Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 10:12 PM JST

PDB ID	:	5Y79
Title	:	Crystal structure of the triose-phosphate/phosphate translocator in complex with 3-phosphoglycerate
Authors	:	Lee, Y.; Nishizawa, T.; Takemoto, M.; Kumazaki, K.; Yamashita, K.; Hirata, K.; Minoda, A.; Nagatoishi, S.; Tsumoto, K.; Ishitani, R.; Nureki, O.
Deposited on	:	2017-08-16
Resolution	:	2.20 Å(reported)

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

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

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

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

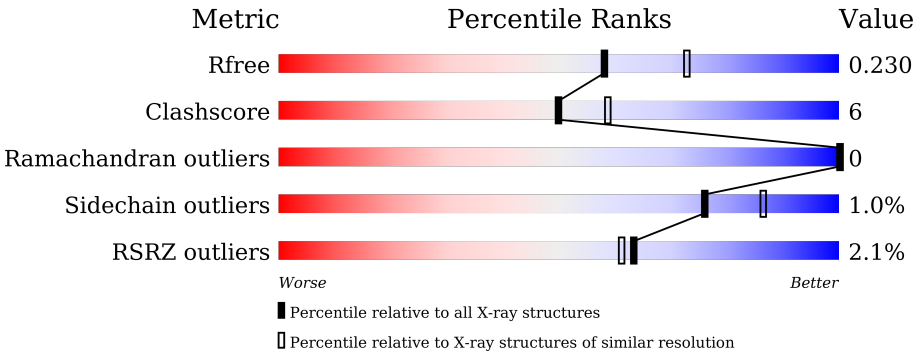
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	329	3% 82% 10% • 7%
1	B	329	. % 82% 11% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

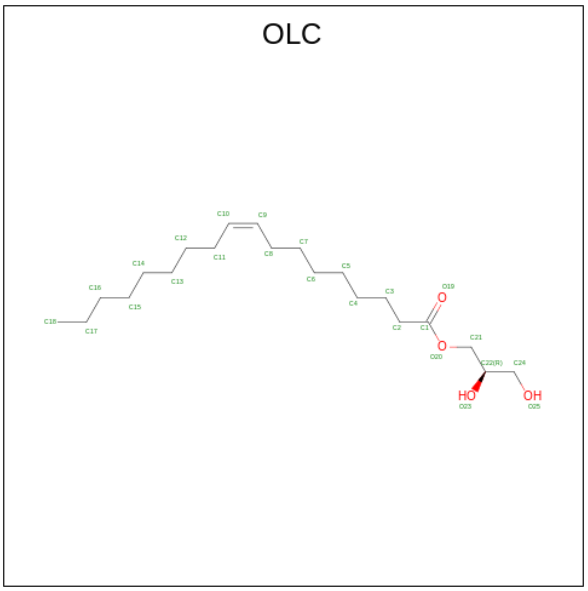
- Molecule 1 is a protein called Putative hexose phosphate translocator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2354	1580	364	398	12			
1	B	305	Total	C	N	O	S	0	0	0
			2359	1586	364	397	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MET	-	initiating methionine	UNP B5AJT1
A	411	GLY	-	expression tag	UNP B5AJT1
A	412	THR	-	expression tag	UNP B5AJT1
A	413	GLU	-	expression tag	UNP B5AJT1
A	414	ASN	-	expression tag	UNP B5AJT1
A	415	LEU	-	expression tag	UNP B5AJT1
A	416	TYR	-	expression tag	UNP B5AJT1
A	417	PHE	-	expression tag	UNP B5AJT1
A	418	GLN	-	expression tag	UNP B5AJT1
B	90	MET	-	initiating methionine	UNP B5AJT1
B	411	GLY	-	expression tag	UNP B5AJT1
B	412	THR	-	expression tag	UNP B5AJT1
B	413	GLU	-	expression tag	UNP B5AJT1
B	414	ASN	-	expression tag	UNP B5AJT1
B	415	LEU	-	expression tag	UNP B5AJT1
B	416	TYR	-	expression tag	UNP B5AJT1
B	417	PHE	-	expression tag	UNP B5AJT1
B	418	GLN	-	expression tag	UNP B5AJT1

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 19 15 4	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 13 13	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 11 7 4	0	0

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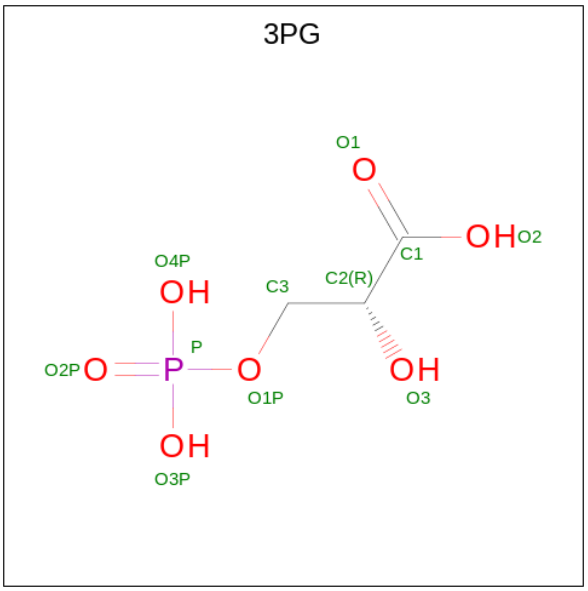
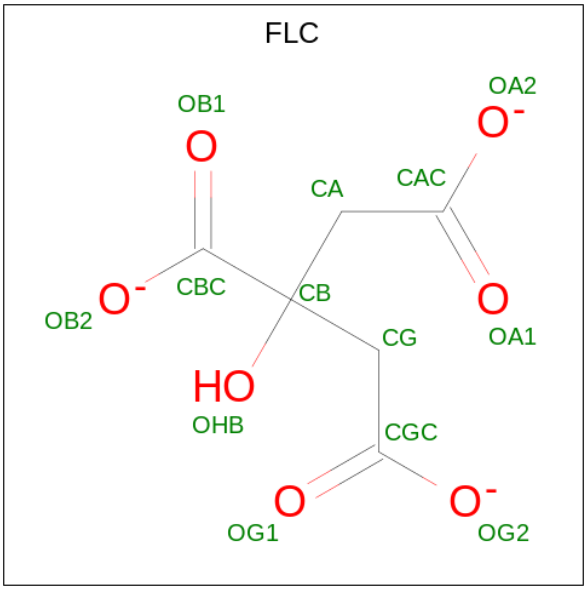
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 13 13	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C O 19 15 4	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 13 13	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C O 20 18 2	0	0
2	B	1	Total C 17 17	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C O 12 8 4	0	0
2	B	1	Total C 12 12	0	0

- Molecule 3 is 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: $C_3H_7O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 11 3 7 1	0	0
3	B	1	Total C O P 11 3 7 1	0	0

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0

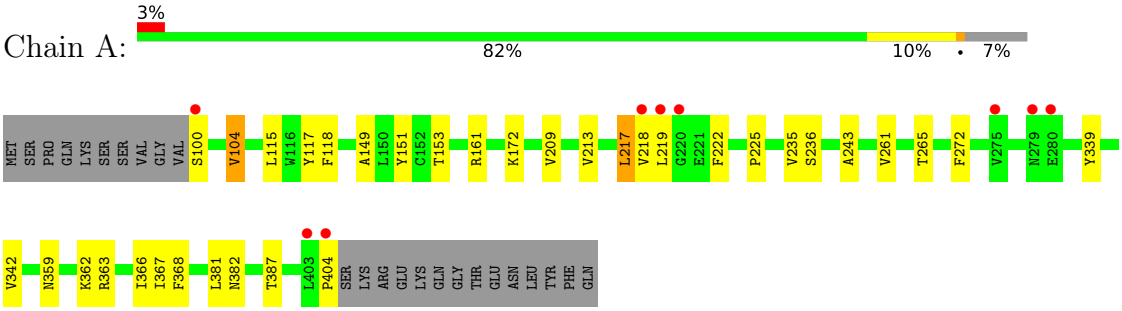
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	95	Total O 95 95	0	0
5	B	127	Total O 127 127	0	0

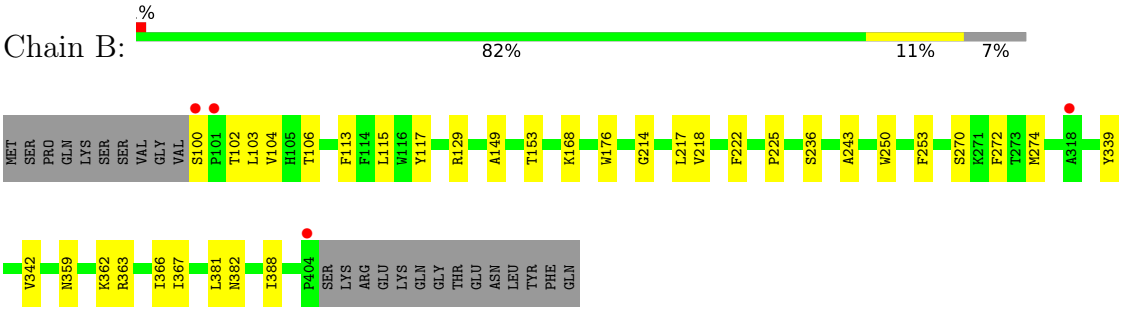
3 Residue-property plots (i)

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: Putative hexose phosphate translocator



• Molecule 1: Putative hexose phosphate translocator



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.05Å 165.33Å 41.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.20 49.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.00-2.20) 92.2 (49.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.191 , 0.229 0.191 , 0.230	Depositor DCC
R_{free} test set	2059 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	1.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.3	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	5396	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 23.51 % 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 4.5984e-03. 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: OLC, FLC, 3PG

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	0.26	0/2423	0.41	0/3313
1	B	0.26	0/2428	0.41	0/3320
All	All	0.26	0/4851	0.41	0/6633

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	2354	0	2375	29	0
1	B	2359	0	2397	31	0
2	A	181	0	272	15	0
2	B	245	0	381	20	0
3	A	11	0	4	0	0
3	B	11	0	4	0	0
4	A	13	0	5	1	0
5	A	95	0	0	0	0
5	B	127	0	0	0	0
All	All	5396	0	5438	61	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 (61) 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)
1:A:218:VAL:HG11	1:A:272:PHE:HZ	1.49	0.77
1:B:113:PHE:HB3	2:B:517:OLC:H9	1.71	0.73
4:A:517:FLC:OA2	4:A:517:FLC:OHB	2.10	0.69
2:A:512:OLC:H5	2:A:515:OLC:H10	1.73	0.69
1:B:129:ARG:HH21	2:B:514:OLC:H5	1.55	0.68
1:A:217:LEU:HD22	1:B:225:PRO:HB2	1.78	0.66
1:A:153:THR:HG21	2:A:504:OLC:H7A	1.78	0.65
1:B:381:LEU:HD21	2:B:504:OLC:H8A	1.80	0.62
1:B:381:LEU:HD11	2:B:504:OLC:H6A	1.82	0.61
1:A:209:VAL:HG11	2:A:501:OLC:H18	1.84	0.59
1:A:243:ALA:HA	2:A:501:OLC:H2A	1.87	0.55
1:B:149:ALA:O	1:B:153:THR:HG23	2.05	0.55
2:A:514:OLC:H24A	2:A:514:OLC:H2A	1.89	0.53
1:B:218:VAL:HG21	2:B:513:OLC:H6	1.92	0.52
1:A:161:ARG:NH2	2:A:514:OLC:H24	2.25	0.51
1:B:388:ILE:HD13	2:B:504:OLC:H15A	1.92	0.51
1:A:225:PRO:HB2	1:B:217:LEU:HD13	1.91	0.51
1:A:218:VAL:HG11	1:A:272:PHE:CZ	2.37	0.51
1:B:382:ASN:OD1	2:B:505:OLC:H22	2.11	0.51
1:A:149:ALA:O	1:A:153:THR:HG23	2.11	0.50
1:B:100:SER:O	1:B:103:LEU:N	2.45	0.50
1:A:261:VAL:O	1:A:265:THR:HG23	2.12	0.49
1:A:387:THR:HG23	2:A:505:OLC:H7	1.94	0.49
1:B:253:PHE:CZ	2:B:501:OLC:H8	2.48	0.49
1:A:382:ASN:OD1	2:A:505:OLC:H22	2.12	0.49
1:B:243:ALA:HA	2:B:501:OLC:H2A	1.95	0.48
1:B:359:ASN:O	1:B:363:ARG:HG3	2.13	0.48
1:A:235:VAL:HG13	2:A:501:OLC:H12A	1.96	0.48
1:A:115:LEU:HB3	1:A:342:VAL:HG11	1.95	0.47
1:B:168:LYS:HE3	1:B:168:LYS:HB2	1.77	0.46
1:A:218:VAL:HG12	1:A:219:LEU:HD12	1.96	0.46
1:B:117:TYR:CE1	1:B:362:LYS:HB2	2.51	0.46
1:A:367:ILE:HG21	2:A:505:OLC:H2A	1.98	0.46
1:A:222:PHE:HB3	1:B:222:PHE:HB3	1.98	0.45
1:A:404:PRO:HB2	1:B:222:PHE:CZ	2.51	0.45
1:B:113:PHE:CB	2:B:517:OLC:H9	2.44	0.45
1:B:236:SER:HA	2:B:502:OLC:H8A	1.98	0.45
1:B:367:ILE:HG21	2:B:505:OLC:H3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:TRP:CD1	2:B:508:OLC:H5A	2.52	0.44
1:B:218:VAL:HG11	1:B:272:PHE:CZ	2.53	0.44
1:A:118:PHE:HA	2:A:510:OLC:H8A	1.99	0.44
1:B:270:SER:O	1:B:274:MET:HG3	2.18	0.44
1:B:153:THR:HG21	2:B:512:OLC:H6A	1.99	0.43
1:B:250:TRP:CZ3	2:B:503:OLC:H4	2.53	0.43
1:A:213:VAL:HG11	2:A:507:OLC:H3A	2.00	0.43
1:A:172:LYS:HE3	1:A:172:LYS:HB3	1.81	0.43
1:A:381:LEU:HD21	2:A:502:OLC:H9	1.99	0.43
2:B:514:OLC:H3A	2:B:514:OLC:H6	1.69	0.42
1:B:250:TRP:CE2	2:B:503:OLC:H2	2.55	0.42
2:B:508:OLC:H5	2:B:513:OLC:H4	2.02	0.42
1:A:151:TYR:HB2	2:A:512:OLC:H10	2.01	0.42
1:B:115:LEU:HB2	1:B:342:VAL:HG11	2.01	0.42
1:B:102:THR:O	1:B:106:THR:HG23	2.20	0.41
1:A:359:ASN:O	1:A:363:ARG:HG3	2.19	0.41
1:A:362:LYS:O	1:A:366:ILE:HG12	2.20	0.41
1:A:236:SER:HA	2:B:503:OLC:H8A	2.02	0.41
1:A:368:PHE:CE1	2:A:505:OLC:H4A	2.56	0.41
1:B:214:GLY:HA3	2:B:513:OLC:H11A	2.01	0.41
1:B:362:LYS:O	1:B:366:ILE:HG12	2.20	0.41
1:A:117:TYR:CE1	1:A:362:LYS:HB2	2.55	0.41
1:A:100:SER:O	1:A:104:VAL:HG13	2.21	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	303/329 (92%)	300 (99%)	3 (1%)	0	100	100
1	B	303/329 (92%)	302 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	606/658 (92%)	602 (99%)	4 (1%)	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	251/286 (88%)	248 (99%)	3 (1%)	71 83
1	B	254/286 (89%)	252 (99%)	2 (1%)	81 90
All	All	505/572 (88%)	500 (99%)	5 (1%)	76 86

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

Mol	Chain	Res	Type
1	A	104	VAL
1	A	217	LEU
1	A	339	TYR
1	B	104	VAL
1	B	339	TYR

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

35 ligands 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	OLC	A	510	-	11,11,24	0.26	0	9,10,25	0.79	0
2	OLC	B	509	-	7,7,24	0.13	0	6,6,25	0.70	0
2	OLC	B	515	-	5,5,24	0.15	0	4,4,25	0.57	0
2	OLC	B	506	-	7,7,24	0.11	0	6,6,25	0.78	0
2	OLC	B	507	-	12,12,24	0.24	0	11,11,25	0.73	0
2	OLC	A	513	-	7,7,24	0.12	0	6,6,25	0.73	0
2	OLC	B	513	2	16,16,24	0.24	0	15,15,25	0.64	0
2	OLC	A	506	-	11,11,24	0.25	0	10,10,25	0.66	0
2	OLC	A	514	-	10,10,24	1.06	1 (10%)	11,11,25	1.29	1 (9%)
2	OLC	B	516	-	11,11,24	0.97	1 (9%)	12,12,25	1.14	1 (8%)
4	FLC	A	517	-	12,12,12	1.08	0	17,17,17	1.29	2 (11%)
2	OLC	A	502	-	13,13,24	0.23	0	12,12,25	0.71	0
2	OLC	B	514	-	8,8,24	0.13	0	7,7,25	0.72	0
2	OLC	B	502	2	24,24,24	0.69	1 (4%)	25,25,25	0.90	1 (4%)
2	OLC	A	504	-	7,7,24	0.12	0	6,6,25	0.74	0
2	OLC	A	505	-	18,18,24	0.79	1 (5%)	18,19,25	1.08	1 (5%)
2	OLC	A	509	-	7,7,24	0.12	0	6,6,25	0.77	0
2	OLC	B	517	-	11,11,24	0.26	0	9,10,25	0.81	0
3	3PG	A	516	-	9,10,10	0.90	0	12,14,14	1.29	2 (16%)
2	OLC	B	505	-	18,18,24	0.78	1 (5%)	18,19,25	1.15	1 (5%)
2	OLC	B	503	2	24,24,24	0.69	1 (4%)	25,25,25	0.85	1 (4%)
2	OLC	B	511	-	7,7,24	0.12	0	6,6,25	0.73	0
2	OLC	A	512	-	10,10,24	0.33	0	9,9,25	0.93	0
2	OLC	B	504	-	13,13,24	0.23	0	12,12,25	0.69	0
2	OLC	A	508	-	13,13,24	0.24	0	12,12,25	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OLC	B	512	-	19,19,24	0.76	1 (5%)	19,19,25	0.97	0
2	OLC	A	507	2	12,12,24	0.25	0	11,11,25	0.76	0
2	OLC	B	501	-	24,24,24	0.67	1 (4%)	25,25,25	0.98	1 (4%)
2	OLC	A	511	-	6,6,24	0.14	0	5,5,25	0.64	0
2	OLC	A	503	-	5,5,24	0.15	0	4,4,25	0.57	0
2	OLC	B	508	-	7,7,24	0.13	0	6,6,25	0.71	0
2	OLC	A	515	-	12,12,24	0.25	0	11,11,25	0.73	0
2	OLC	A	501	-	24,24,24	0.69	1 (4%)	25,25,25	1.06	1 (4%)
3	3PG	B	518	-	9,10,10	0.88	0	12,14,14	1.36	2 (16%)
2	OLC	B	510	-	15,15,24	0.22	0	14,14,25	0.73	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
2	OLC	A	510	-	-	4/9/9/24	-
2	OLC	B	509	-	-	4/5/5/24	-
2	OLC	B	515	-	-	2/3/3/24	-
2	OLC	B	506	-	-	3/5/5/24	-
2	OLC	B	507	-	-	3/10/10/24	-
2	OLC	A	513	-	-	4/5/5/24	-
2	OLC	B	513	2	-	7/14/14/24	-
2	OLC	A	506	-	-	3/9/9/24	-
2	OLC	A	514	-	-	6/10/10/24	-
2	OLC	B	516	-	-	6/11/11/24	-
4	FLC	A	517	-	-	14/16/16/16	-
2	OLC	A	502	-	-	4/11/11/24	-
2	OLC	B	514	-	-	2/6/6/24	-
2	OLC	B	502	2	-	8/24/24/24	-
2	OLC	A	504	-	-	4/5/5/24	-
2	OLC	A	505	-	-	9/18/18/24	-
2	OLC	A	509	-	-	2/5/5/24	-
2	OLC	B	517	-	-	5/9/9/24	-
3	3PG	A	516	-	-	7/10/10/10	-
2	OLC	B	505	-	-	11/18/18/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	503	2	-	11/24/24/24	-
2	OLC	B	511	-	-	3/5/5/24	-
2	OLC	A	512	-	-	2/8/8/24	-
2	OLC	B	504	-	-	6/11/11/24	-
2	OLC	A	508	-	-	6/11/11/24	-
2	OLC	B	512	-	-	6/17/17/24	-
2	OLC	A	507	2	-	3/10/10/24	-
2	OLC	B	501	-	-	8/24/24/24	-
2	OLC	A	511	-	-	2/4/4/24	-
2	OLC	A	503	-	-	1/3/3/24	-
2	OLC	B	508	-	-	3/5/5/24	-
2	OLC	A	515	-	-	4/10/10/24	-
2	OLC	A	501	-	-	11/24/24/24	-
3	3PG	B	518	-	-	5/10/10/10	-
2	OLC	B	510	-	-	8/13/13/24	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	512	OLC	O20-C1	3.10	1.41	1.30
2	A	514	OLC	O20-C1	2.79	1.41	1.33
2	A	501	OLC	O20-C1	2.74	1.41	1.33
2	B	502	OLC	O20-C1	2.71	1.41	1.33
2	B	503	OLC	O20-C1	2.70	1.41	1.33
2	B	501	OLC	O20-C1	2.58	1.40	1.33
2	B	516	OLC	O20-C1	2.57	1.40	1.33
2	A	505	OLC	O20-C1	2.50	1.40	1.33
2	B	505	OLC	O20-C1	2.43	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	514	OLC	O20-C1-C2	3.12	121.71	111.91
2	B	516	OLC	O20-C1-C2	2.69	120.35	111.91
2	A	501	OLC	O20-C1-C2	2.67	120.30	111.91
4	A	517	FLC	OB2-CBC-CB	2.66	117.67	113.05
3	B	518	3PG	O2-C1-C2	2.62	118.48	112.72
2	B	502	OLC	O20-C1-C2	2.58	120.02	111.91
2	B	505	OLC	O20-C1-C2	2.54	119.87	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	516	3PG	O2-C1-C2	2.53	118.28	112.72
2	B	501	OLC	O20-C1-C2	2.48	119.70	111.91
2	A	505	OLC	O20-C1-C2	2.42	119.49	111.91
3	B	518	3PG	O1-C1-C2	-2.22	118.21	122.54
3	A	516	3PG	O1-C1-C2	-2.01	118.61	122.54
4	A	517	FLC	OB1-CBC-CB	-2.01	119.41	122.25
2	B	503	OLC	O20-C1-C2	2.00	118.19	111.91

