Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:56 AM BST

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

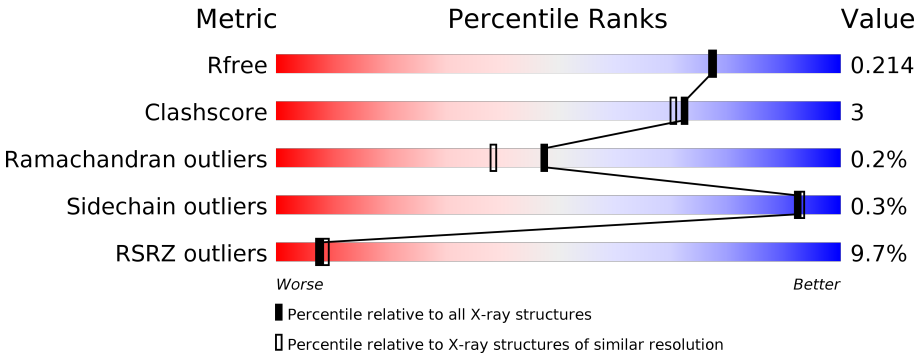
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	12% 62% • 33%
1	B	141	26% 59% 6% • 34%
2	C	422	5% 90% 7% •
2	D	422	5% 90% 8% •
3	E	2	50% 50%
3	I	2	100%

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Mol	Chain	Length	Quality of chain
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%

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
13	MES	D	610	-	-	-	X

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			

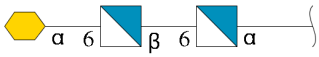
There are 2 discrepancies between the modelled and reference sequences:

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.

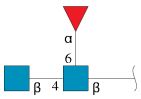
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			
3	I	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			

- 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.

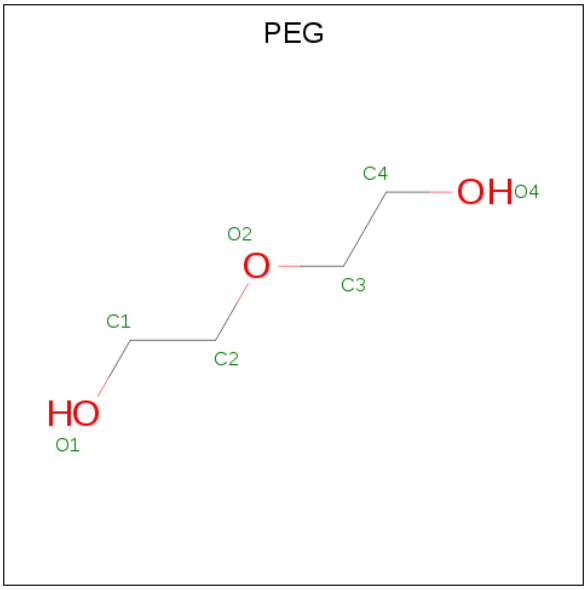


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			
5	K	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			

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

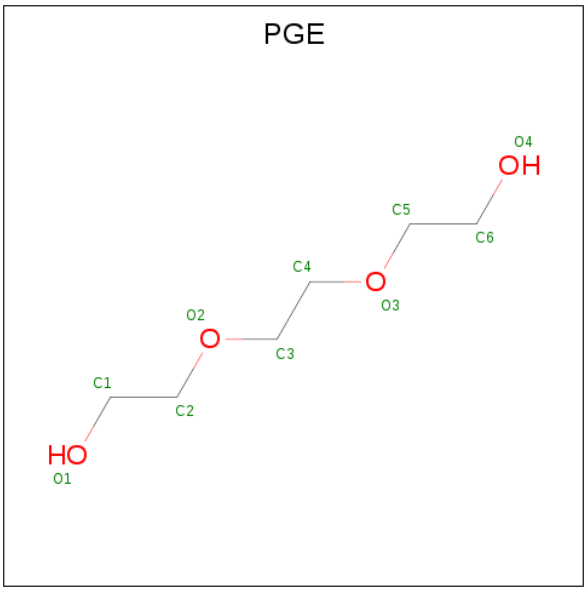
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
6	L	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



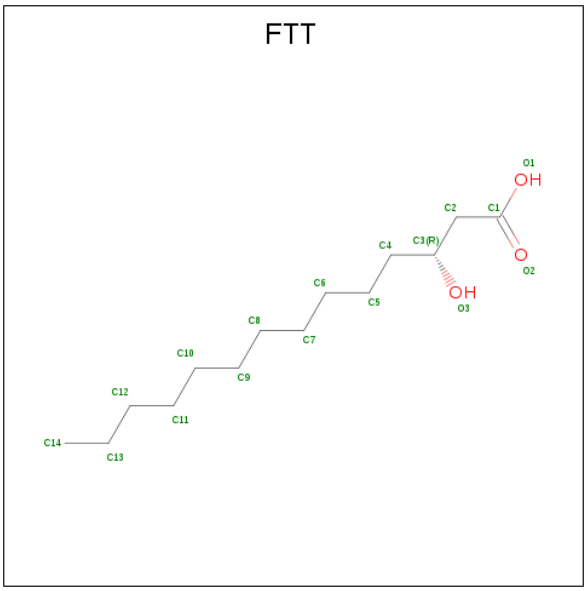
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 17 4 10 3	0	0
7	A	1	Total C H O 17 4 10 3	0	0
7	C	1	Total C H O 17 4 10 3	0	0
7	C	1	Total C H O 17 4 10 3	0	0
7	C	1	Total C H O 17 4 10 3	0	0
7	C	1	Total C H O 17 4 10 3	0	0
7	C	1	Total C H O 17 4 10 3	0	0
7	C	1	Total C H O 17 4 10 3	0	0
7	C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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



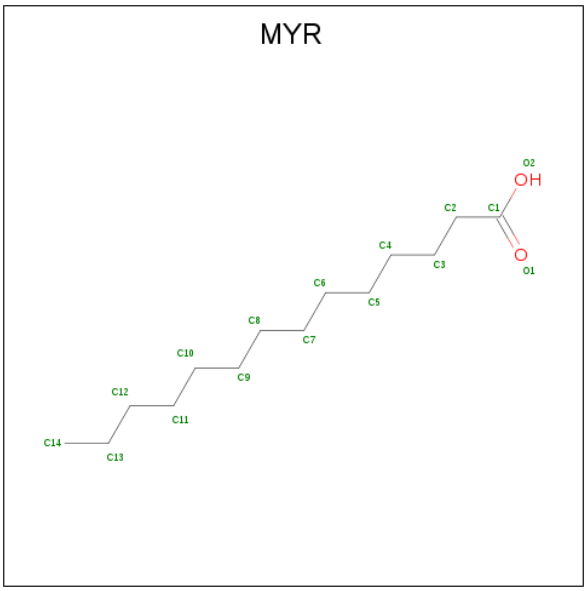
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			24	6	14	4		
8	C	1	Total	C	H	O	0	0
			24	6	14	4		
8	C	1	Total	C	H	O	0	0
			24	6	14	4		
8	C	1	Total	C	H	O	0	0
			24	6	14	4		
8	D	1	Total	C	H	O	0	0
			24	6	14	4		
8	D	1	Total	C	H	O	0	0
			24	6	14	4		
8	D	1	Total	C	H	O	0	0
			24	6	14	4		

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



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: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by author).

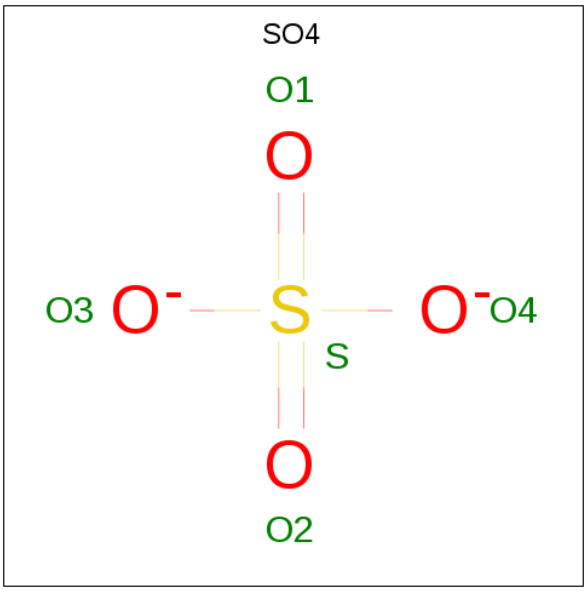


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C H O 43 14 27 2	0	0
10	C	1	Total C H O 42 14 27 1	0	0
10	B	1	Total C H O 43 14 27 2	0	0
10	D	1	Total C H O 42 14 27 1	0	0

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

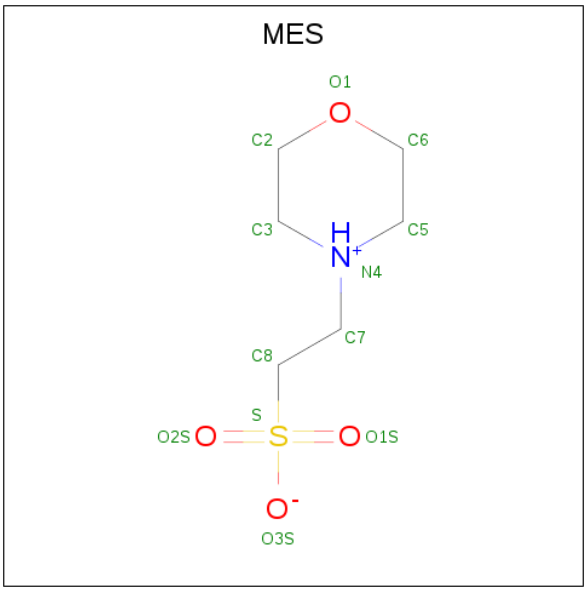
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	3	Total Ca 3 3	0	0
11	C	3	Total Ca 3 3	0	0

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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



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

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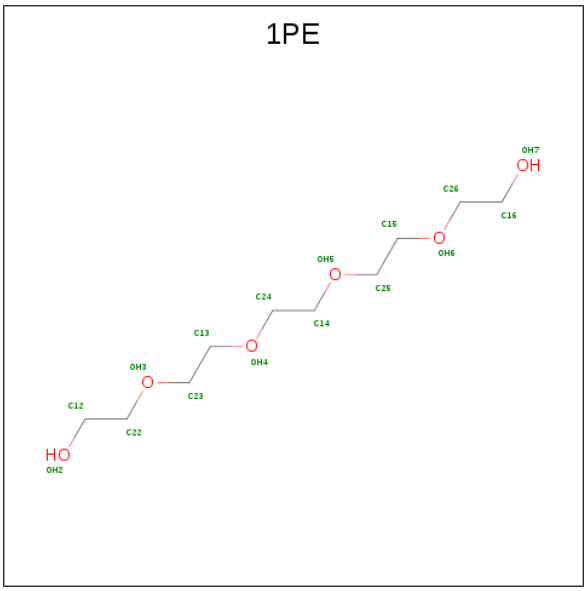
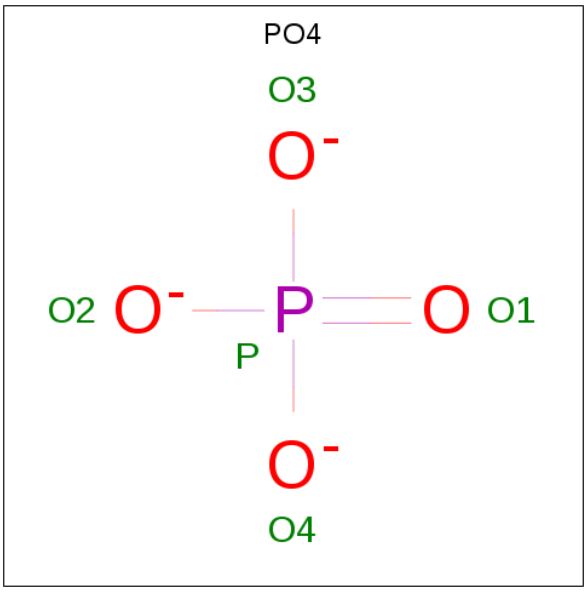
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
13	D	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 14 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by author).



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_4P) (labeled as "Ligand of Interest" by author).



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

- Molecule 16 is water.

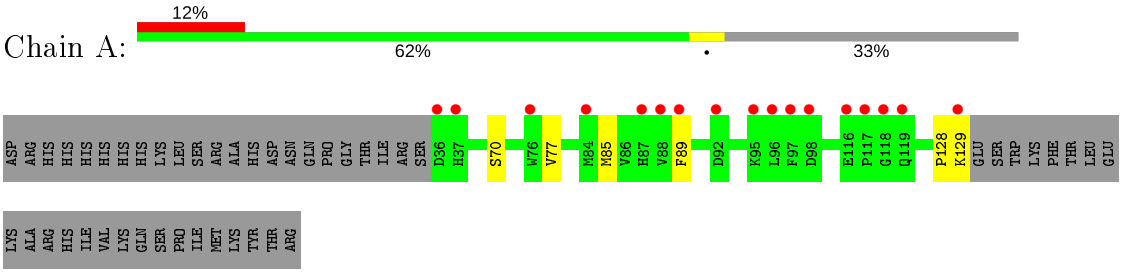
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	24	Total O 24 24	0	0
16	C	236	Total O 236 236	0	0
16	B	17	Total O 17 17	0	0
16	D	171	Total O 171 171	0	0

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.

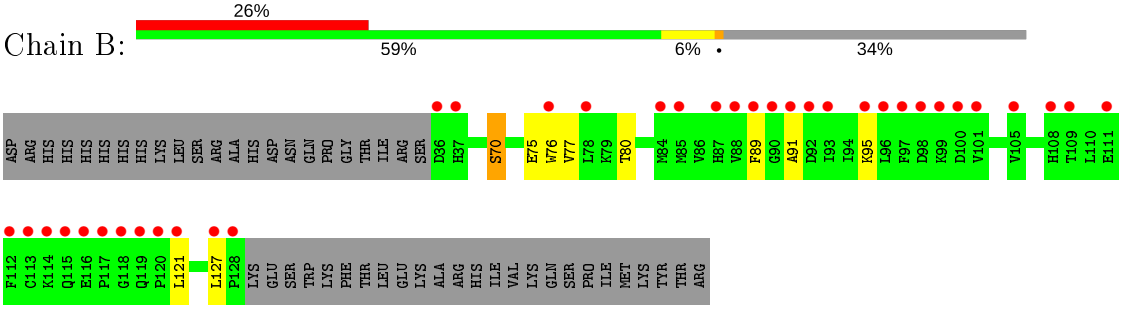
- Molecule 1: Acyloxyacyl hydrolase small subunit

Chain A:



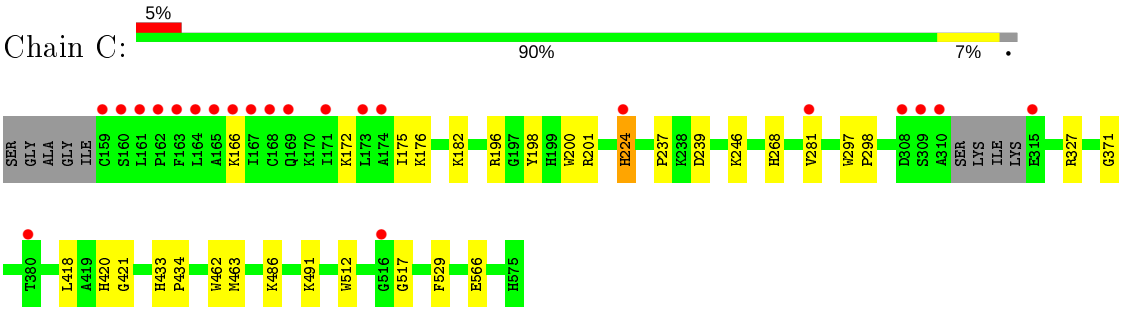
- Molecule 1: Acyloxyacyl hydrolase small subunit

Chain B:



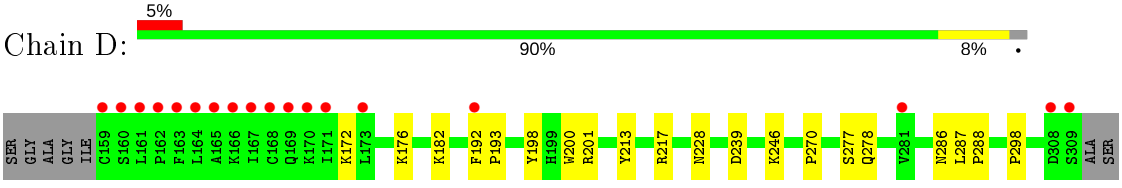
- Molecule 2: Acyloxyacyl hydrolase large subunit

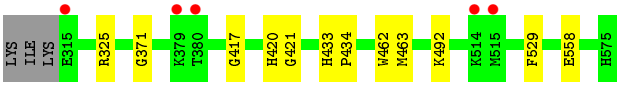
Chain C:



- Molecule 2: Acyloxyacyl hydrolase large subunit

Chain D:



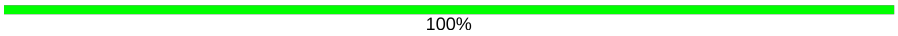


• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

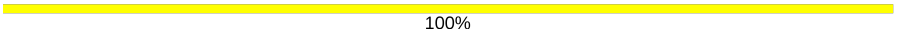
• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• 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:

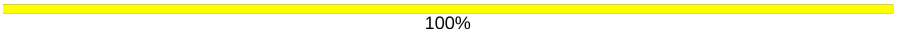


• Molecule 4: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose

Chain J:

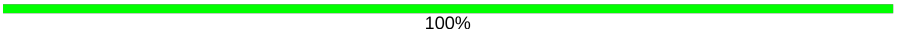
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• 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:



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

Chain H:

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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.95 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.185 , 0.213 0.186 , 0.214	Depositor DCC
R_{free} test set	1912 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[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: PA1, FTT, PGE, NAG, CA, MYR, 1PE, GCS, KDO, SO4, MES, PEG, PO4, 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

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

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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.

All (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

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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:O	1:B:77:VAL:HG12	2.01	0.59
1:A:77:VAL:HG12	1:A:77:VAL:O	2.05	0.56
2:D:277:SER:O	13:D:610:MES:H62	2.04	0.56
2:C:239:ASP:OD2	2:C:246:LYS:NZ	2.37	0.56
2:D:277:SER:OG	2:D:278:GLN:OE1	2.24	0.56
2:C:166:LYS:HD2	1:B:89:PHE:HE2	1.73	0.54
2:D:239:ASP:OD2	2:D:246:LYS:NZ	2.20	0.54
2:C:463:MET:CE	2:C:529:PHE:HB2	2.40	0.52
2:D:463:MET:CE	2:D:529:PHE:HB2	2.40	0.52
2:D:286:ASN:HB3	7:D:613:PEG:H32	1.91	0.52
2:D:421:GLY:HA3	2:D:462:TRP:CD2	2.45	0.52
2:C:418:LEU:O	7:C:620:PEG:H41	2.10	0.51
4:J:3:KDO:O5	4:J:3:KDO:O7	2.18	0.50
2:C:463:MET:HE1	2:C:529:PHE:HB2	1.94	0.50
1:B:77:VAL:HG13	1:B:80:THR:HB	1.93	0.50
2:C:224:HIS:CD2	2:C:224:HIS:H	2.30	0.50
2:C:491:LYS:NZ	16:C:710:HOH:O	2.45	0.49
2:D:217:ARG:HB2	8:D:616:PGE:H12	1.95	0.49
2:C:175:ILE:HG12	7:C:613:PEG:H32	1.96	0.48
2:C:182:LYS:NZ	16:C:711:HOH:O	2.46	0.48
1:A:128:PRO:O	1:A:129:LYS:HB2	2.14	0.48
1:B:75:GLU:O	1:B:76:TRP:HB2	2.14	0.48
2:D:286:ASN:HB3	7:D:613:PEG:H41	1.95	0.47
2:C:418:LEU:O	7:C:620:PEG:C4	2.63	0.47
2:D:433:HIS:CG	2:D:434:PRO:HD2	2.50	0.47
2:D:492:LYS:NZ	16:D:712:HOH:O	2.49	0.46
2:D:270:PRO:HB3	7:D:612:PEG:H42	1.97	0.46
2:D:198:TYR:HA	2:D:201:ARG:O	2.16	0.45
2:D:325:ARG:HG3	2:D:558:GLU:HA	1.98	0.45
2:C:486:LYS:NZ	14:C:624:1PE:OH5	2.49	0.45
2:D:200:TRP:CD2	2:D:298:PRO:HG3	2.52	0.45
2:C:237:PRO:O	7:C:618:PEG:H22	2.17	0.44
2:C:421:GLY:HA3	2:C:462:TRP:CD2	2.52	0.44
2:C:198:TYR:HA	2:C:201:ARG:O	2.17	0.44
1:B:121:LEU:CD2	1:B:127:LEU:HD21	2.47	0.44
2:C:420[A]:HIS:CD2	7:C:620:PEG:H21	2.52	0.44
2:C:268:HIS:HB3	2:C:297:TRP:CD1	2.53	0.44
2:C:433:HIS:CG	2:C:434:PRO:HD2	2.53	0.43
2:D:172:LYS:O	2:D:176:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:ASN:HB3	7:D:613:PEG:C4	2.49	0.43
2:C:327[B]:ARG:NH2	2:C:566:GLU:OE1	2.52	0.42
2:D:287:LEU:HB3	2:D:288:PRO:HD3	2.01	0.42
2:D:213:TYR:O	2:D:228:ASN:HA	2.18	0.42
2:D:192[A]:PHE:CD1	2:D:193:PRO:HD2	2.54	0.42
14:D:619:1PE:H252	16:D:705:HOH:O	2.19	0.42
2:C:166:LYS:CD	1:B:89:PHE:HE2	2.32	0.42
1:A:85:MET:HE3	1:A:89:PHE:CD1	2.55	0.41
1:B:91:ALA:O	1:B:95:LYS:HG3	2.20	0.41
2:D:417:GLY:HA3	7:D:611:PEG:H42	2.02	0.41
1:B:70:SER:OG	16:B:701:HOH:O	2.22	0.41
2:C:224:HIS:HD2	2:C:224:HIS:H	1.69	0.41
2:D:420[A]:HIS:CD2	7:D:611:PEG:H11	2.56	0.41
2:C:196:ARG:HA	2:C:200:TRP:CD1	2.56	0.41
2:D:192[A]:PHE:CG	2:D:193:PRO:HD2	2.56	0.41
2:C:200:TRP:CD2	2:C:298:PRO:HG3	2.56	0.40
2:C:512:TRP:CE2	2:C:517:GLY:HA3	2.56	0.40
15:D:621:PO4:O2	4:J:2:GCS:H62	2.22	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	415/422 (98%)	402 (97%)	12 (3%)	1 (0%)	47 38
2	D	415/422 (98%)	396 (95%)	18 (4%)	1 (0%)	47 38
All	All	1013/1126 (90%)	975 (96%)	36 (4%)	2 (0%)	47 38

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%)	71 70
1	B	85/130 (65%)	84 (99%)	1 (1%)	71 70
2	C	366/366 (100%)	365 (100%)	1 (0%)	92 93
2	D	366/366 (100%)	366 (100%)	0	100 100
All	All	903/992 (91%)	900 (100%)	3 (0%)	92 93

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

Some 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	1,3	14,14,15	1.02	1 (7%)	17,19,21	0.80	1 (5%)
3	FUC	E	2	3	10,10,11	0.83	0	14,14,16	0.86	0
4	PA1	F	1	9,15,4	11,11,12	1.65	3 (27%)	12,15,17	1.12	0
4	GCS	F	2	9,15,4	11,11,12	1.77	2 (18%)	12,15,17	0.91	0
4	KDO	F	3	4	12,15,16	1.58	3 (25%)	16,21,24	2.75	5 (31%)
5	NAG	G	1	2,5	14,14,15	0.85	1 (7%)	17,19,21	0.51	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	0.95	1 (10%)	14,14,16	0.76	0
6	NAG	H	1	2,6	14,14,15	0.44	0	17,19,21	0.49	0
6	NAG	H	2	6	14,14,15	1.16	1 (7%)	17,19,21	1.37	2 (11%)
3	NAG	I	1	1,3	14,14,15	0.29	0	17,19,21	0.40	0
3	FUC	I	2	3	10,10,11	0.72	0	14,14,16	0.82	0
4	PA1	J	1	9,15,4	11,11,12	1.72	3 (27%)	12,15,17	1.23	1 (8%)
4	GCS	J	2	9,15,4	11,11,12	1.79	3 (27%)	12,15,17	1.80	5 (41%)
4	KDO	J	3	4	12,15,16	1.25	2 (16%)	16,21,24	1.83	5 (31%)
5	NAG	K	1	2,5	14,14,15	0.56	0	17,19,21	0.44	0
5	NAG	K	2	5	14,14,15	0.20	0	17,19,21	0.59	0
5	FUC	K	3	5	10,10,11	0.63	0	14,14,16	0.95	0
6	NAG	L	1	2,6	14,14,15	0.24	0	17,19,21	0.83	1 (5%)
6	NAG	L	2	6	14,14,15	0.45	0	17,19,21	1.25	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	1,3	-	0/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
4	PA1	F	1	9,15,4	-	0/2/19/22	0/1/1/1
4	GCS	F	2	9,15,4	-	0/2/19/22	0/1/1/1
4	KDO	F	3	4	-	0/6/26/30	0/1/1/1
5	NAG	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	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	1,3	-	0/6/23/26	0/1/1/1
3	FUC	I	2	3	-	-	0/1/1/1
4	PA1	J	1	9,15,4	-	0/2/19/22	0/1/1/1
4	GCS	J	2	9,15,4	-	0/2/19/22	0/1/1/1
4	KDO	J	3	4	-	2/6/26/30	0/1/1/1
5	NAG	K	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	3/6/23/26	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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	GCS	O5-C1	4.50	1.50	1.43
4	J	1	PA1	O5-C1	4.39	1.50	1.43
4	J	2	GCS	O5-C1	4.25	1.50	1.43
4	F	1	PA1	O5-C1	4.16	1.50	1.43
6	H	2	NAG	O5-C1	-4.15	1.37	1.43
3	E	1	NAG	O5-C1	-3.35	1.38	1.43
4	F	3	KDO	C3-C4	-3.10	1.47	1.52
5	G	1	NAG	O5-C1	-3.07	1.38	1.43
4	F	3	KDO	O6-C2	2.88	1.51	1.43
4	J	2	GCS	C3-C2	-2.86	1.47	1.53
4	F	2	GCS	C3-C2	-2.77	1.47	1.53
4	J	1	PA1	C3-C2	-2.35	1.48	1.53
4	J	2	GCS	O5-C5	2.33	1.48	1.43
4	F	3	KDO	O6-C6	2.31	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	KDO	C3-C4	-2.29	1.48	1.52
4	F	1	PA1	C3-C2	-2.23	1.48	1.53
5	G	3	FUC	O5-C1	-2.20	1.40	1.43
4	J	1	PA1	O5-C5	2.12	1.47	1.43
4	J	3	KDO	O6-C2	2.10	1.49	1.43
4	F	1	PA1	O5-C5	2.01	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	3	KDO	O6-C6-C5	7.33	118.16	107.87
4	F	3	KDO	C7-C6-C5	-4.23	107.02	114.03
6	H	2	NAG	C3-C4-C5	4.16	117.66	110.24
4	F	3	KDO	C6-O6-C2	3.89	119.67	111.34
6	L	2	NAG	C1-O5-C5	3.77	117.30	112.19
4	F	3	KDO	O6-C2-C3	3.45	115.93	109.87
4	J	2	GCS	C1-O5-C5	3.23	116.56	112.19
4	J	3	KDO	C3-C4-C5	3.21	115.34	110.69
4	J	3	KDO	O6-C2-C3	3.14	115.38	109.87
4	J	3	KDO	O6-C6-C5	2.98	112.05	107.87
4	J	2	GCS	O5-C5-C4	2.73	117.46	110.83
6	L	1	NAG	C1-O5-C5	2.71	115.86	112.19
4	F	3	KDO	C4-C5-C6	2.68	115.78	110.41
6	H	2	NAG	C4-C3-C2	2.55	114.76	111.02
4	J	2	GCS	C4-C3-C2	-2.49	107.16	111.37
5	G	2	NAG	C3-C4-C5	2.45	114.60	110.24
5	G	2	NAG	C1-O5-C5	2.40	115.44	112.19
4	J	3	KDO	C6-O6-C2	-2.35	106.32	111.34
4	J	3	KDO	C3-C2-C1	2.29	116.92	111.93
5	G	2	NAG	O5-C1-C2	-2.25	107.74	111.29
4	J	2	GCS	O6-C6-C5	-2.24	103.61	111.29
4	J	1	PA1	C3-C4-C5	2.16	114.10	110.24
4	J	2	GCS	O5-C5-C6	-2.09	103.92	107.20
3	E	1	NAG	C1-O5-C5	-2.02	109.46	112.19

There are no chirality outliers.

All (11) 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
6	L	1	NAG	O5-C5-C6-O6

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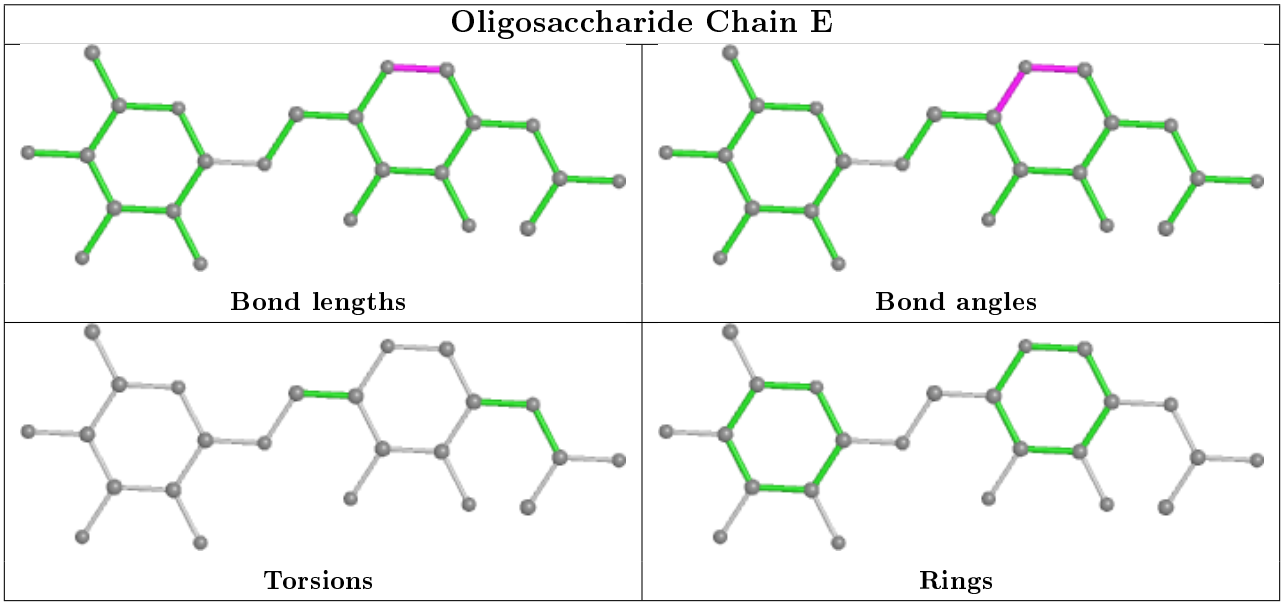
Mol	Chain	Res	Type	Atoms
6	H	2	NAG	C4-C5-C6-O6
4	J	3	KDO	O6-C6-C7-C8
6	H	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C4-C5-C6-O6
4	J	3	KDO	C5-C6-C7-C8

There are no ring outliers.

