



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:43 pm BST

PDB ID : 4E1T
Title : X-ray crystal structure of the transmembrane beta-domain from invasin from *Yersinia pseudotuberculosis*
Authors : Fairman, J.W.; Dautin, N.; Wojtowicz, D.; Wei, L.; Noinaj, N.; Barnard, T.J.; Udho, E.; Finkelstein, A.; Przytycka, T.M.; Cherezov, V.; Buchanan, S.K.
Deposited on : 2012-03-07
Resolution : 2.26 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 : 2.11
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) : 2.11

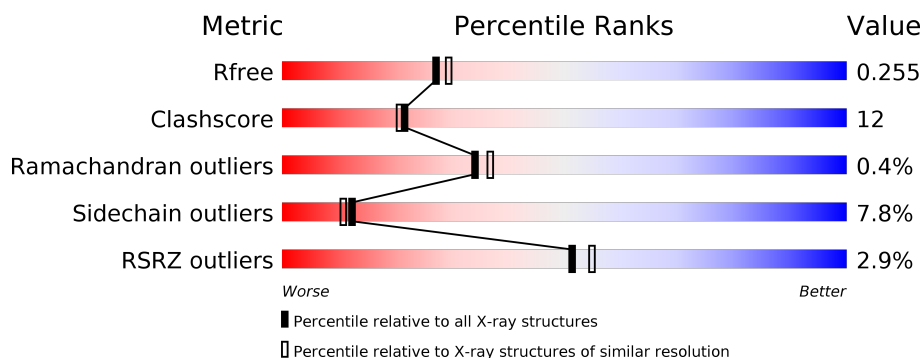
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	245	<div> <div>3%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2360 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.

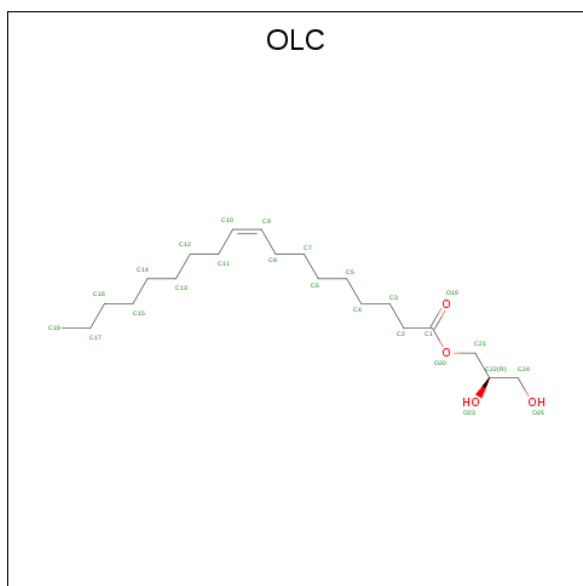
- Molecule 1 is a protein called Invasin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1960	1240	346	370	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	-	INITIATING METHIONINE	UNP P11922
A	352	PHE	LEU	ENGINEERED MUTATION	UNP P11922

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



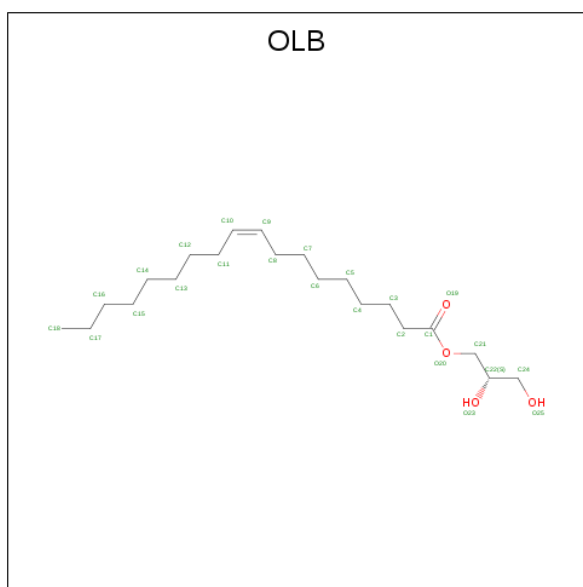
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			19	15	4		

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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 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 17 17	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
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 O 8 4 4	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 21 4	0	0

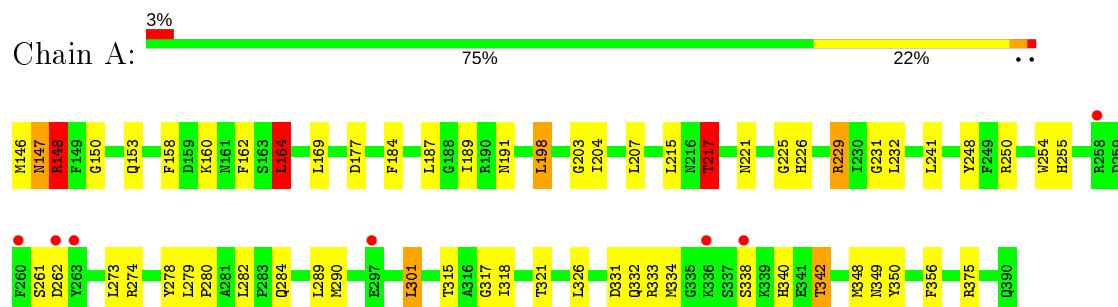
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total 117	O 117	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Invasin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.40 Å 124.89 Å 65.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.26 29.79 – 2.26	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.79-2.26) 90.6 (29.79-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.26 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.188 , 0.260 0.196 , 0.255	Depositor DCC
R_{free} test set	713 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2360	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.88	0/2009	0.90	6/2727 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	148	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	207	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	217	THR	CB-CA-C	-5.90	95.67	111.60
1	A	164	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	229	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	148	ARG	NE-CZ-NH2	5.13	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1960	0	1862	42	0
2	A	258	0	402	24	0
3	A	25	0	40	1	0
4	A	117	0	0	3	0
All	All	2360	0	2304	54	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 12.