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	OLC	C21-C22-C24-O25
2	A	505	OLC	C9-C10-C11-C12
2	A	514	OLC	O20-C21-C22-O23
2	A	515	OLC	C6-C7-C8-C9
2	B	505	OLC	C21-C22-C24-O25
2	B	517	OLC	C9-C10-C11-C12
3	A	516	3PG	C3-O1P-P-O3P
3	A	516	3PG	C3-O1P-P-O4P
3	B	518	3PG	O2-C1-C2-C3
4	A	517	FLC	CAC-CA-CB-CBC
4	A	517	FLC	CAC-CA-CB-CG
4	A	517	FLC	CAC-CA-CB-OHB
4	A	517	FLC	OHB-CB-CBC-OB1
4	A	517	FLC	CA-CB-CG-CGC
4	A	517	FLC	OHB-CB-CG-CGC
2	A	514	OLC	O19-C1-O20-C21
2	A	514	OLC	C2-C1-O20-C21
2	A	505	OLC	C2-C1-O20-C21
2	B	516	OLC	C2-C1-O20-C21
4	A	517	FLC	CBC-CB-CG-CGC
2	B	503	OLC	O20-C21-C22-O23
2	A	501	OLC	C1-C2-C3-C4
2	B	516	OLC	O19-C1-O20-C21
2	B	505	OLC	O23-C22-C24-O25
2	A	505	OLC	C1-C2-C3-C4
2	A	505	OLC	O19-C1-O20-C21
2	B	502	OLC	O20-C21-C22-O23
2	B	504	OLC	C11-C12-C13-C14
2	A	514	OLC	O20-C21-C22-C24
2	A	501	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	A	509	OLC	C5-C6-C7-C8
2	B	503	OLC	C13-C14-C15-C16
2	A	515	OLC	C13-C14-C15-C16
2	B	505	OLC	C4-C5-C6-C7
2	B	513	OLC	C5-C6-C7-C8
2	B	513	OLC	C4-C5-C6-C7
2	A	511	OLC	C4-C5-C6-C7
2	A	505	OLC	C3-C4-C5-C6
2	B	510	OLC	C5-C6-C7-C8
2	A	505	OLC	C5-C6-C7-C8
2	A	514	OLC	C21-C22-C24-O25
2	B	501	OLC	C21-C22-C24-O25
2	B	516	OLC	C21-C22-C24-O25
2	A	501	OLC	C3-C4-C5-C6
2	B	507	OLC	C5-C6-C7-C8
2	B	509	OLC	C2-C3-C4-C5
2	B	502	OLC	C6-C7-C8-C9
2	A	502	OLC	C13-C14-C15-C16
2	B	505	OLC	C5-C6-C7-C8
2	A	501	OLC	C14-C15-C16-C17
2	A	508	OLC	C3-C4-C5-C6
2	B	510	OLC	C3-C4-C5-C6
2	B	516	OLC	C1-C2-C3-C4
4	A	517	FLC	CA-CB-CBC-OB1
2	B	501	OLC	C5-C6-C7-C8
2	A	501	OLC	O23-C22-C24-O25
2	A	514	OLC	O23-C22-C24-O25
2	B	501	OLC	O23-C22-C24-O25
2	B	516	OLC	O23-C22-C24-O25
2	B	512	OLC	C6-C7-C8-C9
2	B	503	OLC	C14-C15-C16-C17
2	B	508	OLC	C5-C6-C7-C8
2	A	501	OLC	C4-C5-C6-C7
2	B	503	OLC	C12-C13-C14-C15
2	B	505	OLC	C2-C3-C4-C5
2	B	501	OLC	C1-C2-C3-C4
2	B	506	OLC	C12-C13-C14-C15
2	B	510	OLC	C10-C11-C12-C13
2	B	509	OLC	C4-C5-C6-C7
2	A	509	OLC	C4-C5-C6-C7
2	B	502	OLC	O20-C21-C22-C24
2	B	515	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	503	OLC	C4-C5-C6-C7
2	B	510	OLC	C2-C3-C4-C5
2	B	502	OLC	C4-C5-C6-C7
2	B	513	OLC	C6-C7-C8-C9
2	A	504	OLC	C3-C4-C5-C6
2	A	506	OLC	C4-C5-C6-C7
2	A	501	OLC	C5-C6-C7-C8
2	A	508	OLC	C2-C3-C4-C5
2	B	511	OLC	C15-C16-C17-C18
2	B	512	OLC	C5-C6-C7-C8
2	B	511	OLC	C11-C12-C13-C14
2	B	506	OLC	C15-C16-C17-C18
2	B	506	OLC	C11-C12-C13-C14
2	B	504	OLC	C5-C6-C7-C8
2	A	508	OLC	C10-C11-C12-C13
2	B	504	OLC	C6-C7-C8-C9
2	B	505	OLC	C6-C7-C8-C9
2	B	509	OLC	C5-C6-C7-C8
3	A	516	3PG	C3-O1P-P-O2P
2	B	517	OLC	C4-C5-C6-C7
2	B	513	OLC	C10-C11-C12-C13
3	A	516	3PG	O2-C1-C2-C3
3	B	518	3PG	O1-C1-C2-C3
3	B	518	3PG	O2-C1-C2-O3
2	B	516	OLC	C2-C3-C4-C5
2	A	504	OLC	C6-C7-C8-C9
2	A	504	OLC	C2-C3-C4-C5
2	B	515	OLC	C1-C2-C3-C4
2	B	501	OLC	C3-C4-C5-C6
2	B	505	OLC	C7-C8-C9-C10
2	A	513	OLC	C6-C7-C8-C9
2	B	509	OLC	C3-C4-C5-C6
2	B	514	OLC	C5-C6-C7-C8
4	A	517	FLC	OHB-CB-CBC-OB2
4	A	517	FLC	CA-CB-CBC-OB2
2	B	502	OLC	C3-C4-C5-C6
2	B	511	OLC	C13-C14-C15-C16
2	B	513	OLC	C15-C16-C17-C18
2	B	510	OLC	C12-C13-C14-C15
2	A	511	OLC	C5-C6-C7-C8
2	B	517	OLC	C1-C2-C3-C4
2	A	515	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	B	517	OLC	C5-C6-C7-C8
2	B	501	OLC	C2-C3-C4-C5
2	A	506	OLC	C3-C4-C5-C6
2	A	501	OLC	C13-C14-C15-C16
2	A	508	OLC	C5-C6-C7-C8
2	B	508	OLC	C2-C3-C4-C5
2	A	510	OLC	C9-C10-C11-C12
2	B	505	OLC	C9-C10-C11-C12
2	B	503	OLC	C2-C1-O20-C21
4	A	517	FLC	CB-CA-CAC-OA1
4	A	517	FLC	CB-CA-CAC-OA2
2	A	507	OLC	C5-C6-C7-C8
2	B	503	OLC	O19-C1-O20-C21
2	A	505	OLC	O23-C22-C24-O25
2	B	510	OLC	C6-C7-C8-C9
2	B	503	OLC	C4-C5-C6-C7
2	A	505	OLC	C21-C22-C24-O25
2	A	510	OLC	C1-C2-C3-C4
2	A	513	OLC	C4-C5-C6-C7
2	B	507	OLC	C6-C7-C8-C9
2	B	514	OLC	C1-C2-C3-C4
2	A	504	OLC	C4-C5-C6-C7
4	A	517	FLC	CG-CB-CBC-OB2
2	A	510	OLC	C7-C8-C9-C10
2	B	502	OLC	C1-C2-C3-C4
2	A	512	OLC	C3-C4-C5-C6
3	A	516	3PG	O1-C1-C2-C3
3	B	518	3PG	O1-C1-C2-O3
2	B	503	OLC	C5-C6-C7-C8
2	B	512	OLC	C12-C13-C14-C15
2	A	507	OLC	C7-C8-C9-C10
2	B	501	OLC	C7-C8-C9-C10
2	B	504	OLC	C7-C8-C9-C10
2	B	503	OLC	C9-C10-C11-C12
2	B	512	OLC	O20-C1-C2-C3
2	B	505	OLC	C3-C4-C5-C6
4	A	517	FLC	CG-CB-CBC-OB1
2	B	503	OLC	O20-C21-C22-C24
2	B	512	OLC	O19-C1-C2-C3
2	B	501	OLC	C4-C5-C6-C7
2	B	503	OLC	C7-C8-C9-C10
2	B	513	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	B	505	OLC	C2-C1-O20-C21
2	B	502	OLC	O23-C22-C24-O25
2	A	512	OLC	C7-C8-C9-C10
3	B	518	3PG	C3-O1P-P-O3P
2	A	508	OLC	C11-C12-C13-C14
2	A	502	OLC	C5-C6-C7-C8
2	B	504	OLC	C9-C10-C11-C12
2	B	507	OLC	C9-C10-C11-C12
2	B	510	OLC	C9-C10-C11-C12
2	A	510	OLC	C6-C7-C8-C9
2	B	510	OLC	C1-C2-C3-C4
2	A	501	OLC	C9-C10-C11-C12
2	A	502	OLC	C7-C8-C9-C10
2	A	508	OLC	C9-C10-C11-C12
2	A	502	OLC	C9-C10-C11-C12
2	A	507	OLC	C9-C10-C11-C12
2	B	517	OLC	C7-C8-C9-C10
3	A	516	3PG	O1-C1-C2-O3
3	A	516	3PG	O2-C1-C2-O3
2	B	502	OLC	C9-C10-C11-C12
2	B	508	OLC	C6-C7-C8-C9
2	A	505	OLC	C4-C5-C6-C7
2	A	513	OLC	C5-C6-C7-C8
2	B	505	OLC	O19-C1-O20-C21
2	A	501	OLC	O20-C1-C2-C3
2	B	512	OLC	C14-C15-C16-C17
2	A	513	OLC	C3-C4-C5-C6
2	B	504	OLC	C14-C15-C16-C17
2	A	515	OLC	C11-C12-C13-C14
2	A	506	OLC	C9-C10-C11-C12
2	B	513	OLC	C14-C15-C16-C17

There are no ring outliers.

20 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	510	OLC	1	0
2	B	513	OLC	3	0
2	A	514	OLC	2	0
4	A	517	FLC	1	0
2	A	502	OLC	1	0
2	B	514	OLC	2	0

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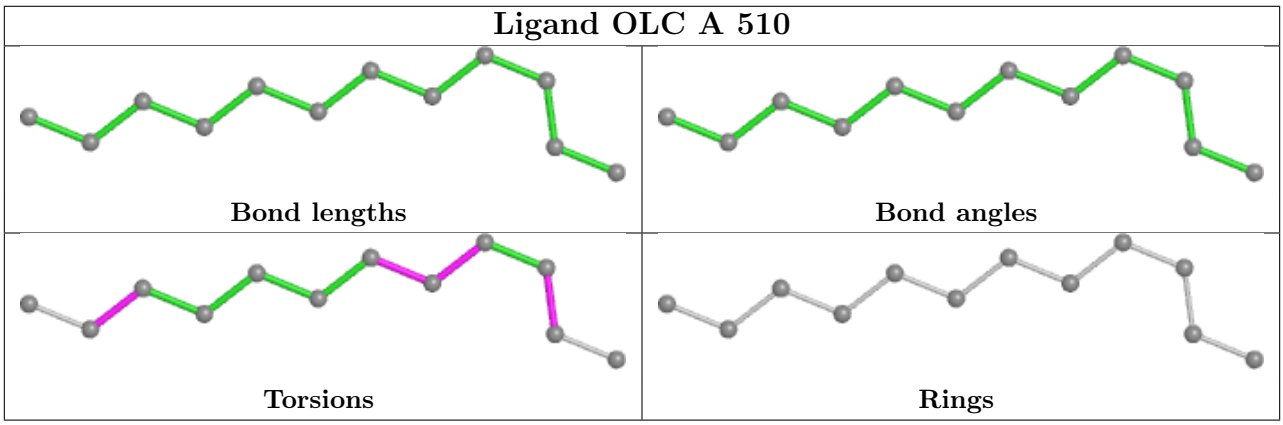
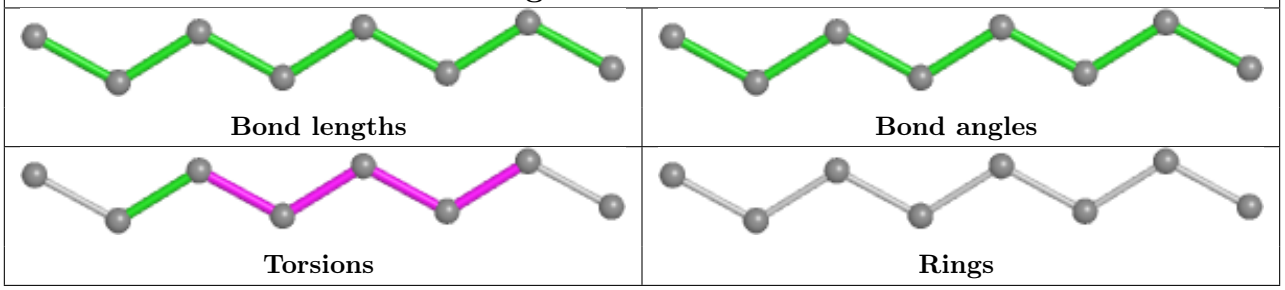
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	OLC	1	0
2	A	504	OLC	1	0
2	A	505	OLC	4	0
2	B	517	OLC	2	0
2	B	505	OLC	2	0
2	B	503	OLC	3	0
2	A	512	OLC	2	0
2	B	504	OLC	3	0
2	B	512	OLC	1	0
2	A	507	OLC	1	0
2	B	501	OLC	2	0
2	B	508	OLC	2	0
2	A	515	OLC	1	0
2	A	501	OLC	3	0

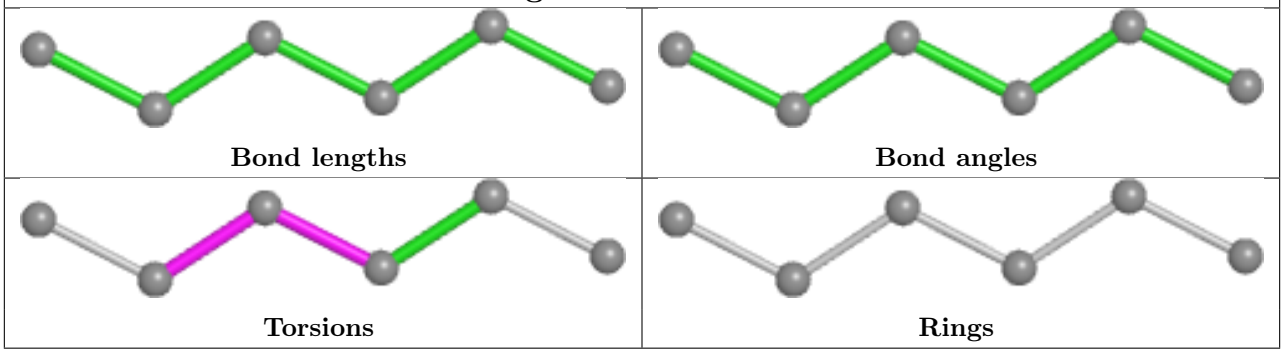
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 OLC B 509



Ligand OLC B 515



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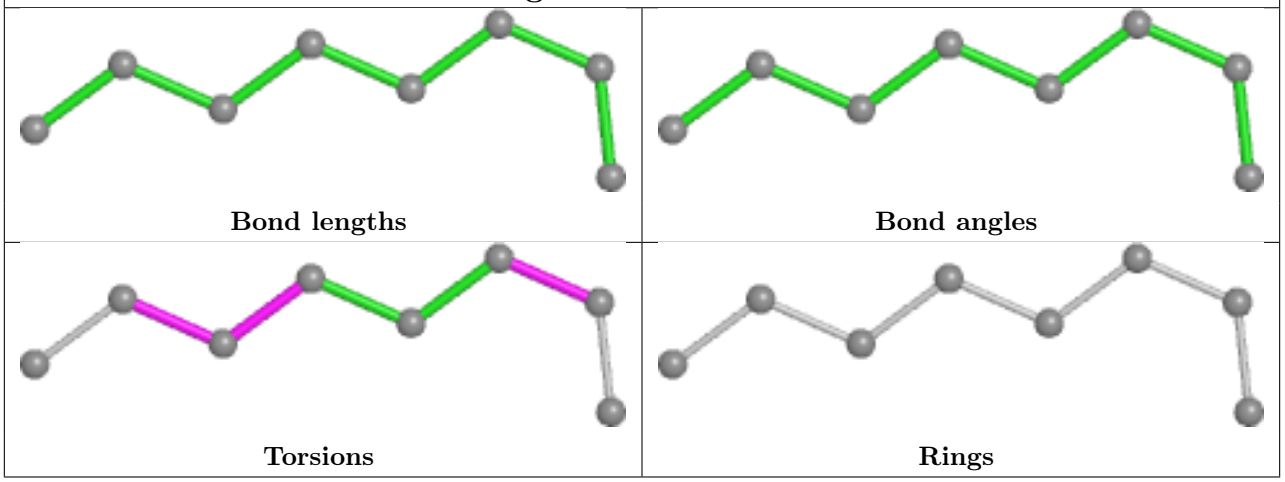
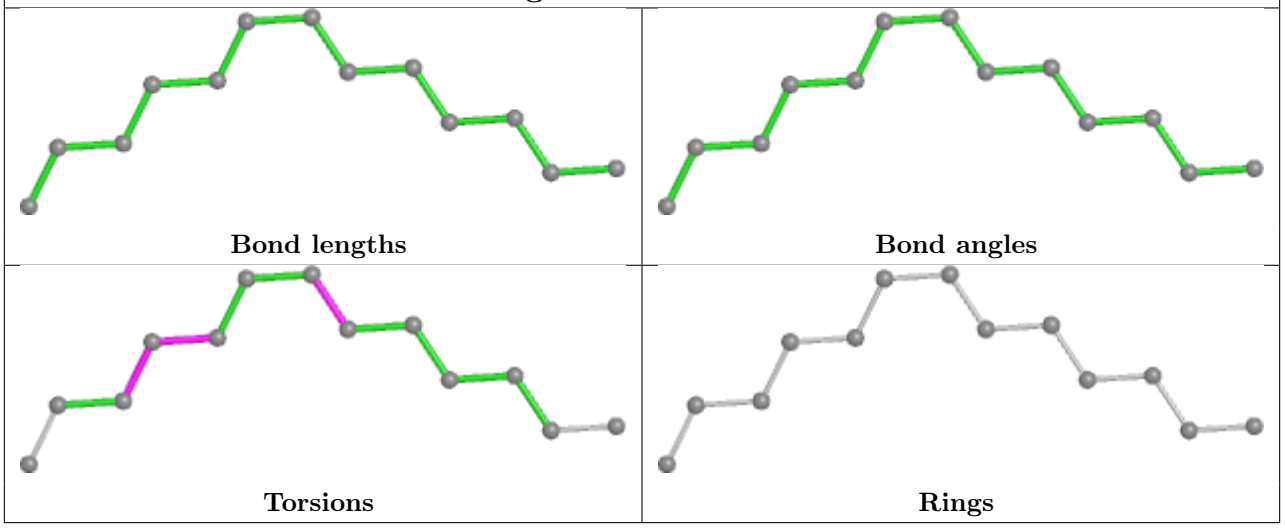
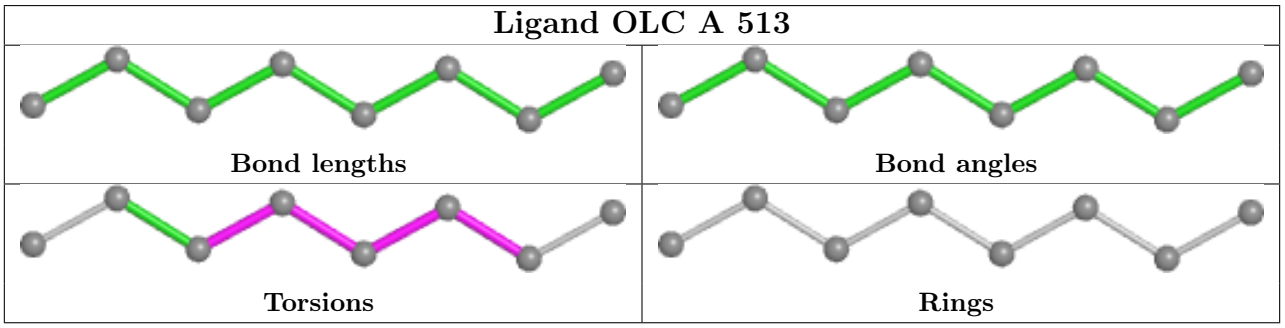


Ligand OLC B 507



Ligand OLC A 513



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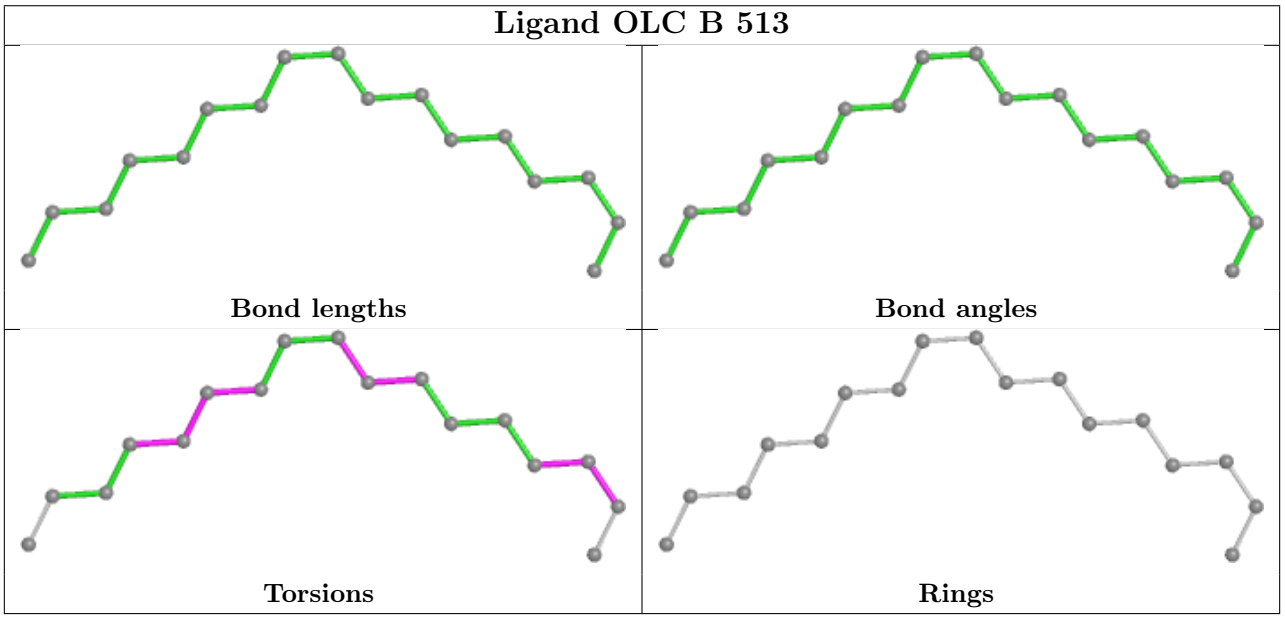

