Full wwPDB X-ray Structure Validation Report (i)

Nov 23, 2023 – 01:53 AM JST

PDB ID	:	7VU1
Title	:	Chitoporin from Escherichia coli complex with chitohexaose
Authors	:	Suginta, W.; Soysa, H.S.M.; Amornloetwattana, R.; van den Berg, B.
Deposited on	:	2021-11-01
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

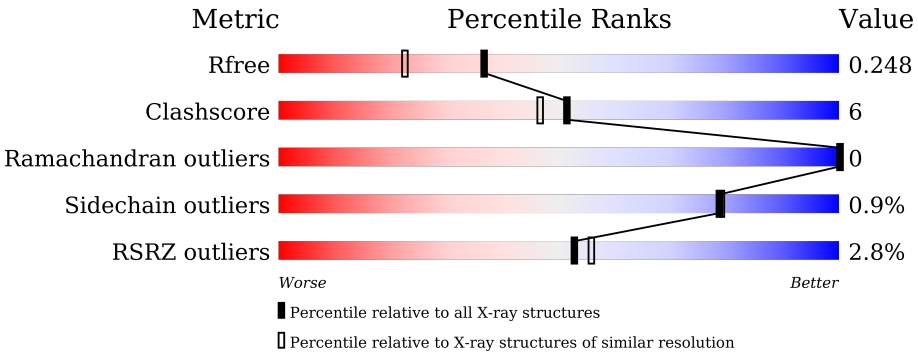
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	3% 90% 9%
1	B	436	3% 89% 10%
2	C	5	20% 80%
2	U	5	20% 80%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	U	3	-	-	X	-
4	C8E	A	505	-	-	-	X
4	C8E	A	512	-	-	-	X

2 Entry composition (i)

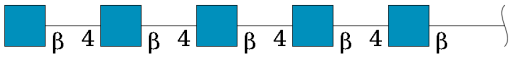
There are 6 unique types of molecules in this entry. The entry contains 14884 atoms, of which 6923 are hydrogens and 0 are deuteriums.

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 Chitoporin.

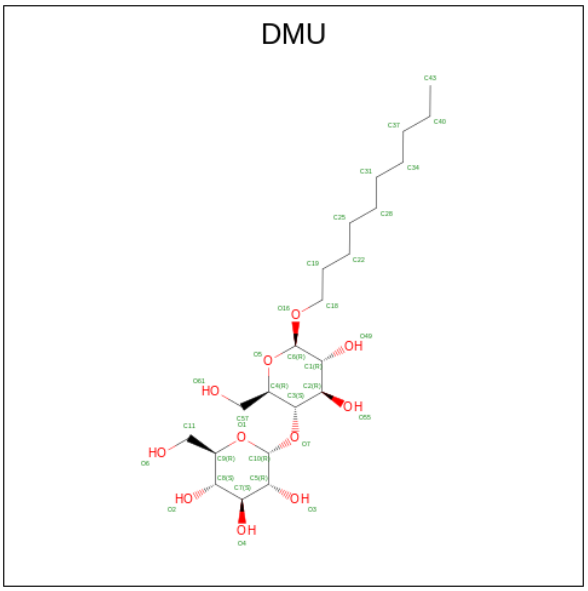
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	H	N	O	S	0	11	0
			6818	2286	3268	569	686	9			
1	B	435	Total	C	H	N	O	S	0	10	0
			6802	2282	3256	569	686	9			

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



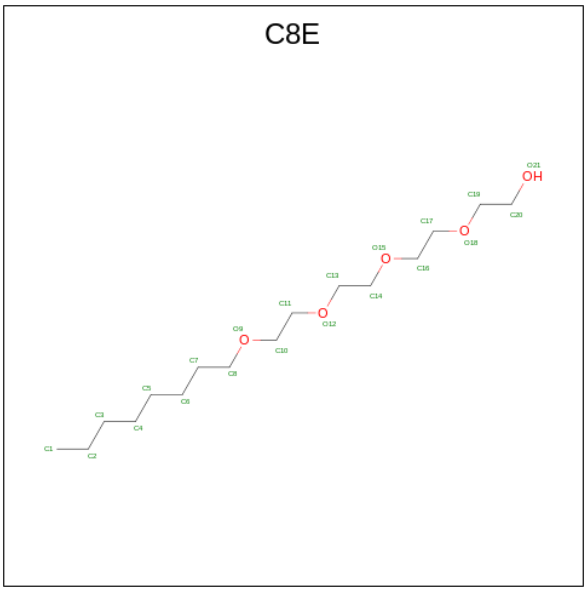
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	5	Total	C	H	N	O	0	0	0
			136	40	65	5	26			
2	C	5	Total	C	H	N	O	0	0	0
			129	40	58	5	26			

- Molecule 3 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			44	12	21	11		
3	A	1	Total	C	H	O	0	0
			62	18	33	11		
3	A	1	Total	C	H	O	0	0
			59	17	31	11		
3	B	1	Total	C	H	O	0	0
			47	13	23	11		
3	B	1	Total	C	H	O	0	0
			62	18	33	11		
3	B	1	Total	C	H	O	0	0
			56	16	29	11		

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H 10 6 4	0	0
4	A	1	Total C H 16 8 8	0	0
4	A	1	Total C H 11 5 6	0	0
4	A	1	Total C H O 10 4 4 2	0	0
4	A	1	Total C H 9 5 4	0	0
4	A	1	Total C H 11 5 6	0	0
4	A	1	Total C H O 9 3 4 2	0	0
4	A	1	Total C H 7 5 2	0	0
4	A	1	Total C H 7 5 2	0	0
4	B	1	Total C H O 26 10 14 2	0	0
4	B	1	Total C H O 24 7 13 4	0	0
4	B	1	Total C H 12 6 6	0	0
4	B	1	Total C H 12 6 6	0	0
4	B	1	Total C H 7 5 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H 12 6 6	0	0
4	B	1	Total C H O 9 3 4 2	0	0
4	B	1	Total C H 12 6 6	0	0
4	B	1	Total C H O 16 4 9 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	B	4	Total Mg 4 4	0	0

- Molecule 6 is water.

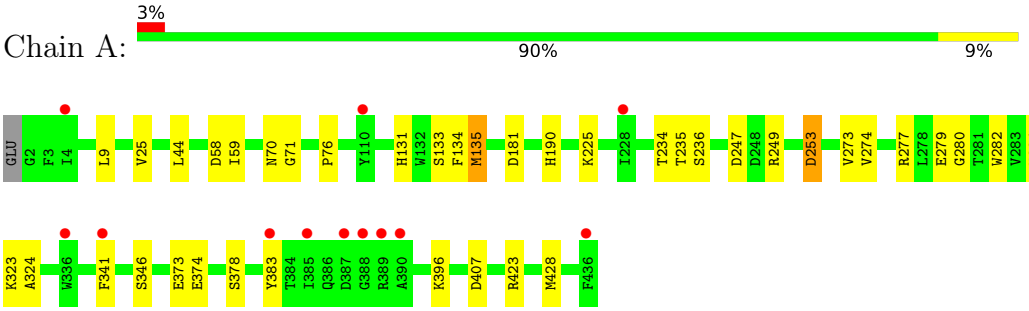
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	204	Total O 204 204	0	0
6	B	239	Total O 239 239	0	0

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.

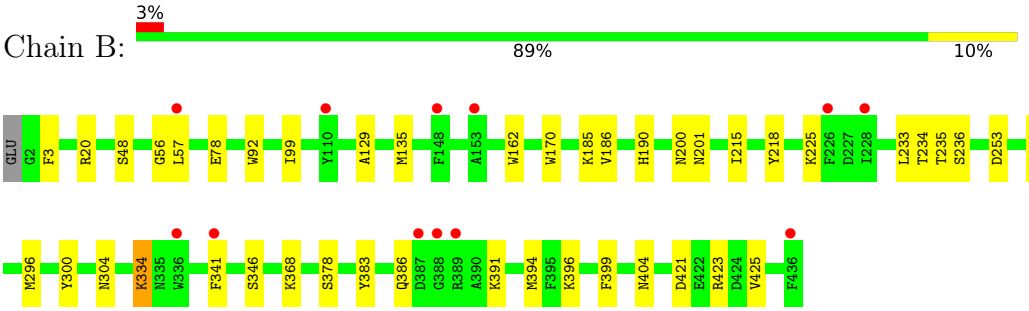
• Molecule 1: Chitoporin

Chain A:



• Molecule 1: Chitoporin

Chain B:



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

Chain U:

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

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.74Å 58.55Å 133.06Å 90.00° 110.71° 90.00°	Depositor
Resolution (Å)	62.34 – 1.90 62.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (62.34-1.90) 91.9 (62.50-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.209 , 0.248 0.209 , 0.248	Depositor DCC
R_{free} test set	5260 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	1.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14884	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 87.32 % 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 7.1216e-08. 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: C8E, MG, NAG, DMU

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	0.53	0/3695	0.70	3/5015 (0.1%)
1	B	0.58	0/3688	0.76	2/5008 (0.0%)
All	All	0.56	0/7383	0.73	5/10023 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	334	LYS	CD-CE-NZ	6.78	127.28	111.70
1	B	135	MET	CG-SD-CE	6.45	110.51	100.20
1	A	135	MET	CG-SD-CE	5.73	109.36	100.20
1	A	253	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	181	ASP	CB-CG-OD1	5.07	122.86	118.30

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	3550	3268	3284	24	0
1	B	3546	3256	3275	37	0
2	C	71	58	63	10	0
2	U	71	65	63	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	80	85	81	0	0
3	B	80	85	79	3	0
4	A	50	40	70	2	0
4	B	64	66	88	10	0
5	A	2	0	0	0	0
5	B	4	0	0	0	0
6	A	204	0	0	3	0
6	B	239	0	0	4	0
All	All	7961	6923	7003	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (81) 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:5:NAG:H82	2:C:5:NAG:O3	1.74	0.87
1:B:284:LYS:NZ	3:B:503:DMU:O4	2.08	0.86
2:C:2:NAG:C6	2:C:3:NAG:H83	2.16	0.75
2:C:2:NAG:H62	2:C:3:NAG:H83	1.67	0.74
1:B:218:TYR:OH	6:B:601:HOH:O	2.06	0.72
4:B:511:C8E:H32	2:U:3:NAG:H5	1.74	0.69
1:A:253:ASP:OD1	6:A:601:HOH:O	2.12	0.68
4:B:511:C8E:C3	2:U:3:NAG:H5	2.24	0.68
1:A:70:ASN:OD1	1:A:71:GLY:N	2.29	0.66
3:B:503:DMU:O61	4:B:509:C8E:H31	1.96	0.66
1:B:394:MET:HE2	1:B:396:LYS:CE	2.27	0.65
1:A:133:SER:O	2:C:1:NAG:H82	1.96	0.65
1:B:346:SER:OG	1:B:378[A]:SER:OG	2.15	0.64
1:A:247:ASP:OD1	6:A:601:HOH:O	2.14	0.64
2:C:2:NAG:O3	2:C:2:NAG:H82	1.95	0.64
2:C:5:NAG:O3	2:C:5:NAG:C8	2.45	0.63
1:A:346:SER:OG	1:A:378[A]:SER:OG	2.17	0.62
1:B:20:ARG:HH22	2:U:3:NAG:C8	2.15	0.59
2:U:4:NAG:O3	2:U:5:NAG:O6	2.21	0.59
1:B:300:TYR:HE1	4:B:511:C8E:H31	1.68	0.58
1:B:20:ARG:HH22	2:U:3:NAG:H82	1.69	0.58
1:B:92:TRP:CZ2	2:U:5:NAG:H5	2.39	0.57
2:C:2:NAG:O3	2:C:2:NAG:C8	2.52	0.56
1:A:134:PHE:HA	2:C:1:NAG:H82	1.90	0.54
1:B:253:ASP:OD1	6:B:602:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:MET:HE2	1:B:396:LYS:HE2	1.89	0.53
2:U:2:NAG:O4	2:U:3:NAG:H83	2.07	0.53
1:A:282:TRP:CD1	1:A:323:LYS:HD3	2.43	0.53
1:B:99:ILE:HD11	4:B:504:C8E:H41	1.91	0.53
1:A:273:VAL:HG13	1:A:274[B]:VAL:HG23	1.92	0.52
1:B:394:MET:HE2	1:B:396:LYS:HE3	1.90	0.52
1:B:78:GLU:OE2	1:B:300:TYR:OH	2.18	0.51
1:B:404:ASN:N	1:B:421:ASP:OD1	2.43	0.51
1:A:373:GLU:OE1	6:A:602:HOH:O	2.19	0.49
1:B:48:SER:HB3	1:B:57[B]:LEU:HD13	1.93	0.49
2:U:3:NAG:O3	2:U:4:NAG:O5	2.28	0.49
3:B:503:DMU:H35	3:B:503:DMU:H30	1.94	0.48
1:B:334:LYS:HB3	1:B:334:LYS:HE3	1.49	0.48
1:B:236:SER:OG	1:B:265[A]:THR:HG22	2.13	0.48
1:A:25:VAL:HG21	1:A:407:ASP:O	2.13	0.47
1:A:133:SER:O	2:C:1:NAG:C8	2.62	0.47
1:A:9:LEU:HD11	1:A:44:LEU:HG	1.97	0.47
4:B:511:C8E:H62	6:B:729:HOH:O	2.14	0.46
1:B:3:PHE:CE2	1:B:57[B]:LEU:HD12	2.51	0.46
1:A:322:GLU:OE1	1:A:374:GLU:OE1	2.34	0.46
1:B:368:LYS:HB3	1:B:368:LYS:HE2	1.74	0.45
1:A:76:PRO:O	4:A:510:C8E:C8	2.65	0.45
1:B:386:GLN:O	1:B:391:LYS:HG3	2.16	0.45
4:B:511:C8E:C2	6:B:706:HOH:O	2.65	0.45
1:A:58:ASP:O	1:A:59[A]:ILE:HD13	2.18	0.44
1:B:185:LYS:HG3	1:B:186:VAL:N	2.31	0.44
1:B:200:ASN:O	1:B:201:ASN:HB2	2.17	0.44
1:A:284:LYS:NZ	1:A:286:ASP:OD2	2.39	0.44
1:B:201:ASN:HB3	1:B:225:LYS:HG3	1.99	0.44
1:B:341[A]:PHE:CE2	1:B:383:TYR:CE1	3.05	0.44
1:A:396:LYS:HB2	1:A:428:MET:HG2	1.98	0.44
1:B:274:VAL:O	1:B:274:VAL:HG13	2.18	0.44
1:A:131:HIS:HD2	4:A:507:C8E:H172	1.83	0.44
1:A:225:LYS:HG2	1:A:234:THR:HG22	2.00	0.44
1:B:225:LYS:HB3	1:B:234:THR:HG22	1.99	0.43
1:B:129:ALA:O	1:B:304:ASN:HB3	2.18	0.43
1:B:394:MET:CE	1:B:396:LYS:CE	2.96	0.43
1:A:341[A]:PHE:CE2	1:A:383:TYR:CE2	3.07	0.43
1:A:277:ARG:HD2	1:A:279:GLU:OE2	2.18	0.43
2:U:2:NAG:HO3	2:U:3:NAG:HO6	1.66	0.42
1:B:215:ILE:HD12	1:B:296:MET:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:TRP:CE2	4:B:505:C8E:H141	2.54	0.42
2:U:1:NAG:H62	2:U:2:NAG:C7	2.50	0.42
1:B:233:LEU:HD13	1:B:235[A]:THR:HG23	2.01	0.41
2:U:2:NAG:O3	2:U:3:NAG:O5	2.38	0.41
1:A:235[B]:THR:HG22	1:A:236:SER:N	2.36	0.41
1:A:280:GLY:HA2	1:A:324:ALA:O	2.21	0.41
2:C:2:NAG:O6	2:C:3:NAG:H83	2.21	0.41
1:B:56:GLY:C	1:B:57[A]:LEU:HD22	2.42	0.41
1:B:399:PHE:HD1	1:B:425:VAL:HG22	1.86	0.41
4:B:511:C8E:C7	2:U:2:NAG:H2	2.51	0.41
1:B:170:TRP:HH2	4:B:511:C8E:H41	1.86	0.41
1:B:236:SER:OG	1:B:265[A]:THR:CG2	2.68	0.40
1:B:3:PHE:CZ	1:B:57[B]:LEU:HD12	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/436 (102%)	425 (96%)	19 (4%)	0	100	100
1	B	443/436 (102%)	427 (96%)	16 (4%)	0	100	100
All	All	887/872 (102%)	852 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	361/351 (103%)	357 (99%)	4 (1%)	73 73
1	B	360/351 (103%)	358 (99%)	2 (1%)	86 87
All	All	721/702 (103%)	715 (99%)	6 (1%)	78 82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	MET
1	A	190	HIS
1	A	249	ARG
1	A	423	ARG
1	B	190	HIS
1	B	423	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	1	2	15,15,15	0.63	0	21,21,21	1.12	2 (9%)
2	NAG	C	2	2	14,14,15	1.40	1 (7%)	17,19,21	1.98	4 (23%)
2	NAG	C	3	2	14,14,15	0.80	1 (7%)	17,19,21	2.46	5 (29%)
2	NAG	C	4	2	14,14,15	0.54	0	17,19,21	0.93	2 (11%)
2	NAG	C	5	2	14,14,15	1.10	2 (14%)	17,19,21	1.71	4 (23%)
2	NAG	U	1	2	15,15,15	0.31	0	21,21,21	0.50	0
2	NAG	U	2	2	14,14,15	0.24	0	17,19,21	1.09	1 (5%)
2	NAG	U	3	2	14,14,15	0.41	0	17,19,21	0.99	2 (11%)
2	NAG	U	4	5,2	14,14,15	0.34	0	17,19,21	0.96	1 (5%)
2	NAG	U	5	2	14,14,15	1.96	2 (14%)	17,19,21	1.90	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	0/6/26/26	0/1/1/1
2	NAG	C	2	2	-	6/6/23/26	0/1/1/1
2	NAG	C	3	2	-	3/6/23/26	0/1/1/1
2	NAG	C	4	2	-	0/6/23/26	0/1/1/1
2	NAG	C	5	2	-	6/6/23/26	0/1/1/1
2	NAG	U	1	2	-	0/6/26/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	3	2	-	4/6/23/26	0/1/1/1
2	NAG	U	4	5,2	-	2/6/23/26	0/1/1/1
2	NAG	U	5	2	-	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	5	NAG	O5-C1	-5.77	1.34	1.43
2	C	2	NAG	O5-C1	-4.97	1.35	1.43
2	U	5	NAG	C1-C2	4.24	1.58	1.52
2	C	5	NAG	C1-C2	3.13	1.57	1.52
2	C	5	NAG	O5-C1	-2.58	1.39	1.43
2	C	3	NAG	O5-C1	2.05	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	NAG	C2-N2-C7	7.70	133.87	122.90
2	C	2	NAG	C2-N2-C7	5.72	131.05	122.90
2	C	5	NAG	C2-N2-C7	4.57	129.41	122.90
2	U	5	NAG	C1-O5-C5	-4.31	106.36	112.19
2	C	3	NAG	C1-O5-C5	4.20	117.88	112.19
2	U	2	NAG	C1-O5-C5	3.95	117.55	112.19
2	U	5	NAG	C2-N2-C7	3.23	127.50	122.90
2	C	1	NAG	C1-C2-N2	-3.15	107.08	110.73
2	C	5	NAG	O3-C3-C4	-3.10	103.18	110.35
2	C	3	NAG	C1-C2-N2	2.97	115.56	110.49
2	C	5	NAG	C1-O5-C5	2.95	116.18	112.19
2	C	2	NAG	C1-C2-N2	-2.93	105.49	110.49
2	U	4	NAG	O4-C4-C5	-2.93	102.03	109.30
2	U	5	NAG	C3-C4-C5	-2.90	105.06	110.24
2	U	5	NAG	C1-C2-N2	-2.85	105.62	110.49
2	U	3	NAG	O4-C4-C5	-2.72	102.54	109.30
2	C	3	NAG	C4-C3-C2	2.54	114.75	111.02
2	C	2	NAG	C1-O5-C5	2.47	115.54	112.19
2	U	5	NAG	C6-C5-C4	2.39	118.60	113.00
2	C	3	NAG	O4-C4-C5	-2.33	103.50	109.30
2	U	5	NAG	O5-C5-C4	-2.30	105.22	110.83
2	U	3	NAG	C2-N2-C7	2.24	126.10	122.90
2	C	4	NAG	O4-C4-C5	-2.20	103.83	109.30
2	C	1	NAG	C1-O5-C5	-2.18	109.55	113.66
2	C	2	NAG	O3-C3-C4	-2.14	105.40	110.35
2	C	5	NAG	O3-C3-C2	2.02	113.64	109.47
2	C	4	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	U	5	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	3	NAG	C8-C7-N2-C2
2	U	5	NAG	O5-C5-C6-O6
2	C	5	NAG	C4-C5-C6-O6
2	U	5	NAG	C4-C5-C6-O6
2	C	5	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	C	5	NAG	C1-C2-N2-C7
2	U	2	NAG	C4-C5-C6-O6
2	U	3	NAG	C8-C7-N2-C2