All (54) 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:254:TRP:HE1	2:A:411:OLC:H24	1.43	0.84
1:A:177:ASP:OD2	1:A:375:ARG:NH2	2.11	0.83
1:A:146:MET:HG2	1:A:147:ASN:N	1.96	0.81
1:A:332:GLN:HG3	2:A:407:OLC:C1	2.14	0.78
1:A:160:LYS:HG3	4:A:541:HOH:O	1.83	0.77
1:A:318:ILE:HD11	2:A:407:OLC:H6	1.70	0.74
1:A:301:LEU:HD22	1:A:333:ARG:HH12	1.52	0.73
1:A:146:MET:HG2	1:A:147:ASN:H	1.51	0.73
2:A:408:OLC:H7	2:A:408:OLC:H3A	1.72	0.72
1:A:146:MET:CG	1:A:147:ASN:N	2.53	0.71
1:A:340:HIS:HE1	1:A:342:THR:HG22	1.58	0.67
1:A:226:HIS:ND1	2:A:401:OLC:H21A	2.13	0.63
1:A:229:ARG:HD2	1:A:248:TYR:HB3	1.80	0.61
1:A:356:PHE:HB2	2:A:408:OLC:H24A	1.83	0.59
1:A:340:HIS:CE1	1:A:342:THR:HG22	2.38	0.57
1:A:189:ILE:HG22	1:A:198:LEU:HD23	1.86	0.57
1:A:261:SER:O	1:A:262:ASP:HB2	2.05	0.57
1:A:148:ARG:NH1	1:A:150:GLY:O	2.36	0.57
1:A:274:ARG:HG2	1:A:290:MET:HE3	1.87	0.56
1:A:164:LEU:HD13	2:A:410:OLC:H24	1.88	0.54
1:A:215:LEU:HG	3:A:405:OLB:H2A	1.89	0.54
1:A:191:ASN:OD1	2:A:410:OLC:H22	2.09	0.52
1:A:217:THR:HG23	1:A:232:LEU:HD23	1.92	0.52
1:A:350:TYR:HB2	2:A:408:OLC:H11	1.92	0.52
2:A:410:OLC:H2	2:A:413:OLC:C1	2.40	0.52
1:A:225:GLY:O	1:A:255:HIS:HE1	1.93	0.51
2:A:401:OLC:H7A	4:A:524:HOH:O	2.11	0.51
1:A:217:THR:HG22	1:A:231:GLY:O	2.12	0.50
1:A:169:LEU:C	1:A:169:LEU:HD13	2.32	0.50
1:A:221:ASN:HD21	2:A:401:OLC:H3A	1.77	0.50
2:A:408:OLC:H7	2:A:408:OLC:C3	2.39	0.49
1:A:158:PHE:HB3	1:A:162:PHE:HA	1.94	0.49
2:A:401:OLC:H10	2:A:404:OLC:H12A	1.94	0.49
1:A:317:GLY:HA3	1:A:331:ASP:OD1	2.13	0.49
1:A:153:GLN:HG3	1:A:349:ASN:OD1	2.13	0.49
2:A:408:OLC:C7	2:A:408:OLC:H3A	2.41	0.48
1:A:301:LEU:HD22	1:A:333:ARG:NH1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD12	2:A:409:OLC:H7A	1.97	0.47
1:A:301:LEU:CD2	1:A:333:ARG:HH12	2.27	0.46
1:A:250:ARG:HD3	4:A:522:HOH:O	2.16	0.46
1:A:225:GLY:O	1:A:255:HIS:CE1	2.69	0.46
1:A:321:THR:HG23	1:A:326:LEU:O	2.17	0.45
2:A:404:OLC:O19	2:A:409:OLC:H2	2.18	0.44
1:A:232:LEU:HD21	2:A:402:OLC:H6	1.98	0.44
1:A:318:ILE:HD11	2:A:407:OLC:C6	2.45	0.42
2:A:410:OLC:H2	2:A:413:OLC:O19	2.19	0.42
2:A:409:OLC:H8	2:A:409:OLC:H11A	1.69	0.42
1:A:278:TYR:O	1:A:280:PRO:HD3	2.20	0.41
2:A:402:OLC:H21	2:A:411:OLC:H12A	2.02	0.41
2:A:408:OLC:H13A	2:A:408:OLC:H10	1.60	0.41
1:A:184:PHE:CZ	1:A:203:GLY:HA3	2.56	0.41
1:A:160:LYS:HG2	1:A:342:THR:HG23	2.02	0.41
2:A:411:OLC:H13	2:A:411:OLC:H10	1.71	0.41
1:A:315:THR:OG1	1:A:333:ARG:HG3	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	243/245 (99%)	236 (97%)	6 (2%)	1 (0%)	34 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASN

5.3.2 Protein sidechains ⓘ

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	204/206 (99%)	188 (92%)	16 (8%)	12	11

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	164	LEU
1	A	198	LEU
1	A	204	ILE
1	A	217	THR
1	A	241	LEU
1	A	273	LEU
1	A	279	LEU
1	A	282	LEU
1	A	284	GLN
1	A	289	LEU
1	A	301	LEU
1	A	334	MET
1	A	338	SER
1	A	342	THR
1	A	348	MET

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	408	-	24,24,24	1.04	1 (4%)	25,25,25	0.83	0
2	OLC	A	403	-	24,24,24	0.99	1 (4%)	25,25,25	0.97	2 (8%)
2	OLC	A	409	-	24,24,24	1.03	1 (4%)	25,25,25	1.03	1 (4%)
2	OLC	A	413	-	7,7,24	1.49	1 (14%)	6,7,25	1.33	0
2	OLC	A	407	-	16,16,24	0.32	0	15,15,25	0.56	0
3	OLB	A	405	-	24,24,24	1.16	1 (4%)	25,25,25	1.14	2 (8%)
2	OLC	A	411	-	24,24,24	0.92	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	A	404	-	24,24,24	1.22	1 (4%)	25,25,25	1.15	3 (12%)
2	OLC	A	401	-	24,24,24	1.35	1 (4%)	25,25,25	1.07	2 (8%)
2	OLC	A	402	-	18,18,24	1.22	1 (5%)	18,19,25	0.95	1 (5%)
2	OLC	A	406	-	24,24,24	1.13	1 (4%)	25,25,25	0.77	2 (8%)
2	OLC	A	412	-	13,13,24	0.42	0	12,12,25	0.57	0
2	OLC	A	410	-	24,24,24	1.17	1 (4%)	25,25,25	1.18	4 (16%)

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	408	-	-	14/24/24/24	-
2	OLC	A	403	-	-	12/24/24/24	-
2	OLC	A	409	-	-	14/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	413	-	-	3/6/6/24	-
2	OLC	A	407	-	-	8/14/14/24	-
3	OLB	A	405	-	-	15/24/24/24	-
2	OLC	A	411	-	-	18/24/24/24	-
2	OLC	A	404	-	-	11/24/24/24	-
2	OLC	A	401	-	-	13/24/24/24	-
2	OLC	A	402	-	-	6/18/18/24	-
2	OLC	A	406	-	-	11/24/24/24	-
2	OLC	A	412	-	-	5/11/11/24	-
2	OLC	A	410	-	-	15/24/24/24	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	OLC	O20-C1	6.26	1.51	1.33
2	A	404	OLC	O20-C1	5.51	1.49	1.33
3	A	405	OLB	O20-C1	5.24	1.48	1.33
2	A	410	OLC	O20-C1	5.22	1.48	1.33
2	A	406	OLC	O20-C1	4.93	1.47	1.33
2	A	402	OLC	O20-C1	4.91	1.47	1.33
2	A	409	OLC	O20-C1	4.70	1.47	1.33
2	A	408	OLC	O20-C1	4.49	1.46	1.33
2	A	403	OLC	O20-C1	4.31	1.45	1.33
2	A	411	OLC	O20-C1	4.29	1.45	1.33
2	A	413	OLC	O20-C1	3.57	1.47	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	404	OLC	O20-C1-C2	4.02	124.52	111.91
3	A	405	OLB	O20-C1-C2	3.85	123.99	111.91
2	A	403	OLC	O20-C1-C2	3.38	122.52	111.91
2	A	410	OLC	O20-C1-C2	3.30	122.27	111.91
2	A	409	OLC	O20-C1-C2	3.20	121.95	111.91
2	A	402	OLC	O20-C1-C2	2.97	121.23	111.91
2	A	411	OLC	O20-C1-C2	2.61	120.11	111.91
3	A	405	OLB	O20-C21-C22	2.60	118.31	105.77
2	A	403	OLC	O20-C1-O19	-2.58	117.07	123.59
2	A	410	OLC	O20-C1-O19	-2.56	117.14	123.59
2	A	401	OLC	O20-C1-C2	2.40	119.43	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	404	OLC	O20-C21-C22	2.37	117.21	105.77
2	A	410	OLC	C21-O20-C1	2.27	125.54	117.12
2	A	406	OLC	O20-C1-C2	2.14	118.62	111.91
2	A	406	OLC	O20-C1-O19	-2.09	118.32	123.59
2	A	404	OLC	O20-C1-O19	-2.06	118.38	123.59
2	A	401	OLC	C21-O20-C1	2.05	124.73	117.12
2	A	410	OLC	O20-C21-C22	2.00	115.45	105.77