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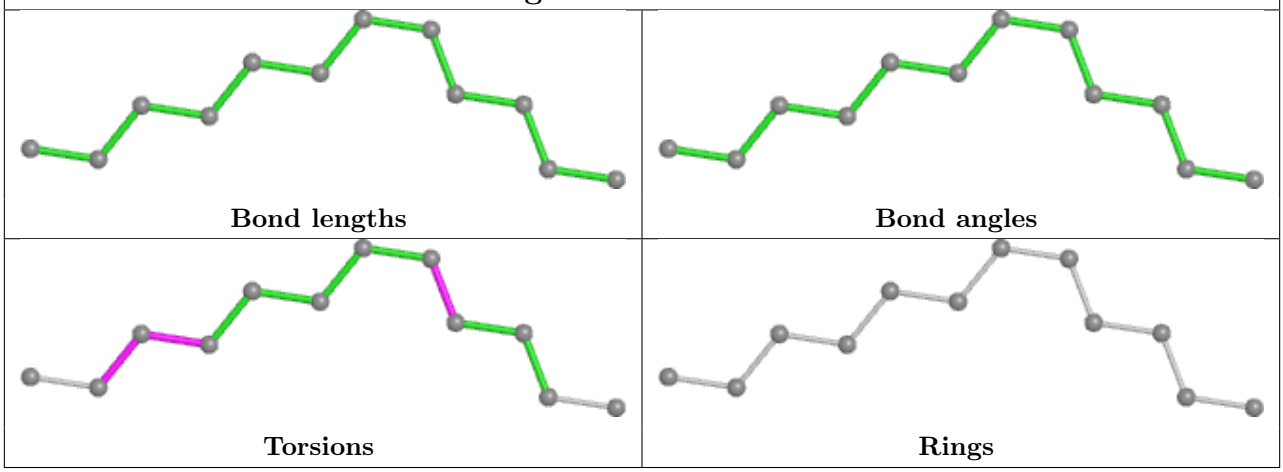

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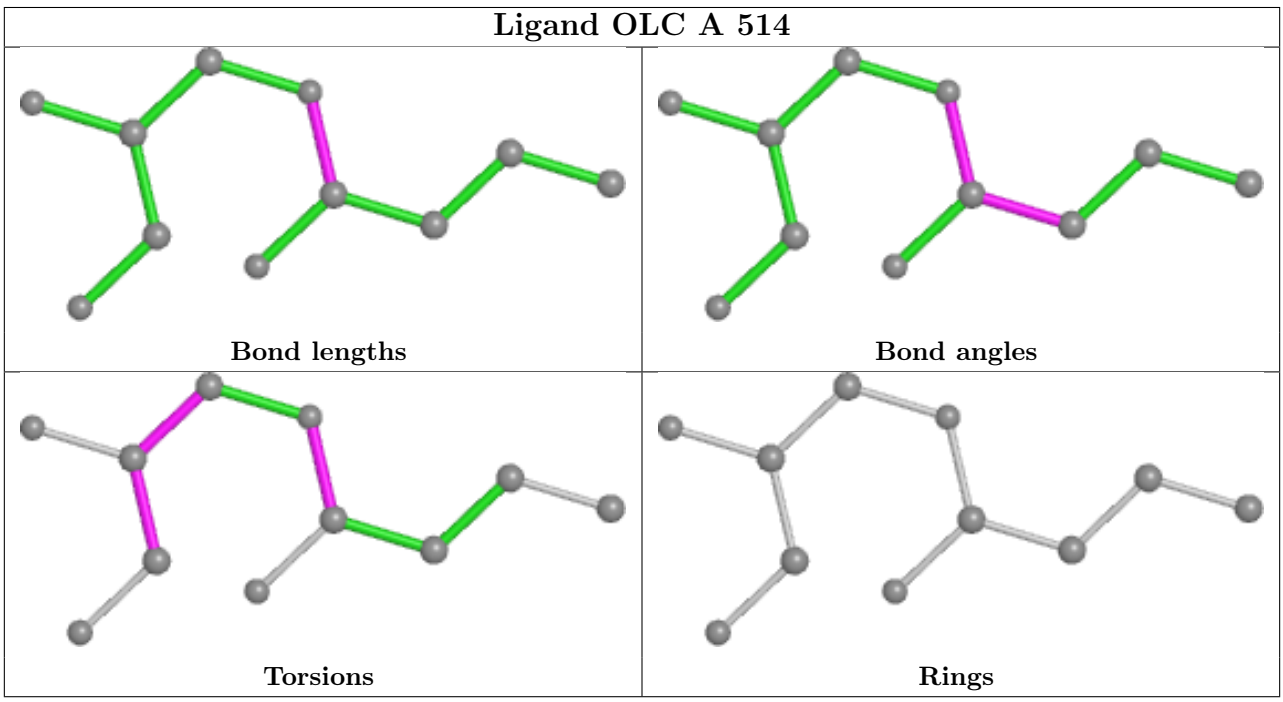

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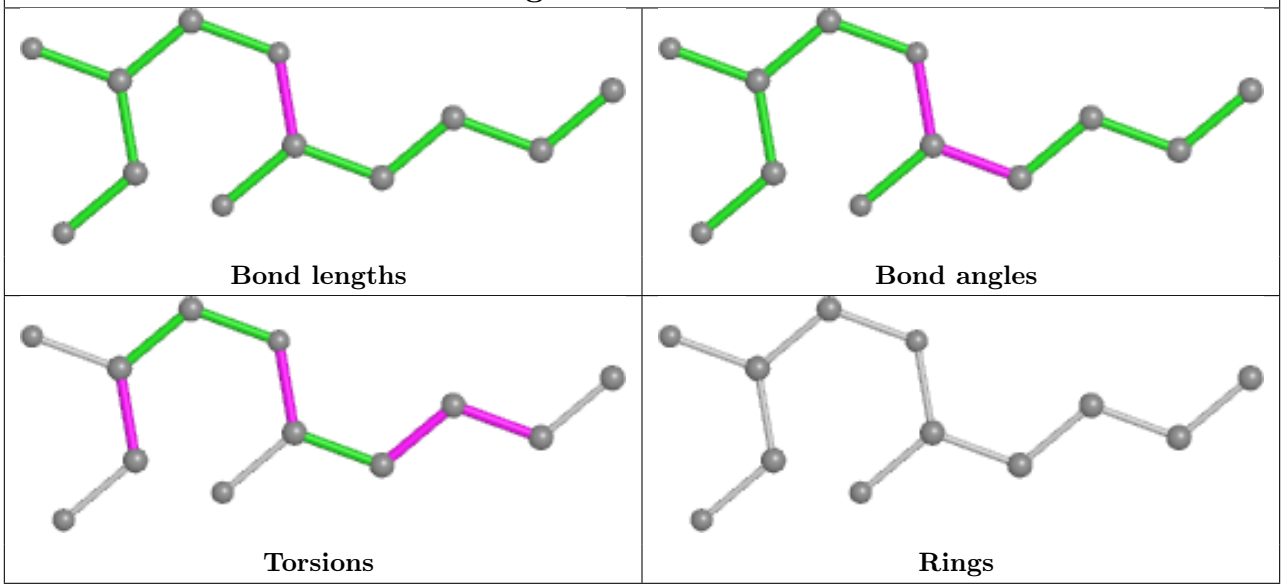

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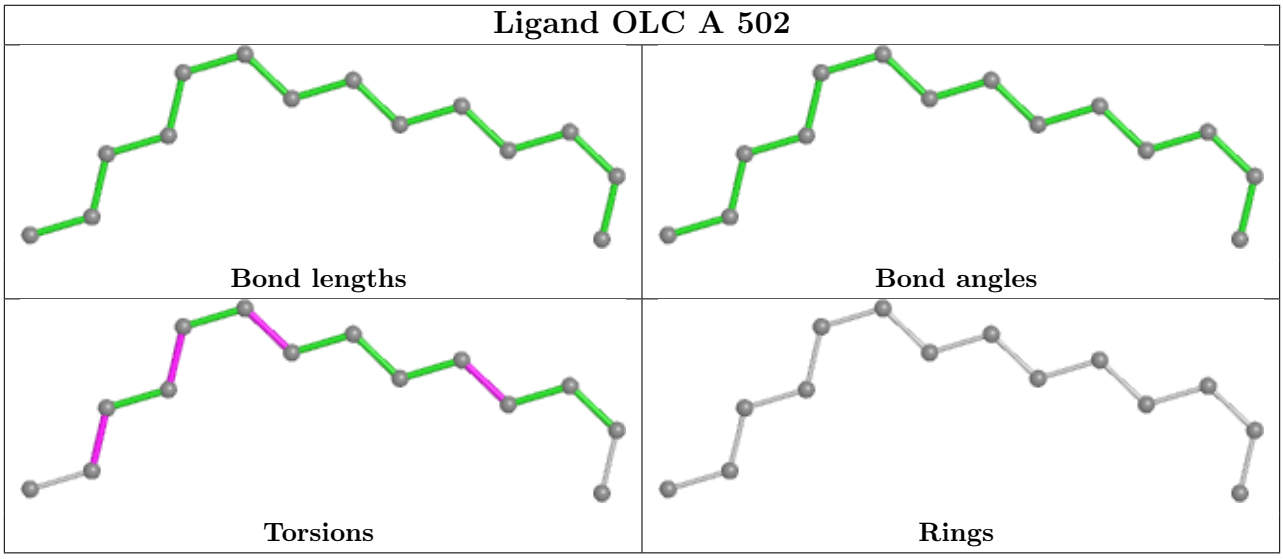

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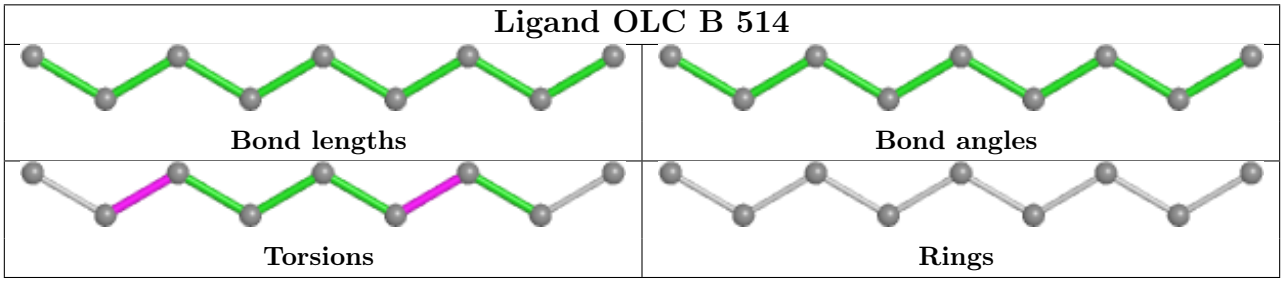

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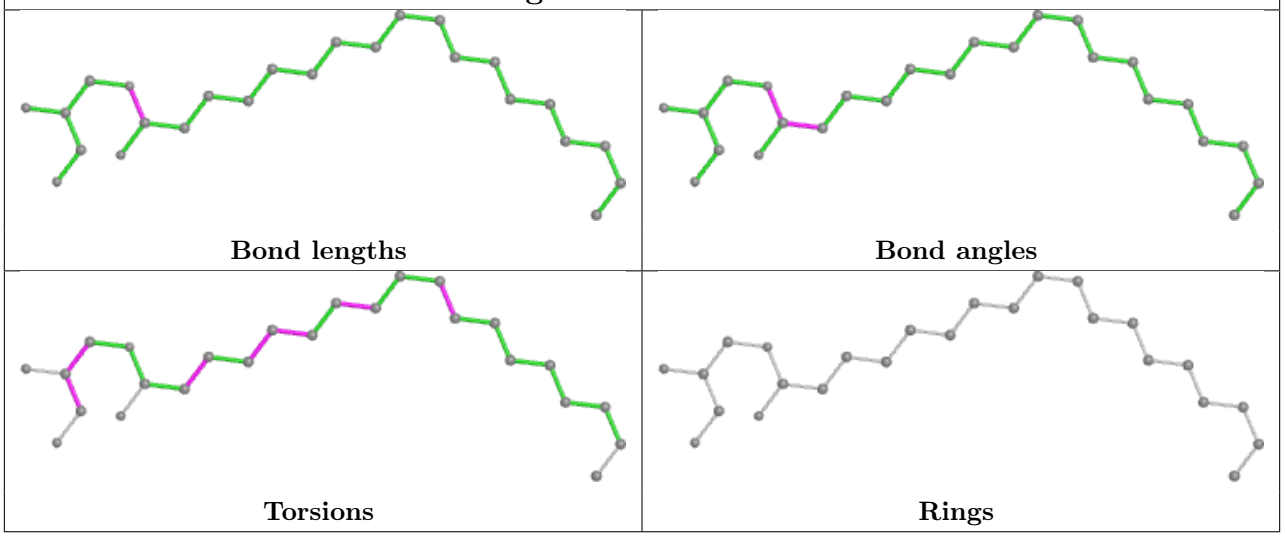
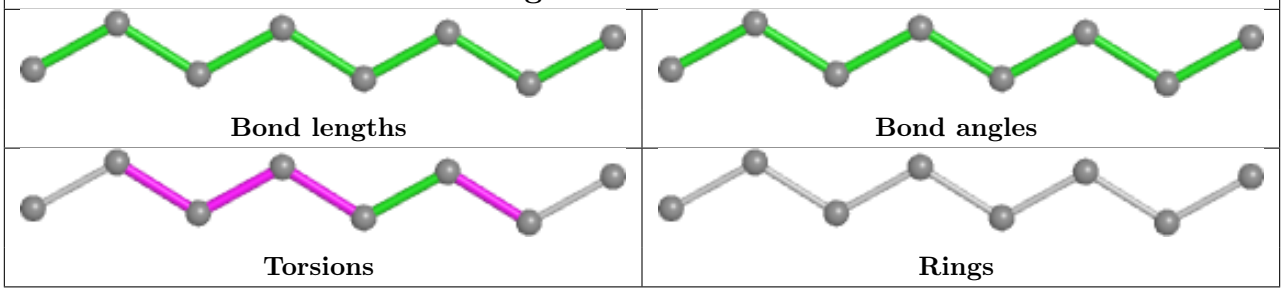
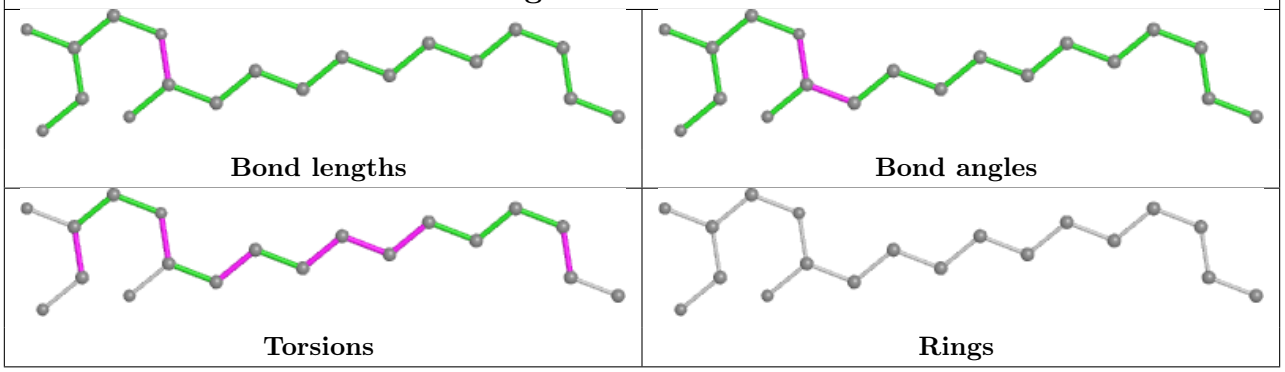


