



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:27 AM BST

PDB ID : 5ZIH
Title : Crystal structure of the red light-activated channelrhodopsin Chrimson.
Authors : Oda, K.; Vierock, J.; Oishi, S.; Taniguchi, R.; Yamashita, K.; Nishizawa, T.; Hegemann, P.; Nureki, O.
Deposited on : 2018-03-15
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

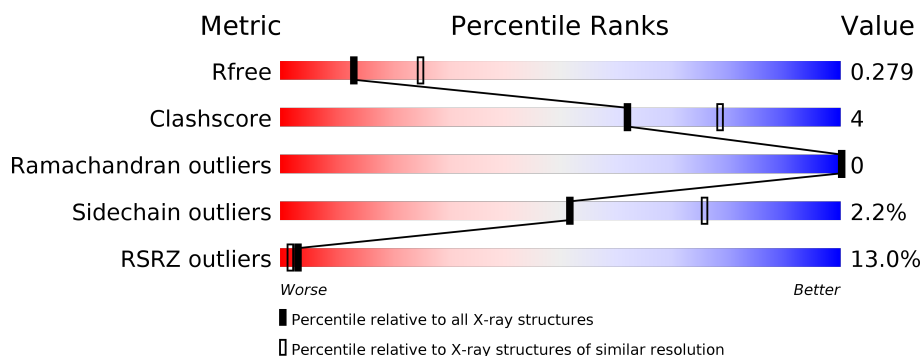
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	347	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>5%</div> <div>20%</div> </div> </div>
1	B	347	<div> <div>12%</div> <div> <div></div> <div>72%</div> <div>8%</div> <div>18%</div> </div> </div>

2 Entry composition [i](#)

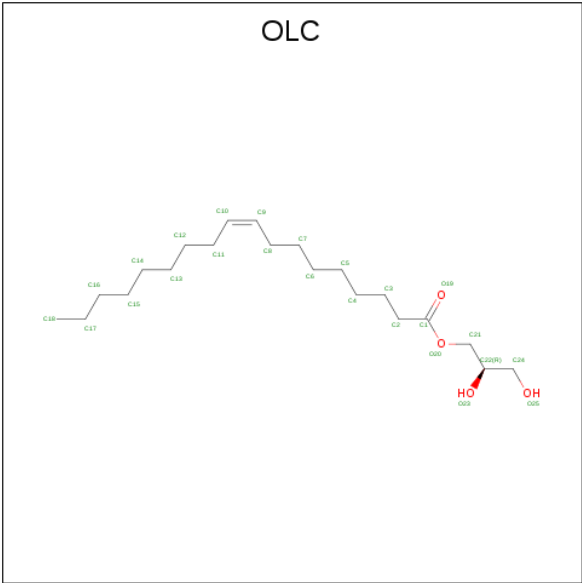
There are 3 unique types of molecules in this entry. The entry contains 4821 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sensory opsin A,Chrimson.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2179	1443	349	366	21			
1	B	285	Total	C	N	O	S	0	0	0
			2231	1471	355	384	21			

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	15	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			18	14	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 20 18 2	0	0
2	A	1	Total C O 15 11 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 O 20 16 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C O 23 19 4	0	0
2	B	1	Total C O 20 18 2	0	0
2	B	1	Total C O 20 18 2	0	0
2	B	1	Total C O 15 11 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C O 21 17 4	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 14 12 2	0	0

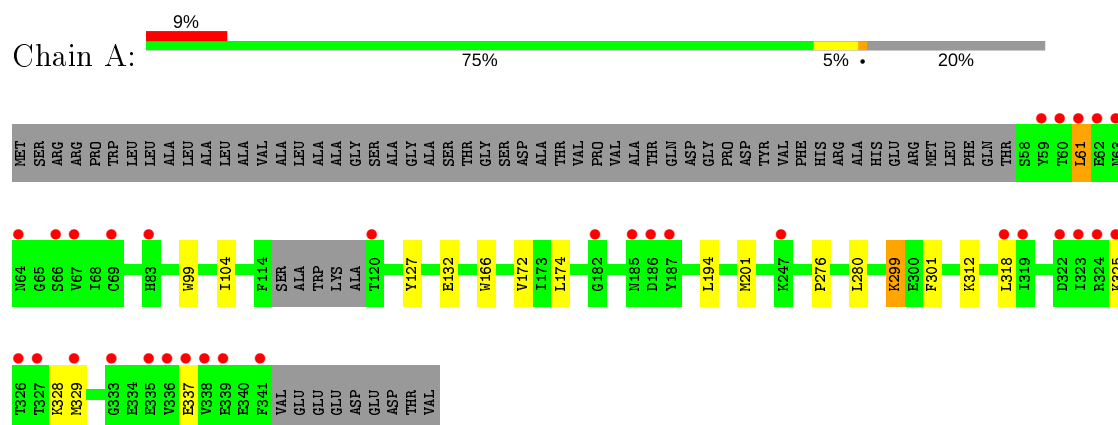
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	20	Total O 20 20	0	0

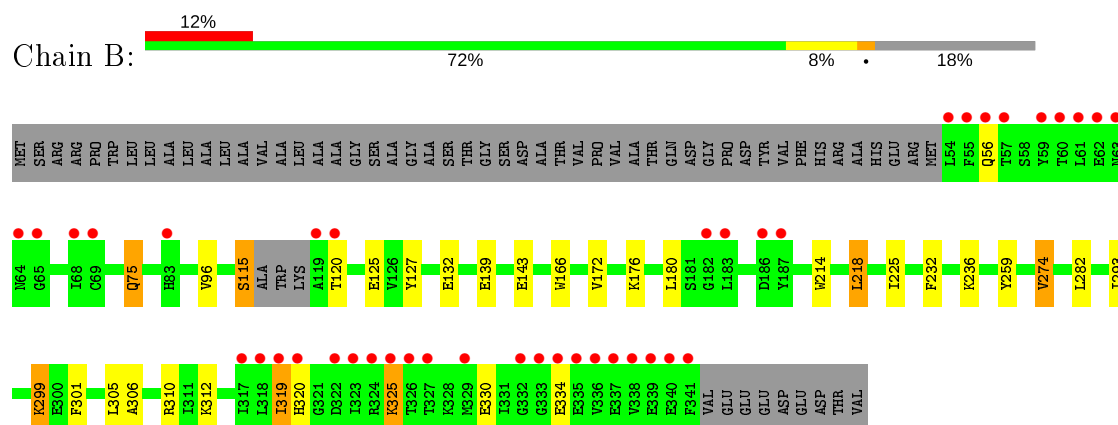
3 Residue-property plots [i](#)

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: Sensory opsin A,Chrimson



- Molecule 1: Sensory opsin A,Chrimson



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.99 Å 81.44 Å 170.14 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 2.60 48.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.82-2.60) 99.6 (48.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.61 Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.228 , 0.279 0.228 , 0.279	Depositor DCC
R_{free} test set	2671 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.964	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4821	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1718e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, LYR

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	0/2213	0.40	0/3011
1	B	0.26	0/2266	0.42	0/3083
All	All	0.26	0/4479	0.41	0/6094

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	2179	0	2128	13	0
1	B	2231	0	2152	22	0
2	A	147	0	220	9	0
2	B	227	0	338	5	0
3	A	17	0	0	0	0
3	B	20	0	0	0	0
All	All	4821	0	4838	42	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 4.

All (42) 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:104:ILE:HD13	2:A:403:OLC:H10	1.61	0.83
2:B:410:OLC:H6	2:B:412:OLC:H9	1.60	0.83
1:B:176:LYS:HE2	1:B:306:ALA:HB1	1.74	0.69
1:A:299:LYR:H9	1:A:299:LYR:H183	1.81	0.62
1:B:166:TRP:CD1	1:B:299:LYR:HC2	2.34	0.61
1:B:132:GLU:HG2	1:B:299:LYR:HD2	1.82	0.61
1:B:299:LYR:H9	1:B:299:LYR:H183	1.86	0.58
1:A:166:TRP:CD1	1:A:299:LYR:HC2	2.41	0.56
1:B:115:SER:O	1:B:120:THR:HG21	2.05	0.55
1:A:132:GLU:HG2	1:A:299:LYR:HD2	1.89	0.55
1:A:174:LEU:HD22	1:A:194:LEU:HD23	1.88	0.54
1:B:330:GLU:HA	1:B:334:GLU:O	2.08	0.53
1:A:301:PHE:HA	2:A:403:OLC:H8	1.90	0.52
1:B:125:GLU:OE2	1:B:310:ARG:NH2	2.41	0.51
1:A:127:TYR:CD2	1:A:172:VAL:HG21	2.44	0.51
1:A:201:MET:SD	1:A:299:LYR:H133	2.51	0.50
2:A:402:OLC:H24A	2:A:406:OLC:H3	1.94	0.50
1:B:274:VAL:HG13	1:B:282:LEU:HG	1.94	0.49
1:B:96:VAL:HG22	2:B:401:OLC:H5A	1.95	0.49
1:B:127:TYR:CD2	1:B:172:VAL:HG21	2.48	0.48
1:B:56:GLN:HG2	1:B:75:GLN:HB3	1.94	0.48
1:A:276:PRO:HA	1:A:280:LEU:HD13	1.96	0.47
1:B:325:LYS:HE3	1:B:325:LYS:HB2	1.81	0.47
1:B:293:ILE:HG23	2:B:410:OLC:H12A	1.98	0.46
2:A:406:OLC:H2A	2:A:406:OLC:H5	1.79	0.46
1:B:139:GLU:O	1:B:143:GLU:HB2	2.15	0.46
1:A:328:LYS:HA	1:A:337:GLU:HA	1.98	0.46
1:B:214:TRP:HZ3	1:B:218:LEU:HD12	1.80	0.46
1:B:319:ILE:HG13	1:B:320:HIS:N	2.31	0.45
2:A:406:OLC:H11	2:A:406:OLC:H8	1.72	0.45
1:B:232:PHE:CZ	1:B:236:LYS:HD2	2.51	0.45
2:A:406:OLC:H15A	2:A:406:OLC:H12A	1.75	0.43
1:A:312:LYS:HD3	1:A:312:LYS:HA	1.85	0.43
1:A:61:LEU:H	1:A:61:LEU:HD23	1.83	0.43
1:B:259:TYR:CD1	2:B:408:OLC:H2	2.53	0.43
1:B:225:ILE:HA	2:B:405:OLC:H8A	2.01	0.42
2:A:402:OLC:H8A	2:A:402:OLC:H11	1.74	0.42
1:A:99:TRP:HB3	2:A:405:OLC:H7A	2.02	0.42
2:A:402:OLC:H9	2:A:406:OLC:H16A	2.03	0.41
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.81	0.41
1:B:301:PHE:O	1:B:305:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:HA	1:B:312:LYS:HD3	1.92	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	274/347 (79%)	263 (96%)	11 (4%)	0	100	100
1	B	280/347 (81%)	267 (95%)	13 (5%)	0	100	100
All	All	554/694 (80%)	530 (96%)	24 (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	221/286 (77%)	217 (98%)	4 (2%)	59	80
1	B	226/286 (79%)	220 (97%)	6 (3%)	44	71
All	All	447/572 (78%)	437 (98%)	10 (2%)	52	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	318	LEU
1	A	325	LYS
1	A	329	MET
1	B	75	GLN
1	B	115	SER
1	B	218	LEU
1	B	274	VAL
1	B	319	ILE
1	B	325	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	B	56	GLN
1	B	287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LYR	B	299	1	27,29,30	0.61	0	30,37,39	2.01	9 (30%)
1	LYR	A	299	1	27,29,30	0.62	0	30,37,39	1.94	9 (30%)

