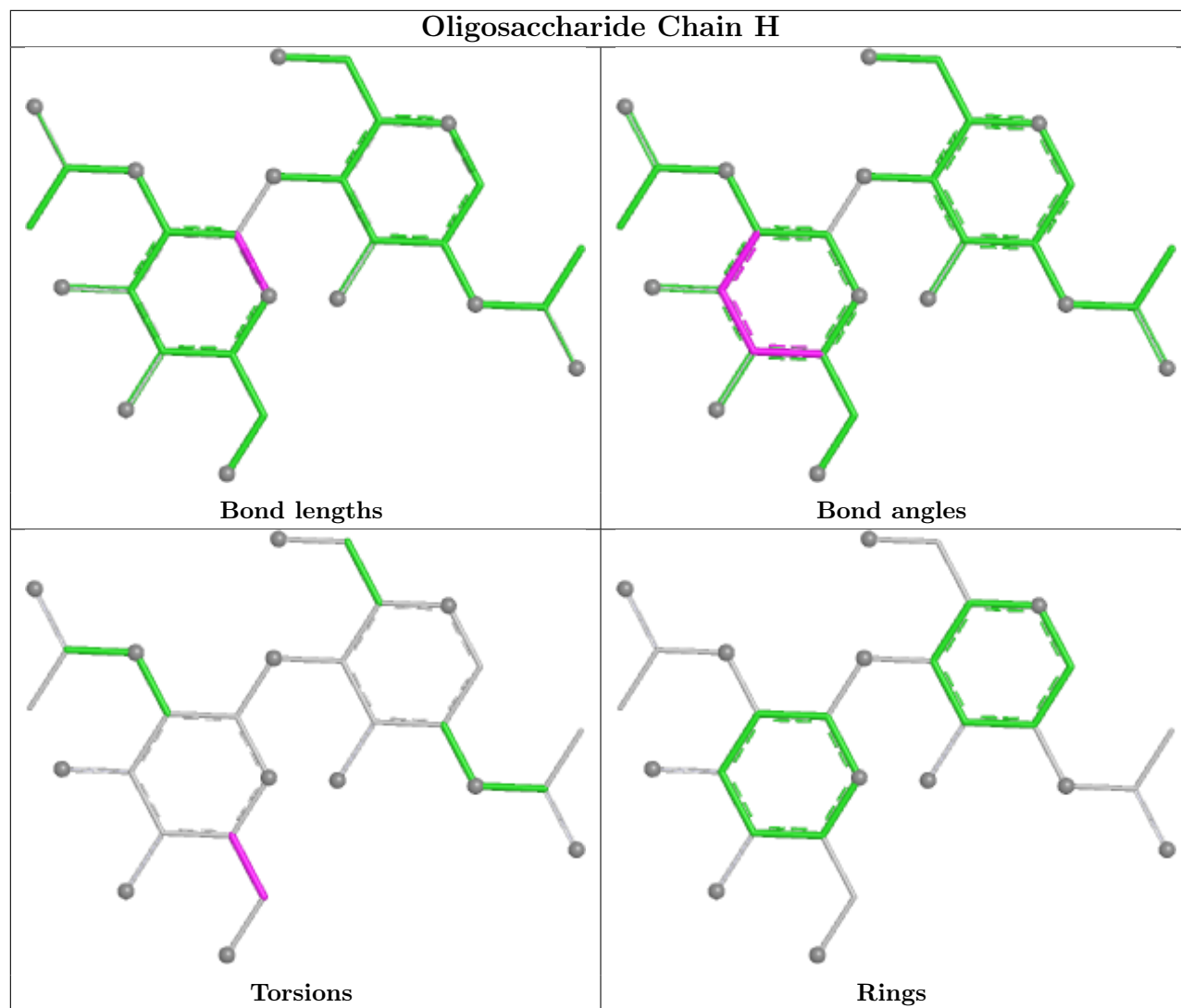


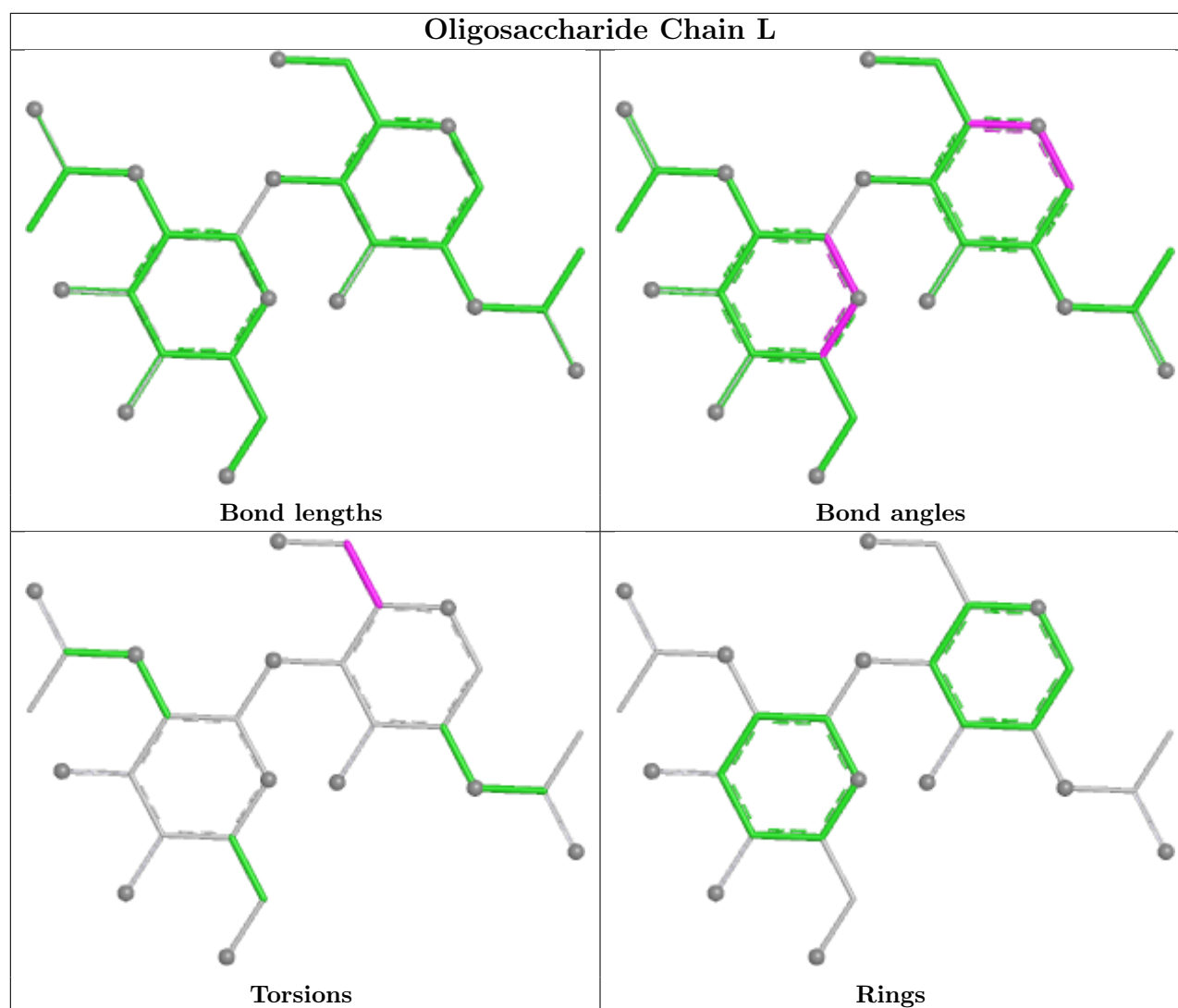












## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 6 are monoatomic - leaving 46 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	$\# Z  > 2$
9	FTT	D	623	4	14,15,16	0.50	0	15,15,17	1.33	2 (13%)
7	PEG	C	611	-	6,6,6	0.49	0	5,5,5	0.48	0
15	PO4	C	627	4	0,3,4	-	-	0,3,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PEG	C	615	-	6,6,6	0.52	0	5,5,5	0.28	0
13	MES	C	610	-	12,12,12	2.21	1 (8%)	15,16,16	1.69	5 (33%)
7	PEG	D	612	-	6,6,6	0.48	0	5,5,5	0.24	0
13	MES	D	610	-	12,12,12	2.40	1 (8%)	15,16,16	1.47	1 (6%)
10	MYR	A	210	-	15,15,15	0.56	0	15,15,15	0.90	0
7	PEG	D	613	-	6,6,6	0.54	0	5,5,5	0.34	0
15	PO4	D	621	4	0,3,4	-	-	0,3,6	-	-
9	FTT	A	209	4,10	14,15,16	0.57	0	15,15,17	1.15	1 (6%)
10	MYR	C	630	9	13,14,15	0.33	0	12,13,15	0.66	0
15	PO4	D	620	4	4,4,4	0.98	0	6,6,6	0.46	0
7	PEG	C	613	-	6,6,6	0.47	0	5,5,5	0.59	0
7	PEG	C	612	-	6,6,6	0.49	0	5,5,5	0.36	0
7	PEG	C	618	-	6,6,6	0.52	0	5,5,5	0.38	0
7	PEG	C	617	-	6,6,6	0.48	0	5,5,5	0.30	0
7	PEG	A	203	-	6,6,6	0.49	0	5,5,5	0.45	0
8	PGE	D	616	-	9,9,9	0.31	0	8,8,8	0.31	0
9	FTT	C	628	4	14,15,16	0.60	0	15,15,17	0.90	0
9	FTT	D	622	4	14,15,16	0.64	0	15,15,17	0.86	0
9	FTT	C	629	4	14,15,16	0.60	0	15,15,17	1.20	2 (13%)
8	PGE	D	615	-	9,9,9	0.31	0	8,8,8	0.25	0
14	1PE	C	625	-	15,15,15	0.55	0	14,14,14	0.43	0
13	MES	B	203	-	12,12,12	2.33	1 (8%)	15,16,16	1.50	2 (13%)
12	SO4	C	609	-	4,4,4	0.24	0	6,6,6	0.10	0
10	MYR	B	208	-	15,15,15	0.56	0	15,15,15	1.01	1 (6%)
14	1PE	C	624	-	15,15,15	0.55	0	14,14,14	0.45	0
7	PEG	C	619	-	6,6,6	0.52	0	5,5,5	1.01	0
8	PGE	A	205	-	9,9,9	0.33	0	8,8,8	0.33	0
7	PEG	A	204	-	6,6,6	0.45	0	5,5,5	0.44	0
8	PGE	C	623	-	9,9,9	0.36	0	8,8,8	0.48	0
7	PEG	C	620	-	6,6,6	0.45	0	5,5,5	0.48	0
8	PGE	C	621	-	9,9,9	0.32	0	8,8,8	0.39	0
7	PEG	C	614	-	6,6,6	0.48	0	5,5,5	0.36	0
14	1PE	D	618	-	15,15,15	0.53	0	14,14,14	0.33	0
9	FTT	B	207	4,10	14,15,16	0.52	0	15,15,17	1.26	2 (13%)
15	PO4	C	626	4	4,4,4	0.94	0	6,6,6	0.59	0
12	SO4	D	609	-	4,4,4	0.24	0	6,6,6	0.07	0
7	PEG	D	611	-	6,6,6	0.49	0	5,5,5	0.36	0
10	MYR	D	624	9	13,14,15	0.39	0	12,13,15	0.71	0
8	PGE	D	617	-	9,9,9	0.31	0	8,8,8	0.45	0
7	PEG	D	614	-	6,6,6	0.50	0	5,5,5	0.43	0
8	PGE	C	622	-	9,9,9	0.32	0	8,8,8	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PEG	C	616	-	6,6,6	0.50	0	5,5,5	0.27	0
14	1PE	D	619	-	15,15,15	0.53	0	14,14,14	0.46	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	D	623	4	-	11/14/14/15	-
7	PEG	C	611	-	-	3/4/4/4	-
7	PEG	C	615	-	-	1/4/4/4	-
13	MES	C	610	-	-	0/6/14/14	0/1/1/1
7	PEG	D	612	-	-	2/4/4/4	-
13	MES	D	610	-	-	4/6/14/14	0/1/1/1
10	MYR	A	210	-	-	6/13/13/13	-
7	PEG	D	613	-	-	2/4/4/4	-
9	FTT	A	209	4,10	-	6/14/14/15	-
10	MYR	C	630	9	-	4/12/12/13	-
7	PEG	C	613	-	-	1/4/4/4	-
7	PEG	C	612	-	-	2/4/4/4	-
7	PEG	C	618	-	-	2/4/4/4	-
7	PEG	C	617	-	-	1/4/4/4	-
7	PEG	A	203	-	-	3/4/4/4	-
8	PGE	D	616	-	-	4/7/7/7	-
9	FTT	C	628	4	-	1/14/14/15	-
9	FTT	D	622	4	-	0/14/14/15	-
9	FTT	C	629	4	-	8/14/14/15	-
8	PGE	D	615	-	-	0/7/7/7	-
14	1PE	C	625	-	-	3/13/13/13	-
13	MES	B	203	-	-	3/6/14/14	0/1/1/1
10	MYR	B	208	-	-	3/13/13/13	-
14	1PE	C	624	-	-	4/13/13/13	-
7	PEG	C	619	-	-	2/4/4/4	-
8	PGE	A	205	-	-	6/7/7/7	-
7	PEG	A	204	-	-	1/4/4/4	-
8	PGE	C	623	-	-	3/7/7/7	-
7	PEG	C	620	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PGE	C	621	-	-	4/7/7/7	-
7	PEG	C	614	-	-	2/4/4/4	-
14	1PE	D	618	-	-	7/13/13/13	-
9	FTT	B	207	4,10	-	10/14/14/15	-
7	PEG	D	611	-	-	1/4/4/4	-
10	MYR	D	624	9	-	1/12/12/13	-
8	PGE	D	617	-	-	2/7/7/7	-
7	PEG	D	614	-	-	2/4/4/4	-
8	PGE	C	622	-	-	6/7/7/7	-
7	PEG	C	616	-	-	2/4/4/4	-
14	1PE	D	619	-	-	9/13/13/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	610	MES	C8-S	-8.08	1.66	1.77
13	B	203	MES	C8-S	-7.80	1.66	1.77
13	C	610	MES	C8-S	-7.36	1.67	1.77

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	203	MES	C5-N4-C3	4.31	118.12	108.84
13	D	610	MES	C5-N4-C3	3.60	116.60	108.84
13	C	610	MES	C5-N4-C3	3.17	115.67	108.84
9	D	623	FTT	C3-C2-C1	-2.92	107.73	112.70
9	C	629	FTT	C5-C4-C3	-2.86	106.81	114.68

There are no chirality outliers.

5 of 135 torsion outliers are listed below:

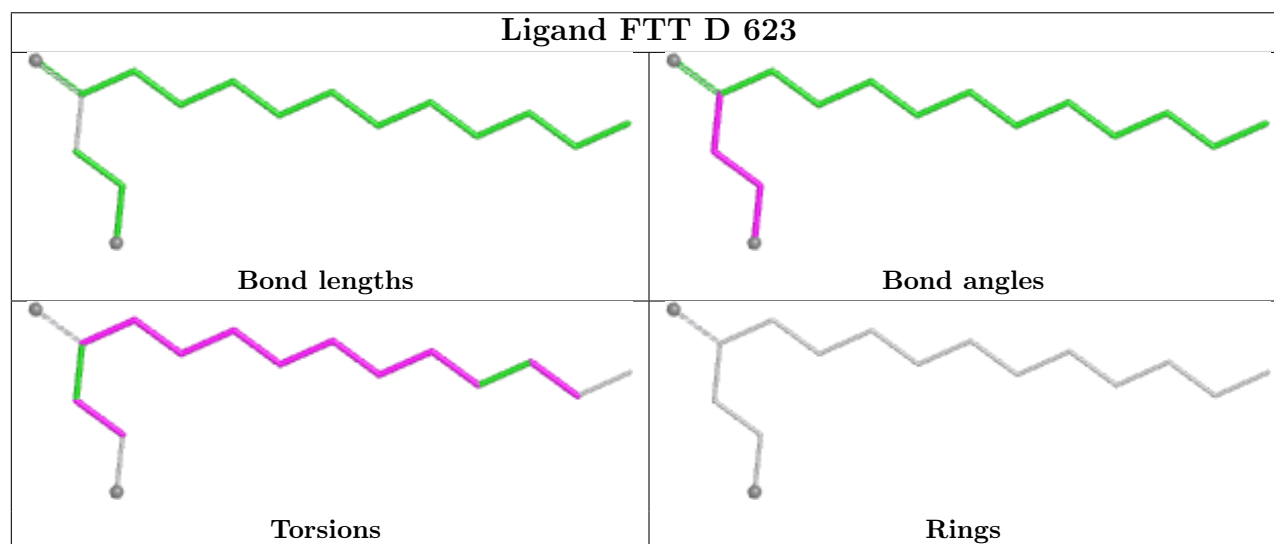
Mol	Chain	Res	Type	Atoms
9	A	209	FTT	O2-C1-C2-C3
9	C	629	FTT	C1-C2-C3-O3
9	B	207	FTT	O2-C1-C2-C3
9	B	207	FTT	C1-C2-C3-C4
9	B	207	FTT	C1-C2-C3-O3

There are no ring outliers.