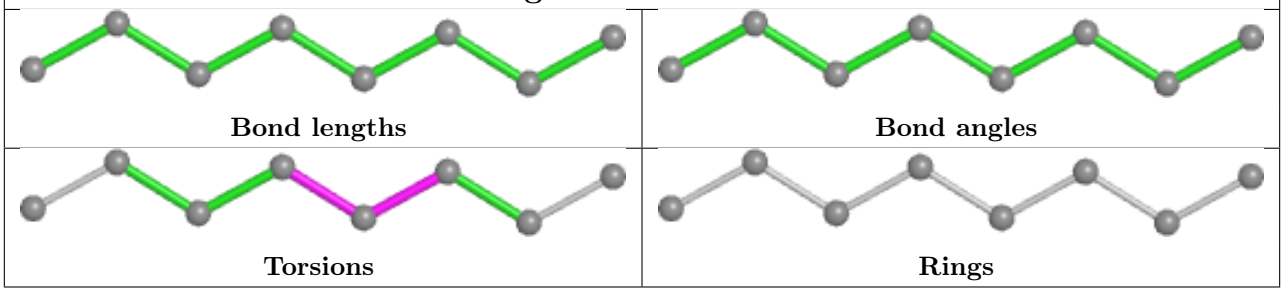
Ligand OLC A 504



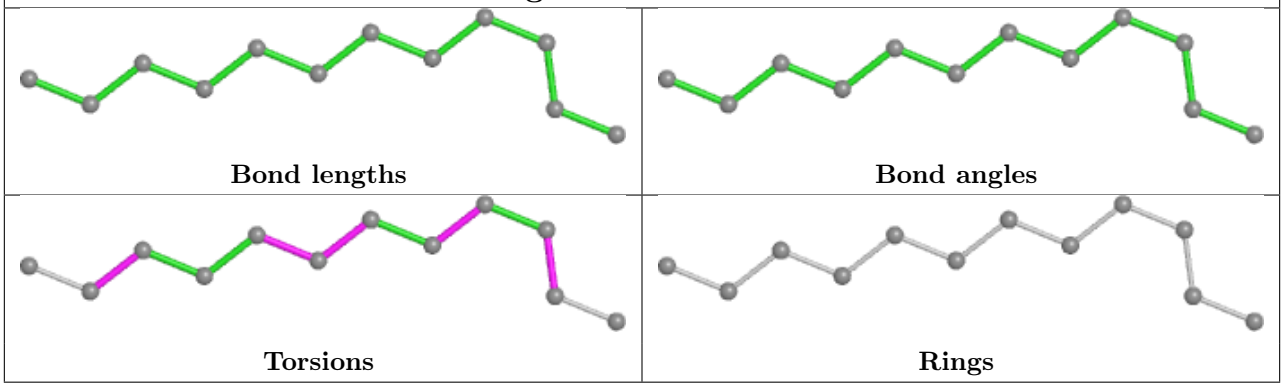
Ligand OLC A 505



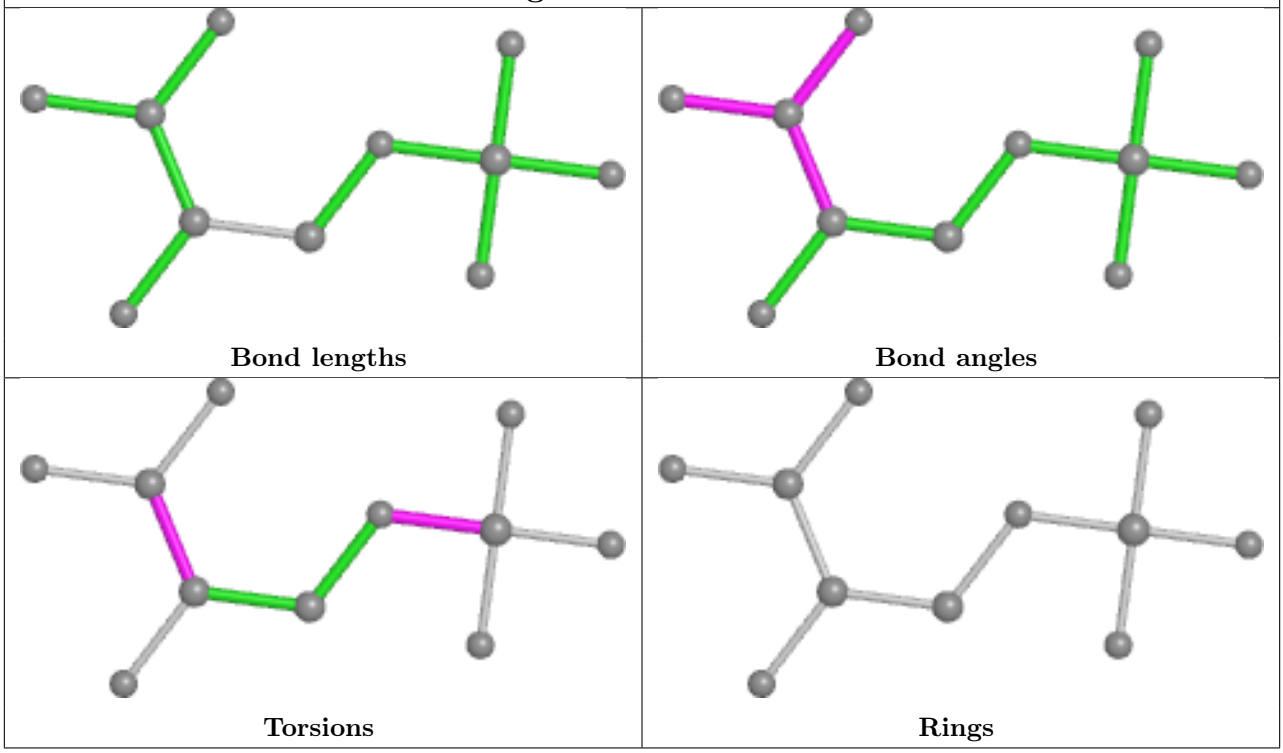
Ligand OLC A 509



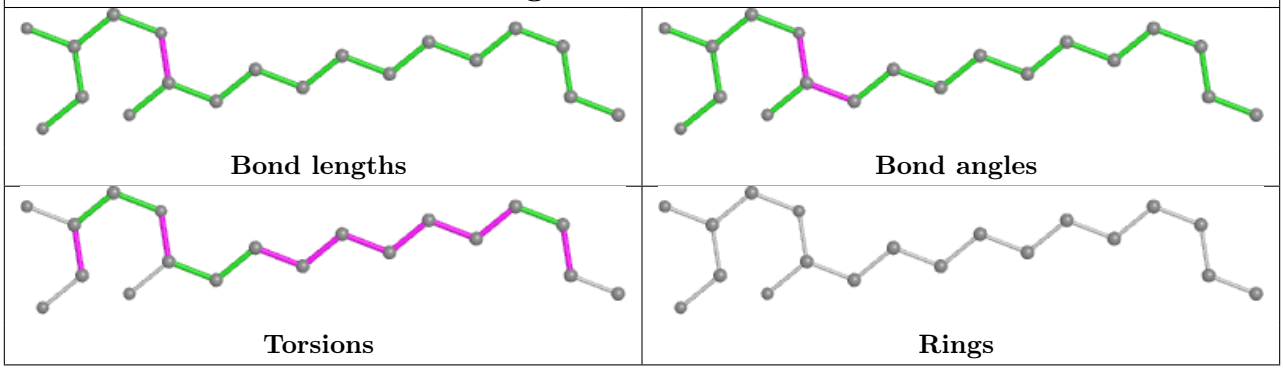
Ligand OLC B 517



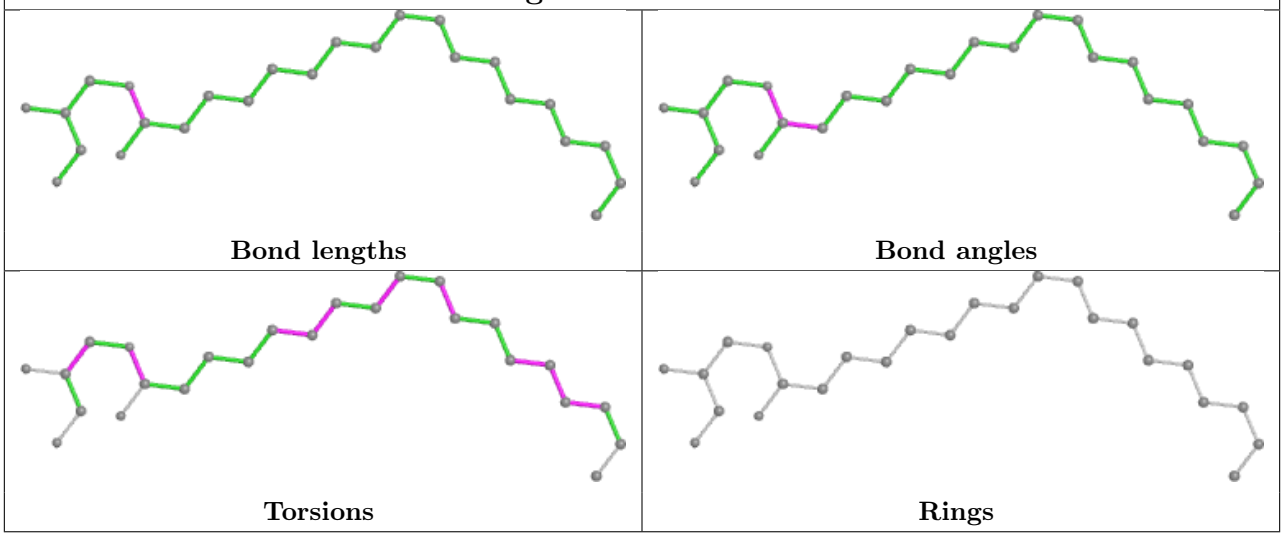
Ligand 3PG A 516



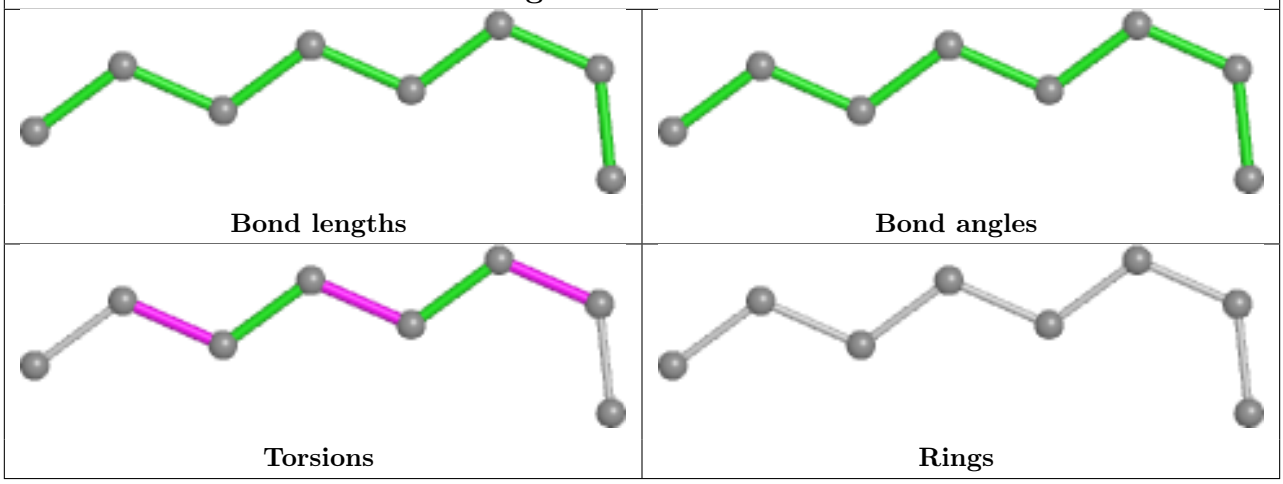
Ligand OLC B 505



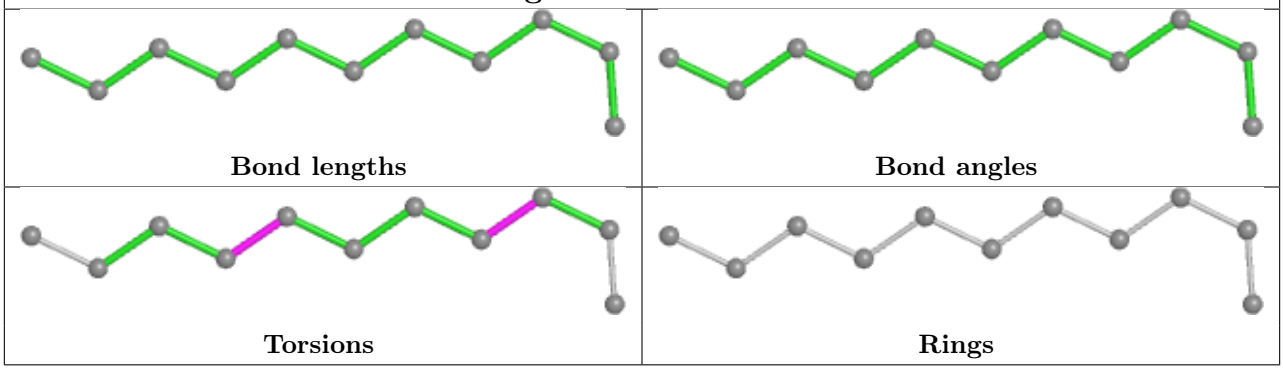
Ligand OLC B 503



Ligand OLC B 511



Ligand OLC A 512



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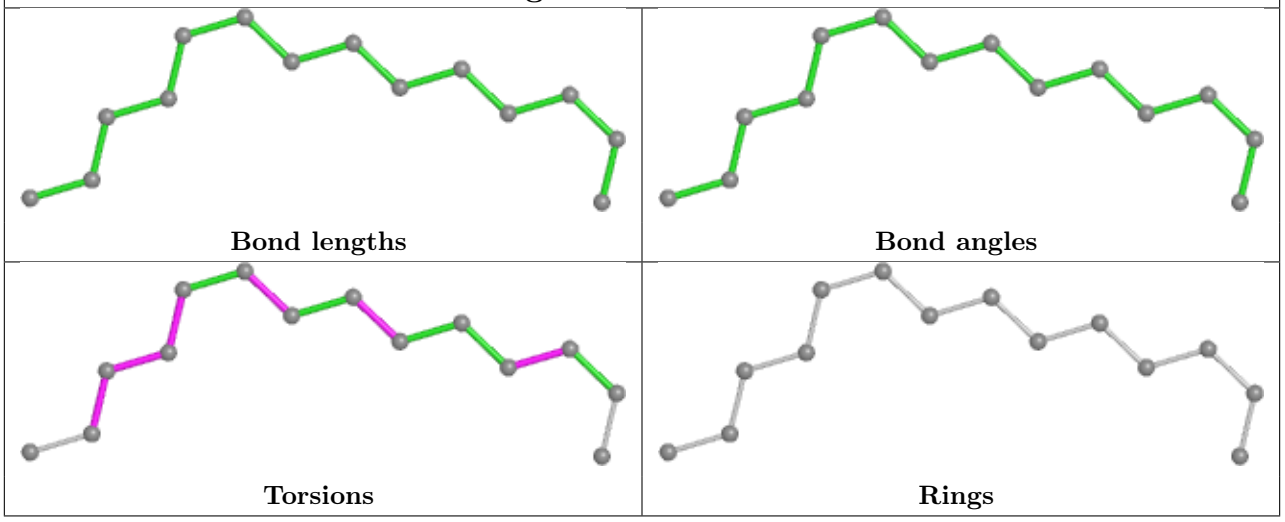

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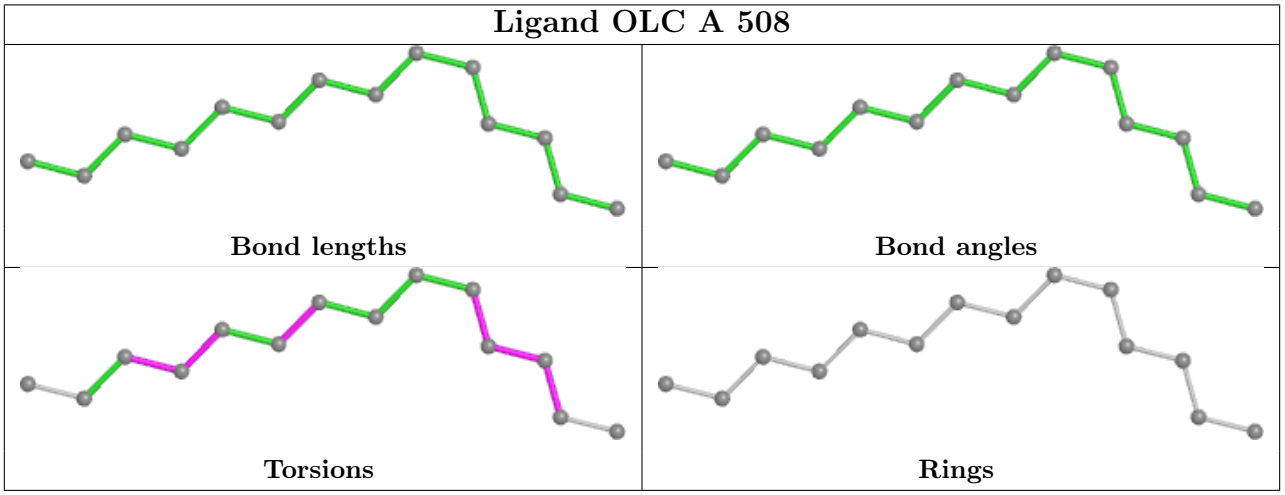

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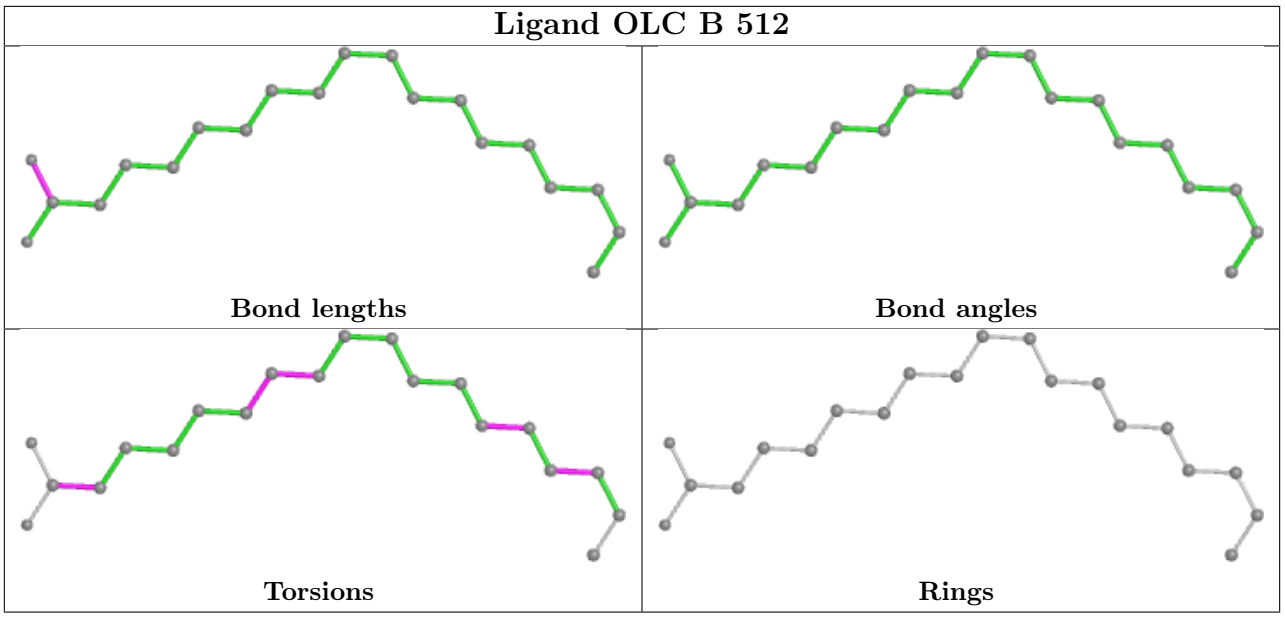

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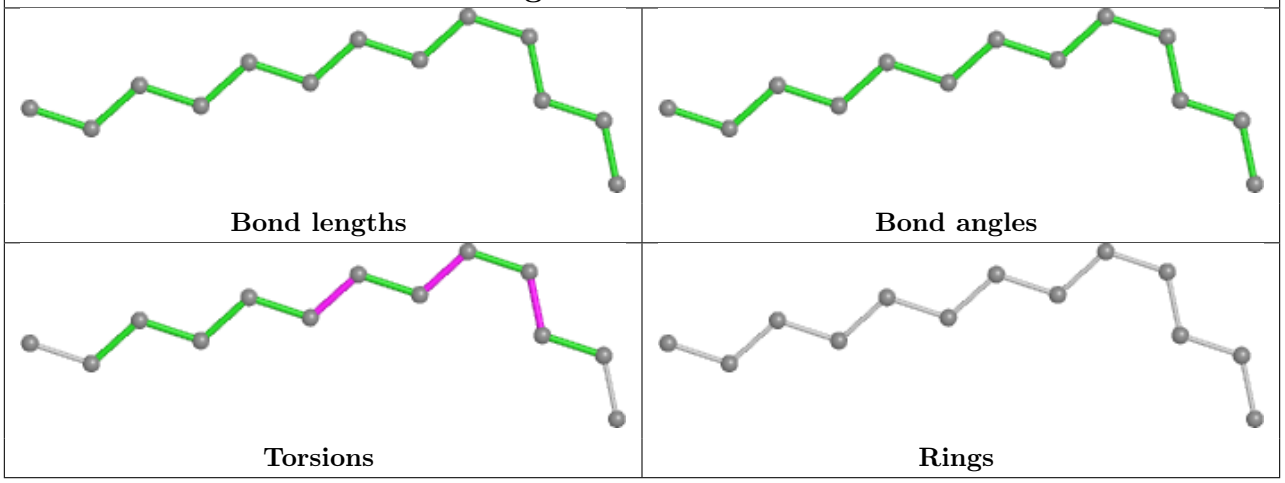

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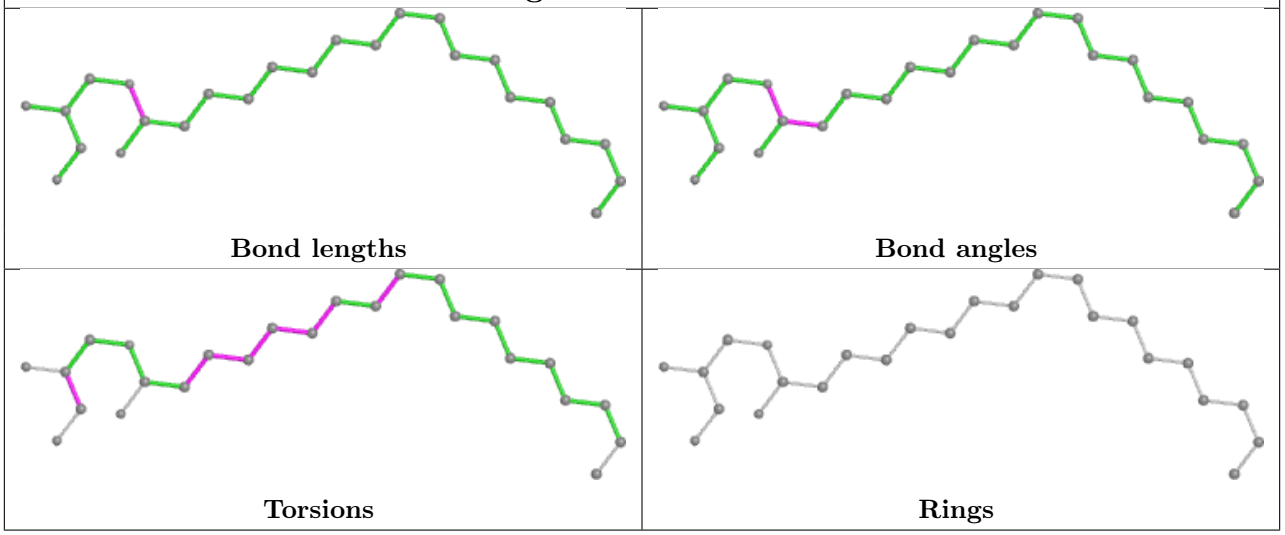
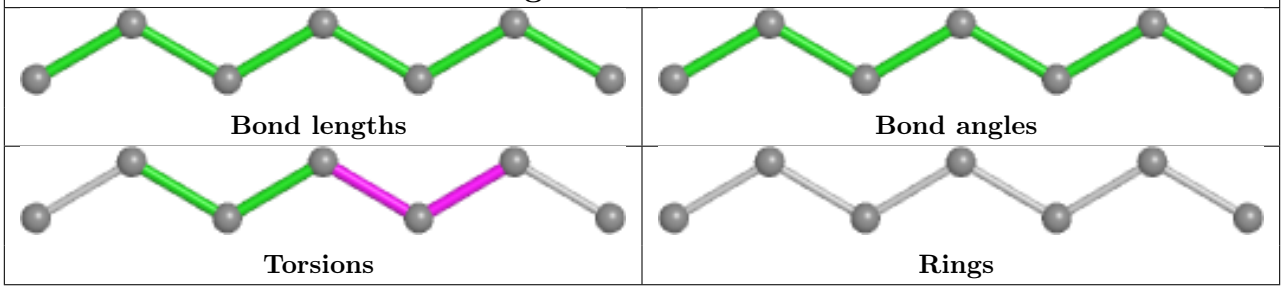
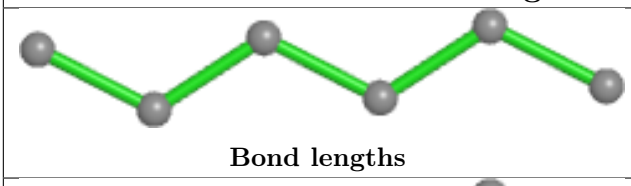