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
1	LYR	B	299	1	-	1/22/40/42	0/1/1/1
1	LYR	A	299	1	-	3/22/40/42	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	LYR	C13-C12-C11	-5.10	118.80	124.53
1	A	299	LYR	C1-NZ-CE	4.89	121.07	113.33
1	B	299	LYR	C1-NZ-CE	4.85	121.02	113.33
1	A	299	LYR	C13-C12-C11	-4.36	119.64	124.53
1	A	299	LYR	C17-C11-C10	2.77	123.61	115.78
1	B	299	LYR	C17-C11-C10	2.77	123.61	115.78
1	A	299	LYR	C15-C14-C12	-2.67	109.31	114.08
1	B	299	LYR	C10-C11-C12	-2.67	115.00	121.46
1	A	299	LYR	C6-C7-C80	-2.63	123.56	127.31
1	A	299	LYR	C10-C11-C12	-2.62	115.13	121.46
1	B	299	LYR	C8-C80-C9	2.60	122.18	118.08
1	B	299	LYR	C1-C2-C3	-2.56	122.06	126.97
1	B	299	LYR	C7-C6-C5	-2.39	115.74	123.22
1	A	299	LYR	C4-C3-C5	2.39	121.85	118.08
1	B	299	LYR	C13-C12-C14	2.18	117.80	113.62
1	A	299	LYR	C16-C17-C11	2.15	113.79	110.48
1	B	299	LYR	C15-C14-C12	-2.11	110.30	114.08
1	A	299	LYR	C8-C80-C9	2.03	121.27	118.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	299	LYR	C-CA-CB-CG
1	A	299	LYR	CG-CD-CE-NZ
1	B	299	LYR	CG-CD-CE-NZ
1	A	299	LYR	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	299	LYR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	299	LYR	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	B	403	-	19,19,24	0.92	1 (5%)	20,20,25	0.93	1 (5%)
2	OLC	B	404	-	13,13,24	0.35	0	12,12,25	0.64	0
2	OLC	B	407	-	16,19,24	0.35	0	15,19,25	0.78	0
2	OLC	A	403	-	24,24,24	0.83	2 (8%)	25,25,25	0.98	1 (4%)
2	OLC	B	402	-	24,24,24	0.82	2 (8%)	25,25,25	0.89	1 (4%)
2	OLC	B	410	-	20,20,24	0.91	2 (10%)	21,21,25	0.89	1 (4%)
2	OLC	A	407	-	14,14,24	1.03	2 (14%)	15,15,25	0.99	1 (6%)
2	OLC	B	406	-	16,19,24	0.32	0	15,19,25	0.85	0
2	OLC	A	404	-	17,17,24	0.97	2 (11%)	18,18,25	1.06	1 (5%)
2	OLC	B	409	-	13,13,24	0.34	0	12,12,25	0.71	0
2	OLC	B	401	-	24,24,24	0.82	2 (8%)	25,25,25	0.96	1 (4%)
2	OLC	A	401	-	18,18,24	0.96	1 (5%)	18,19,25	1.09	1 (5%)
2	OLC	B	405	-	22,22,24	0.86	2 (9%)	23,23,25	1.02	1 (4%)
2	OLC	A	405	-	24,24,24	0.83	2 (8%)	25,25,25	0.91	1 (4%)
2	OLC	B	412	-	10,13,24	0.35	0	8,13,25	1.00	0
2	OLC	A	402	-	24,24,24	0.81	2 (8%)	25,25,25	0.91	1 (4%)
2	OLC	A	406	-	16,19,24	0.31	0	15,19,25	0.88	0
2	OLC	B	411	-	12,15,24	0.30	0	11,15,25	0.97	0
2	OLC	B	408	-	14,14,24	1.03	2 (14%)	15,15,25	0.94	1 (6%)

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	B	403	-	-	9/19/19/24	-
2	OLC	B	404	-	-	2/11/11/24	-
2	OLC	B	407	-	-	8/15/17/24	-
2	OLC	A	403	-	-	10/24/24/24	-
2	OLC	B	402	-	-	7/24/24/24	-
2	OLC	B	410	-	-	7/20/20/24	-
2	OLC	A	407	-	-	4/14/14/24	-
2	OLC	B	406	-	-	3/15/17/24	-
2	OLC	A	404	-	-	10/17/17/24	-
2	OLC	B	409	-	-	7/11/11/24	-
2	OLC	B	401	-	-	12/24/24/24	-
2	OLC	A	401	-	-	5/18/18/24	-
2	OLC	B	405	-	-	11/22/22/24	-
2	OLC	A	405	-	-	9/24/24/24	-
2	OLC	B	412	-	-	5/9/11/24	-
2	OLC	A	402	-	-	12/24/24/24	-
2	OLC	A	406	-	-	3/15/17/24	-
2	OLC	B	411	-	-	3/11/13/24	-
2	OLC	B	408	-	-	3/14/14/24	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	OLC	O20-C1	2.61	1.41	1.33
2	B	403	OLC	O20-C1	2.56	1.40	1.33
2	B	410	OLC	O20-C1	2.54	1.40	1.33
2	B	408	OLC	O20-C1	2.50	1.40	1.33
2	A	404	OLC	O20-C1	2.47	1.40	1.33
2	A	405	OLC	O20-C1	2.46	1.40	1.33
2	B	405	OLC	O20-C1	2.45	1.40	1.33
2	A	403	OLC	O20-C1	2.43	1.40	1.33
2	A	407	OLC	O20-C1	2.42	1.40	1.33
2	B	401	OLC	O20-C1	2.41	1.40	1.33
2	A	402	OLC	O20-C1	2.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	OLC	O20-C1	2.39	1.40	1.33
2	B	401	OLC	O20-C21	-2.17	1.40	1.45
2	A	403	OLC	O20-C21	-2.13	1.40	1.45
2	A	407	OLC	O20-C21	-2.08	1.40	1.45
2	A	402	OLC	O20-C21	-2.07	1.40	1.45
2	B	402	OLC	O20-C21	-2.07	1.40	1.45
2	B	410	OLC	O20-C21	-2.02	1.40	1.45
2	A	405	OLC	O20-C21	-2.02	1.40	1.45
2	B	408	OLC	O20-C21	-2.02	1.40	1.45
2	A	404	OLC	O20-C21	-2.01	1.40	1.45
2	B	405	OLC	O20-C21	-2.01	1.40	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	405	OLC	O20-C1-C2	3.13	121.72	111.91
2	A	401	OLC	O20-C1-C2	3.04	121.46	111.91
2	A	404	OLC	O20-C1-C2	2.83	120.79	111.91
2	A	403	OLC	O20-C1-C2	2.77	120.59	111.91
2	A	405	OLC	O20-C1-C2	2.76	120.56	111.91
2	B	401	OLC	O20-C1-C2	2.74	120.52	111.91
2	B	403	OLC	O20-C1-C2	2.74	120.51	111.91
2	B	410	OLC	O20-C1-C2	2.61	120.11	111.91
2	A	402	OLC	O20-C1-C2	2.50	119.76	111.91
2	A	407	OLC	O20-C1-C2	2.47	119.67	111.91
2	B	408	OLC	O20-C1-C2	2.41	119.47	111.91
2	B	402	OLC	O20-C1-C2	2.39	119.40	111.91

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	OLC	C21-C22-C24-O25
2	A	404	OLC	C21-C22-C24-O25
2	A	404	OLC	O23-C22-C24-O25
2	A	401	OLC	C9-C10-C11-C12
2	A	401	OLC	C21-C22-C24-O25
2	B	405	OLC	O20-C21-C22-O23
2	B	412	OLC	C9-C10-C11-C12
2	B	412	OLC	C1-C2-C3-C4
2	A	402	OLC	C21-C22-C24-O25
2	B	408	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
2	B	402	OLC	O19-C1-O20-C21
2	A	405	OLC	O19-C1-O20-C21
2	A	405	OLC	C2-C1-O20-C21
2	B	402	OLC	C2-C1-O20-C21
2	B	403	OLC	O19-C1-O20-C21
2	A	402	OLC	O19-C1-O20-C21
2	B	403	OLC	C2-C1-O20-C21
2	A	402	OLC	C2-C1-O20-C21
2	B	405	OLC	C2-C1-O20-C21
2	B	401	OLC	C6-C7-C8-C9
2	B	408	OLC	O20-C21-C22-O23
2	B	405	OLC	O19-C1-O20-C21
2	A	403	OLC	C1-C2-C3-C4
2	A	402	OLC	C1-C2-C3-C4
2	B	412	OLC	C6-C7-C8-C9
2	B	401	OLC	C5-C6-C7-C8
2	B	401	OLC	C3-C4-C5-C6
2	B	405	OLC	O20-C21-C22-C24
2	B	406	OLC	C4-C5-C6-C7
2	B	409	OLC	C11-C12-C13-C14
2	B	409	OLC	C5-C6-C7-C8
2	B	412	OLC	C4-C5-C6-C7
2	A	404	OLC	C1-C2-C3-C4
2	B	401	OLC	C12-C13-C14-C15
2	A	402	OLC	O20-C21-C22-O23
2	B	407	OLC	C4-C5-C6-C7
2	A	407	OLC	C2-C3-C4-C5
2	B	404	OLC	C4-C5-C6-C7
2	B	405	OLC	C2-C3-C4-C5
2	B	401	OLC	C1-C2-C3-C4
2	A	407	OLC	C2-C1-O20-C21
2	B	407	OLC	C5-C6-C7-C8
2	A	403	OLC	O23-C22-C24-O25
2	A	402	OLC	O23-C22-C24-O25
2	B	401	OLC	C4-C5-C6-C7
2	B	406	OLC	C10-C11-C12-C13
2	A	406	OLC	C10-C11-C12-C13
2	A	403	OLC	C4-C5-C6-C7
2	A	407	OLC	O19-C1-O20-C21
2	B	411	OLC	C6-C7-C8-C9
2	B	409	OLC	C12-C13-C14-C15
2	B	402	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	404	OLC	C6-C7-C8-C9
2	B	403	OLC	C1-C2-C3-C4
2	B	405	OLC	C4-C5-C6-C7
2	B	412	OLC	C3-C4-C5-C6
2	B	407	OLC	C11-C12-C13-C14
2	B	402	OLC	C5-C6-C7-C8
2	B	410	OLC	C10-C11-C12-C13
2	B	401	OLC	C2-C1-O20-C21
2	A	401	OLC	O23-C22-C24-O25
2	A	406	OLC	C13-C14-C15-C16
2	B	402	OLC	C6-C7-C8-C9
2	B	410	OLC	C6-C7-C8-C9
2	A	404	OLC	O20-C21-C22-C24
2	A	403	OLC	C2-C3-C4-C5
2	B	401	OLC	O19-C1-O20-C21
2	A	404	OLC	O20-C21-C22-O23
2	B	408	OLC	C2-C3-C4-C5
2	A	404	OLC	C4-C5-C6-C7
2	B	410	OLC	C11-C12-C13-C14
2	A	405	OLC	C5-C6-C7-C8
2	B	405	OLC	C5-C6-C7-C8
2	B	401	OLC	C15-C16-C17-C18
2	B	406	OLC	C3-C4-C5-C6
2	A	402	OLC	C12-C13-C14-C15
2	B	411	OLC	C2-C3-C4-C5
2	B	410	OLC	O23-C22-C24-O25
2	A	406	OLC	C5-C6-C7-C8
2	B	410	OLC	C21-C22-C24-O25
2	B	407	OLC	C1-C2-C3-C4
2	A	401	OLC	C4-C5-C6-C7
2	B	405	OLC	C10-C11-C12-C13
2	A	407	OLC	C4-C5-C6-C7
2	A	402	OLC	C2-C3-C4-C5
2	A	405	OLC	C4-C5-C6-C7
2	B	407	OLC	C12-C13-C14-C15
2	A	402	OLC	C13-C14-C15-C16
2	B	409	OLC	C6-C7-C8-C9
2	B	401	OLC	C13-C14-C15-C16
2	B	409	OLC	C9-C10-C11-C12
2	A	402	OLC	C3-C4-C5-C6
2	A	404	OLC	C5-C6-C7-C8
2	B	401	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
2	A	404	OLC	C2-C3-C4-C5
2	B	409	OLC	C13-C14-C15-C16
2	A	405	OLC	C7-C8-C9-C10
2	B	405	OLC	C9-C10-C11-C12
2	B	407	OLC	C9-C10-C11-C12
2	B	402	OLC	C9-C10-C11-C12
2	B	410	OLC	C9-C10-C11-C12
2	A	405	OLC	O20-C1-C2-C3
2	B	404	OLC	C7-C8-C9-C10
2	B	410	OLC	C7-C8-C9-C10
2	B	403	OLC	C6-C7-C8-C9
2	B	402	OLC	C10-C11-C12-C13
2	B	409	OLC	C10-C11-C12-C13
2	B	405	OLC	C7-C8-C9-C10
2	B	411	OLC	C9-C10-C11-C12
2	B	407	OLC	C7-C8-C9-C10
2	A	403	OLC	C2-C1-O20-C21
2	B	401	OLC	O20-C21-C22-O23
2	A	403	OLC	O20-C1-C2-C3
2	A	403	OLC	C15-C16-C17-C18
2	B	403	OLC	C7-C8-C9-C10
2	B	403	OLC	O20-C21-C22-C24
2	B	407	OLC	C3-C4-C5-C6
2	A	405	OLC	O19-C1-C2-C3
2	A	405	OLC	C9-C10-C11-C12
2	A	405	OLC	C21-C22-C24-O25
2	A	404	OLC	O20-C1-C2-C3
2	A	403	OLC	O19-C1-O20-C21
2	A	401	OLC	C7-C8-C9-C10
2	B	403	OLC	O20-C1-C2-C3
2	B	405	OLC	C6-C7-C8-C9
2	A	402	OLC	O20-C1-C2-C3
2	B	403	OLC	C9-C10-C11-C12
2	B	403	OLC	O19-C1-C2-C3
2	A	403	OLC	O19-C1-C2-C3
2	A	402	OLC	O19-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 14 short contacts:

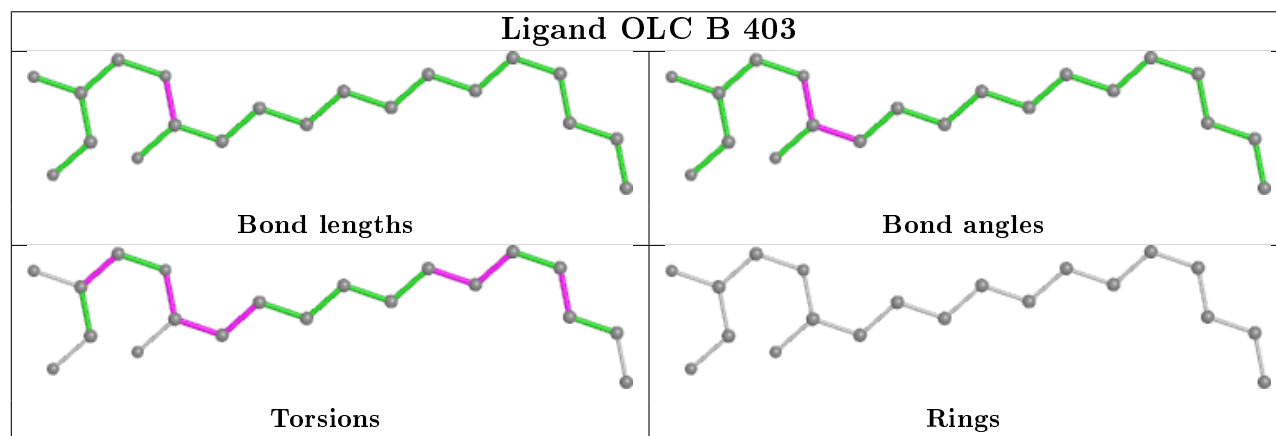
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	OLC	2	0