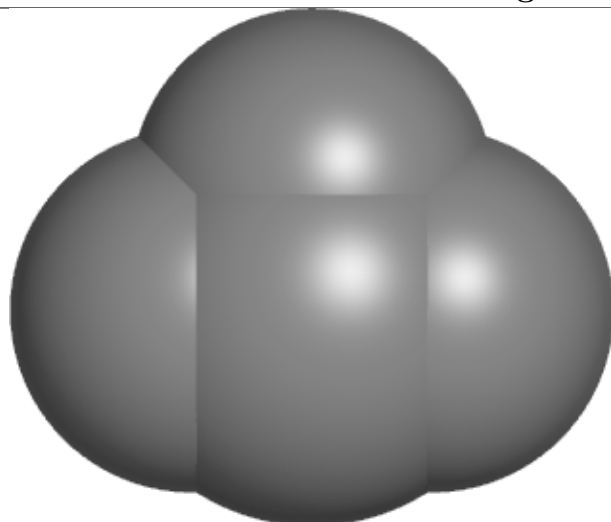
11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	612	PEG	1	0
13	D	610	MES	1	0
7	D	613	PEG	3	0
15	D	621	PO4	1	0
7	C	613	PEG	1	0
7	C	618	PEG	1	0
8	D	616	PGE	1	0
14	C	624	1PE	1	0
7	C	620	PEG	3	0
7	D	611	PEG	2	0
14	D	619	1PE	1	0

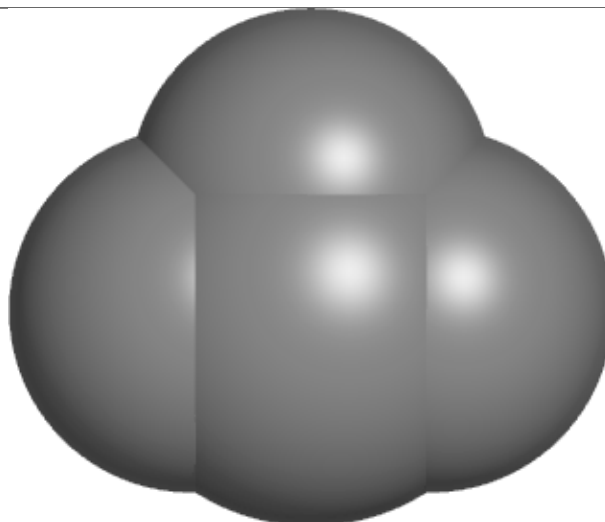
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



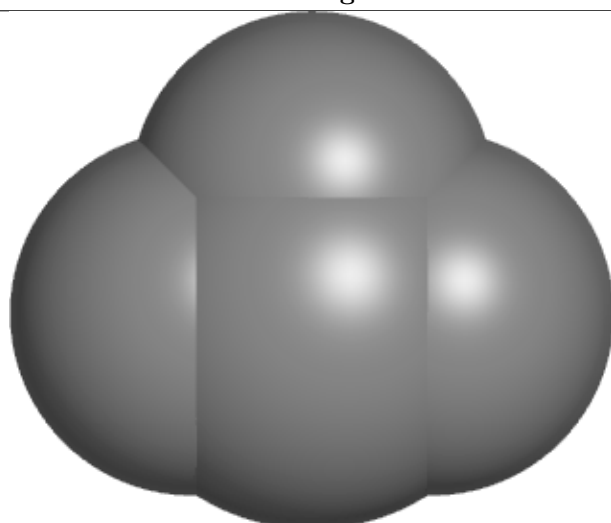
## Ligand PO4 C 627



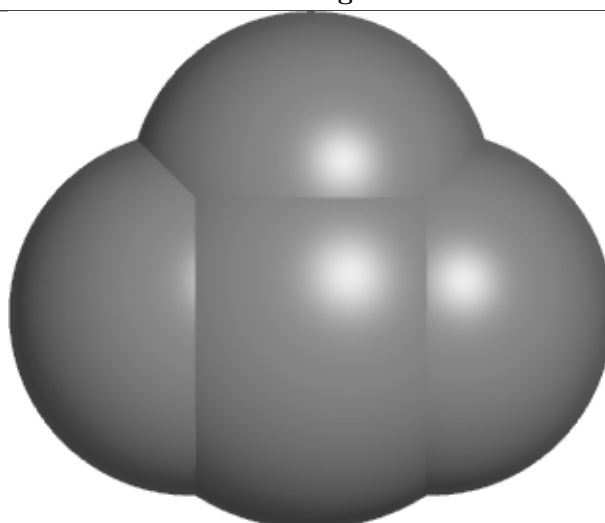
Bond lengths



Bond angles

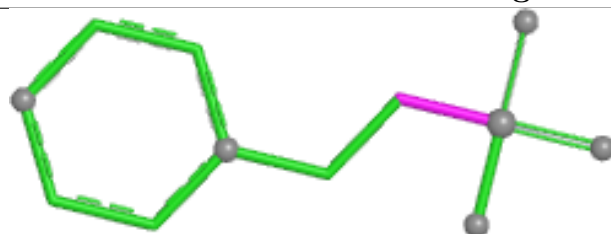


Torsions

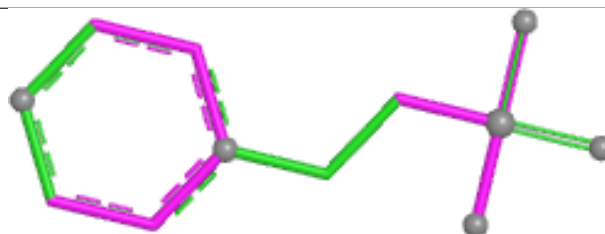


Rings

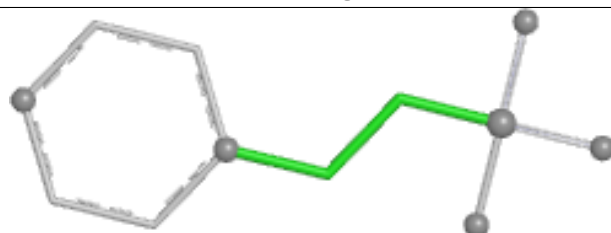
## Ligand MES C 610



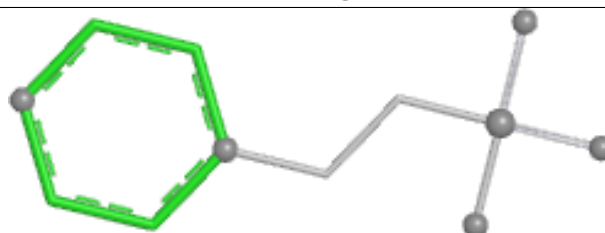
Bond lengths



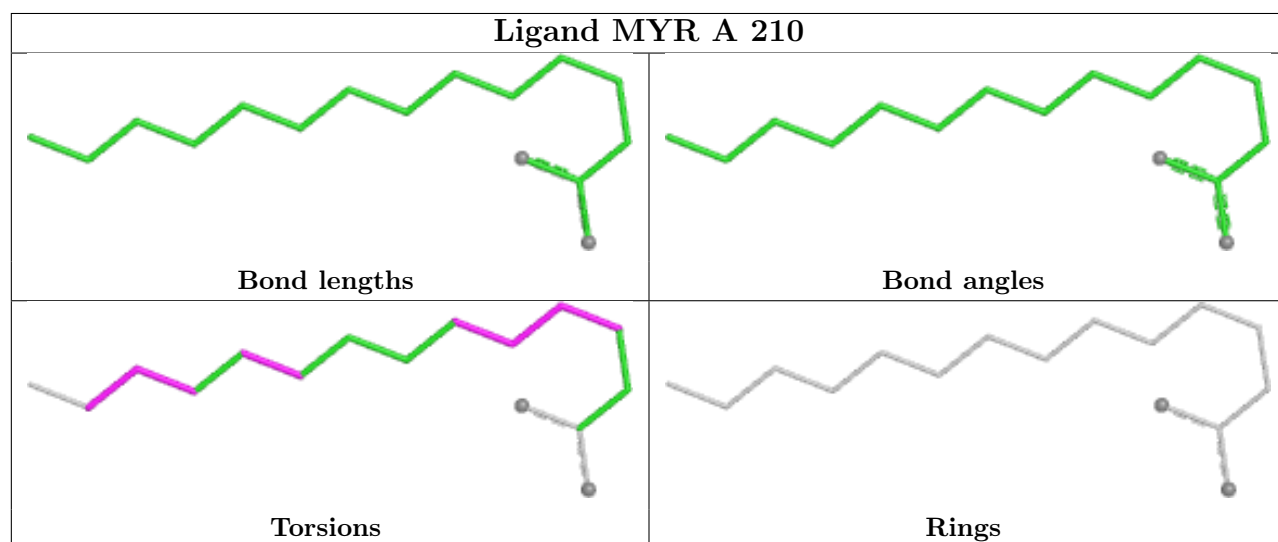
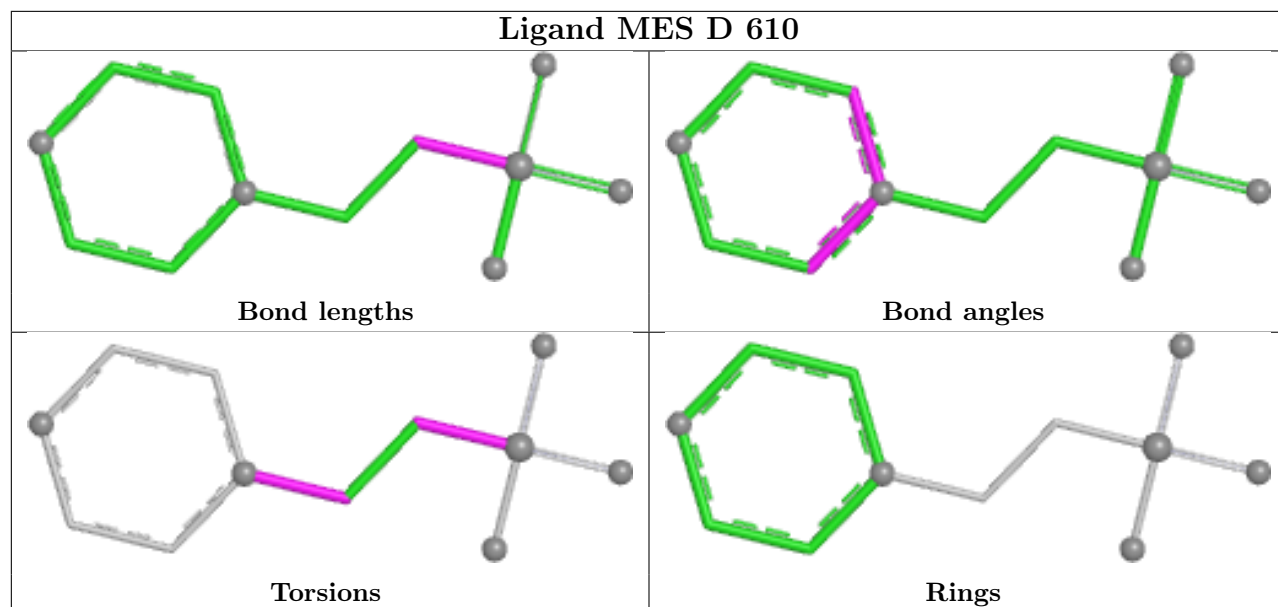
Bond angles



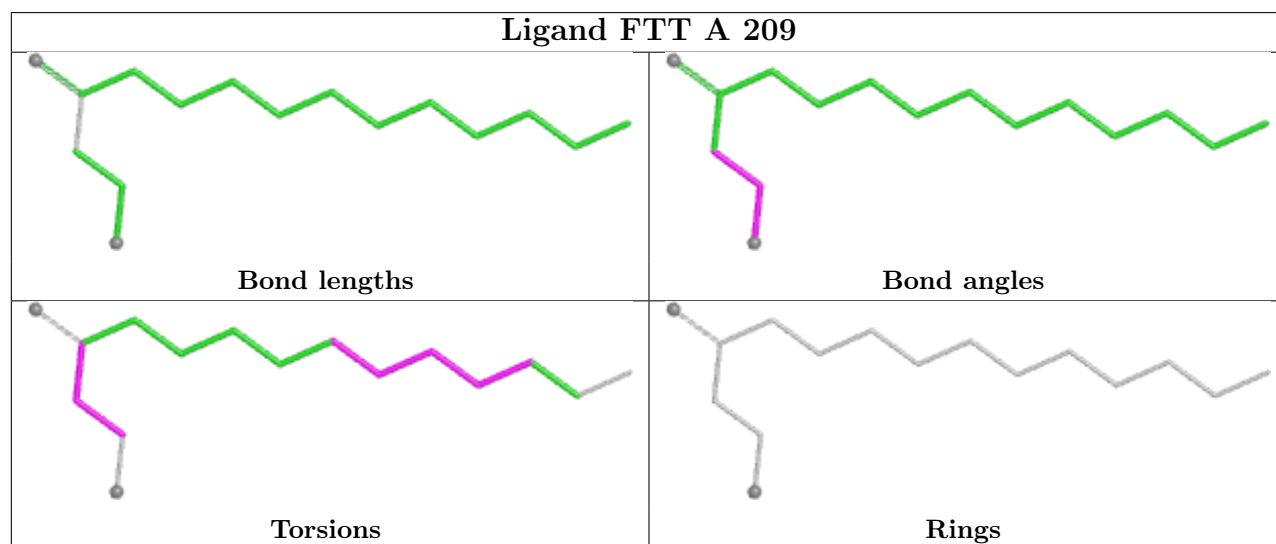
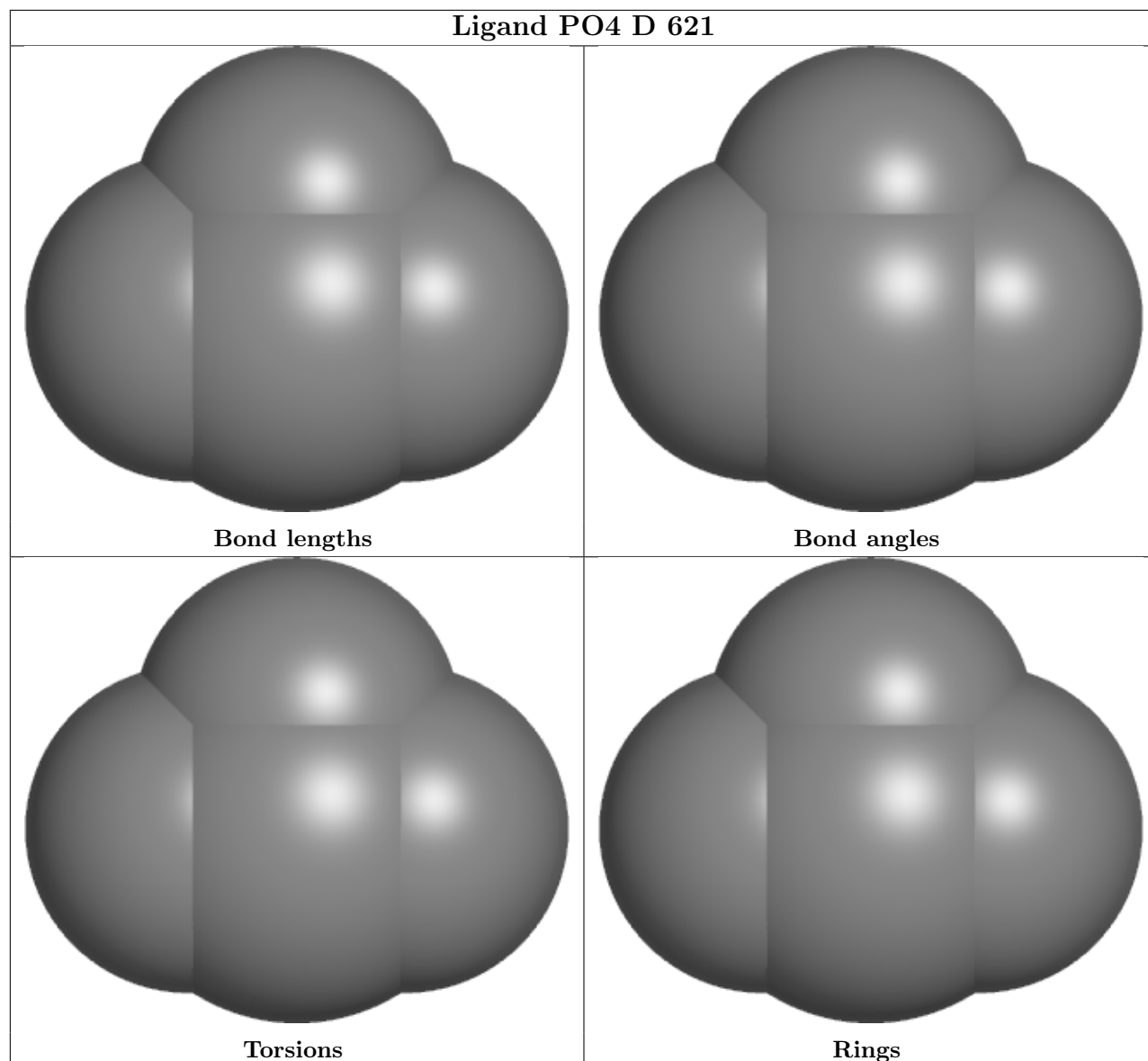
Torsions