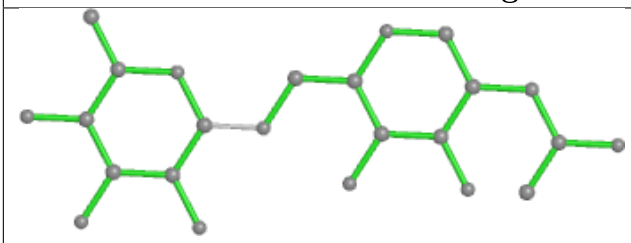
2 monomers are involved in 2 short contacts:

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

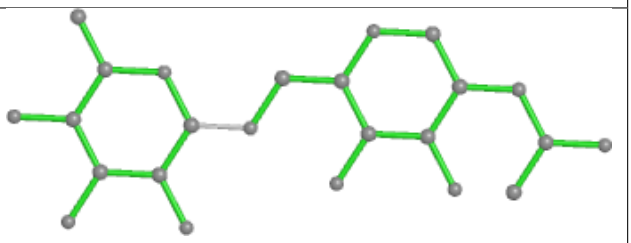
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



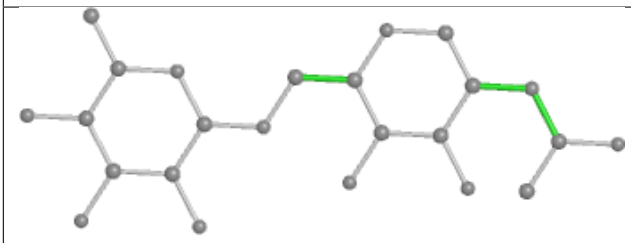
Oligosaccharide Chain I



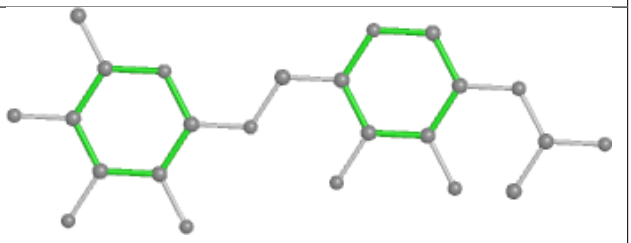
Bond lengths



Bond angles

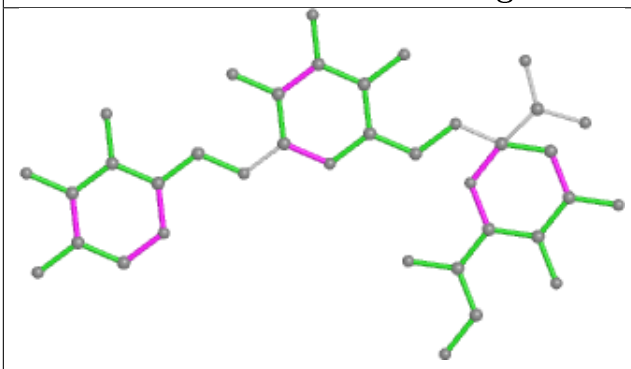


Torsions

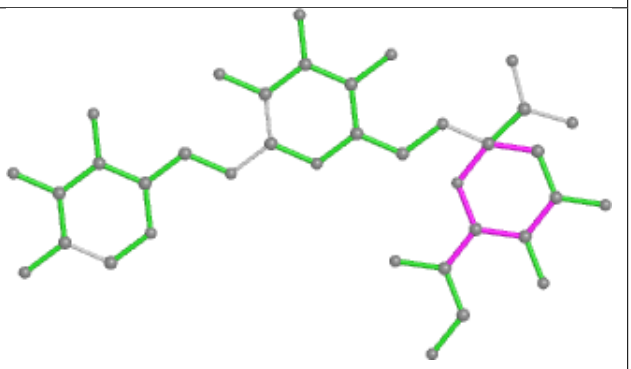


Rings

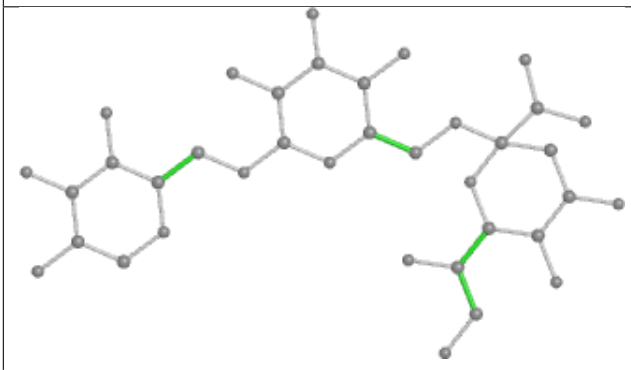
Oligosaccharide Chain F



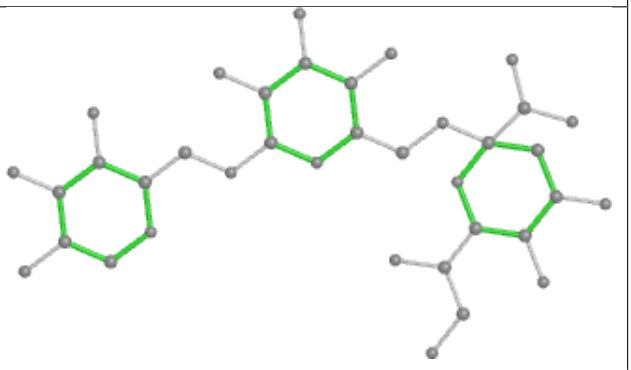
Bond lengths



Bond angles

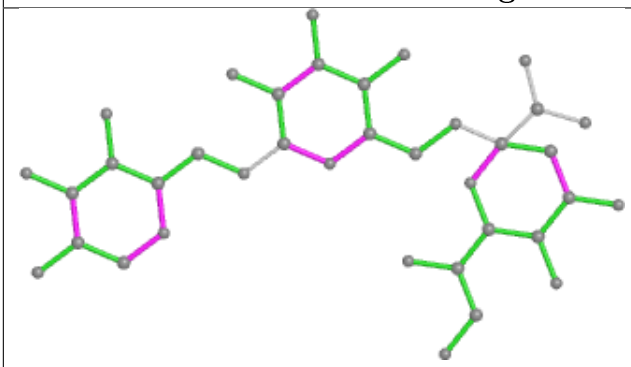


Torsions

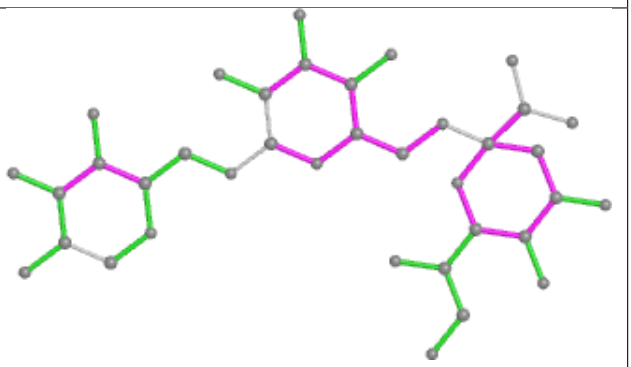


Rings

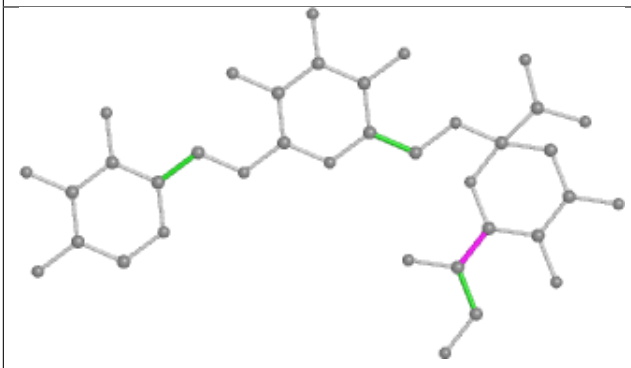
Oligosaccharide Chain J



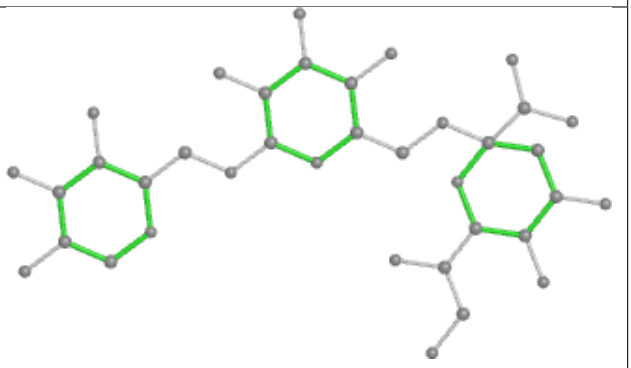
Bond lengths



Bond angles

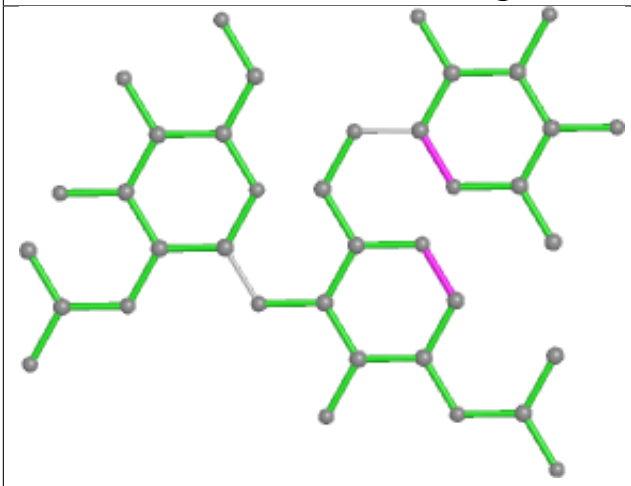


Torsions

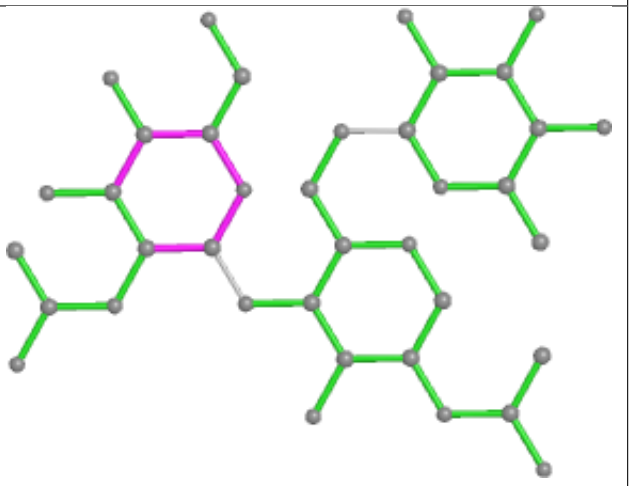


Rings

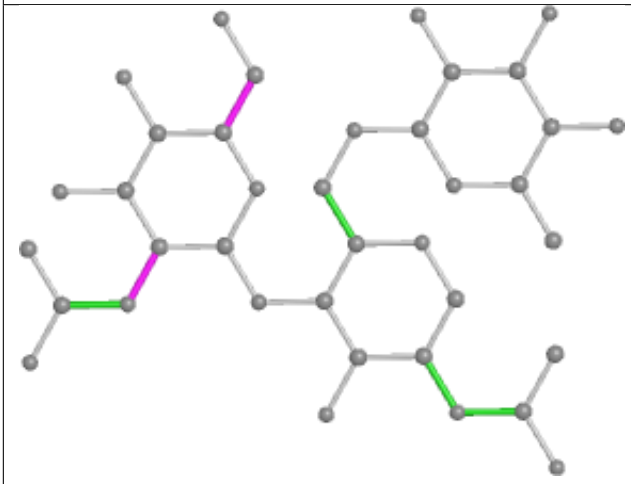
Oligosaccharide Chain G



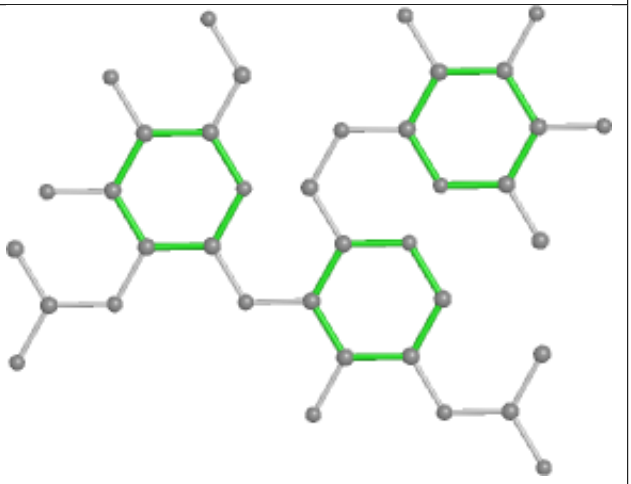
Bond lengths



Bond angles

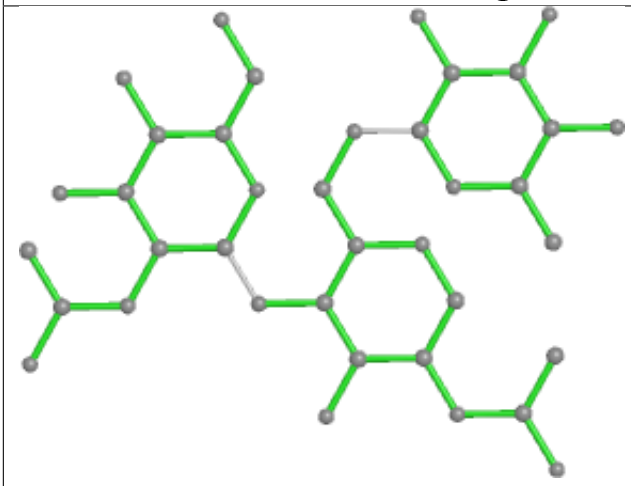


Torsions

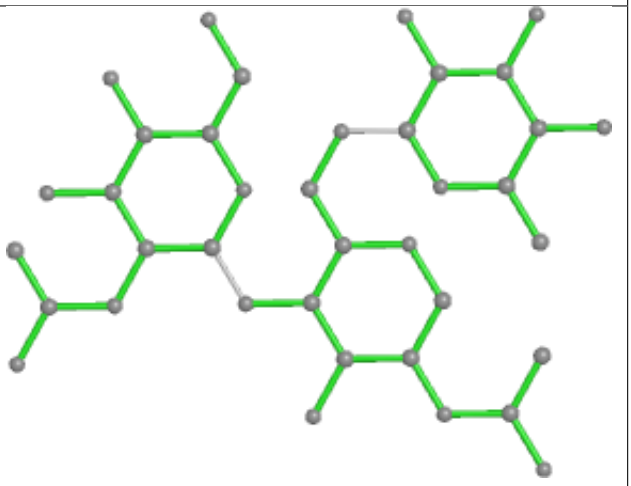


Rings

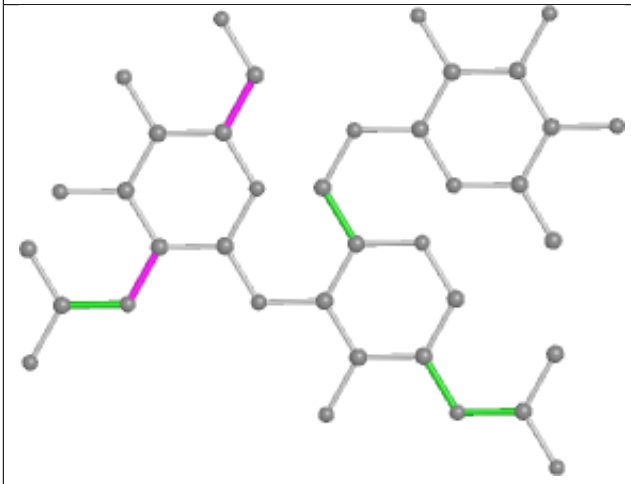
Oligosaccharide Chain K



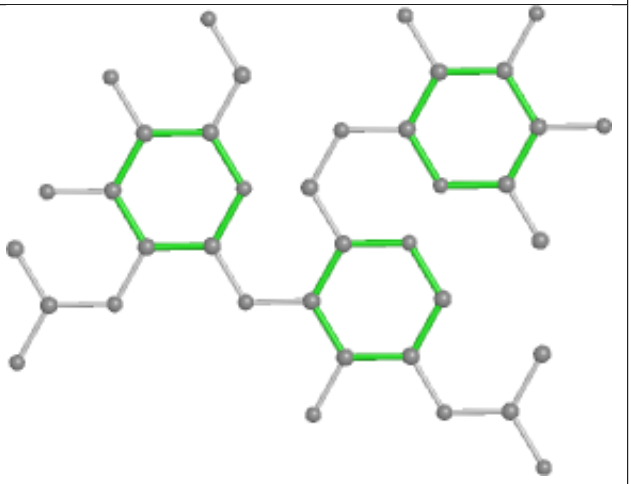
Bond lengths



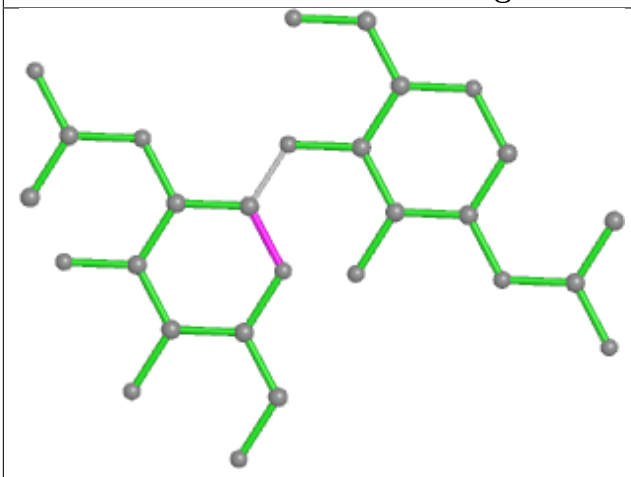
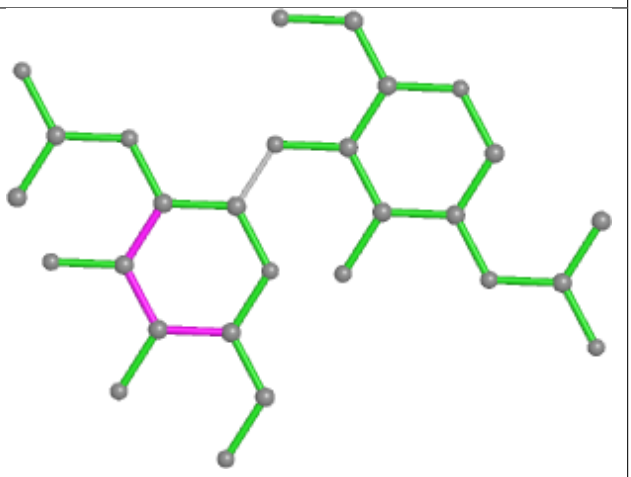
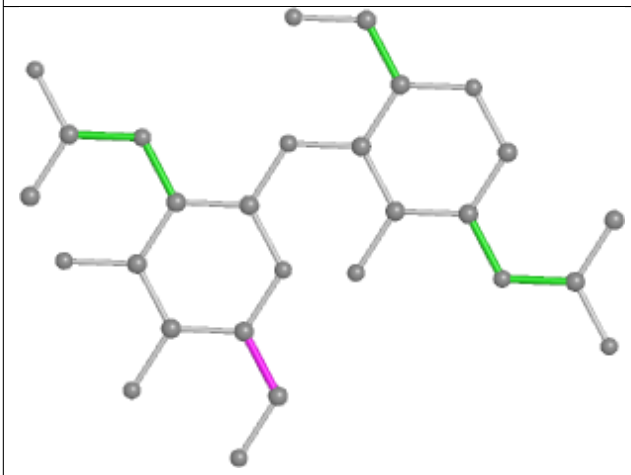
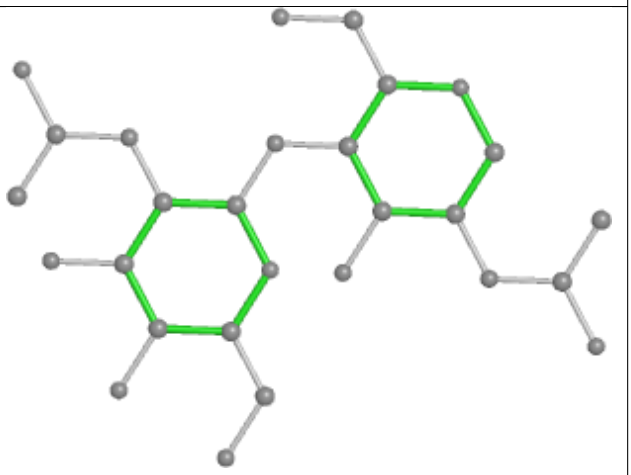
Bond angles



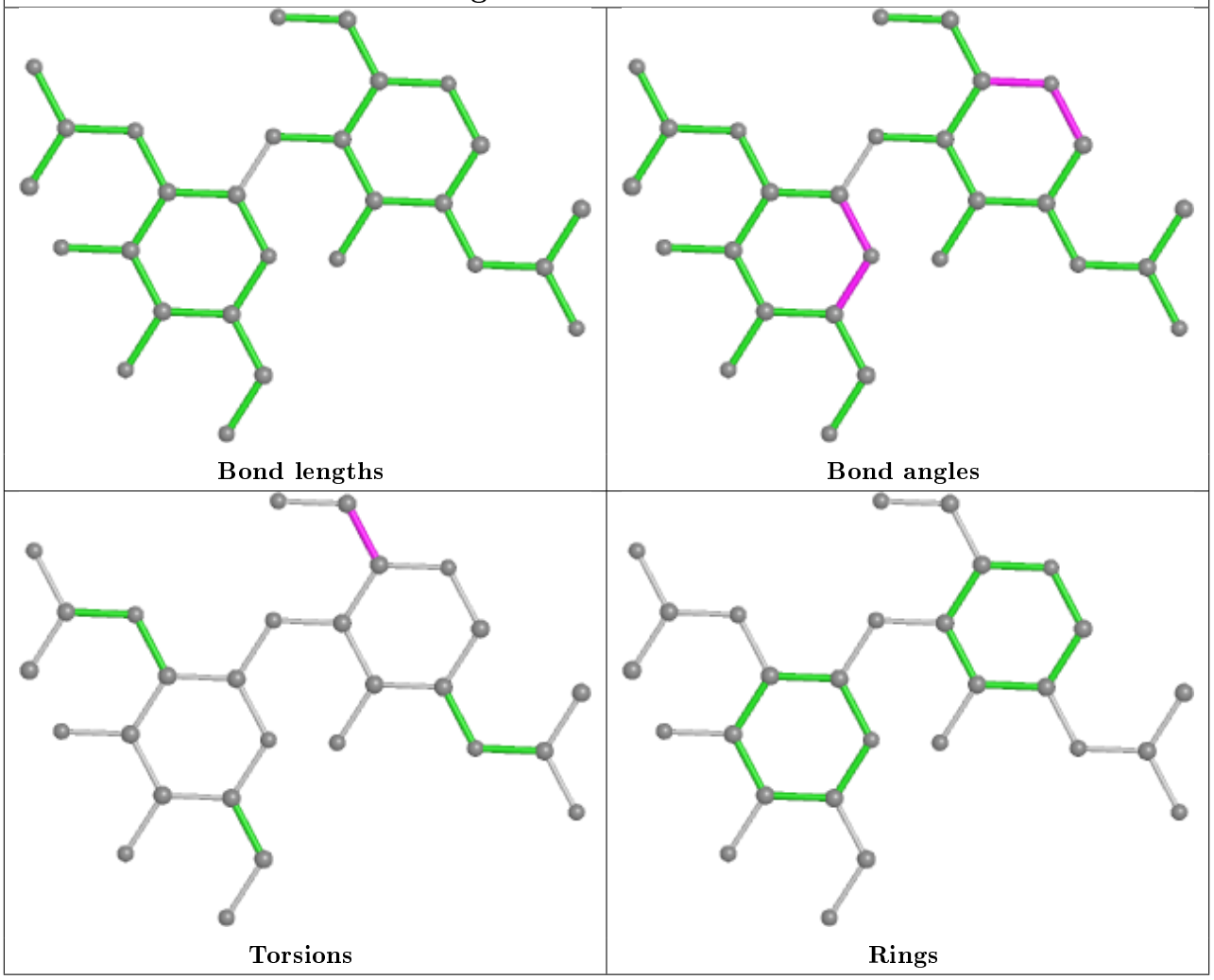
Torsions



Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain L



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	$\#\|Z\| > 2$
8	PGE	D	615	-	9,9,9	0.31	0	8,8,8	0.26	0
15	PO4	C	626	4	4,4,4	0.89	0	6,6,6	0.55	0
7	PEG	C	618	-	6,6,6	0.51	0	5,5,5	0.38	0
9	FTT	D	622	4	15,15,16	0.64	0	15,15,17	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	FTT	D	623	4	15,15,16	0.52	0	15,15,17	1.31	2 (13%)
7	PEG	C	617	-	6,6,6	0.46	0	5,5,5	0.30	0
14	1PE	C	625	-	15,15,15	0.54	0	14,14,14	0.42	0
9	FTT	C	628	4	15,15,16	0.60	0	15,15,17	0.90	0
7	PEG	C	614	-	6,6,6	0.47	0	5,5,5	0.36	0
12	SO4	D	609	-	4,4,4	0.14	0	6,6,6	0.13	0
8	PGE	C	623	-	9,9,9	0.36	0	8,8,8	0.48	0
7	PEG	D	613	-	6,6,6	0.53	0	5,5,5	0.34	0
9	FTT	C	629	4	15,15,16	0.59	0	15,15,17	1.19	2 (13%)
7	PEG	C	619	-	6,6,6	0.51	0	5,5,5	1.02	0
7	PEG	C	616	-	6,6,6	0.49	0	5,5,5	0.27	0
15	PO4	C	627	4	0,3,4	0.00	-	0,3,6	0.00	-
7	PEG	C	612	-	6,6,6	0.48	0	5,5,5	0.35	0
15	PO4	D	620	4	4,4,4	0.94	0	6,6,6	0.43	0
7	PEG	D	611	-	6,6,6	0.48	0	5,5,5	0.37	0
7	PEG	C	613	-	6,6,6	0.46	0	5,5,5	0.60	0
15	PO4	D	621	4	0,3,4	0.00	-	0,3,6	0.00	-
7	PEG	C	611	-	6,6,6	0.48	0	5,5,5	0.48	0
14	1PE	D	618	-	15,15,15	0.52	0	14,14,14	0.34	0
10	MYR	D	624	9	14,14,15	0.41	0	13,13,15	0.74	0
14	1PE	C	624	-	15,15,15	0.53	0	14,14,14	0.46	0
10	MYR	C	630	9	14,14,15	0.35	0	13,13,15	0.78	0
12	SO4	C	609	-	4,4,4	0.14	0	6,6,6	0.07	0
8	PGE	C	622	-	9,9,9	0.31	0	8,8,8	0.40	0
10	MYR	A	210	-	12,15,15	0.29	0	11,15,15	0.60	0
13	MES	D	610	-	12,12,12	2.34	1 (8%)	14,16,16	1.58	4 (28%)
9	FTT	A	209	10,4	15,15,16	0.56	0	15,15,17	1.14	1 (6%)
14	1PE	D	619	-	15,15,15	0.52	0	14,14,14	0.47	0
13	MES	C	610	-	12,12,12	2.16	1 (8%)	14,16,16	1.84	5 (35%)
10	MYR	B	208	-	12,15,15	0.27	0	11,15,15	0.61	0
8	PGE	D	617	-	9,9,9	0.30	0	8,8,8	0.45	0
8	PGE	D	616	-	9,9,9	0.31	0	8,8,8	0.32	0
7	PEG	D	614	-	6,6,6	0.49	0	5,5,5	0.42	0
13	MES	B	203	-	12,12,12	2.28	1 (8%)	14,16,16	1.61	2 (14%)
7	PEG	A	204	-	6,6,6	0.44	0	5,5,5	0.44	0
8	PGE	A	205	-	9,9,9	0.32	0	8,8,8	0.34	0
7	PEG	C	620	-	6,6,6	0.44	0	5,5,5	0.48	0
7	PEG	A	203	-	6,6,6	0.48	0	5,5,5	0.44	0
7	PEG	C	615	-	6,6,6	0.50	0	5,5,5	0.29	0
8	PGE	C	621	-	9,9,9	0.31	0	8,8,8	0.39	0
7	PEG	D	612	-	6,6,6	0.47	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	FTT	B	207	10,4	15,15,16	0.52	0	15,15,17	1.25	2 (13%)