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	OLC	O20-C21-C22-O23
2	A	409	OLC	O20-C21-C22-C24
2	A	409	OLC	O20-C21-C22-O23
2	A	413	OLC	O20-C21-C22-O23
2	A	413	OLC	O19-C1-O20-C21
3	A	405	OLB	O20-C21-C22-C24
3	A	405	OLB	C21-C22-C24-O25
2	A	411	OLC	C21-C22-C24-O25
2	A	411	OLC	C2-C1-O20-C21
2	A	411	OLC	O19-C1-O20-C21
2	A	404	OLC	O20-C21-C22-O23
2	A	402	OLC	C21-C22-C24-O25
2	A	402	OLC	O23-C22-C24-O25
2	A	410	OLC	C21-C22-C24-O25
2	A	410	OLC	O23-C22-C24-O25
2	A	410	OLC	O20-C21-C22-C24
2	A	410	OLC	O20-C21-C22-O23
2	A	410	OLC	C2-C1-O20-C21
2	A	410	OLC	O19-C1-O20-C21
2	A	404	OLC	O19-C1-O20-C21
2	A	406	OLC	O19-C1-O20-C21
2	A	404	OLC	C2-C1-O20-C21
2	A	406	OLC	C2-C1-O20-C21
2	A	401	OLC	C2-C1-O20-C21
2	A	401	OLC	O19-C1-O20-C21
2	A	404	OLC	C10-C11-C12-C13
2	A	408	OLC	C1-C2-C3-C4
2	A	411	OLC	O20-C21-C22-C24
2	A	409	OLC	C1-C2-C3-C4
2	A	404	OLC	C1-C2-C3-C4

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

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

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Mol	Chain	Res	Type	Atoms
2	A	401	OLC	C6-C7-C8-C9
2	A	404	OLC	C14-C15-C16-C17
2	A	413	OLC	O20-C21-C22-C24
2	A	411	OLC	C15-C16-C17-C18
2	A	403	OLC	C13-C14-C15-C16
2	A	412	OLC	C6-C7-C8-C9
2	A	410	OLC	C3-C4-C5-C6
2	A	403	OLC	O19-C1-O20-C21
2	A	403	OLC	C2-C1-O20-C21
2	A	407	OLC	C3-C4-C5-C6
2	A	407	OLC	C7-C8-C9-C10
2	A	401	OLC	C3-C4-C5-C6
2	A	411	OLC	C7-C8-C9-C10
2	A	403	OLC	C14-C15-C16-C17
2	A	404	OLC	C5-C6-C7-C8
2	A	401	OLC	C5-C6-C7-C8
3	A	405	OLB	C7-C8-C9-C10
2	A	403	OLC	C7-C8-C9-C10
2	A	411	OLC	C9-C10-C11-C12
2	A	406	OLC	C15-C16-C17-C18
3	A	405	OLB	O19-C1-O20-C21
2	A	408	OLC	C9-C10-C11-C12
3	A	405	OLB	C2-C1-O20-C21
3	A	405	OLB	C9-C10-C11-C12
2	A	408	OLC	O23-C22-C24-O25
2	A	402	OLC	C5-C6-C7-C8
2	A	411	OLC	C12-C13-C14-C15
2	A	406	OLC	C7-C8-C9-C10
2	A	406	OLC	C9-C10-C11-C12
2	A	408	OLC	C3-C4-C5-C6
2	A	401	OLC	C9-C10-C11-C12

There are no ring outliers.

10 monomers are involved in 25 short contacts:

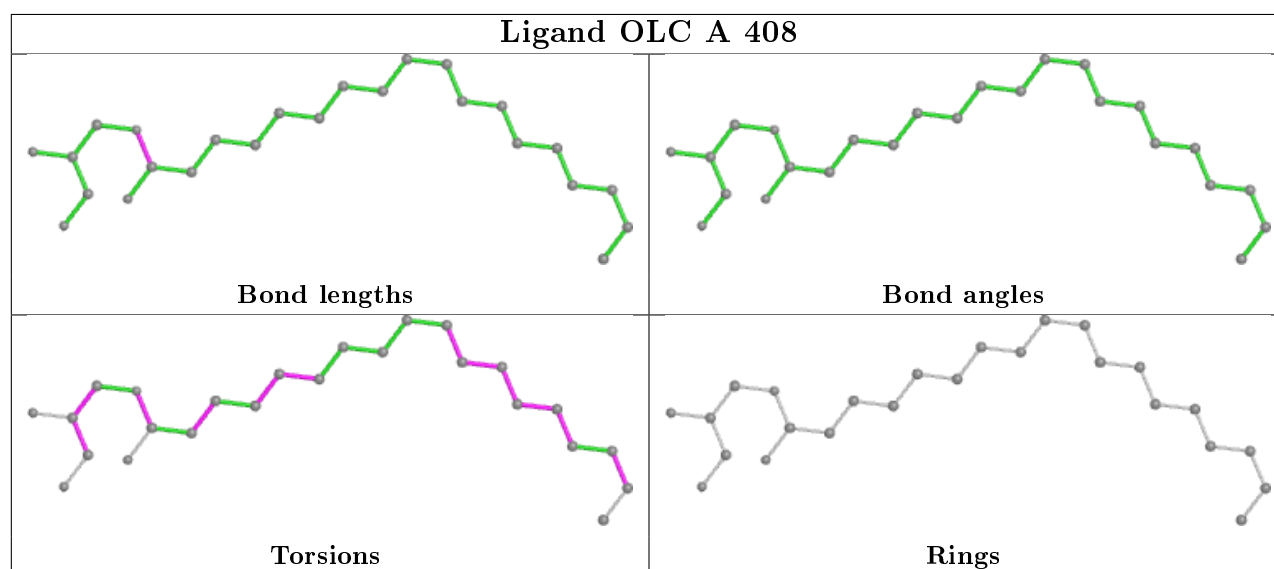
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	408	OLC	6	0
2	A	409	OLC	3	0
2	A	413	OLC	2	0
2	A	407	OLC	3	0
3	A	405	OLB	1	0
2	A	411	OLC	3	0