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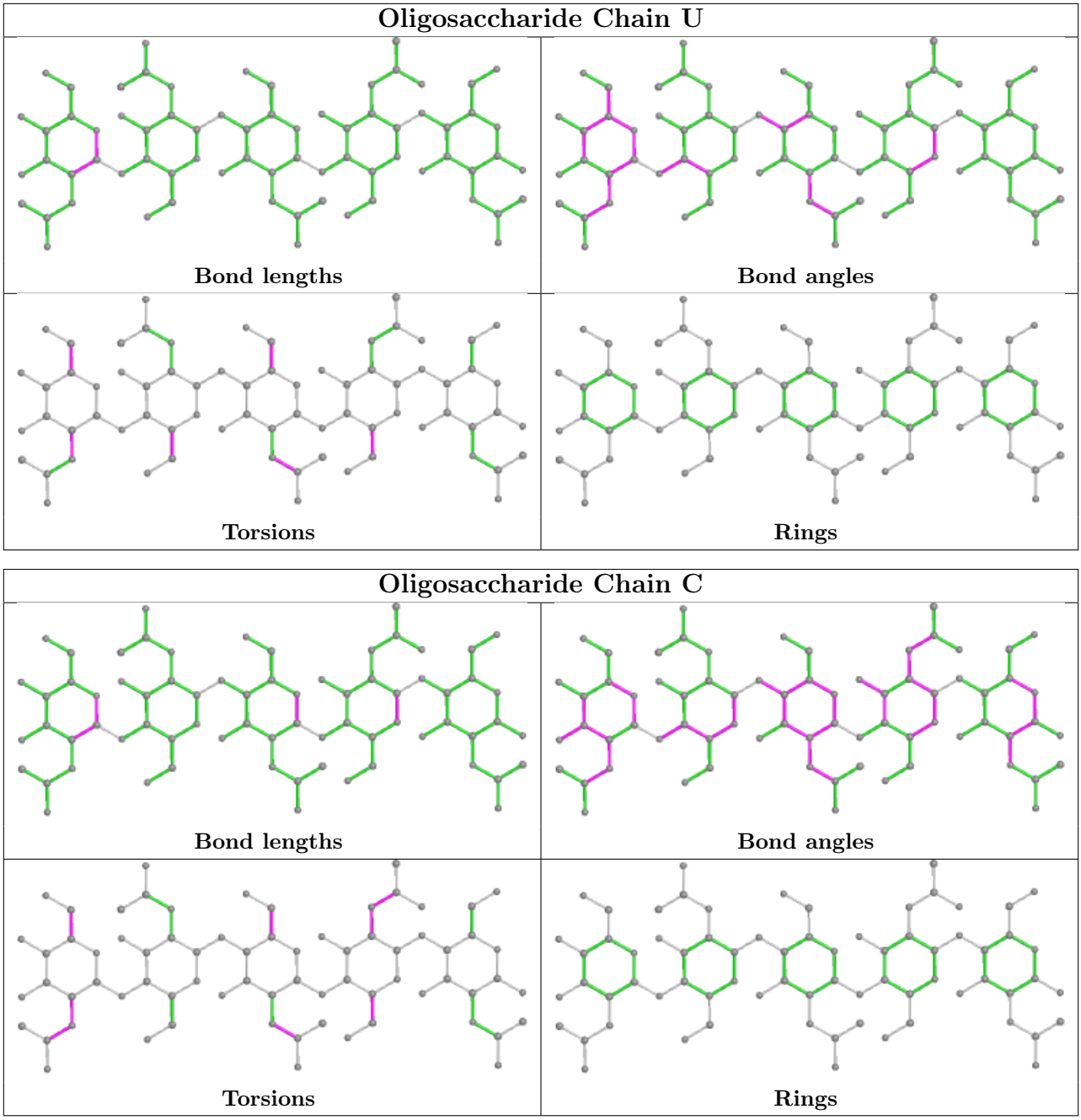
Mol	Chain	Res	Type	Atoms
2	U	3	NAG	O7-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	3	NAG	O7-C7-N2-C2
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	U	4	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	U	3	NAG	O5-C5-C6-O6
2	C	3	NAG	O5-C5-C6-O6
2	U	4	NAG	C4-C5-C6-O6
2	U	5	NAG	C1-C2-N2-C7
2	C	5	NAG	C3-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7
2	U	3	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	U	1	NAG	1	0
2	U	3	NAG	8	0
2	C	3	NAG	3	0
2	C	5	NAG	2	0
2	U	5	NAG	2	0
2	U	4	NAG	2	0
2	C	2	NAG	5	0
2	C	1	NAG	3	0
2	U	2	NAG	5	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 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 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	$\#\|Z\|>2$
4	C8E	A	506	-	4,4,20	0.30	0	3,3,19	0.30	0
4	C8E	A	505	-	7,7,20	0.31	0	6,6,19	0.35	0
4	C8E	A	510	-	4,4,20	0.35	0	3,3,19	0.51	0
3	DMU	B	503	-	28,28,34	1.66	6 (21%)	39,39,45	1.22	4 (10%)
3	DMU	A	502	-	30,30,34	1.57	6 (20%)	41,41,45	1.19	4 (9%)
4	C8E	A	511	-	4,4,20	0.27	0	3,3,19	0.39	0
4	C8E	B	505	-	10,10,20	0.43	0	9,9,19	0.28	0
4	C8E	A	507	5	5,5,20	0.38	0	4,4,19	0.31	0
3	DMU	A	503	-	29,29,34	1.65	6 (20%)	40,40,45	1.04	1 (2%)
3	DMU	A	501	-	24,24,34	1.65	5 (20%)	35,35,45	0.90	1 (2%)
4	C8E	B	509	-	5,5,20	0.26	0	4,4,19	0.41	0
4	C8E	B	508	-	4,4,20	0.29	0	3,3,19	0.35	0
4	C8E	B	510	-	4,4,20	0.41	0	3,3,19	0.21	0
4	C8E	B	507	-	5,5,20	0.27	0	4,4,19	0.39	0
4	C8E	B	511	-	5,5,20	0.26	0	4,4,19	0.43	0
4	C8E	A	509	-	4,4,20	0.32	0	3,3,19	0.29	0
4	C8E	A	508	-	4,4,20	0.31	0	3,3,19	0.33	0
4	C8E	B	504	-	11,11,20	0.32	0	10,10,19	0.40	0
3	DMU	B	501	-	25,25,34	1.64	7 (28%)	36,36,45	1.15	2 (5%)
4	C8E	A	504	-	5,5,20	0.34	0	4,4,19	0.28	0
3	DMU	B	502	-	30,30,34	1.54	6 (20%)	41,41,45	1.15	4 (9%)
4	C8E	B	506	-	5,5,20	0.29	0	4,4,19	0.38	0
4	C8E	B	512	-	6,6,20	0.39	0	5,5,19	0.29	0
4	C8E	A	512	-	4,4,20	0.33	0	3,3,19	0.37	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
4	C8E	A	506	-	-	1/2/2/18	-
4	C8E	A	505	-	-	5/5/5/18	-
4	C8E	A	510	-	-	1/2/2/18	-
3	DMU	B	503	-	-	2/13/53/59	0/2/2/2
3	DMU	A	502	-	-	0/15/55/59	0/2/2/2
4	C8E	A	511	-	-	1/2/2/18	-
4	C8E	B	505	-	-	6/8/8/18	-
4	C8E	A	507	5	-	3/3/3/18	-
3	DMU	A	503	-	-	4/14/54/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMU	A	501	-	-	0/8/48/59	0/2/2/2
4	C8E	B	509	-	-	2/3/3/18	-
4	C8E	B	508	-	-	0/2/2/18	-
4	C8E	B	510	-	-	0/2/2/18	-
4	C8E	B	507	-	-	2/3/3/18	-
4	C8E	B	511	-	-	1/3/3/18	-
4	C8E	A	509	-	-	2/2/2/18	-
4	C8E	A	508	-	-	0/2/2/18	-
4	C8E	B	504	-	-	7/9/9/18	-
3	DMU	B	501	-	-	0/10/50/59	0/2/2/2
4	C8E	A	504	-	-	2/3/3/18	-
3	DMU	B	502	-	-	0/15/55/59	0/2/2/2
4	C8E	B	506	-	-	3/3/3/18	-
4	C8E	B	512	-	-	2/4/4/18	-
4	C8E	A	512	-	-	1/2/2/18	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	DMU	O1-C9	4.05	1.54	1.44
3	A	503	DMU	O1-C9	3.99	1.54	1.44
3	A	502	DMU	O1-C9	3.92	1.53	1.44
3	B	502	DMU	O1-C9	3.83	1.53	1.44
3	A	501	DMU	O1-C9	3.42	1.52	1.44
3	B	501	DMU	C11-C9	-3.28	1.40	1.51
3	A	501	DMU	O4-C7	3.23	1.50	1.43
3	B	501	DMU	O4-C7	3.22	1.50	1.43
3	A	502	DMU	C7-C5	-3.21	1.44	1.52
3	B	503	DMU	C11-C9	-3.18	1.41	1.51
3	A	501	DMU	C11-C9	-3.13	1.41	1.51
3	B	502	DMU	C7-C5	-3.05	1.44	1.52
3	A	503	DMU	C11-C9	-3.02	1.41	1.51
3	B	501	DMU	O1-C9	2.96	1.51	1.44
3	A	503	DMU	O4-C7	2.88	1.49	1.43
3	A	502	DMU	O4-C7	2.86	1.49	1.43
3	B	502	DMU	C11-C9	-2.70	1.42	1.51
3	B	502	DMU	O4-C7	2.64	1.49	1.43
3	B	503	DMU	O55-C2	2.64	1.49	1.43
3	A	503	DMU	O55-C2	2.63	1.49	1.43
3	A	502	DMU	C11-C9	-2.62	1.43	1.51
3	B	503	DMU	O4-C7	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	DMU	C8-C9	2.52	1.58	1.53
3	B	502	DMU	O55-C2	2.46	1.48	1.43
3	A	502	DMU	O55-C2	2.39	1.48	1.43
3	A	503	DMU	C7-C5	-2.38	1.46	1.52
3	B	503	DMU	C7-C5	-2.37	1.46	1.52
3	B	501	DMU	O5-C6	2.26	1.47	1.41
3	A	501	DMU	C8-C9	2.21	1.57	1.53
3	A	502	DMU	O5-C4	2.15	1.49	1.44
3	B	502	DMU	C8-C7	-2.12	1.46	1.52
3	A	503	DMU	O5-C6	2.10	1.47	1.41
3	A	501	DMU	O5-C4	2.06	1.49	1.44
3	B	501	DMU	O3-C5	2.05	1.47	1.43
3	B	503	DMU	O5-C6	2.04	1.47	1.41
3	B	501	DMU	O5-C4	2.04	1.49	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	DMU	O16-C6-C1	3.78	112.58	108.15
3	B	502	DMU	O49-C1-C6	-2.85	103.12	110.05
3	A	502	DMU	C10-O7-C3	-2.84	110.95	117.96
3	A	502	DMU	O49-C1-C6	-2.79	103.26	110.05
3	A	502	DMU	C7-C8-C9	2.62	114.91	110.24
3	B	502	DMU	C6-C1-C2	2.58	115.36	110.00
3	A	502	DMU	C6-C1-C2	2.55	115.31	110.00
3	A	503	DMU	C1-C2-C3	2.53	115.46	109.68
3	B	502	DMU	C10-O7-C3	-2.46	111.88	117.96
3	B	503	DMU	C7-C8-C9	-2.41	105.95	110.24
3	B	501	DMU	O2-C8-C7	2.26	115.56	110.35
3	A	501	DMU	O1-C9-C8	-2.12	105.83	109.69
3	B	503	DMU	C1-C2-C3	2.04	114.35	109.68
3	B	502	DMU	C11-C9-C8	-2.04	108.22	113.00
3	B	503	DMU	C6-O5-C4	-2.03	109.69	113.69
3	B	503	DMU	O5-C4-C57	2.03	111.48	106.44

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	DMU	O6-C11-C9-C8
4	B	505	C8E	O12-C13-C14-O15
3	B	503	DMU	O6-C11-C9-O1

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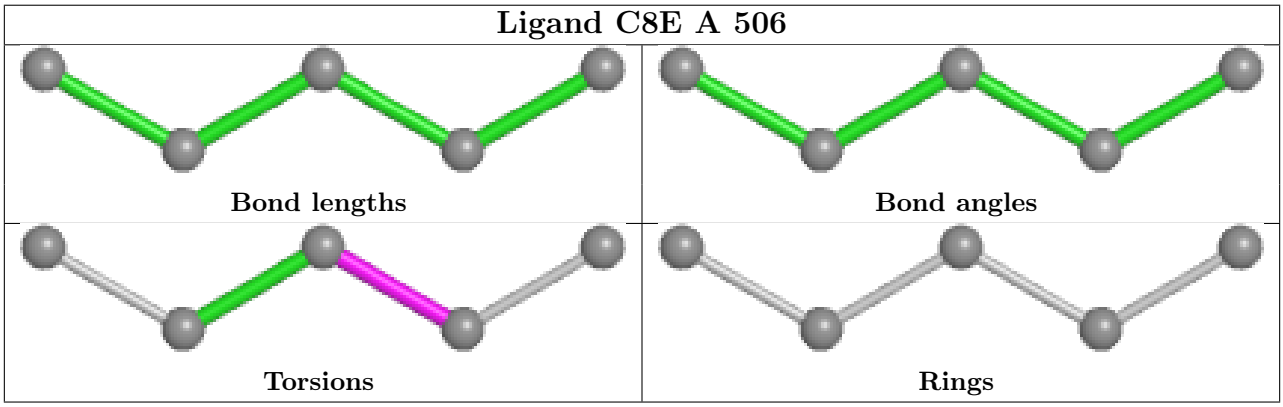
Mol	Chain	Res	Type	Atoms
3	A	503	DMU	O6-C11-C9-C8
4	A	507	C8E	O15-C16-C17-O18
4	B	504	C8E	C6-C7-C8-O9
4	B	512	C8E	O18-C19-C20-O21
4	B	507	C8E	C3-C4-C5-C6
3	A	503	DMU	O6-C11-C9-O1
4	B	506	C8E	C3-C4-C5-C6
4	B	504	C8E	O9-C10-C11-O12
4	A	504	C8E	C2-C3-C4-C5
4	A	505	C8E	C3-C4-C5-C6
4	A	506	C8E	C3-C4-C5-C6
4	B	504	C8E	C5-C6-C7-C8
4	A	507	C8E	C17-C16-O15-C14
4	B	504	C8E	C2-C3-C4-C5
4	B	505	C8E	O18-C19-C20-O21
4	A	511	C8E	C2-C3-C4-C5
4	A	505	C8E	C5-C6-C7-C8
4	B	504	C8E	C4-C5-C6-C7
4	B	504	C8E	C1-C2-C3-C4
4	A	505	C8E	C2-C3-C4-C5
4	A	512	C8E	C2-C3-C4-C5
4	B	509	C8E	C3-C4-C5-C6
4	B	505	C8E	C14-C13-O12-C11
4	B	511	C8E	C2-C3-C4-C5
4	A	504	C8E	C1-C2-C3-C4
4	B	505	C8E	C20-C19-O18-C17
4	B	512	C8E	C16-C17-O18-C19
4	A	510	C8E	O9-C10-C11-O12
4	B	505	C8E	C16-C17-O18-C19
4	A	509	C8E	C4-C5-C6-C7
4	B	505	C8E	C13-C14-O15-C16
4	A	505	C8E	C4-C5-C6-C7
4	A	507	C8E	C16-C17-O18-C19
3	A	503	DMU	C19-C18-O16-C6
4	B	506	C8E	C4-C5-C6-C7
4	B	507	C8E	C2-C3-C4-C5
4	A	505	C8E	C1-C2-C3-C4
3	A	503	DMU	C3-C4-C57-O61
4	A	509	C8E	C3-C4-C5-C6
4	B	506	C8E	C2-C3-C4-C5
4	B	509	C8E	C2-C3-C4-C5
4	B	504	C8E	C7-C8-O9-C10

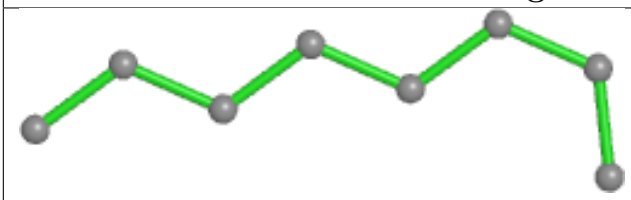
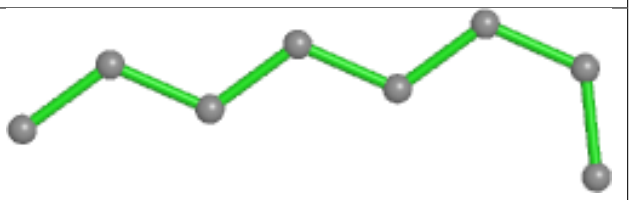
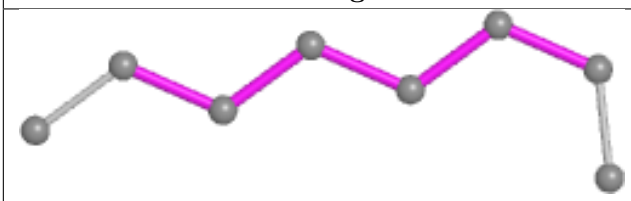
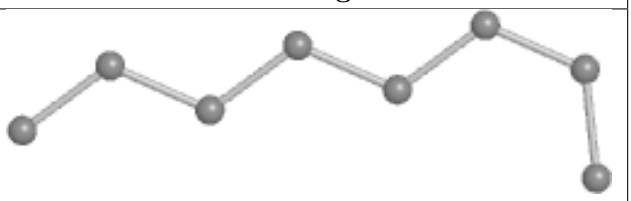
There are no ring outliers.