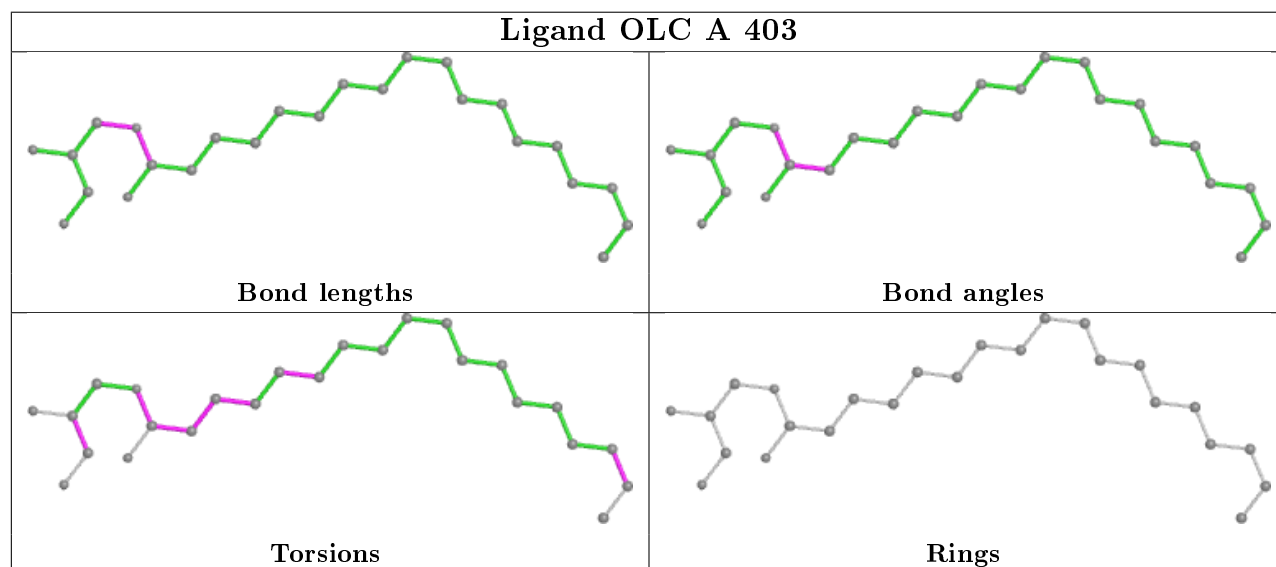
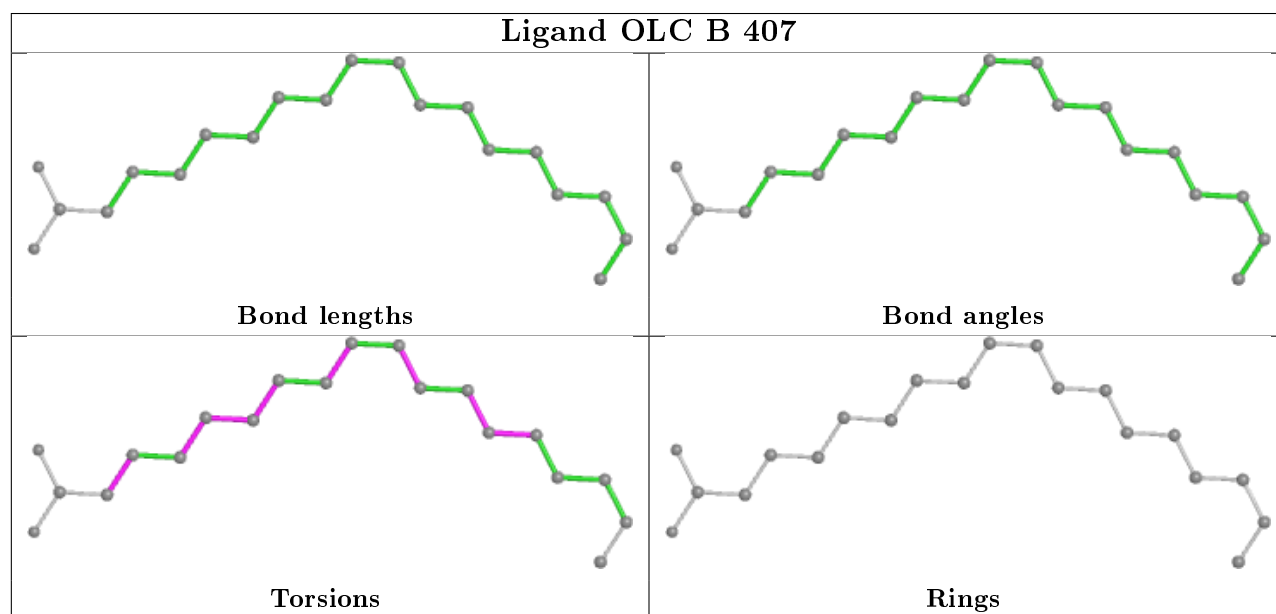
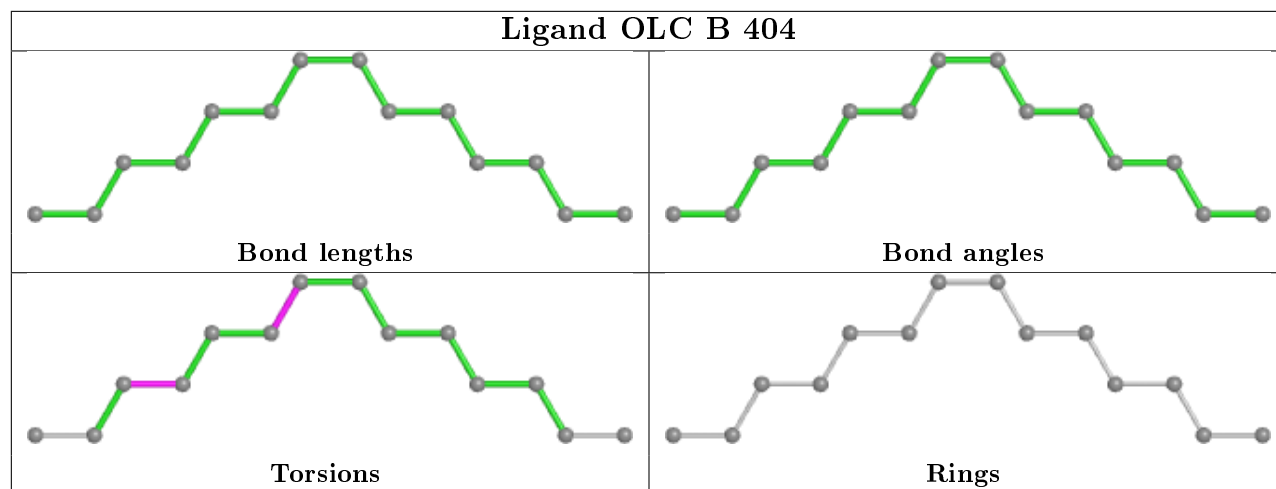
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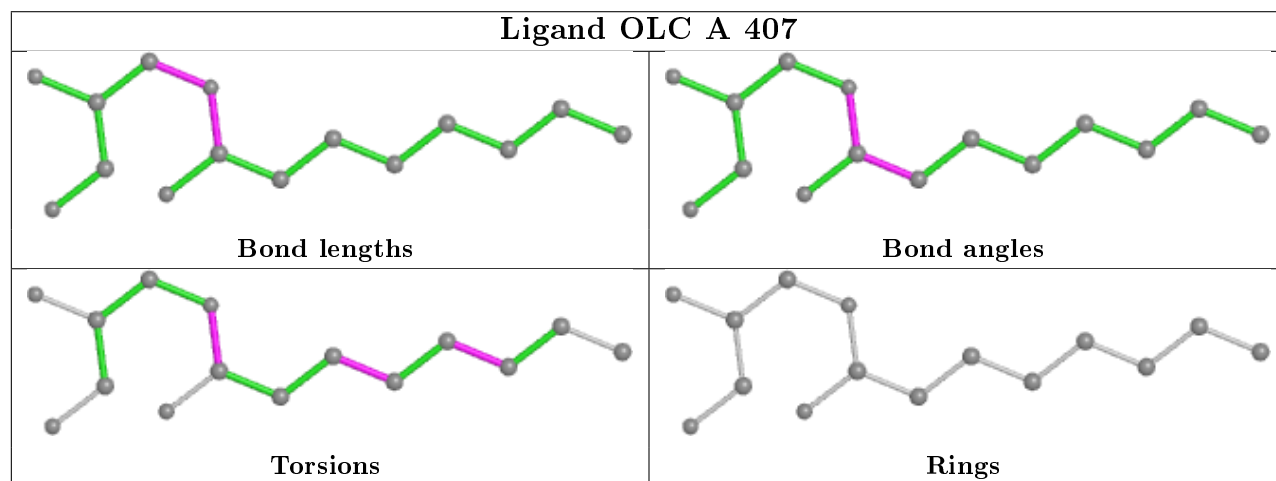
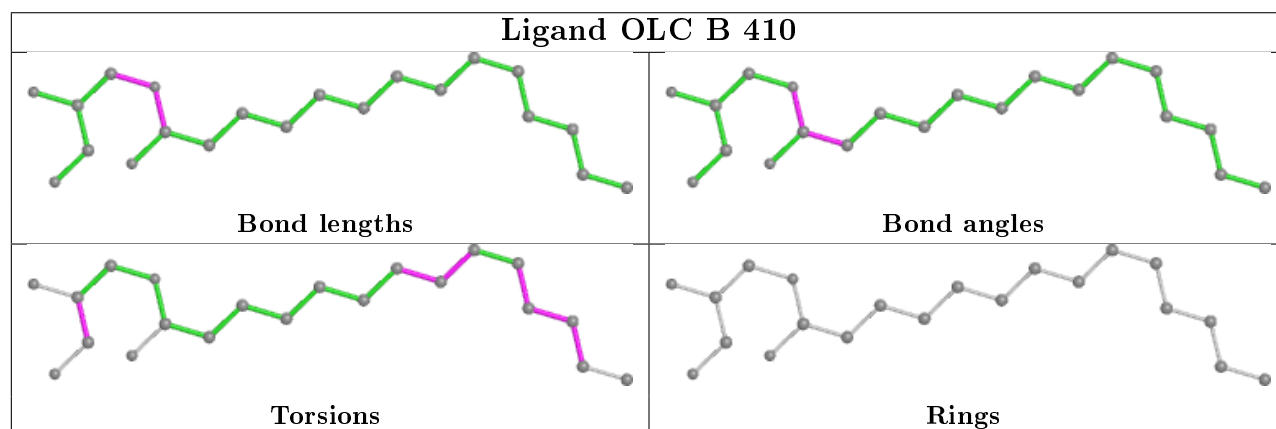
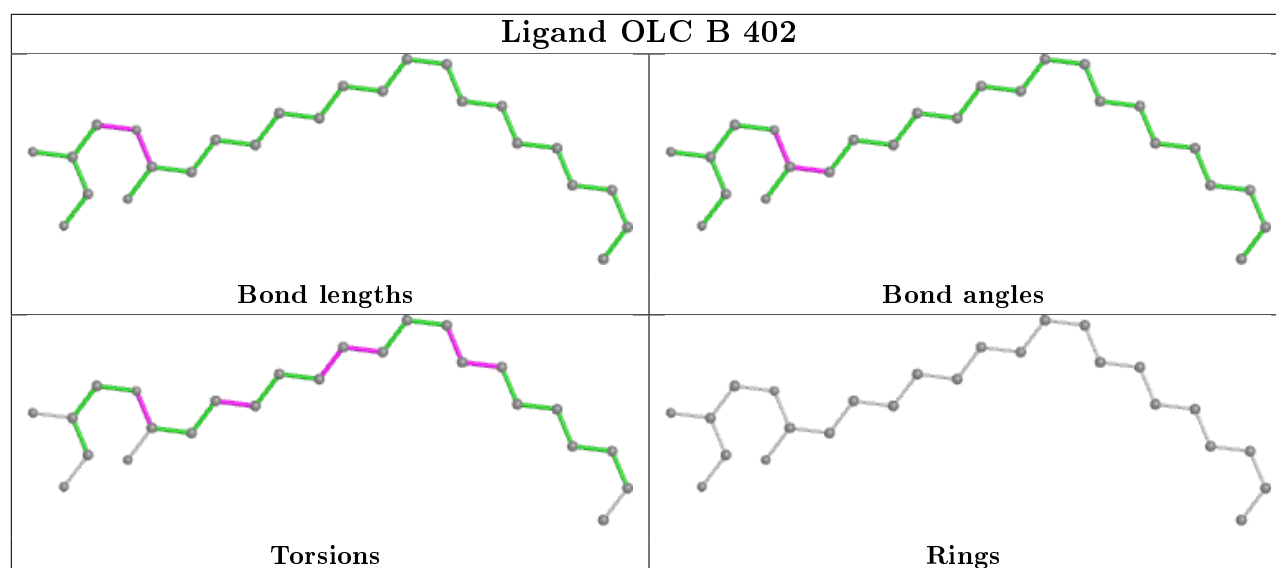
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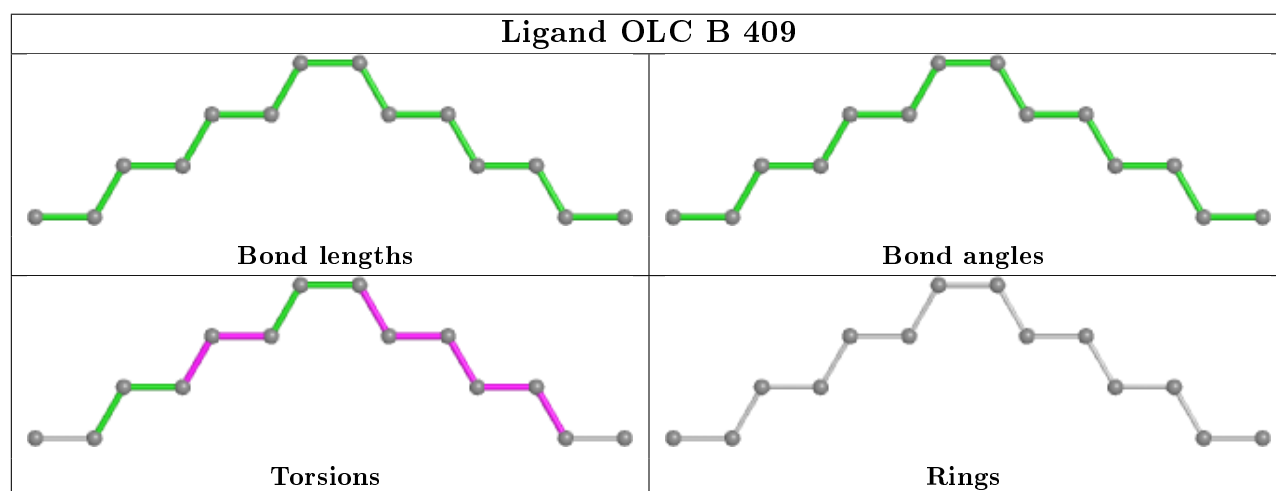
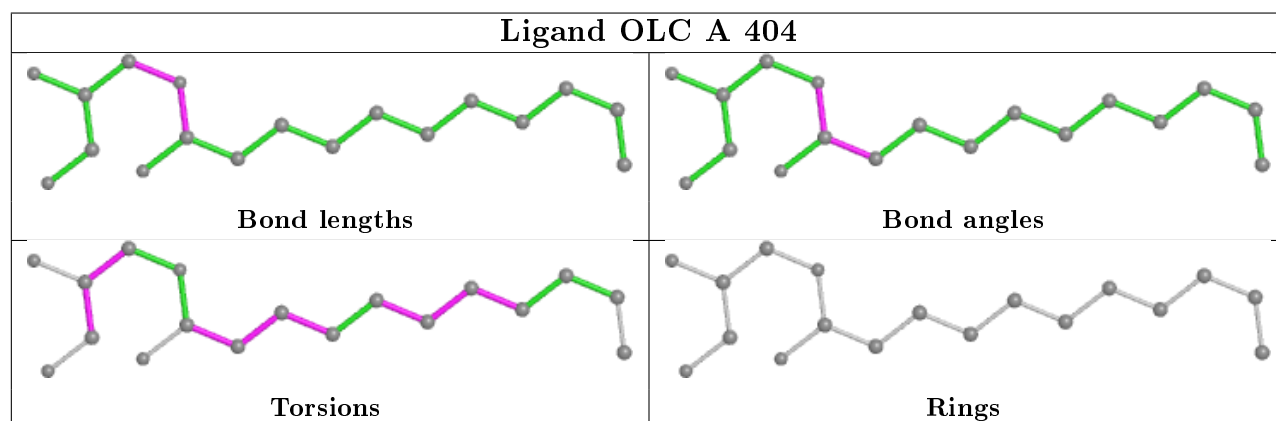
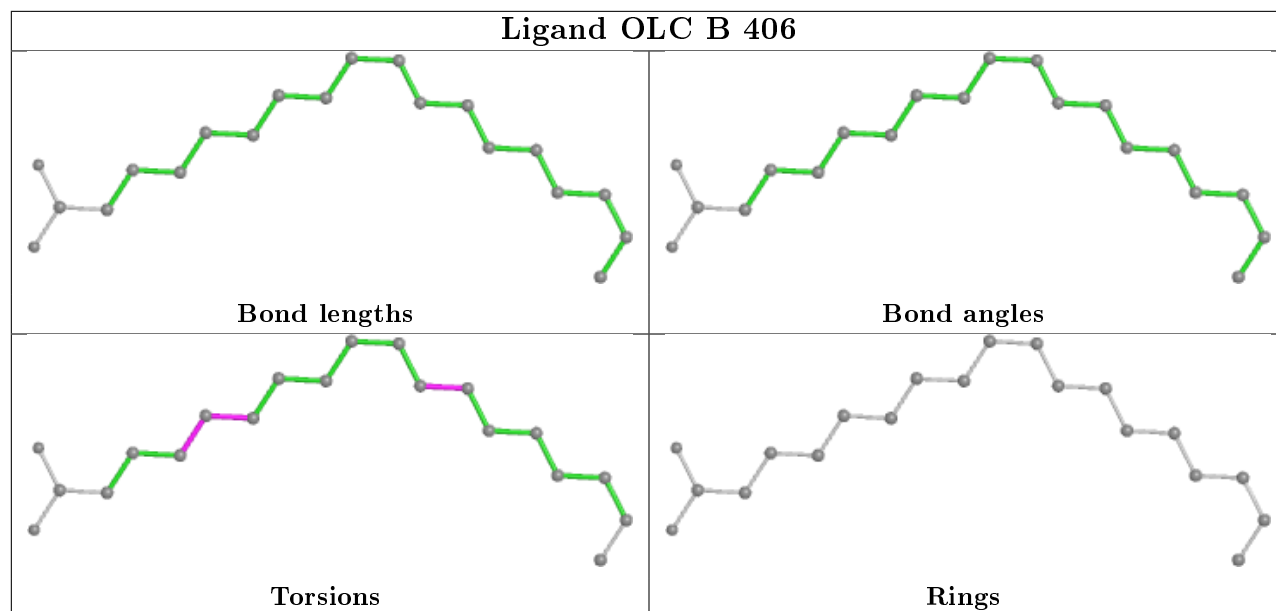
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	410	OLC	2	0
2	B	401	OLC	1	0
2	B	405	OLC	1	0
2	A	405	OLC	1	0
2	B	412	OLC	1	0
2	A	402	OLC	3	0
2	A	406	OLC	5	0
2	B	408	OLC	1	0