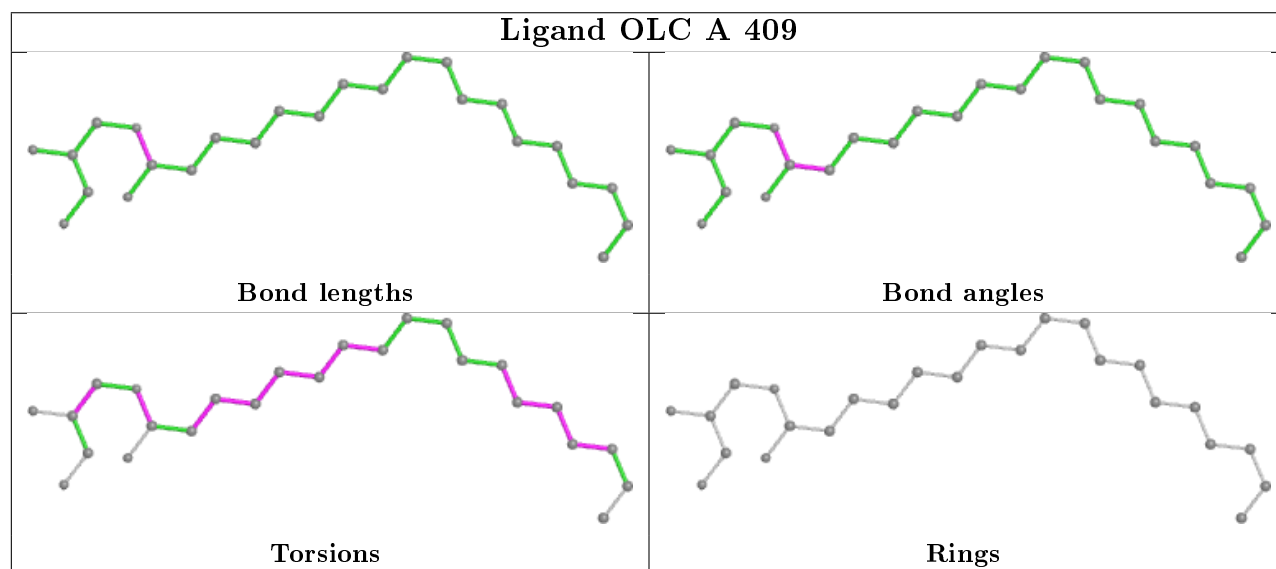
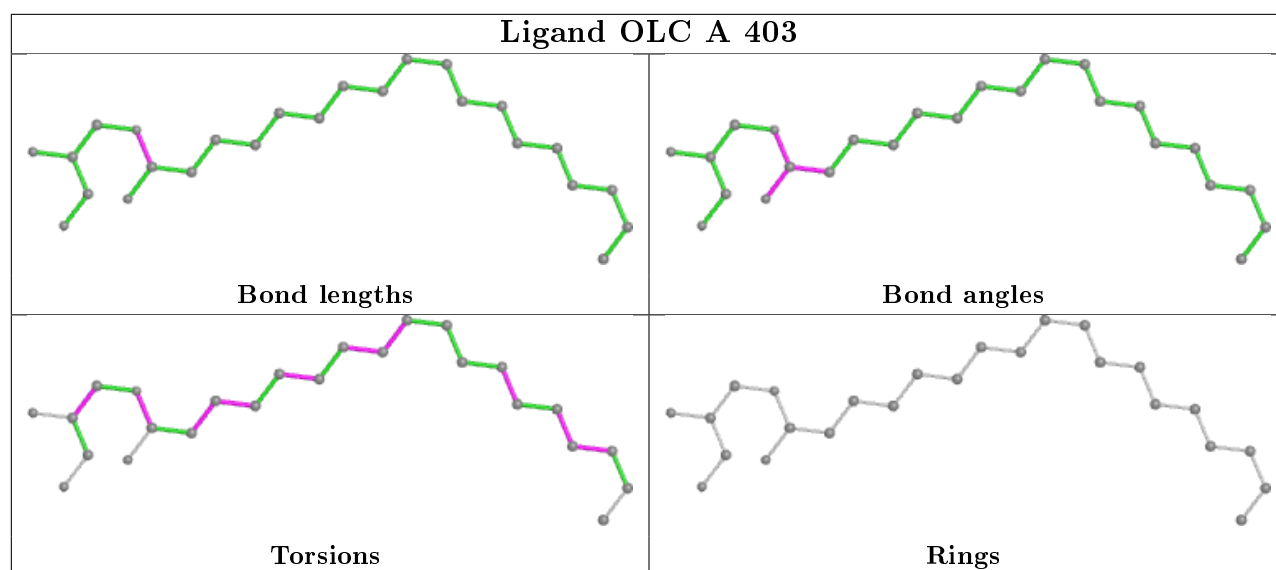
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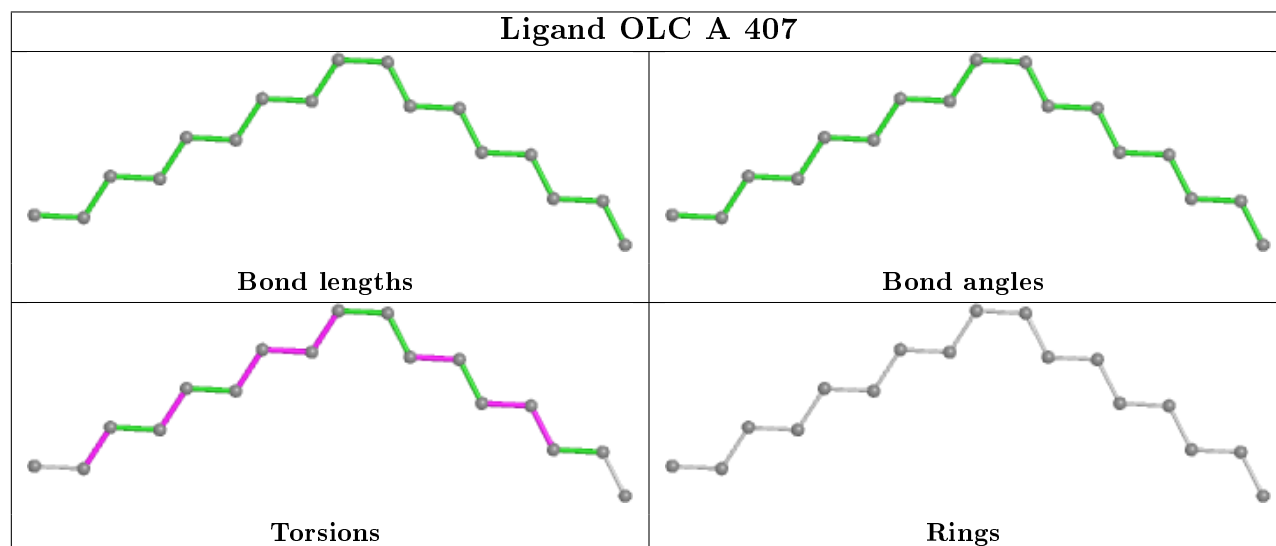
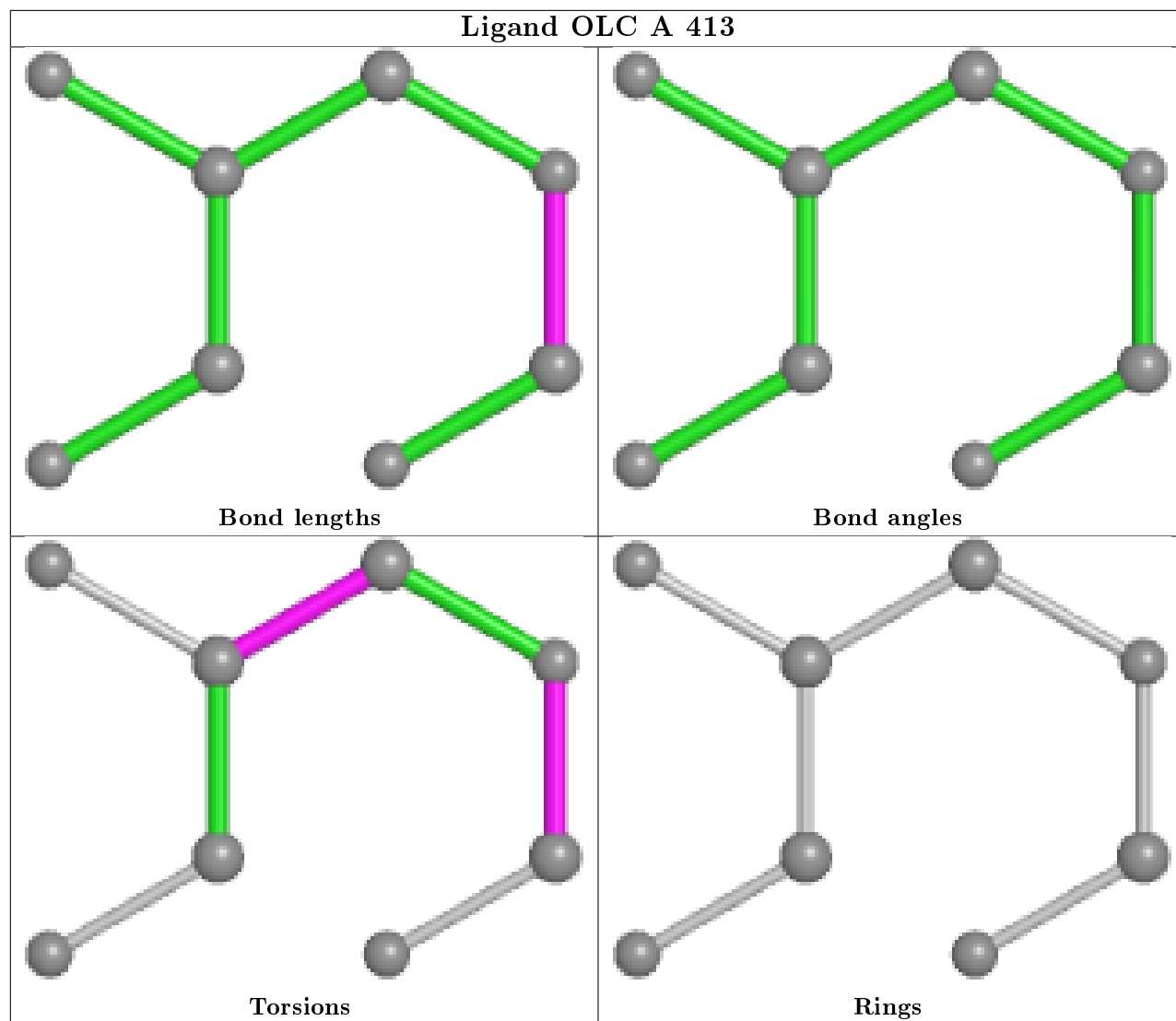