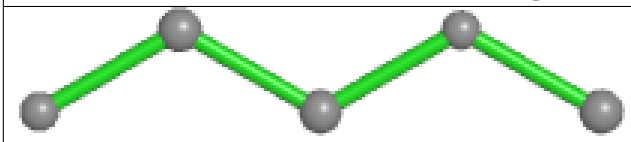
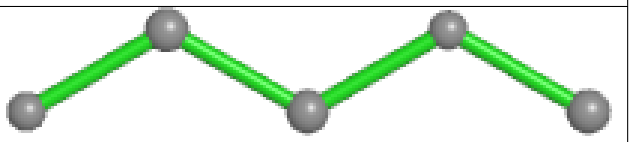
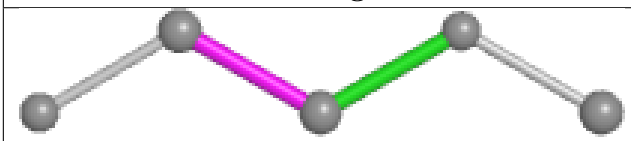
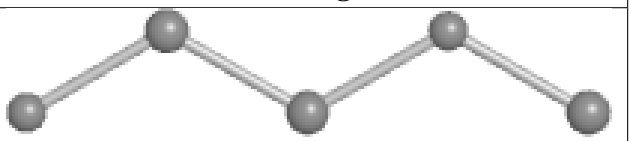
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	510	C8E	1	0
3	B	503	DMU	3	0
4	B	505	C8E	1	0
4	A	507	C8E	1	0
4	B	509	C8E	1	0
4	B	511	C8E	7	0
4	B	504	C8E	1	0

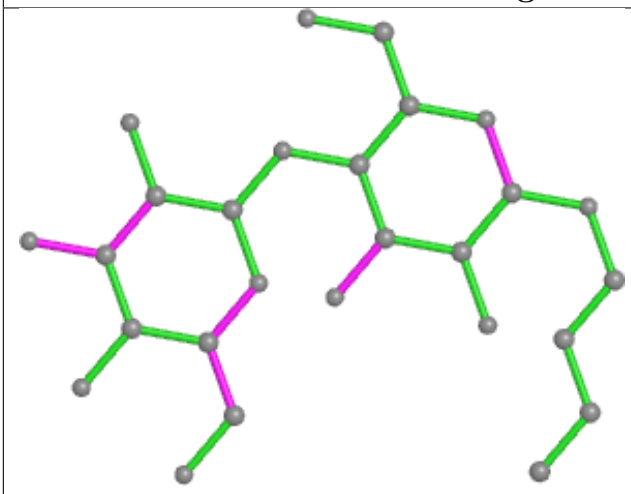
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



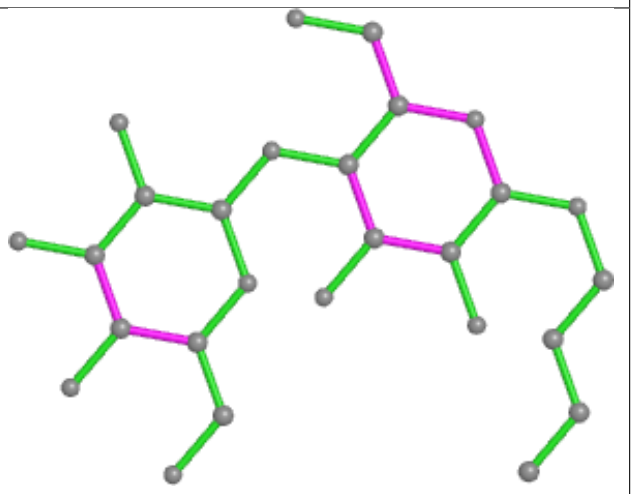
Ligand C8E A 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand C8E A 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

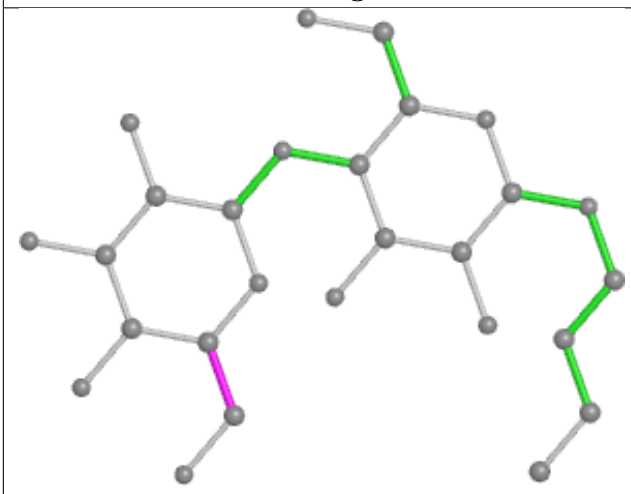
Ligand DMU B 503



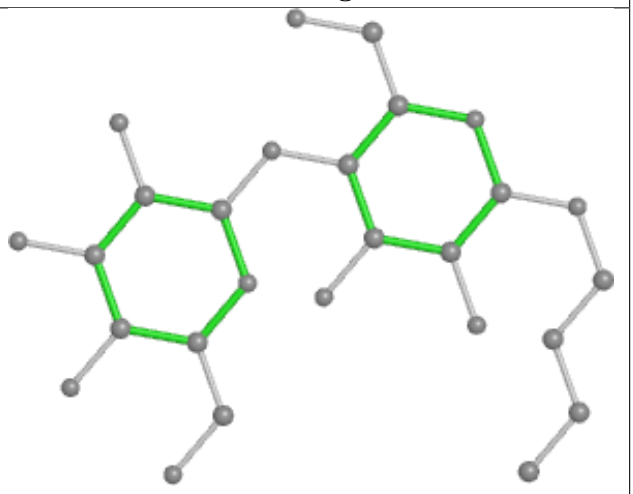
Bond lengths



Bond angles

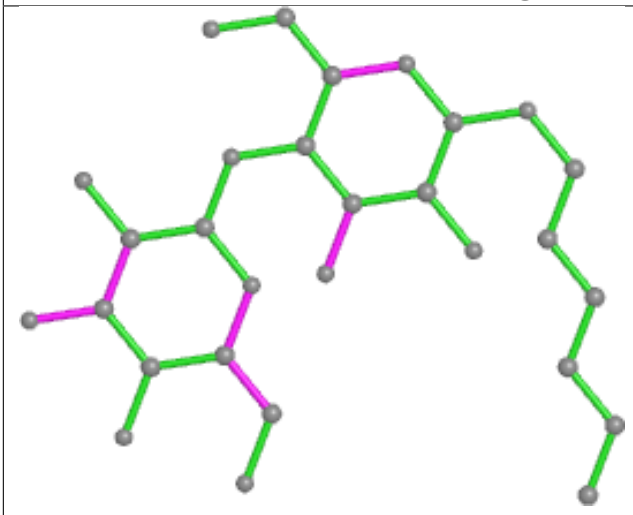


Torsions



Rings

Ligand DMU A 502



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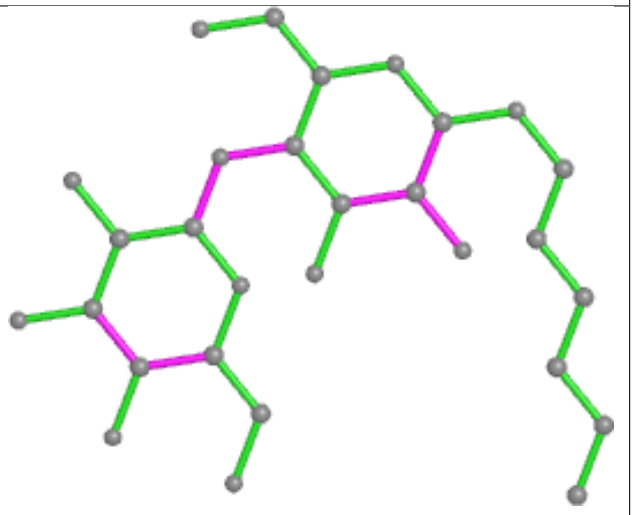

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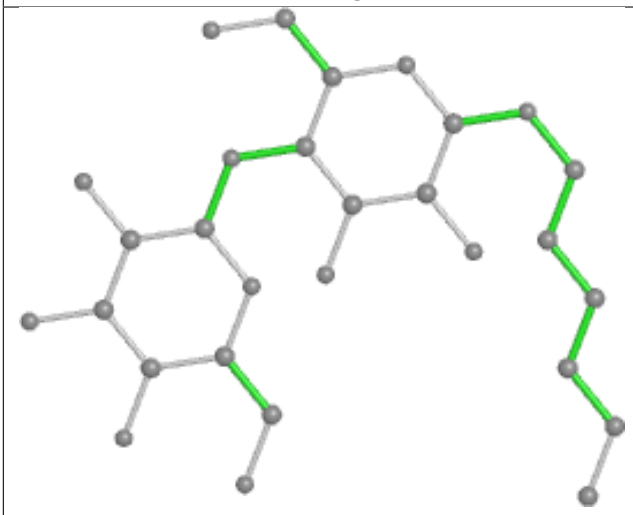

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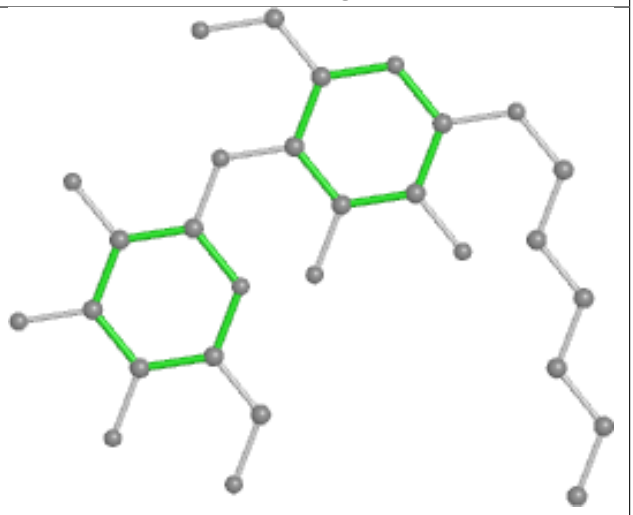
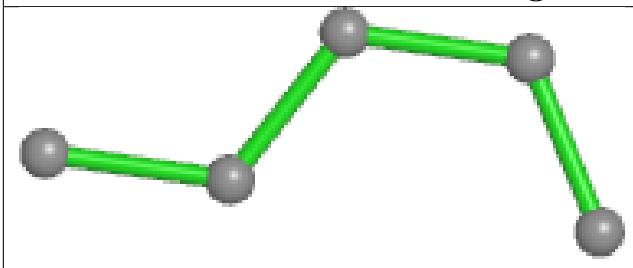


Rings

Ligand C8E A 511



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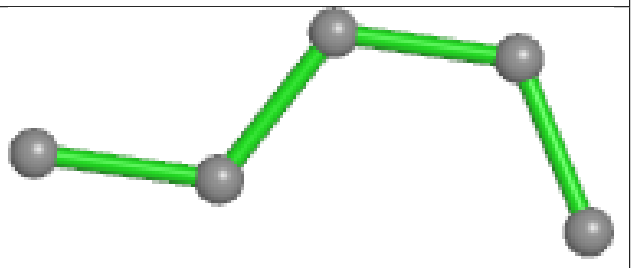

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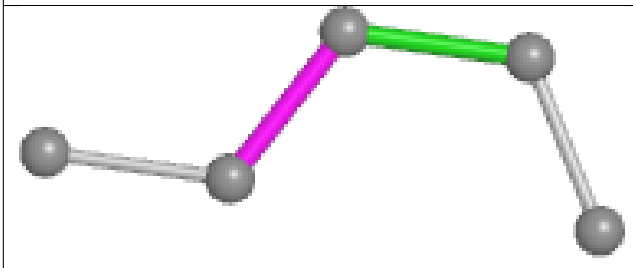

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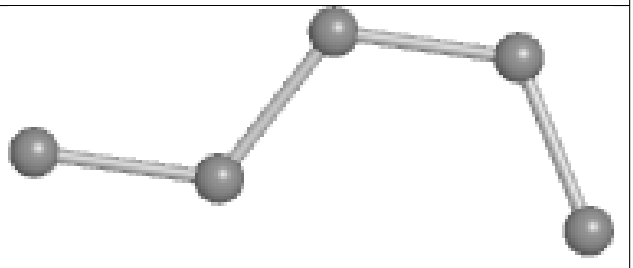
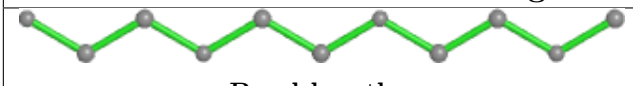


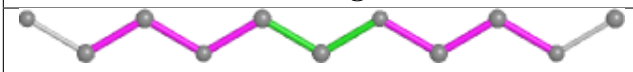
Rings

Ligand C8E B 505



Bond lengths

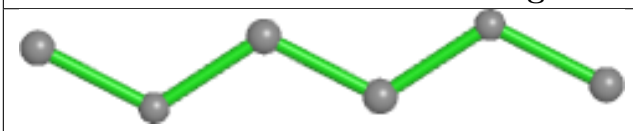
Bond angles



Torsions

Rings

Ligand C8E A 507



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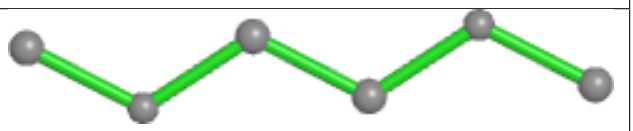

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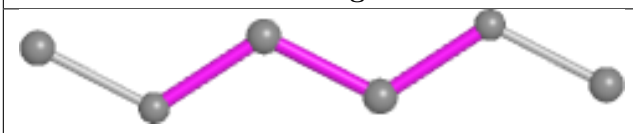

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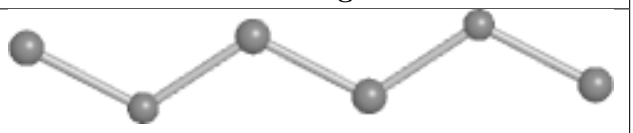
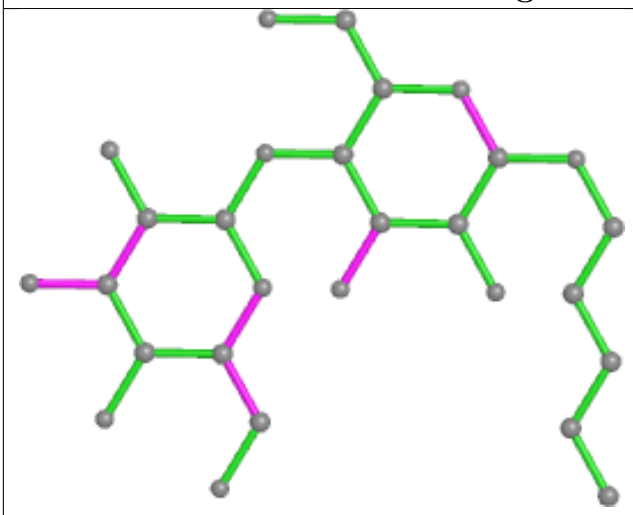


Rings

Ligand DMU A 503



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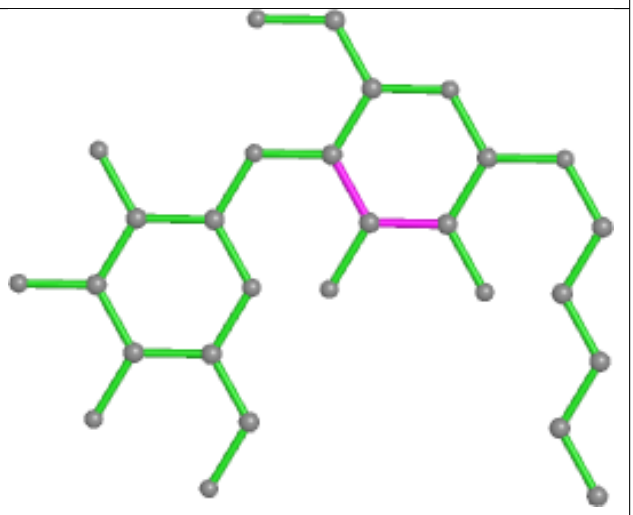

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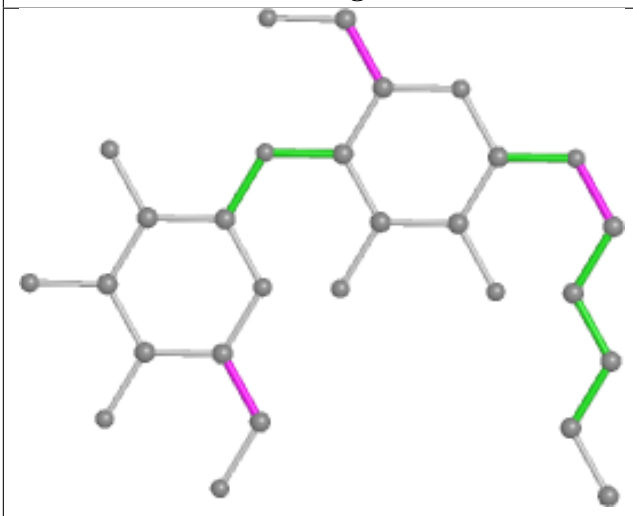

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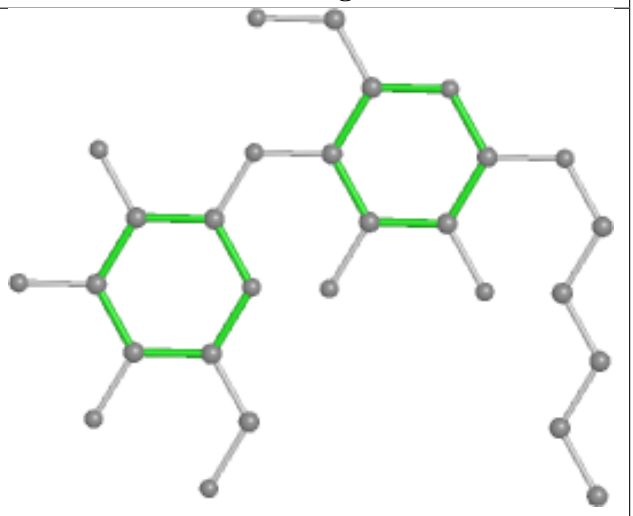
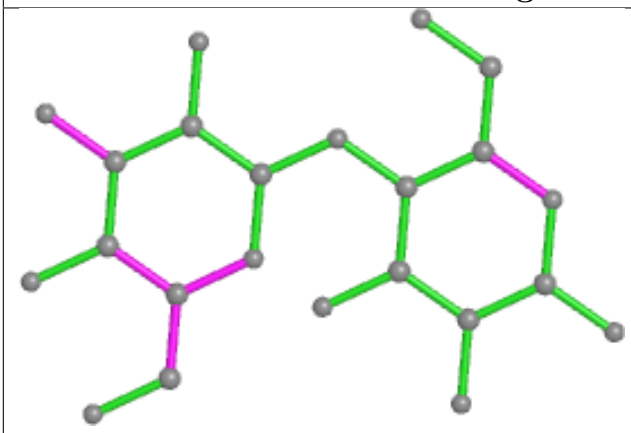