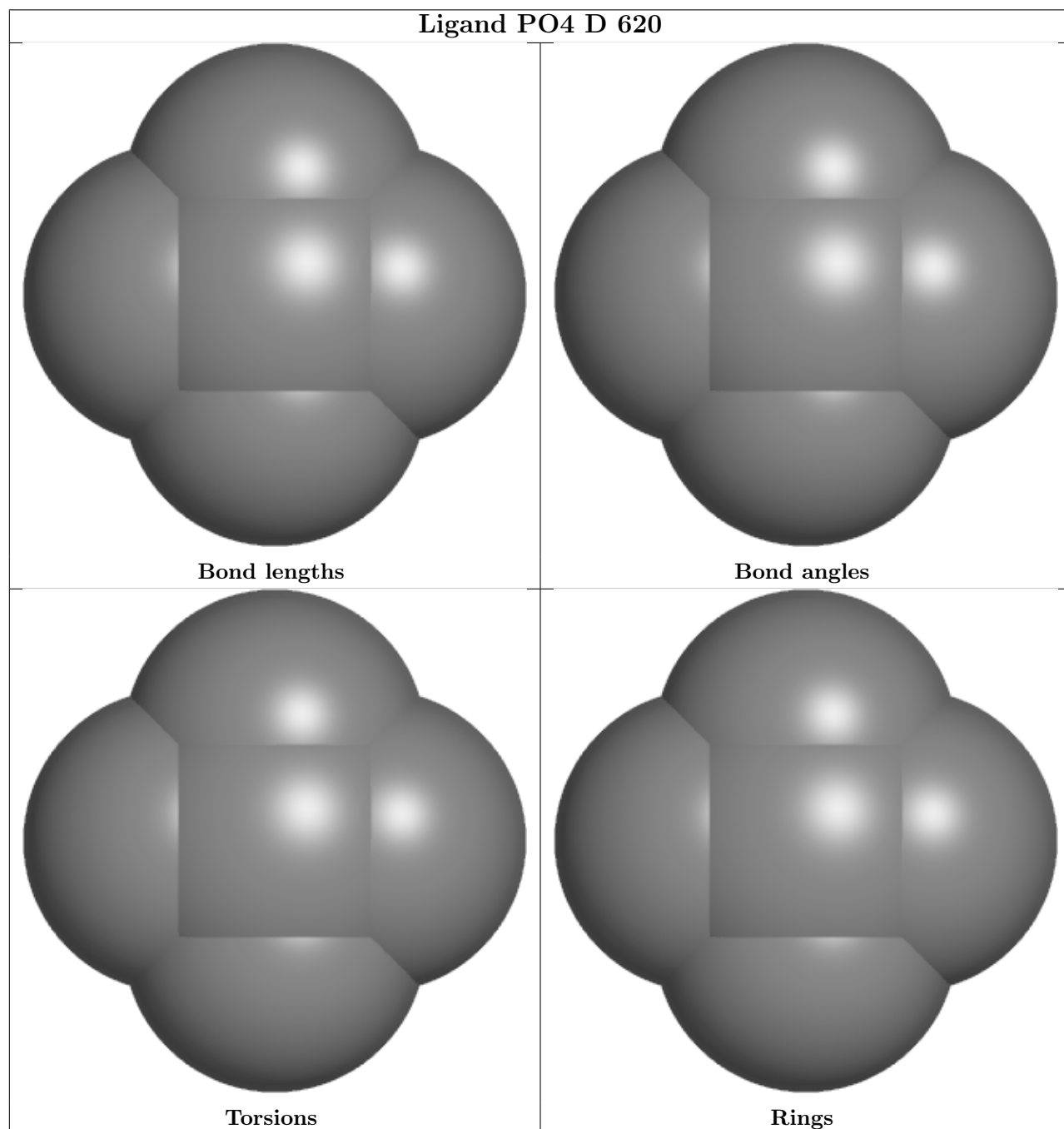
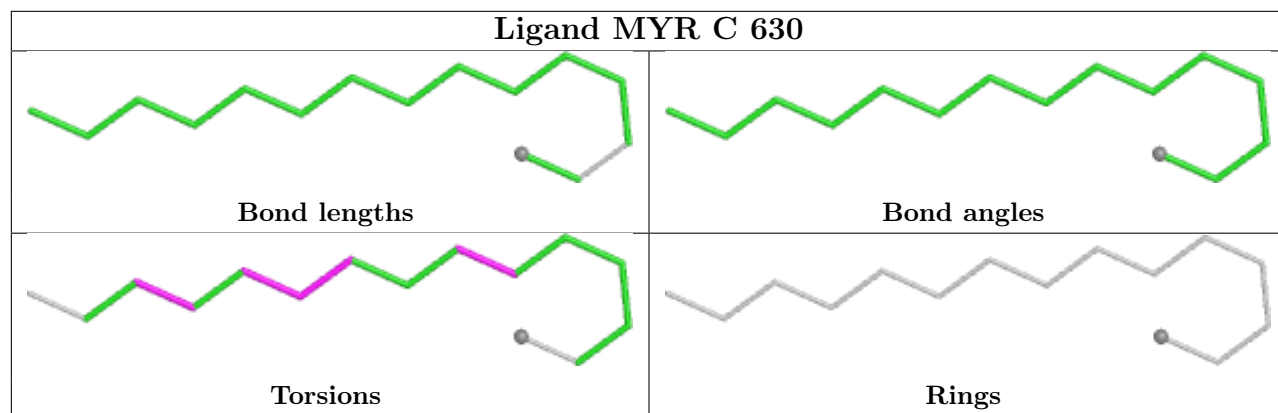


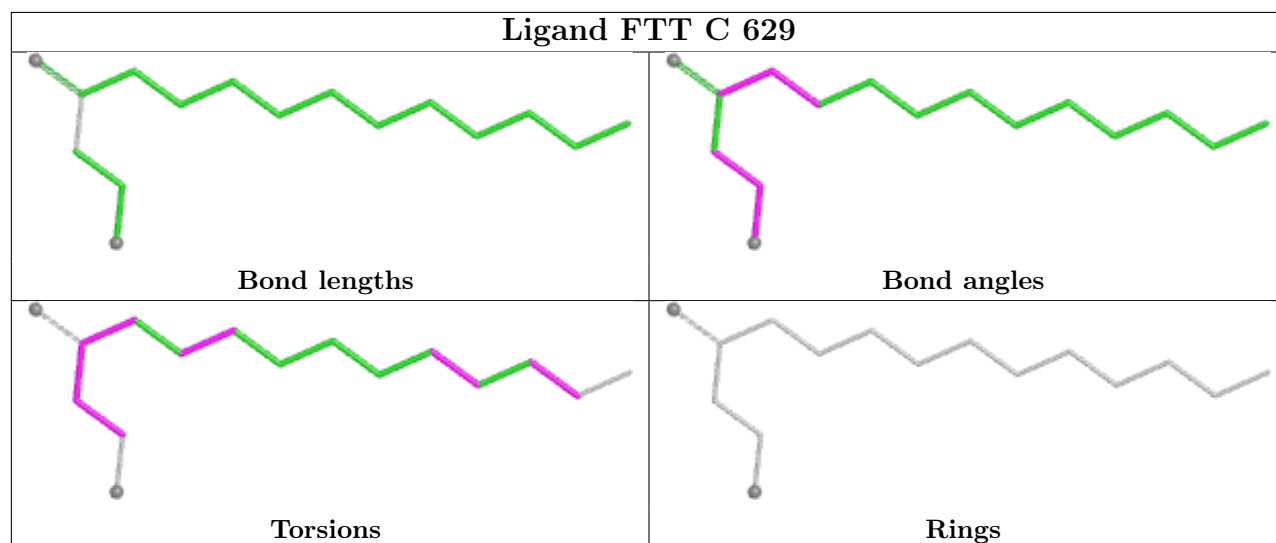
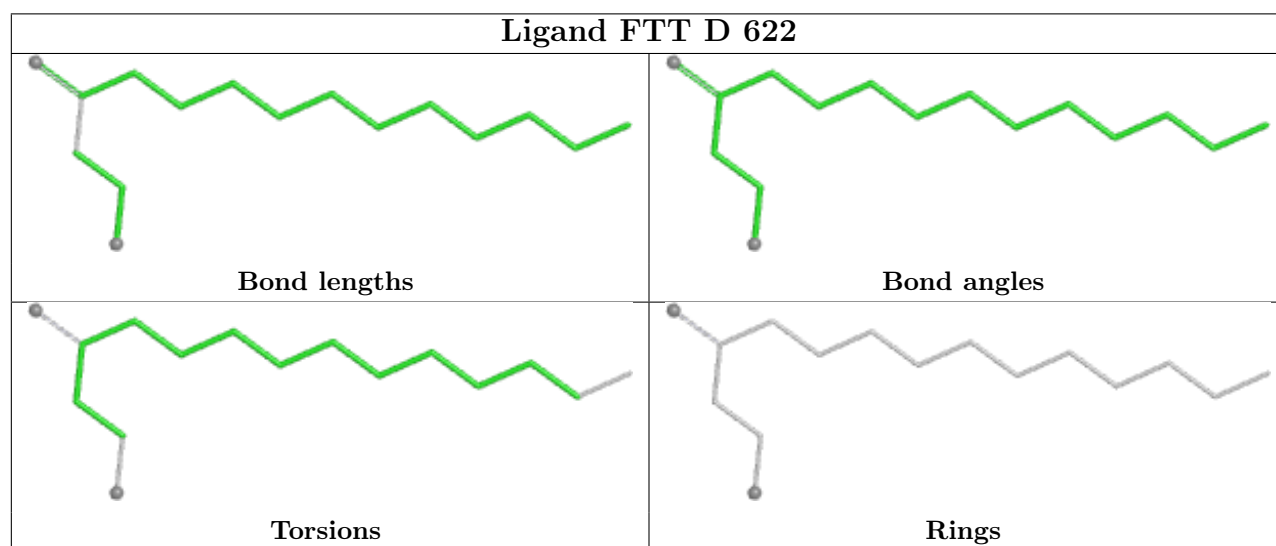
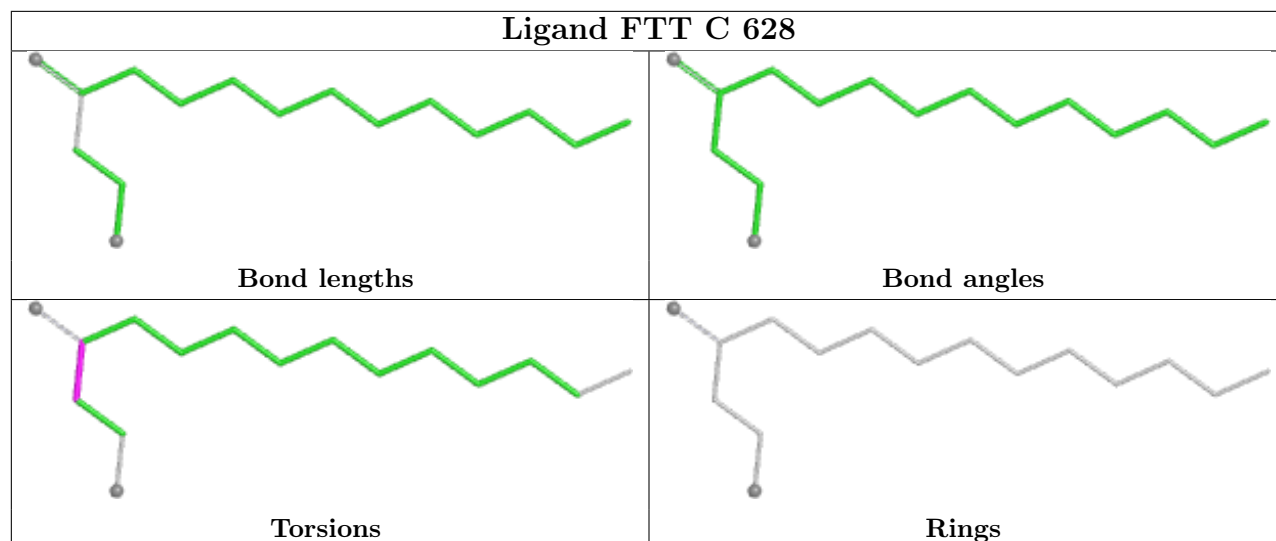
Rings

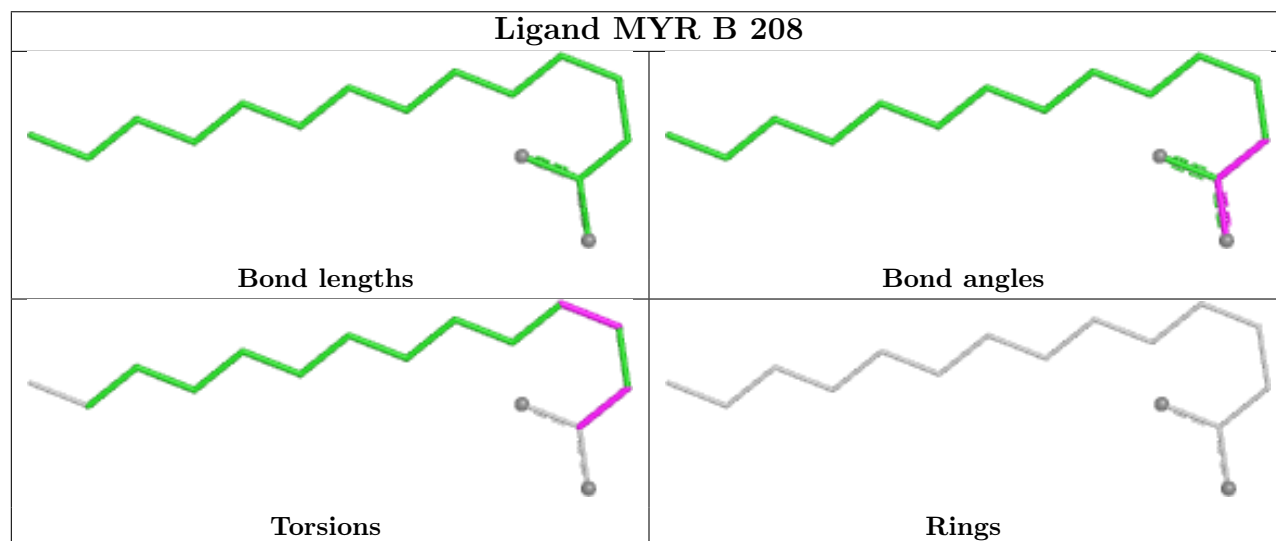
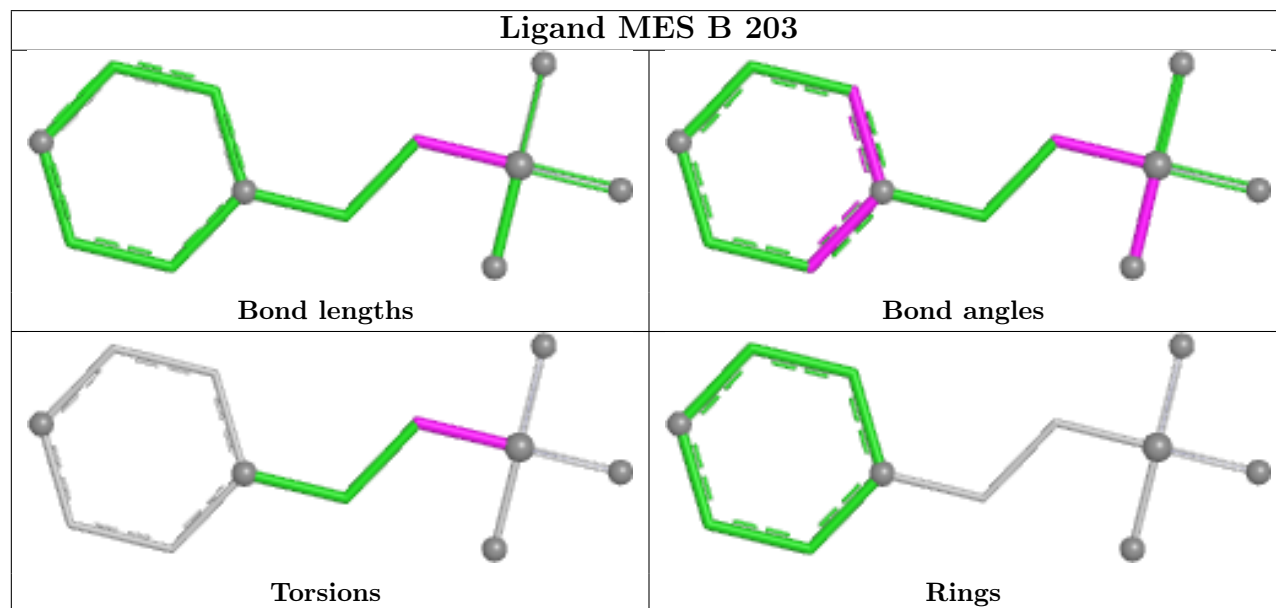
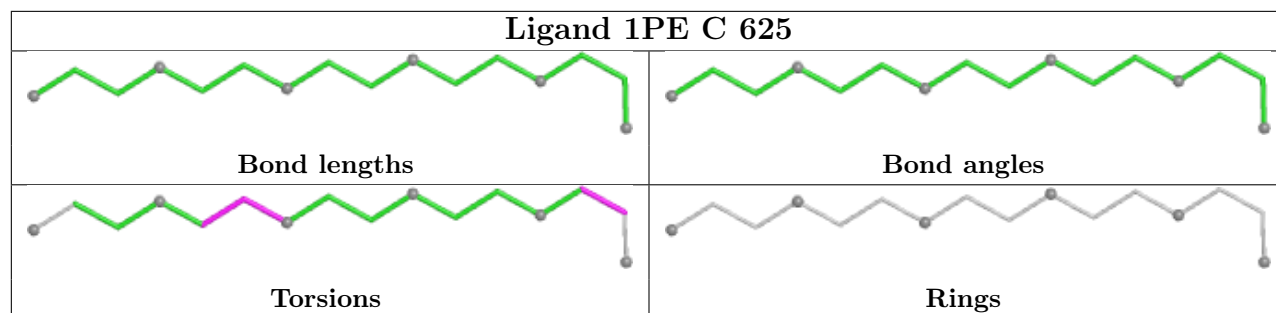