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
8	PGE	D	615	-	-	0/7/7/7	-
7	PEG	C	618	-	-	2/4/4/4	-
9	FTT	D	622	4	-	0/14/14/15	-
9	FTT	D	623	4	-	10/14/14/15	-
7	PEG	C	617	-	-	1/4/4/4	-
14	1PE	C	625	-	-	3/13/13/13	-
9	FTT	C	628	4	-	1/14/14/15	-
7	PEG	C	614	-	-	2/4/4/4	-
8	PGE	C	623	-	-	3/7/7/7	-
7	PEG	D	613	-	-	2/4/4/4	-
9	FTT	C	629	4	-	8/14/14/15	-
7	PEG	C	619	-	-	2/4/4/4	-
7	PEG	C	616	-	-	2/4/4/4	-
7	PEG	C	612	-	-	2/4/4/4	-
7	PEG	D	611	-	-	1/4/4/4	-
7	PEG	C	613	-	-	1/4/4/4	-
8	PGE	A	205	-	-	6/7/7/7	-
7	PEG	C	611	-	-	3/4/4/4	-
14	1PE	D	618	-	-	7/13/13/13	-
10	MYR	D	624	9	-	1/11/12/13	-
14	1PE	C	624	-	-	4/13/13/13	-
10	MYR	C	630	9	-	4/11/12/13	-
8	PGE	C	622	-	-	6/7/7/7	-
10	MYR	A	210	-	-	6/11/13/13	-
13	MES	D	610	-	-	3/6/14/14	0/1/1/1
9	FTT	A	209	10,4	-	6/14/14/15	-
14	1PE	D	619	-	-	9/13/13/13	-
13	MES	C	610	-	-	0/6/14/14	0/1/1/1
10	MYR	B	208	-	-	1/11/13/13	-
8	PGE	D	617	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PGE	D	616	-	-	4/7/7/7	-
7	PEG	D	614	-	-	2/4/4/4	-
13	MES	B	203	-	-	3/6/14/14	0/1/1/1
7	PEG	A	204	-	-	1/4/4/4	-
7	PEG	C	620	-	-	3/4/4/4	-
7	PEG	A	203	-	-	3/4/4/4	-
7	PEG	C	615	-	-	1/4/4/4	-
8	PGE	C	621	-	-	4/7/7/7	-
7	PEG	D	612	-	-	2/4/4/4	-
9	FTT	B	207	10,4	-	10/14/14/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	610	MES	C8-S	-7.91	1.66	1.77
13	B	203	MES	C8-S	-7.64	1.66	1.77
13	C	610	MES	C8-S	-7.20	1.67	1.77

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	203	MES	C5-N4-C3	4.13	118.12	108.83
13	D	610	MES	C5-N4-C3	3.45	116.60	108.83
13	C	610	MES	C5-N4-C3	3.04	115.67	108.83
9	D	623	FTT	C3-C2-C1	-2.86	107.73	112.75
9	C	629	FTT	C5-C4-C3	-2.79	106.81	114.85
13	C	610	MES	O3S-S-C8	2.78	110.27	105.77
13	C	610	MES	O1S-S-C8	2.74	110.21	106.92
9	B	207	FTT	O2-C1-C2	-2.63	117.77	125.43
9	B	207	FTT	C5-C4-C3	-2.57	107.46	114.85
13	B	203	MES	O1S-S-C8	2.56	109.99	106.92
13	C	610	MES	C6-C5-N4	-2.55	106.23	110.10
9	A	209	FTT	O2-C1-C2	-2.53	118.06	125.43
9	C	629	FTT	O2-C1-C2	-2.26	118.84	125.43
13	C	610	MES	C2-C3-N4	2.25	113.51	110.10
13	D	610	MES	O3S-S-C8	2.06	109.09	105.77
13	D	610	MES	O1S-S-C8	2.04	109.37	106.92
9	D	623	FTT	O2-C1-C2	-2.03	119.50	125.43
13	D	610	MES	C7-N4-C5	2.02	116.40	111.23

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	623	FTT	C2-C3-C4-C5
9	C	629	FTT	C1-C2-C3-O3
13	D	610	MES	C8-C7-N4-C5
13	D	610	MES	C7-C8-S-O2S
9	A	209	FTT	O2-C1-C2-C3
13	B	203	MES	C7-C8-S-O1S
13	B	203	MES	C7-C8-S-O2S
9	B	207	FTT	O2-C1-C2-C3
9	B	207	FTT	C1-C2-C3-C4
9	B	207	FTT	C1-C2-C3-O3
9	B	207	FTT	C2-C3-C4-C5
7	C	619	PEG	C4-C3-O2-C2
8	C	622	PGE	O1-C1-C2-O2
8	C	621	PGE	O3-C5-C6-O4
14	D	618	1PE	OH6-C15-C25-OH5
9	C	629	FTT	C4-C5-C6-C7
7	C	611	PEG	O2-C3-C4-O4
14	D	619	1PE	OH6-C15-C25-OH5
9	B	207	FTT	O3-C3-C4-C5
7	C	614	PEG	O1-C1-C2-O2
7	C	614	PEG	O2-C3-C4-O4
7	C	619	PEG	O1-C1-C2-O2
7	C	616	PEG	O2-C3-C4-O4
7	C	612	PEG	O2-C3-C4-O4
14	D	618	1PE	OH7-C16-C26-OH6
14	D	619	1PE	OH7-C16-C26-OH6
7	A	203	PEG	O2-C3-C4-O4
8	C	623	PGE	O2-C3-C4-O3
14	D	618	1PE	OH4-C13-C23-OH3
8	A	205	PGE	O2-C3-C4-O3
7	C	618	PEG	O1-C1-C2-O2
7	D	611	PEG	O1-C1-C2-O2
14	D	618	1PE	OH2-C12-C22-OH3
8	C	622	PGE	O3-C5-C6-O4
8	D	616	PGE	O3-C5-C6-O4
7	D	614	PEG	O2-C3-C4-O4
7	A	204	PEG	O1-C1-C2-O2
9	D	623	FTT	C6-C7-C8-C9
9	A	209	FTT	C9-C10-C11-C12
10	A	210	MYR	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
14	D	619	1PE	OH5-C14-C24-OH4
9	A	209	FTT	C10-C11-C12-C13
14	C	624	1PE	OH7-C16-C26-OH6
7	A	203	PEG	O1-C1-C2-O2
8	C	621	PGE	O1-C1-C2-O2
7	D	612	PEG	O1-C1-C2-O2
10	B	208	MYR	C2-C3-C4-C5
9	B	207	FTT	C9-C10-C11-C12
9	C	629	FTT	O3-C3-C4-C5
9	D	623	FTT	C4-C5-C6-C7
7	C	612	PEG	O1-C1-C2-O2
8	A	205	PGE	O3-C5-C6-O4
14	C	625	1PE	OH6-C15-C25-OH5
9	A	209	FTT	C7-C8-C9-C10
9	B	207	FTT	C6-C7-C8-C9
8	C	622	PGE	O2-C3-C4-O3
10	A	210	MYR	C10-C11-C12-C13
13	B	203	MES	C7-C8-S-O3S
9	D	623	FTT	C7-C8-C9-C10
9	C	628	FTT	C1-C2-C3-O3
7	C	617	PEG	O1-C1-C2-O2
7	D	613	PEG	O2-C3-C4-O4
7	C	616	PEG	O1-C1-C2-O2
7	C	613	PEG	O1-C1-C2-O2
8	A	205	PGE	O1-C1-C2-O2
9	D	623	FTT	C11-C12-C13-C14
9	B	207	FTT	C11-C12-C13-C14
7	D	613	PEG	C4-C3-O2-C2
8	D	616	PGE	O2-C3-C4-O3
10	A	210	MYR	C4-C5-C6-C7
9	D	623	FTT	O3-C3-C4-C5
9	C	629	FTT	C2-C3-C4-C5
14	D	619	1PE	OH4-C13-C23-OH3
14	D	618	1PE	OH5-C14-C24-OH4
9	D	623	FTT	C5-C6-C7-C8
7	C	620	PEG	O2-C3-C4-O4
10	C	630	MYR	C7-C8-C9-C10
10	C	630	MYR	C11-C10-C9-C8
9	A	209	FTT	C11-C10-C9-C8
9	C	629	FTT	C11-C12-C13-C14
14	C	624	1PE	OH4-C13-C23-OH3
8	C	623	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
14	C	625	1PE	OH2-C12-C22-OH3
14	D	619	1PE	C24-C14-OH5-C25
9	D	623	FTT	C9-C10-C11-C12
14	D	618	1PE	C25-C15-OH6-C26
7	A	203	PEG	C1-C2-O2-C3
8	C	621	PGE	C1-C2-O2-C3
14	D	619	1PE	C25-C15-OH6-C26
14	C	624	1PE	C13-C23-OH3-C22
14	D	619	1PE	C23-C13-OH4-C24
7	C	620	PEG	C1-C2-O2-C3
7	C	611	PEG	C4-C3-O2-C2
7	C	618	PEG	C1-C2-O2-C3
9	D	623	FTT	C3-C4-C5-C6
9	C	629	FTT	C1-C2-C3-C4
7	C	611	PEG	O1-C1-C2-O2
7	D	614	PEG	O1-C1-C2-O2
8	D	616	PGE	C1-C2-O2-C3
8	D	616	PGE	C6-C5-O3-C4
13	D	610	MES	C7-C8-S-O1S
8	A	205	PGE	C1-C2-O2-C3
7	C	620	PEG	O1-C1-C2-O2
14	D	618	1PE	C12-C22-OH3-C23
8	A	205	PGE	C3-C4-O3-C5
10	A	210	MYR	C11-C10-C9-C8
10	D	624	MYR	C2-C3-C4-C5
8	C	622	PGE	C3-C4-O3-C5
9	B	207	FTT	C11-C10-C9-C8
10	C	630	MYR	C10-C11-C12-C13
7	D	612	PEG	O2-C3-C4-O4
8	C	622	PGE	C1-C2-O2-C3
10	A	210	MYR	C2-C3-C4-C5
8	C	622	PGE	C6-C5-O3-C4
10	C	630	MYR	C4-C5-C6-C7
14	C	624	1PE	C23-C13-OH4-C24
9	C	629	FTT	C9-C10-C11-C12
8	D	617	PGE	C1-C2-O2-C3
9	D	623	FTT	C11-C10-C9-C8
9	A	209	FTT	C1-C2-C3-O3
14	C	625	1PE	C15-C25-OH5-C14
10	A	210	MYR	C11-C12-C13-C14
14	D	619	1PE	C16-C26-OH6-C15
9	C	629	FTT	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
14	D	619	1PE	C14-C24-OH4-C13
8	C	623	PGE	C1-C2-O2-C3
7	C	615	PEG	O1-C1-C2-O2
9	B	207	FTT	C4-C5-C6-C7
8	D	617	PGE	O2-C3-C4-O3
8	C	621	PGE	O2-C3-C4-O3
8	A	205	PGE	C4-C3-O2-C2

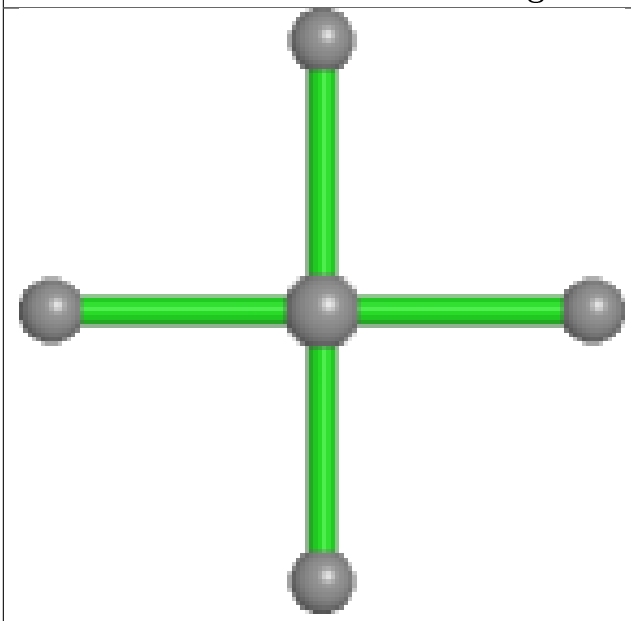
There are no ring outliers.

11 monomers are involved in 16 short contacts:

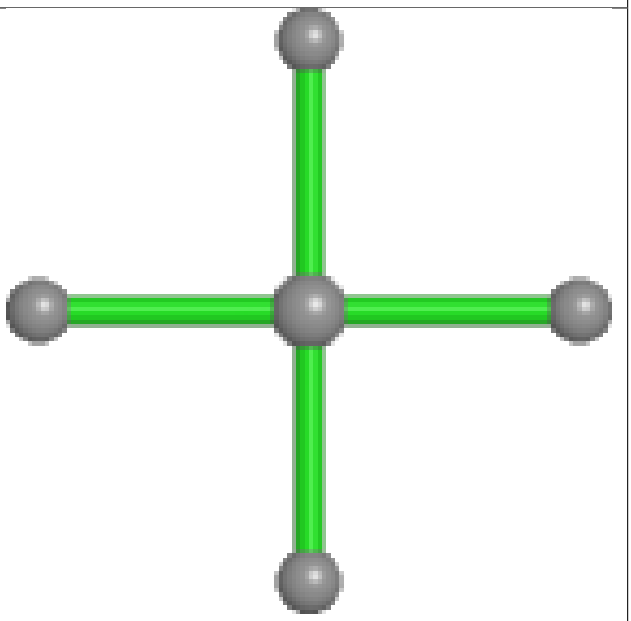
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	618	PEG	1	0
7	D	613	PEG	3	0
7	D	611	PEG	2	0
7	C	613	PEG	1	0
15	D	621	PO4	1	0
14	C	624	1PE	1	0
13	D	610	MES	1	0
14	D	619	1PE	1	0
8	D	616	PGE	1	0
7	C	620	PEG	3	0
7	D	612	PEG	1	0

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 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.