Rings

Ligand DMU A 501



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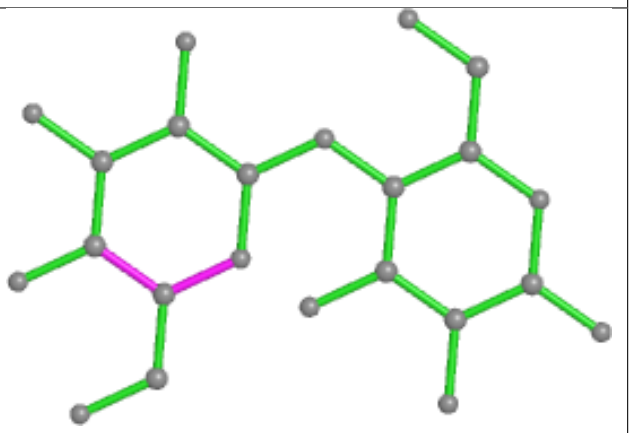
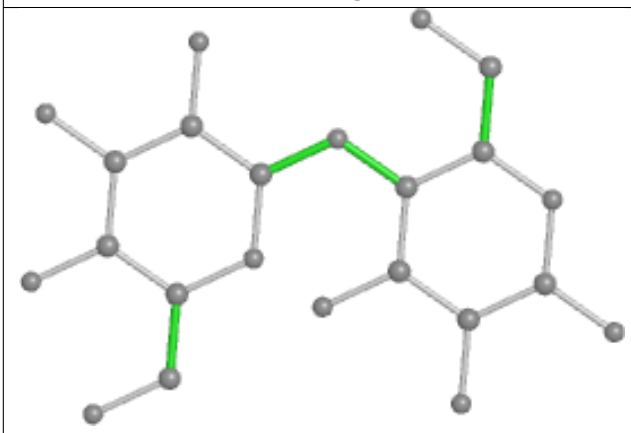


Bond angles



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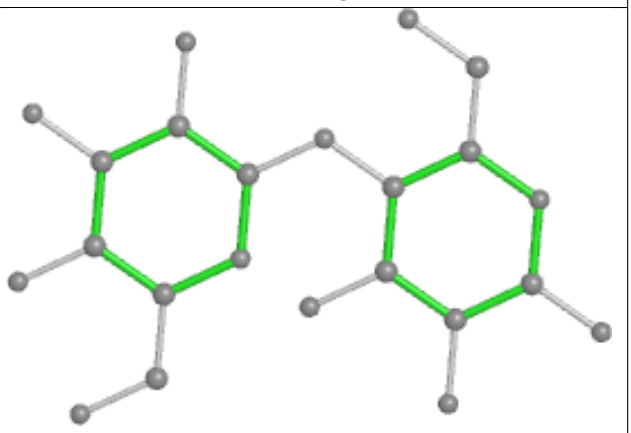
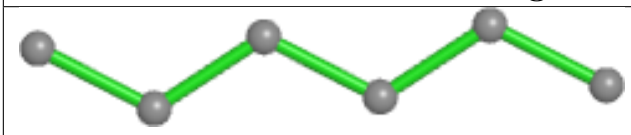


Rings

Ligand C8E B 509



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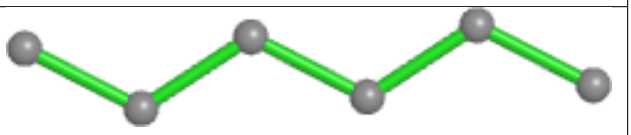
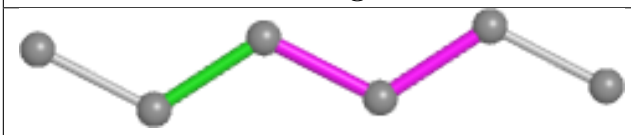
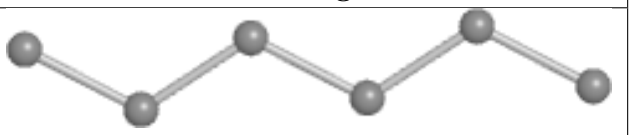


Bond angles

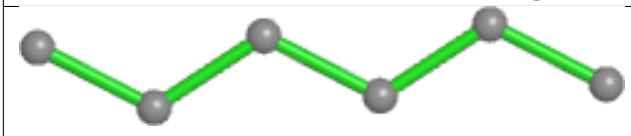


Torsions



Rings

Ligand C8E B 507



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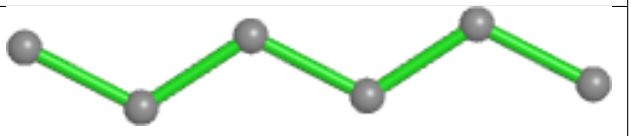

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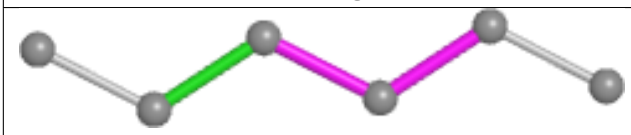

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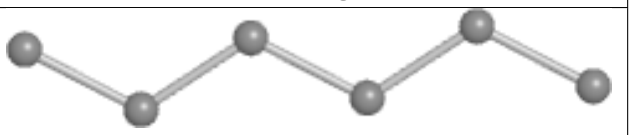

Rings

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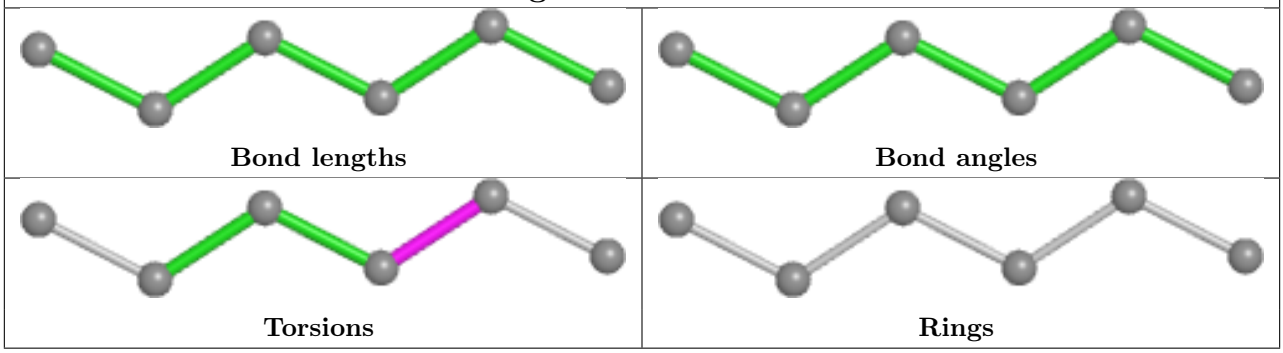

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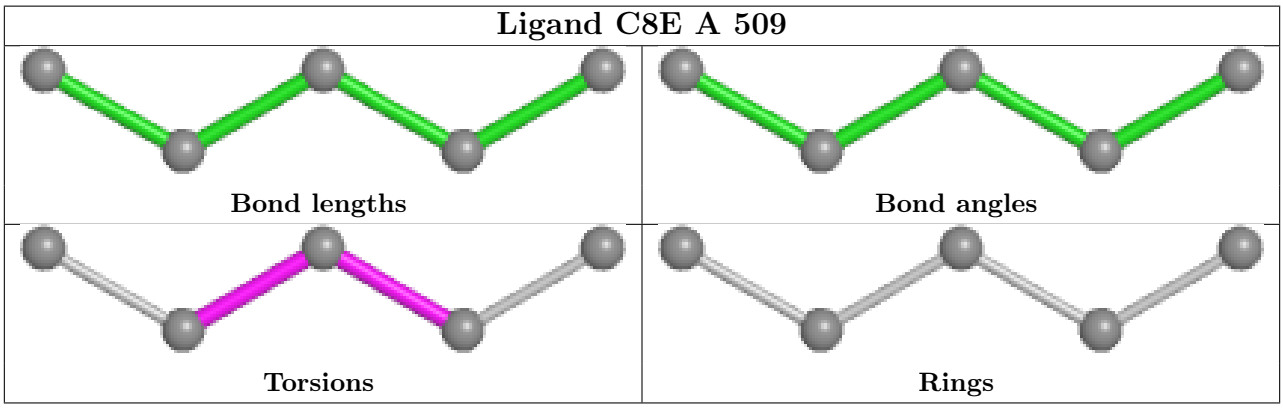

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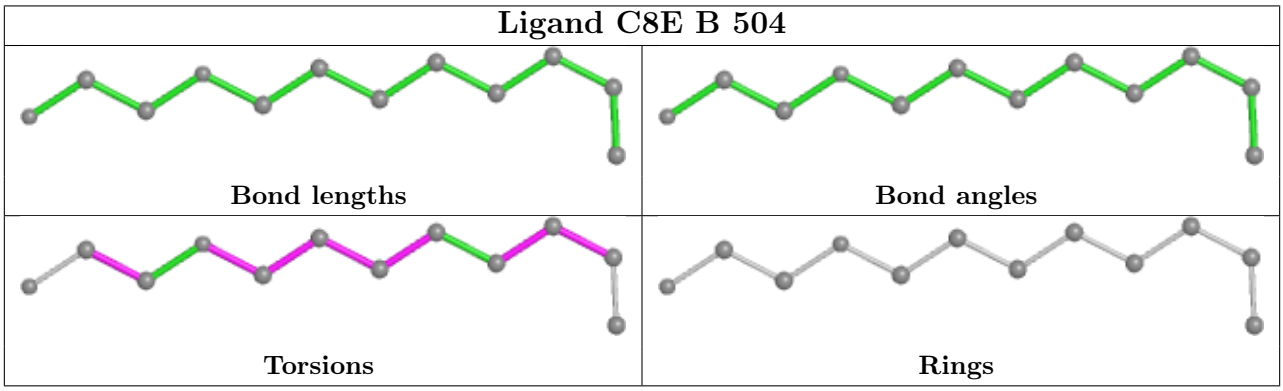
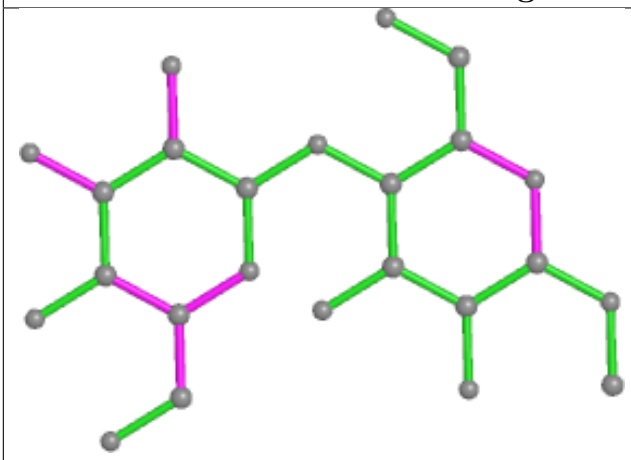
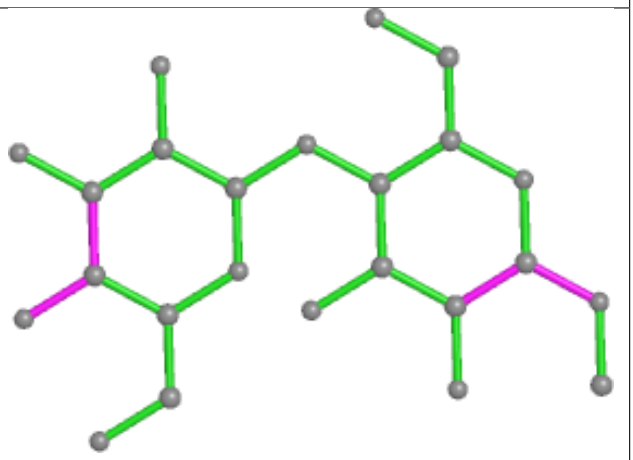


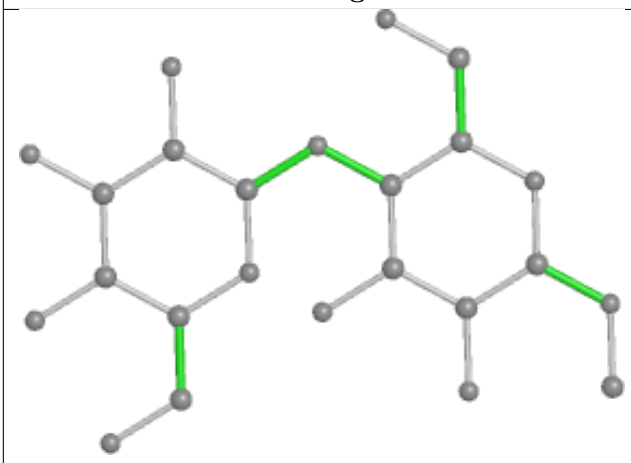
Ligand DMU B 501



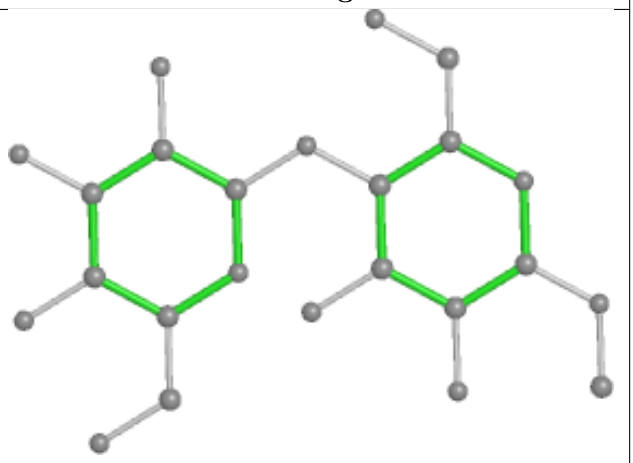
Bond lengths



Bond angles

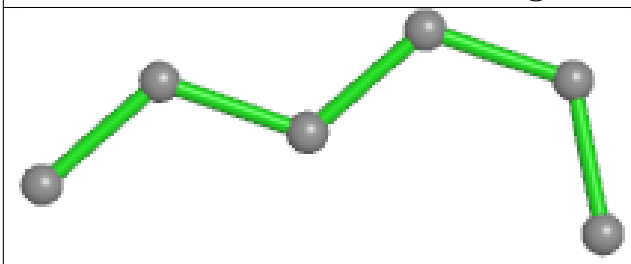


Torsions



Rings

Ligand C8E A 504



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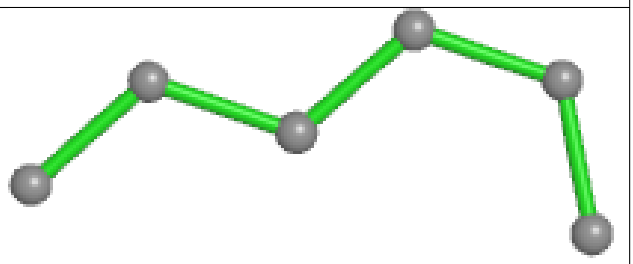
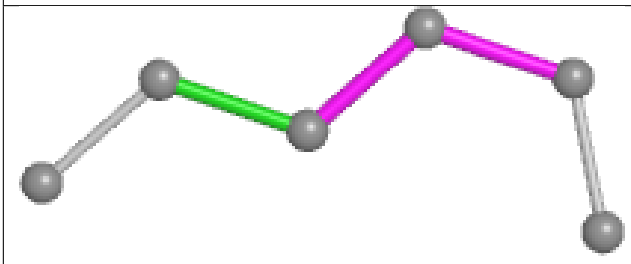
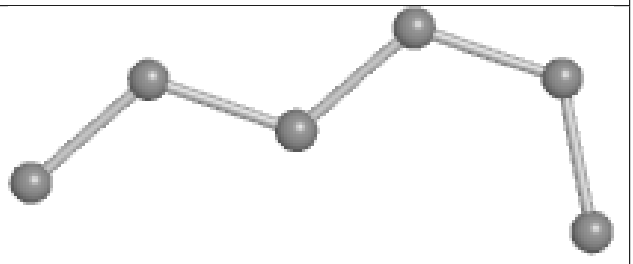