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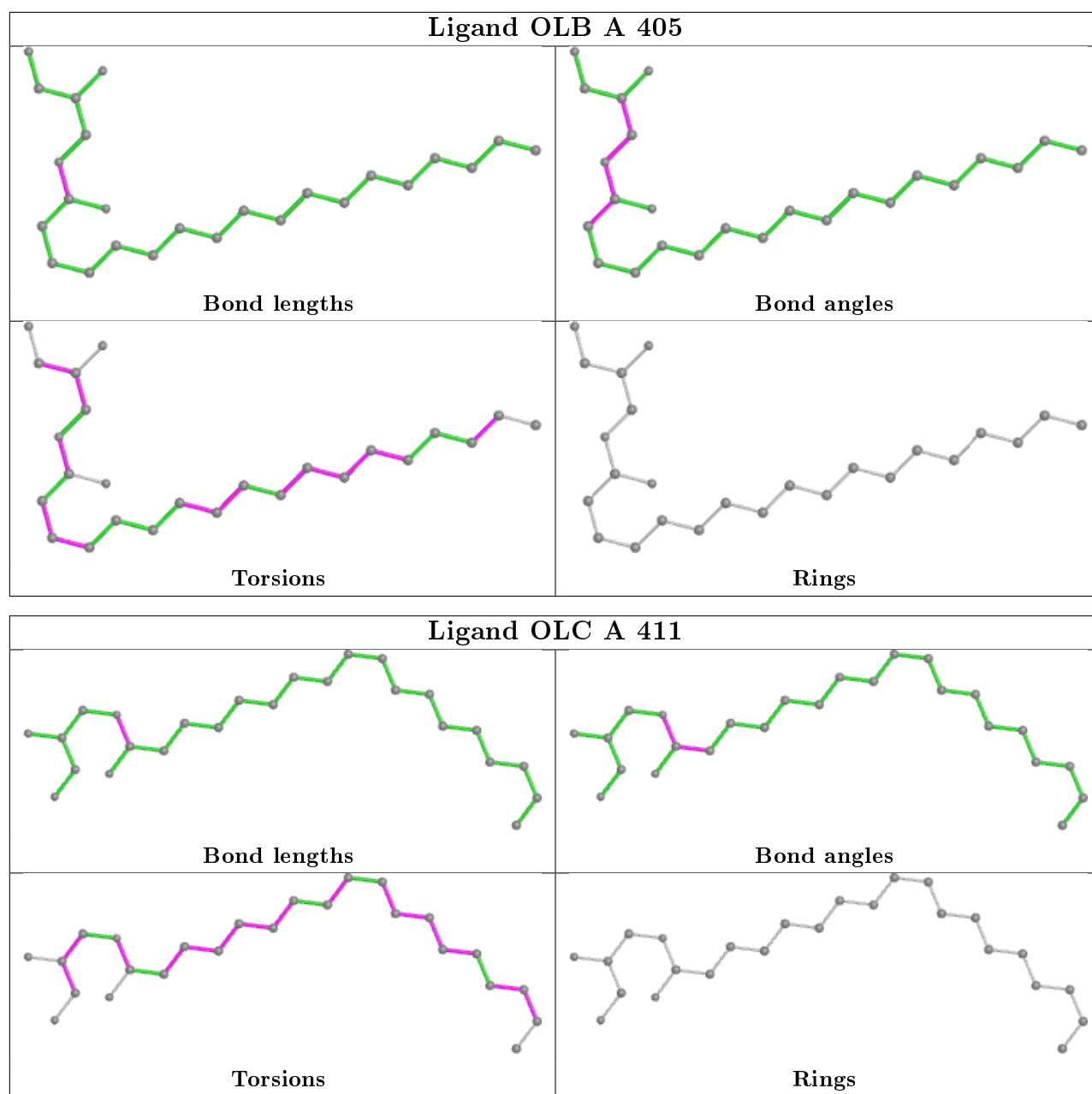
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	OLC	2	0
2	A	401	OLC	4	0
2	A	402	OLC	2	0
2	A	410	OLC	4	0