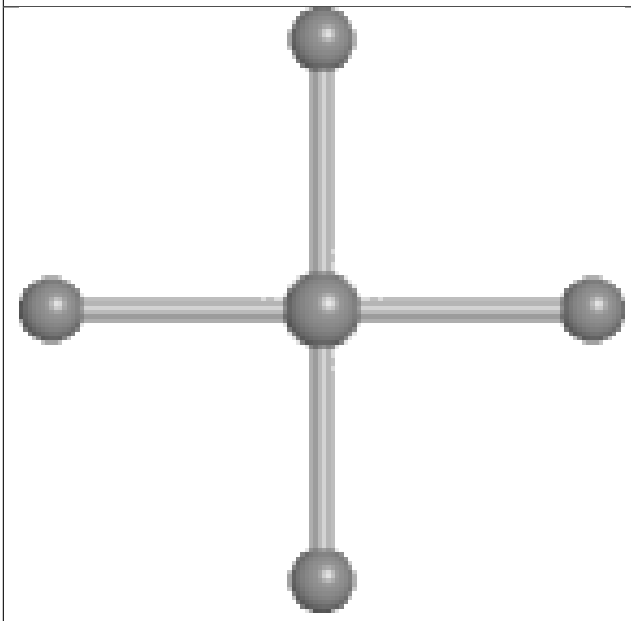
Ligand PO4 C 626



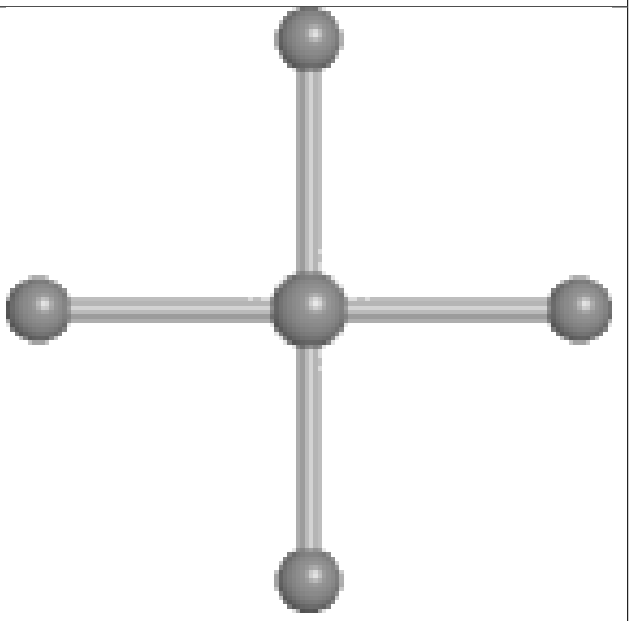
Bond lengths



Bond angles

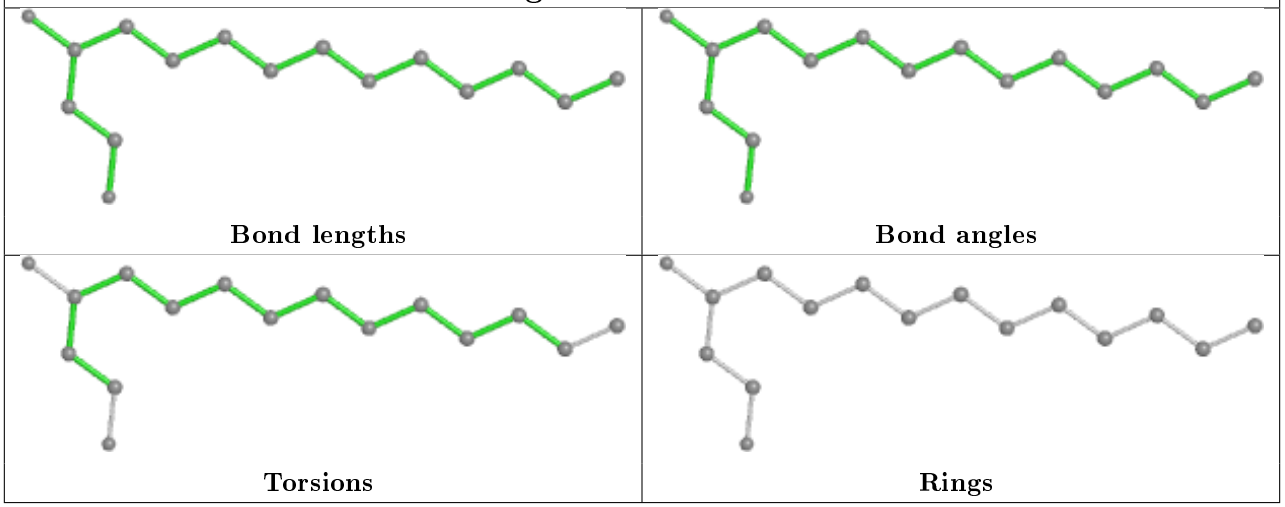


Torsions

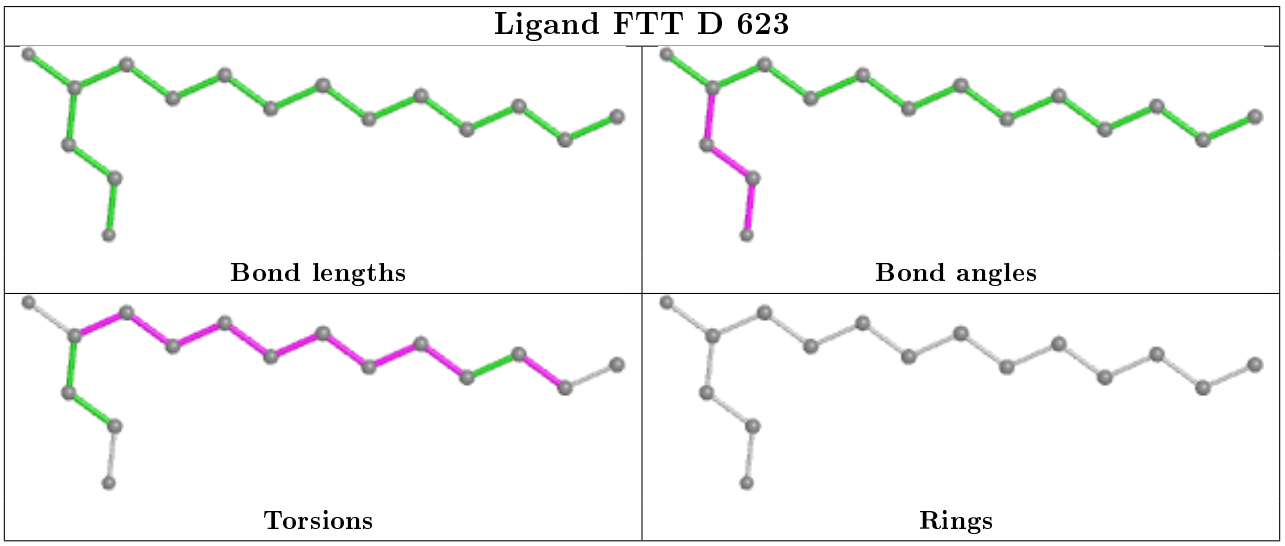


Rings

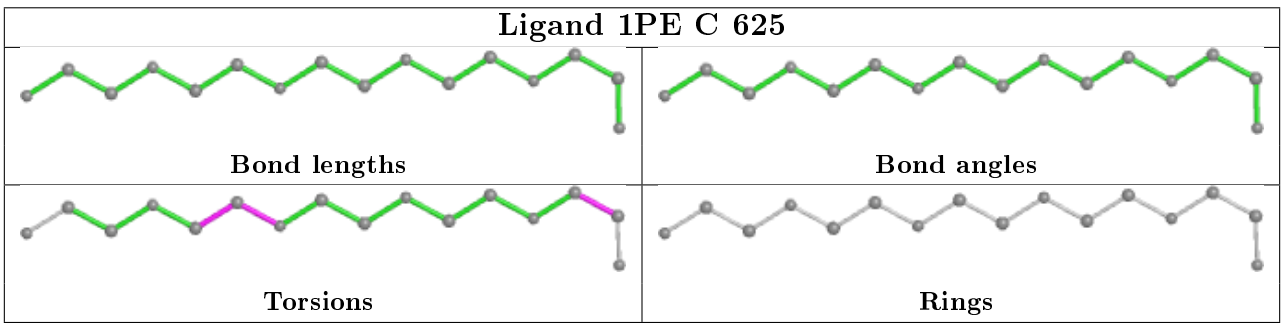
Ligand FTT D 622



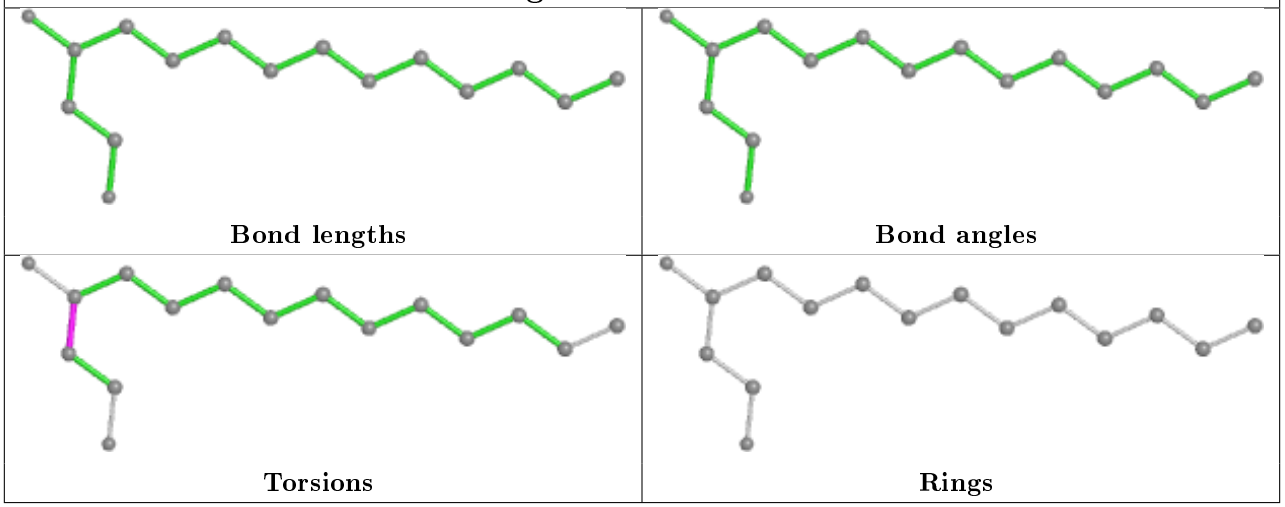
Ligand FTT D 623



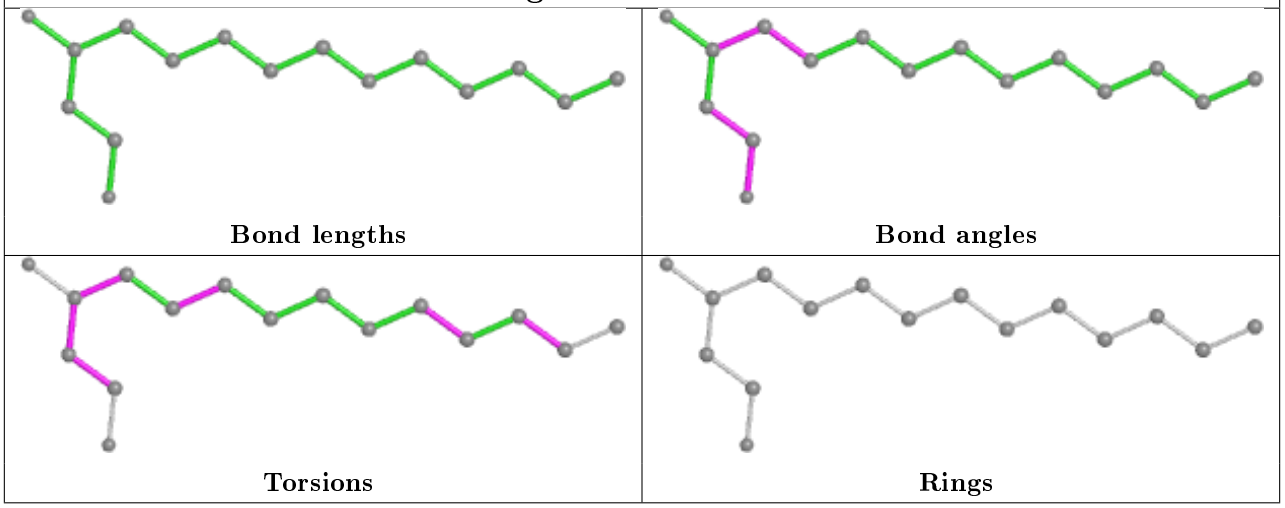
Ligand 1PE C 625



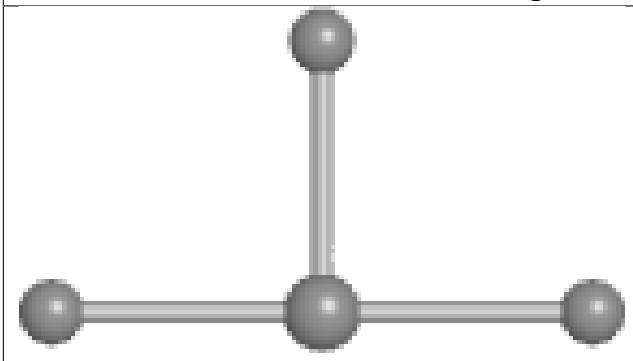
Ligand FTT C 628



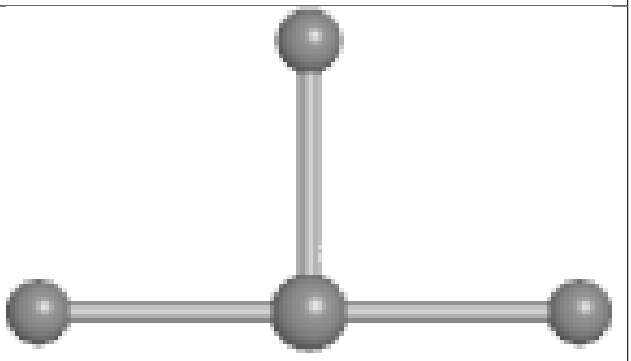
Ligand FTT C 629



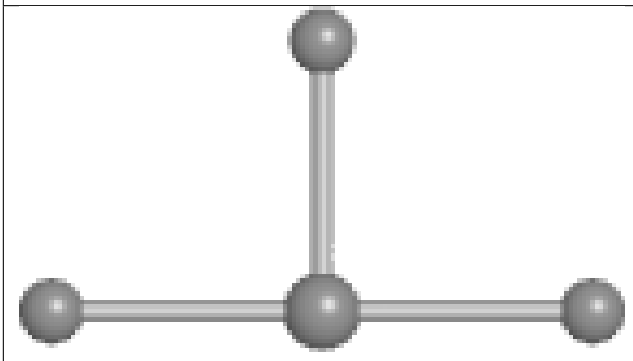
Ligand PO4 C 627



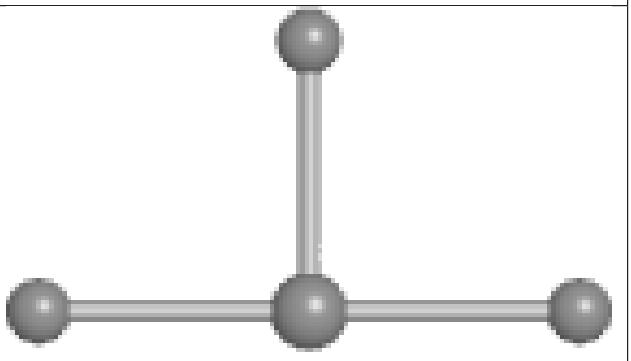
Bond lengths



Bond angles

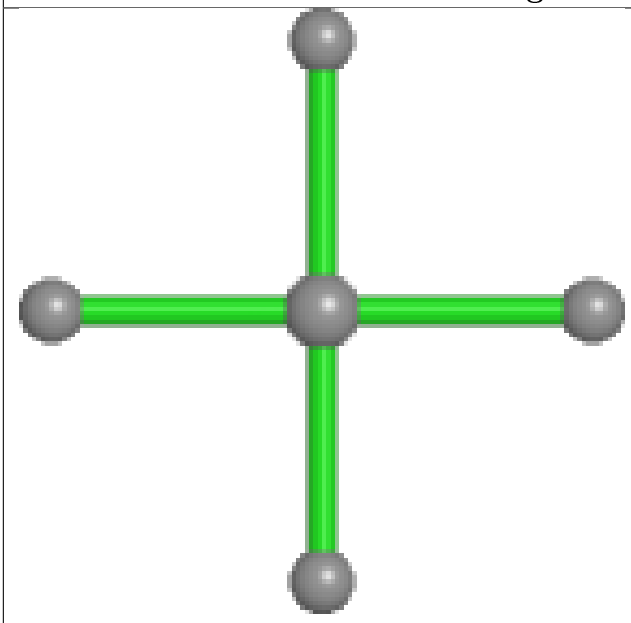


Torsions

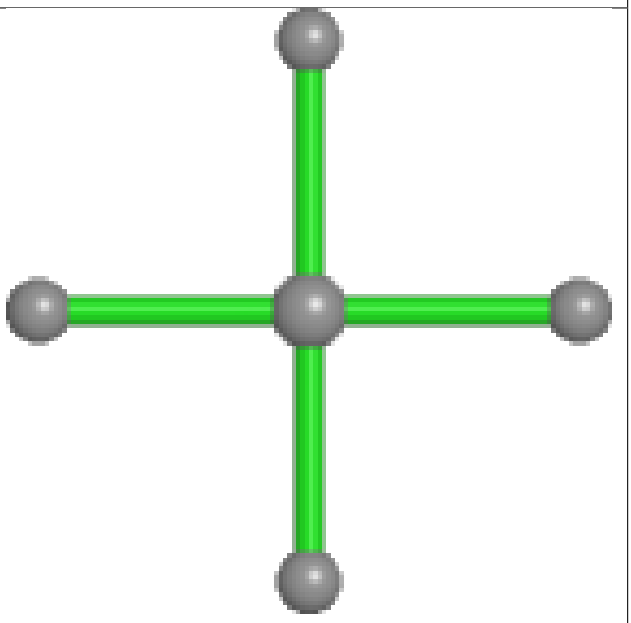


Rings

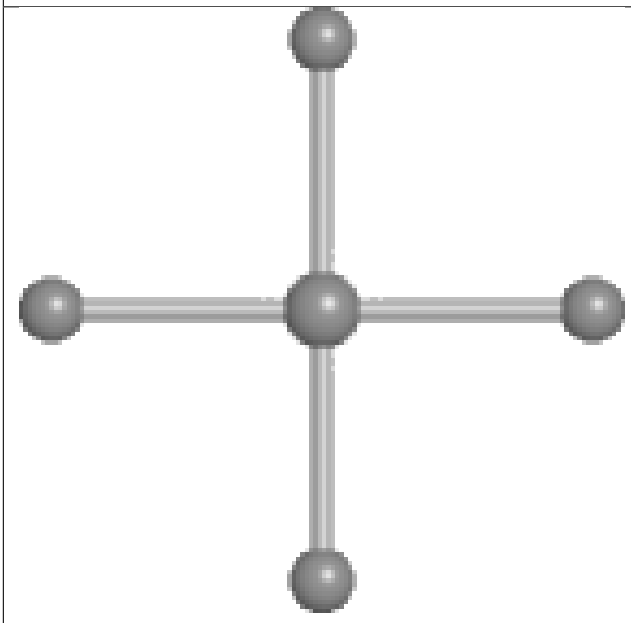
Ligand PO4 D 620



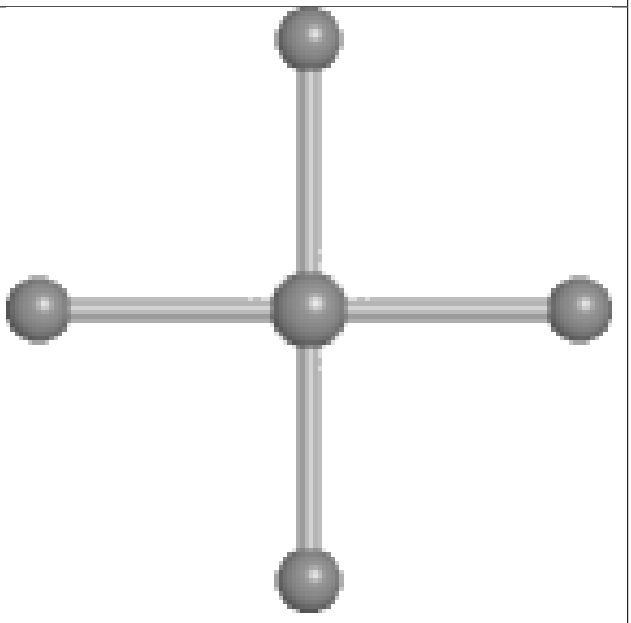
Bond lengths



Bond angles

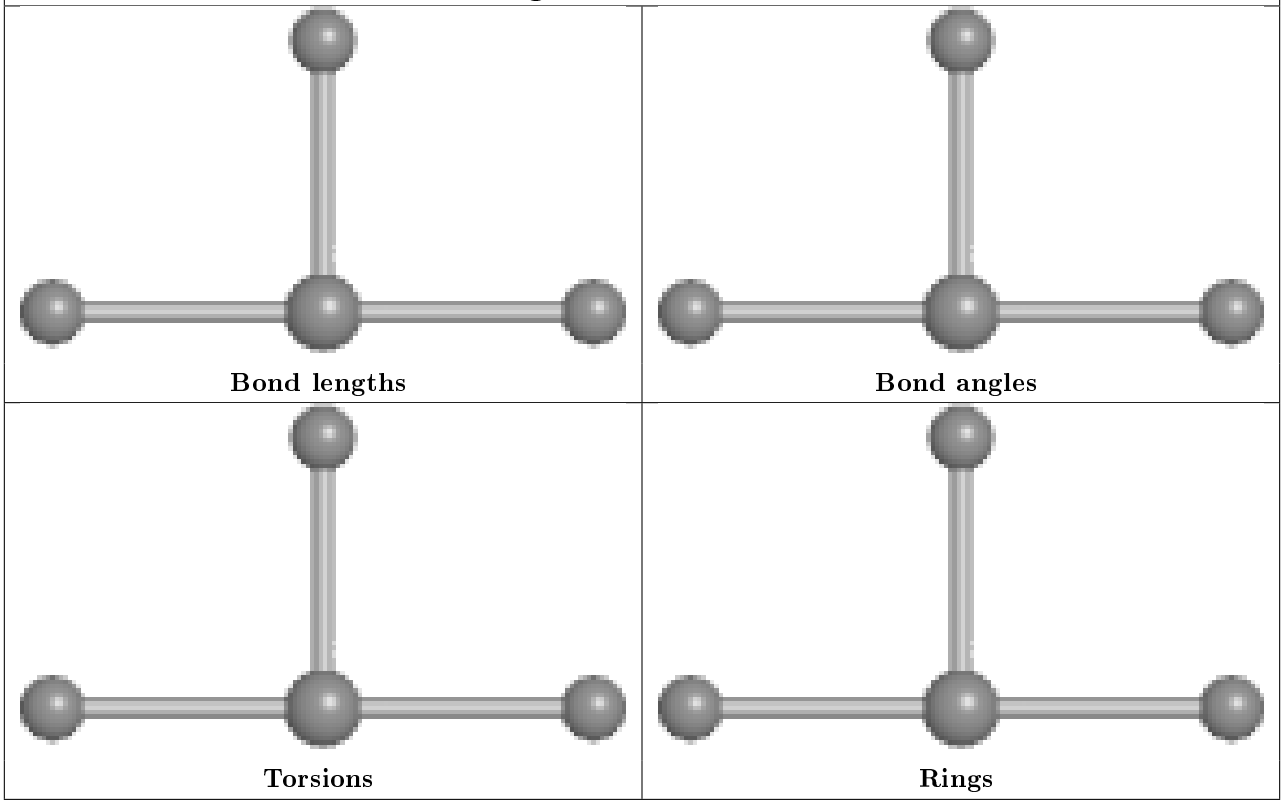


Torsions

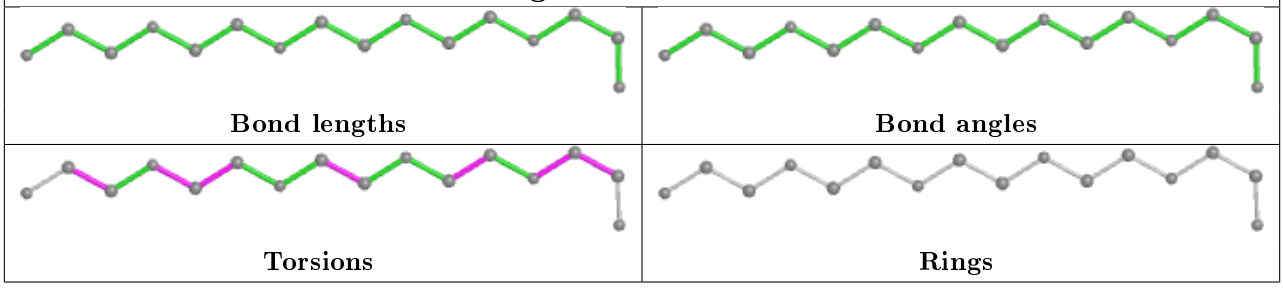


Rings

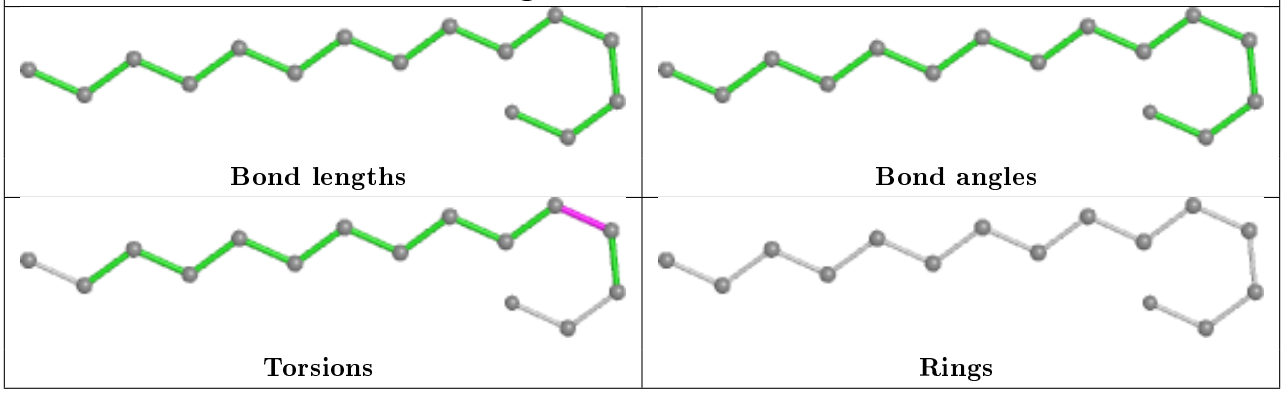
Ligand PO4 D 621



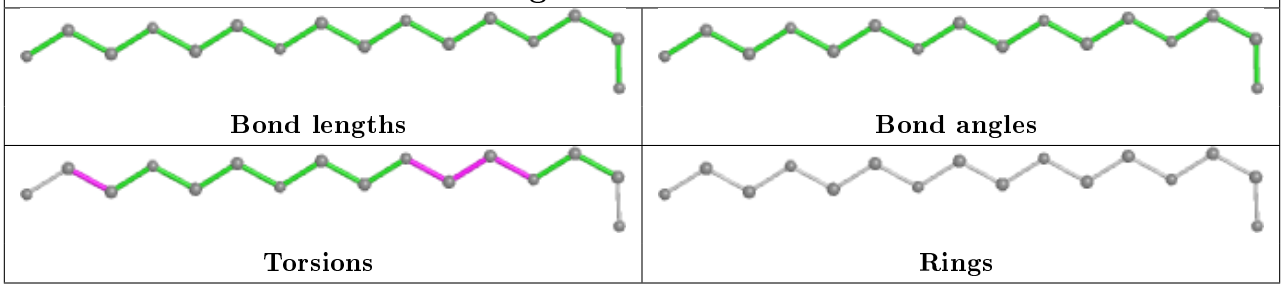
Ligand 1PE D 618



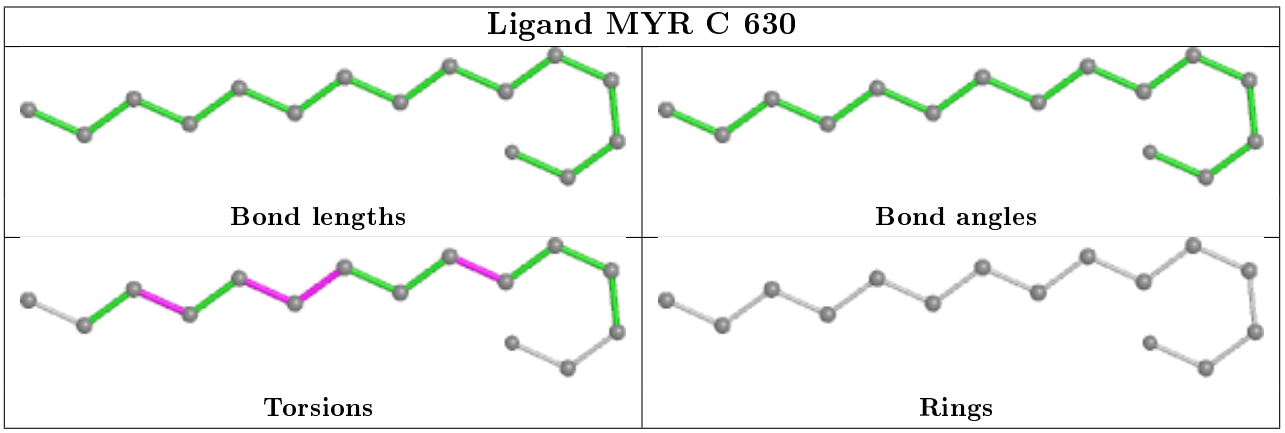
Ligand MYR D 624



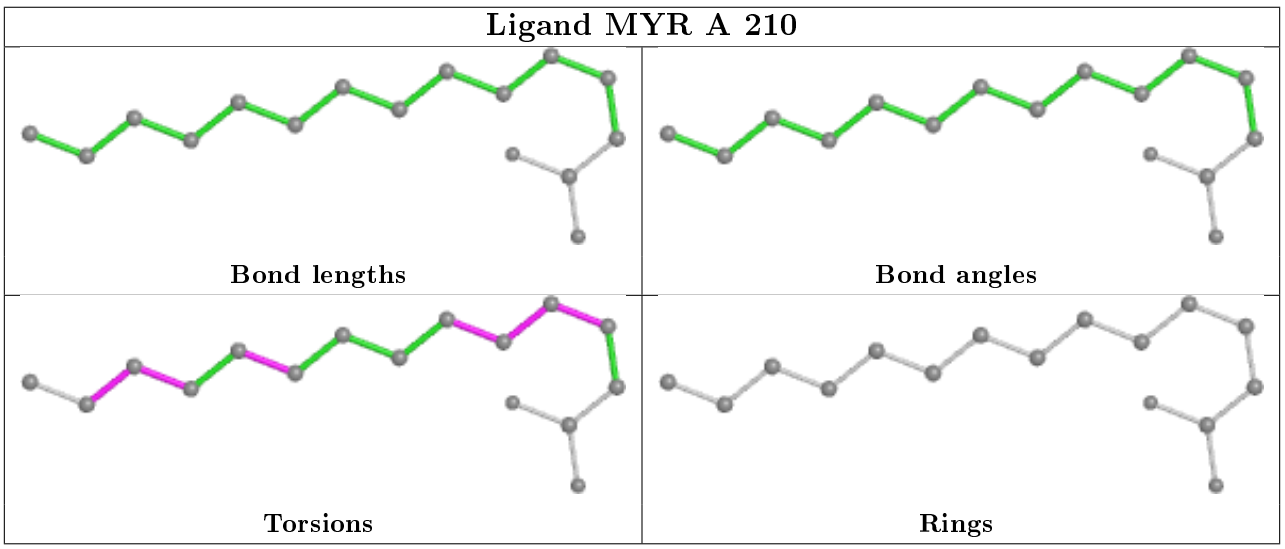
Ligand 1PE C 624



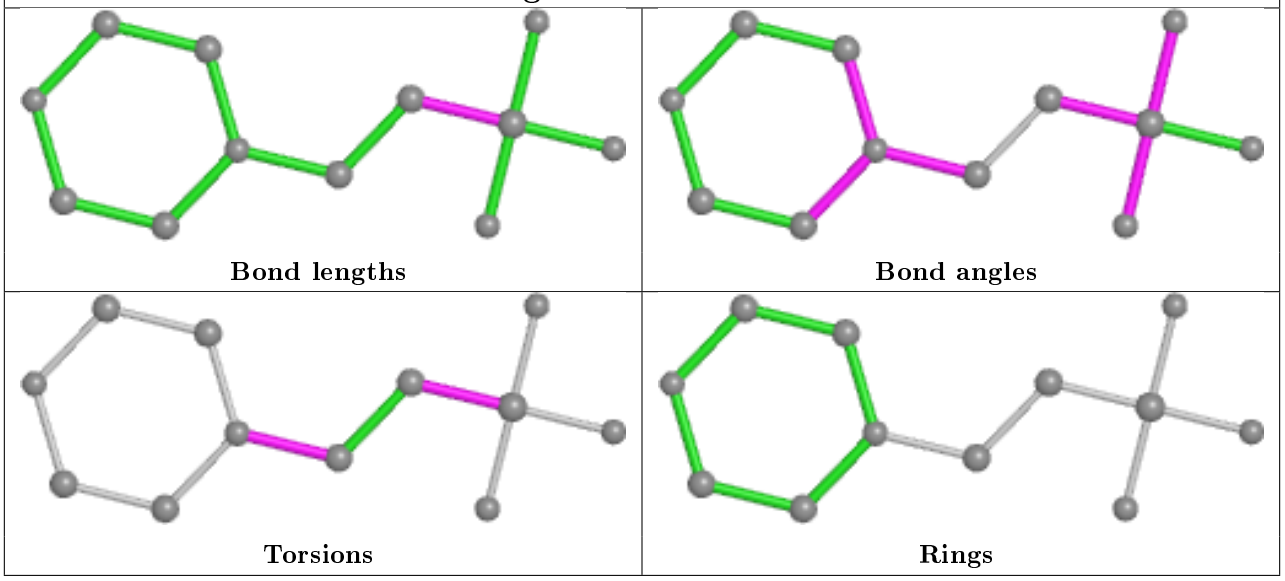
Ligand MYR C 630



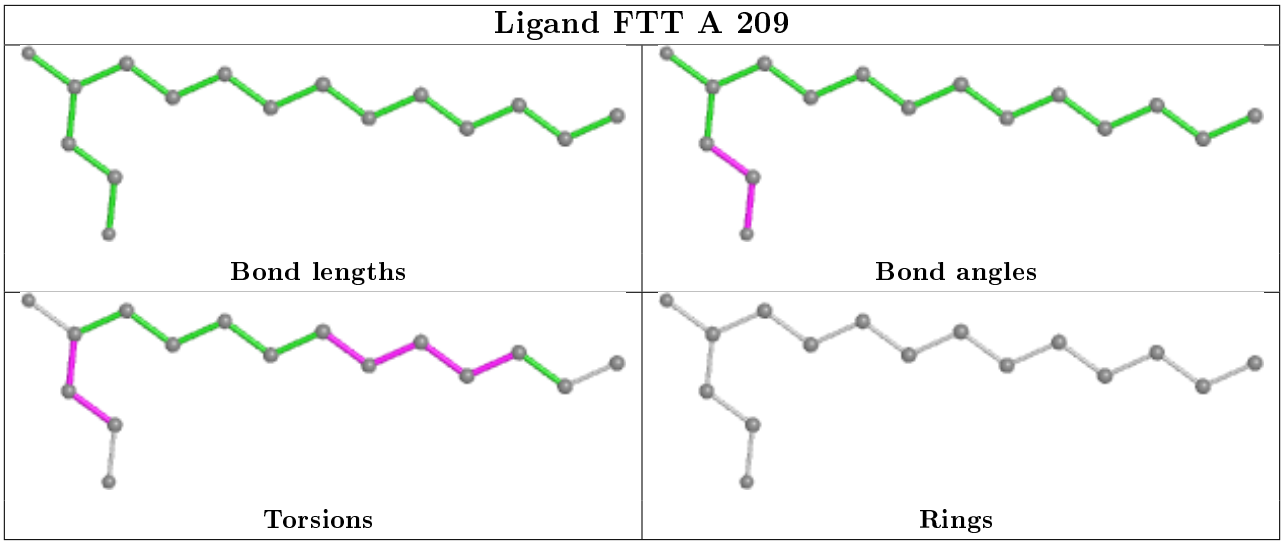
Ligand MYR A 210



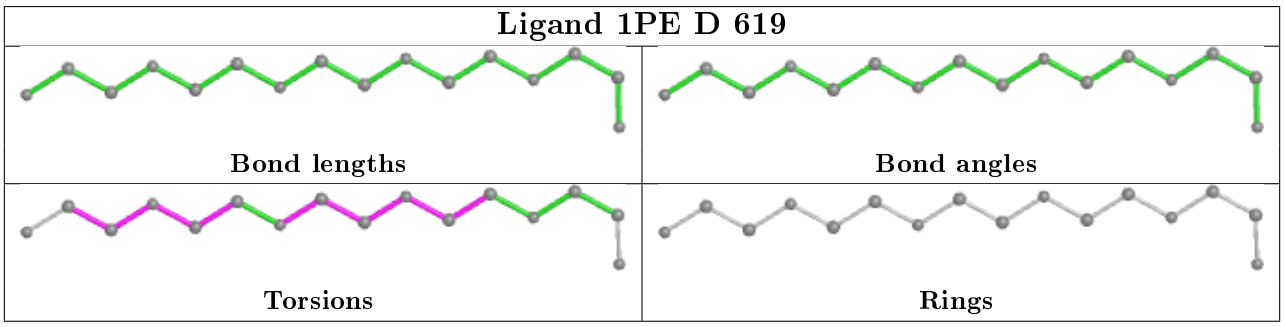
Ligand MES D 610



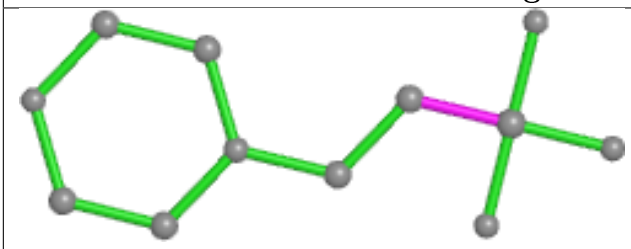
Ligand FTT A 209



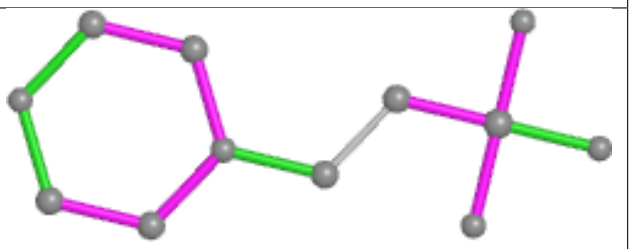
Ligand 1PE D 619



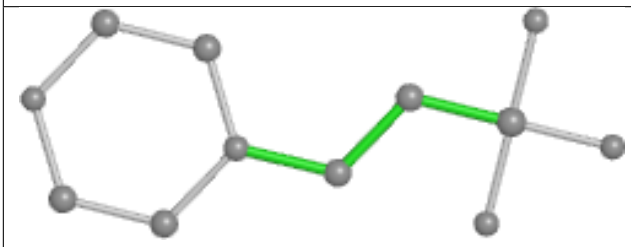
Ligand MES C 610



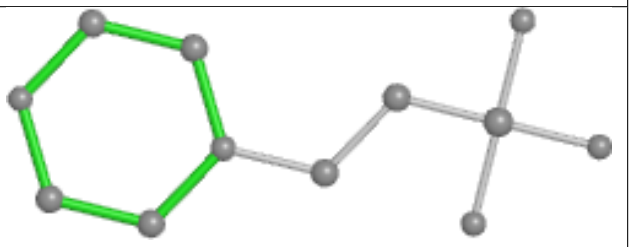
Bond lengths



Bond angles

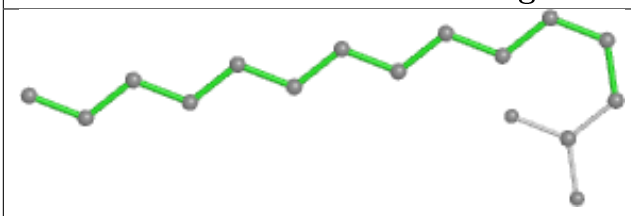


Torsions

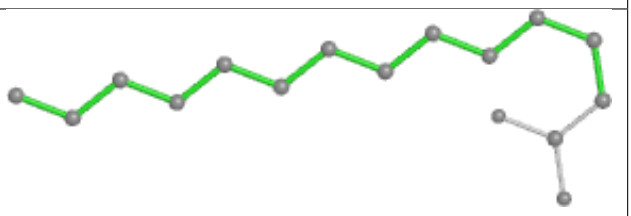


Rings

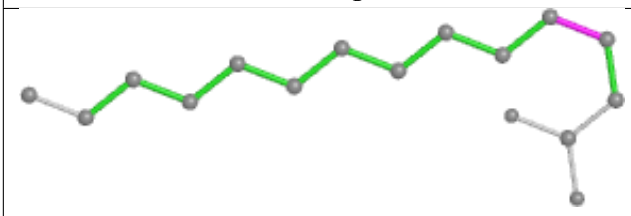
Ligand MYR B 208



Bond lengths



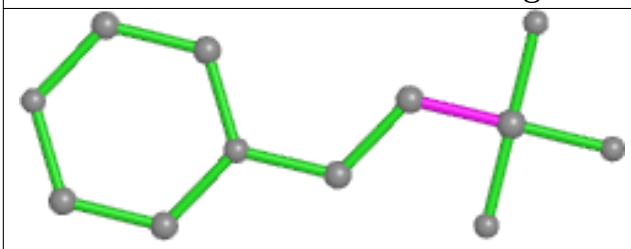
Bond angles



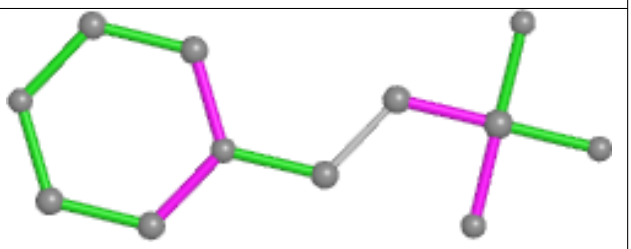
Torsions

Rings

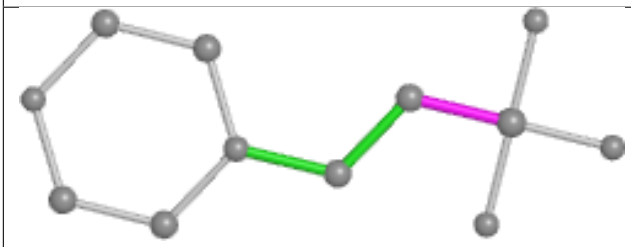
Ligand MES B 203



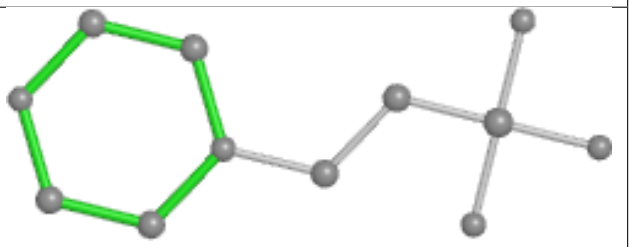
Bond lengths



Bond angles

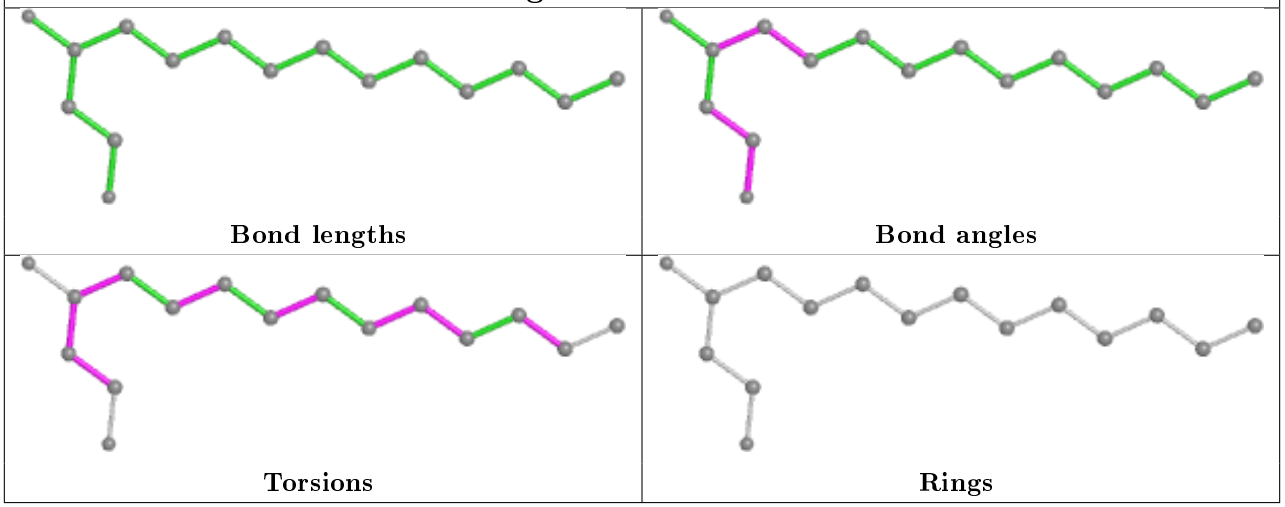


Torsions



Rings

Ligand FTT B 207



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	94/141 (66%)	0.74	17 (18%) 1 1	17, 38, 74, 96	0
1	B	93/141 (65%)	1.94	36 (38%) 0 0	25, 50, 84, 94	0
2	C	413/422 (97%)	0.36	22 (5%) 26 29	12, 22, 62, 112	0
2	D	412/422 (97%)	0.41	23 (5%) 24 27	15, 26, 64, 104	0
All	All	1012/1126 (89%)	0.56	98 (9%) 7 9	12, 26, 72, 112	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	161	LEU	10.8
2	C	163	PHE	9.9
1	B	98	ASP	8.9
2	D	161	LEU	8.6
2	D	162	PRO	8.4
2	D	163	PHE	8.4
2	C	162	PRO	7.9
2	C	310	ALA	7.9
2	C	159	CYS	7.7
2	C	165	ALA	7.5
1	B	117	PRO	7.4
1	B	96	LEU	7.4
2	C	164	LEU	7.1
2	D	160	SER	7.0
1	A	98	ASP	6.9
2	C	309	SER	6.8
2	D	173	LEU	6.7
2	D	168	CYS	6.6
2	C	168	CYS	6.5
1	B	121	LEU	6.4
2	C	160	SER	6.3