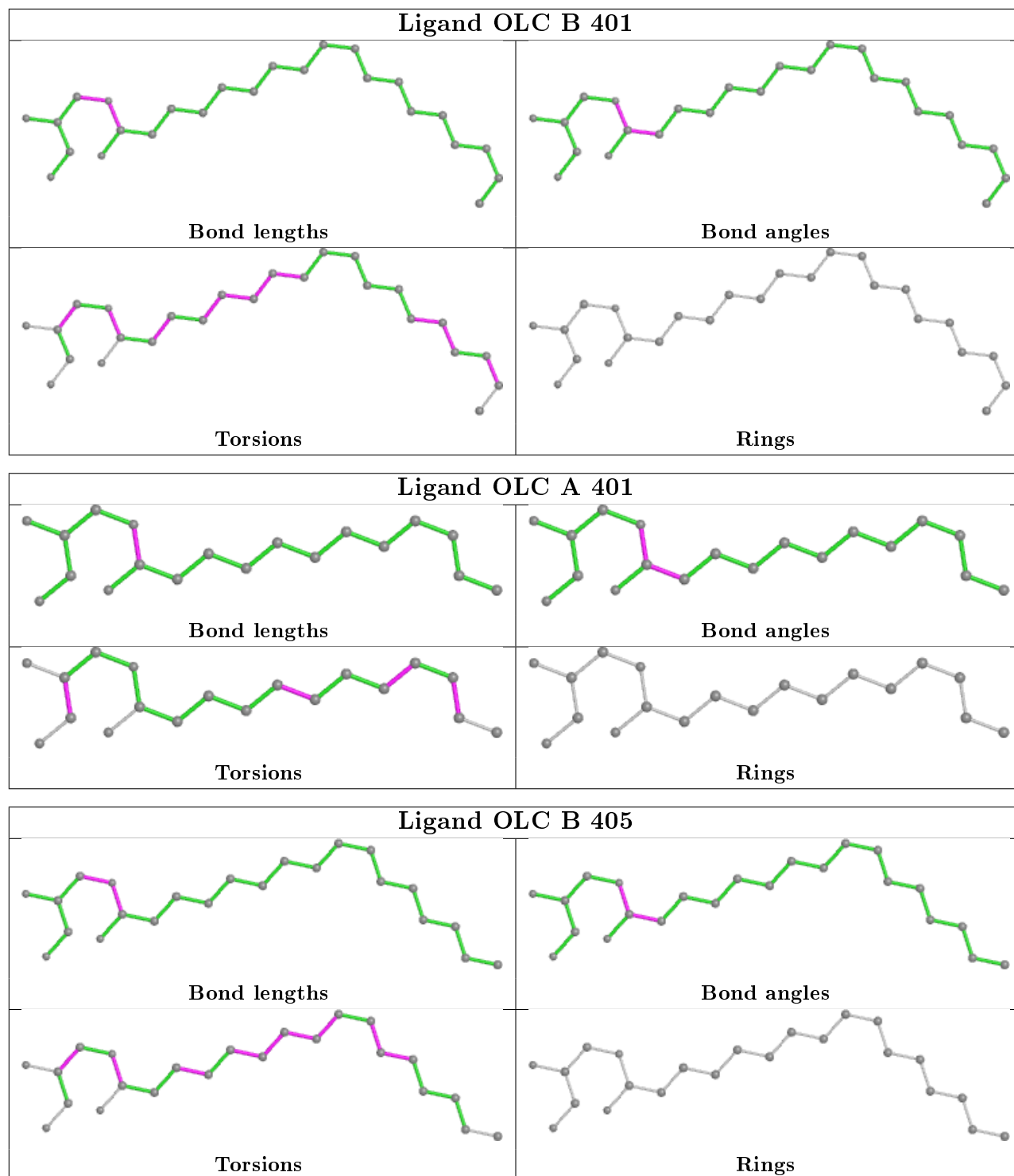
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

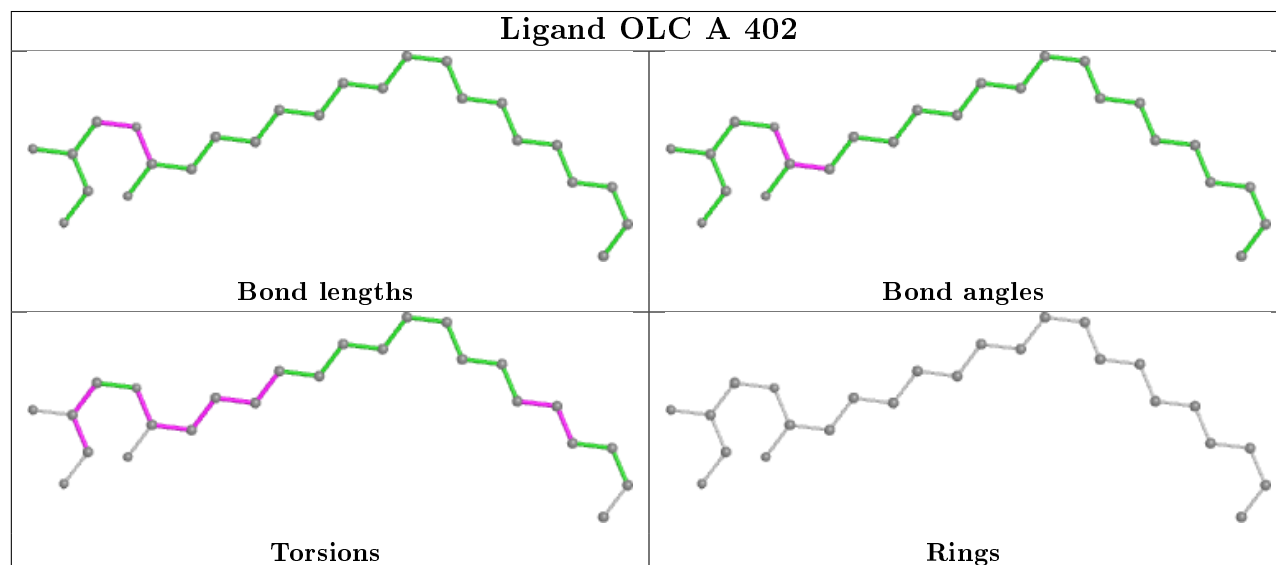
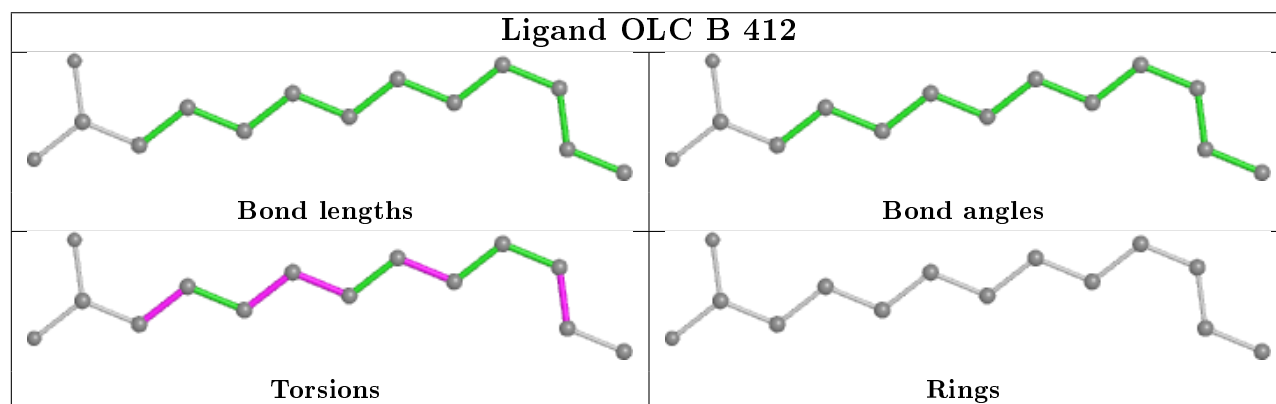
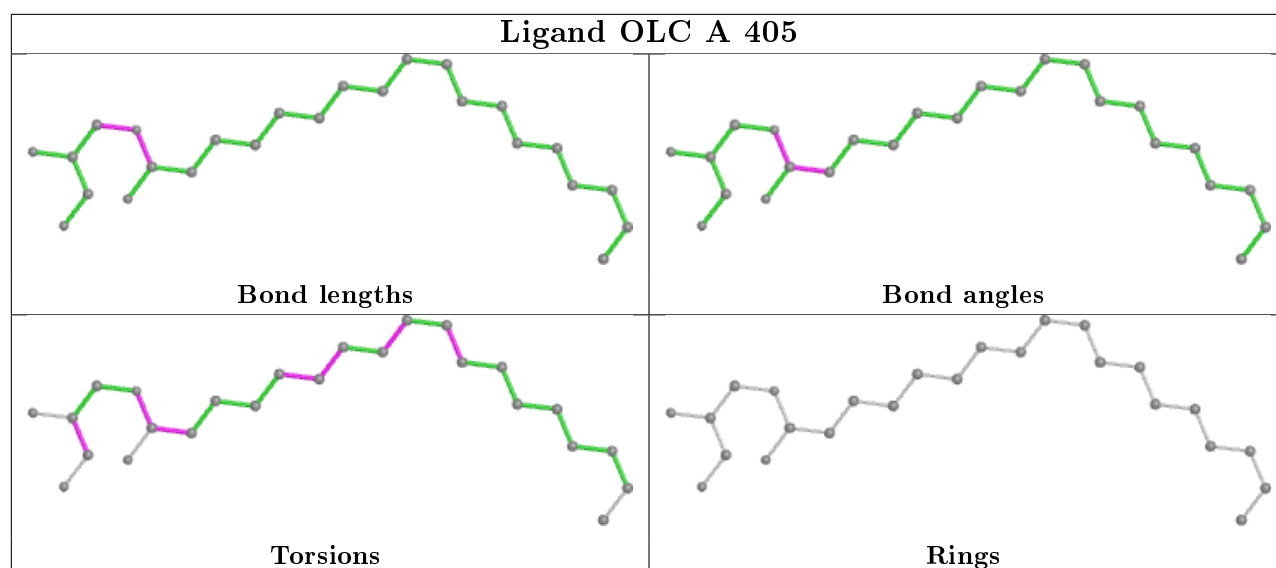