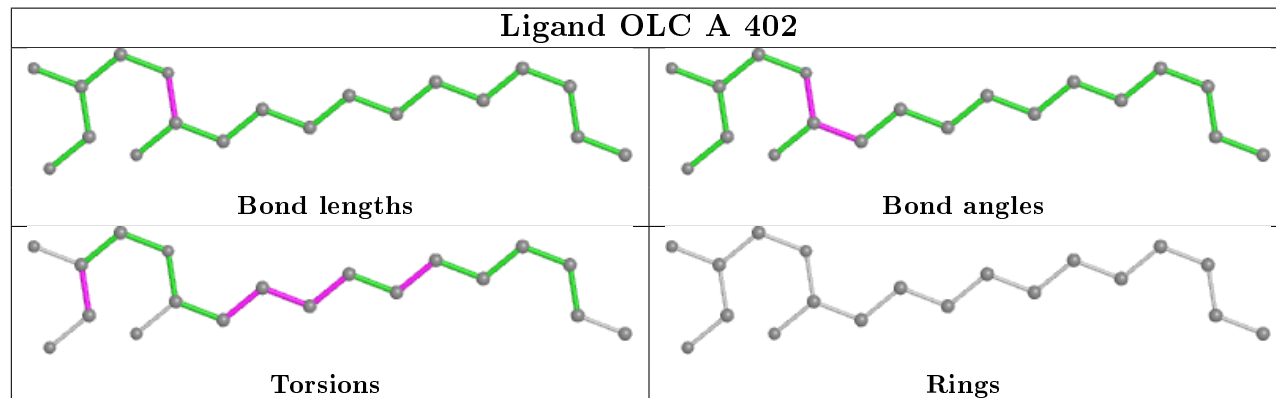
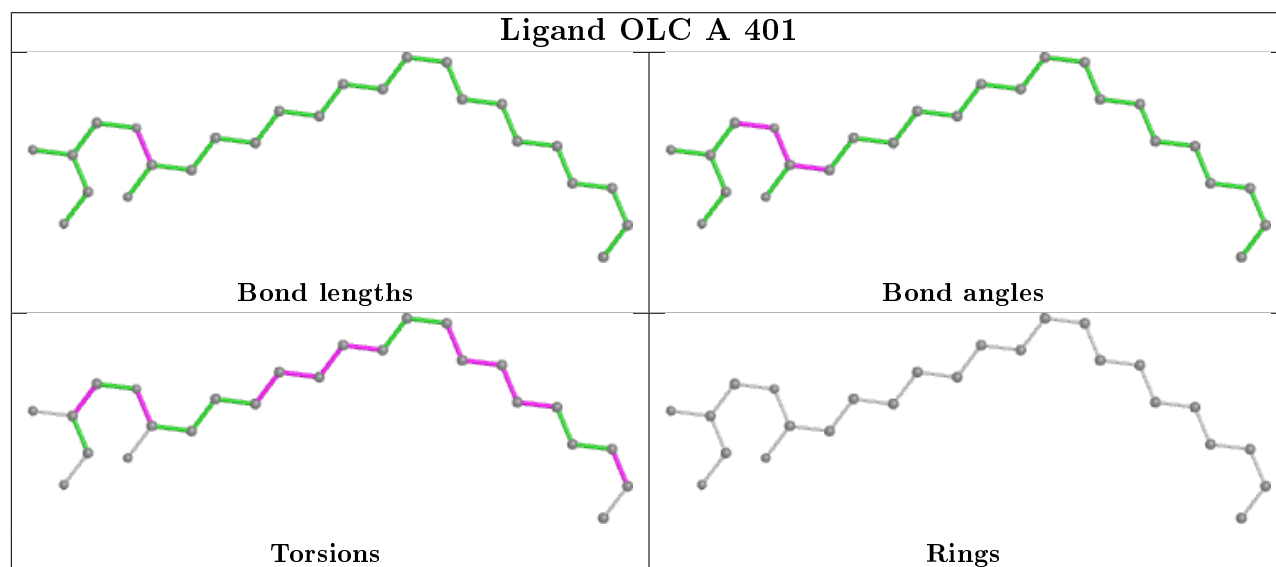
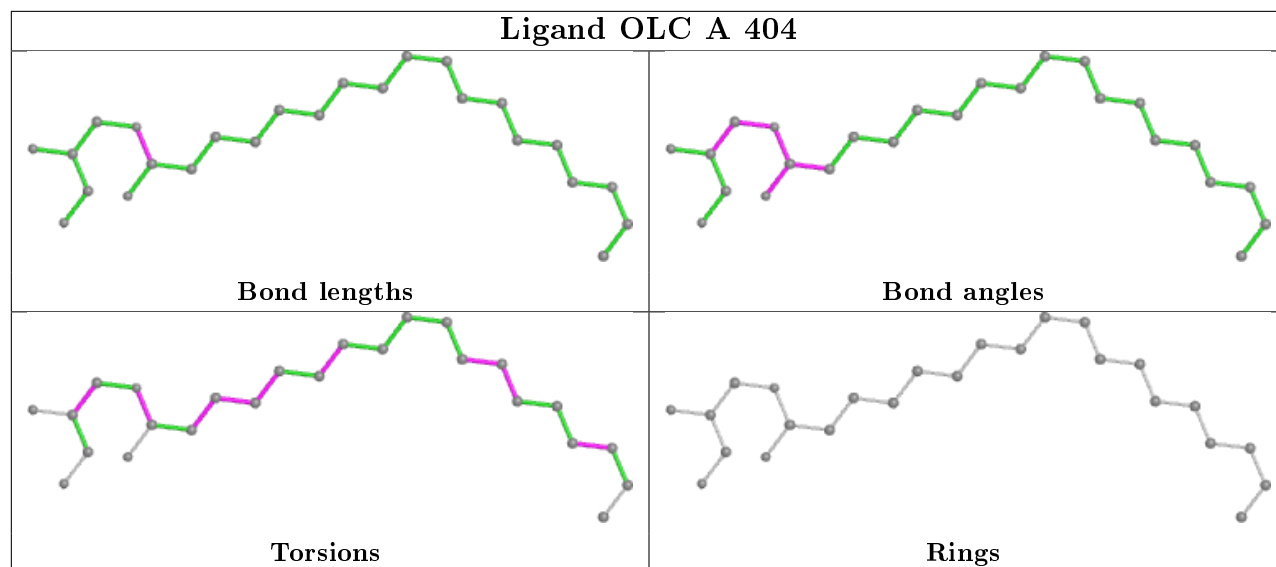
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