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Mol	Chain	Res	Type	RSRZ
2	D	159	CYS	6.2
1	B	115	GLN	6.2
1	A	96	LEU	5.9
1	B	91	ALA	5.6
2	D	165	ALA	5.3
1	B	120	PRO	5.3
1	B	93	ILE	5.2
1	B	116	GLU	5.2
1	A	92	ASP	5.1
1	B	87	HIS	5.0
1	B	101	VAL	4.9
1	B	95	LYS	4.8
2	C	308	ASP	4.8
2	D	167	ILE	4.7
1	B	36	ASP	4.7
2	C	173	LEU	4.6
1	B	84	MET	4.6
2	D	166	LYS	4.5
1	B	85	MET	4.5
2	D	171	ILE	4.5
1	B	97	PHE	4.5
1	A	88	VAL	4.3
2	C	171	ILE	4.2
2	D	164	LEU	4.2
1	B	89	PHE	4.1
1	B	90	GLY	4.0
2	C	166	LYS	3.9
1	B	105	VAL	3.8
1	B	111	GLU	3.8
2	D	315	GLU	3.8
1	B	92	ASP	3.7
2	C	380	THR	3.6
1	A	89	PHE	3.6
1	A	117	PRO	3.6
1	B	119	GLN	3.5
1	B	78	LEU	3.4
1	A	84	MET	3.4
1	B	99	LYS	3.4
2	D	170	LYS	3.3
1	B	128	PRO	3.3
1	B	127	LEU	3.3
1	A	36	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	281	VAL	3.2
1	A	95	LYS	3.2
1	A	119	GLN	3.2
2	C	315	GLU	3.2
2	D	379	LYS	3.1
1	A	118	GLY	3.1
2	D	169	GLN	3.0
2	D	308	ASP	3.0
1	B	114	LYS	3.0
1	B	112	PHE	3.0
1	B	113	CYS	3.0
1	B	88	VAL	2.9
1	A	116	GLU	2.9
2	C	167	ILE	2.9
1	B	118	GLY	2.9
2	D	515	MET	2.8
1	A	129	LYS	2.8
2	C	169	GLN	2.8
1	A	37	HIS	2.7
1	B	76	TRP	2.6
1	B	109	THR	2.5
1	B	37	HIS	2.5
2	D	192[A]	PHE	2.4
1	B	108	HIS	2.4
1	B	100	ASP	2.2
2	C	224	HIS	2.2
2	D	514	LYS	2.2
2	C	174	ALA	2.2
2	D	309	SER	2.1
2	C	281	VAL	2.1
2	D	380	THR	2.1
2	C	516	GLY	2.1
1	A	97	PHE	2.1
1	A	76	TRP	2.0
1	A	87	HIS	2.0

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

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

6.3 Carbohydrates (i)

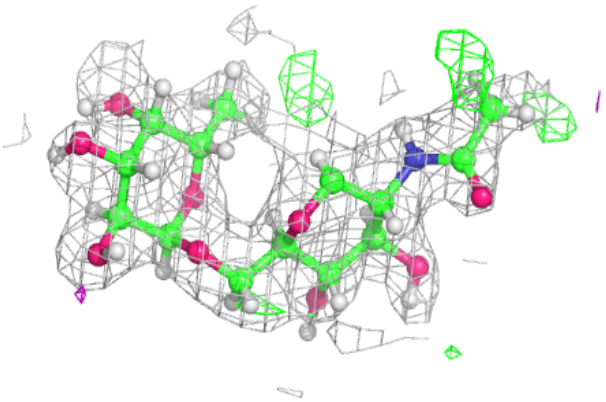
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

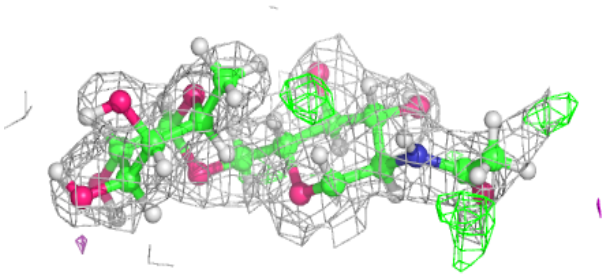
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	KDO	J	3	15/16	0.65	0.34	73,95,112,114	0
4	GCS	J	2	11/12	0.65	0.22	59,90,128,128	0
4	KDO	F	3	15/16	0.70	0.24	59,82,106,110	0
5	NAG	K	2	14/15	0.70	0.33	60,88,113,123	0
5	NAG	G	2	14/15	0.72	0.26	56,73,88,100	0
4	GCS	F	2	11/12	0.72	0.17	48,73,91,91	0
6	NAG	H	2	14/15	0.76	0.27	41,74,110,127	0
3	NAG	I	1	14/15	0.78	0.20	48,59,71,75	0
3	NAG	E	1	14/15	0.82	0.20	48,61,78,84	0
5	FUC	G	3	10/11	0.83	0.24	45,55,67,72	0
3	FUC	E	2	10/11	0.83	0.24	41,57,64,71	0
5	FUC	K	3	10/11	0.83	0.29	49,65,78,90	0
6	NAG	H	1	14/15	0.84	0.20	36,55,88,88	0
5	NAG	K	1	14/15	0.85	0.23	45,57,70,72	0
5	NAG	G	1	14/15	0.87	0.22	38,55,74,74	0
3	FUC	I	2	10/11	0.88	0.29	53,63,73,75	0
6	NAG	L	2	14/15	0.88	0.13	37,63,92,93	0
6	NAG	L	1	14/15	0.91	0.13	39,53,90,90	0
4	PA1	F	1	11/12	0.94	0.11	26,38,46,50	0
4	PA1	J	1	11/12	0.96	0.10	31,39,62,64	0

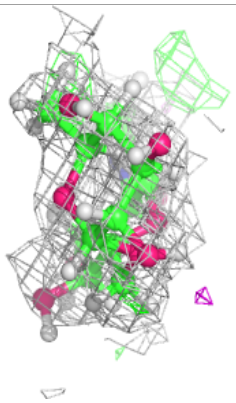
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

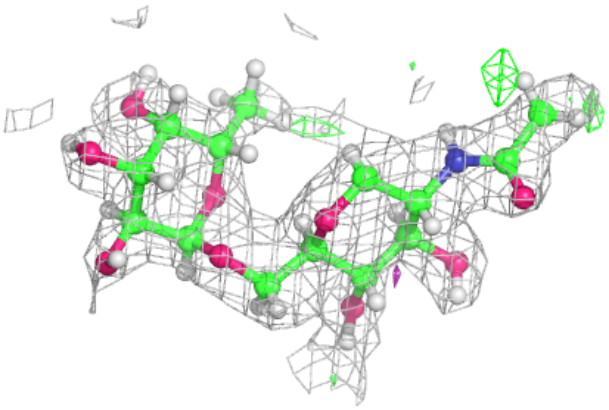


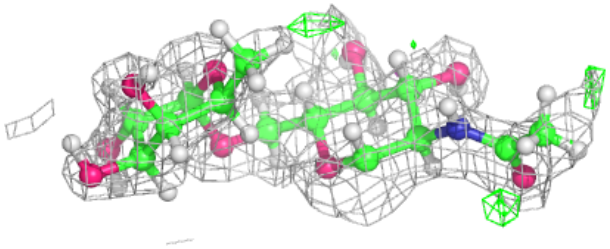


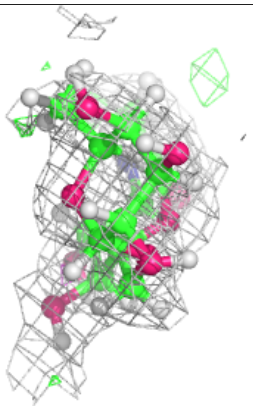


Electron density around Chain I:

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

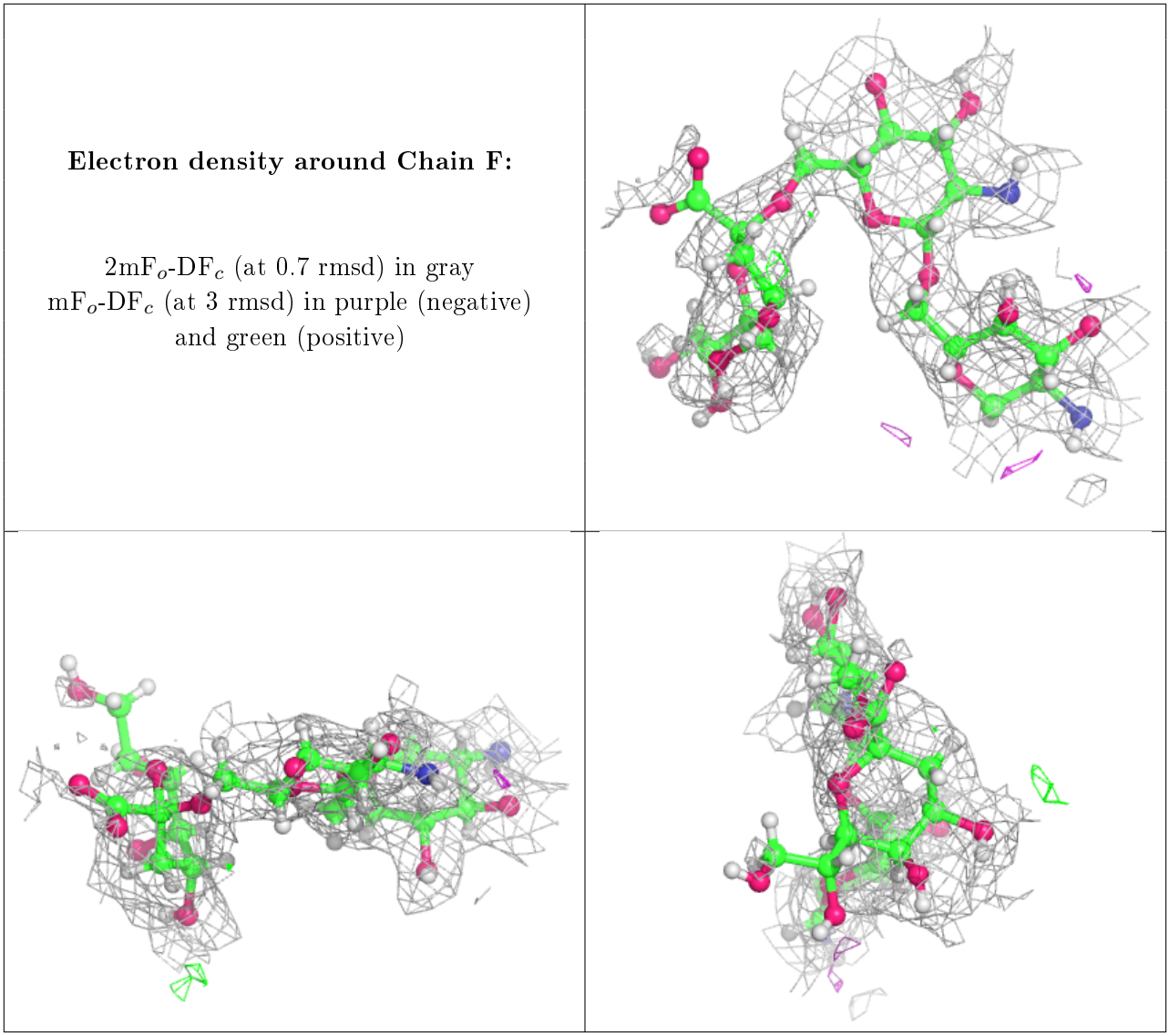






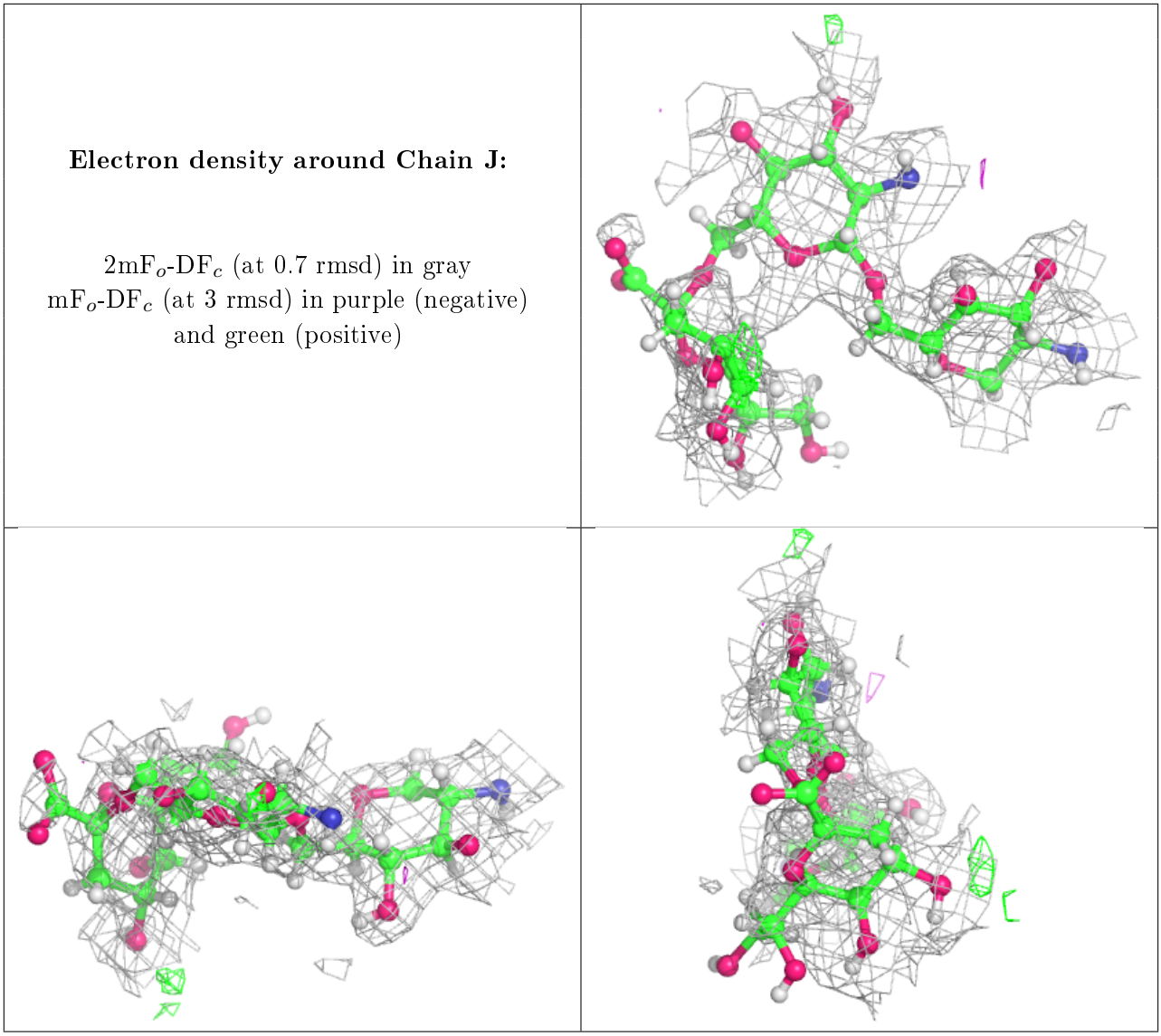
Electron density around Chain F:

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



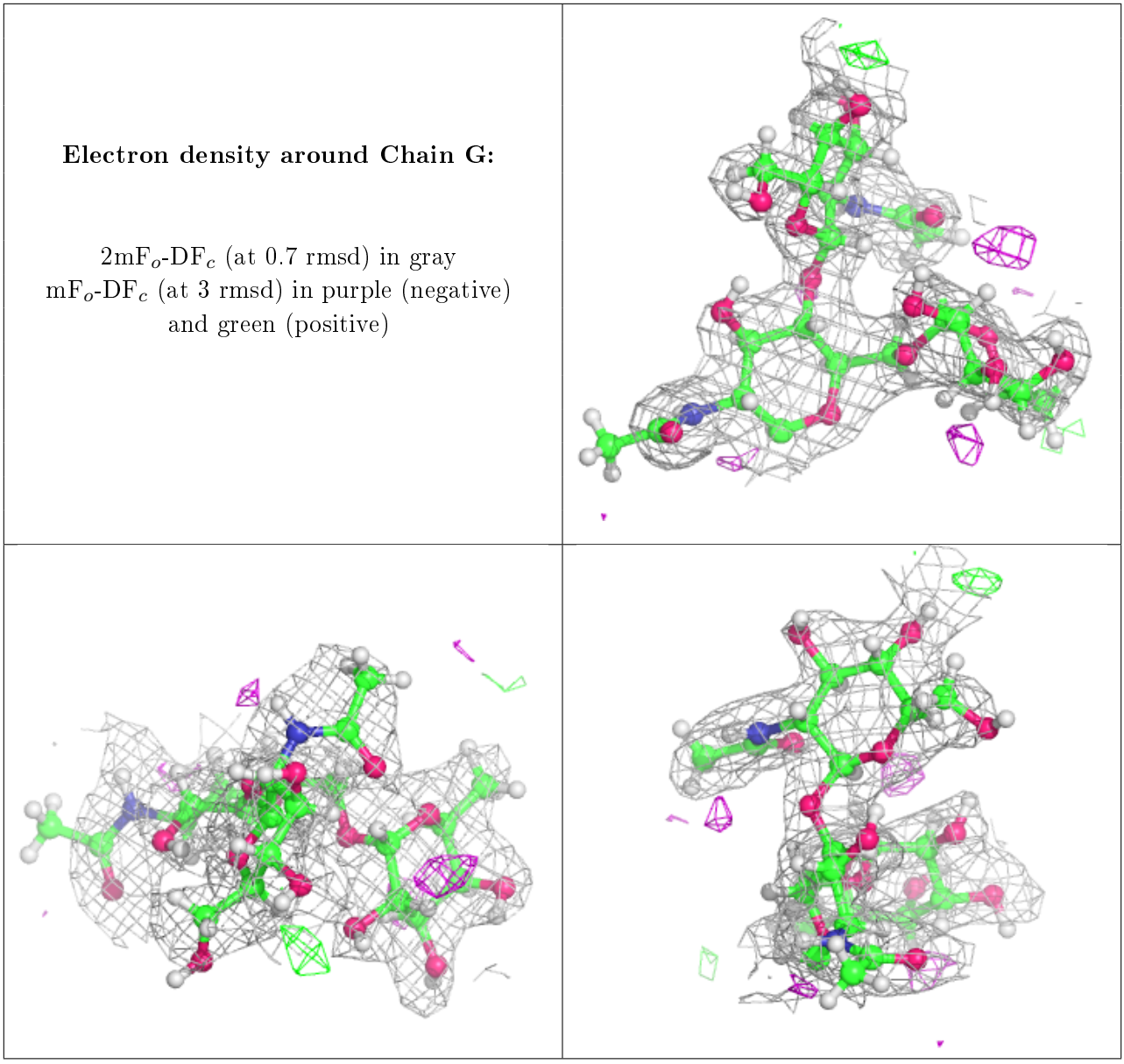
Electron density around Chain J:

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



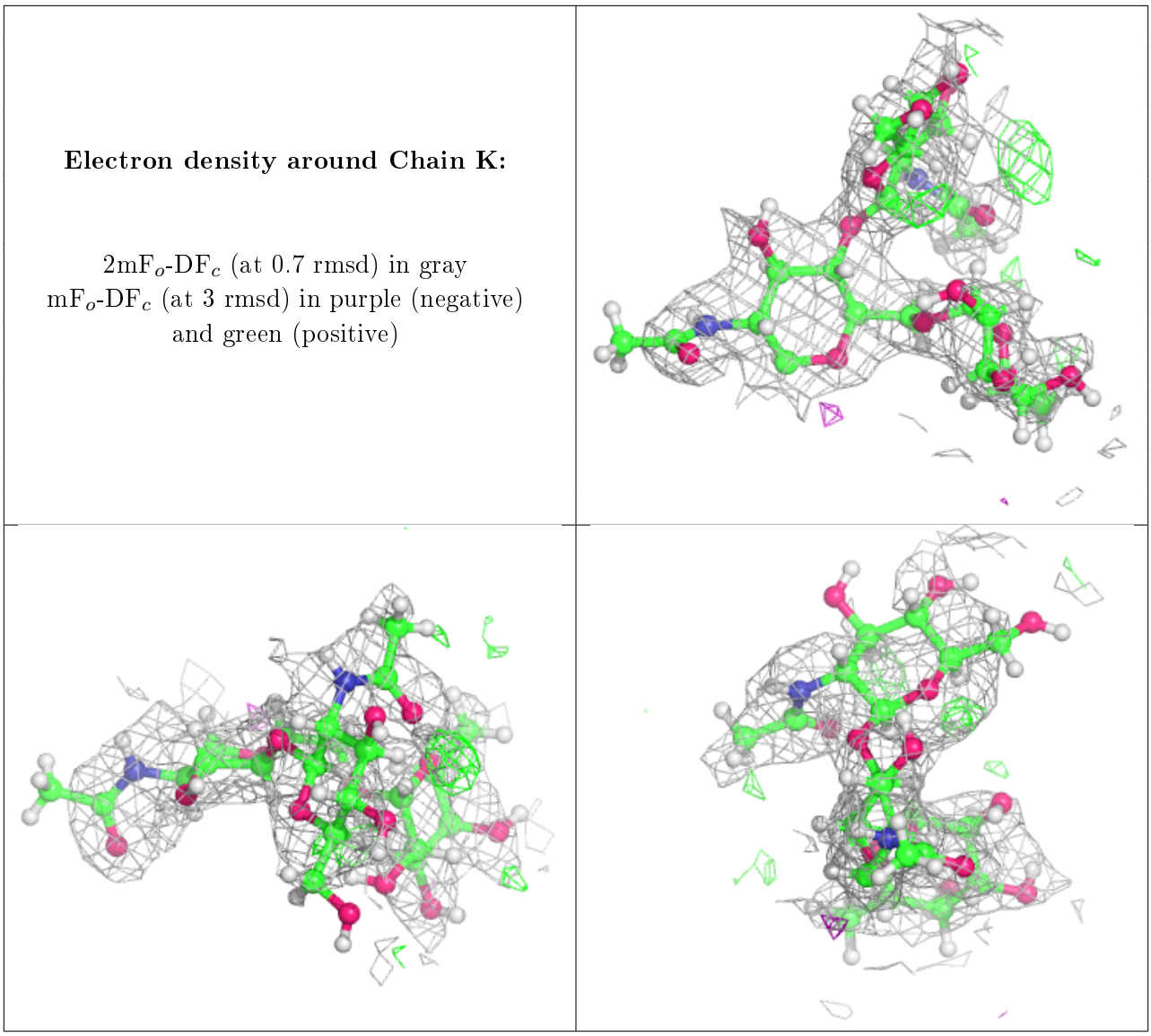
Electron density around Chain G:

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



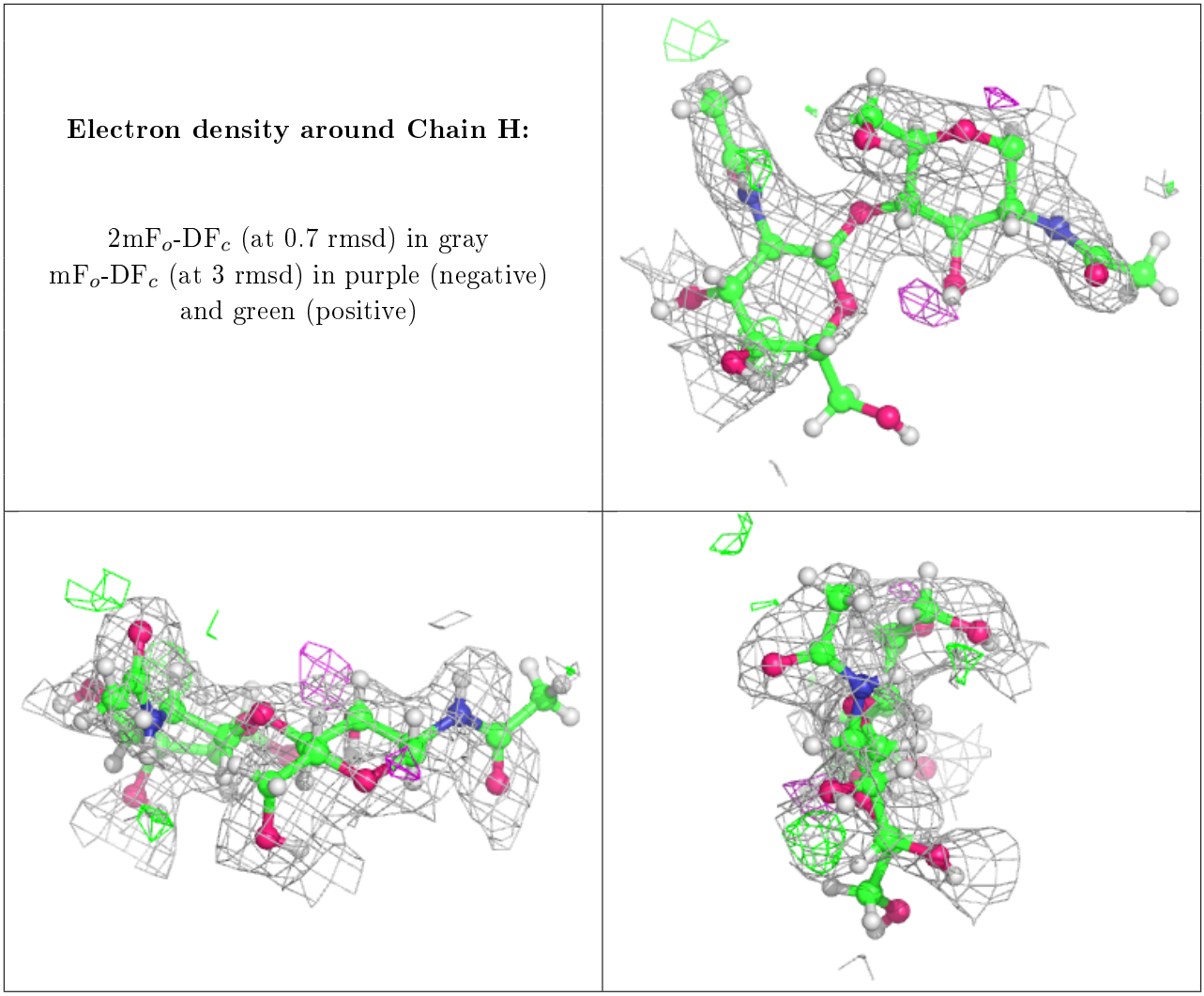
Electron density around Chain K:

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



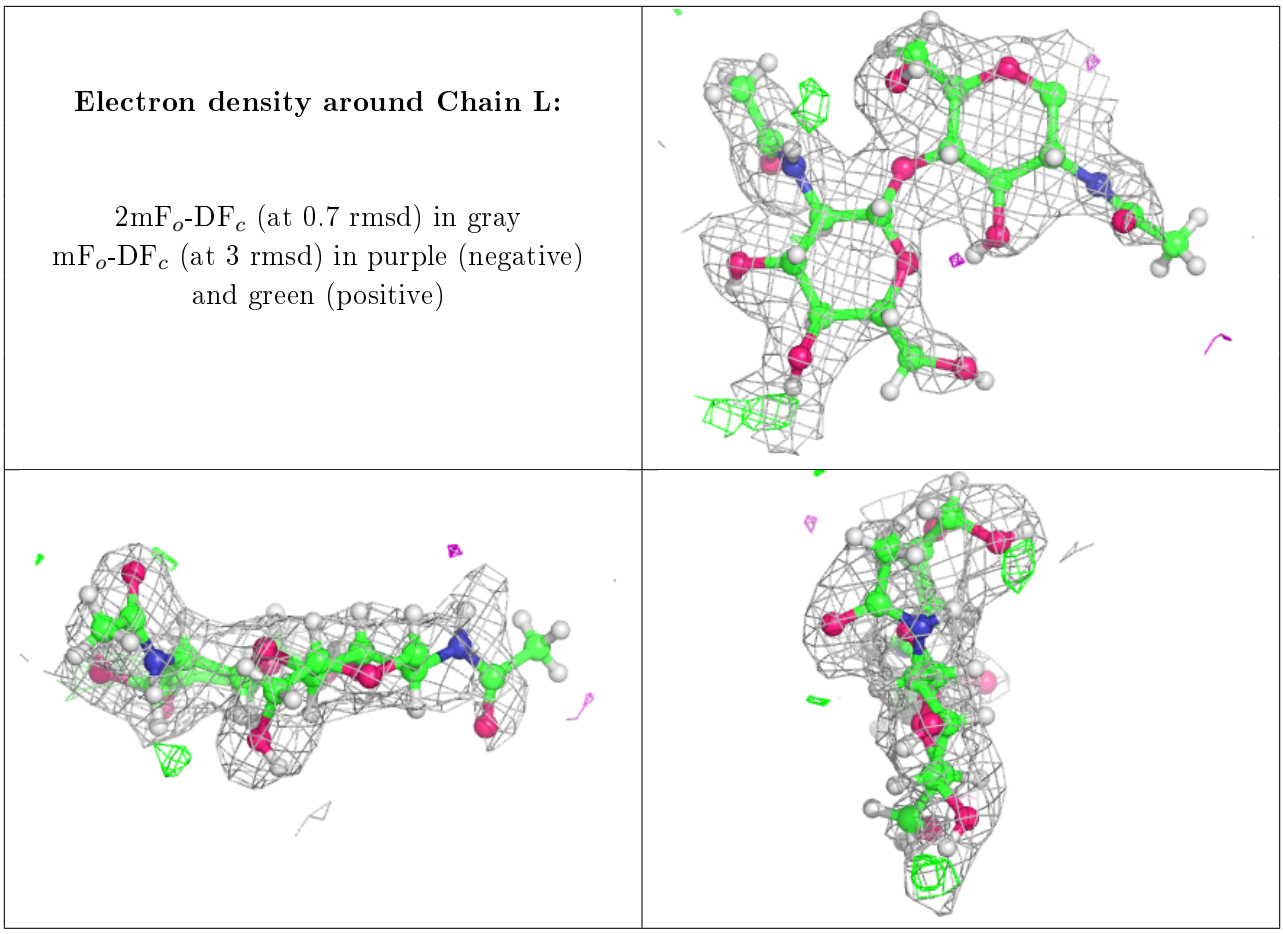
Electron density around Chain H:

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



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)



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
7	PEG	C	618	7/7	0.61	0.22	60,72,83,85	0
7	PEG	A	204	7/7	0.72	0.19	66,80,90,90	0
15	PO4	C	627	4/5	0.75	0.17	71,75,76,93	0
7	PEG	C	613	7/7	0.78	0.20	41,54,67,67	0
7	PEG	D	613	7/7	0.78	0.22	49,60,74,82	0
7	PEG	C	615	7/7	0.78	0.18	42,61,79,79	0
13	MES	D	610	12/12	0.79	0.41	73,91,105,111	0
7	PEG	C	620	7/7	0.80	0.23	27,38,46,46	0
7	PEG	C	614	7/7	0.80	0.40	51,63,74,89	0
7	PEG	C	619	7/7	0.81	0.19	23,35,43,44	0
7	PEG	C	616	7/7	0.81	0.16	53,64,72,75	0
10	MYR	C	630	15/16	0.81	0.16	36,50,73,74	0