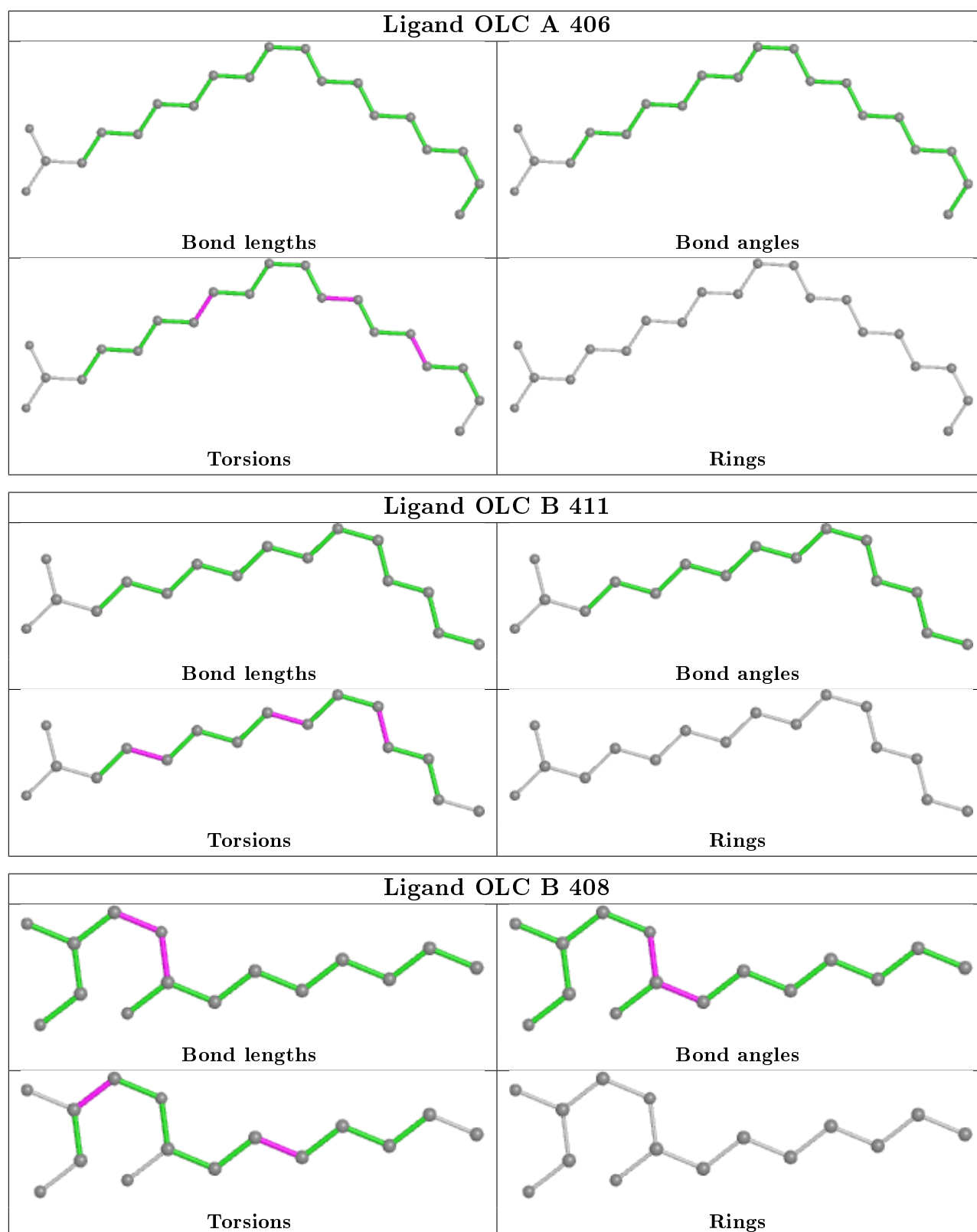












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	278/347 (80%)	0.35	32 (11%) 4 3	12, 25, 100, 114	0
1	B	284/347 (81%)	0.42	41 (14%) 2 1	12, 27, 101, 134	0
All	All	562/694 (80%)	0.38	73 (12%) 3 2	12, 26, 101, 134	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	VAL	7.2
1	B	327	THR	6.6
1	A	338	VAL	6.4
1	A	329	MET	5.6
1	B	335	GLU	5.5
1	B	61	LEU	5.5
1	B	63	ASN	5.4
1	B	341	PHE	5.2
1	A	339	GLU	5.0
1	B	325	LYS	5.0
1	A	322	ASP	5.0
1	B	329	MET	4.9
1	B	324	ARG	4.7
1	A	323	ILE	4.7
1	A	326	THR	4.6
1	B	183	LEU	4.6
1	B	323	ILE	4.5
1	B	64	ASN	4.5
1	A	324	ARG	4.5
1	A	59	TYR	4.5
1	A	341	PHE	4.3
1	A	182	GLY	4.2
1	A	335	GLU	4.1
1	B	318	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	336	VAL	4.0
1	B	322	ASP	3.9
1	A	327	THR	3.9
1	B	339	GLU	3.9
1	A	319	ILE	3.9
1	B	319	ILE	3.8
1	B	337	GLU	3.7
1	A	61	LEU	3.7
1	A	325	LYS	3.7
1	B	119	ALA	3.6
1	B	332	GLY	3.6
1	A	186	ASP	3.6
1	B	54	LEU	3.6
1	B	320	HIS	3.6
1	B	317	ILE	3.6
1	B	340	GLU	3.6
1	A	318	LEU	3.5
1	B	62	GLU	3.5
1	B	182	GLY	3.4
1	B	336	VAL	3.3
1	B	120	THR	3.2
1	B	56	GLN	3.2
1	B	186	ASP	3.1
1	B	333	GLY	3.1
1	B	59	TYR	3.1
1	B	326	THR	3.0
1	A	83	HIS	2.9
1	B	83	HIS	2.9
1	B	69	CYS	2.9
1	B	60	THR	2.8
1	A	69	CYS	2.8
1	A	63	ASN	2.7
1	B	68	ILE	2.7
1	A	67	VAL	2.7
1	A	337	GLU	2.4
1	A	333	GLY	2.4
1	B	187	TYR	2.4
1	A	64	ASN	2.4
1	A	120	THR	2.3
1	B	57	THR	2.3
1	B	334	GLU	2.2
1	A	247	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	66	SER	2.2
1	A	60	THR	2.1
1	B	65	GLY	2.1
1	A	62	GLU	2.1
1	A	185	ASN	2.1
1	B	55	PHE	2.0
1	A	187	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
1	LYR	A	299	29/30	0.91	0.19	7,25,39,43	0
1	LYR	B	299	29/30	0.92	0.17	9,21,32,37	0

6.3 Carbohydrates [i](#)

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, 95th 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.

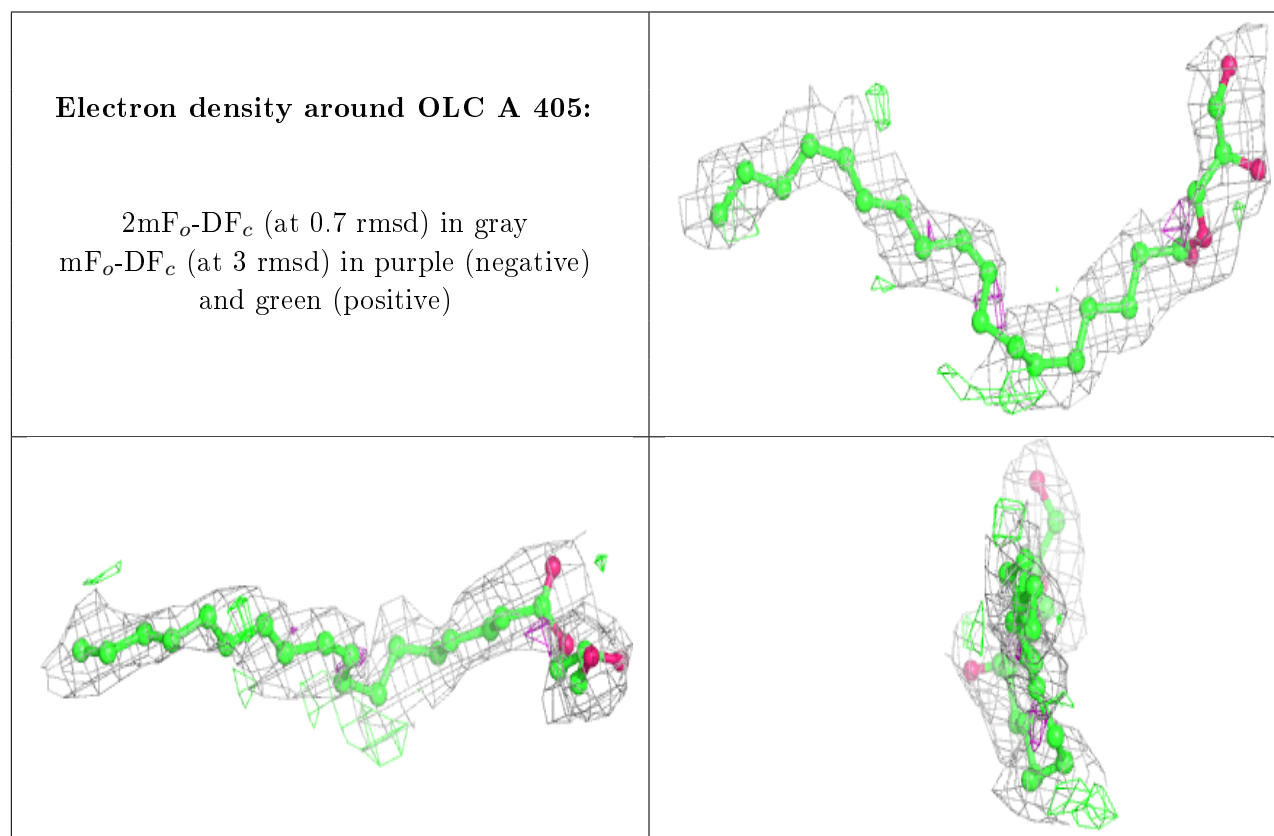
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	A	405	25/25	0.73	0.27	10,38,63,74	0
2	OLC	B	412	14/25	0.73	0.28	29,40,63,64	0
2	OLC	B	408	15/25	0.73	0.22	35,55,69,75	0
2	OLC	B	406	20/25	0.74	0.33	33,56,82,82	0
2	OLC	B	407	20/25	0.76	0.28	22,38,54,56	0
2	OLC	A	407	15/25	0.76	0.26	42,57,69,71	0
2	OLC	A	406	20/25	0.79	0.28	33,48,65,68	0
2	OLC	B	410	21/25	0.81	0.29	29,45,54,78	0
2	OLC	B	411	16/25	0.83	0.29	11,36,55,66	0

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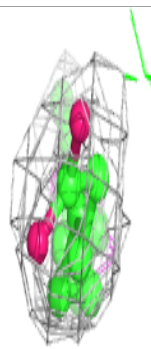
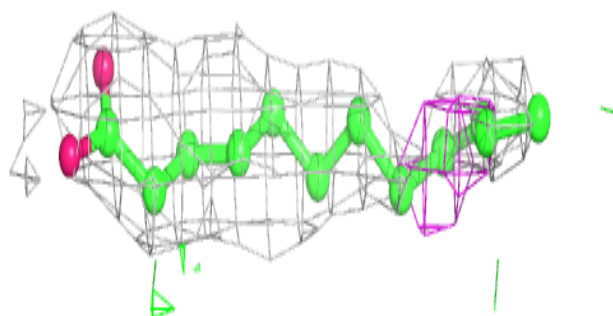
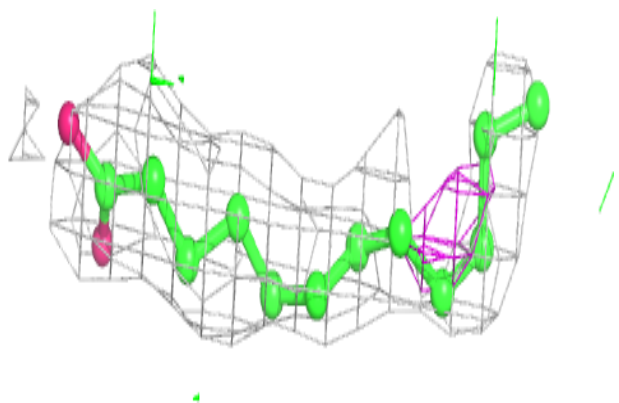
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	B	405	23/25	0.83	0.24	15,35,72,74	0
2	OLC	B	402	25/25	0.85	0.28	22,35,46,54	0
2	OLC	A	401	19/25	0.85	0.22	15,27,49,55	0
2	OLC	A	402	25/25	0.86	0.20	17,45,63,74	0
2	OLC	A	403	25/25	0.87	0.20	22,36,63,66	0
2	OLC	A	404	18/25	0.87	0.19	25,41,61,62	0
2	OLC	B	403	20/25	0.88	0.22	19,35,70,85	0
2	OLC	B	404	14/25	0.89	0.25	18,30,38,41	0
2	OLC	B	409	14/25	0.93	0.23	10,27,35,45	0
2	OLC	B	401	25/25	0.93	0.16	11,28,38,49	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.

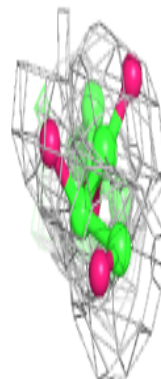
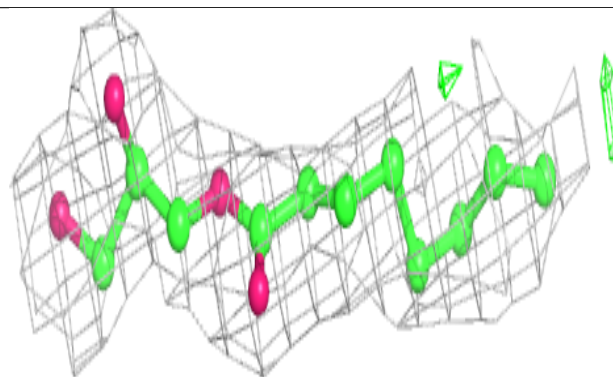
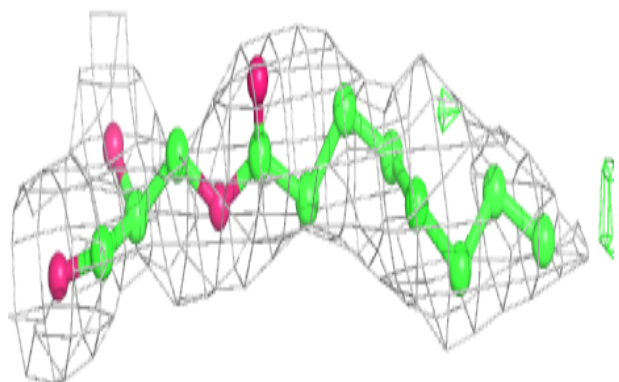


Electron density around OLC B 412:

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

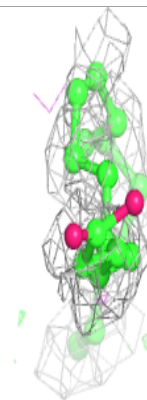
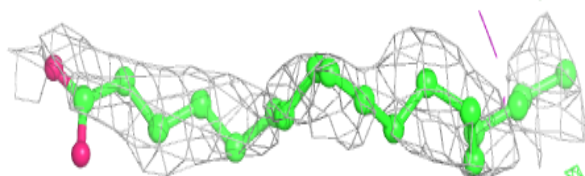
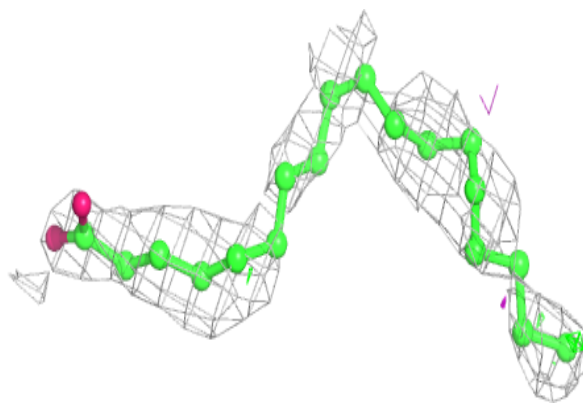
**Electron density around OLC B 408:**