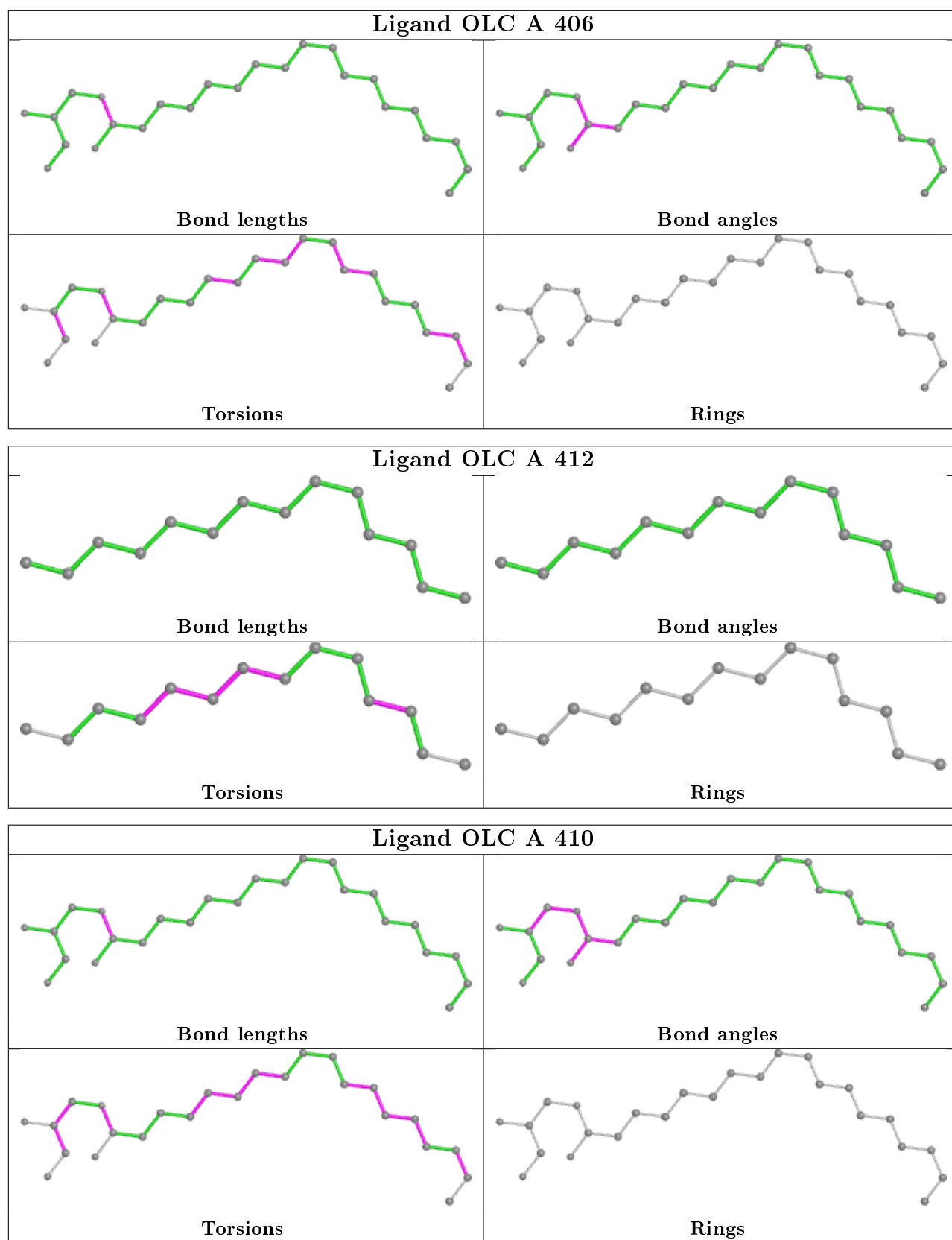












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	245/245 (100%)	-0.15	7 (2%) 51 55	30, 45, 63, 84	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	GLU	2.7
1	A	260	PHE	2.4
1	A	258	ARG	2.4
1	A	338	SER	2.2
1	A	336	LYS	2.2
1	A	262	ASP	2.2
1	A	263	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

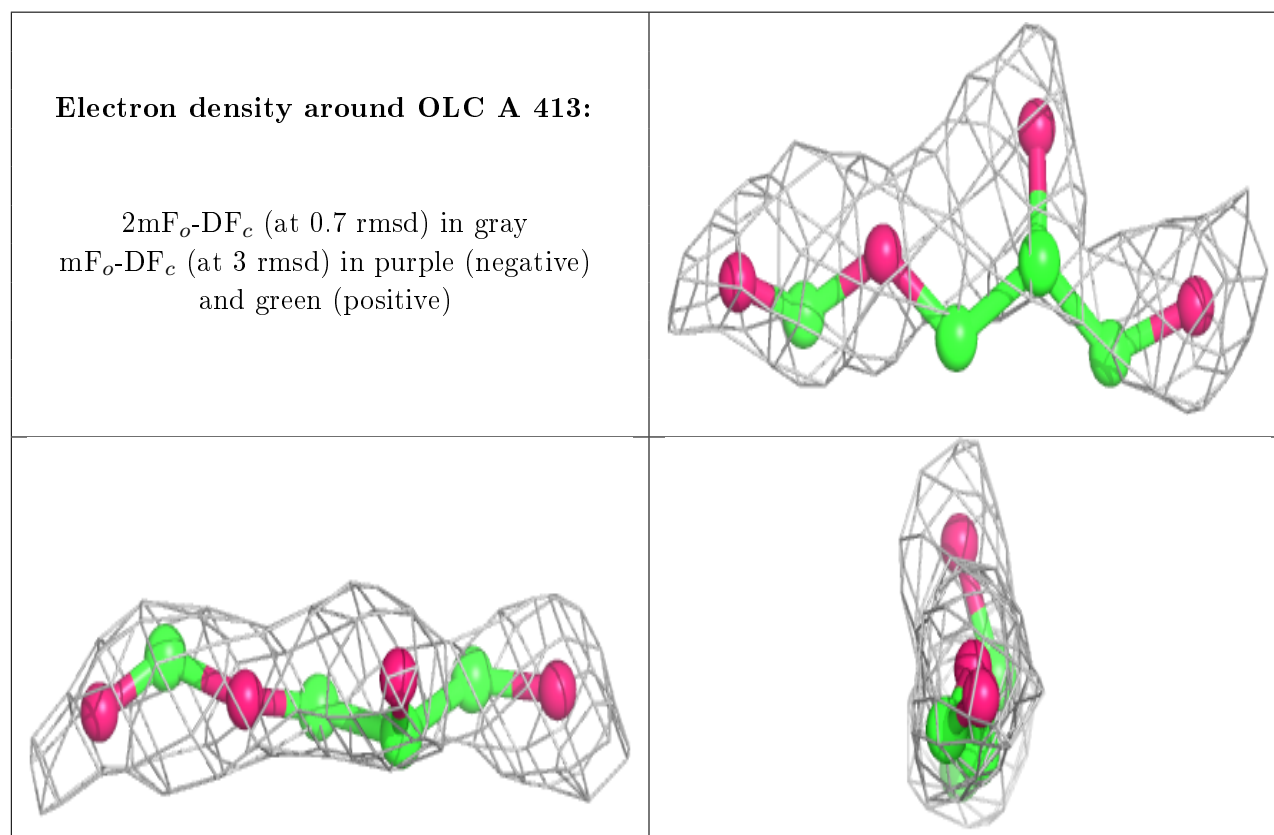
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	A	413	8/25	0.61	0.39	72,77,83,84	0