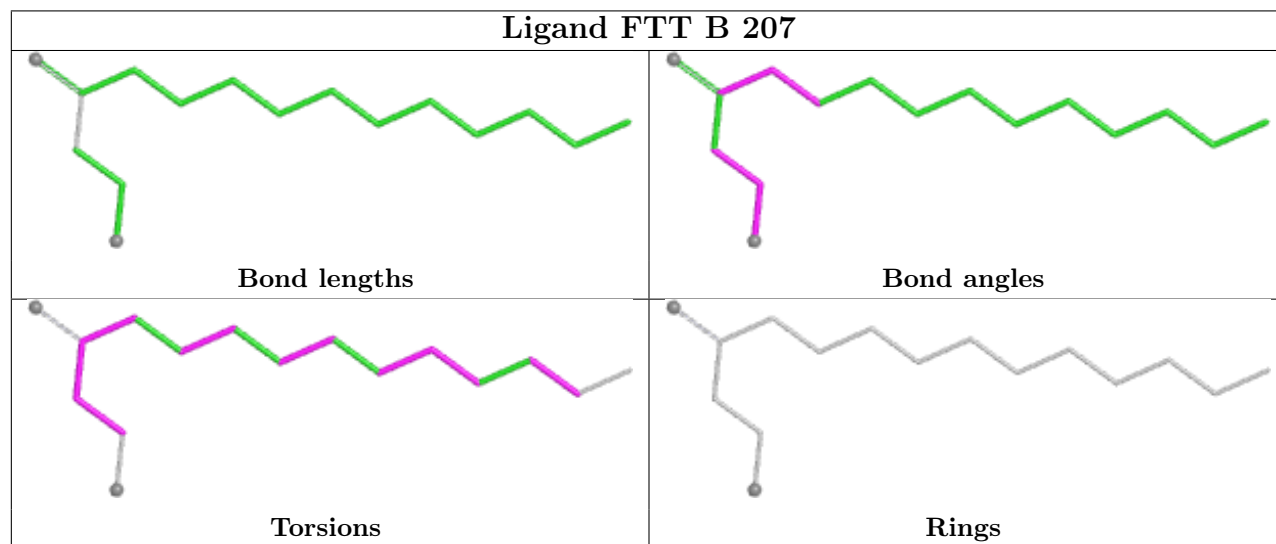
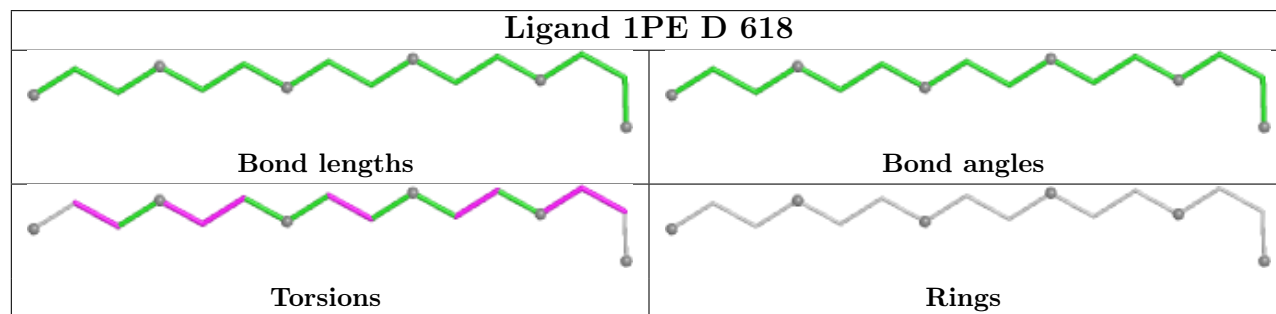
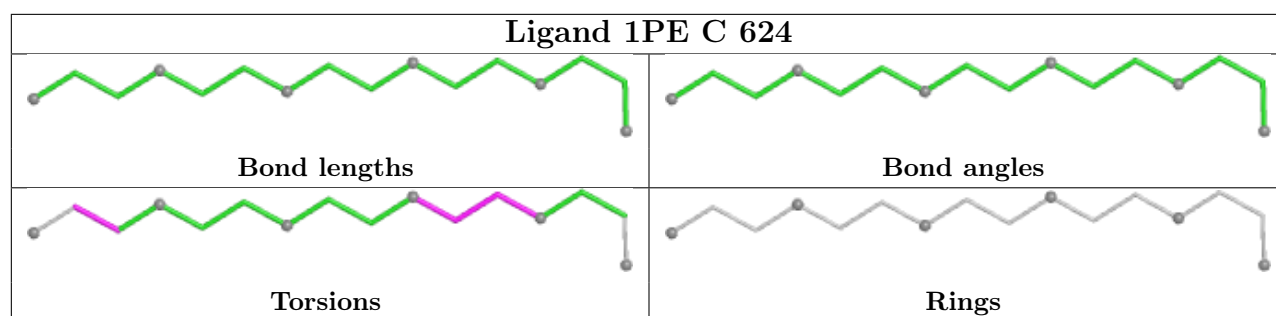




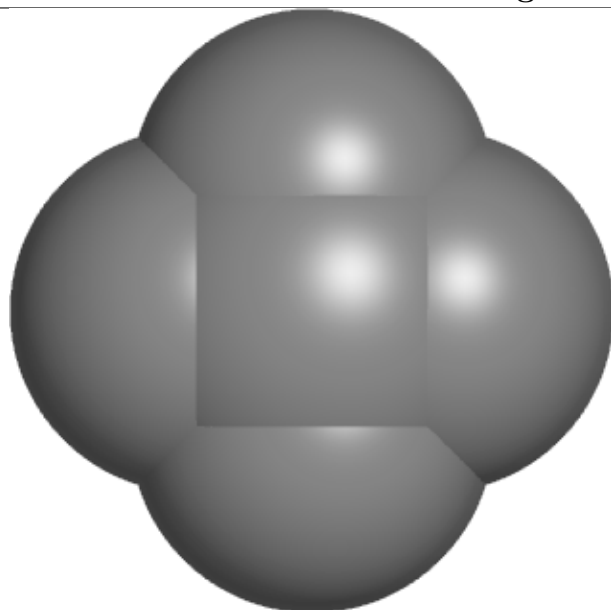




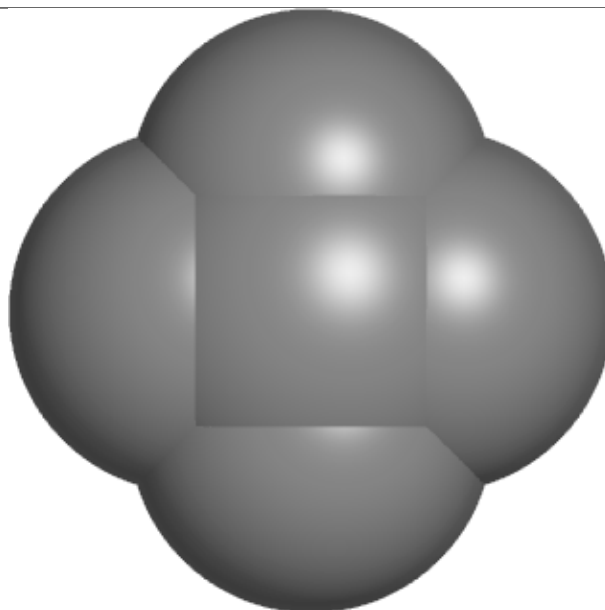




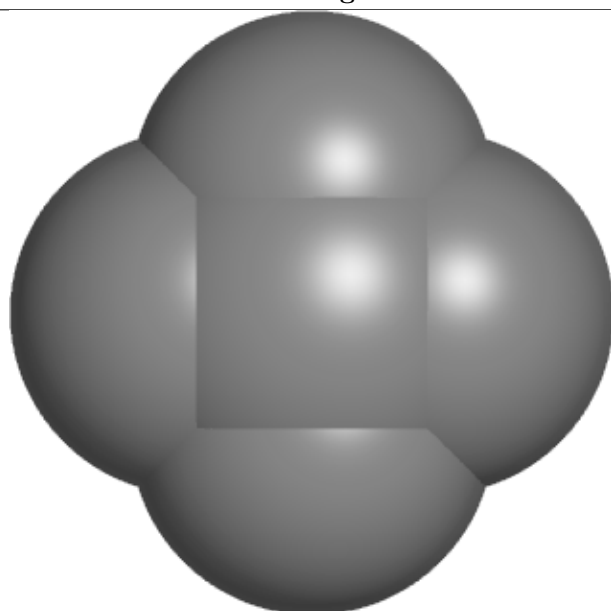
## Ligand PO4 C 626



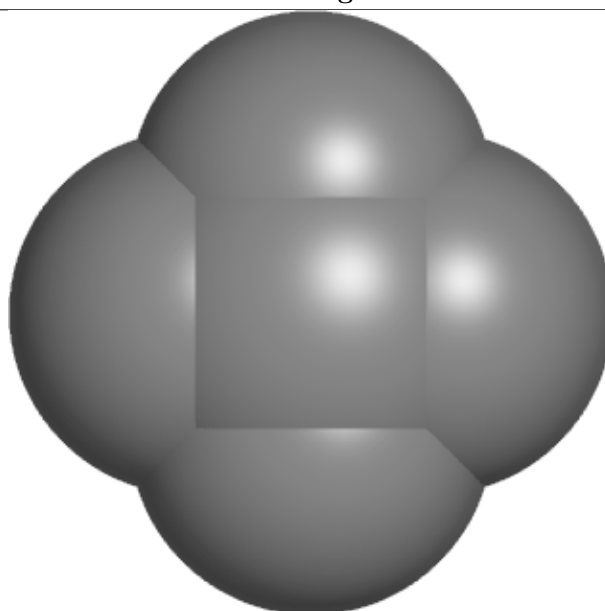
Bond lengths



Bond angles

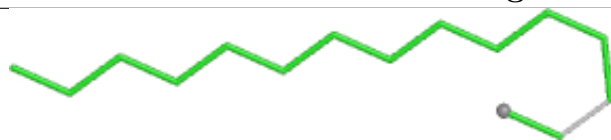


Torsions

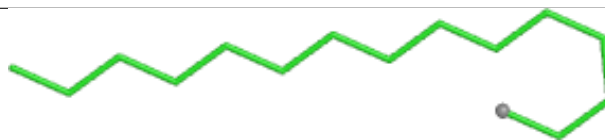


Rings

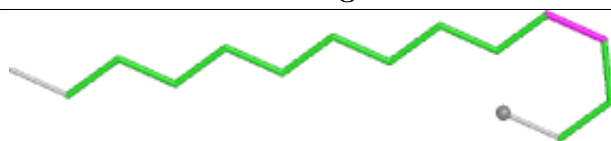
## Ligand MYR D 624



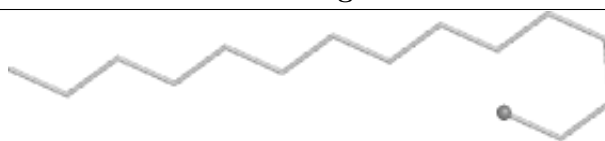
Bond lengths



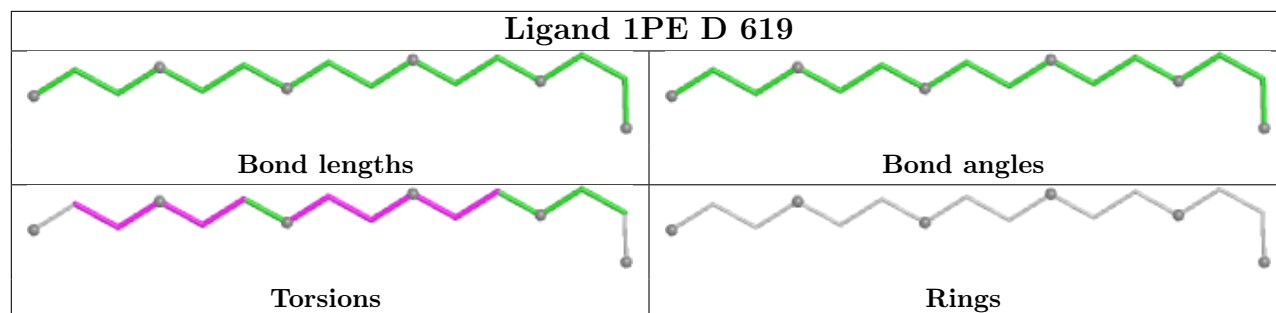
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	94/141 (66%)	1.01	25 (26%) 2 1	19, 41, 80, 102	0
1	B	93/141 (65%)	1.75	37 (39%) 1 1	26, 54, 91, 100	0
2	C	413/422 (97%)	-0.05	27 (6%) 26 27	13, 24, 67, 123	6 (1%)
2	D	412/422 (97%)	0.28	26 (6%) 27 28	13, 29, 72, 113	7 (1%)
All	All	1012/1126 (89%)	0.35	115 (11%) 11 11	13, 29, 79, 123	13 (1%)

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	310	ALA	5.9
1	B	120	PRO	5.9
2	D	161	LEU	5.8
2	D	163	PHE	5.6
2	C	163	PHE	5.3

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

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	K	2	14/15	0.45	0.20	60,88,113,123	0
4	KDO	J	3	15/16	0.58	0.18	73,95,112,114	0

*Continued on next page...*



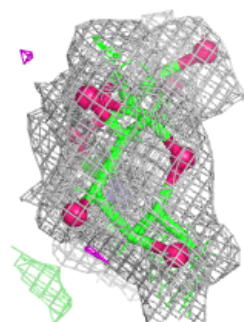
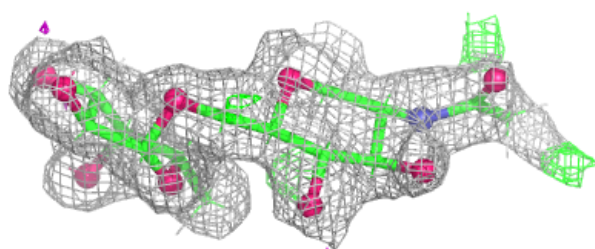
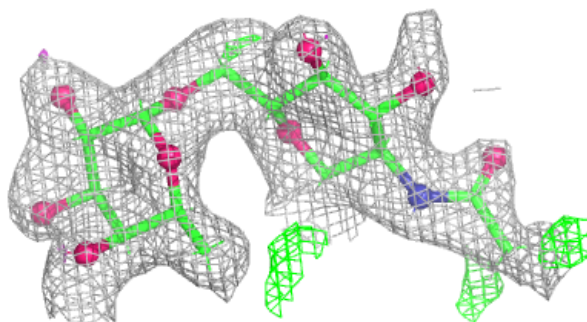
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	G	2	14/15	0.67	0.19	56,73,88,100	0
4	KDO	F	3	15/16	0.67	0.16	59,82,106,110	0
4	GCS	J	2	11/12	0.73	0.14	59,90,128,128	0
3	NAG	E	1	14/15	0.74	0.16	48,61,78,84	0
6	NAG	H	2	14/15	0.76	0.17	41,74,110,127	0
4	GCS	F	2	11/12	0.78	0.12	48,73,91,91	0
3	NAG	I	1	14/15	0.79	0.13	48,59,71,75	0
5	FUC	G	3	10/11	0.80	0.15	45,55,67,72	0
5	FUC	K	3	10/11	0.81	0.17	49,65,78,90	0
3	FUC	E	2	10/11	0.81	0.13	41,57,64,71	0
3	FUC	I	2	10/11	0.82	0.13	53,63,73,75	0
6	NAG	L	2	14/15	0.85	0.12	37,63,92,93	0
5	NAG	G	1	14/15	0.86	0.13	38,55,74,74	0
6	NAG	H	1	14/15	0.86	0.14	36,55,88,88	0
5	NAG	K	1	14/15	0.88	0.12	45,57,70,72	0
6	NAG	L	1	14/15	0.89	0.12	39,53,90,90	0
4	PA1	F	1	11/12	0.93	0.09	26,38,46,50	0
4	PA1	J	1	11/12	0.95	0.08	31,39,62,64	0

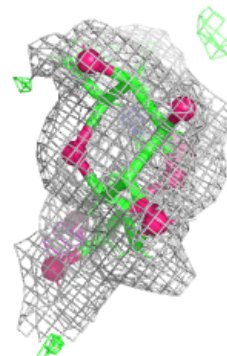
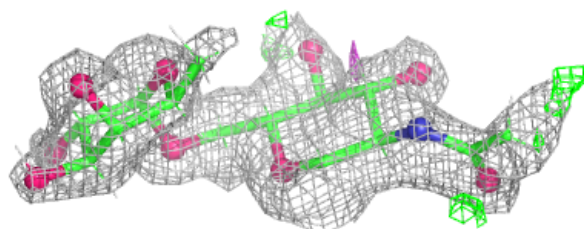
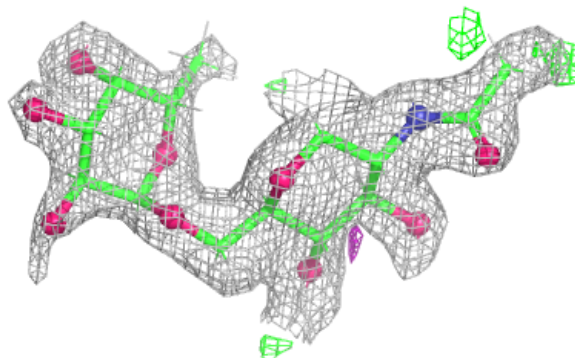
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