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

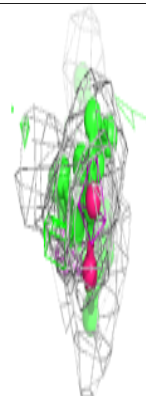
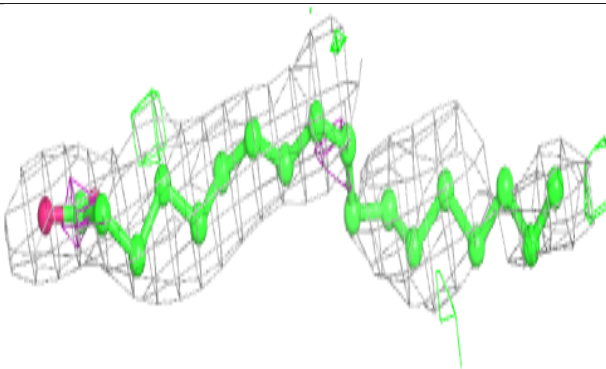
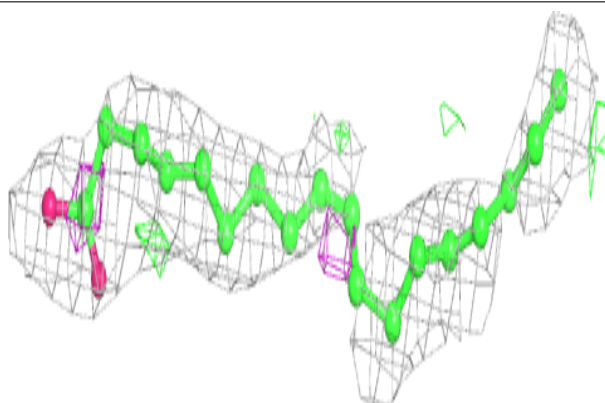


Electron density around OLC B 406:

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

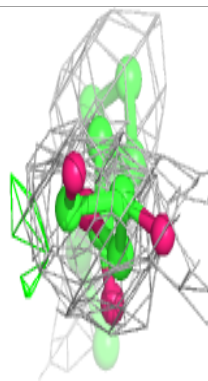
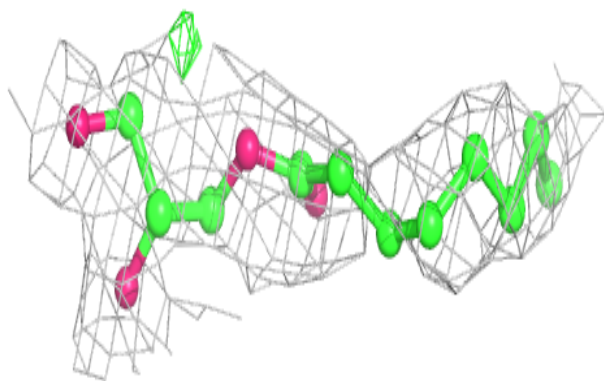
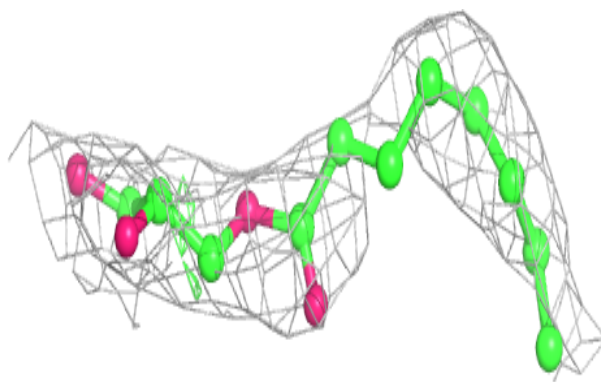
**Electron density around OLC B 407:**

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

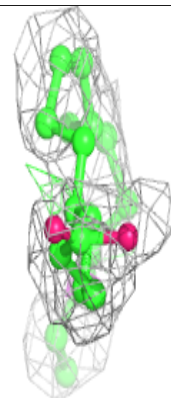
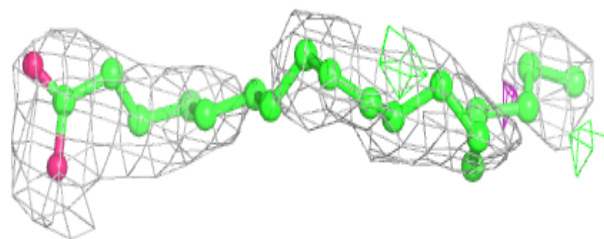
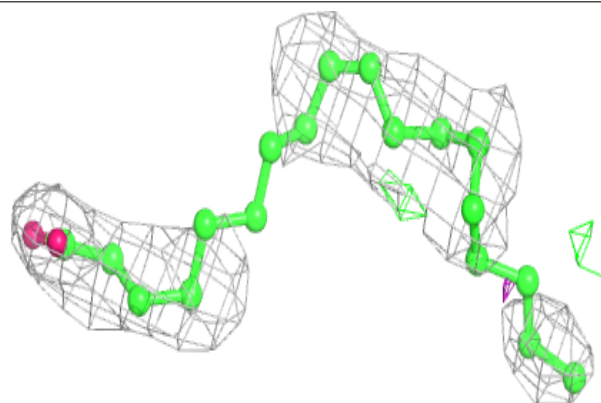


Electron density around OLC A 407:

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

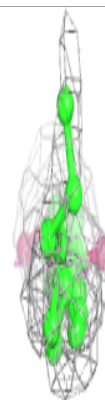
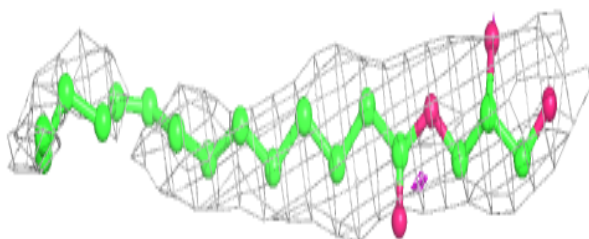
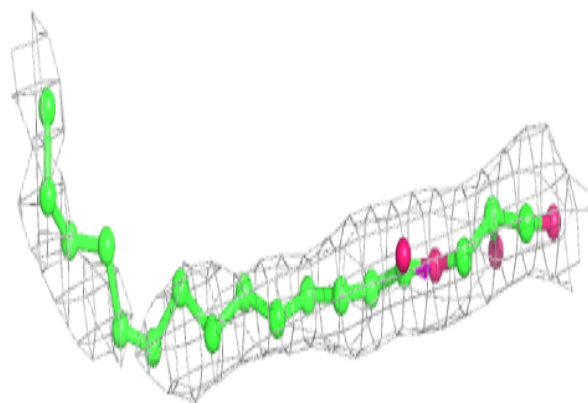
**Electron density around OLC A 406:**

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

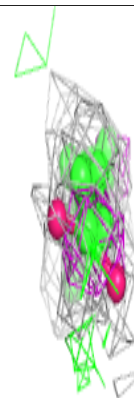
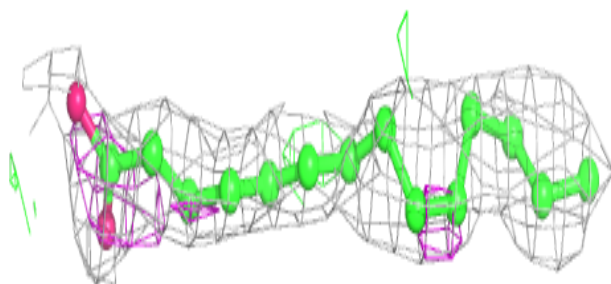
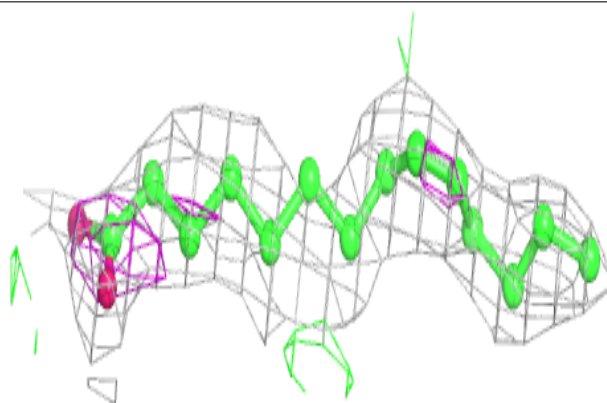


Electron density around OLC B 410:

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

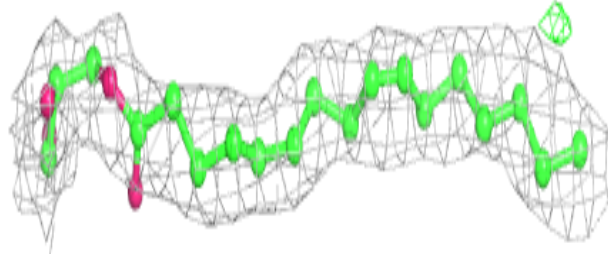
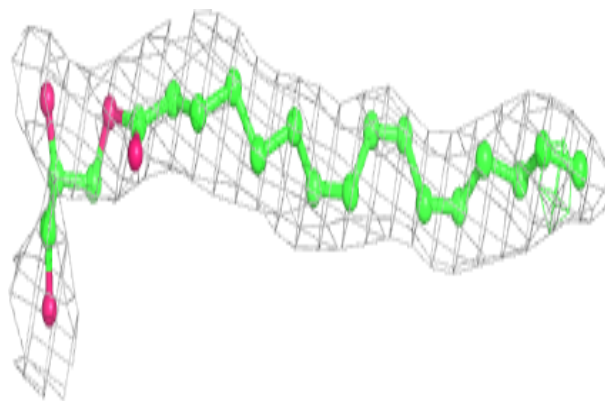
**Electron density around OLC B 411:**

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

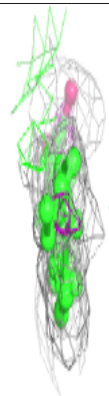
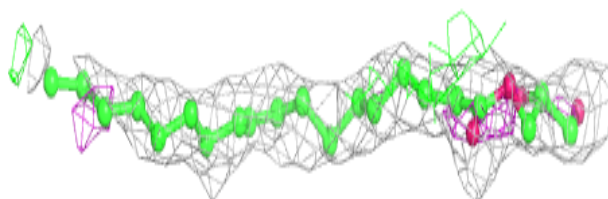
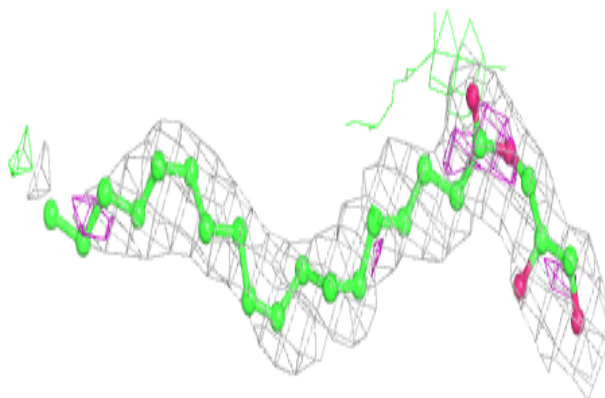


Electron density around OLC B 405:

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

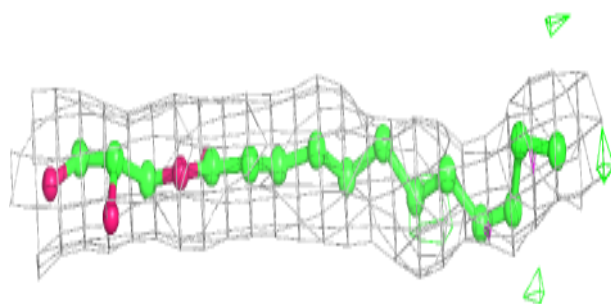
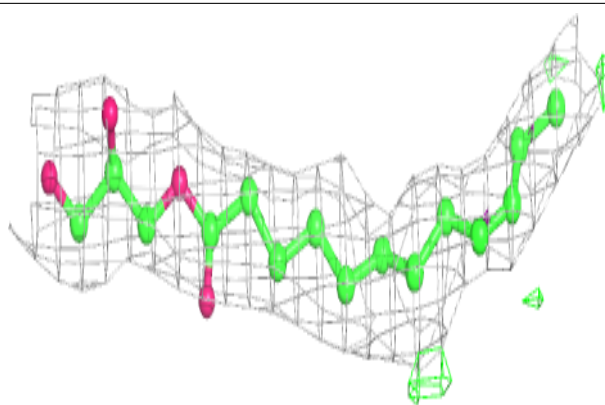
**Electron density around OLC B 402:**

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

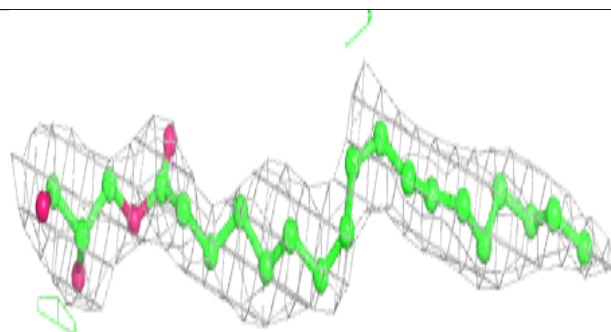
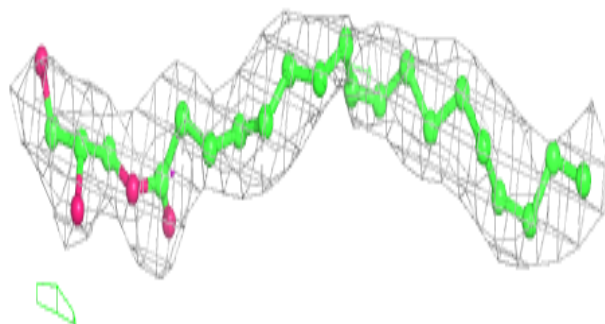


Electron density around OLC A 401:

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

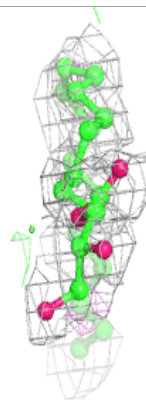
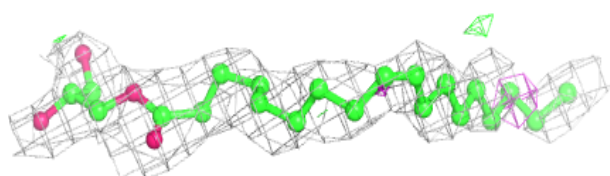
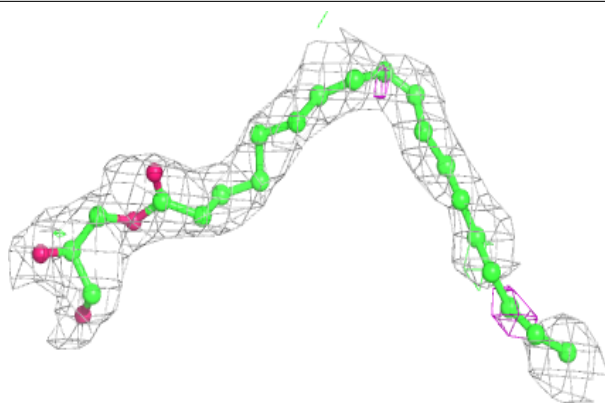
**Electron density around OLC A 402:**

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

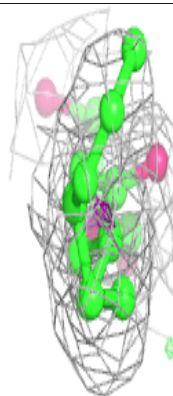
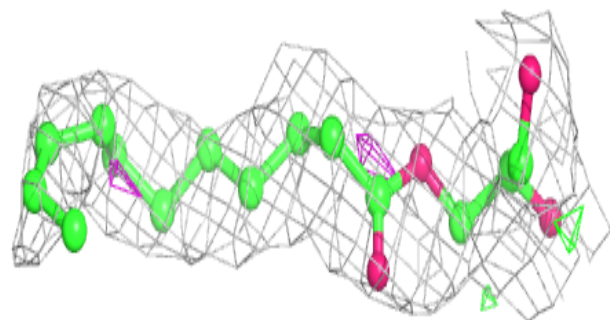
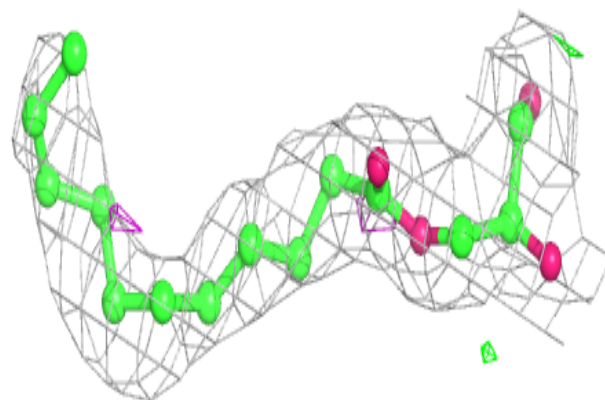


Electron density around OLC A 403:

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

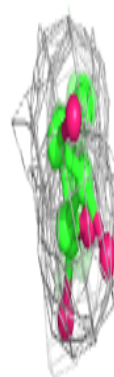
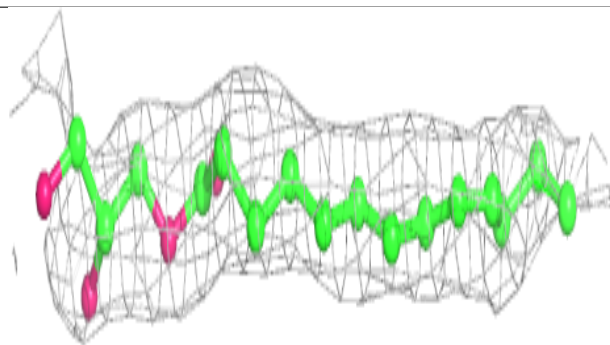
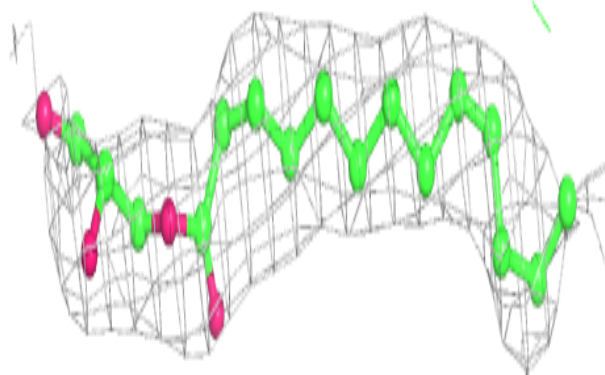
**Electron density around OLC A 404:**

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

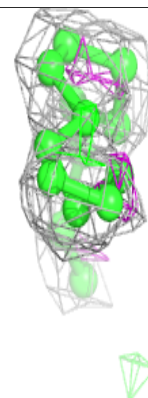
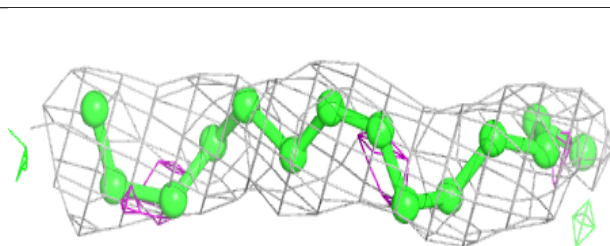
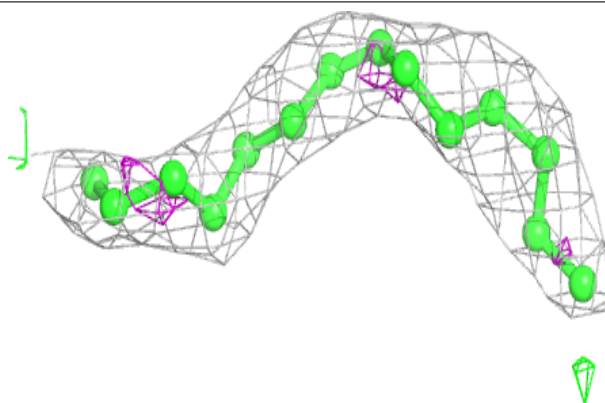


Electron density around OLC B 403:

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

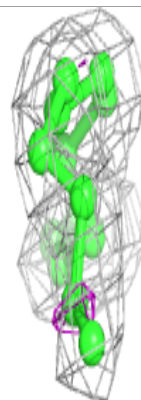
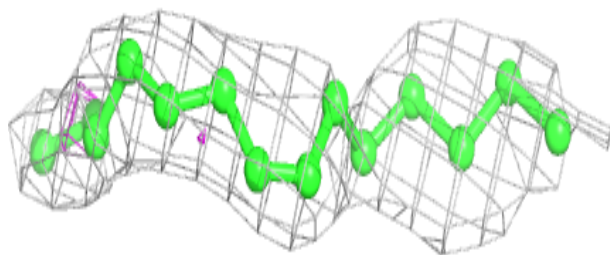
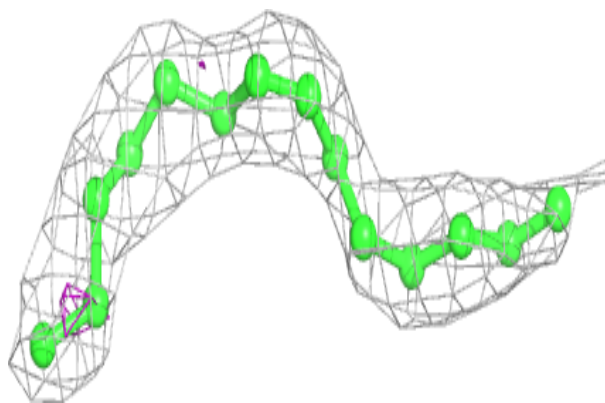
**Electron density around OLC B 404:**

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

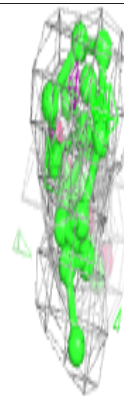
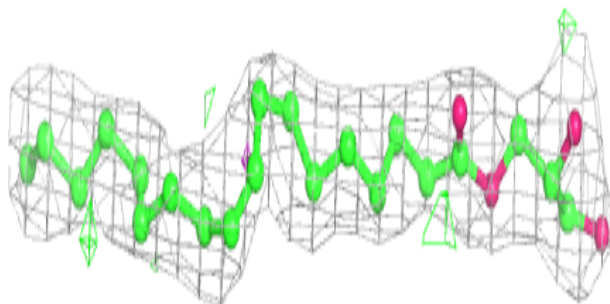
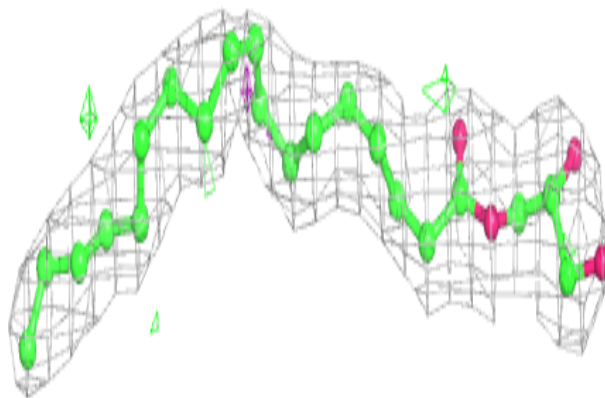


Electron density around OLC B 409:

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

**Electron density around OLC B 401:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.