Bond angles

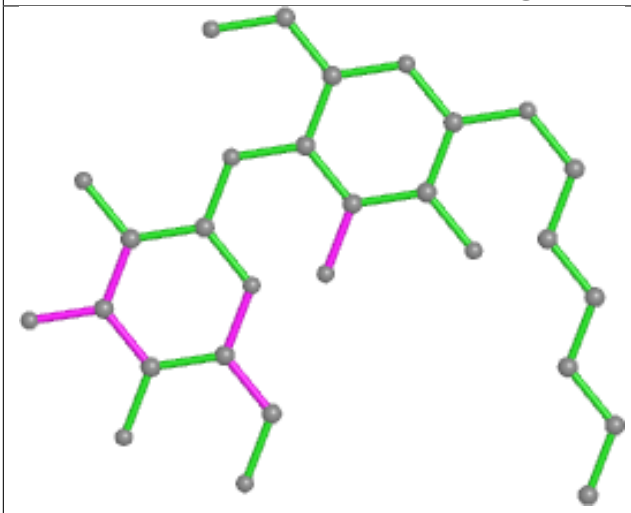


Torsions

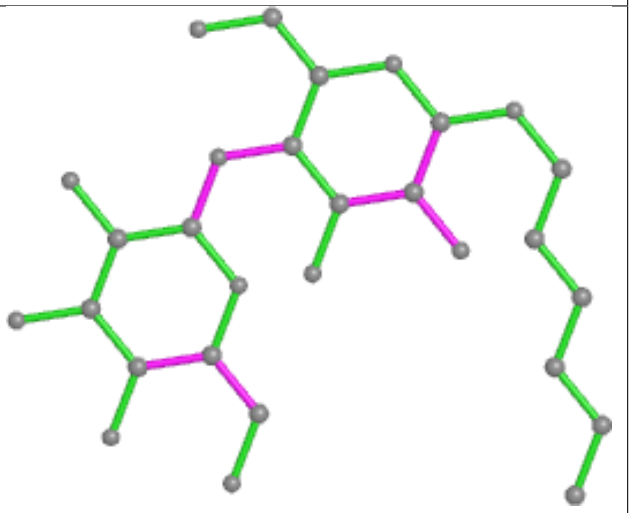


Rings

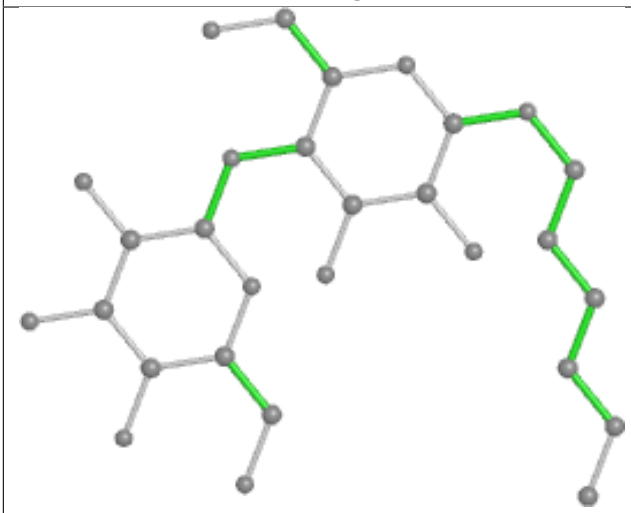
Ligand DMU B 502



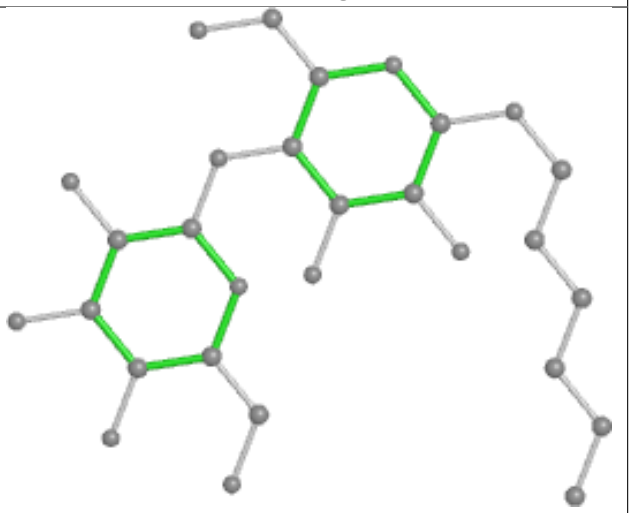
Bond lengths



Bond angles

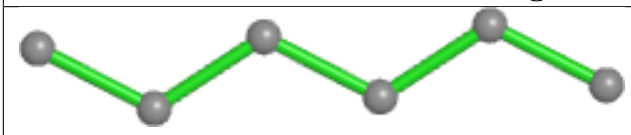


Torsions

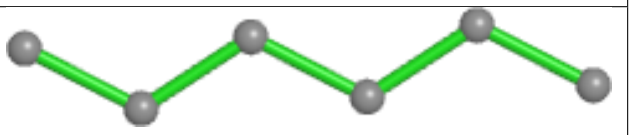


Rings

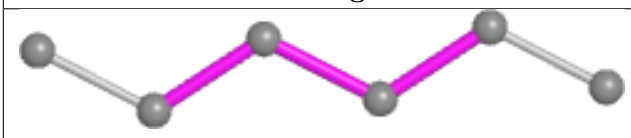
Ligand C8E B 506



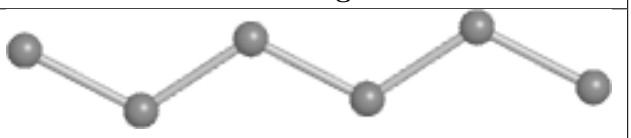
Bond lengths



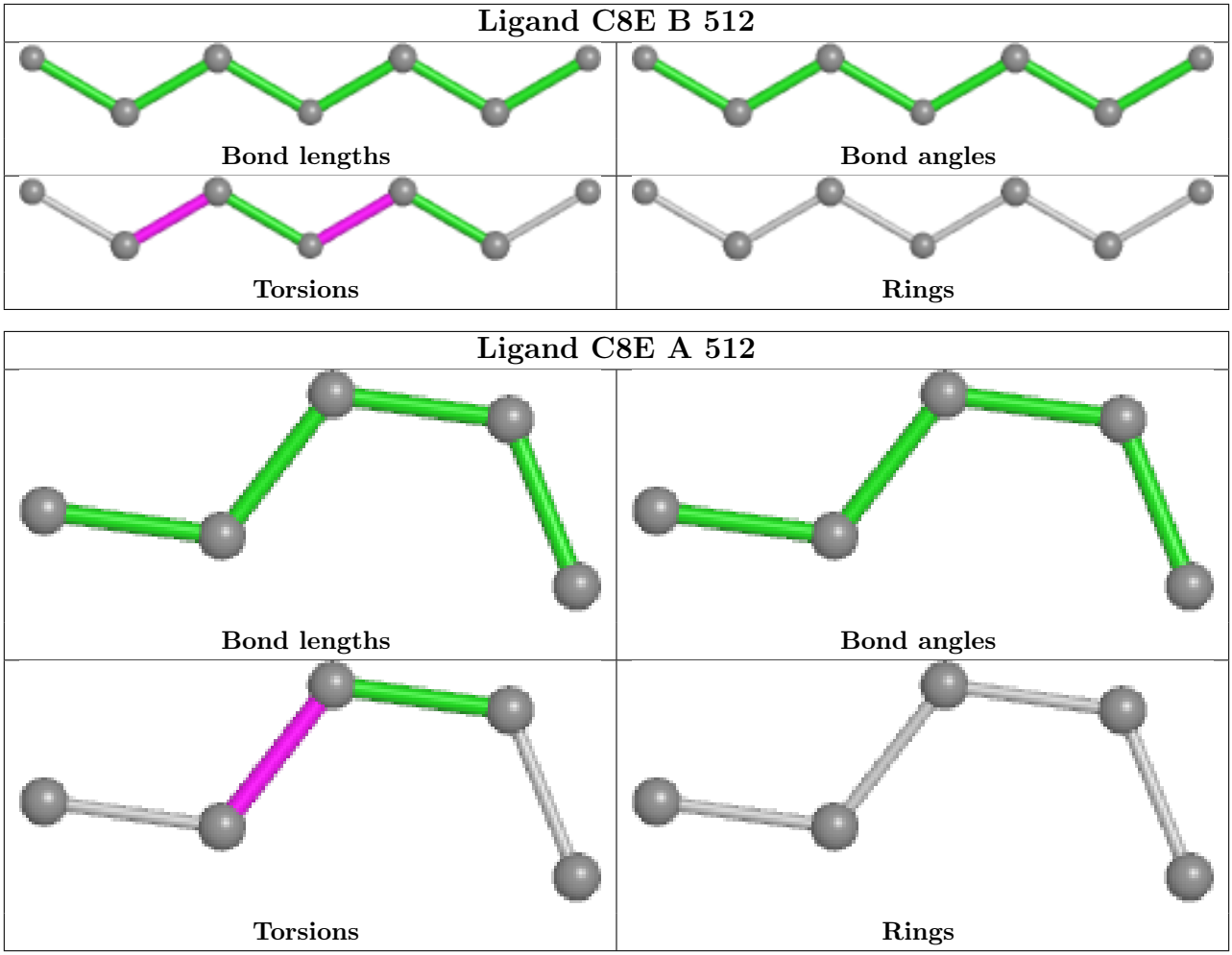
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	435/436 (99%)	0.30	12 (2%) 53 56	20, 36, 62, 88	0
1	B	435/436 (99%)	0.21	12 (2%) 53 56	18, 32, 57, 82	0
All	All	870/872 (99%)	0.26	24 (2%) 53 56	18, 34, 59, 88	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341[A]	PHE	5.5
1	B	110	TYR	4.8
1	A	389	ARG	4.8
1	A	387	ASP	4.2
1	A	110	TYR	4.0
1	A	390	ALA	3.8
1	B	226	PHE	3.3
1	A	436	PHE	3.1
1	B	436	PHE	3.1
1	A	385	ILE	3.0
1	B	341[A]	PHE	2.9
1	B	387	ASP	2.8
1	A	228	ILE	2.8
1	A	336	TRP	2.7
1	A	4	ILE	2.6
1	B	389	ARG	2.6
1	B	336	TRP	2.5
1	B	57[A]	LEU	2.5
1	B	148	PHE	2.4
1	A	383	TYR	2.3
1	B	228	ILE	2.3
1	B	388	GLY	2.2
1	B	153	ALA	2.2
1	A	388	GLY	2.0

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

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

6.3 Carbohydrates (i)

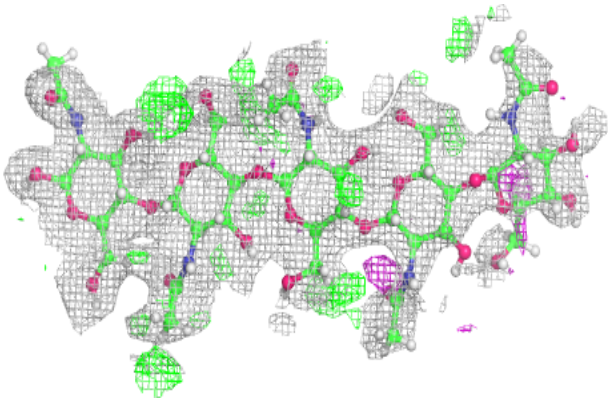
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

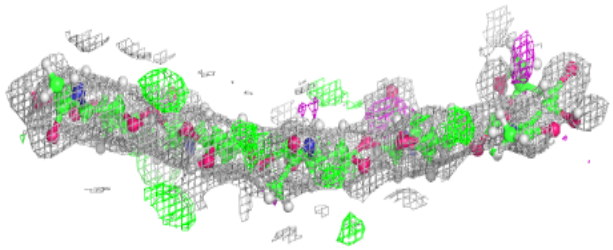
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	U	5	14/15	0.56	0.33	62,75,91,93	0
2	NAG	C	1	15/15	0.70	0.17	58,70,82,85	0
2	NAG	C	5	14/15	0.70	0.28	70,85,103,107	0
2	NAG	U	4	14/15	0.71	0.20	52,63,74,86	0
2	NAG	C	4	14/15	0.74	0.15	56,70,77,84	0
2	NAG	C	2	14/15	0.81	0.16	50,62,80,80	0
2	NAG	C	3	14/15	0.81	0.15	43,64,72,76	0
2	NAG	U	1	15/15	0.82	0.11	53,64,73,87	0
2	NAG	U	3	14/15	0.86	0.12	42,56,70,71	0
2	NAG	U	2	14/15	0.87	0.13	49,61,74,76	0

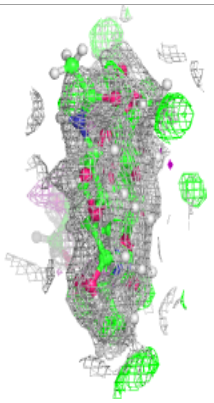
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

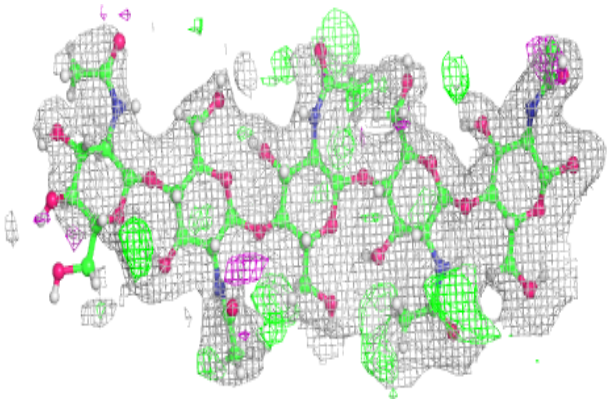


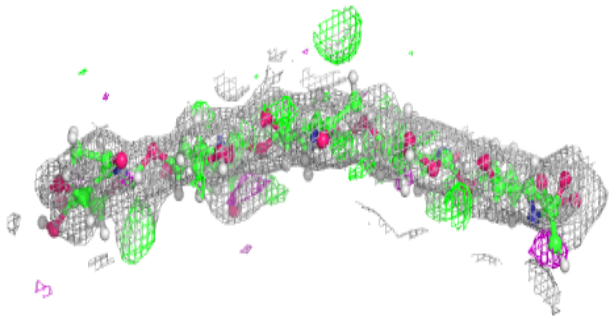


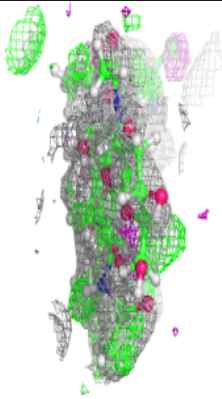


Electron density around Chain C:

$2mF_o$-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)

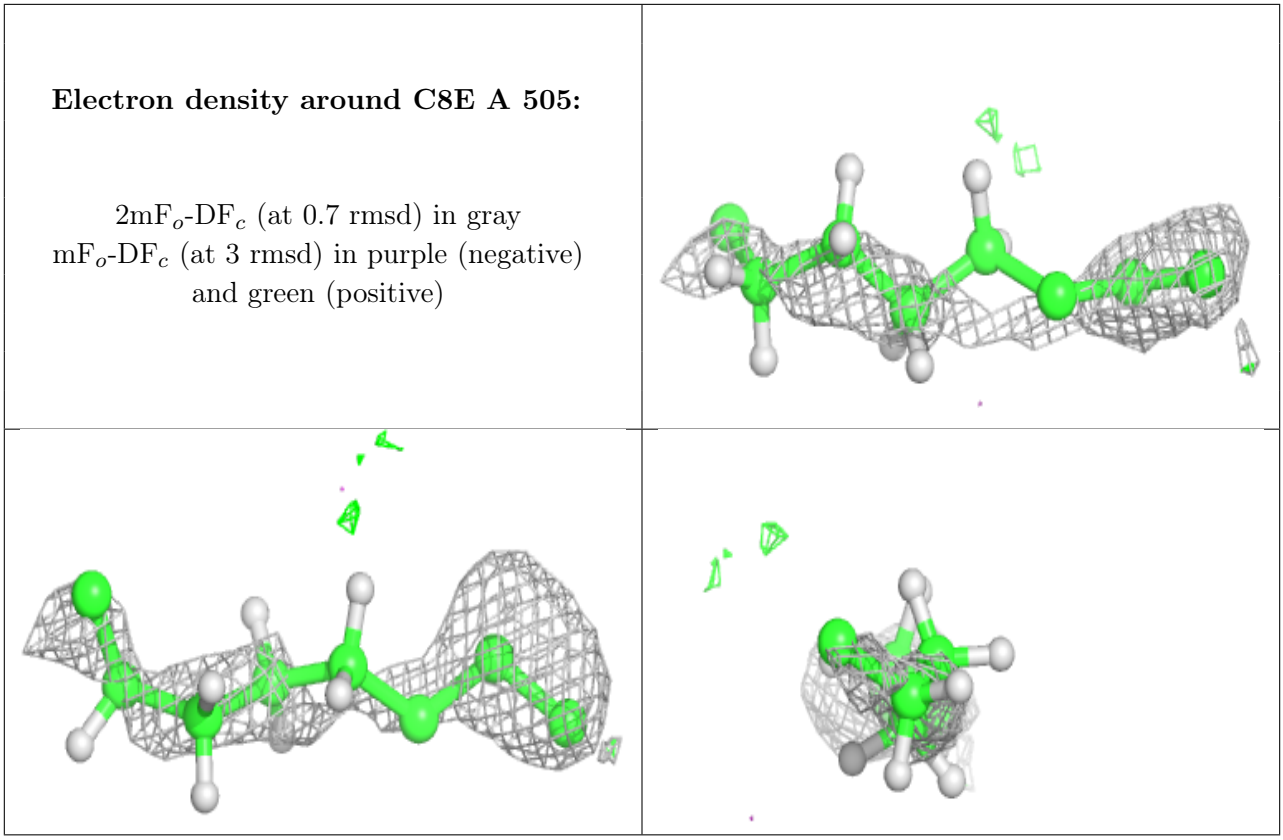
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	C8E	A	505	8/21	0.44	0.42	59,74,92,92	0
4	C8E	A	508	5/21	0.62	0.20	53,62,88,88	0
4	C8E	A	507	6/21	0.64	0.29	40,48,58,61	0
4	C8E	B	510	5/21	0.65	0.32	61,67,81,81	0
3	DMU	A	503	28/33	0.70	0.29	47,85,110,114	0
4	C8E	A	512	5/21	0.71	0.58	51,56,77,77	0
3	DMU	B	503	27/33	0.71	0.24	48,77,98,118	0
4	C8E	B	511	6/21	0.72	0.25	35,43,53,53	0
4	C8E	B	505	11/21	0.76	0.23	49,64,79,82	0
4	C8E	B	506	6/21	0.77	0.18	46,53,62,62	0
4	C8E	A	506	5/21	0.78	0.17	46,68,81,81	0
4	C8E	B	509	6/21	0.78	0.18	41,61,89,89	0
4	C8E	B	508	5/21	0.79	0.18	46,54,65,65	0
4	C8E	B	504	12/21	0.79	0.30	45,61,73,74	0
4	C8E	A	504	6/21	0.80	0.13	38,54,70,70	0
4	C8E	A	509	5/21	0.83	0.22	46,60,66,66	0
5	MG	A	513	1/1	0.84	0.11	32,32,32,32	0
4	C8E	B	507	6/21	0.86	0.20	43,56,64,64	0
4	C8E	A	510	5/21	0.87	0.38	48,58,73,74	0
4	C8E	B	512	7/21	0.88	0.45	50,68,78,88	0
4	C8E	A	511	5/21	0.89	0.17	37,43,54,63	0
3	DMU	A	501	23/33	0.89	0.13	30,53,68,75	0
3	DMU	B	501	24/33	0.89	0.12	24,48,66,79	0
5	MG	B	513	1/1	0.89	0.10	30,30,30,30	0
5	MG	B	516	1/1	0.92	0.10	44,44,44,44	0
3	DMU	A	502	29/33	0.93	0.10	27,40,55,64	0
3	DMU	B	502	29/33	0.95	0.09	24,36,47,59	0
5	MG	B	515	1/1	0.96	0.10	46,46,46,46	0
5	MG	B	514	1/1	0.97	0.12	34,34,34,34	0
5	MG	A	514	1/1	0.99	0.15	41,41,41,41	0

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

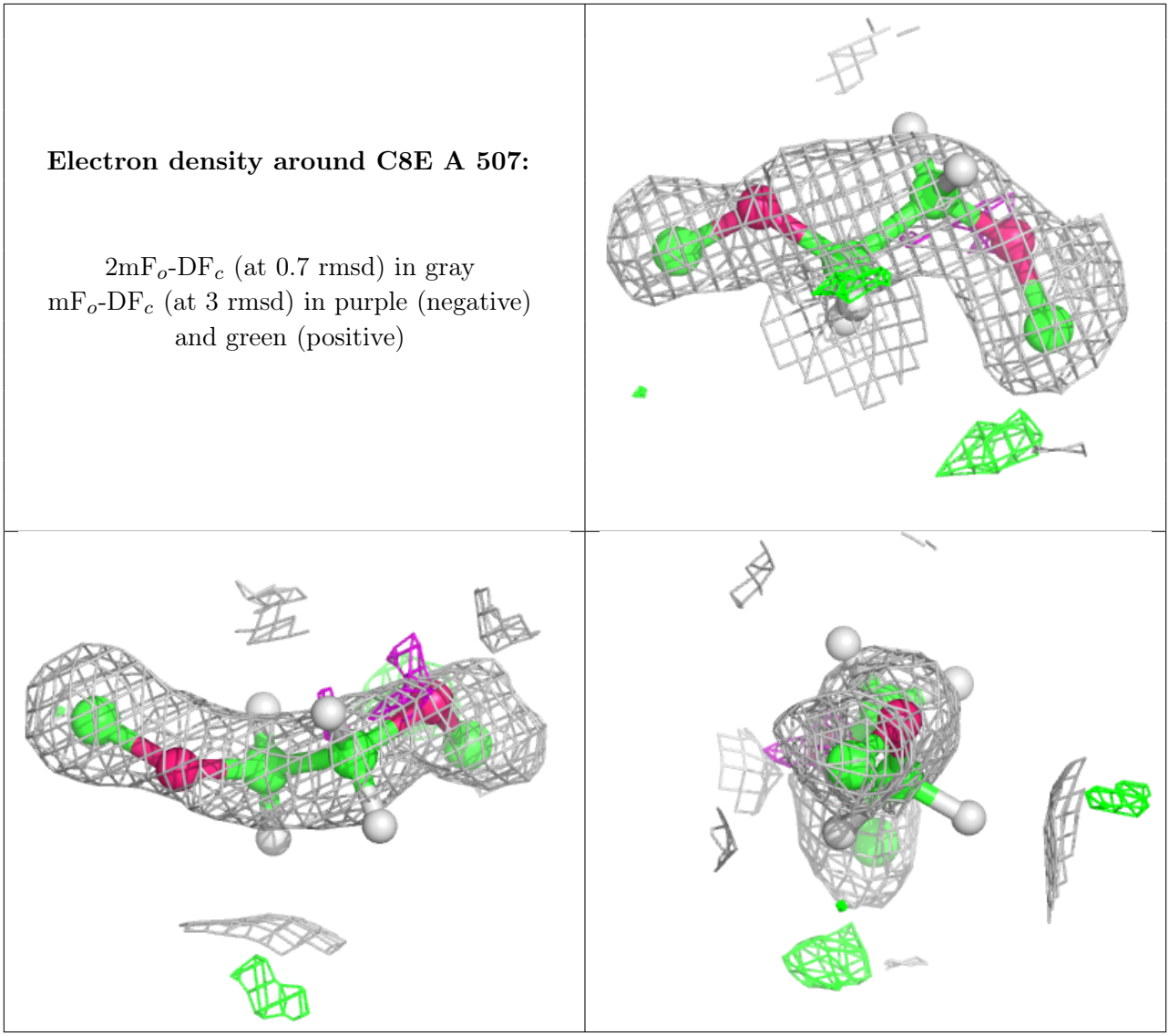
Electron density around C8E A 505:

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



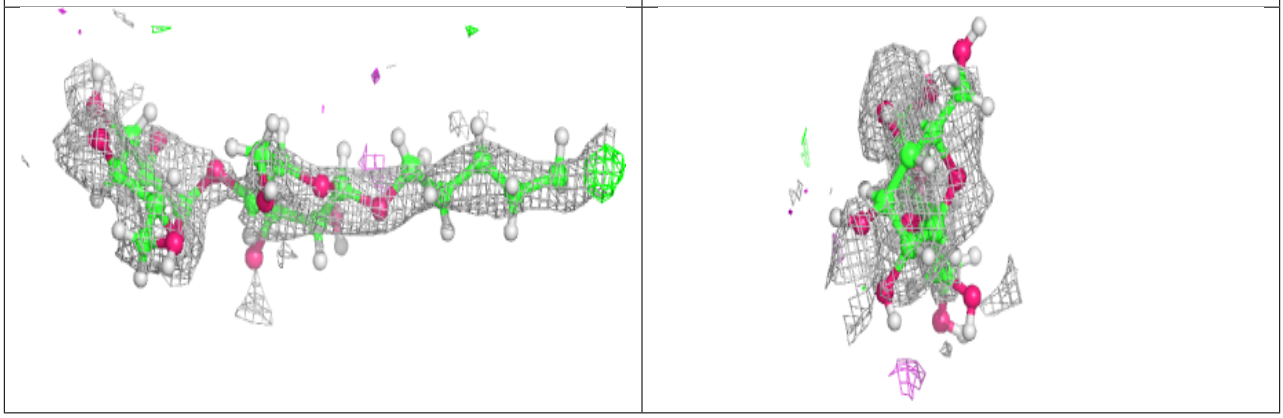
Electron density around C8E A 507:

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



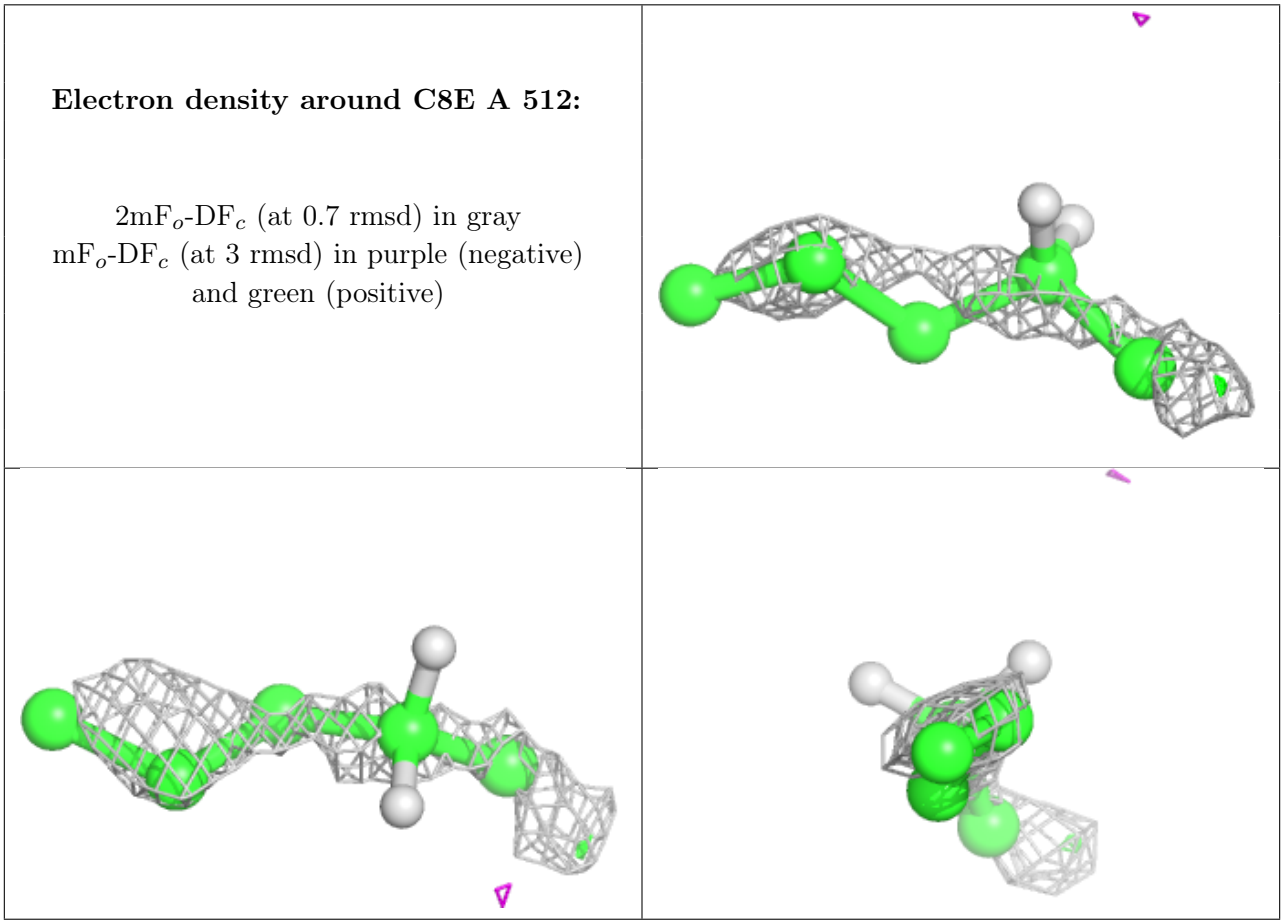
Electron density around DMU A 503:

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



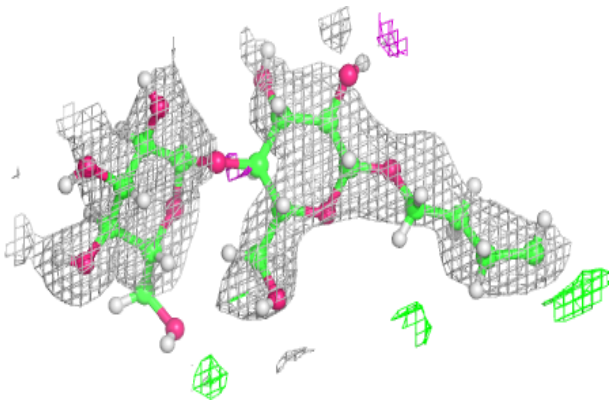
Electron density around C8E A 512:

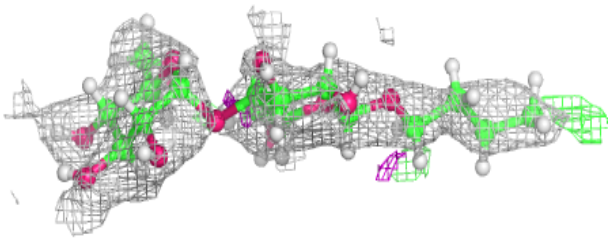
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

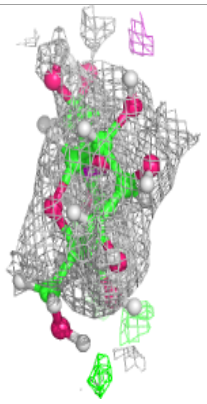


Electron density around DMU B 503:

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

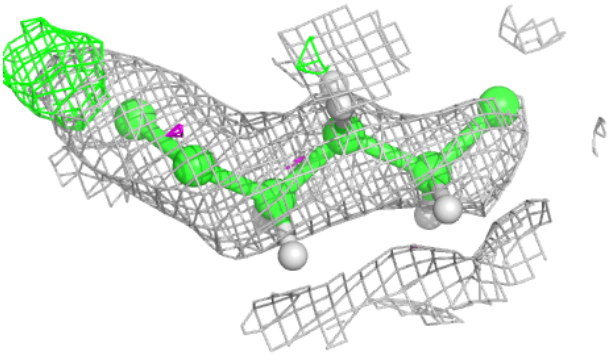


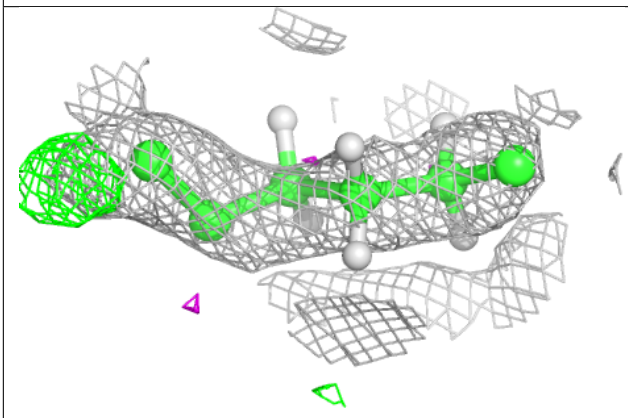


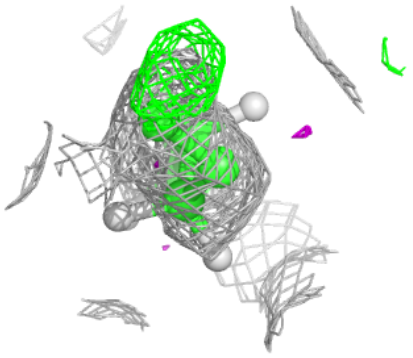


Electron density around C8E B 511:

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

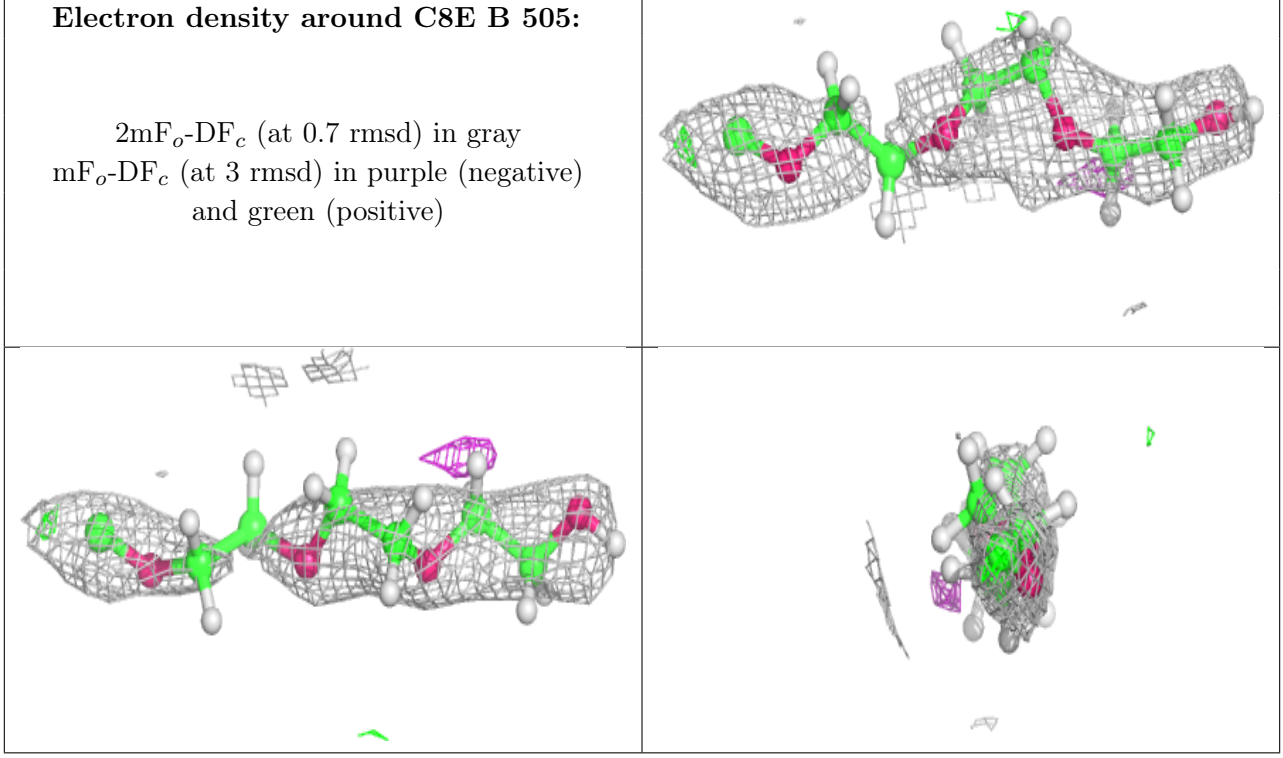






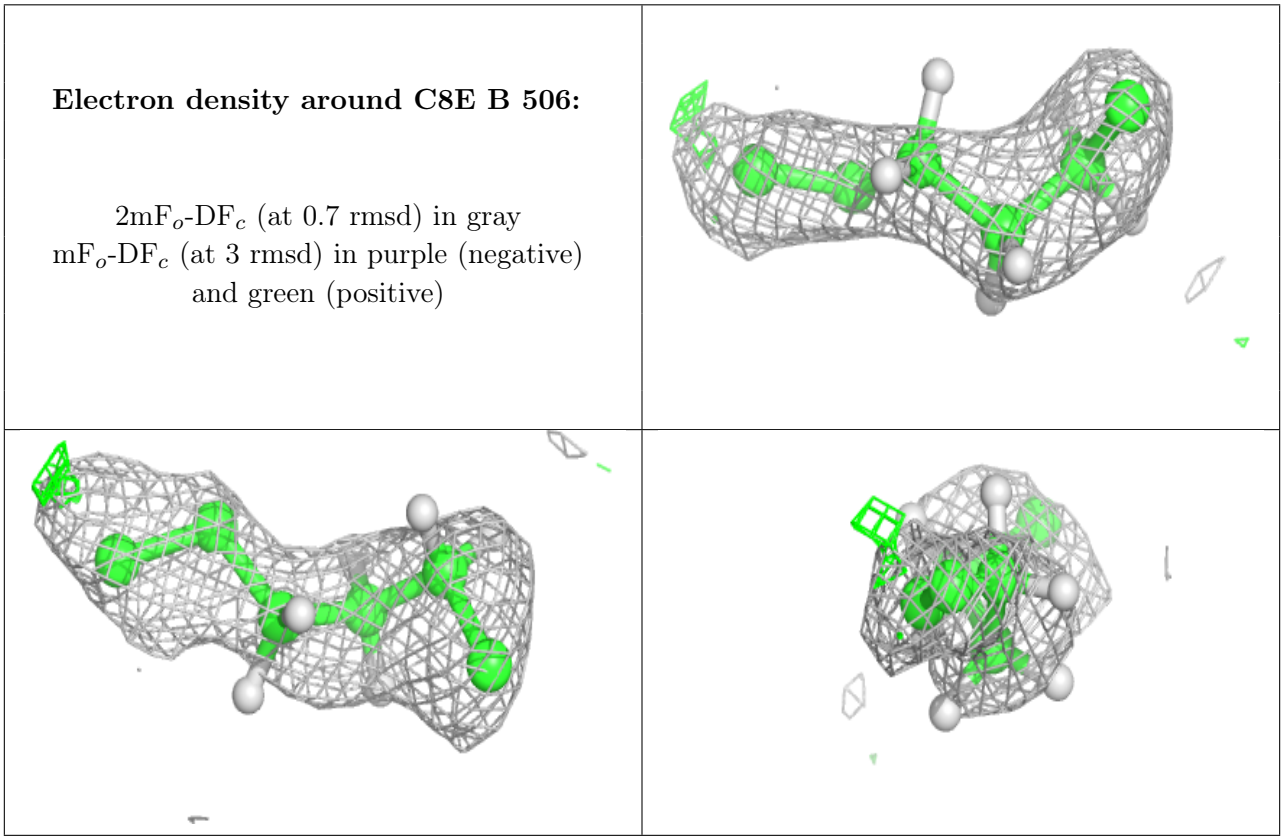
Electron density around C8E B 505:

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



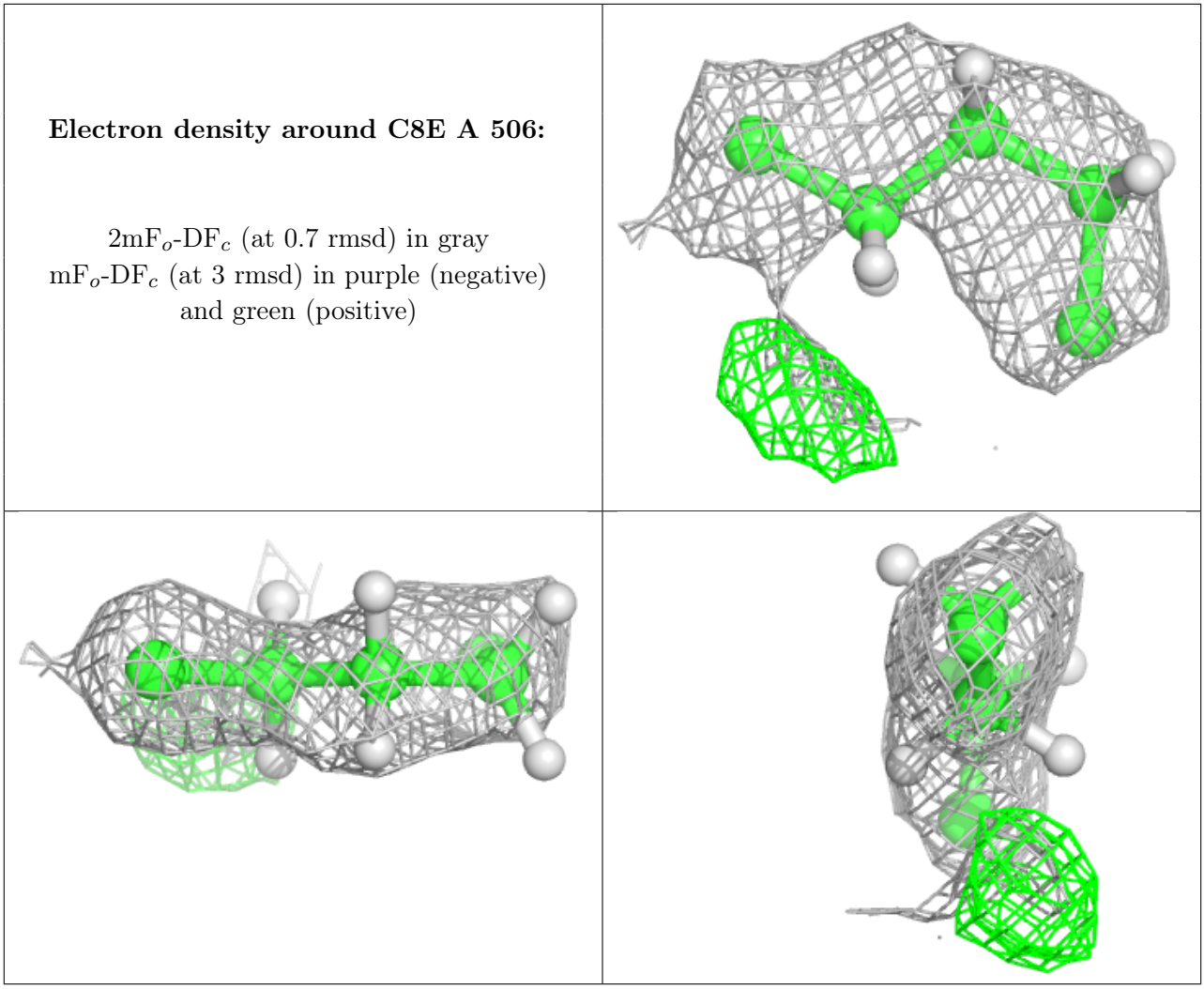
Electron density around C8E B 506:

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



Electron density around C8E A 506:

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



Electron density around C8E B 509:

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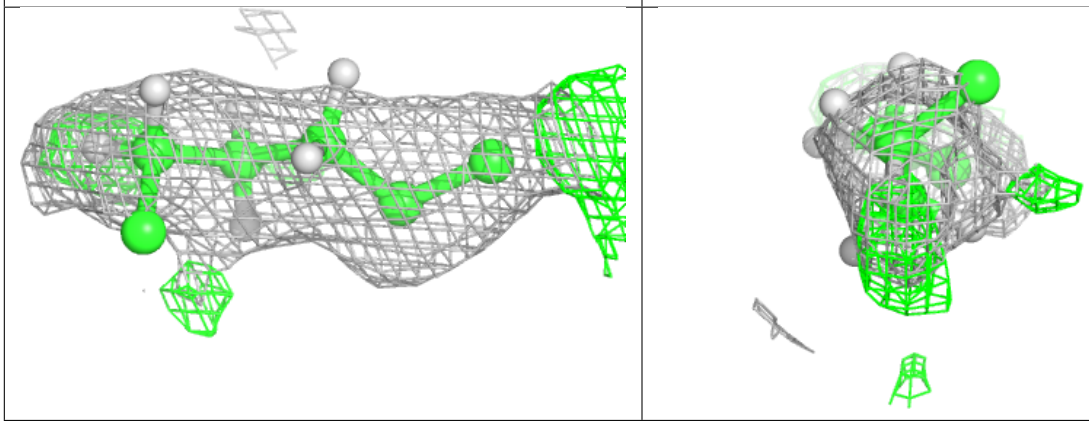
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around C8E B 504:

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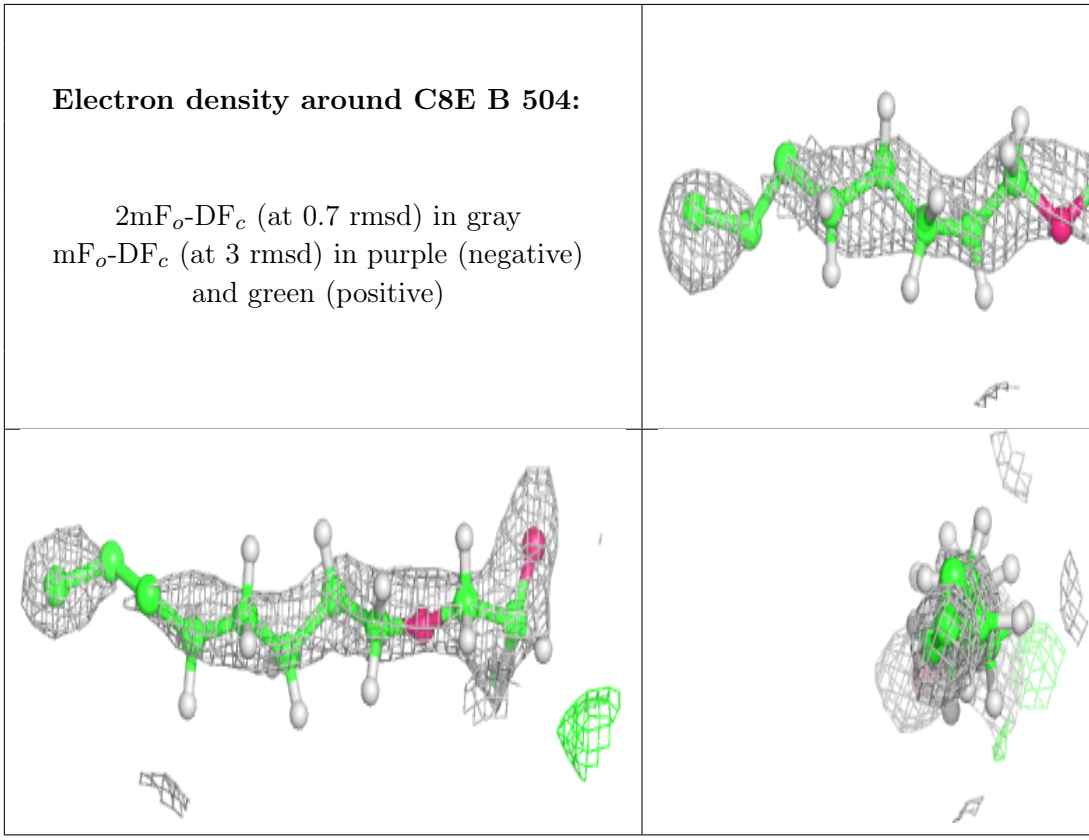
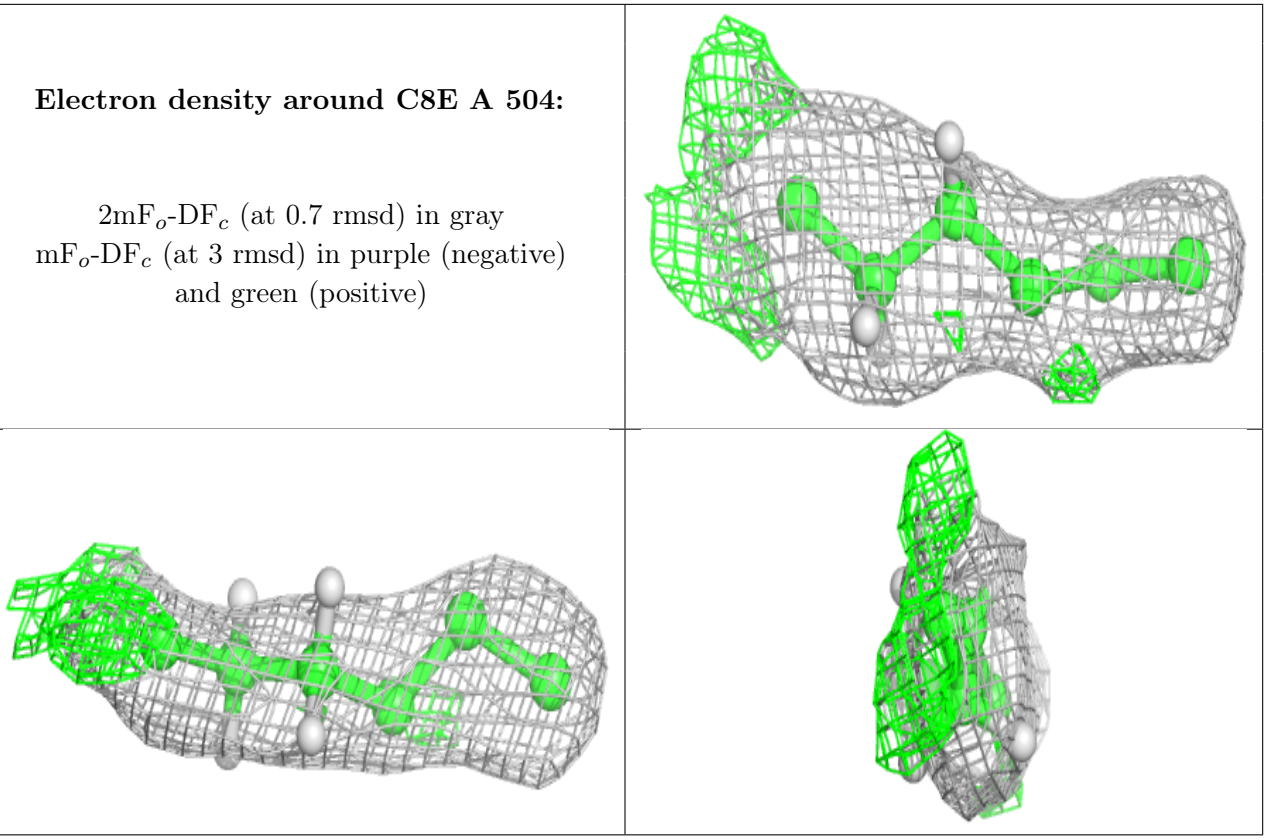
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



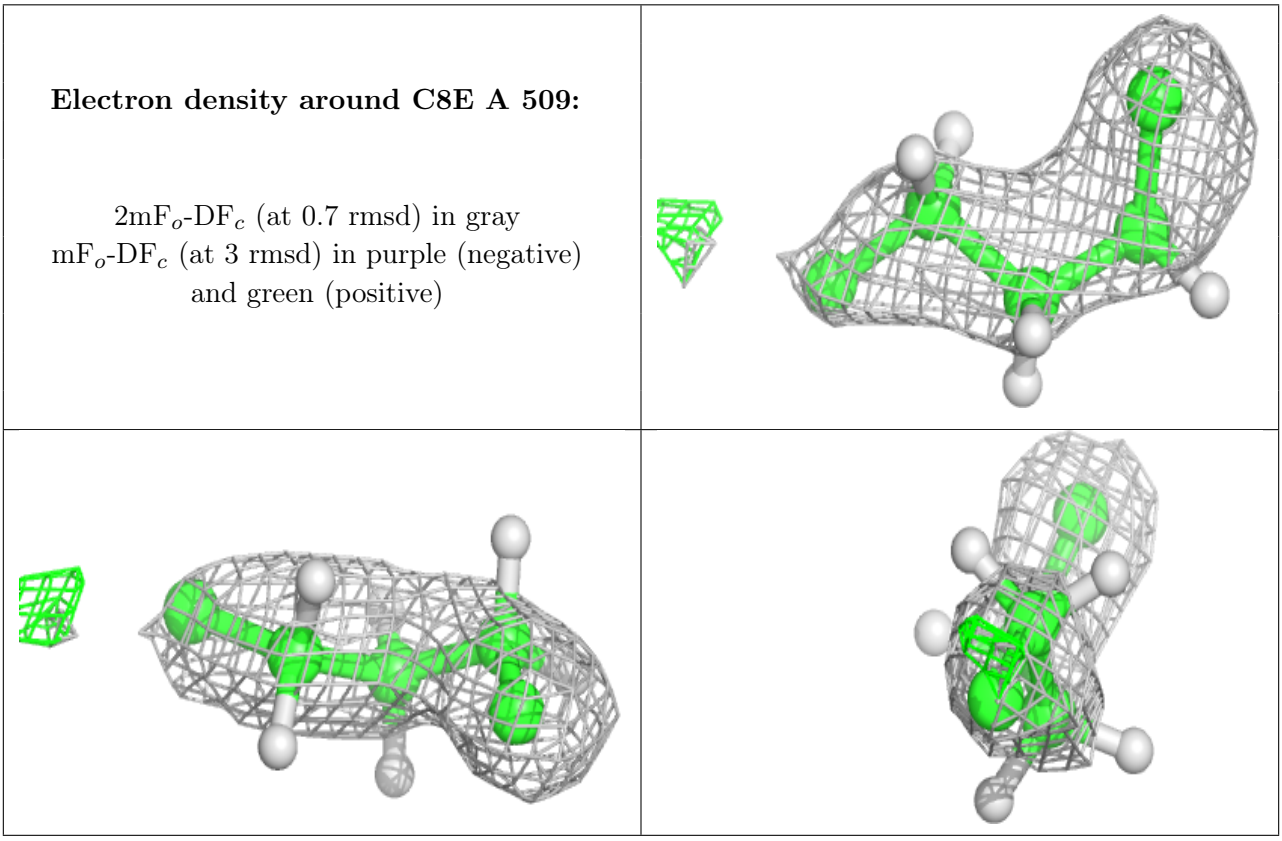
Electron density around C8E A 504:

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



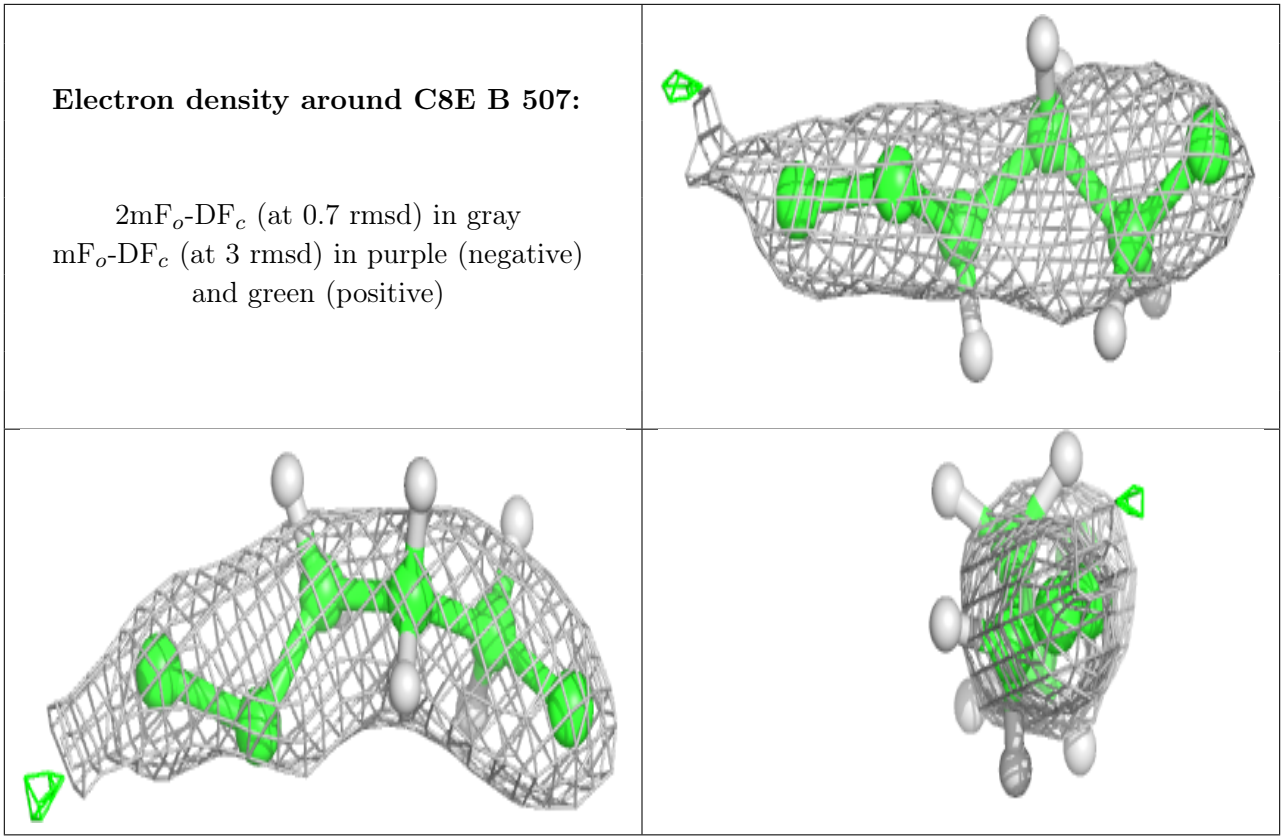
Electron density around C8E A 509:

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



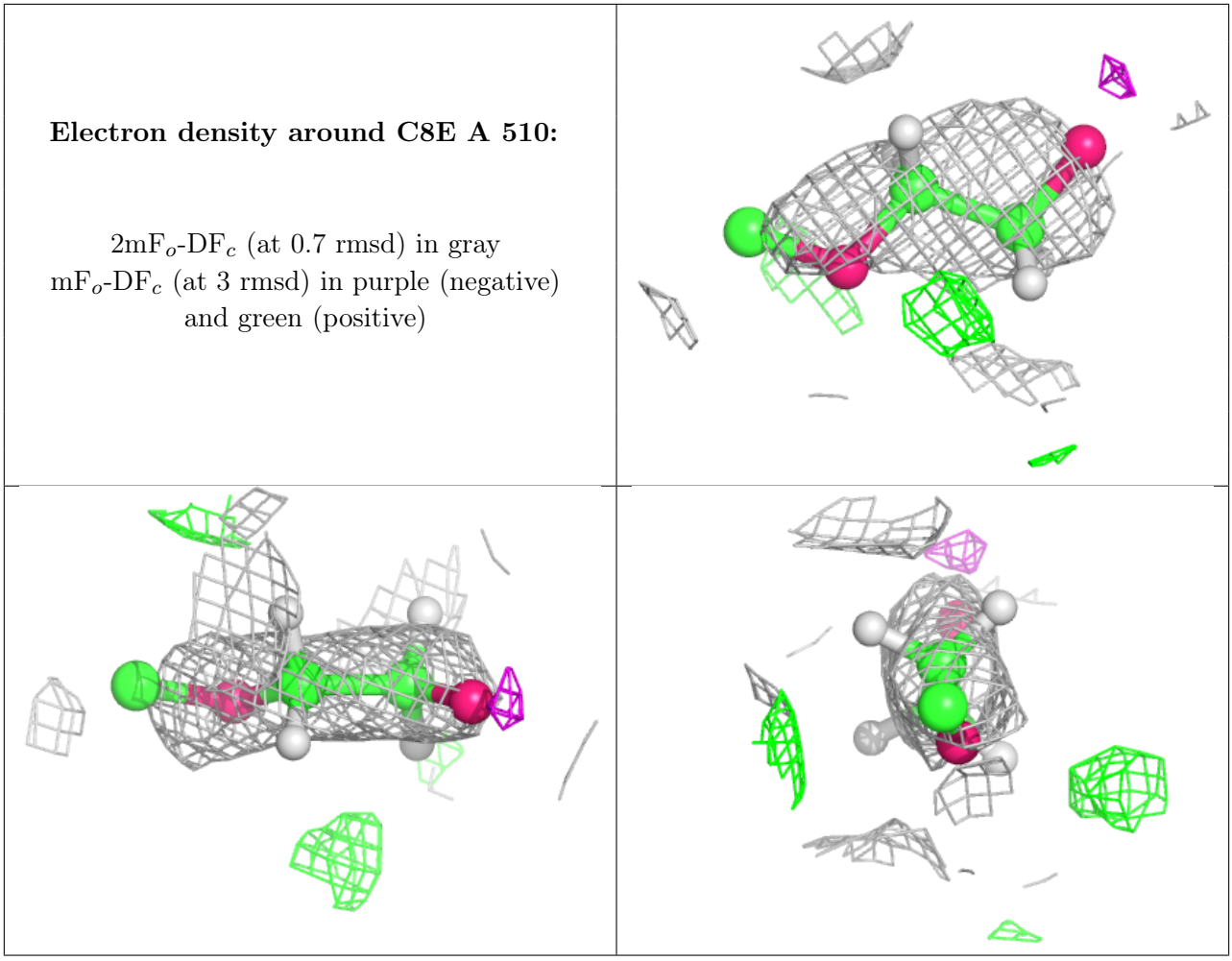
Electron density around C8E B 507:

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



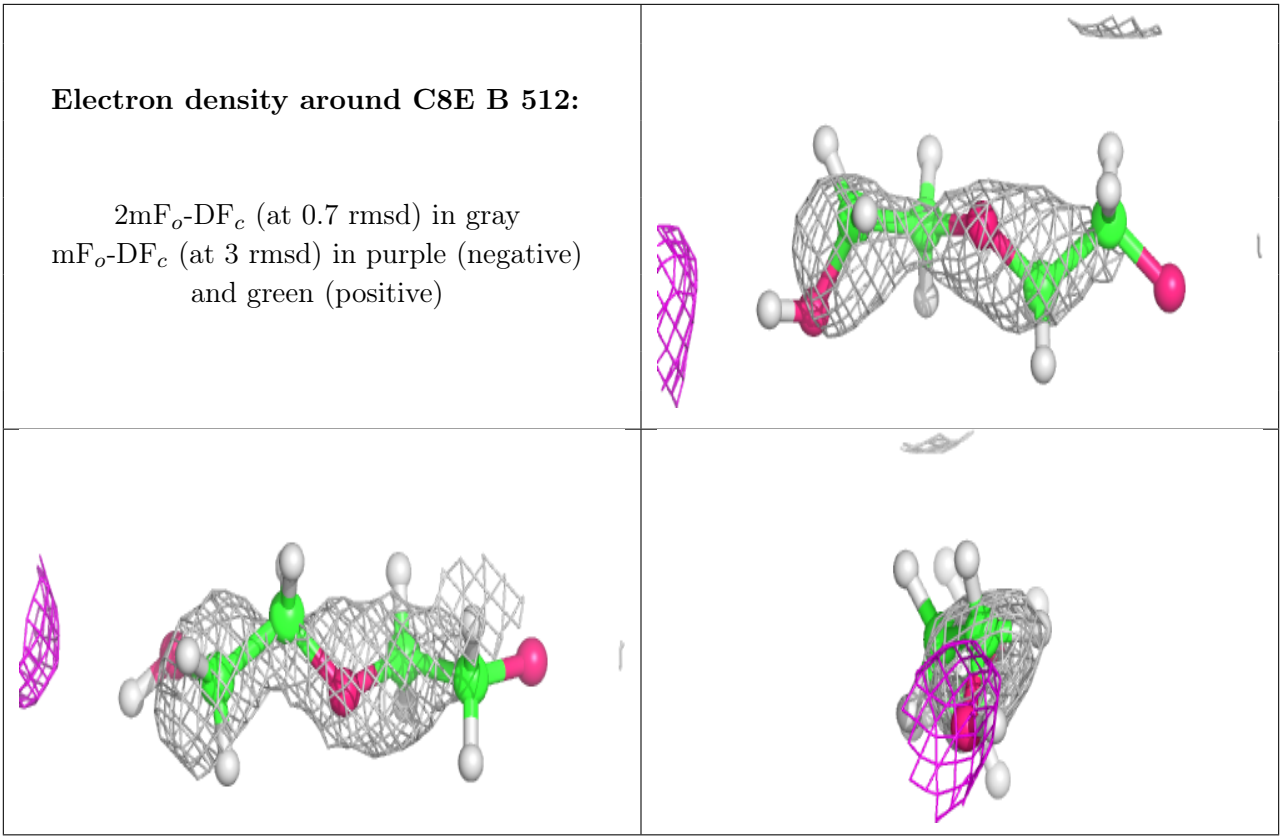
Electron density around C8E A 510:

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



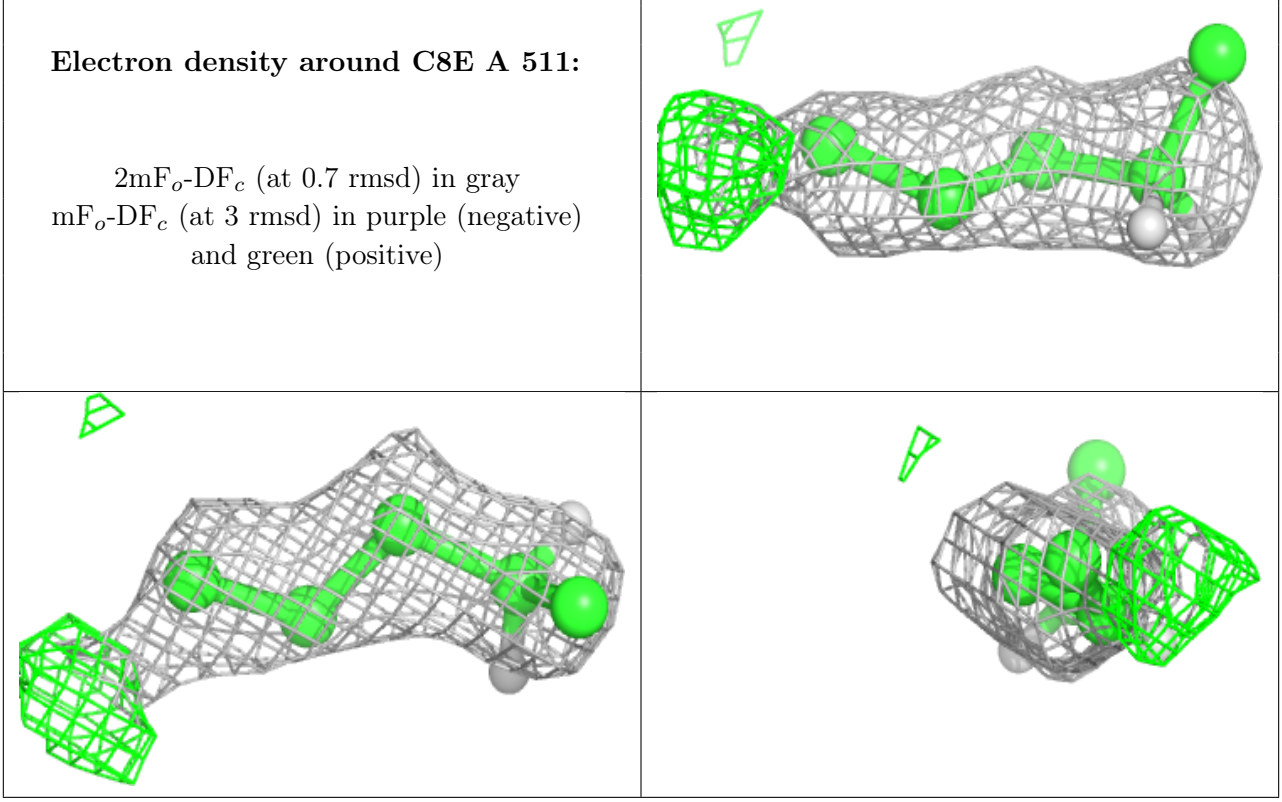
Electron density around C8E B 512:

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



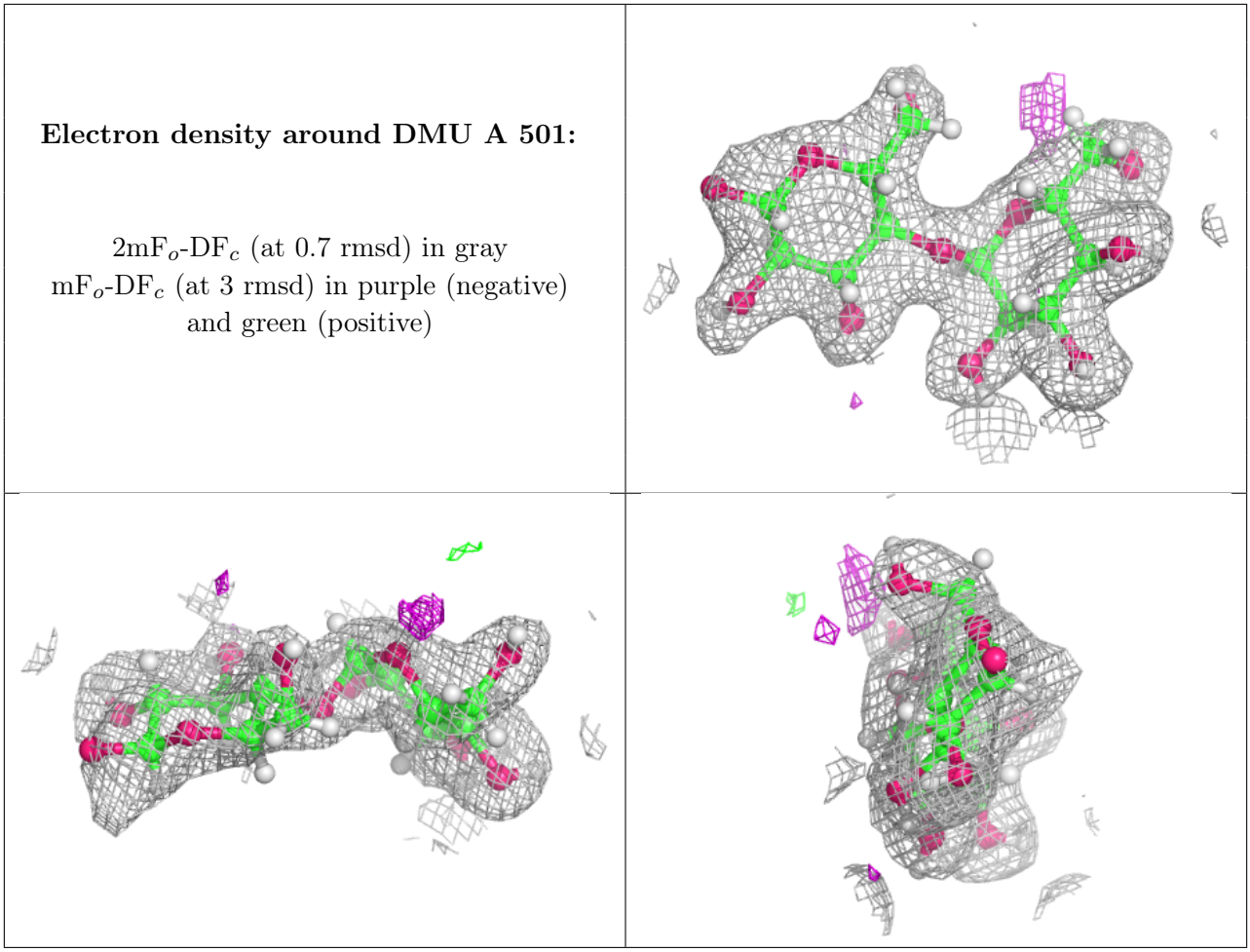
Electron density around C8E A 511:

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



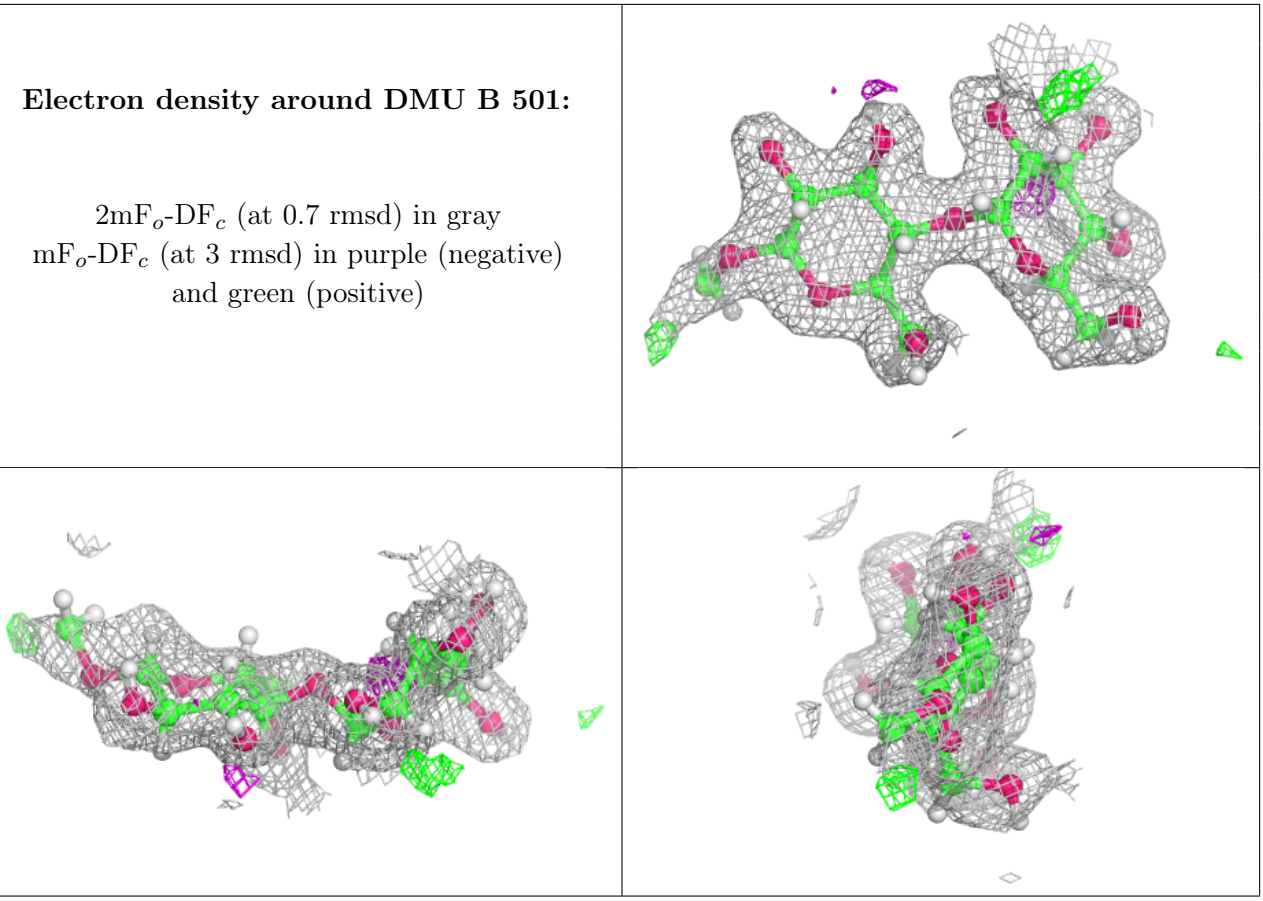
Electron density around DMU A 501:

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



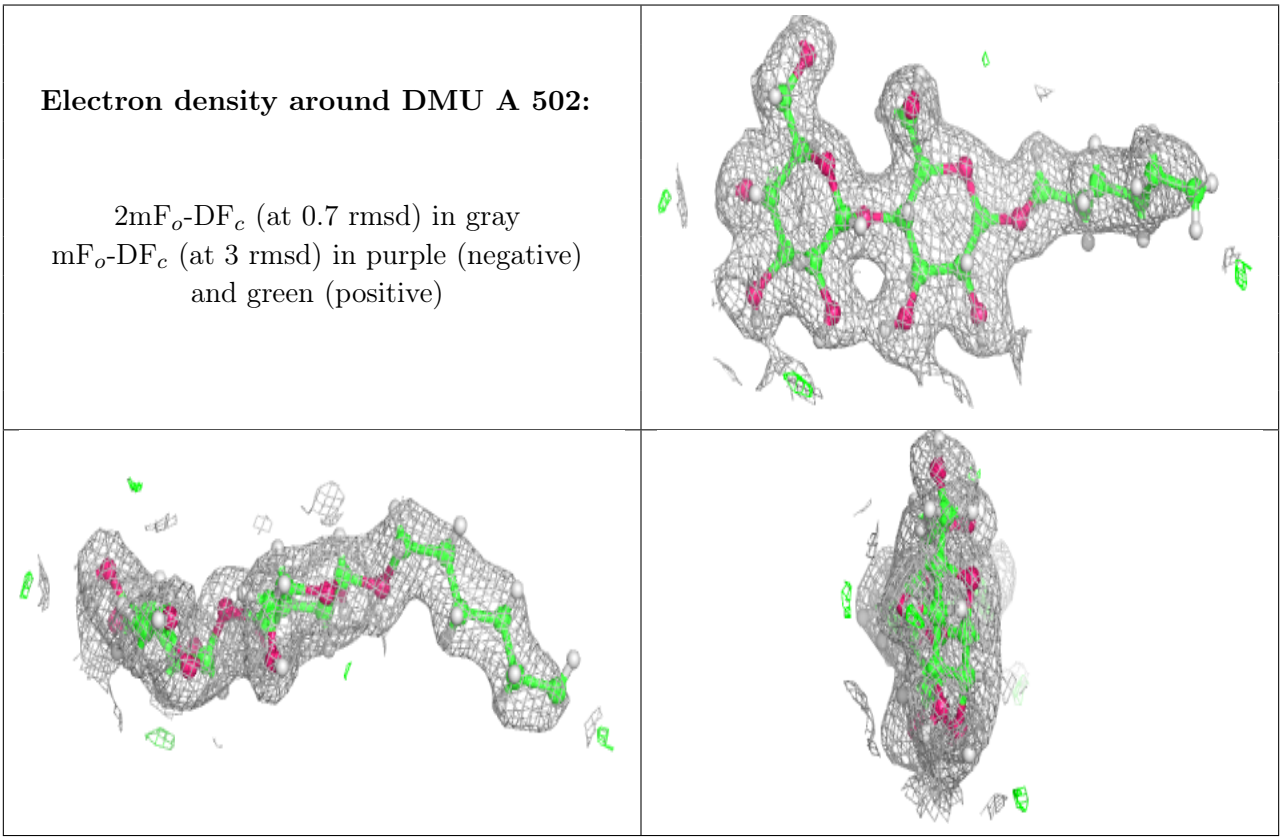
Electron density around DMU B 501:

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



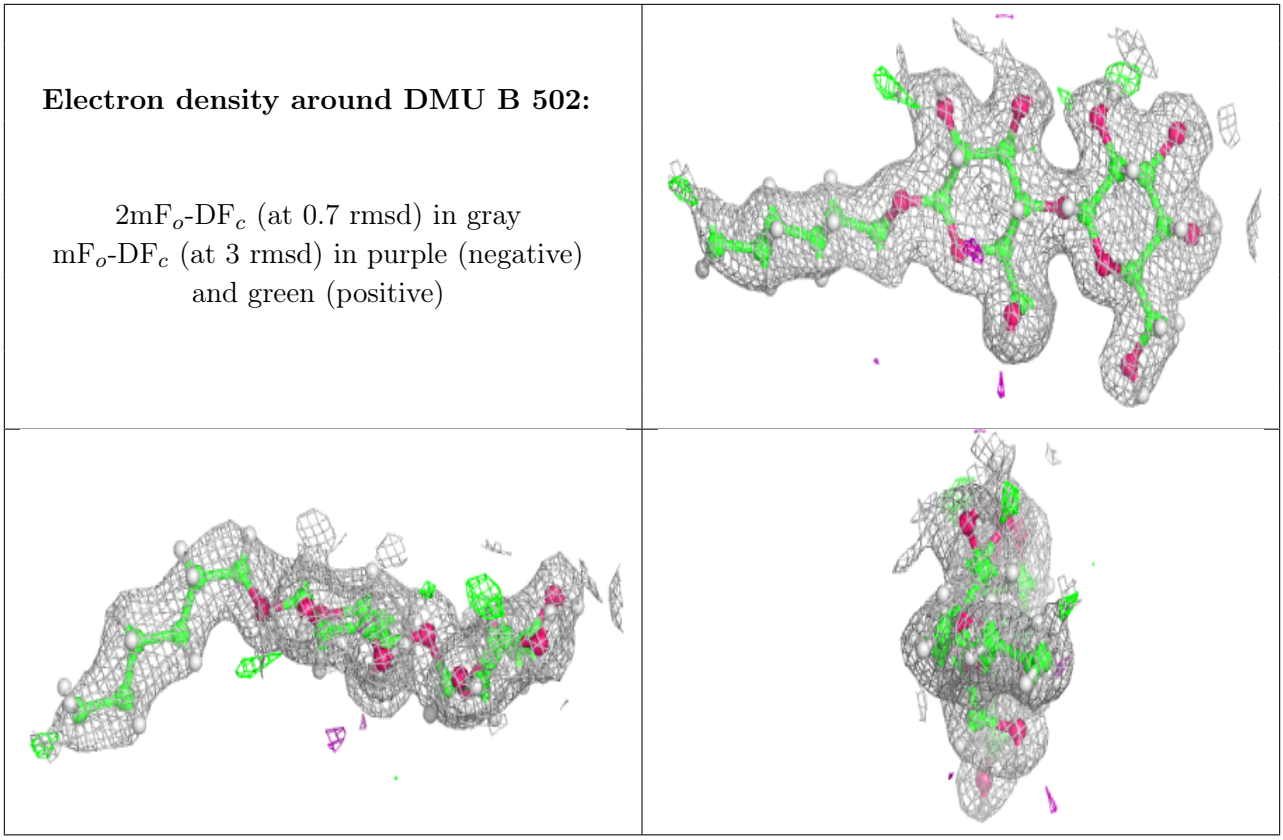
Electron density around DMU A 502:

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



Electron density around DMU B 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.