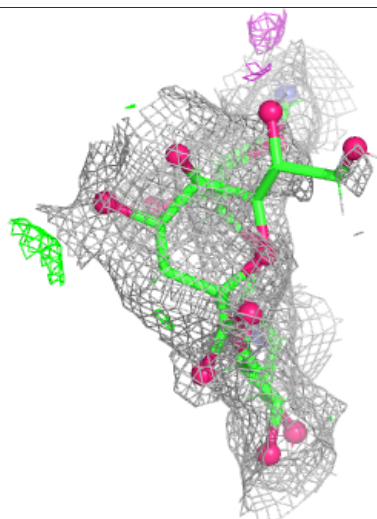
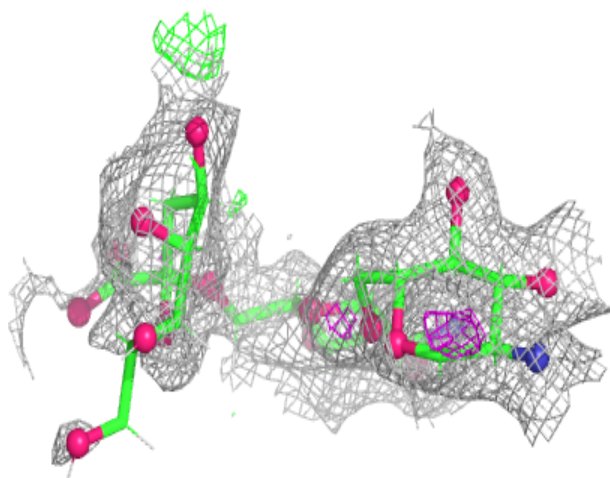
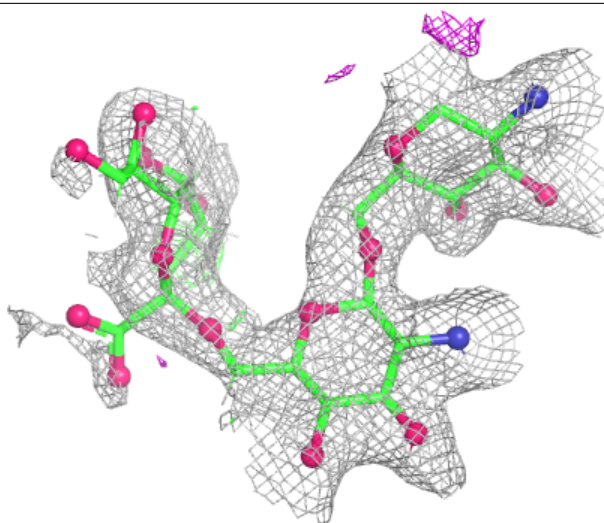
**Electron density around Chain I:**

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



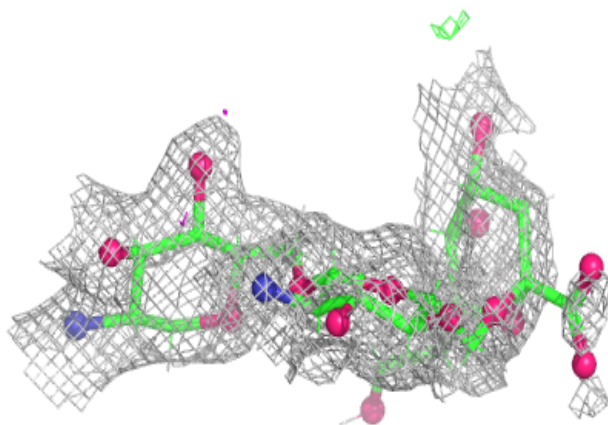
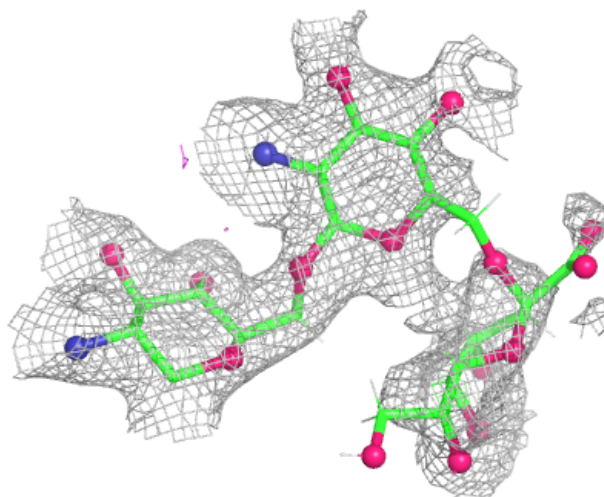
**Electron density around Chain F:**

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



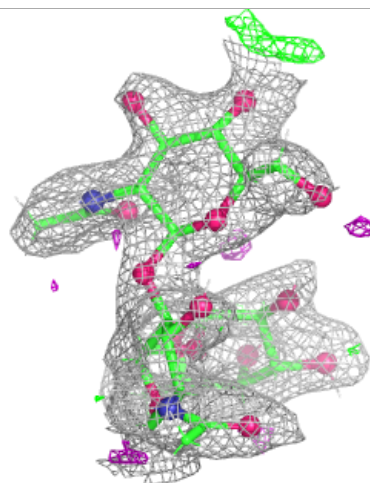
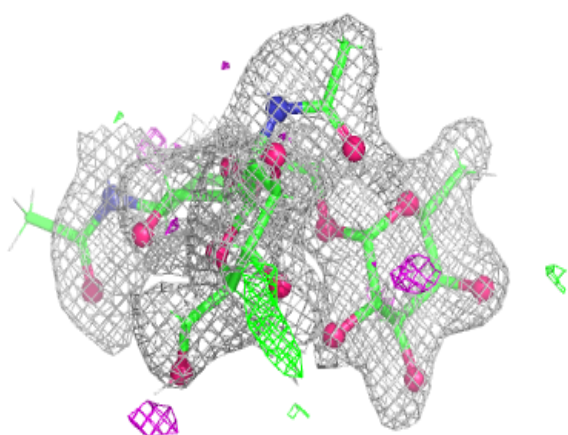
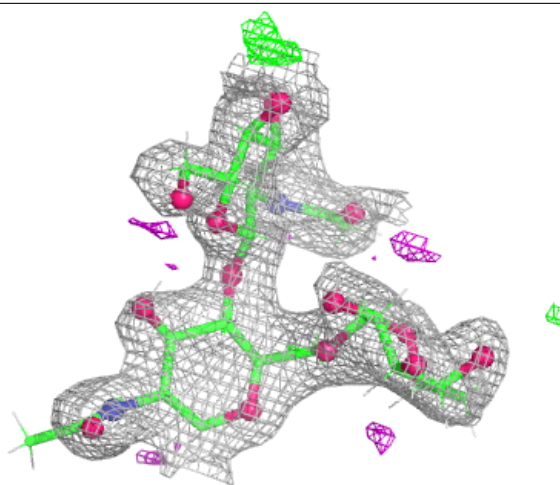
**Electron density around Chain J:**

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



**Electron density around Chain G:**

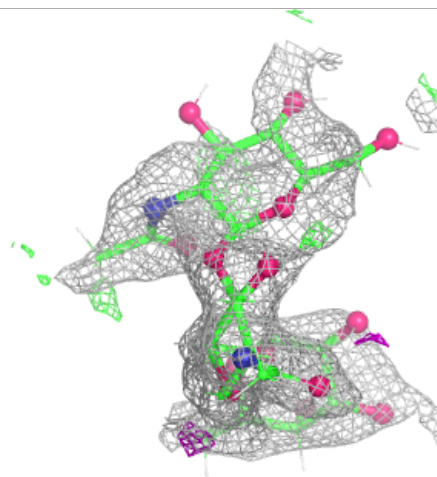
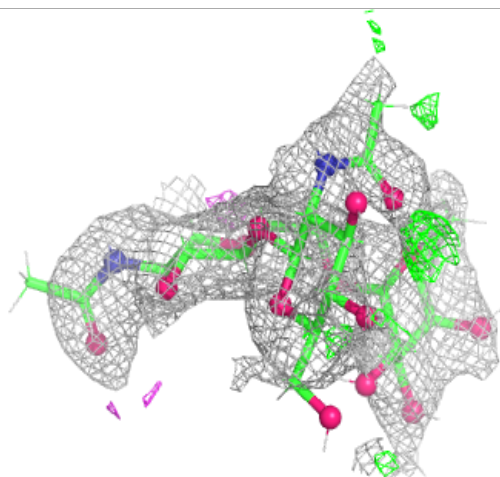
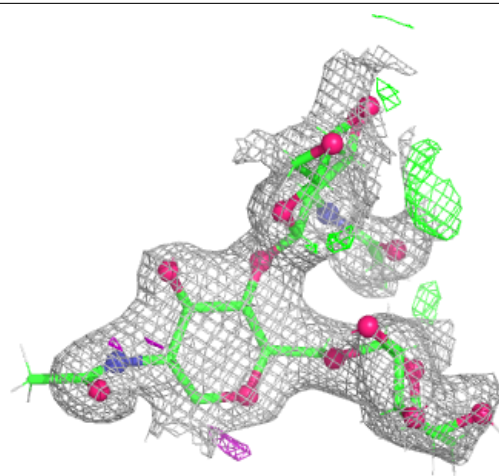
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





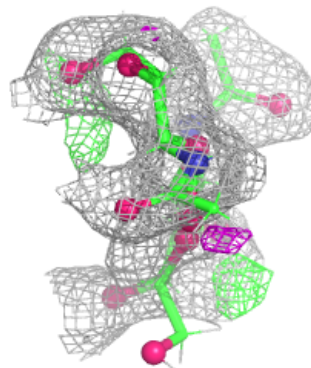
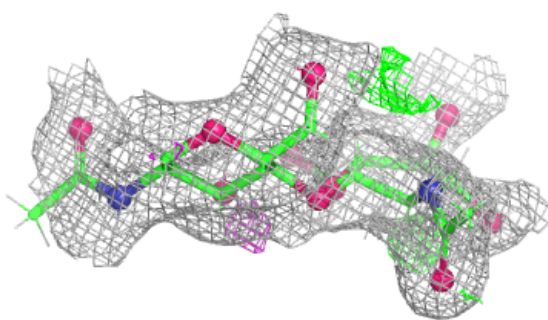
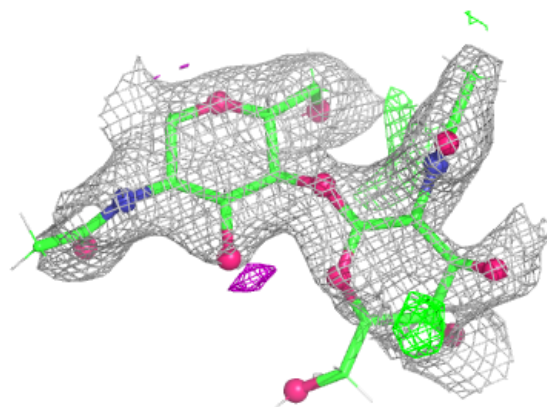
**Electron density around Chain K:**

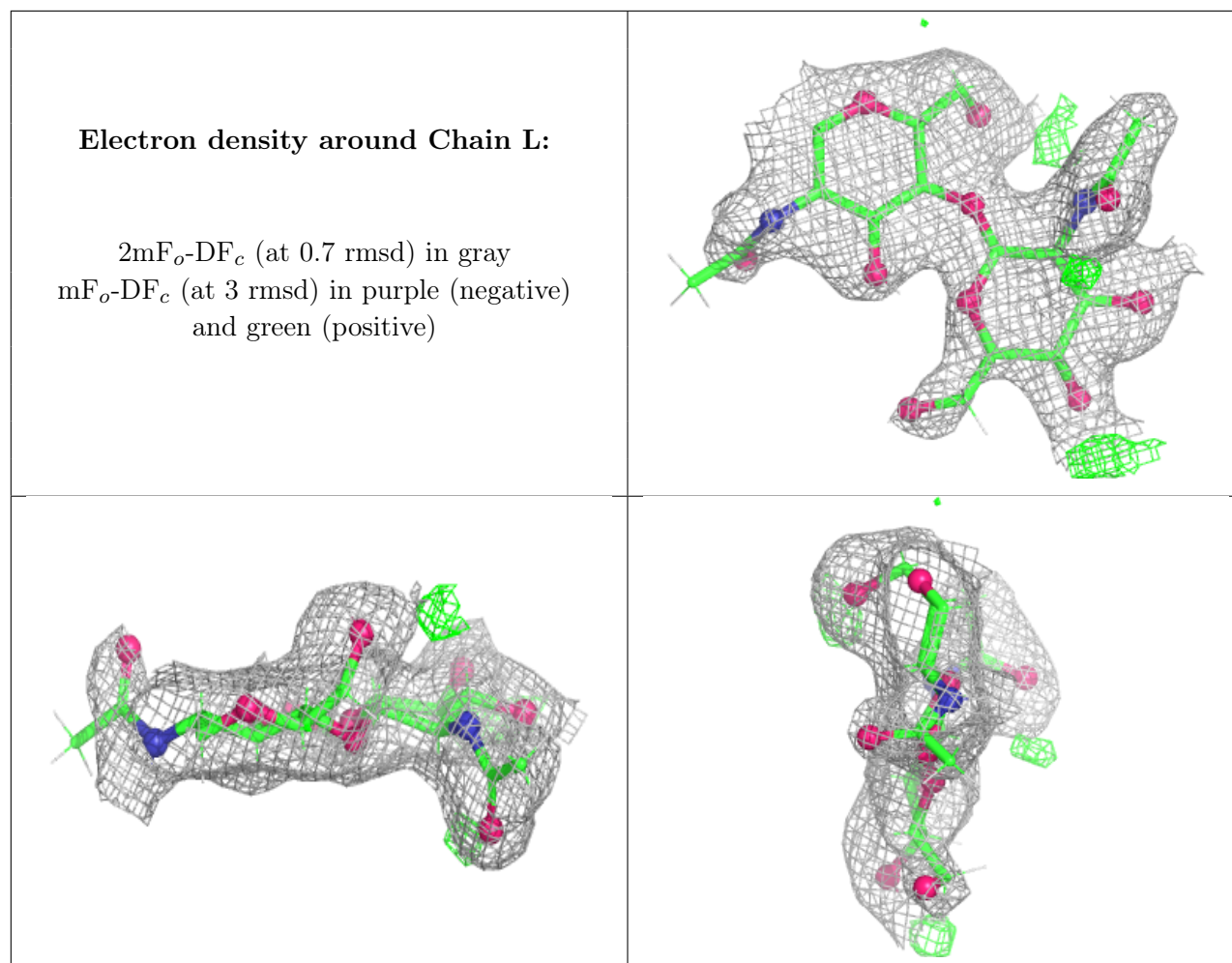
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain H:**

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





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	MES	D	610	12/12	0.50	0.21	73,91,105,111	0
15	PO4	D	621	4/5	0.56	0.15	93,99,111,116	0
15	PO4	C	627	4/5	0.62	0.13	71,75,76,93	0
7	PEG	C	618	7/7	0.68	0.21	60,72,83,85	0
7	PEG	A	204	7/7	0.69	0.16	66,80,90,90	0
13	MES	B	203	12/12	0.71	0.21	45,79,92,93	0
7	PEG	D	613	7/7	0.73	0.17	49,60,74,82	0
7	PEG	C	612	7/7	0.76	0.17	45,62,78,78	0
13	MES	C	610	12/12	0.76	0.20	39,73,88,89	0
7	PEG	C	615	7/7	0.77	0.18	42,61,79,79	0