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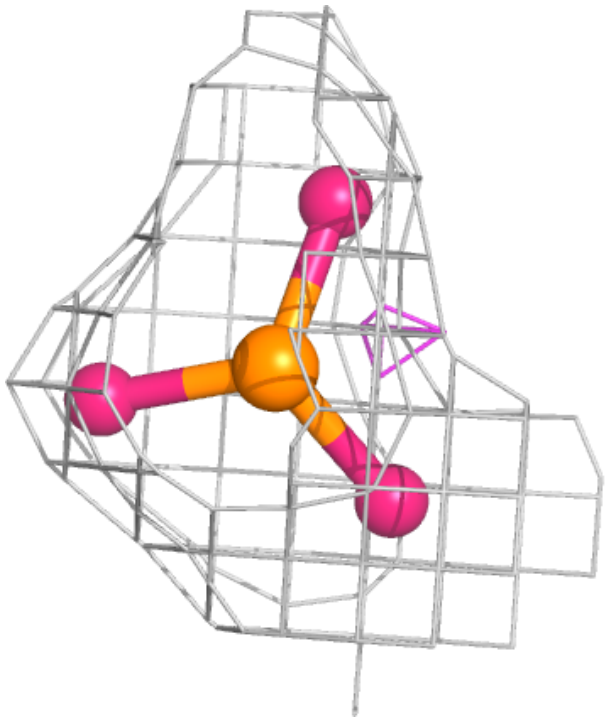
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MYR	B	208	16/16	0.82	0.34	41,59,75,87	0
10	MYR	A	210	16/16	0.84	0.22	40,54,90,94	0
9	FTT	A	209	16/17	0.84	0.17	45,61,76,76	0
15	PO4	D	621	4/5	0.84	0.34	93,99,111,116	0
10	MYR	D	624	15/16	0.85	0.17	34,55,76,78	0
7	PEG	A	203	7/7	0.85	0.19	35,59,72,72	0
7	PEG	C	612	7/7	0.85	0.25	45,62,78,78	0
9	FTT	B	207	16/17	0.85	0.20	49,64,83,89	0
8	PGE	C	623	10/10	0.86	0.12	41,53,60,64	0
7	PEG	C	617	7/7	0.86	0.13	42,54,70,73	0
7	PEG	D	614	7/7	0.86	0.22	42,53,64,64	0
7	PEG	C	611	7/7	0.86	0.19	30,38,53,53	0
8	PGE	C	622	10/10	0.87	0.23	34,49,70,77	0
7	PEG	D	612	7/7	0.87	0.16	38,54,66,66	0
7	PEG	D	611	7/7	0.87	0.19	29,42,47,52	0
13	MES	C	610	12/12	0.88	0.29	39,73,88,89	0
14	1PE	C	624	16/16	0.89	0.12	31,44,58,70	0
8	PGE	D	616	10/10	0.89	0.20	41,51,60,62	0
14	1PE	D	618	16/16	0.89	0.12	29,43,52,62	0
13	MES	B	203	12/12	0.89	0.30	45,79,92,93	0
8	PGE	A	205	10/10	0.89	0.35	42,59,74,77	0
8	PGE	C	621	10/10	0.91	0.17	29,38,50,68	0
9	FTT	D	622	16/17	0.92	0.12	21,32,51,53	0
9	FTT	D	623	16/17	0.92	0.14	30,59,80,85	0
14	1PE	D	619	16/16	0.92	0.14	24,36,52,62	0
8	PGE	D	617	10/10	0.93	0.14	30,37,46,55	0
14	1PE	C	625	16/16	0.95	0.12	20,29,42,45	0
9	FTT	C	628	16/17	0.95	0.12	14,25,42,46	0
8	PGE	D	615	10/10	0.95	0.10	23,34,52,53	0
12	SO4	D	609	5/5	0.95	0.11	42,42,50,57	0
9	FTT	C	629	16/17	0.96	0.12	26,46,69,69	0
15	PO4	C	626	5/5	0.96	0.12	31,33,48,52	0
15	PO4	D	620	5/5	0.97	0.09	35,37,44,45	0
11	CA	D	602	1/1	0.98	0.10	19,19,19,19	0
12	SO4	C	609	5/5	0.98	0.11	31,35,37,50	0
11	CA	D	603	1/1	0.98	0.10	21,21,21,21	0
11	CA	C	602	1/1	0.99	0.10	18,18,18,18	0
11	CA	C	601	1/1	0.99	0.13	17,17,17,17	0
11	CA	C	603	1/1	0.99	0.13	20,20,20,20	0
11	CA	D	601	1/1	1.00	0.13	18,18,18,18	0

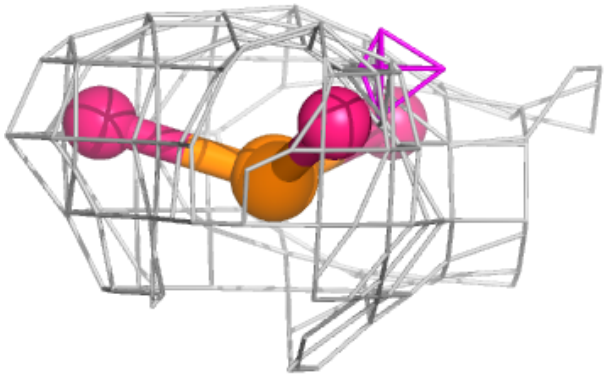
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

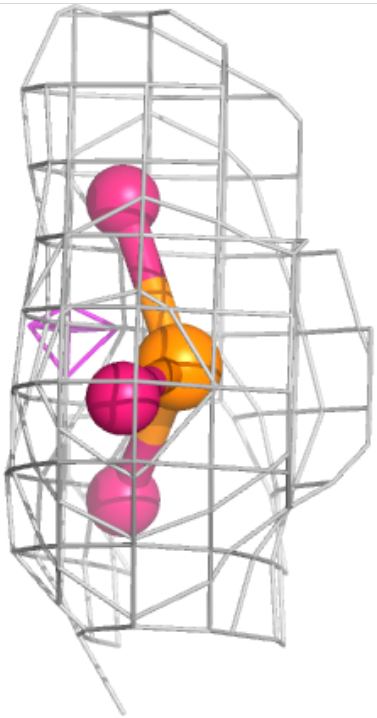
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

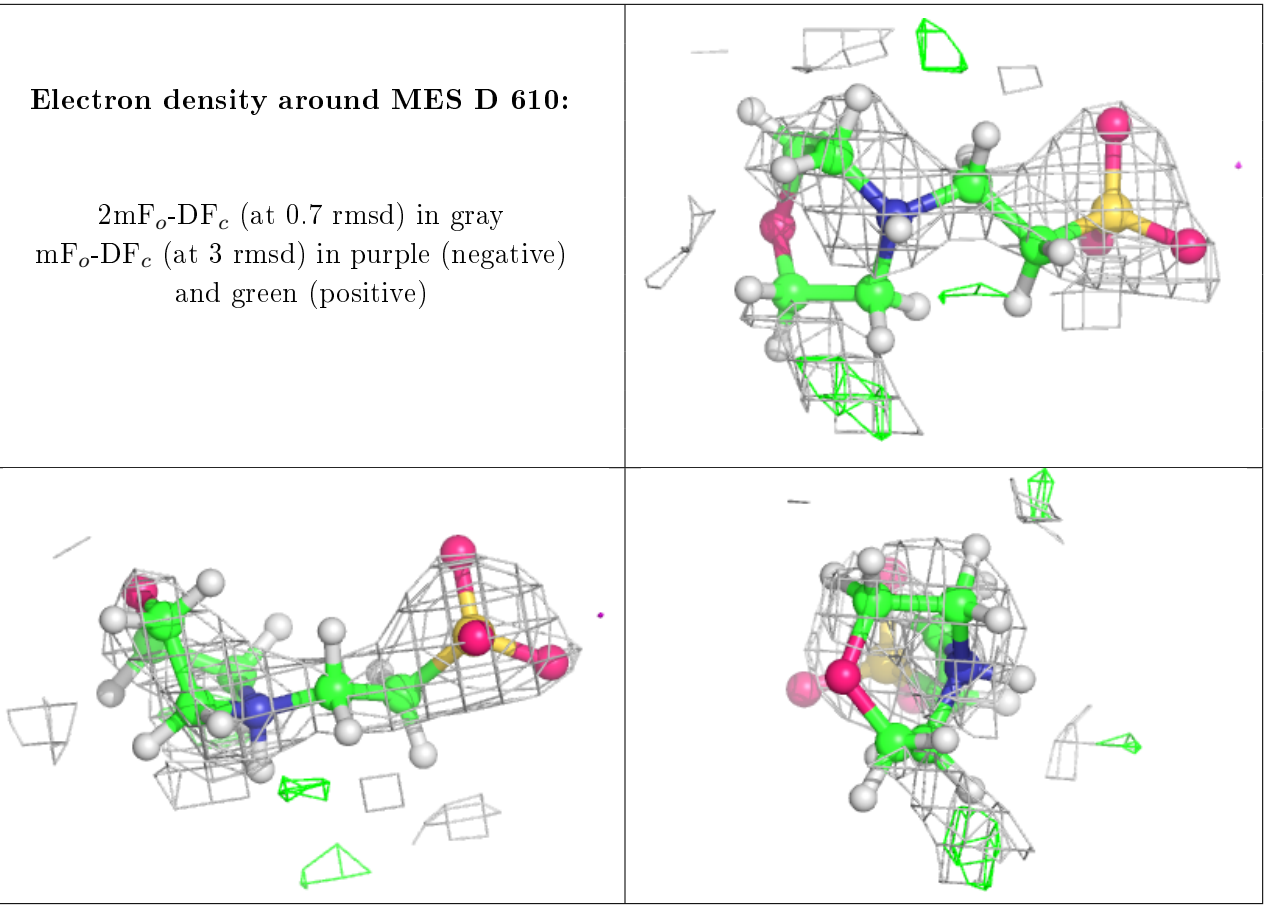






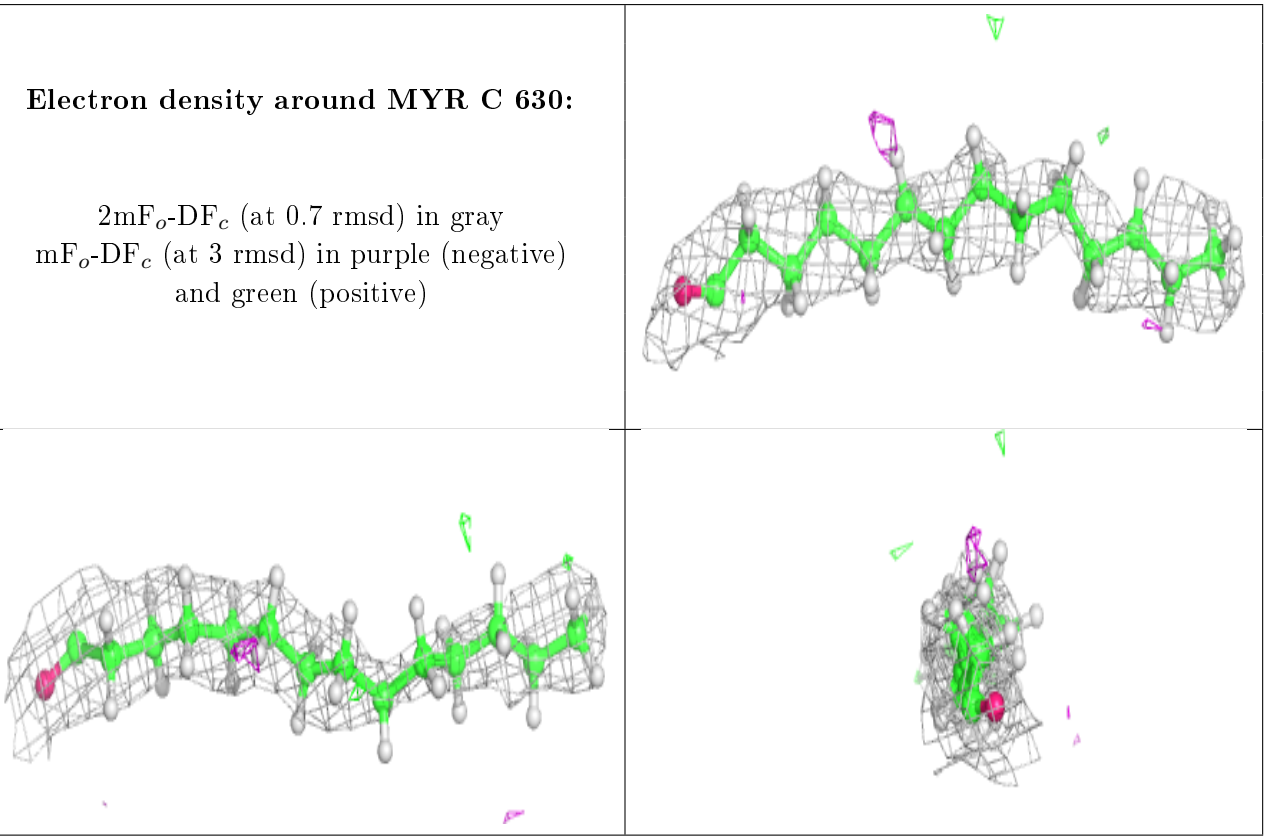
Electron density around MES D 610:

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



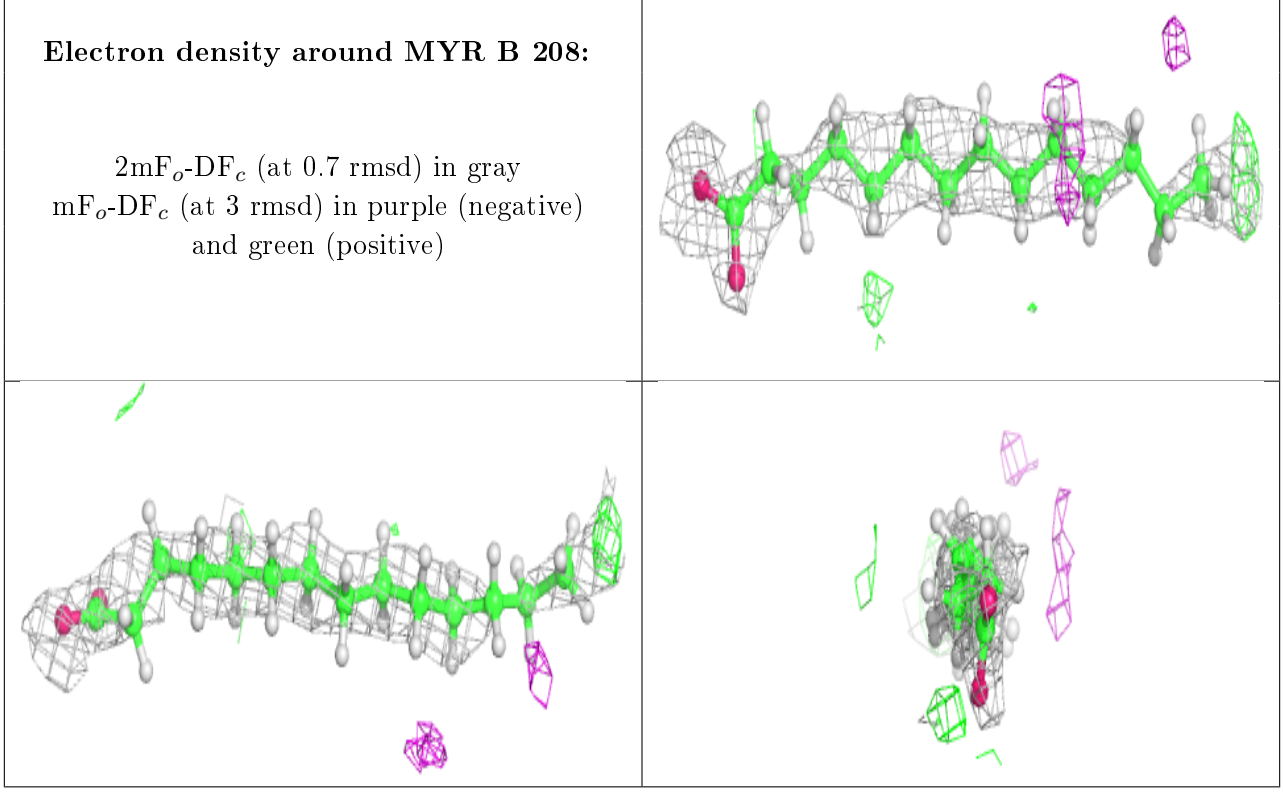
Electron density around MYR C 630:

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



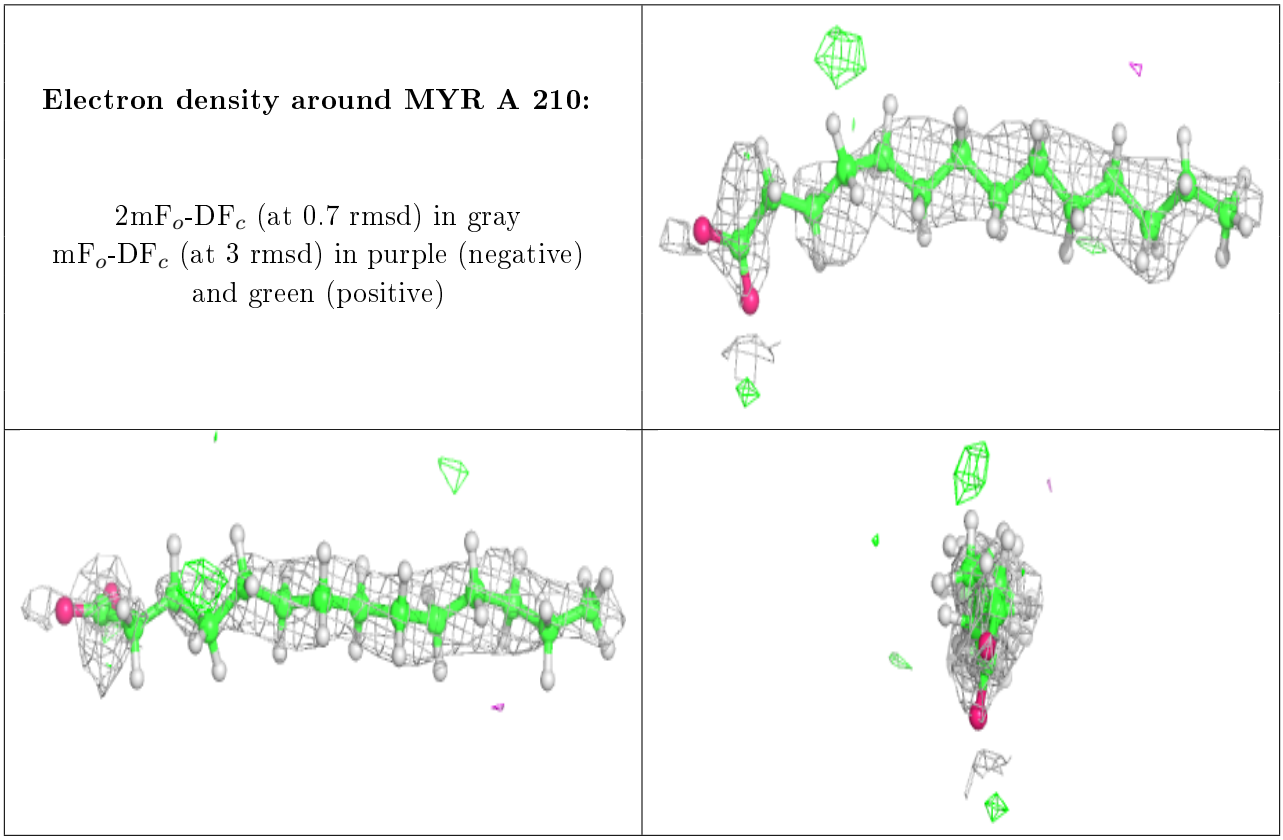
Electron density around MYR B 208:

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



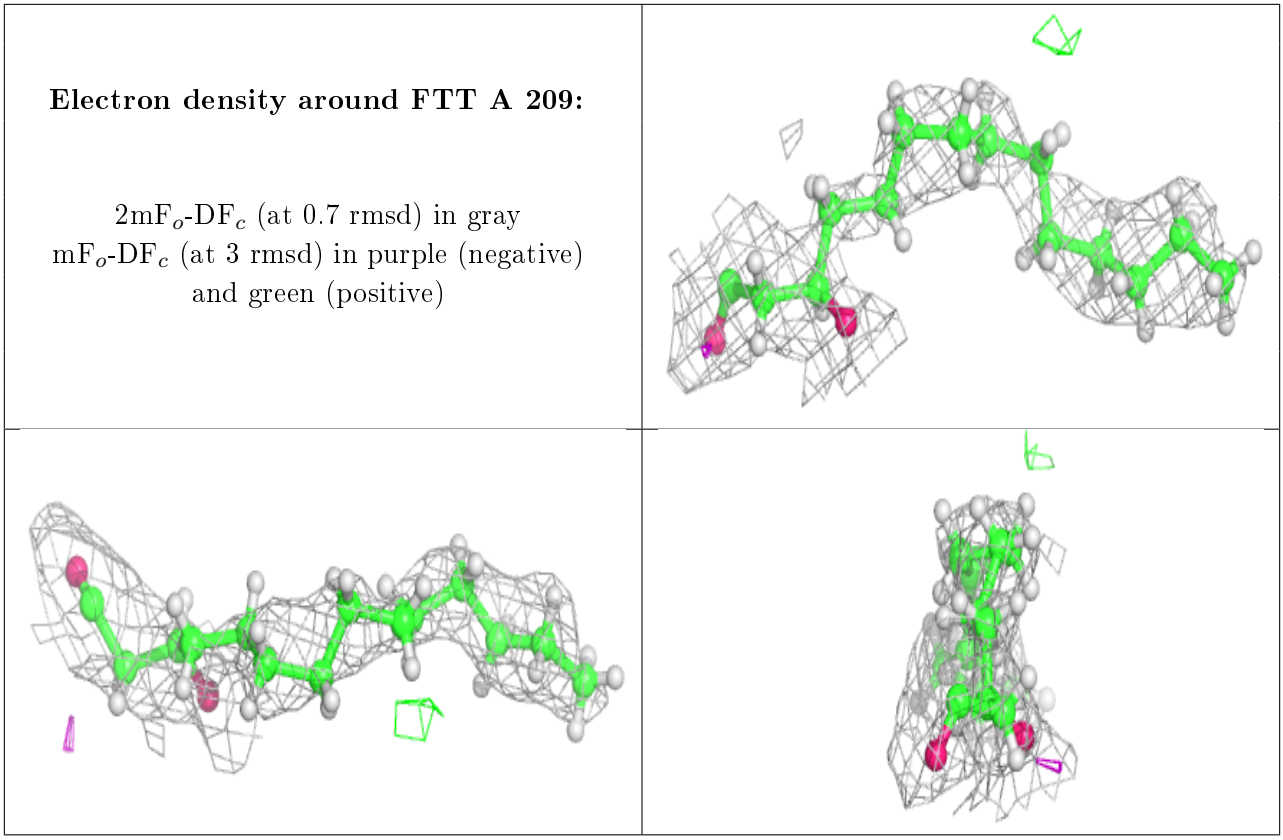
Electron density around MYR A 210:

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



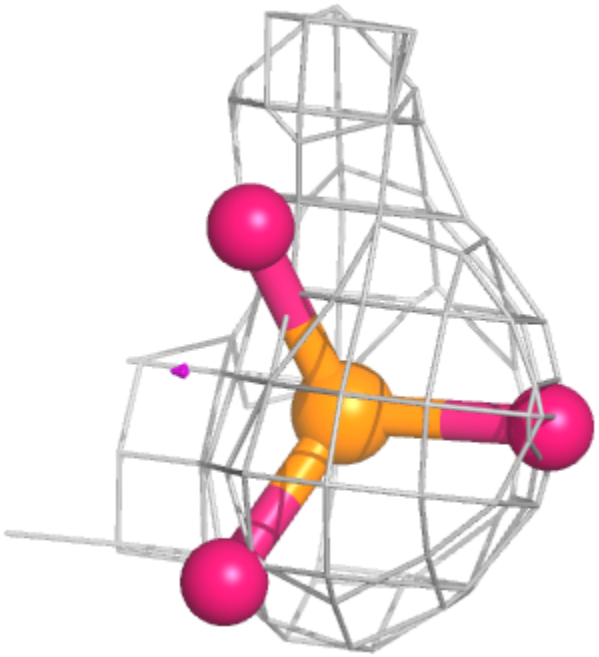
Electron density around FTT A 209:

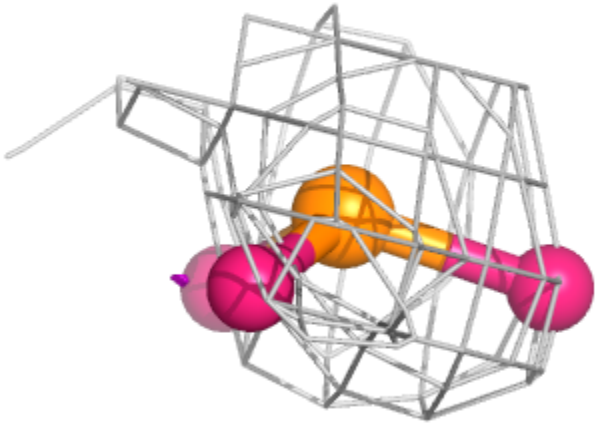
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

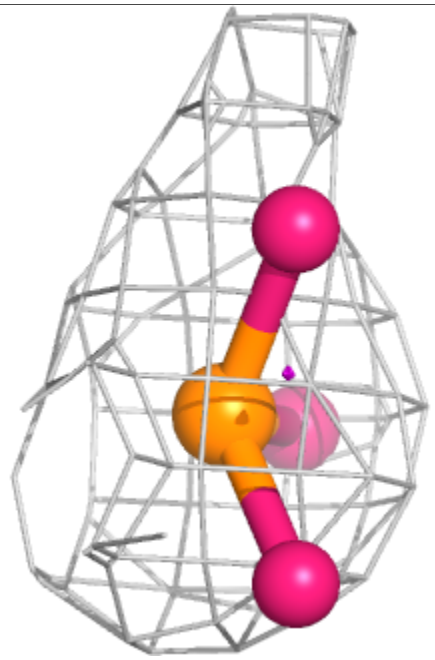


Electron density around PO4 D 621:

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

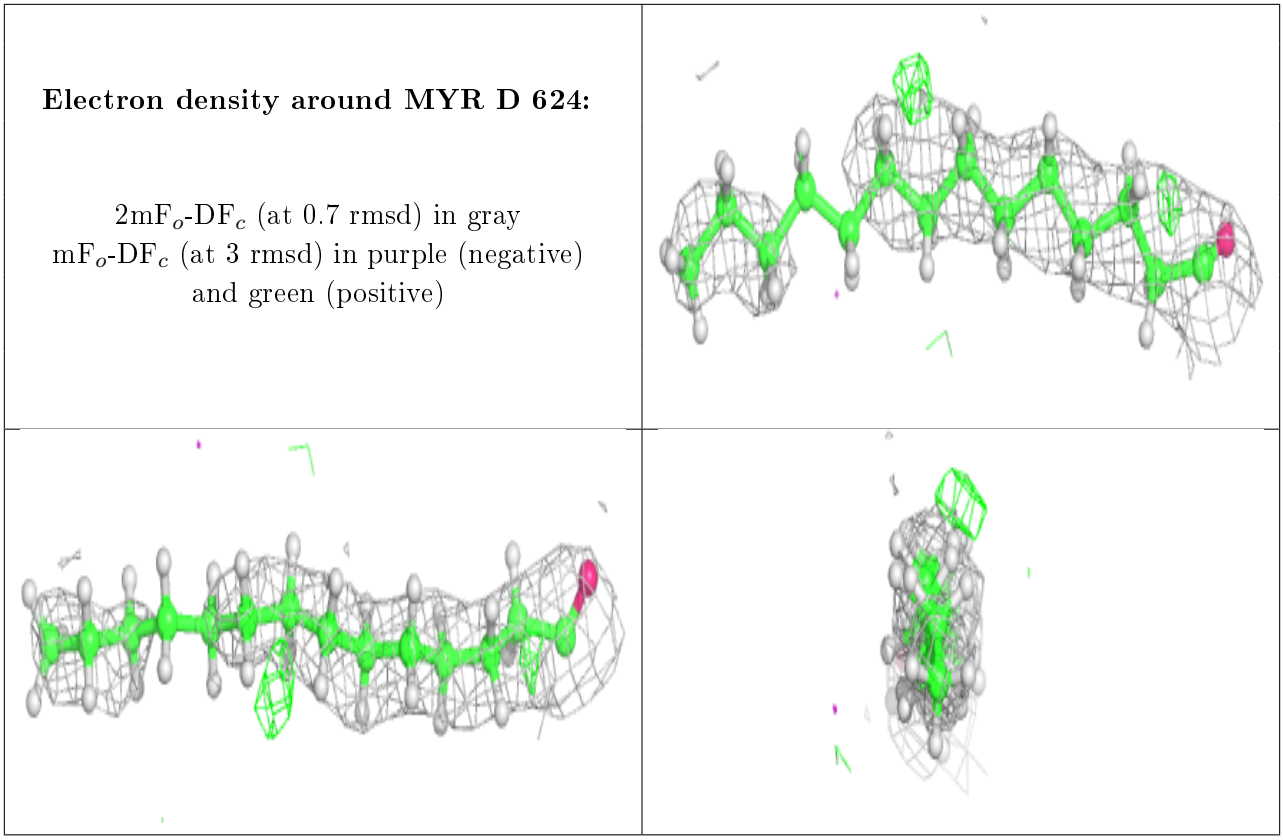






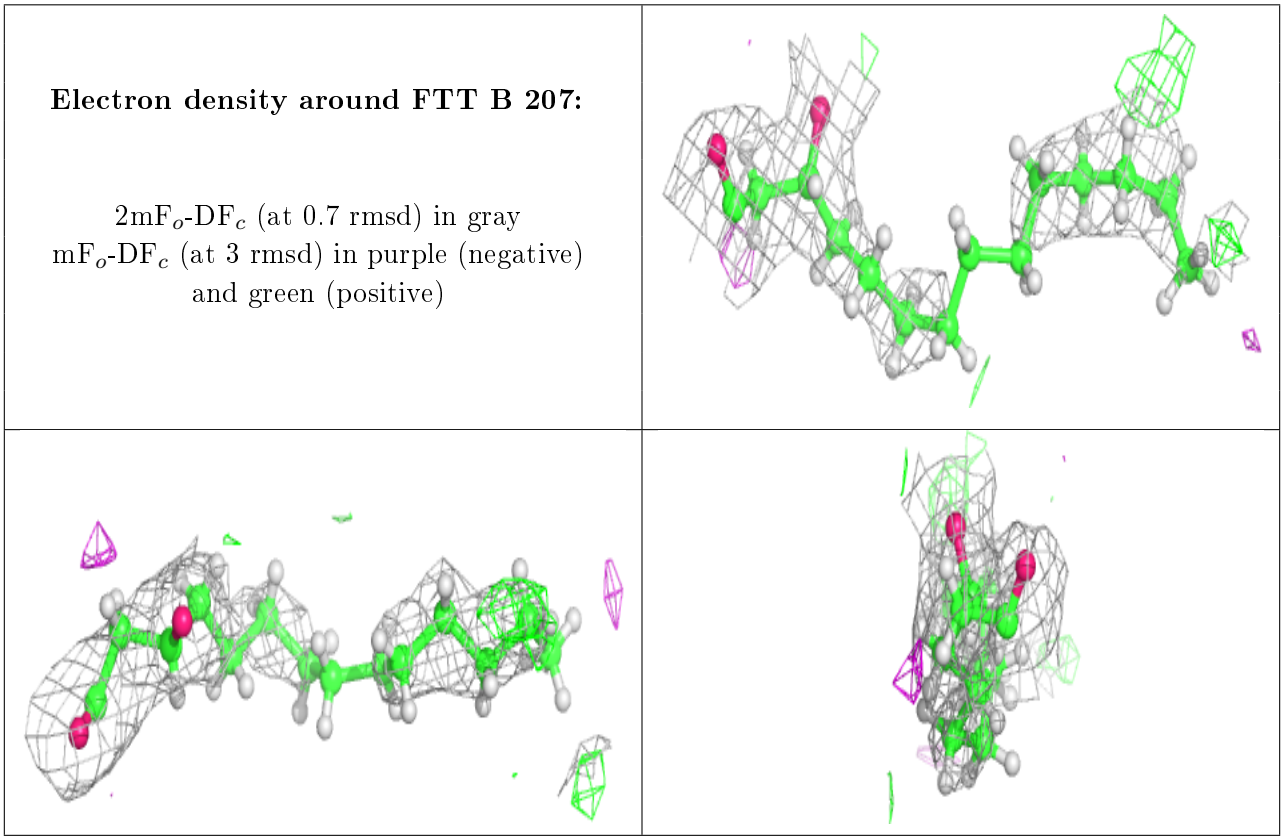
Electron density around MYR D 624:

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



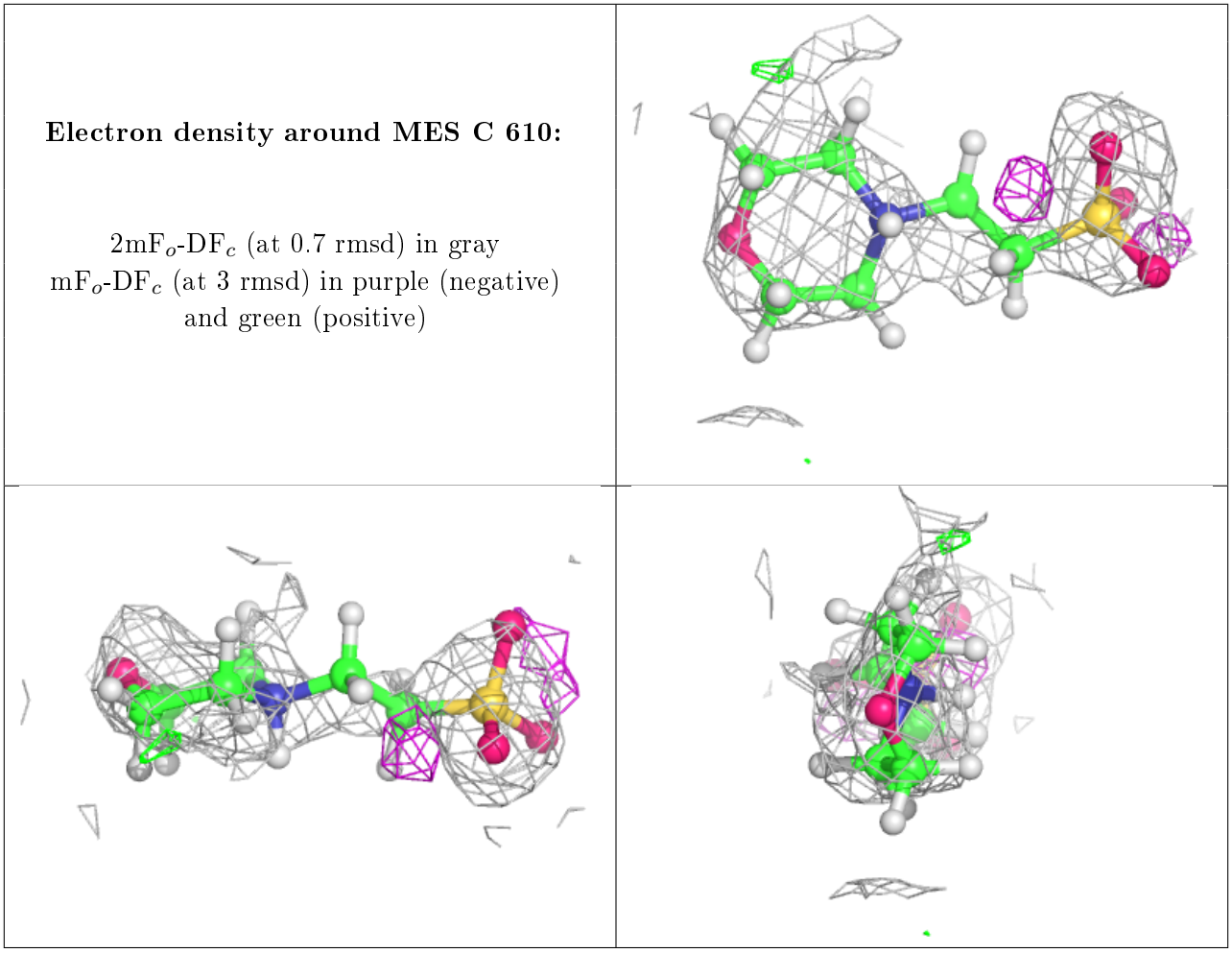
Electron density around FTT B 207:

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



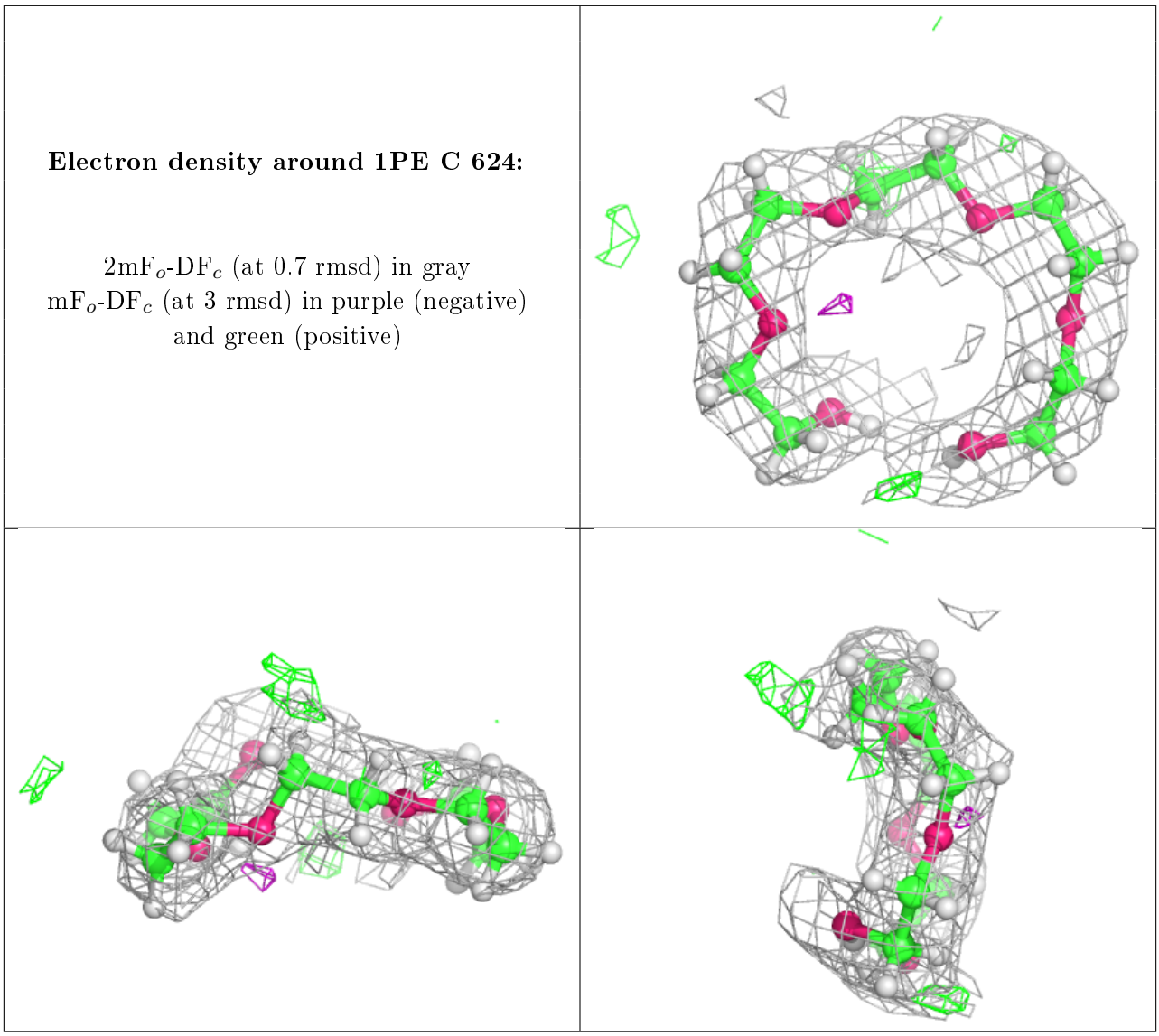
Electron density around MES C 610:

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



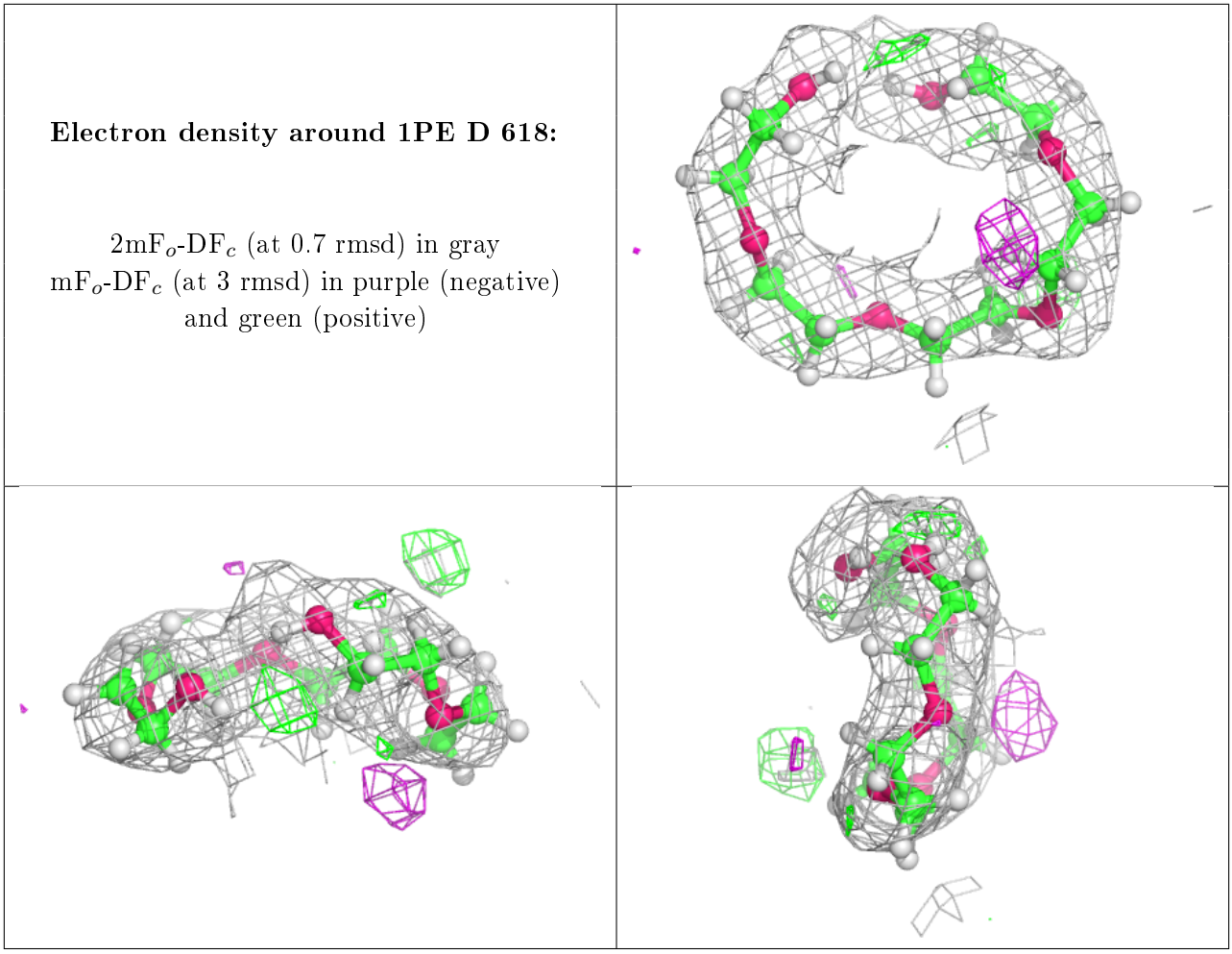
Electron density around 1PE C 624:

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



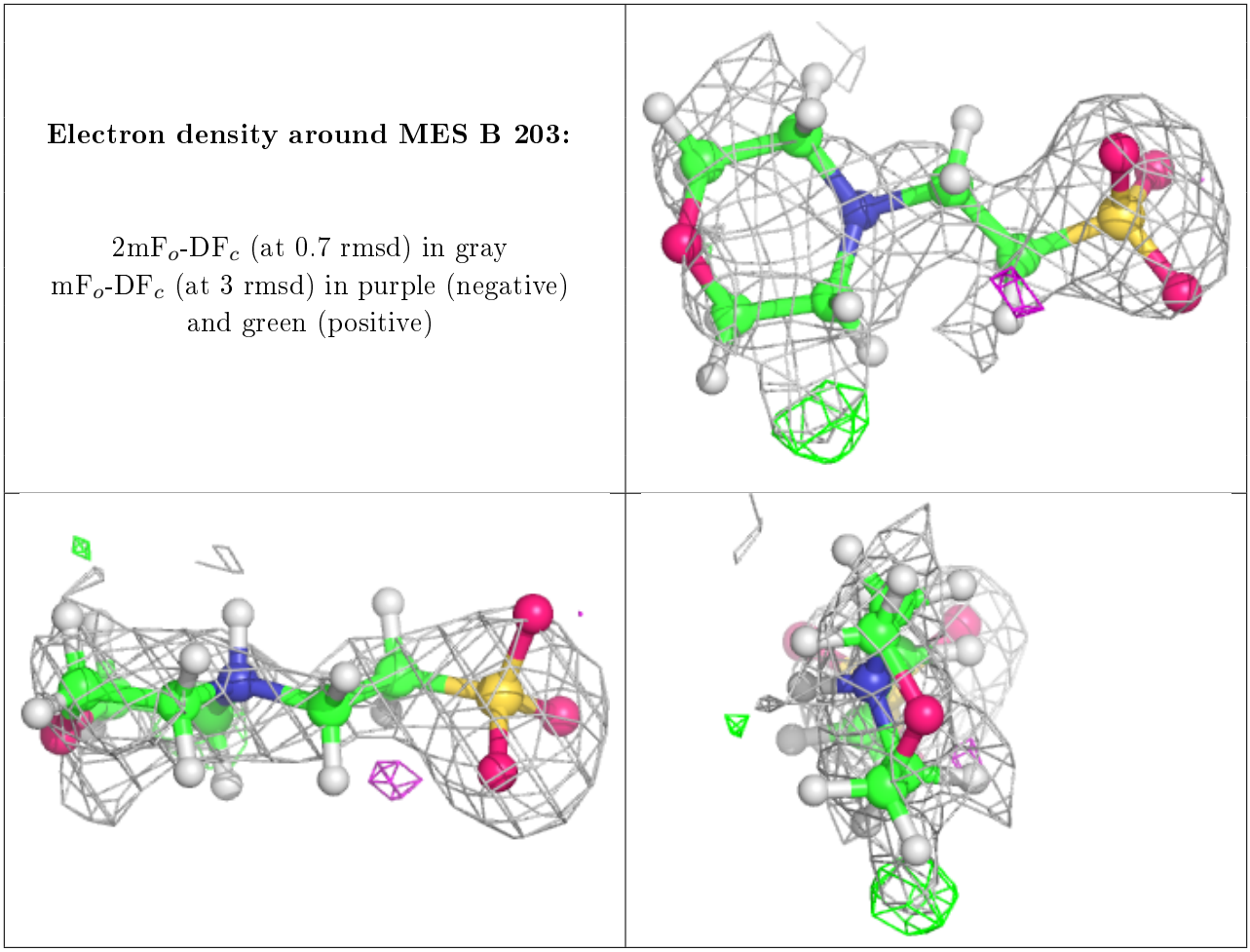
Electron density around 1PE D 618:

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



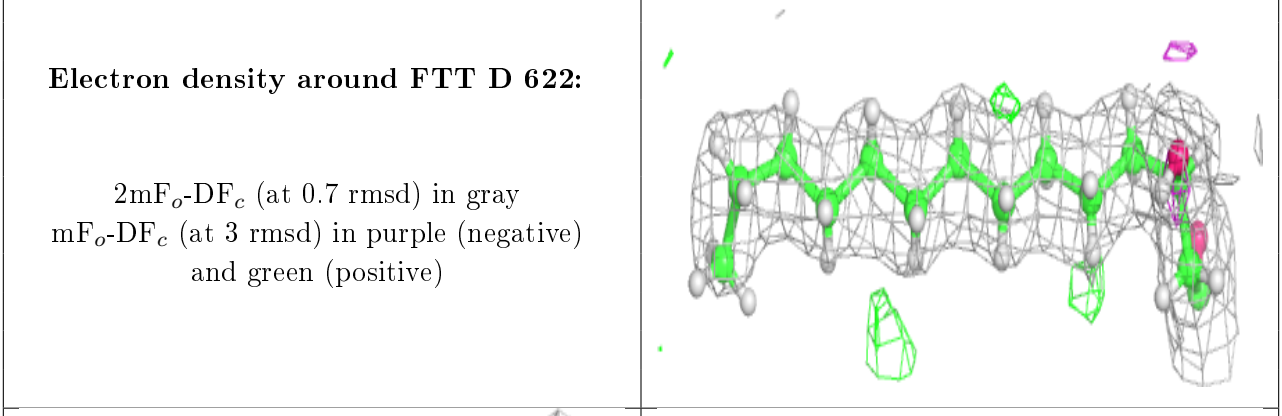
Electron density around MES B 203:

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



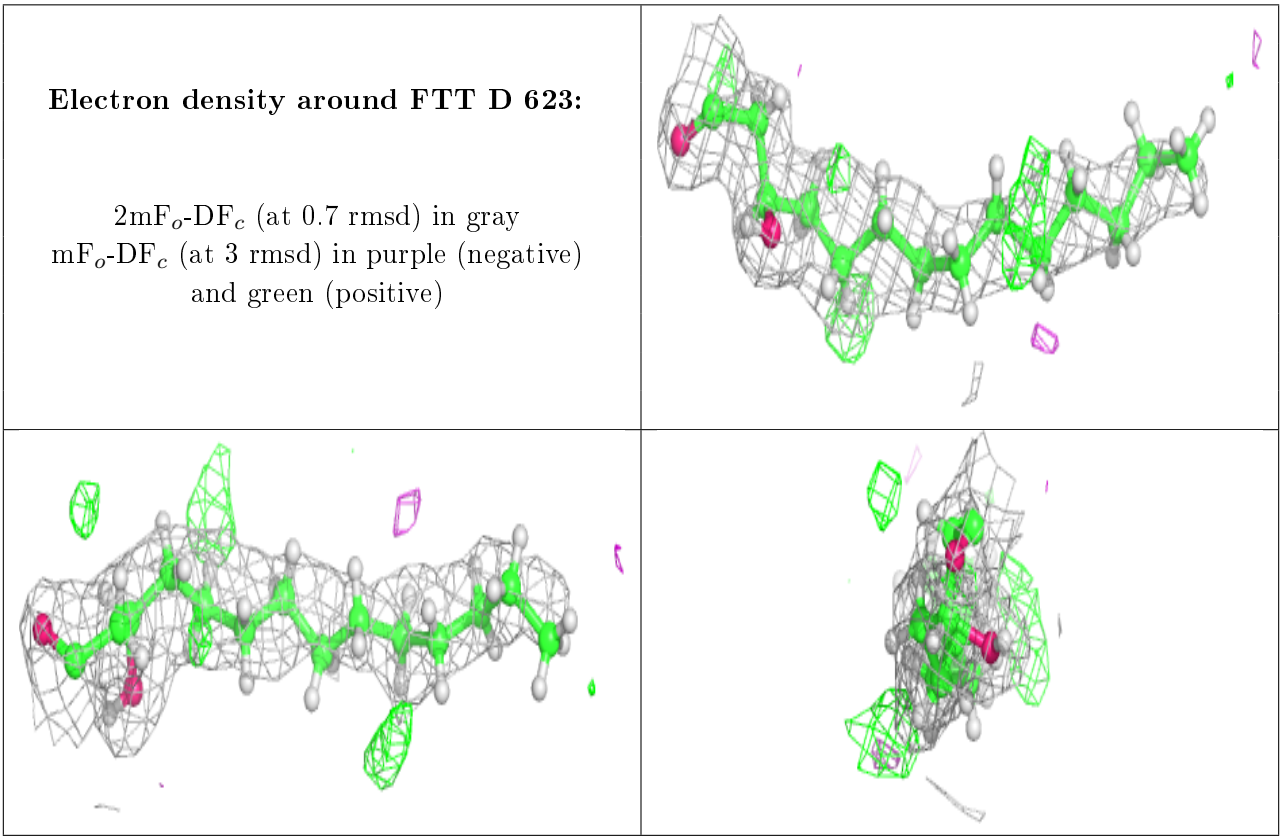
Electron density around FTT D 622:

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



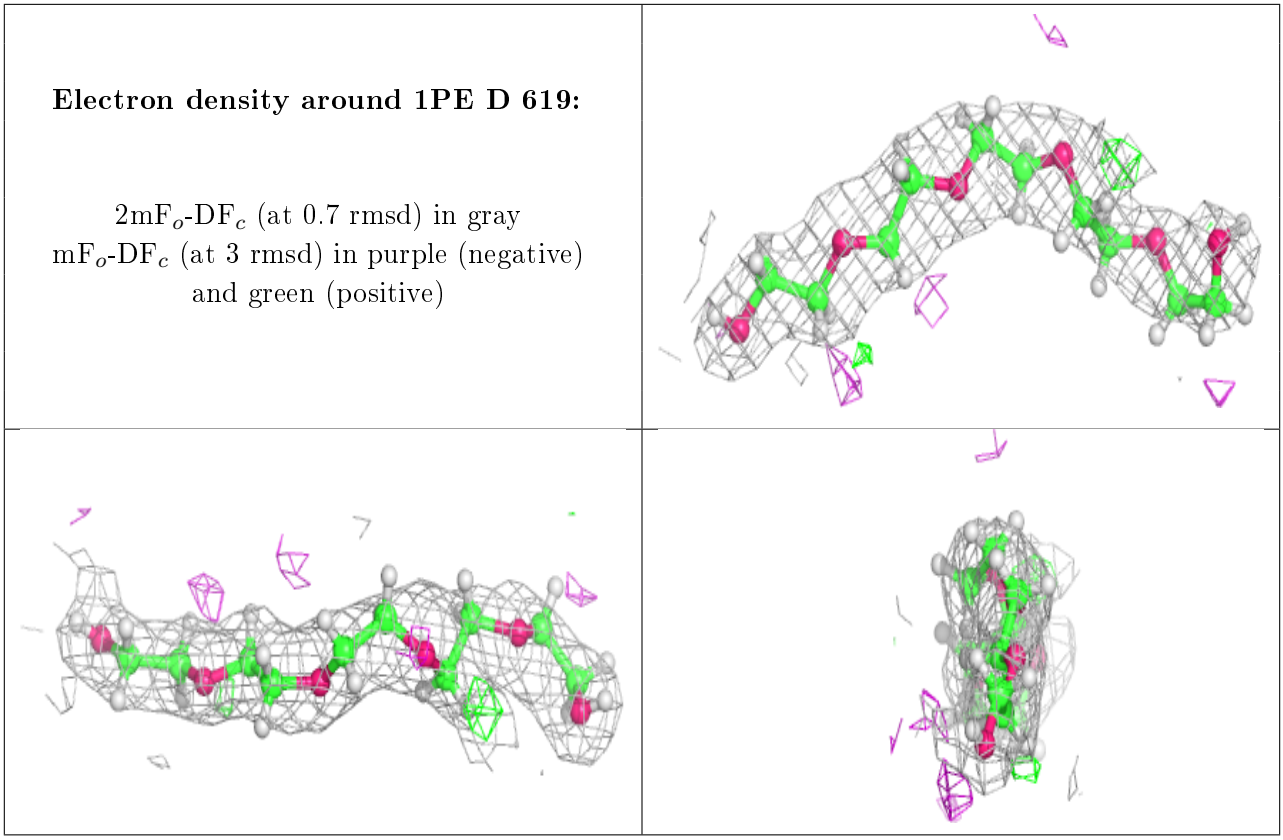
Electron density around FTT D 623:

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



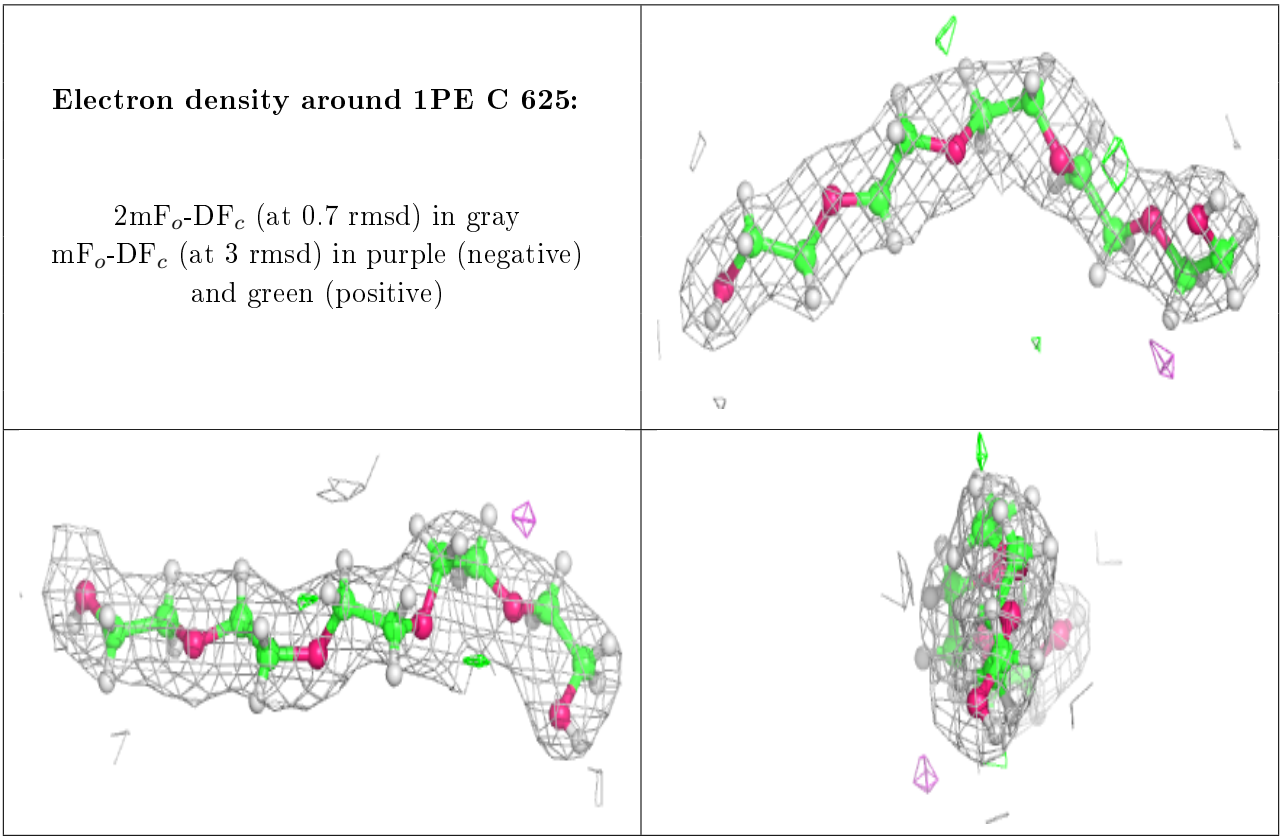
Electron density around 1PE D 619:

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



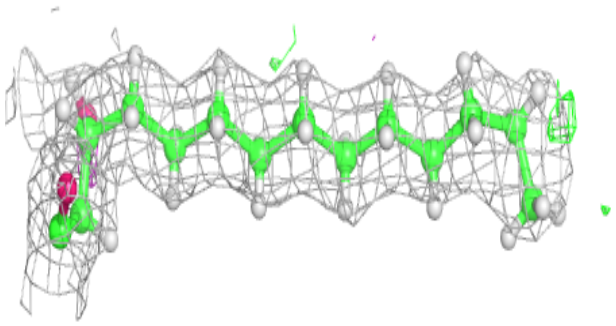
Electron density around 1PE C 625:

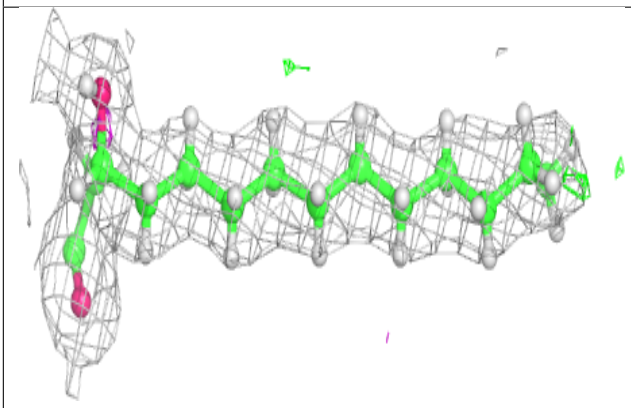
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