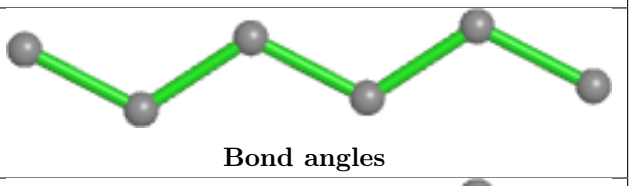
Ligand OLC A 511



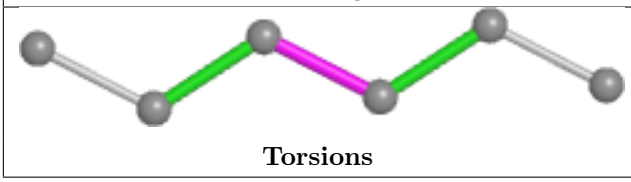
Ligand OLC A 503



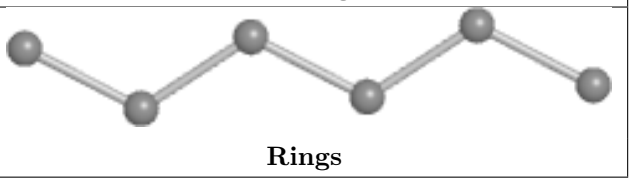
Bond lengths



Bond angles

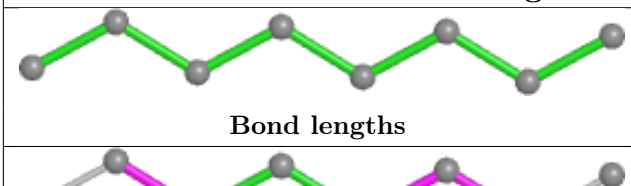


Torsions

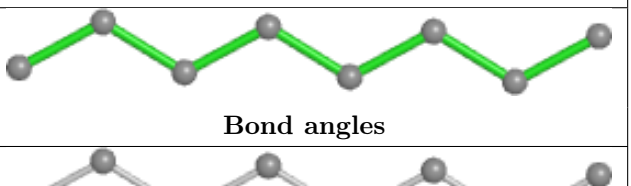


Rings

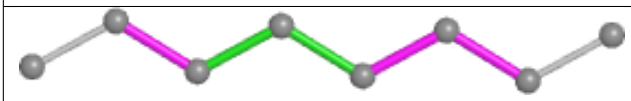
Ligand OLC B 508



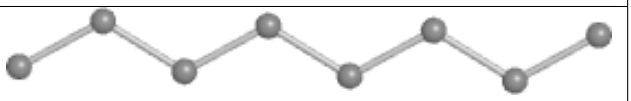
Bond lengths



Bond angles

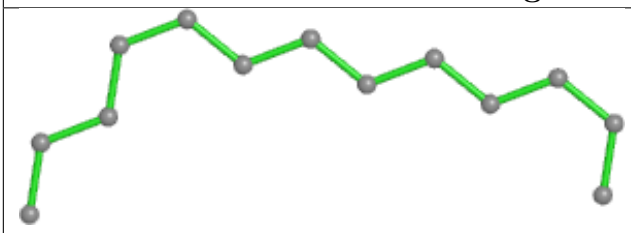


Torsions

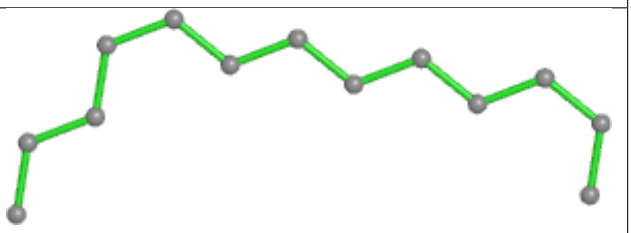


Rings

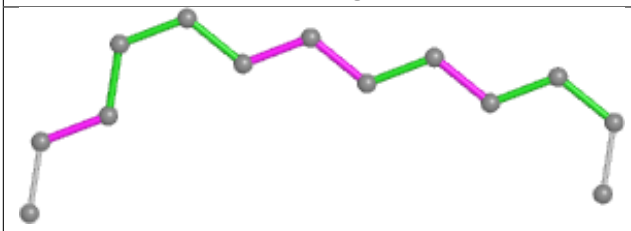
Ligand OLC A 515



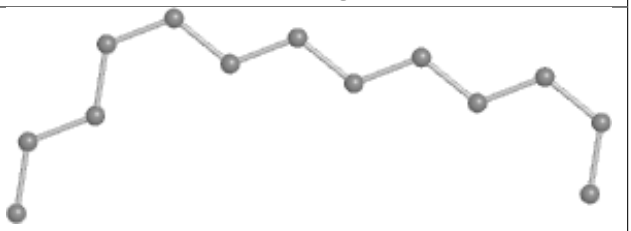
Bond lengths



Bond angles

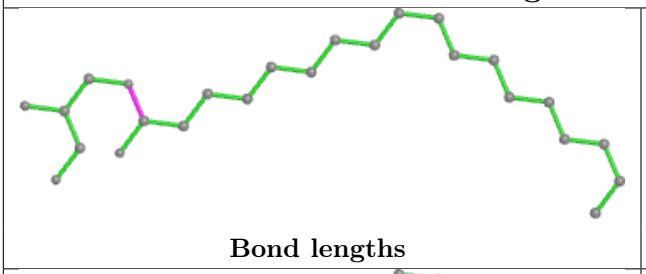


Torsions

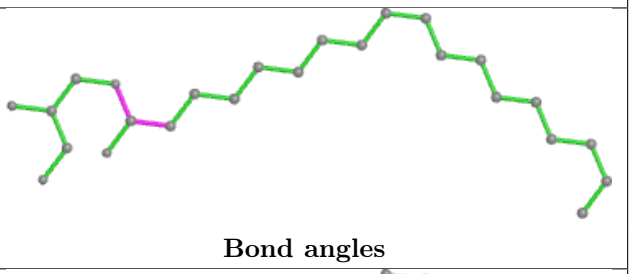


Rings

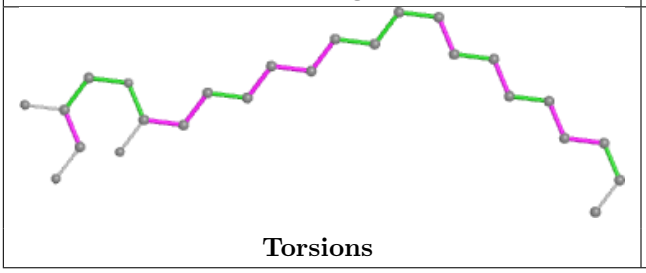
Ligand OLC A 501



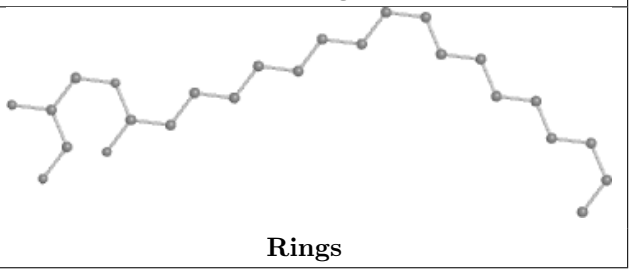
Bond lengths



Bond angles

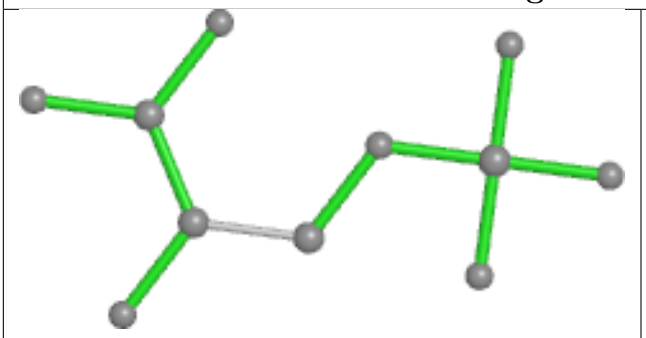


Torsions

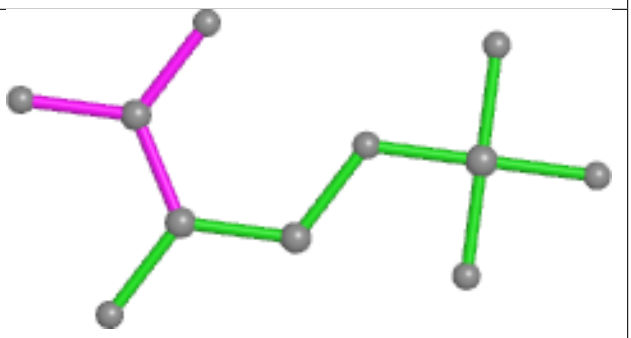


Rings

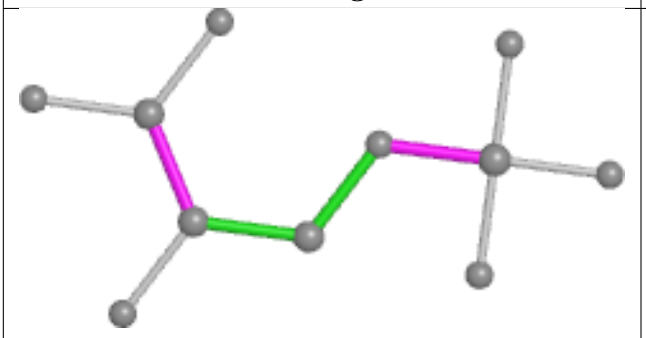
Ligand 3PG B 518



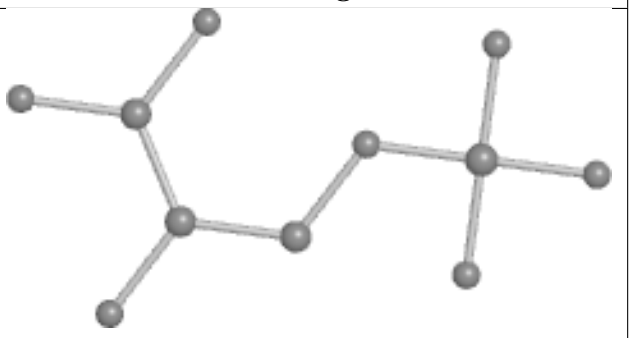
Bond lengths



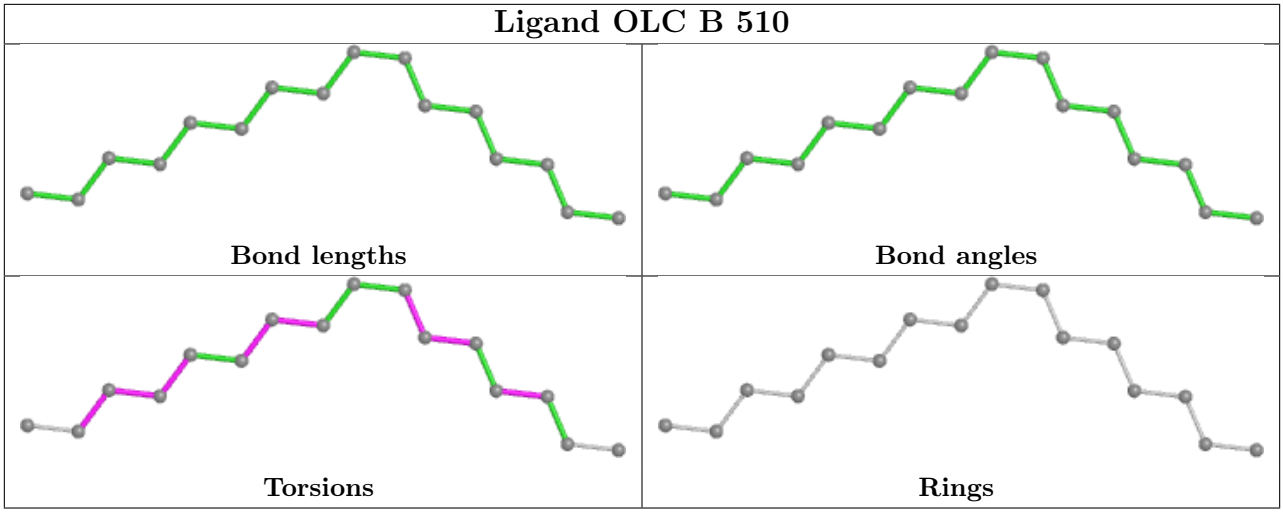
Bond angles



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	305/329 (92%)	-0.22	9 (2%)	50	48	16, 27, 47, 66	0
1	B	305/329 (92%)	-0.35	4 (1%)	77	75	18, 26, 43, 70	0
All	All	610/658 (92%)	-0.28	13 (2%)	63	61	16, 26, 46, 70	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	PRO	4.9
1	A	218	VAL	4.4
1	A	279	ASN	3.8
1	A	100	SER	3.7
1	A	275	VAL	3.5
1	B	404	PRO	3.5
1	B	100	SER	2.7
1	A	220	GLY	2.7
1	B	318	ALA	2.5
1	A	404	PRO	2.5
1	A	219	LEU	2.4
1	A	280	GLU	2.1
1	A	403	LEU	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

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.

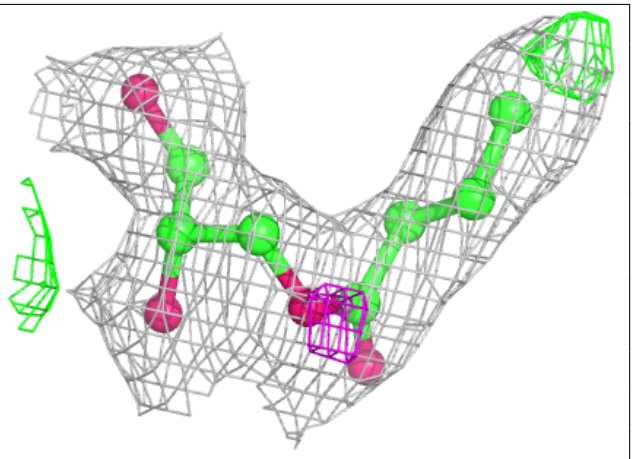
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OLC	A	514	11/25	0.67	0.25	35,49,56,59	0
2	OLC	B	501	25/25	0.71	0.22	27,37,57,62	0
2	OLC	A	507	13/25	0.74	0.22	34,38,43,46	0
2	OLC	A	501	25/25	0.75	0.23	30,38,49,51	0
2	OLC	A	512	11/25	0.76	0.19	37,40,45,46	0
2	OLC	B	504	14/25	0.76	0.19	35,43,48,48	0
2	OLC	B	510	16/25	0.77	0.18	43,48,51,52	0
2	OLC	B	507	13/25	0.78	0.16	31,43,48,51	0
2	OLC	A	508	14/25	0.78	0.20	29,39,46,47	0
2	OLC	B	515	6/25	0.79	0.17	36,42,42,44	0
2	OLC	B	517	12/25	0.79	0.21	38,43,47,48	0
2	OLC	A	511	7/25	0.80	0.20	33,39,42,44	0
2	OLC	A	502	14/25	0.80	0.19	36,44,47,49	0
2	OLC	A	506	12/25	0.80	0.17	38,42,51,51	0
2	OLC	B	512	20/25	0.81	0.19	23,42,51,52	0
2	OLC	B	514	9/25	0.81	0.17	31,38,42,44	0
2	OLC	A	513	8/25	0.82	0.21	32,43,49,51	0
2	OLC	B	503	25/25	0.82	0.19	34,41,47,58	0
2	OLC	A	515	13/25	0.82	0.21	36,42,47,47	0
2	OLC	B	513	17/25	0.83	0.20	33,38,45,45	0
2	OLC	B	511	8/25	0.86	0.22	29,37,42,43	0
2	OLC	B	502	25/25	0.86	0.17	28,40,48,55	0
2	OLC	B	506	8/25	0.88	0.24	30,39,46,47	0
2	OLC	A	510	12/25	0.88	0.13	35,41,46,49	0
2	OLC	B	516	12/25	0.88	0.16	52,54,61,63	0
2	OLC	B	505	19/25	0.88	0.17	29,32,42,48	0
4	FLC	A	517	13/13	0.88	0.36	35,42,50,54	0
2	OLC	A	504	8/25	0.89	0.13	33,36,39,43	0
2	OLC	B	508	8/25	0.89	0.10	41,43,45,52	0
2	OLC	B	509	8/25	0.89	0.15	34,38,42,42	0
2	OLC	A	505	19/25	0.91	0.16	26,32,42,47	0
2	OLC	A	503	6/25	0.92	0.10	30,36,40,49	0
2	OLC	A	509	8/25	0.93	0.11	32,36,41,43	0
3	3PG	B	518	11/11	0.97	0.11	19,21,27,28	0
3	3PG	A	516	11/11	0.98	0.10	19,22,27,27	0

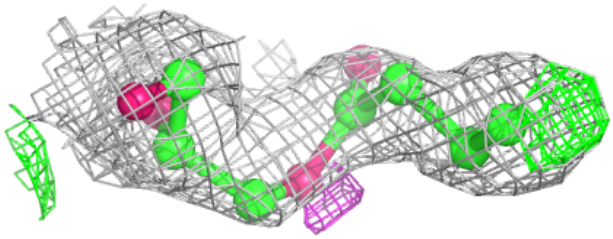
The following is a graphical depiction of the model fit to experimental electron density of all

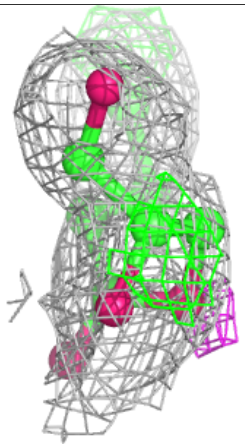
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OLC A 514:

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

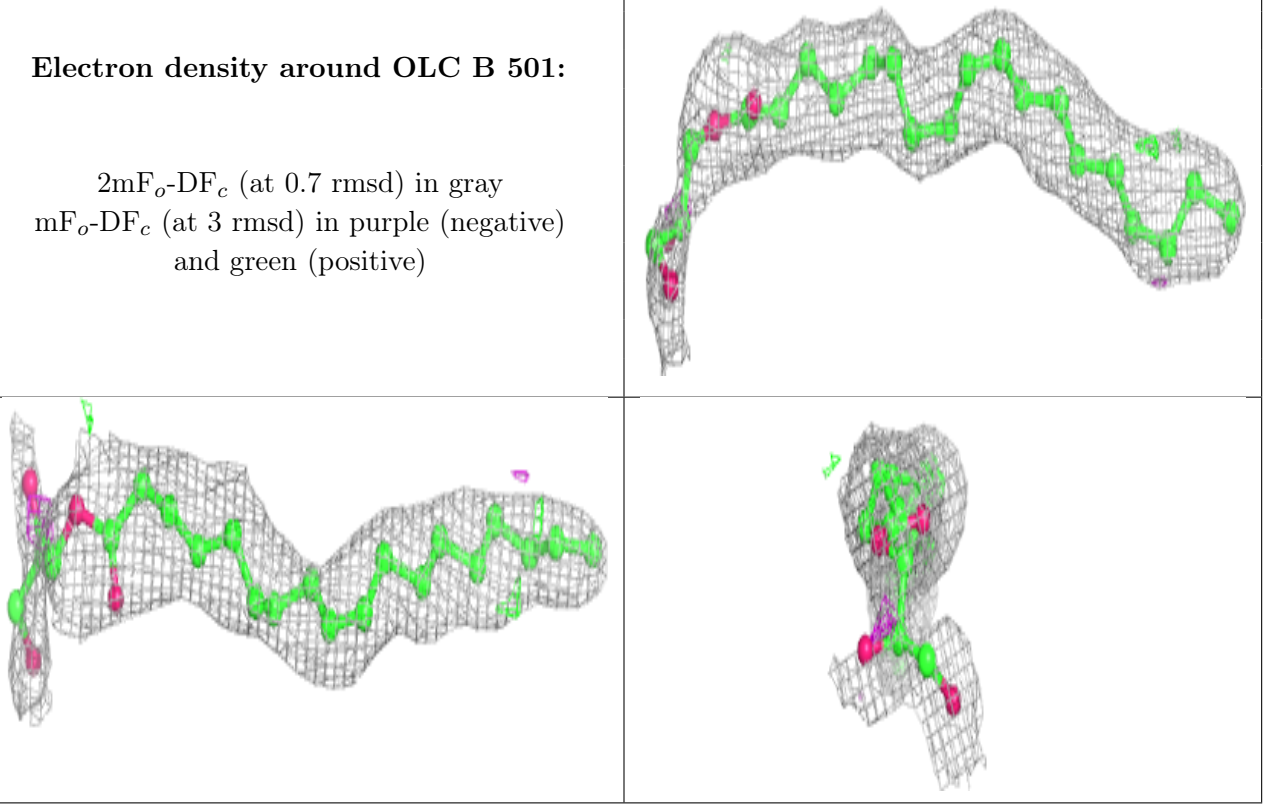






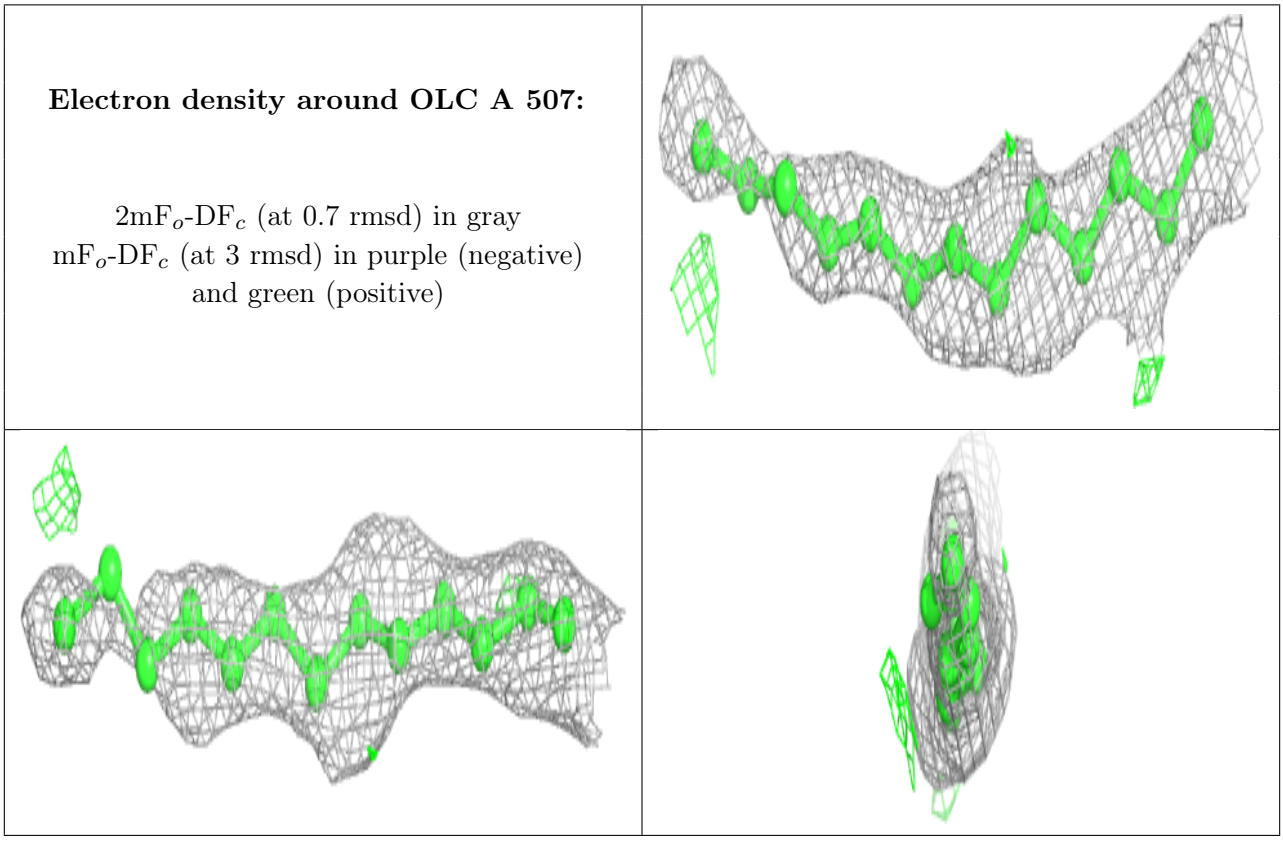
Electron density around OLC B 501:

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



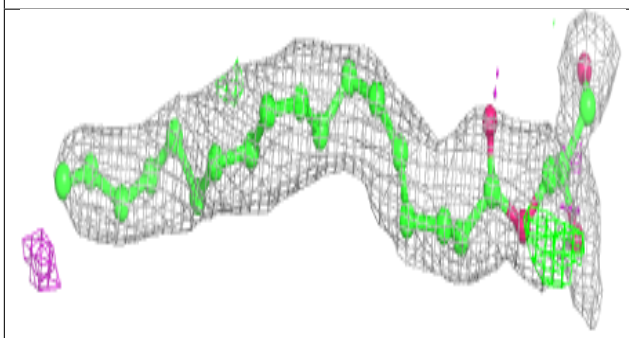
Electron density around OLC A 507:

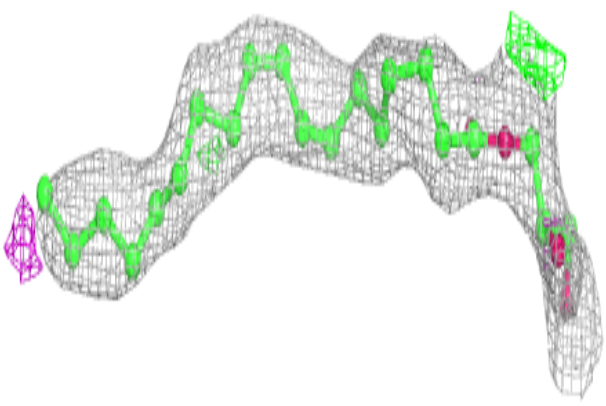
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

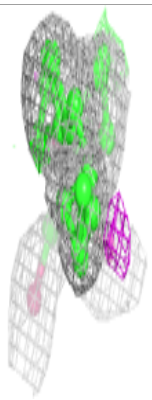


Electron density around OLC A 501:

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

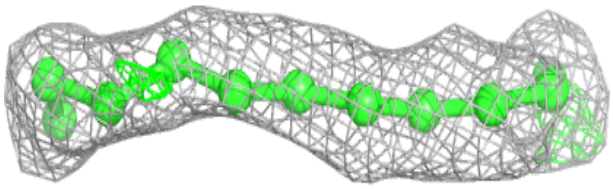


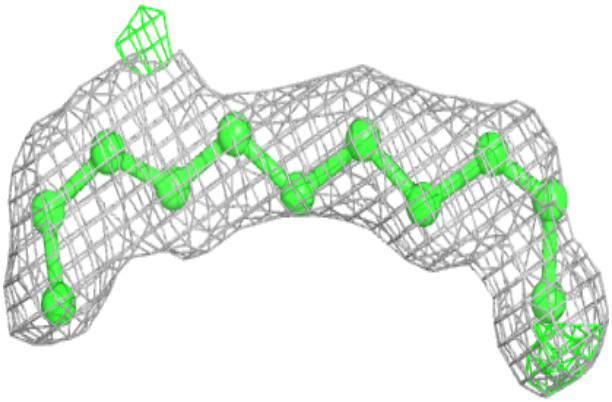


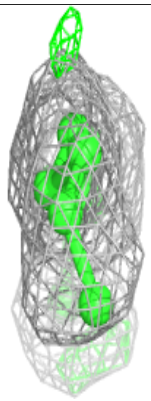


Electron density around OLC A 512:

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

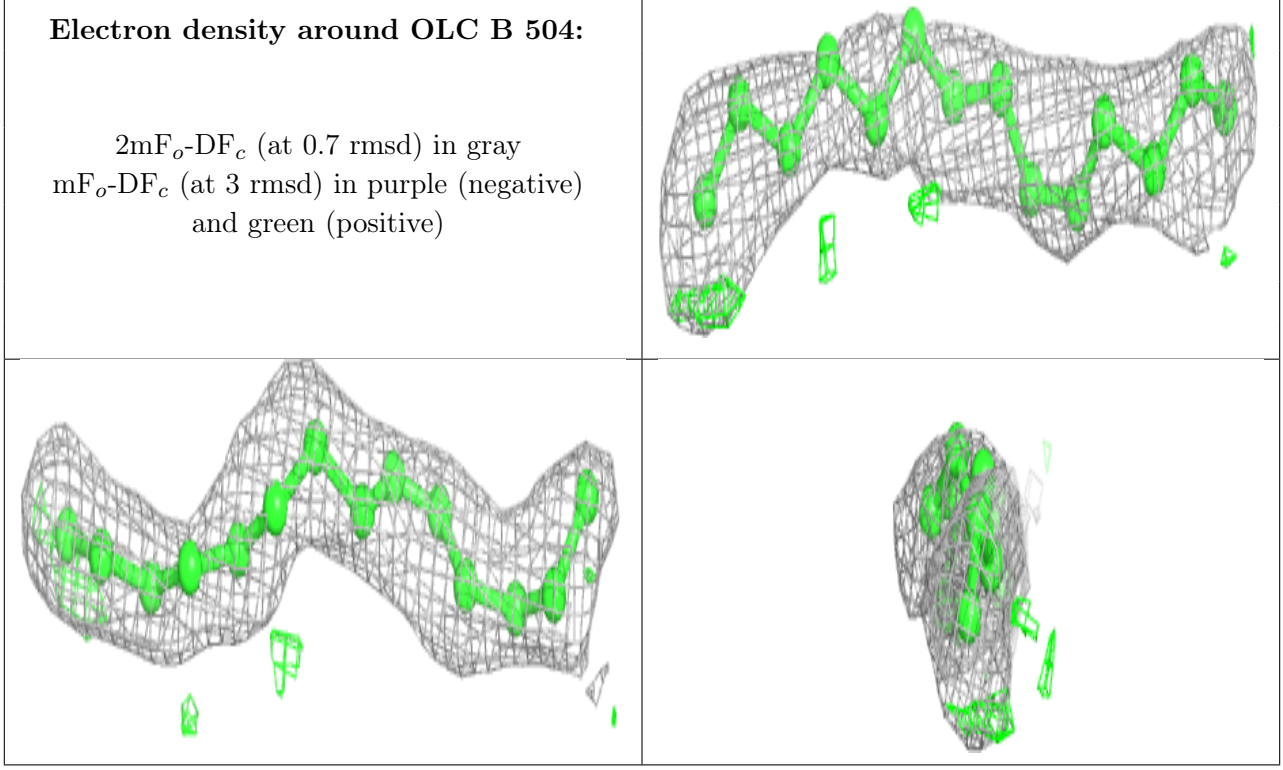






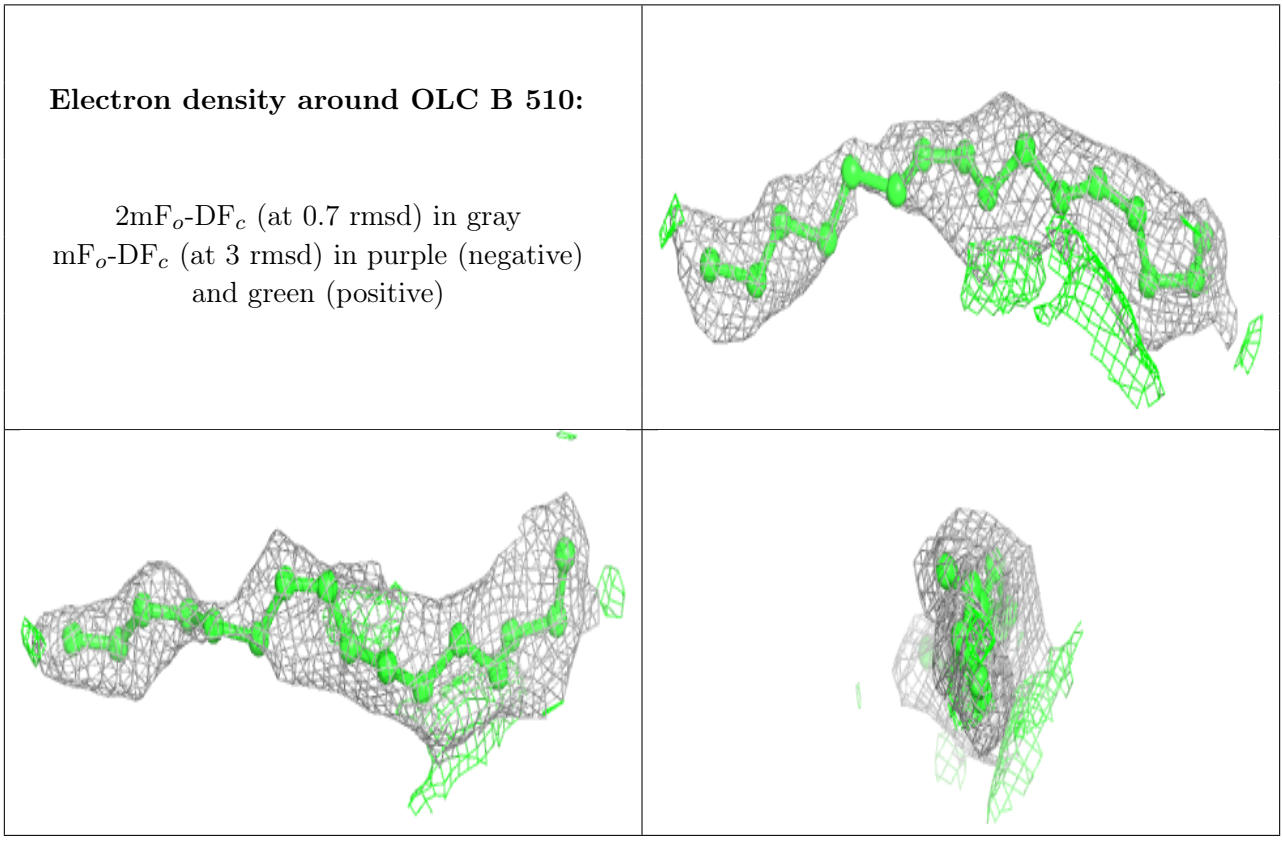
Electron density around OLC B 504:

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



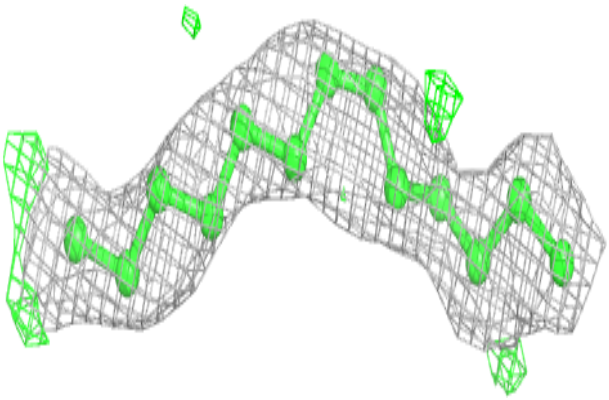
Electron density around OLC B 510:

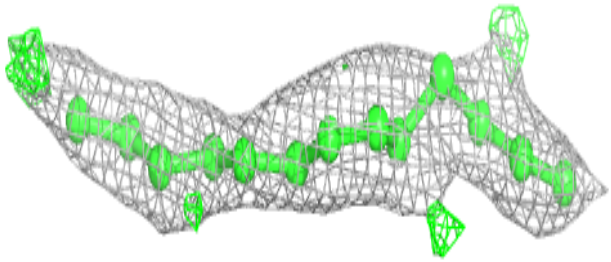
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

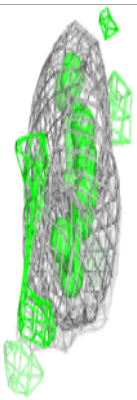


Electron density around OLC B 507:

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

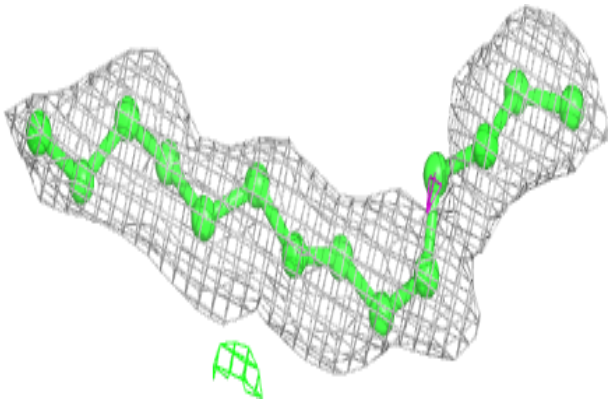


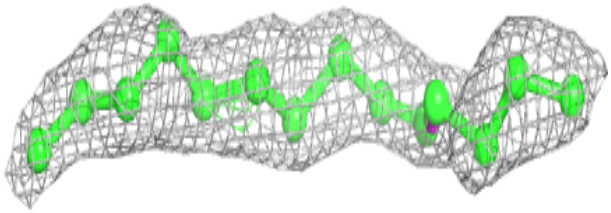


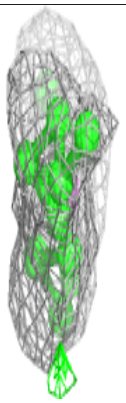


Electron density around OLC A 508:

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

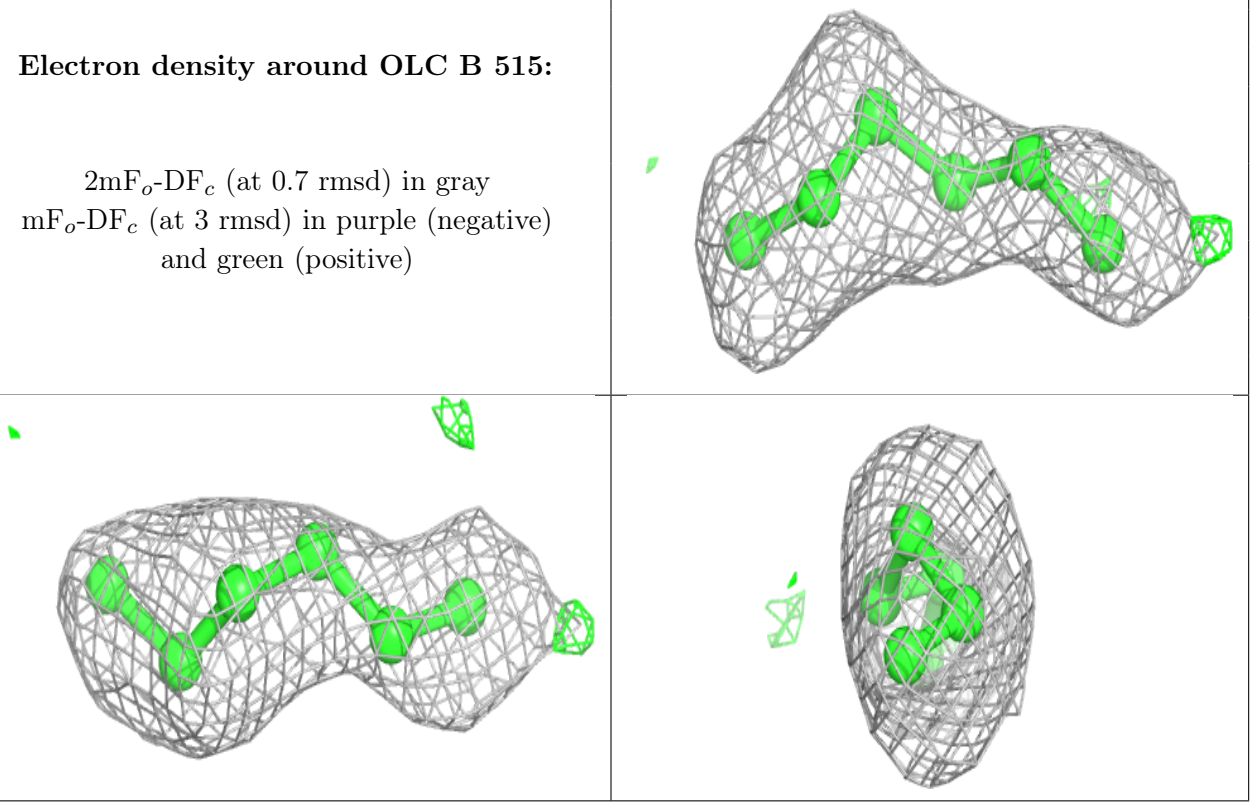






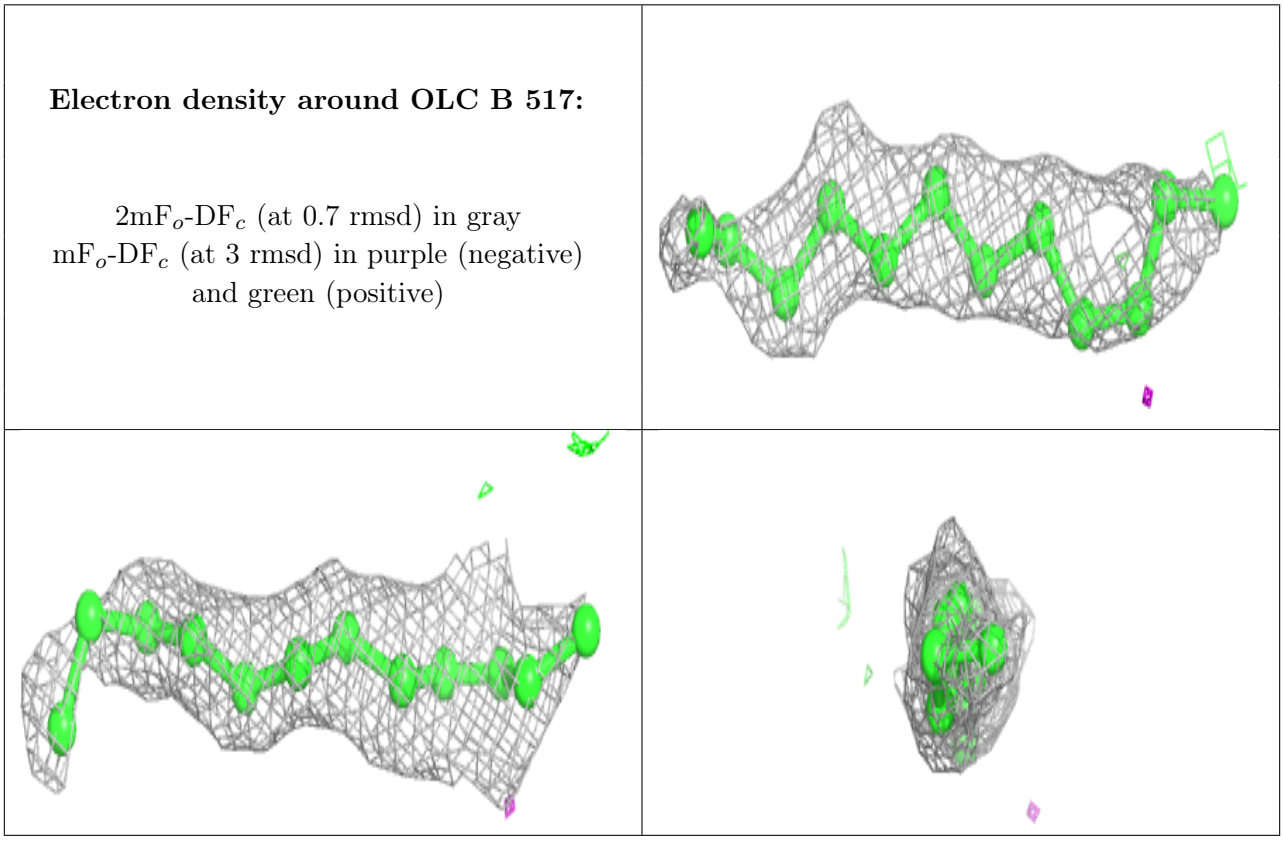
Electron density around OLC B 515:

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



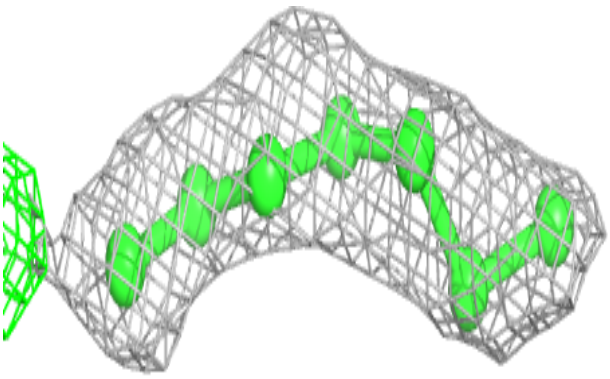
Electron density around OLC B 517:

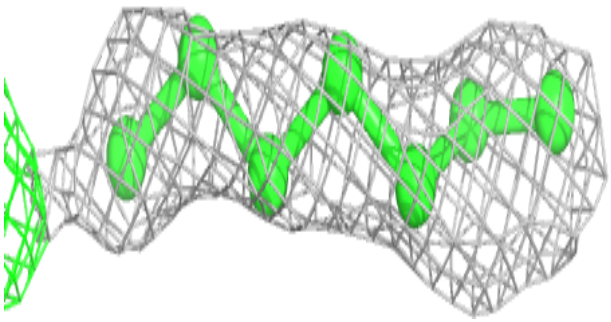
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

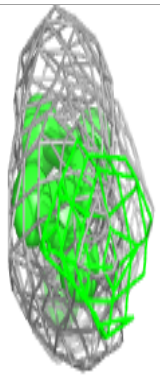


Electron density around OLC A 511:

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

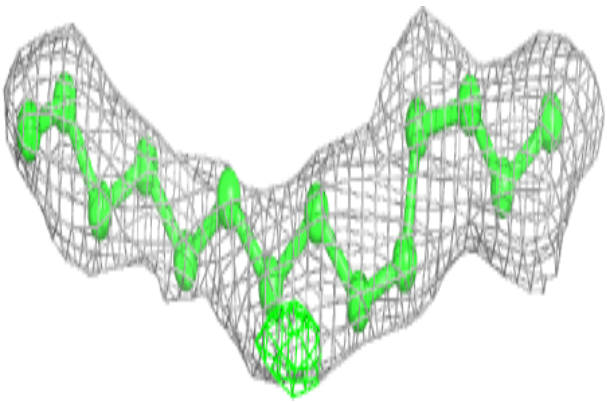


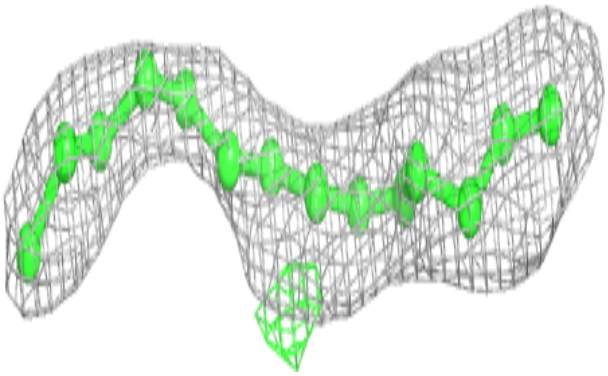


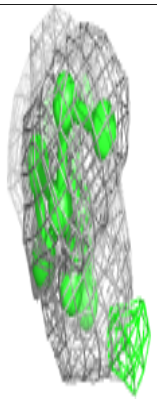


Electron density around OLC A 502:

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

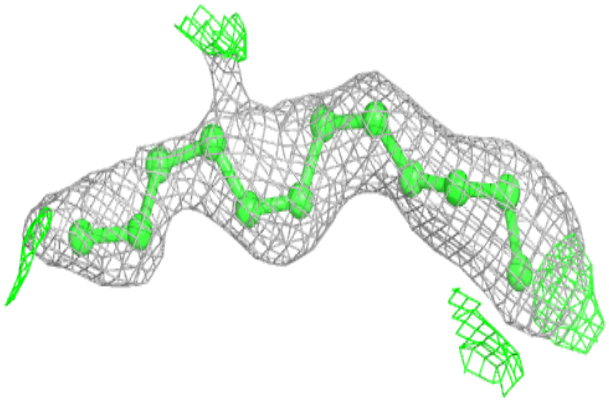


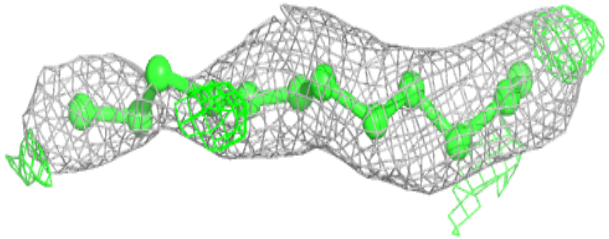


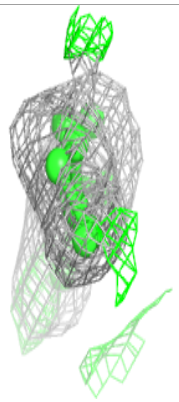


Electron density around OLC A 506:

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

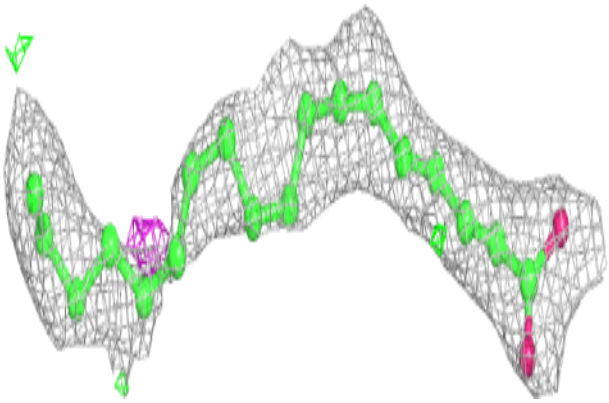


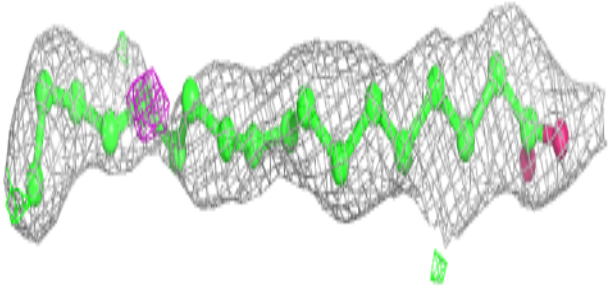


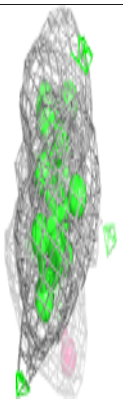


Electron density around OLC B 512:

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

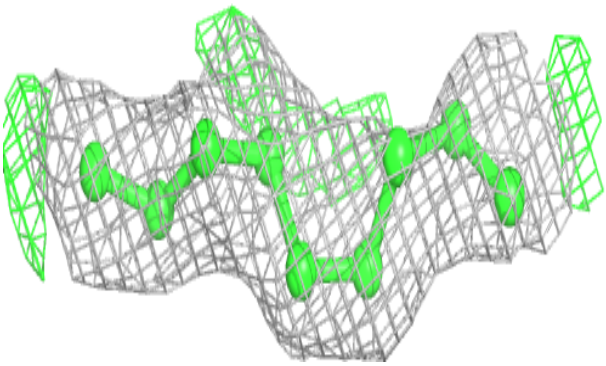


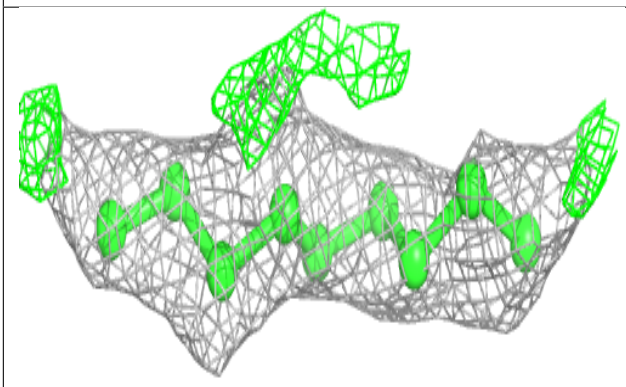


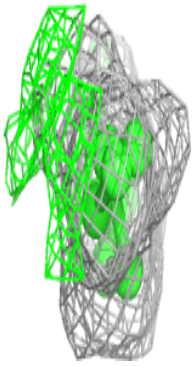


Electron density around OLC B 514:

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

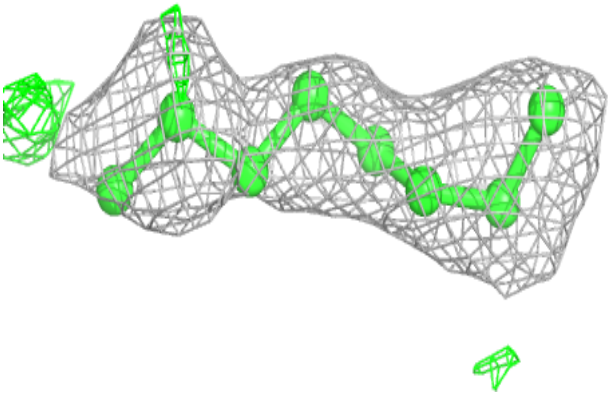


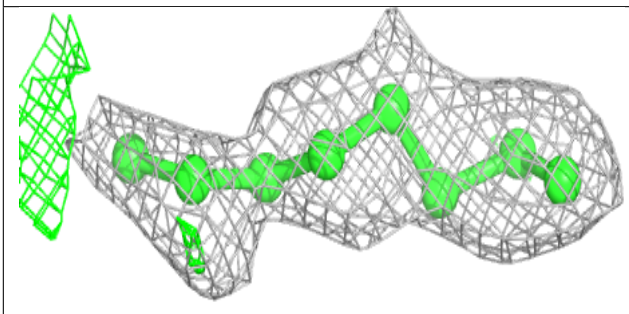


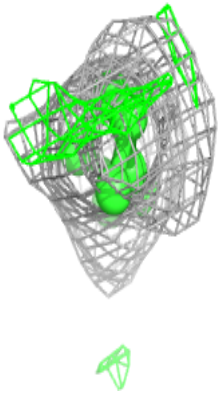


Electron density around OLC A 513:

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

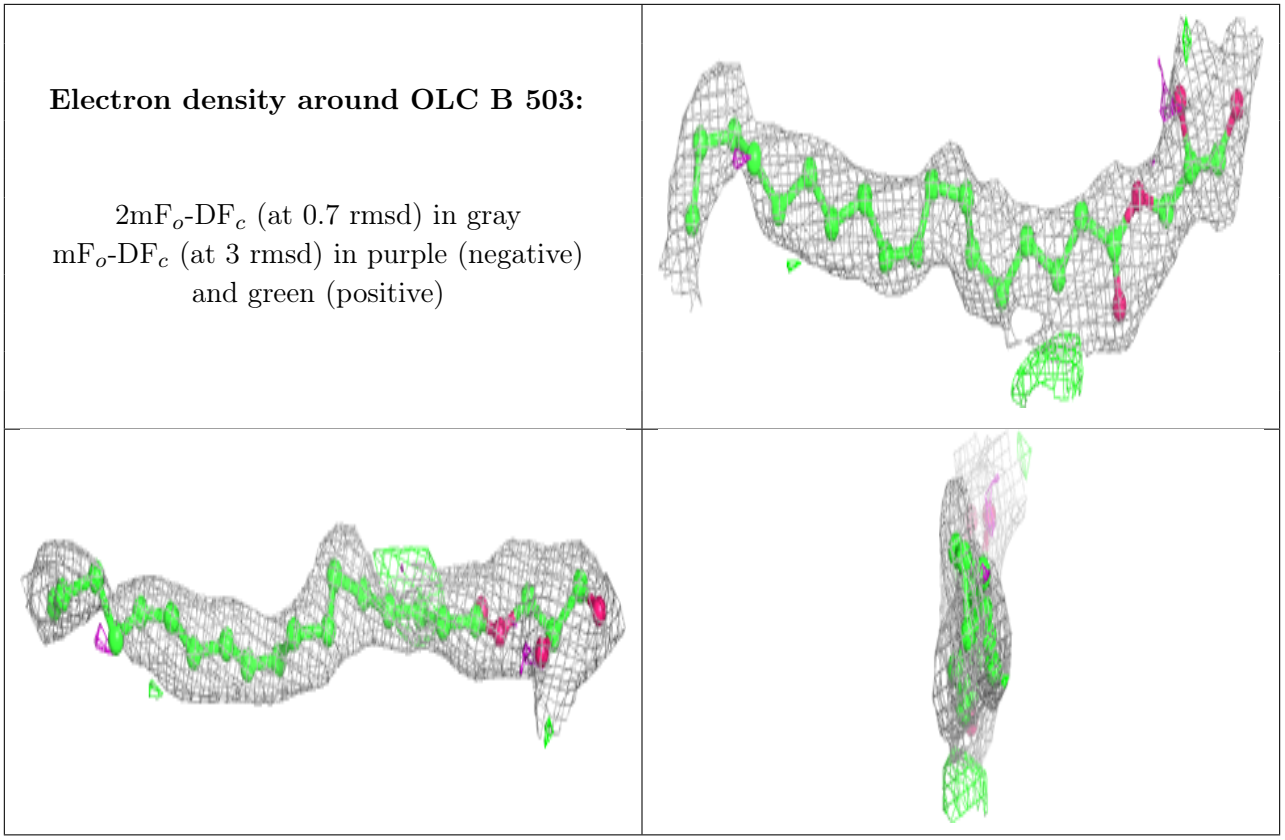






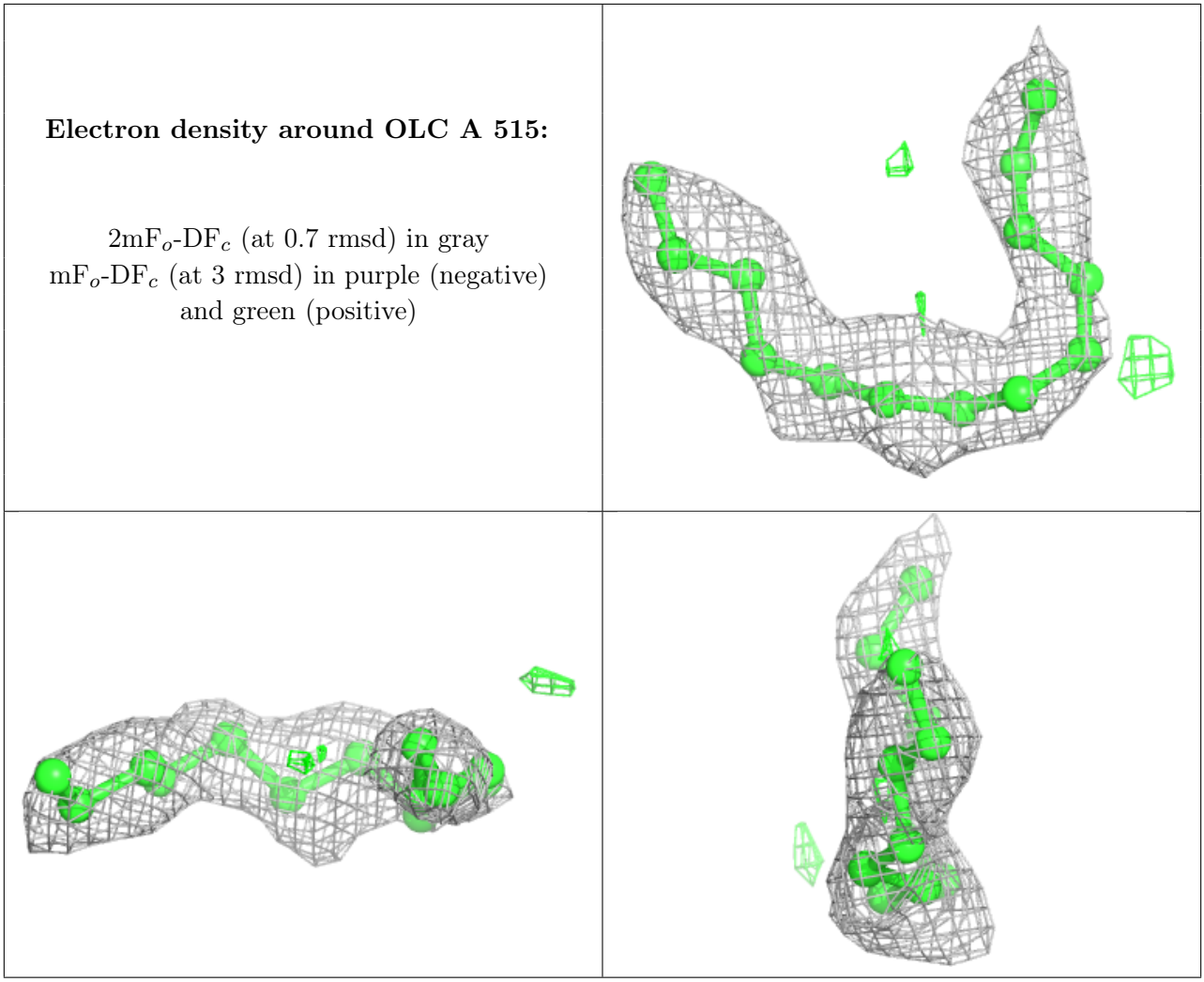
Electron density around OLC B 503:

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



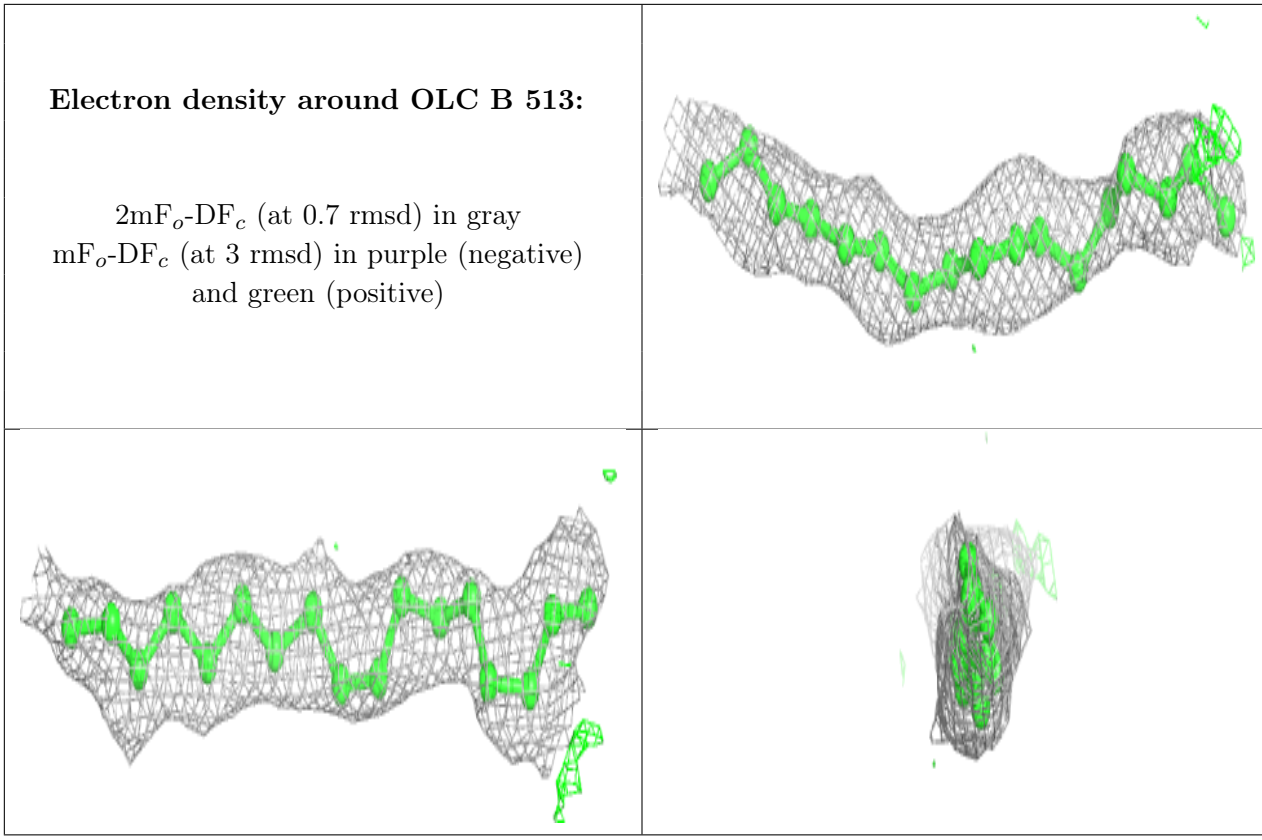
Electron density around OLC A 515:

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



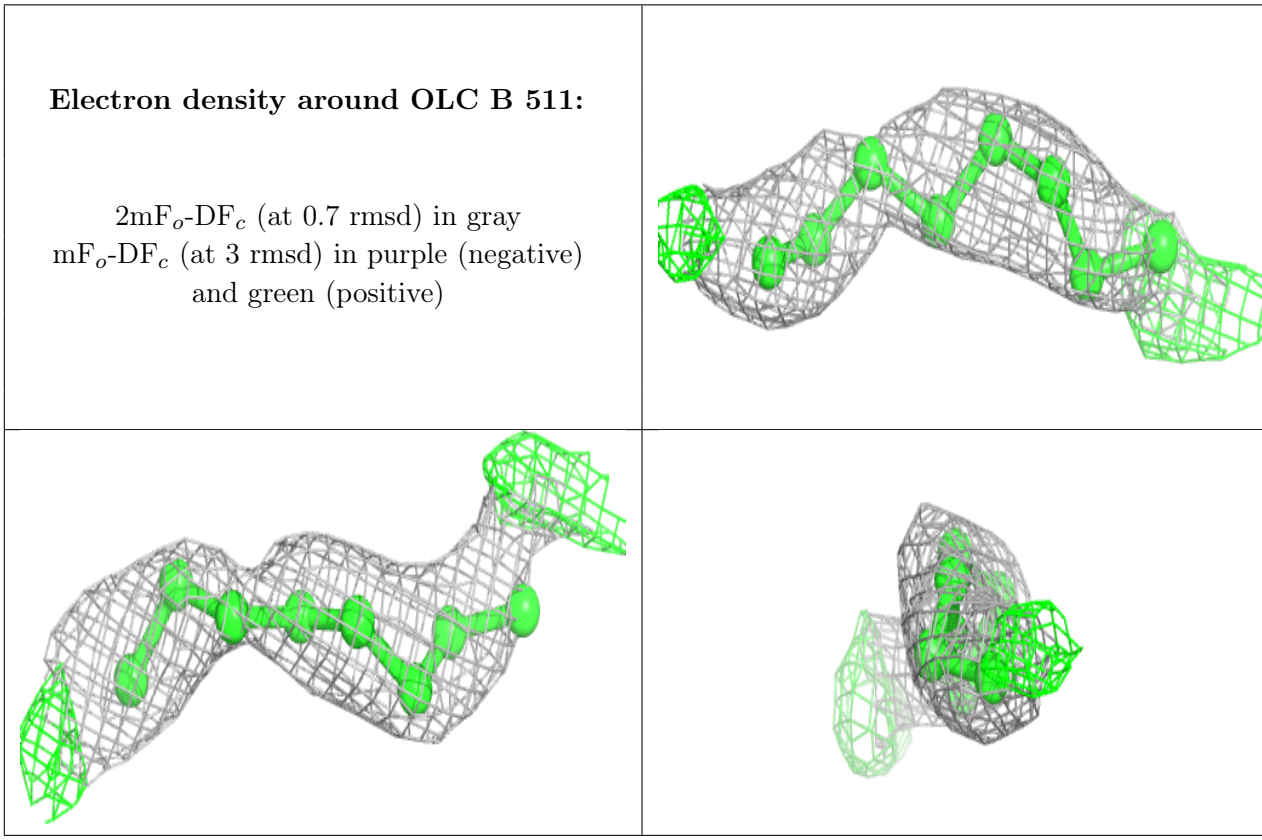
Electron density around OLC B 513:

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



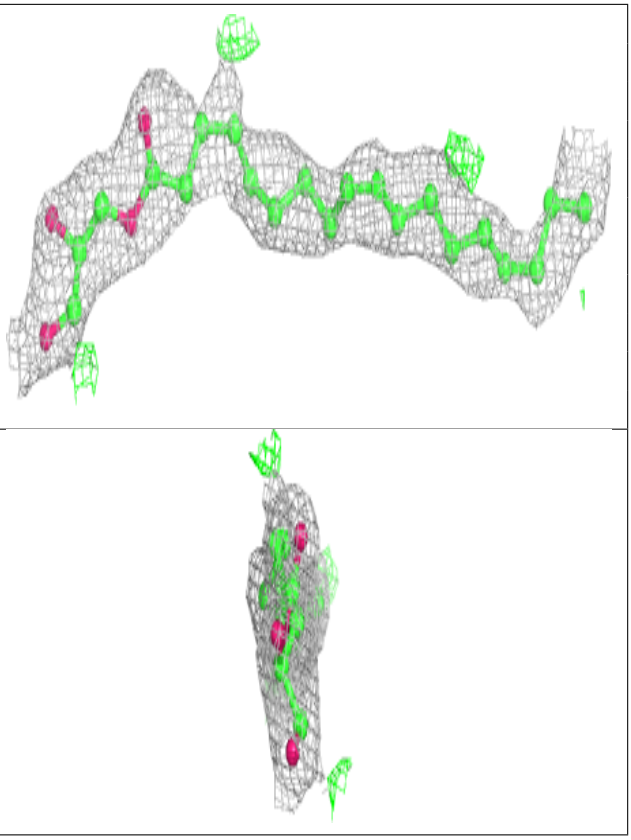
Electron density around OLC B 511:

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



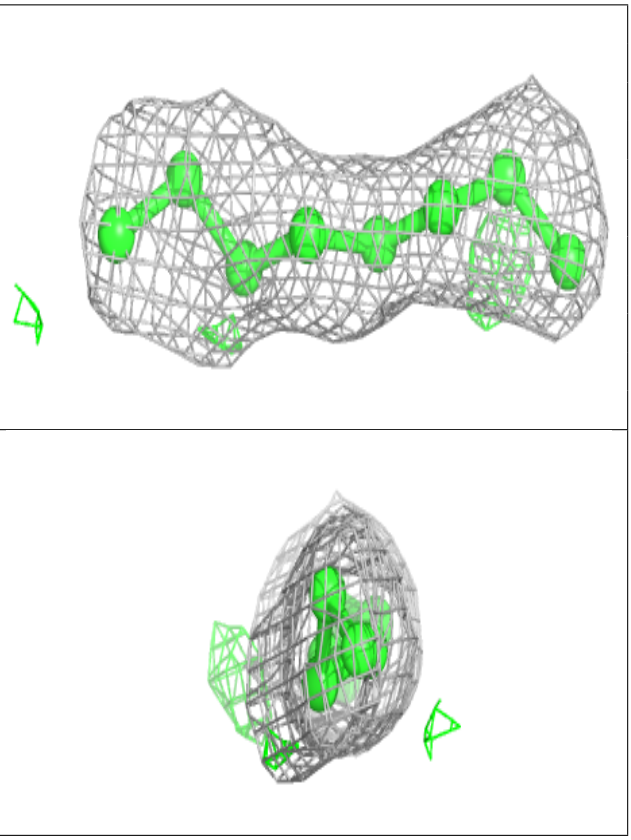
Electron density around OLC B 502:

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



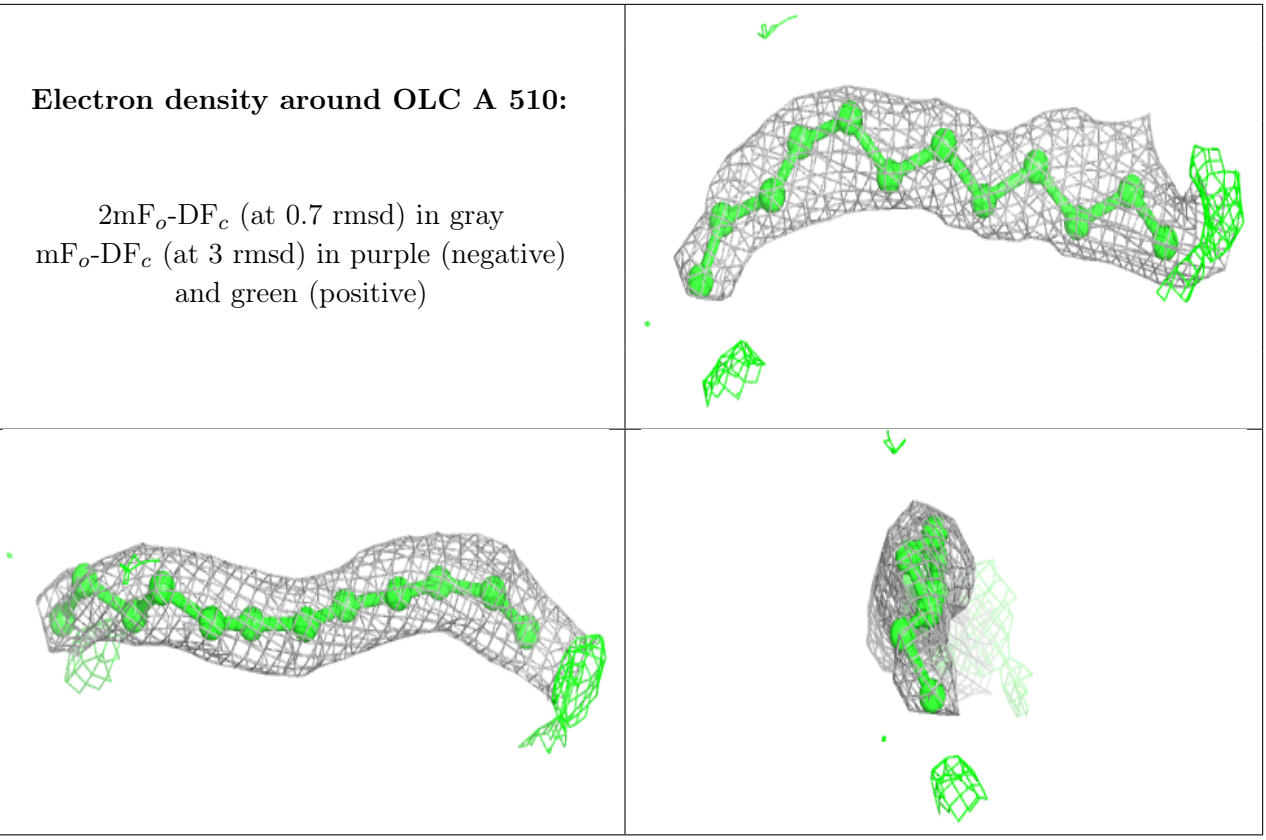
Electron density around OLC B 506:

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



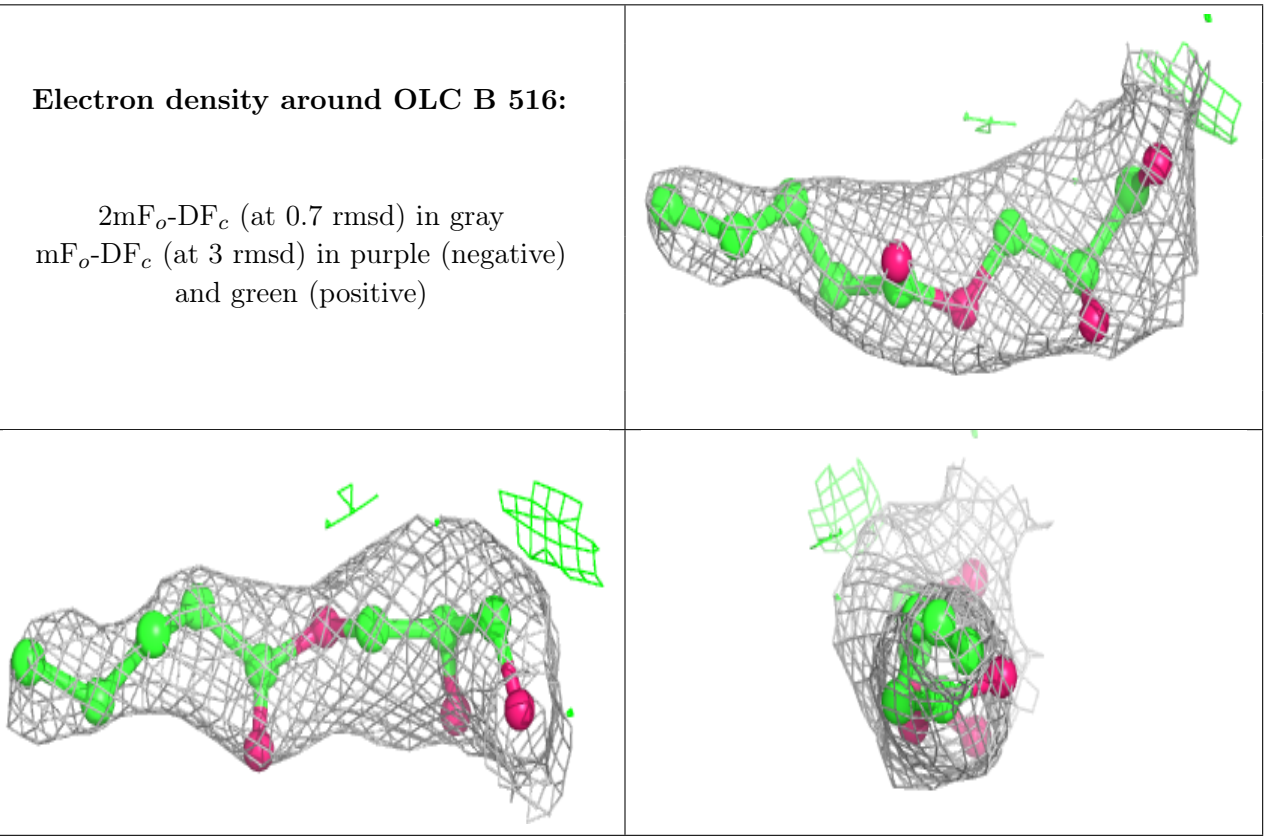
Electron density around OLC A 510:

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



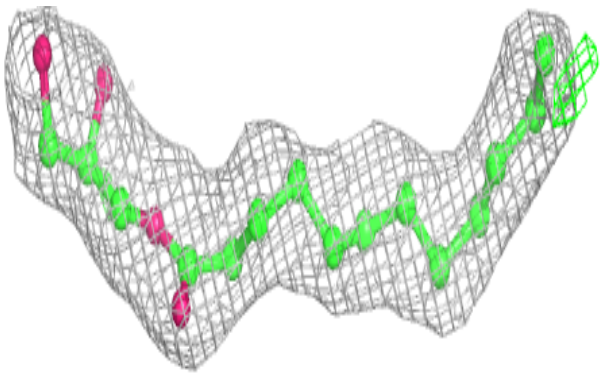
Electron density around OLC B 516:

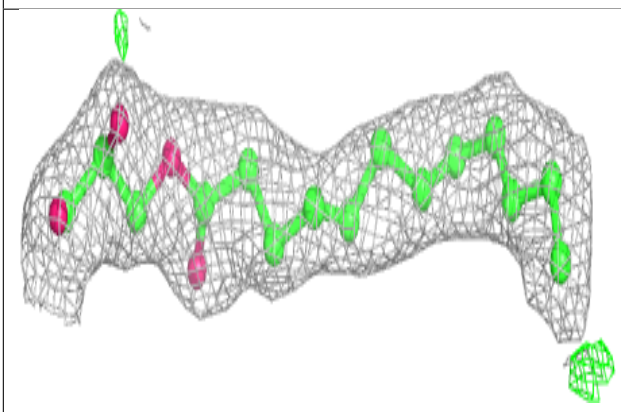
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

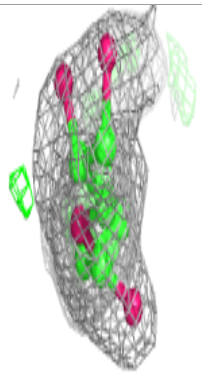


Electron density around OLC B 505:

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

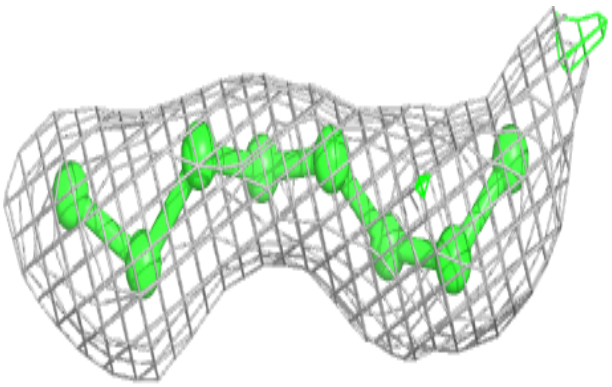


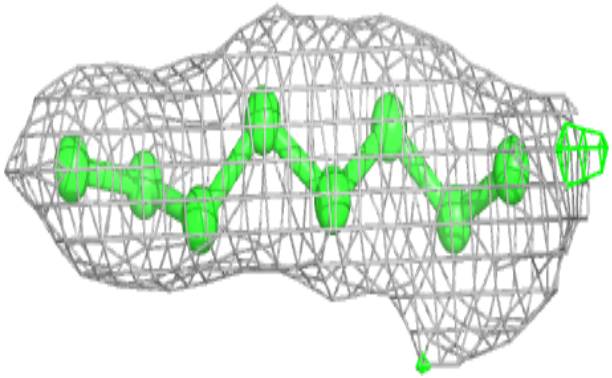


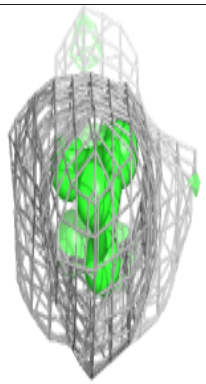


Electron density around OLC A 504:

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

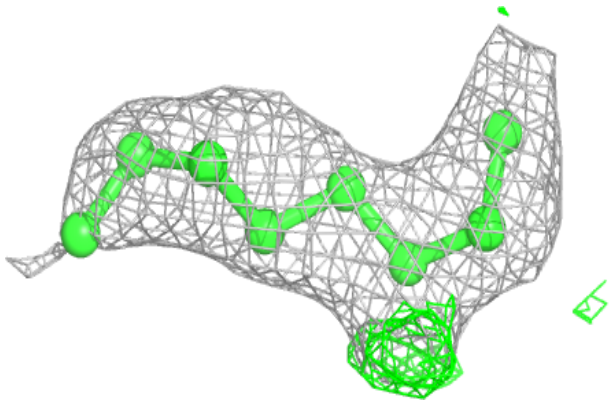


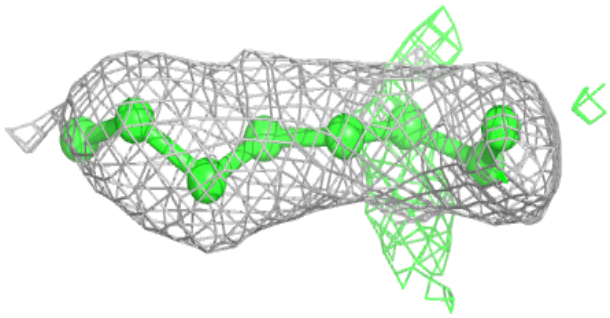


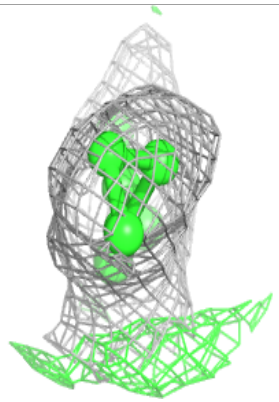


Electron density around OLC B 508:

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

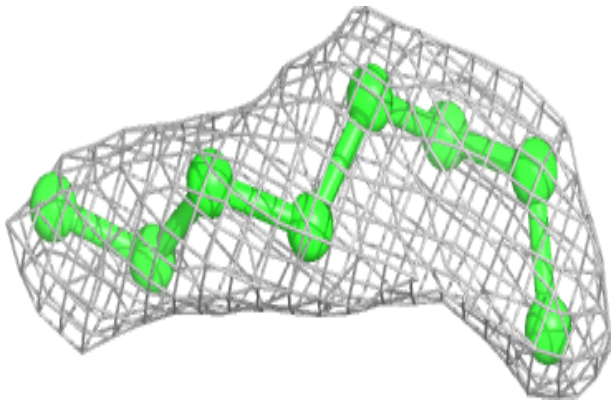


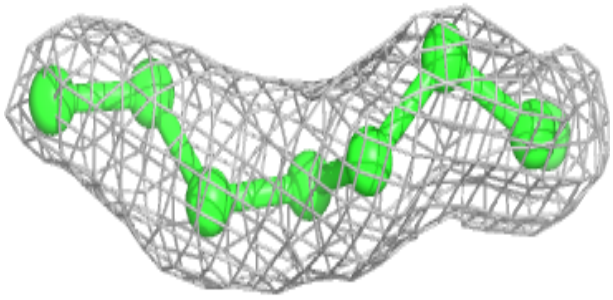


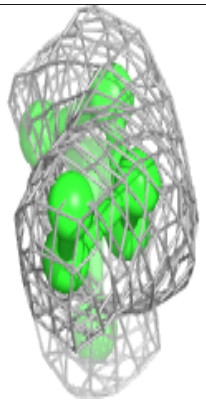


Electron density around OLC B 509:

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

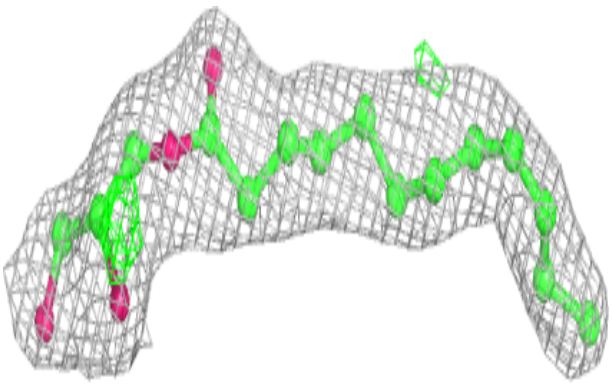


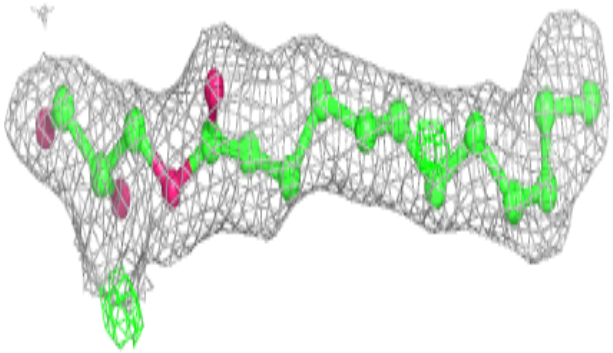


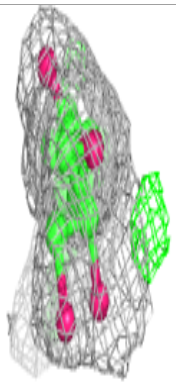


Electron density around OLC A 505:

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

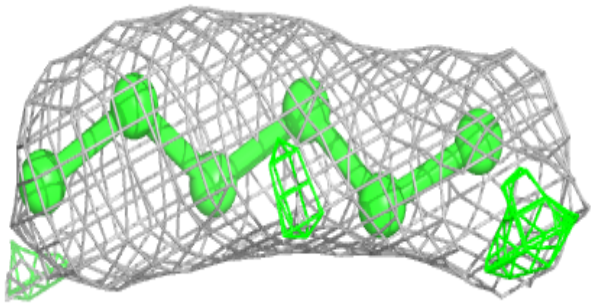


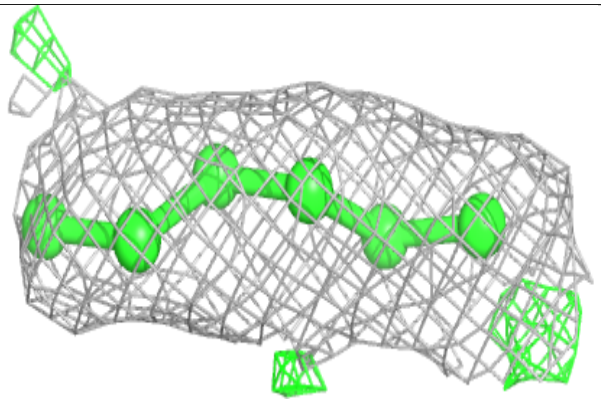


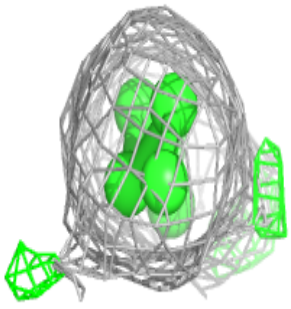


Electron density around OLC A 503:

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

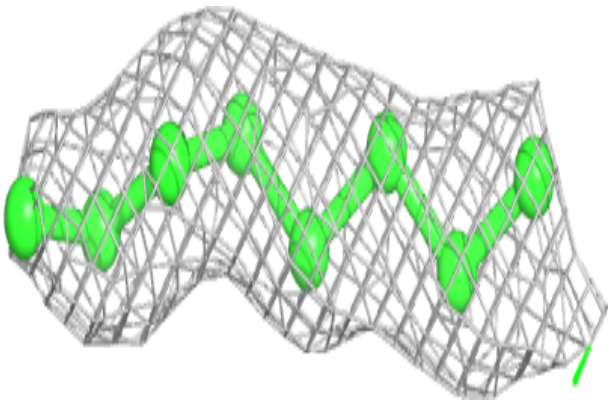


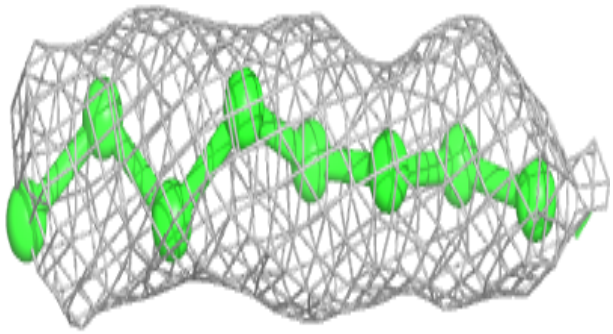


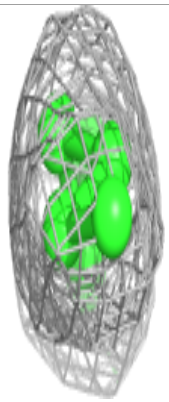


Electron density around OLC A 509:

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

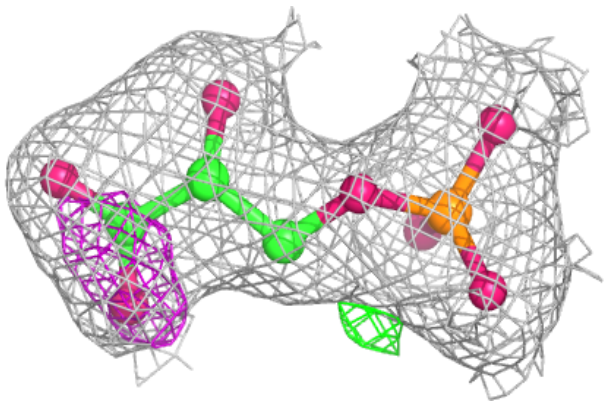


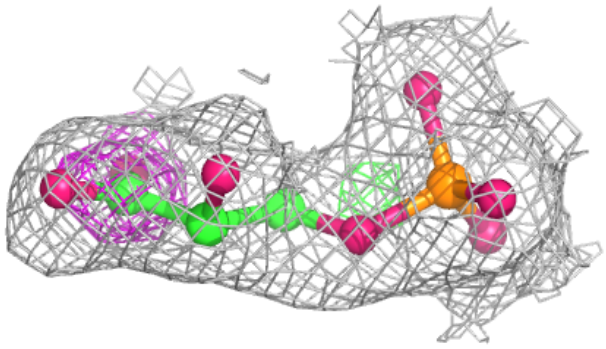


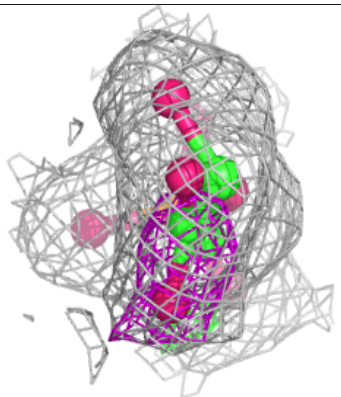


Electron density around 3PG B 518:

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

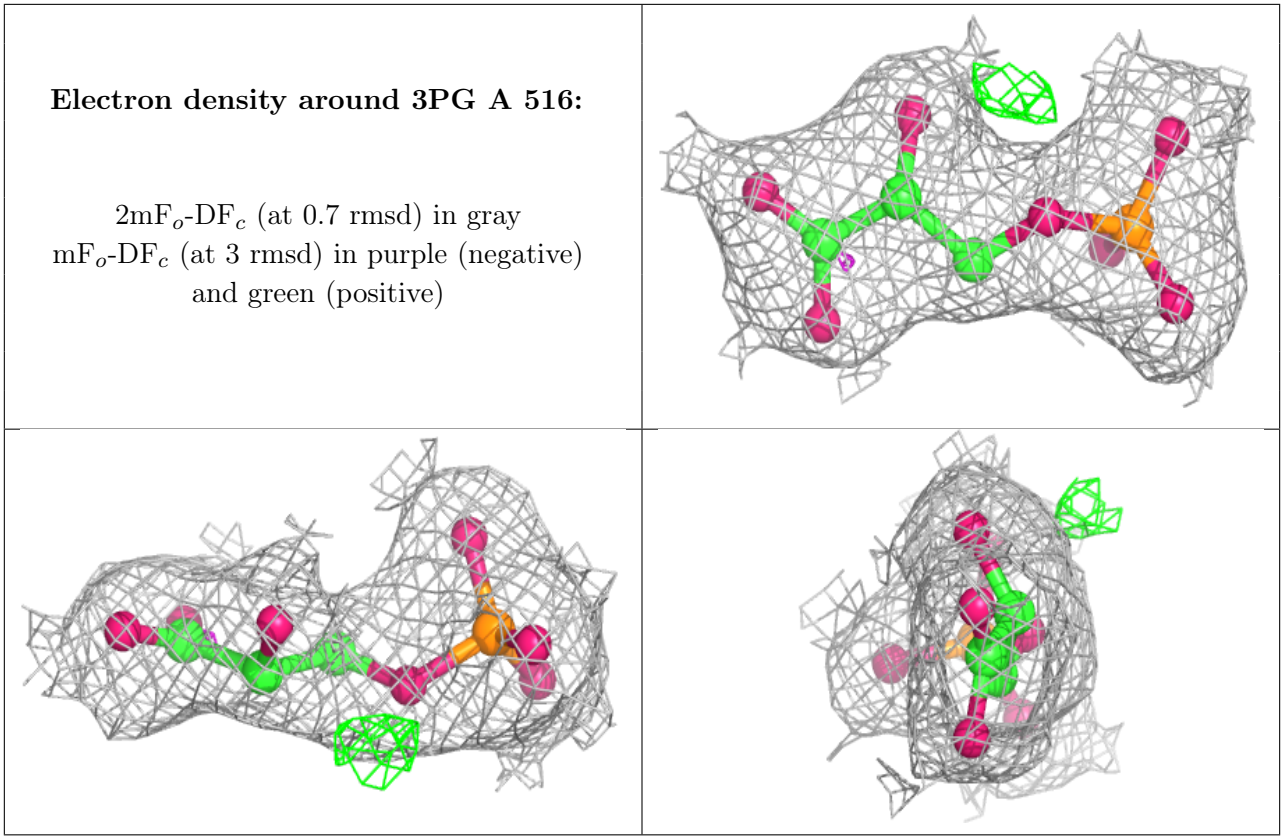






Electron density around 3PG A 516:

$2mF_o$-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.