*Continued on next page...*



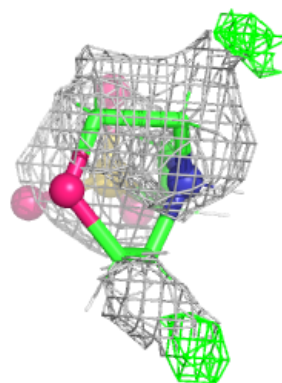
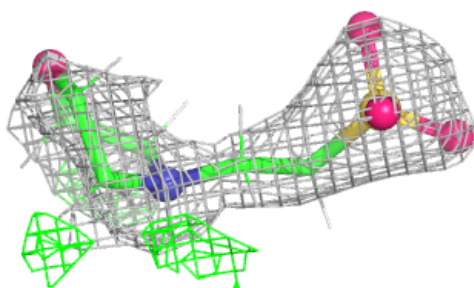
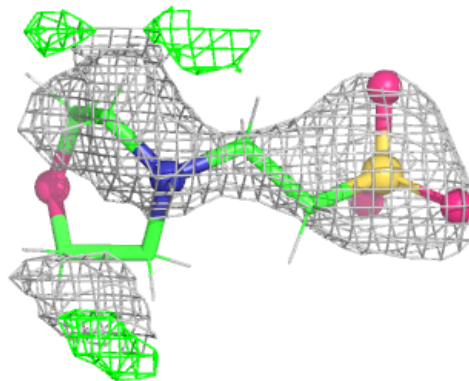
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PEG	A	203	7/7	0.78	0.19	35,59,72,72	0
7	PEG	C	614	7/7	0.78	0.16	51,63,74,89	0
10	MYR	A	210	16/16	0.79	0.17	40,54,90,94	0
7	PEG	C	620	7/7	0.79	0.15	27,38,46,46	0
7	PEG	C	616	7/7	0.80	0.16	53,64,72,75	0
8	PGE	C	622	10/10	0.80	0.17	34,49,70,77	0
7	PEG	C	617	7/7	0.80	0.15	42,54,70,73	0
7	PEG	D	611	7/7	0.80	0.14	29,42,47,52	0
10	MYR	B	208	16/16	0.81	0.16	41,59,75,87	0
9	FTT	B	207	16/17	0.82	0.17	49,64,83,89	0
7	PEG	C	619	7/7	0.82	0.15	23,35,43,44	0
7	PEG	D	614	7/7	0.84	0.15	42,53,64,64	0
9	FTT	A	209	16/17	0.85	0.15	45,61,76,76	0
8	PGE	A	205	10/10	0.85	0.13	42,59,74,77	0
7	PEG	D	612	7/7	0.85	0.13	38,54,66,66	0
10	MYR	C	630	15/16	0.85	0.16	36,50,73,74	0
8	PGE	C	623	10/10	0.85	0.14	41,53,60,64	0
7	PEG	C	613	7/7	0.86	0.14	41,54,67,67	0
14	1PE	C	624	16/16	0.86	0.12	31,44,58,70	0
8	PGE	D	616	10/10	0.86	0.14	41,51,60,62	0
7	PEG	C	611	7/7	0.86	0.12	30,38,53,53	0
10	MYR	D	624	15/16	0.87	0.15	34,55,76,78	0
14	1PE	D	618	16/16	0.87	0.12	29,43,52,62	0
8	PGE	C	621	10/10	0.89	0.12	29,38,50,68	0
9	FTT	D	623	16/17	0.90	0.15	30,59,80,85	0
12	SO4	D	609	5/5	0.90	0.10	42,42,50,57	0
8	PGE	D	617	10/10	0.90	0.12	30,37,46,55	0
9	FTT	D	622	16/17	0.91	0.10	21,32,51,53	0
15	PO4	C	626	5/5	0.91	0.17	31,33,48,52	0
14	1PE	D	619	16/16	0.92	0.10	24,36,52,62	0
9	FTT	C	629	16/17	0.92	0.11	26,46,69,69	0
8	PGE	D	615	10/10	0.94	0.08	23,34,52,53	0
14	1PE	C	625	16/16	0.95	0.07	20,29,42,45	0
15	PO4	D	620	5/5	0.95	0.11	35,37,44,45	0
9	FTT	C	628	16/17	0.95	0.07	14,25,42,46	0
12	SO4	C	609	5/5	0.96	0.11	31,35,37,50	0
11	CA	D	602	1/1	0.97	0.04	19,19,19,19	0
11	CA	D	603	1/1	0.98	0.03	21,21,21,21	0
11	CA	C	603	1/1	0.99	0.04	20,20,20,20	0
11	CA	C	601	1/1	0.99	0.03	17,17,17,17	0
11	CA	D	601	1/1	1.00	0.02	18,18,18,18	0
11	CA	C	602	1/1	1.00	0.02	18,18,18,18	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.

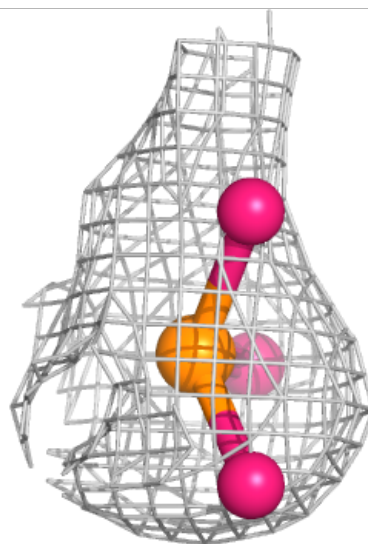
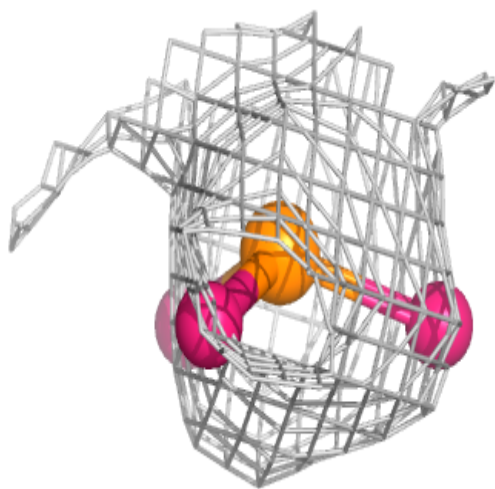
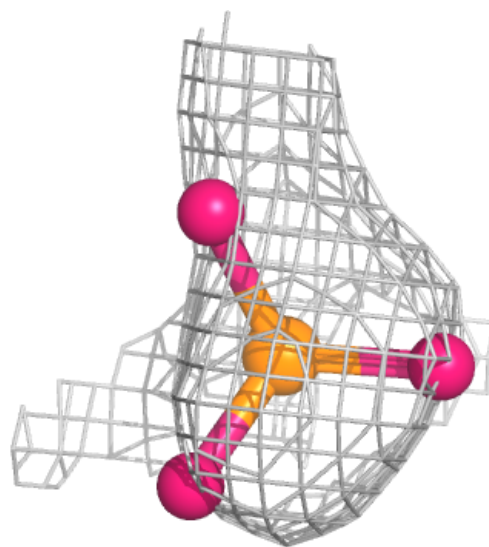
**Electron density around MES D 610:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



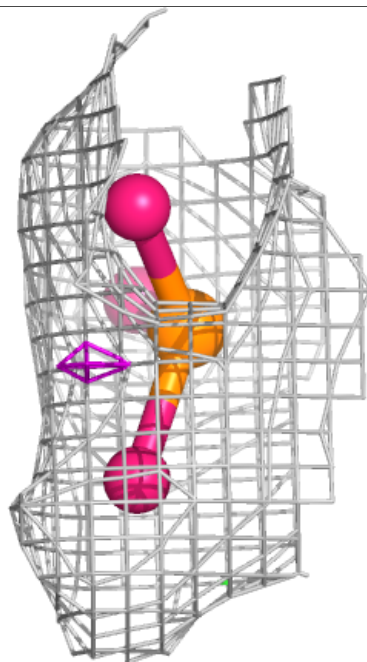
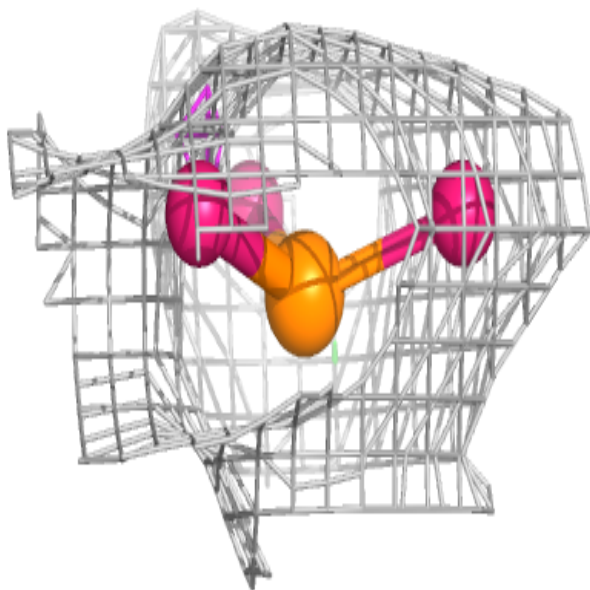
**Electron density around PO4 D 621:**

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



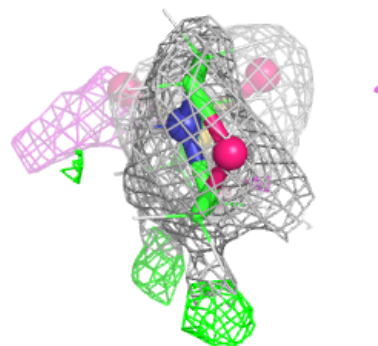
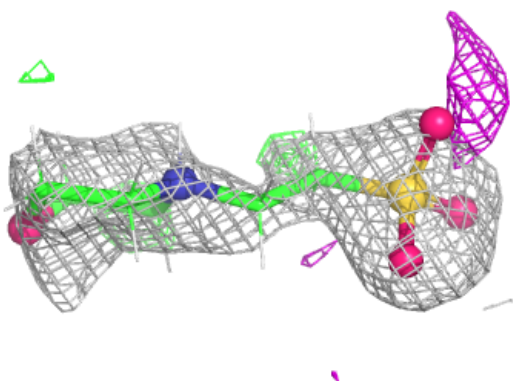
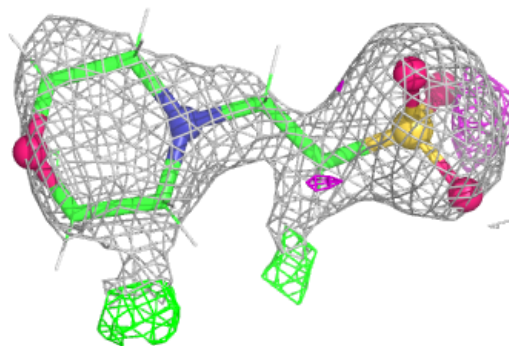
**Electron density around PO4 C 627:**

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

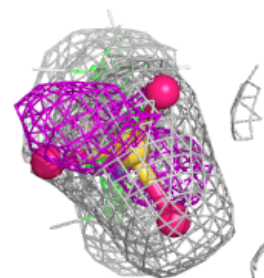
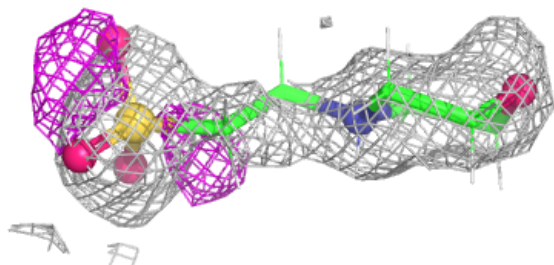
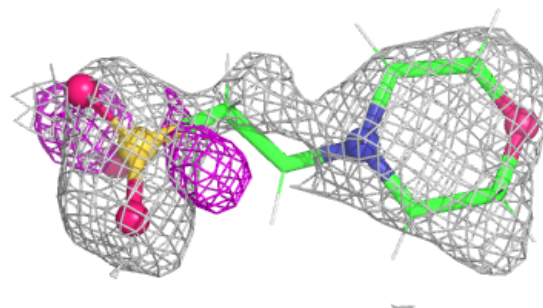


**Electron density around MES B 203:**

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

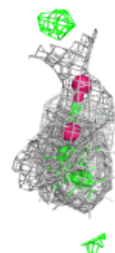
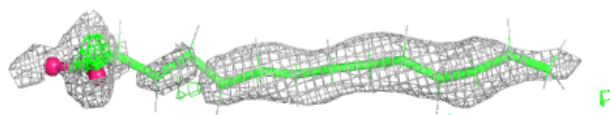
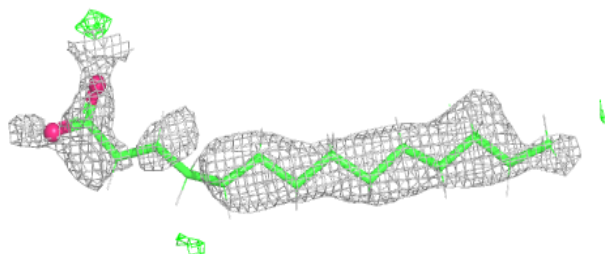
**Electron density around MES C 610:**

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

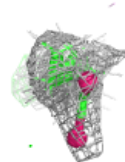
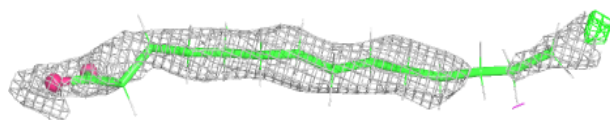
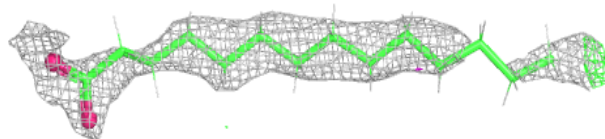


**Electron density around MYR A 210:**

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

**Electron density around MYR B 208:**

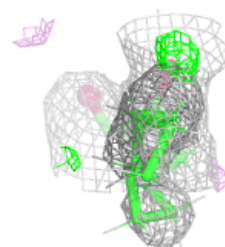
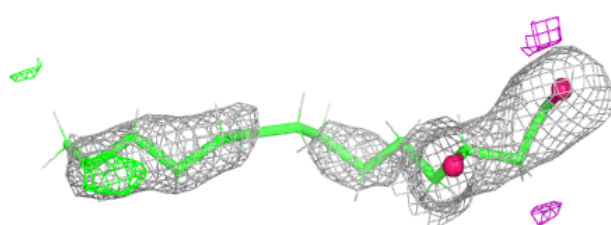
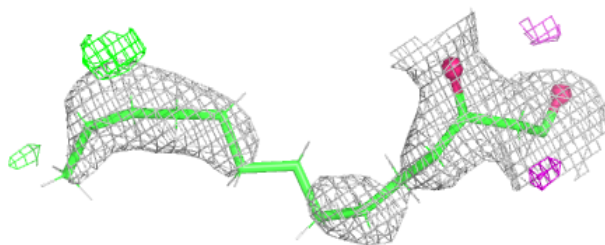
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



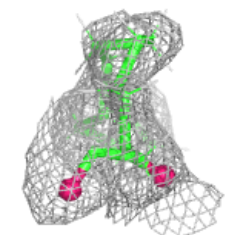
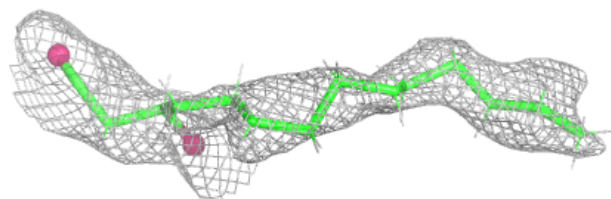


**Electron density around FTT B 207:**

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

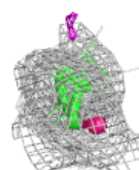
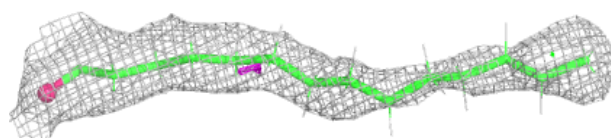
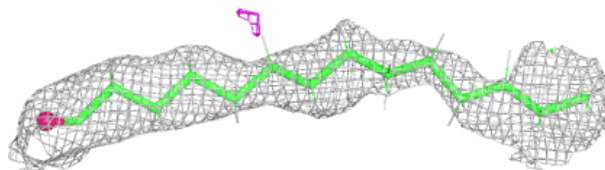
**Electron density around FTT A 209:**

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



**Electron density around MYR C 630:**

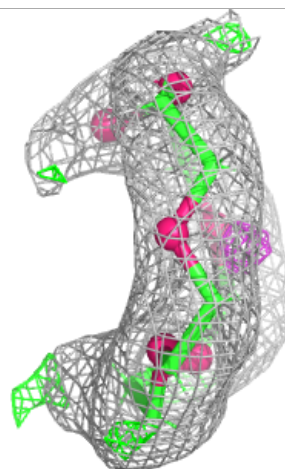
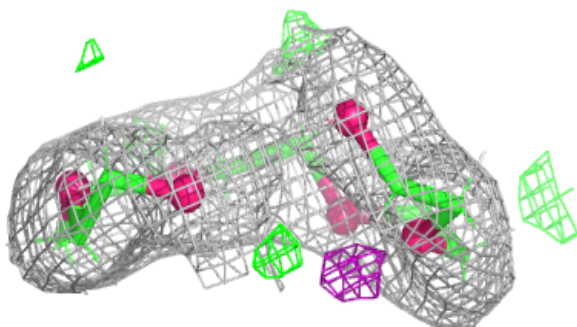
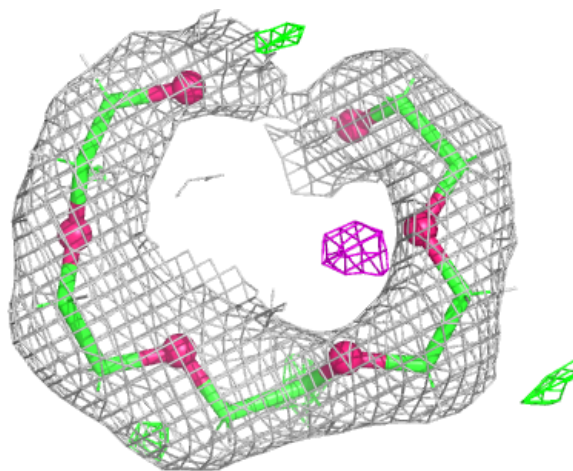
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





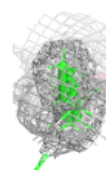
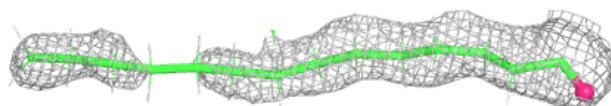
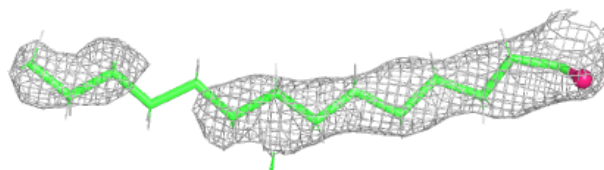
**Electron density around 1PE C 624:**