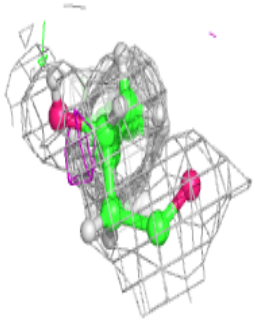


Electron density around FTT C 628:

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

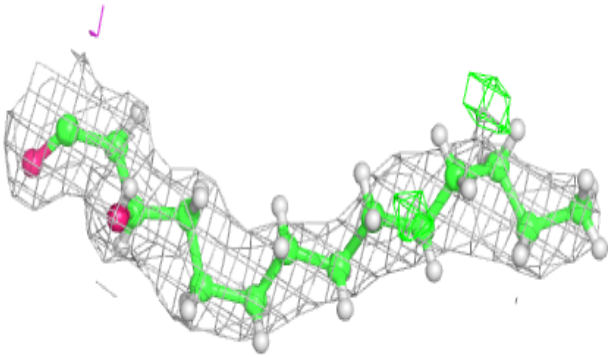


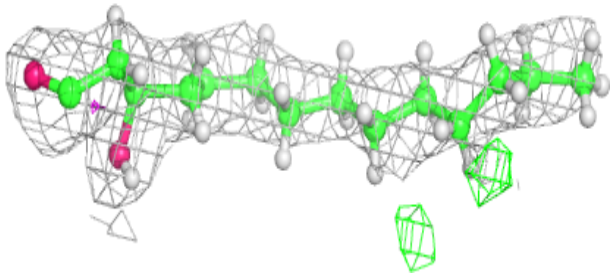


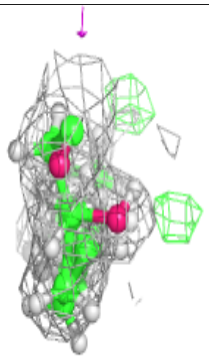


Electron density around FTT C 629:

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

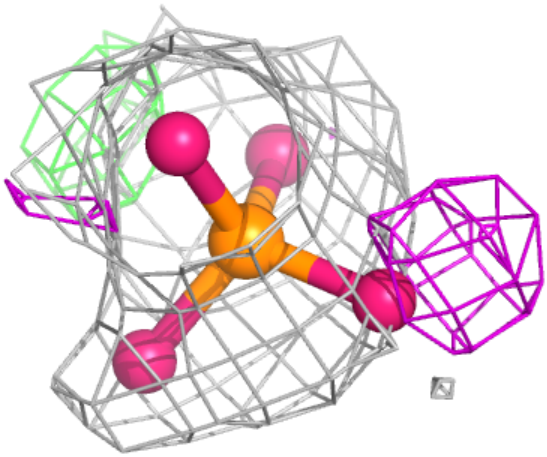


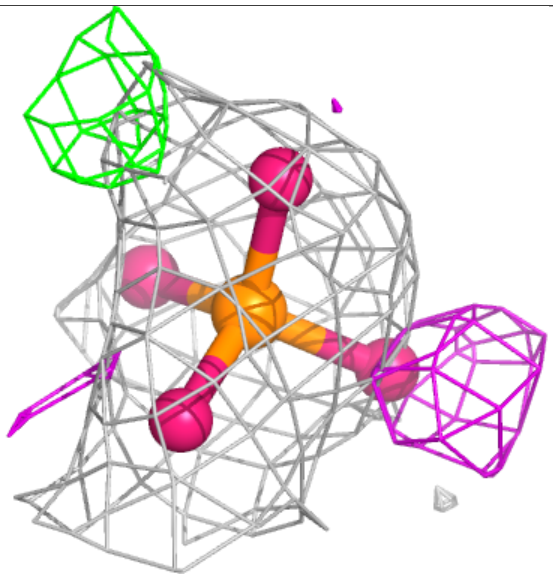


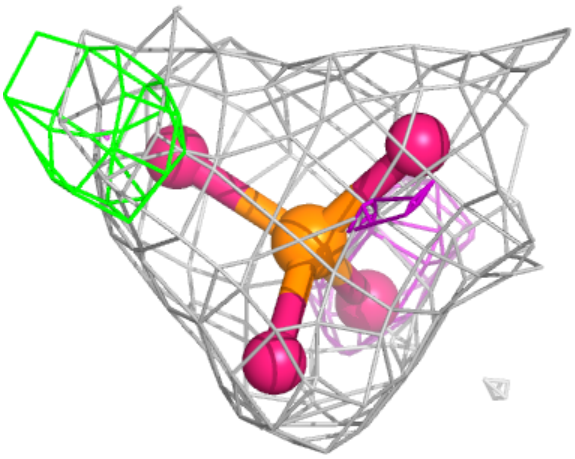


Electron density around PO4 C 626:

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

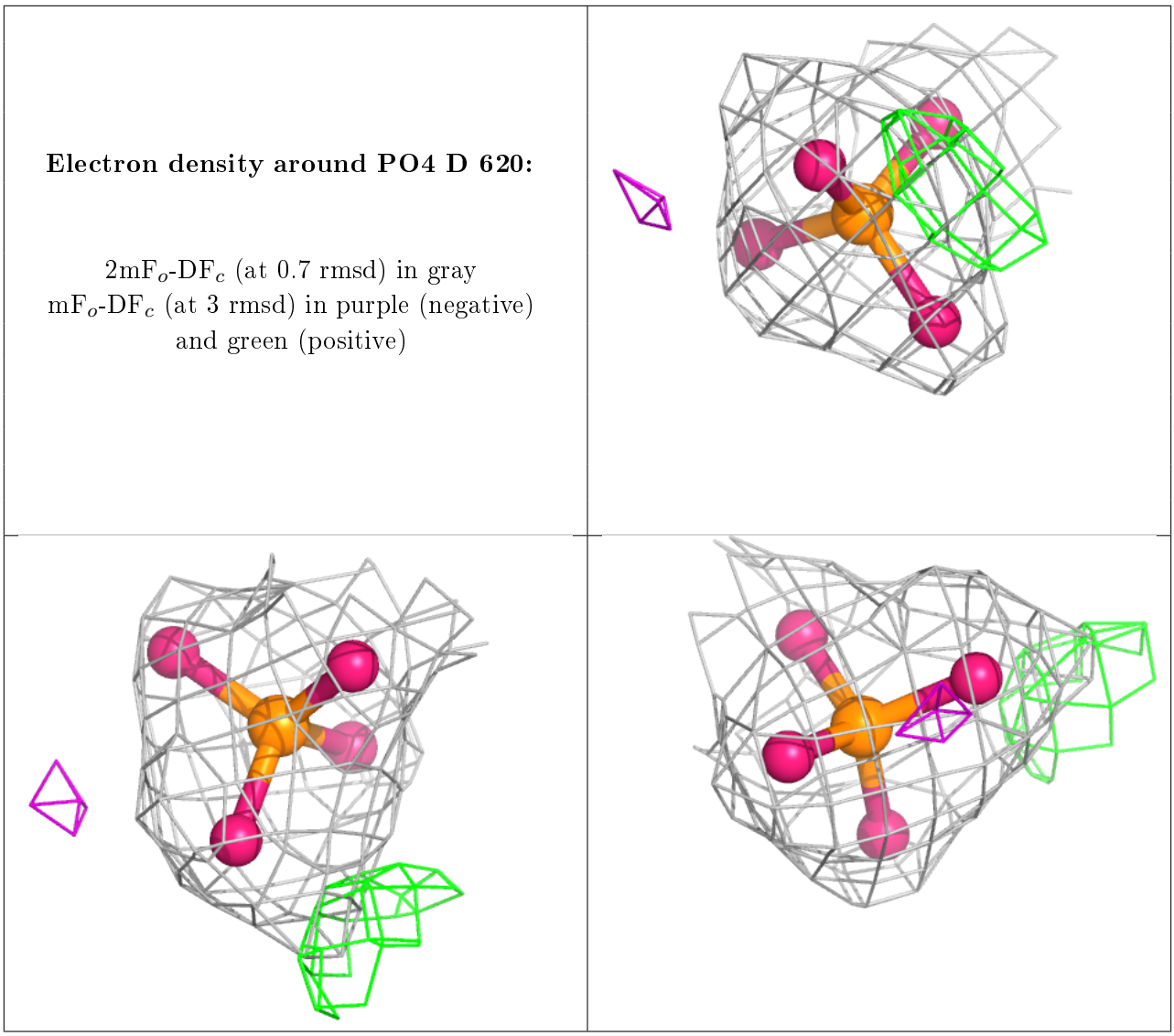






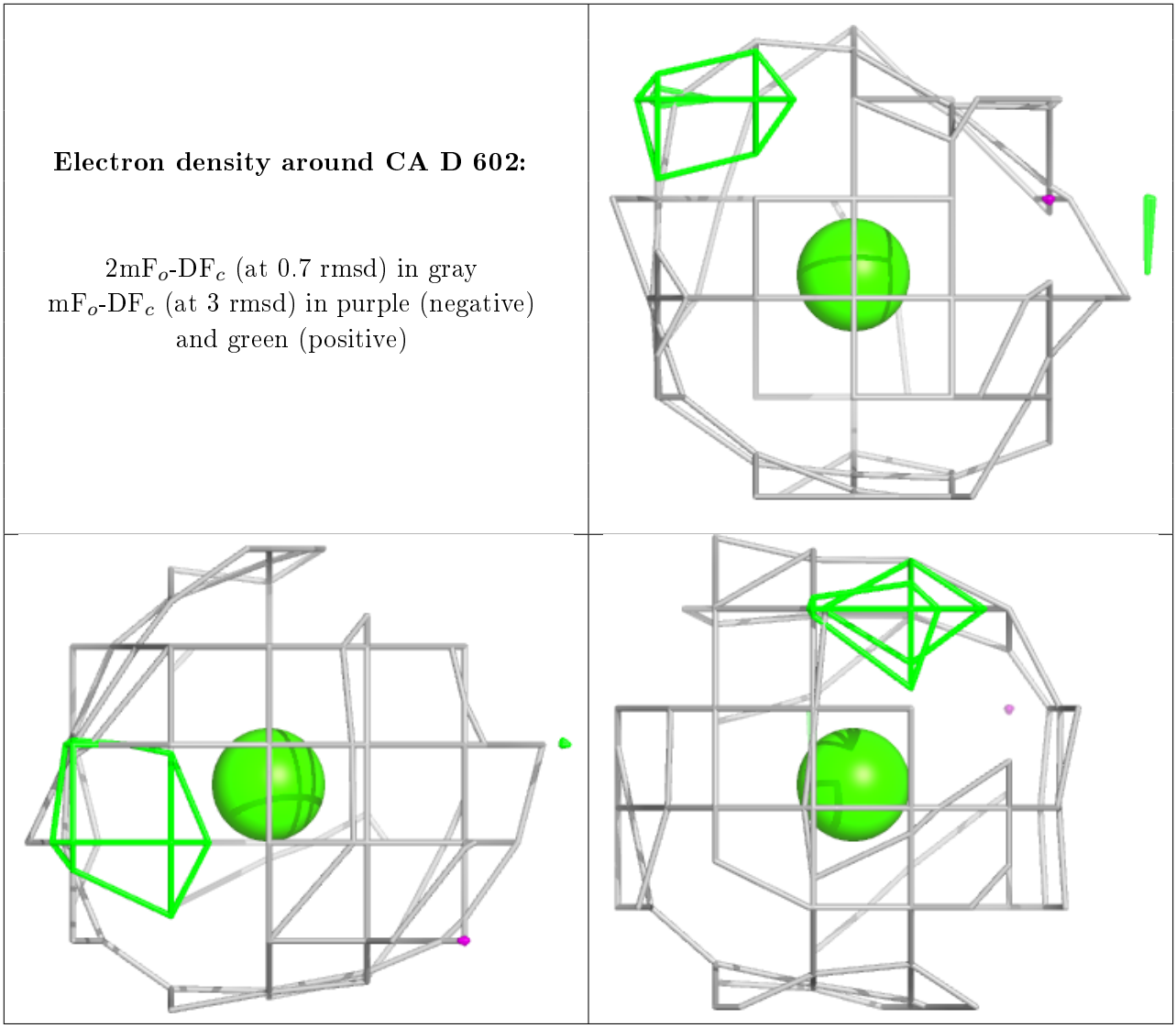
Electron density around PO4 D 620:

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



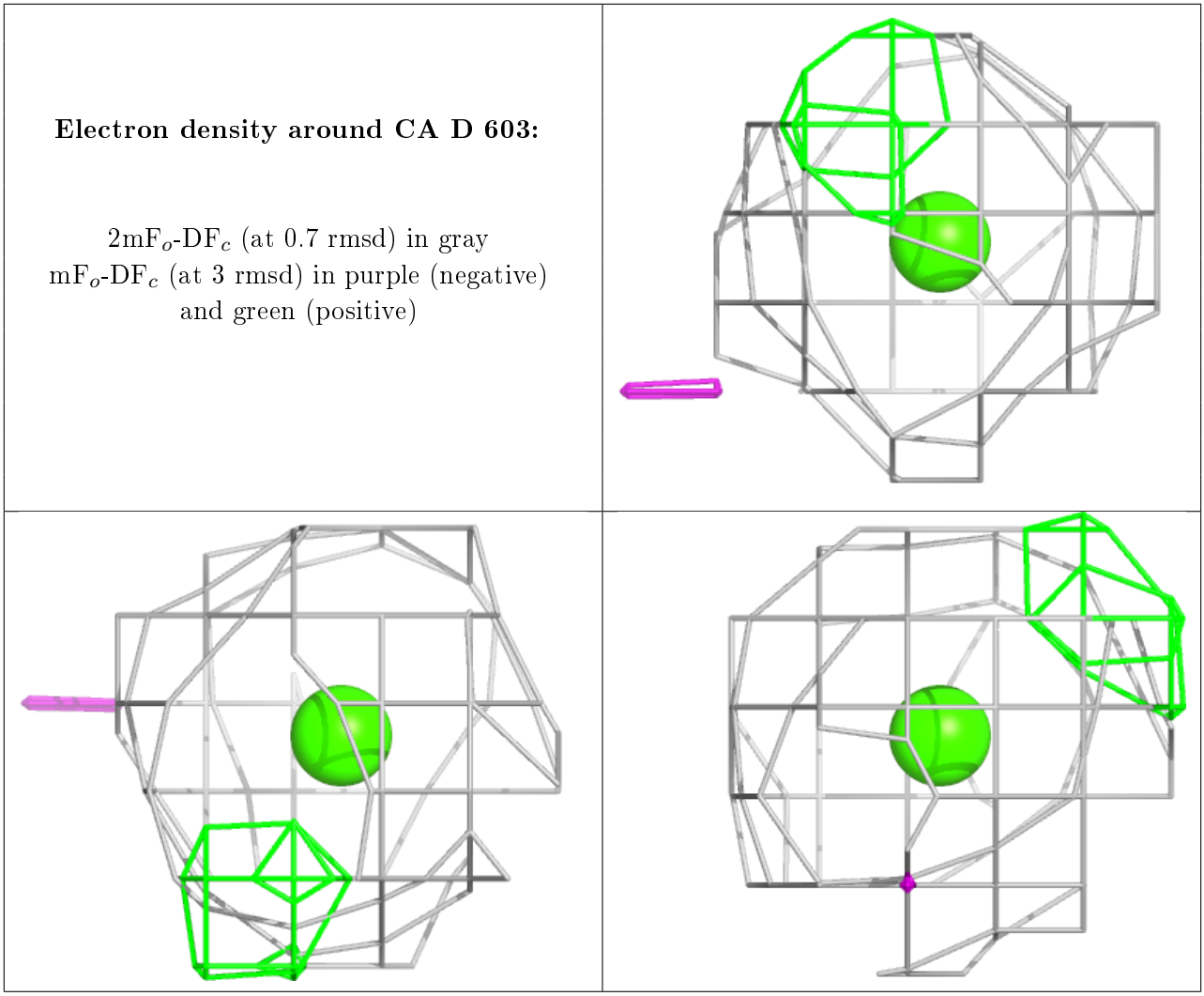
Electron density around CA D 602:

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



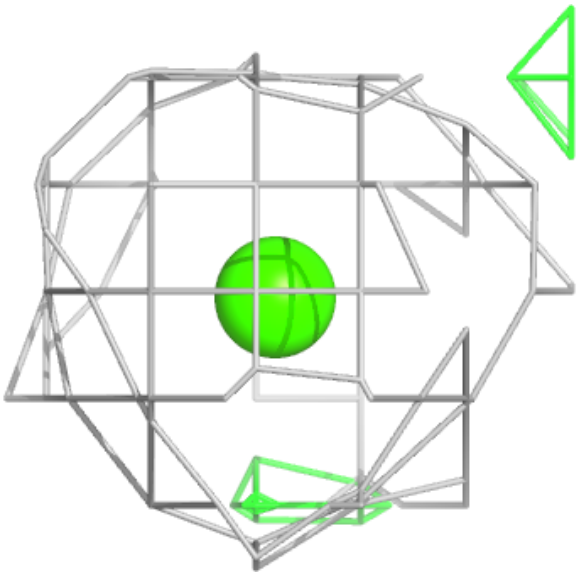
Electron density around CA D 603:

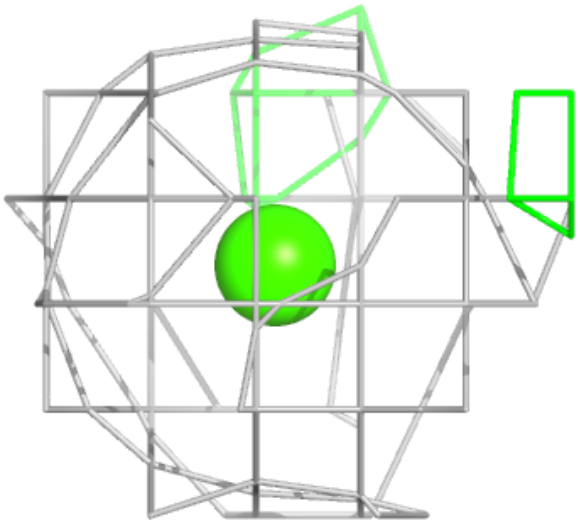
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

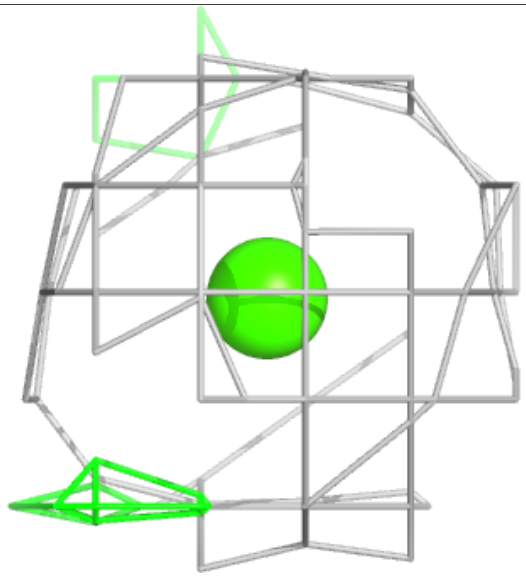


Electron density around CA C 602:

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

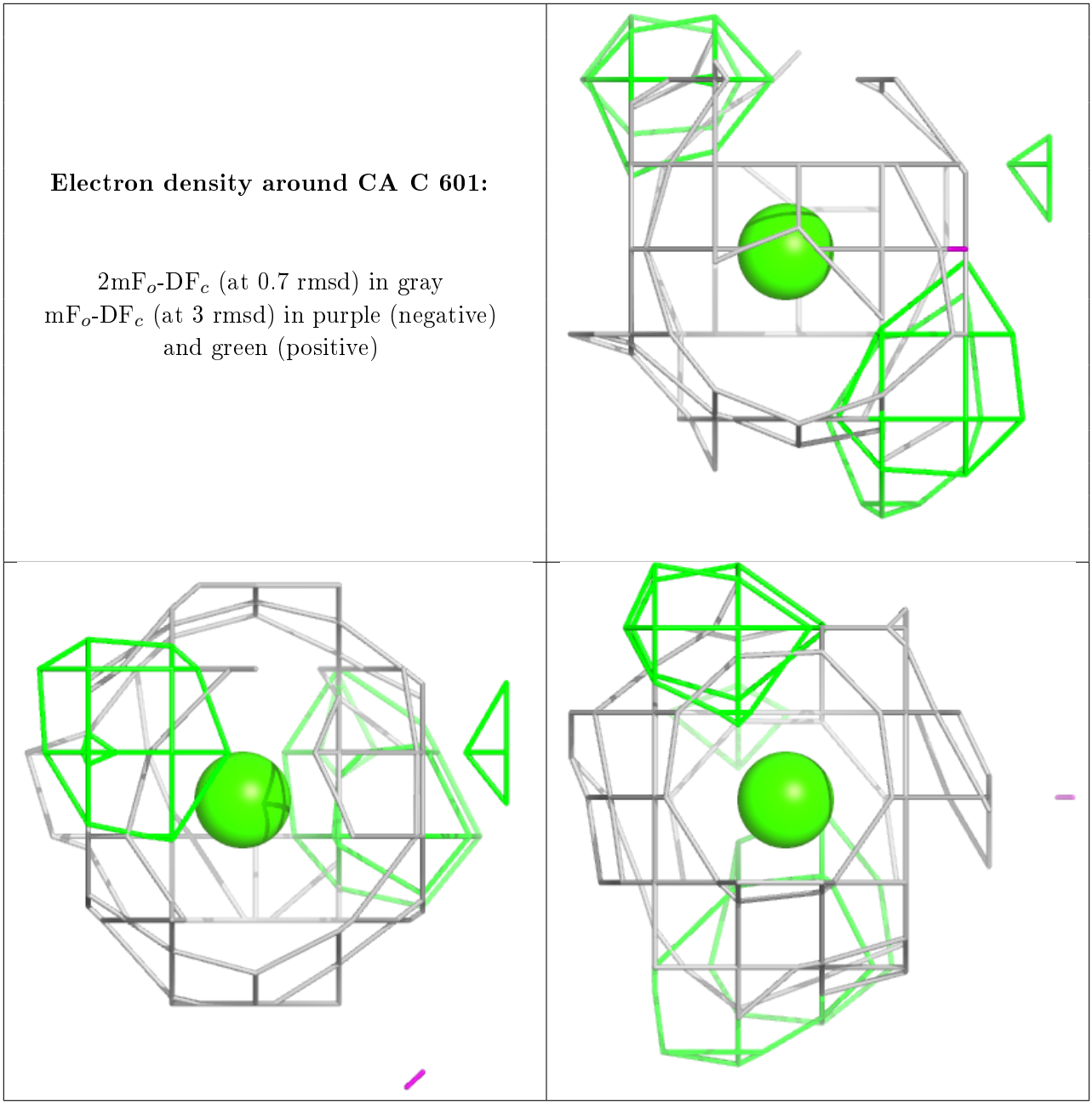






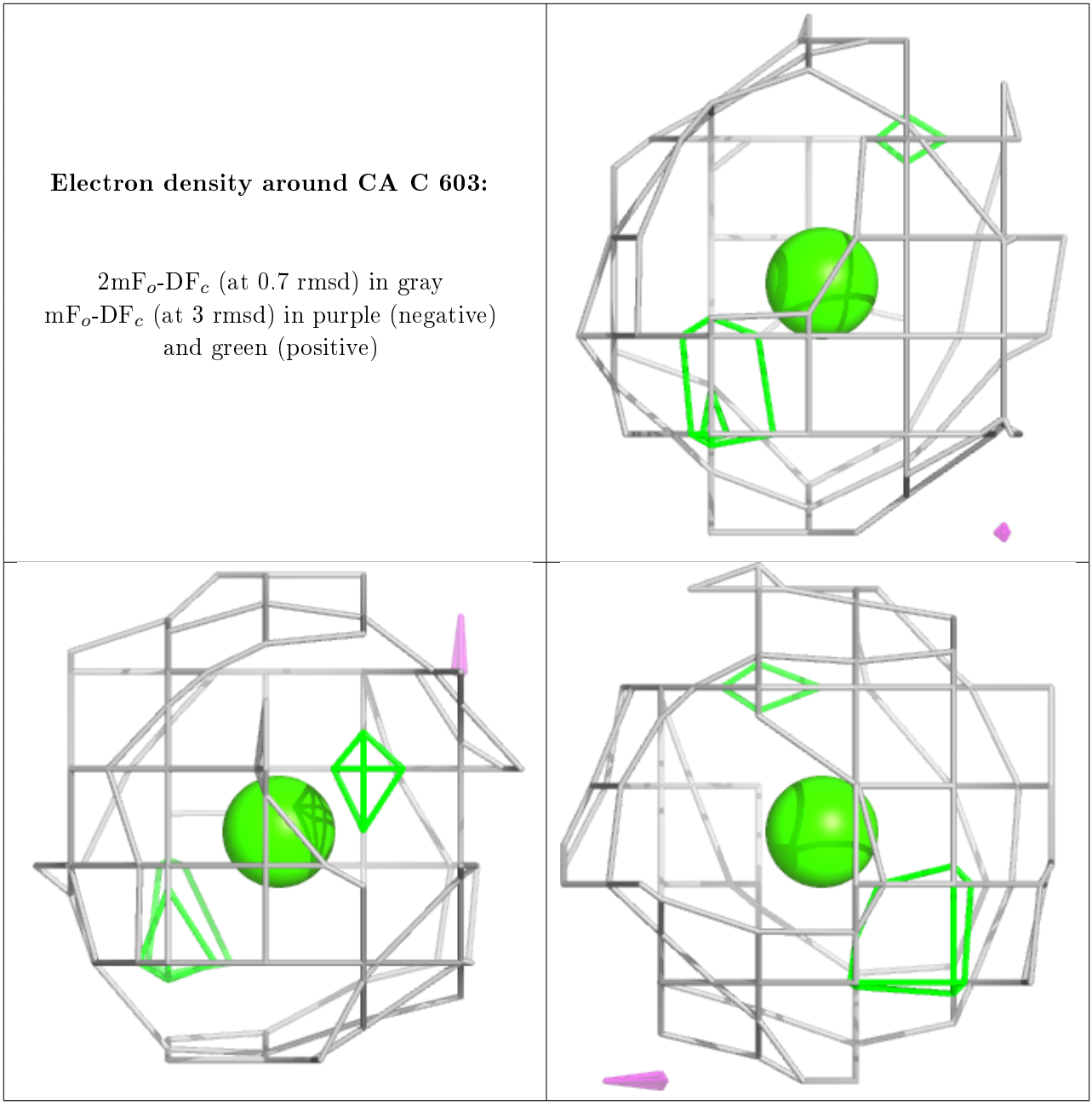
Electron density around CA C 601:

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



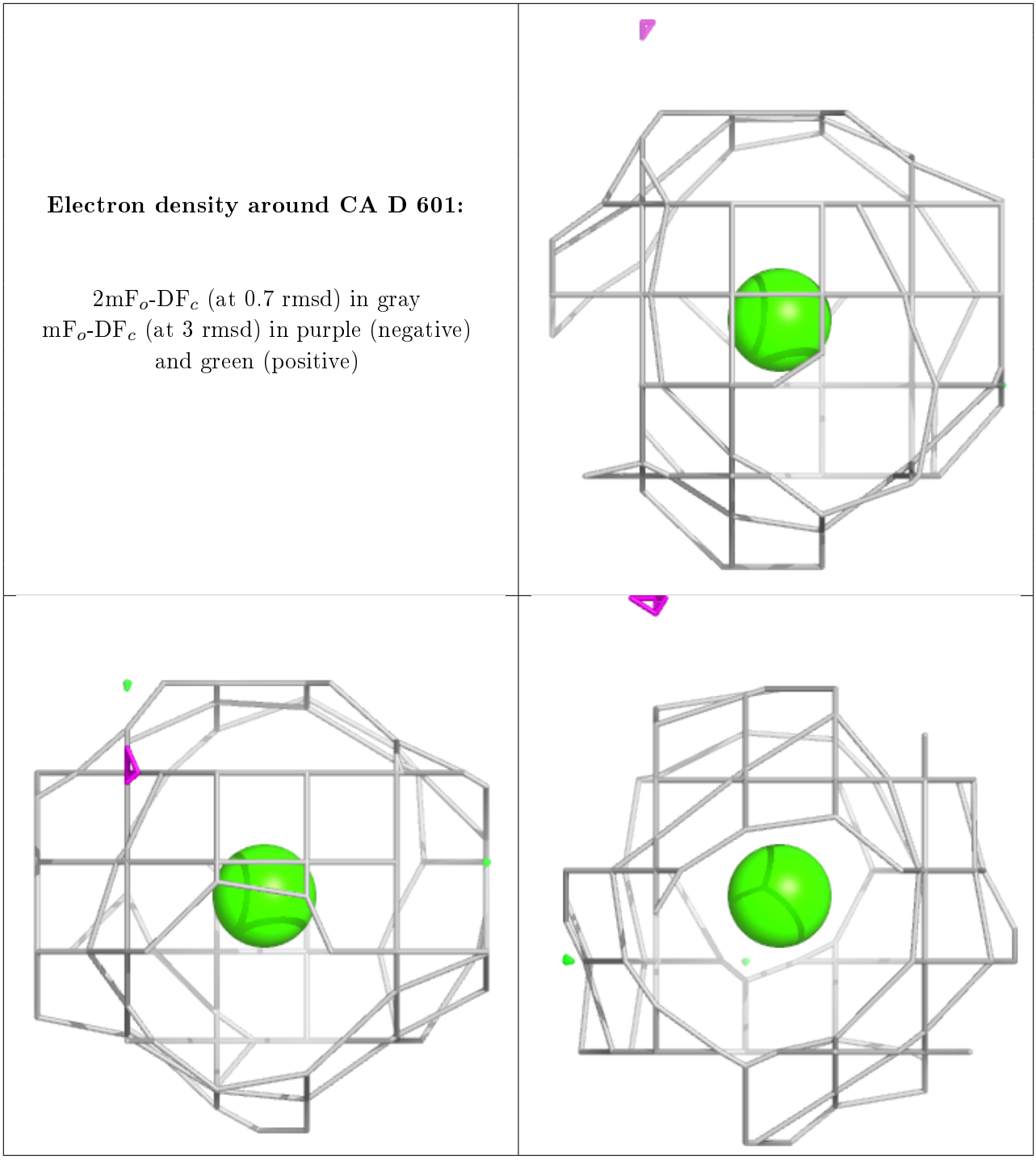
Electron density around CA C 603:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.