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

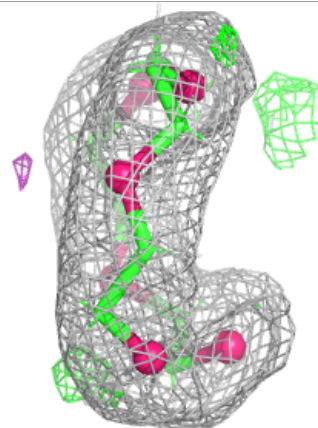
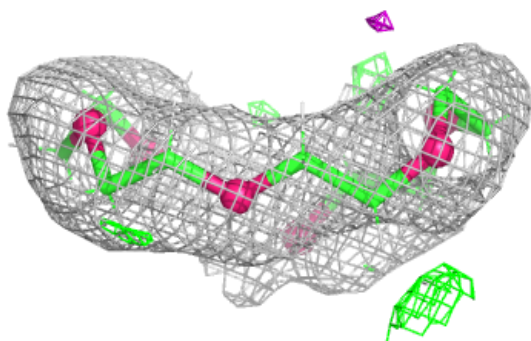
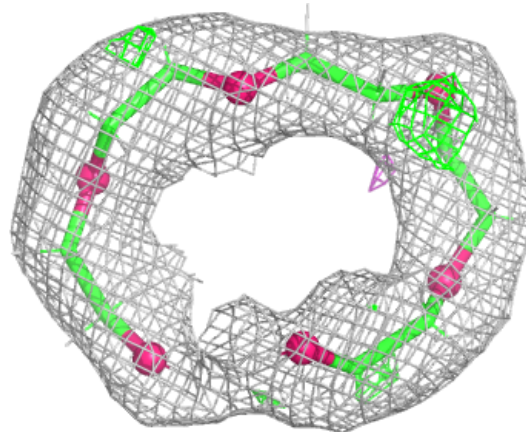


**Electron density around MYR D 624:**

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

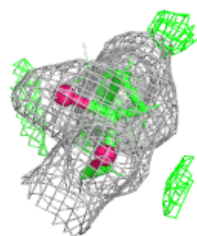
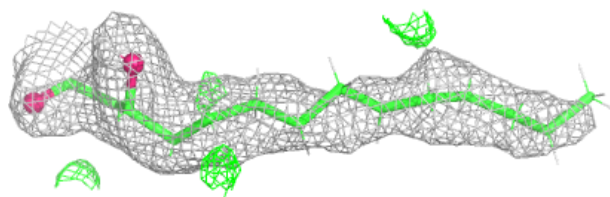
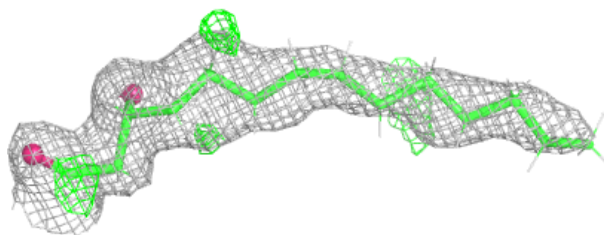
**Electron density around 1PE D 618:**

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

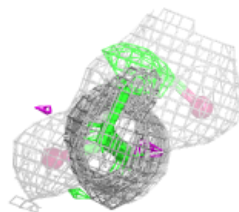
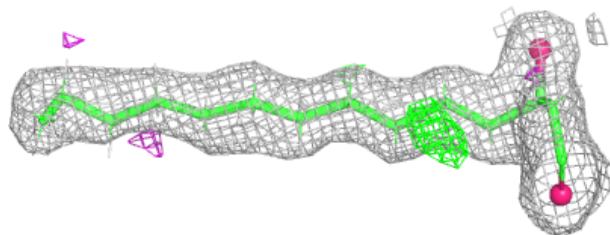
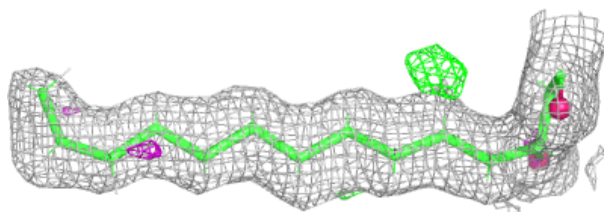


**Electron density around FTT D 623:**

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

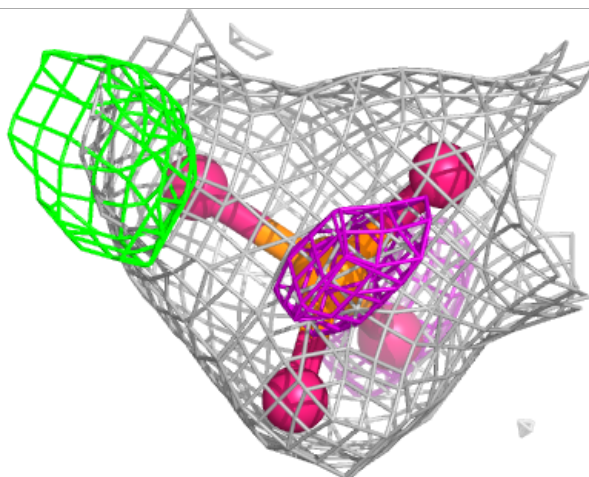
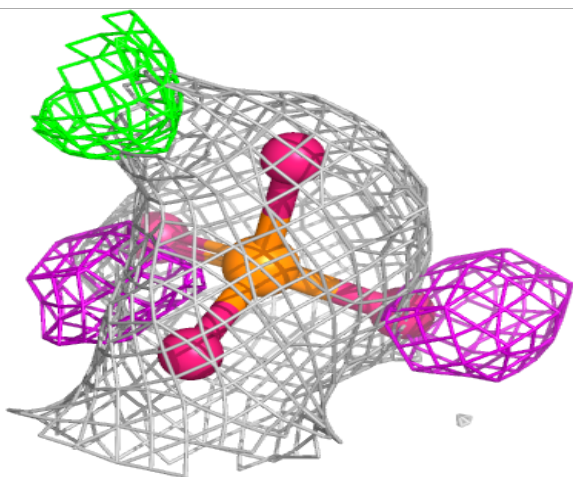
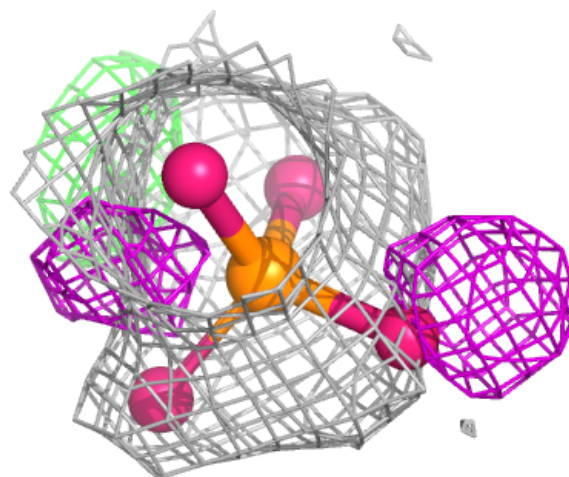
**Electron density around FTT D 622:**

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



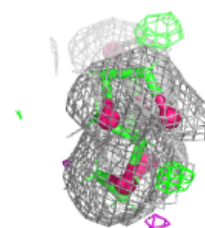
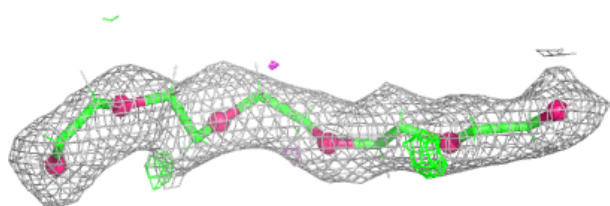
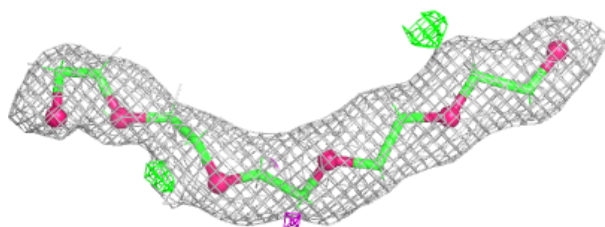
**Electron density around PO4 C 626:**

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

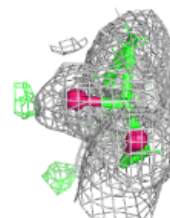
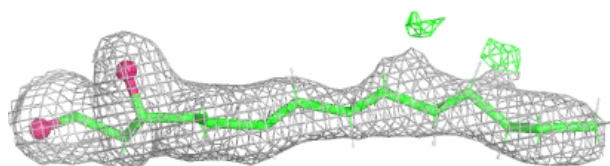
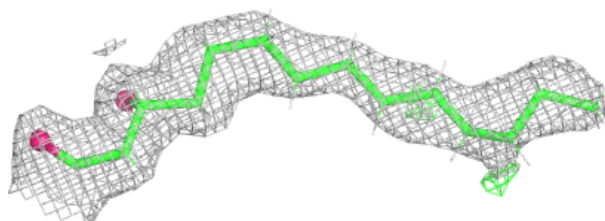


**Electron density around 1PE D 619:**

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

**Electron density around FTT C 629:**

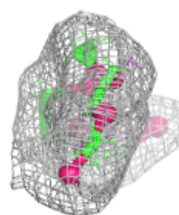
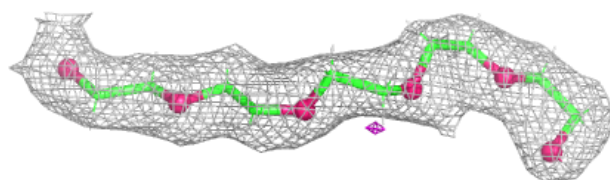
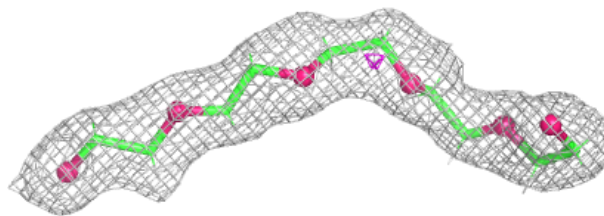
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





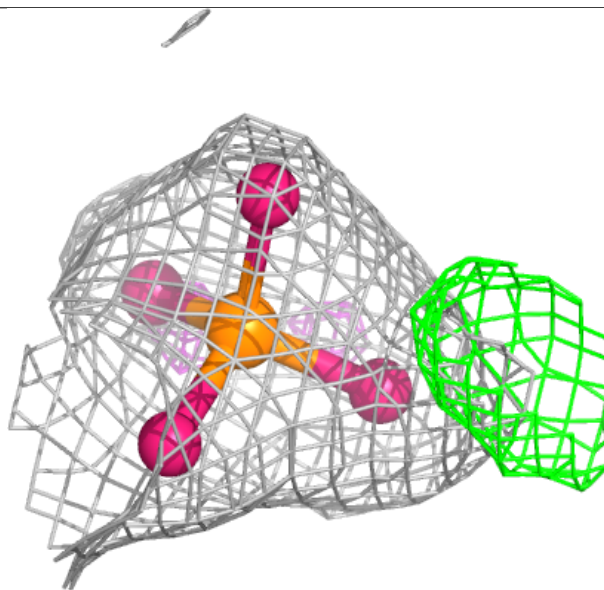
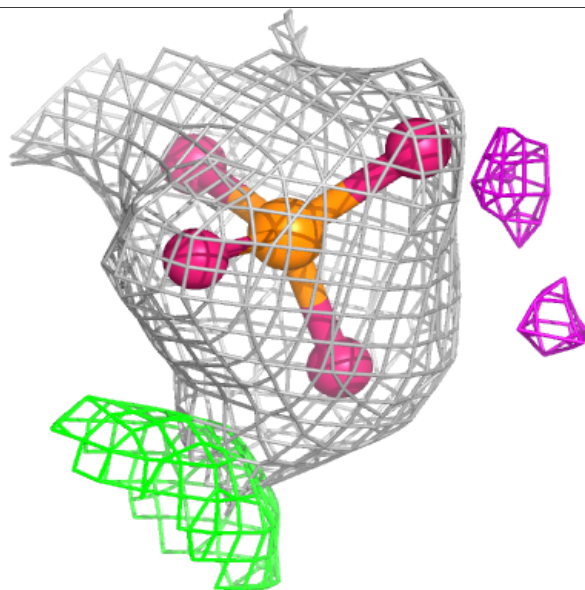
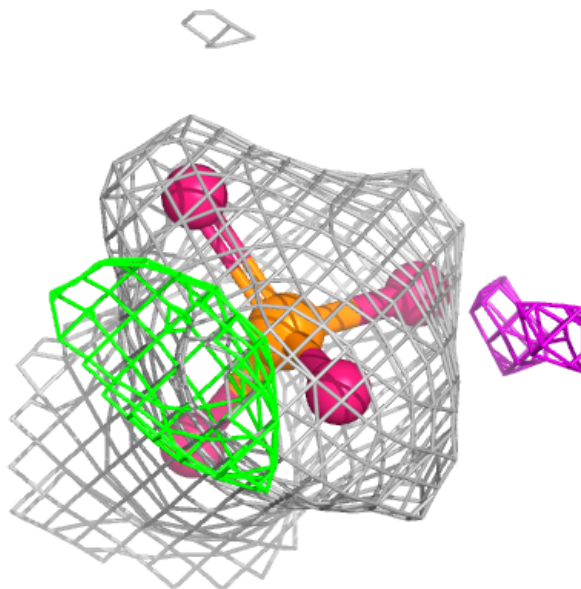
**Electron density around 1PE C 625:**

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



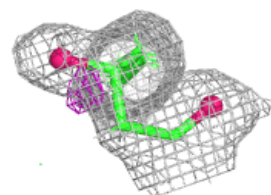
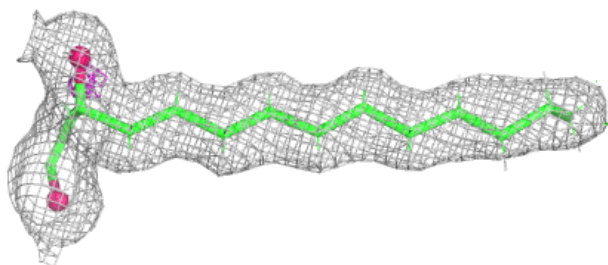
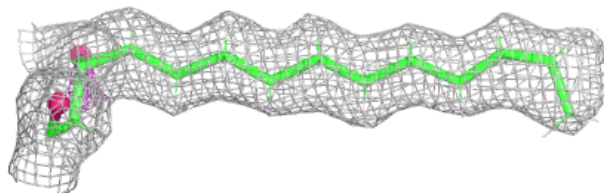
**Electron density around PO4 D 620:**

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



**Electron density around FTT C 628:**

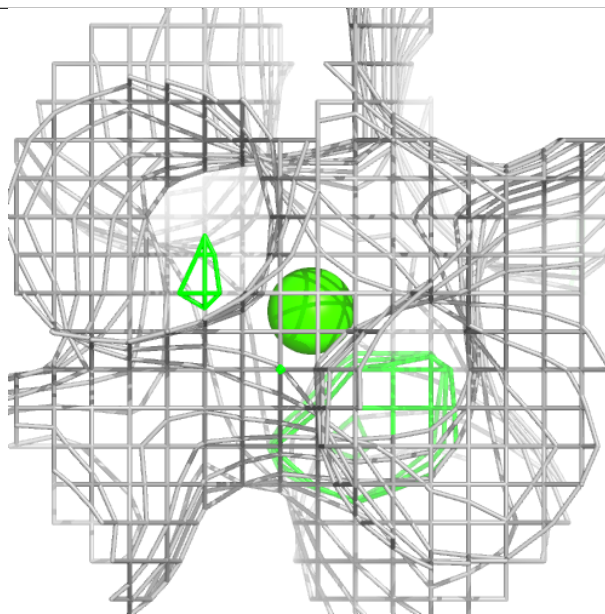
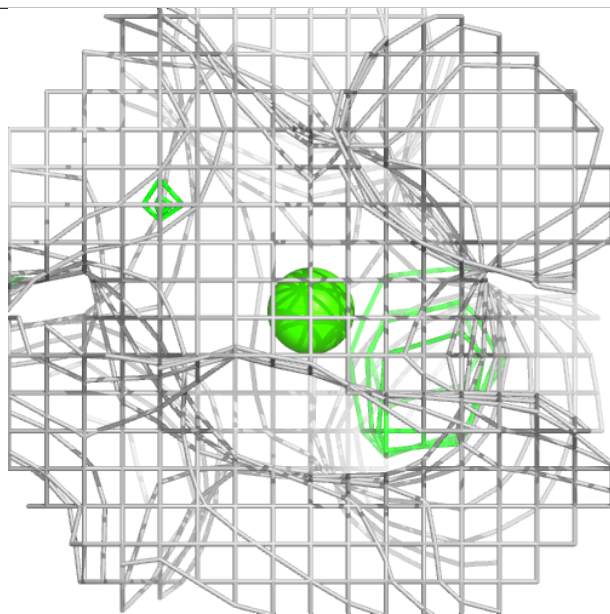
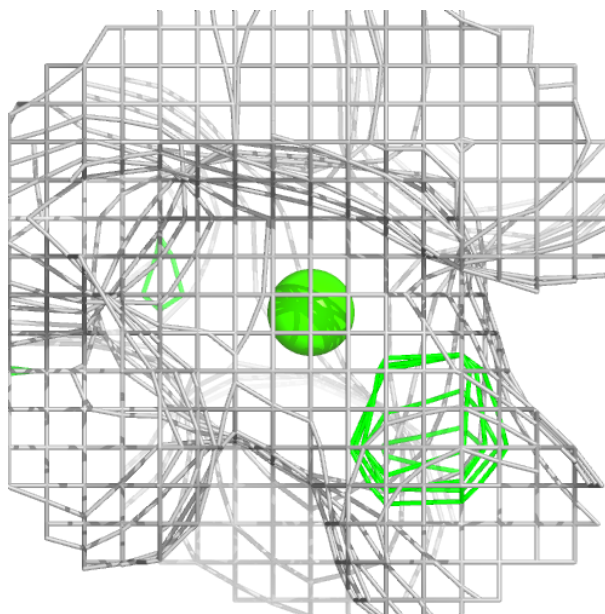
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





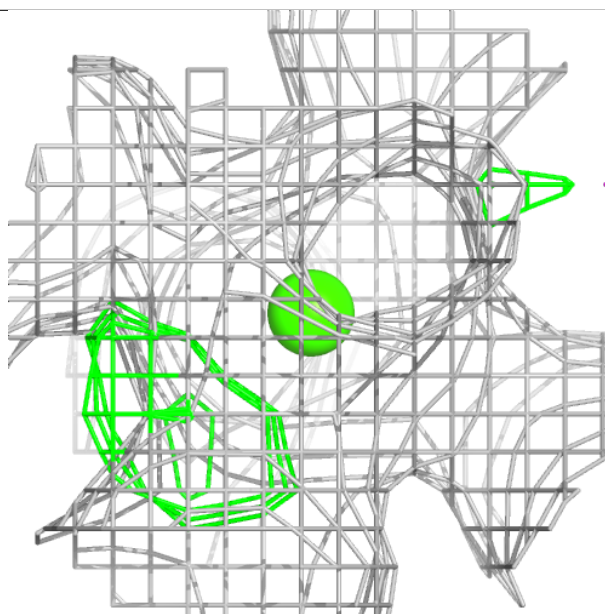
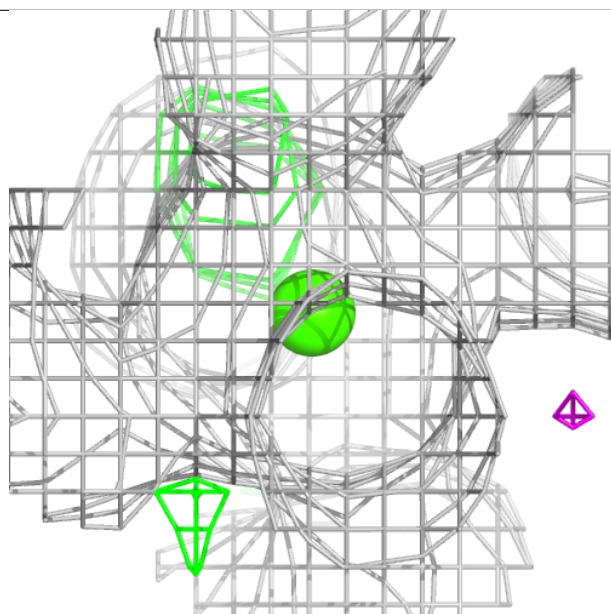
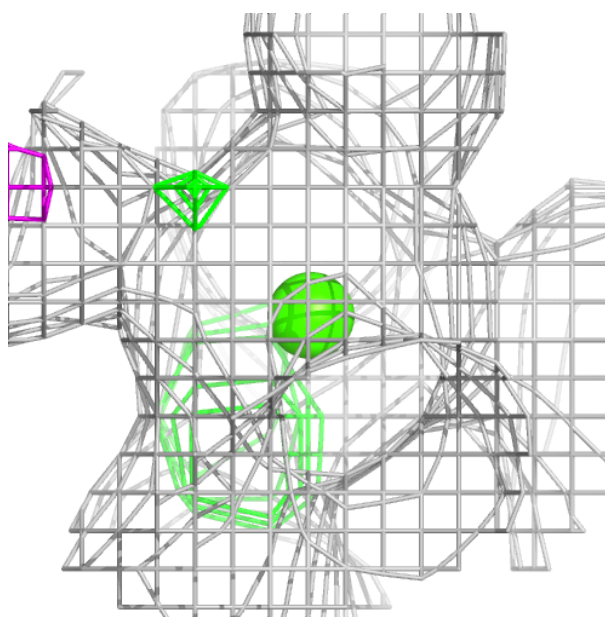
**Electron density around CA D 602:**

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



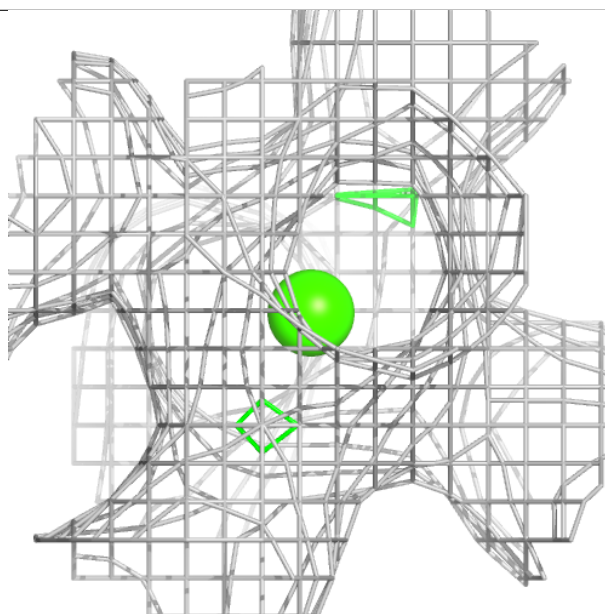
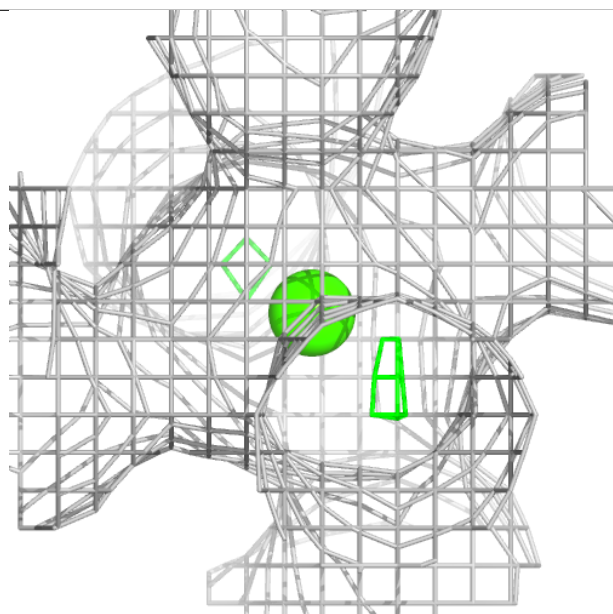
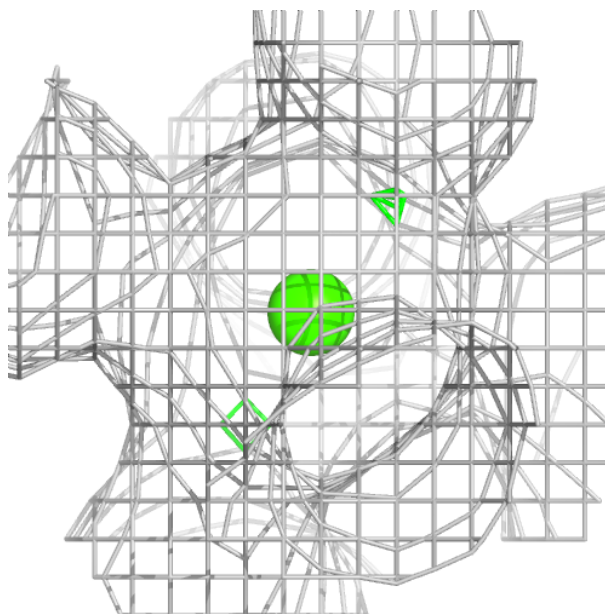
**Electron density around CA D 603:**

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



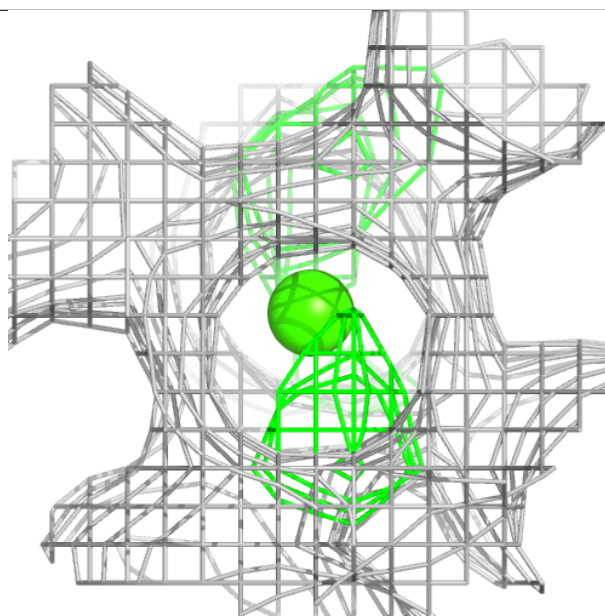
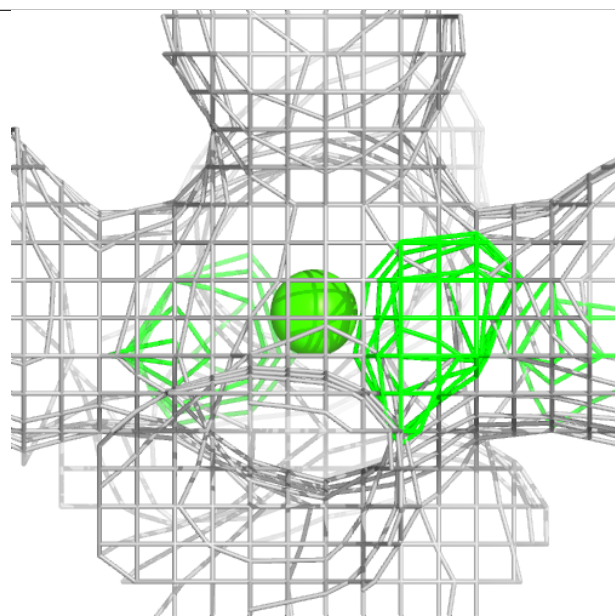
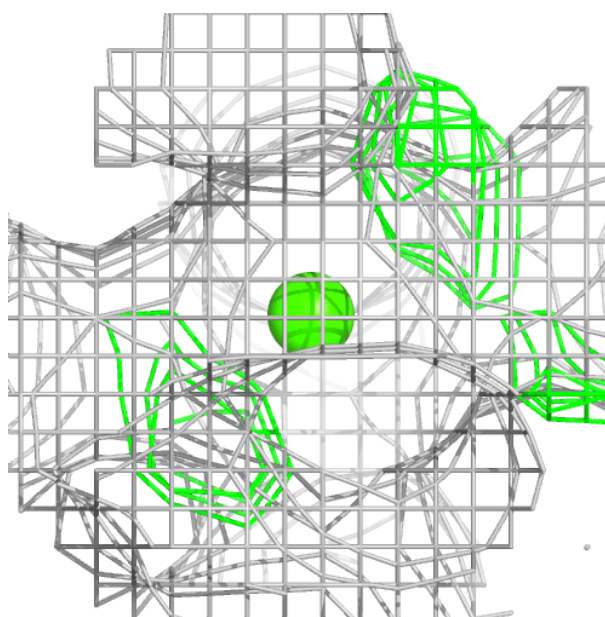
**Electron density around CA C 603:**

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



**Electron density around CA C 601:**

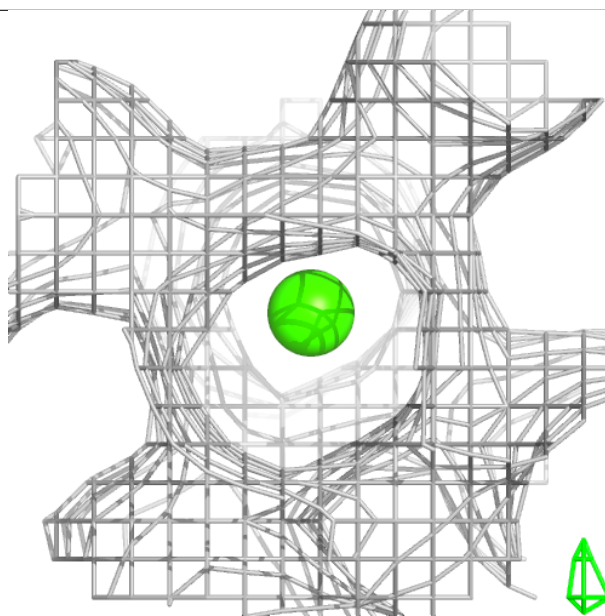
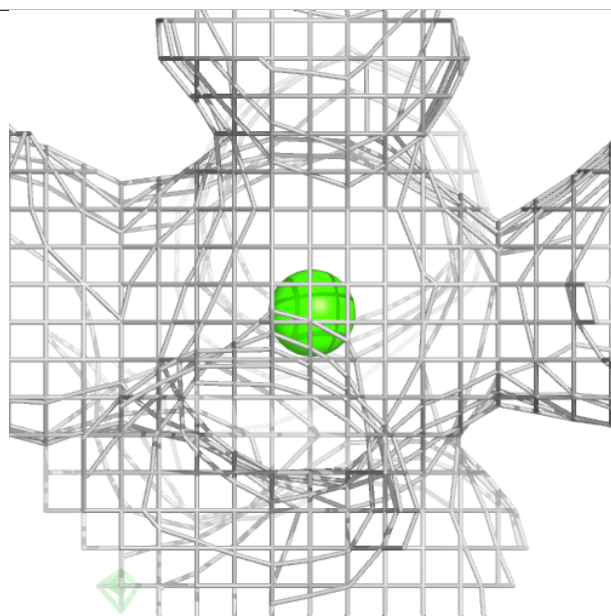
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





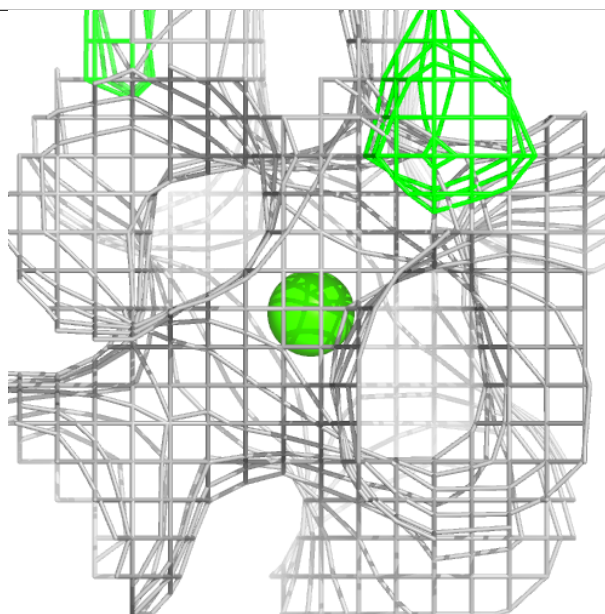
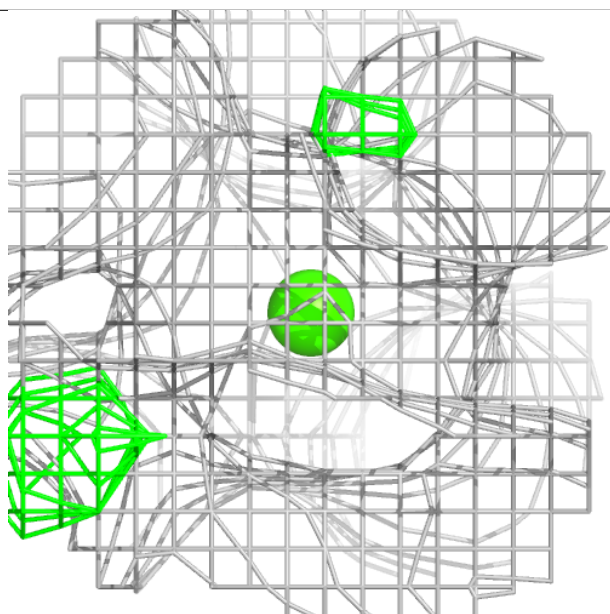
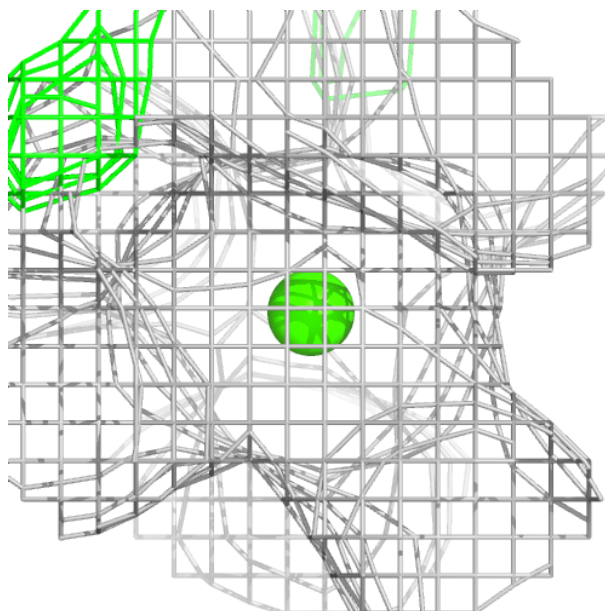
**Electron density around CA D 601:**

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



**Electron density around CA C 602:**

$2mF_o-DF_c$  (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.