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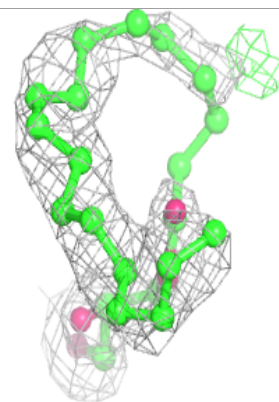
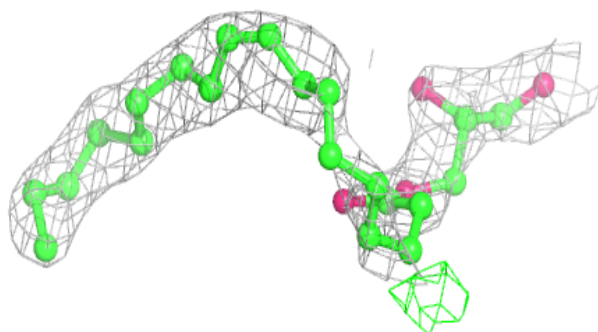
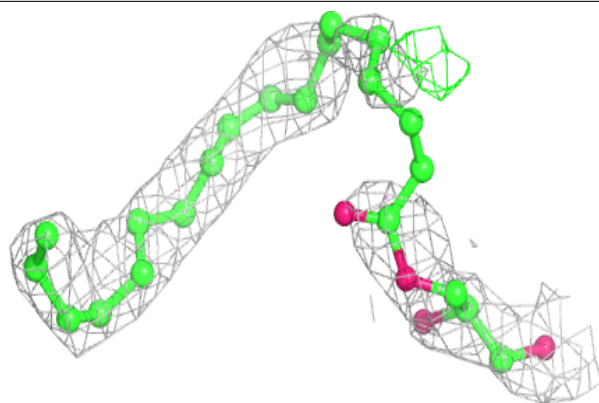
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	A	410	25/25	0.65	0.28	63,78,81,81	0
2	OLC	A	406	25/25	0.66	0.26	66,73,89,89	0
2	OLC	A	401	25/25	0.72	0.21	54,62,71,72	0
2	OLC	A	403	25/25	0.72	0.28	79,86,95,96	0
2	OLC	A	408	25/25	0.72	0.23	63,74,78,78	0
2	OLC	A	412	14/25	0.73	0.25	57,60,67,68	0
2	OLC	A	404	25/25	0.73	0.24	74,78,81,81	0
2	OLC	A	411	25/25	0.74	0.21	78,87,92,93	0
3	OLB	A	405	25/25	0.77	0.25	68,74,76,77	0
2	OLC	A	407	17/25	0.79	0.24	56,63,69,70	0
2	OLC	A	402	19/25	0.91	0.17	52,61,66,69	0
2	OLC	A	409	25/25	0.91	0.15	43,55,66,67	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.

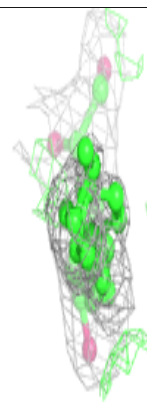
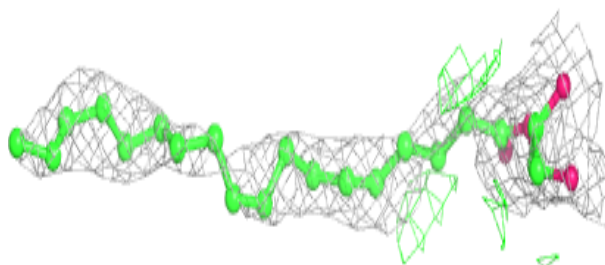
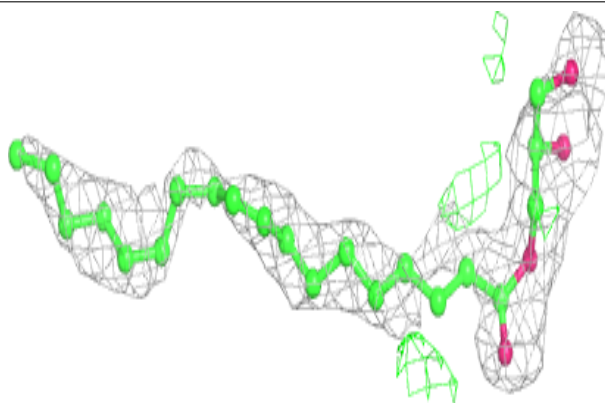


Electron density around OLC A 410:

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

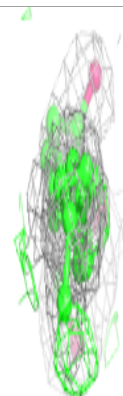
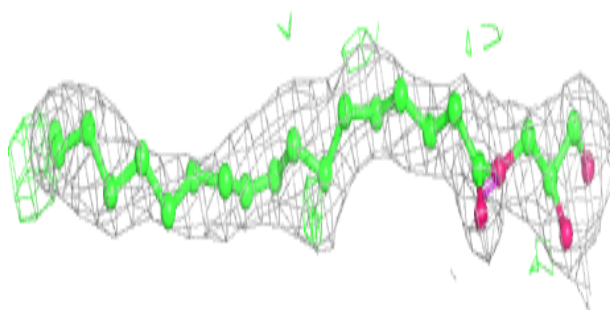
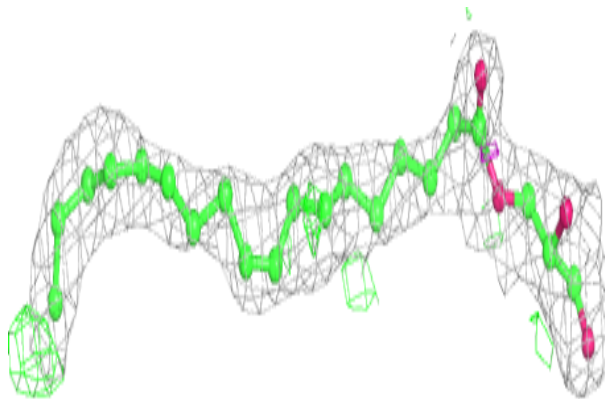
**Electron density around OLC A 406:**

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

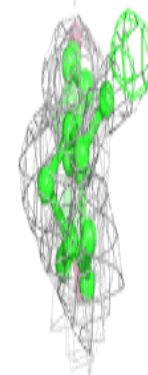
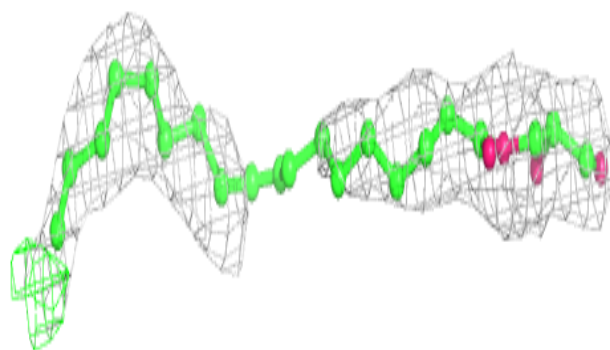
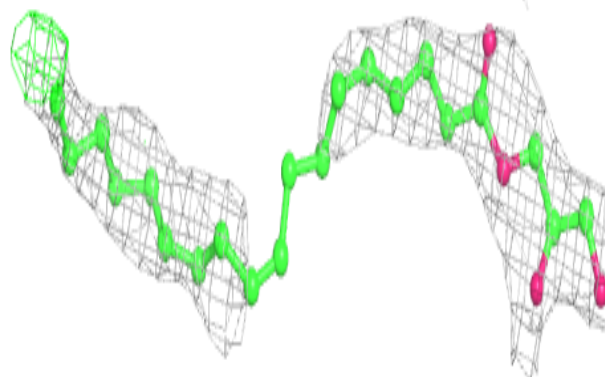


Electron density around OLC A 401:

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

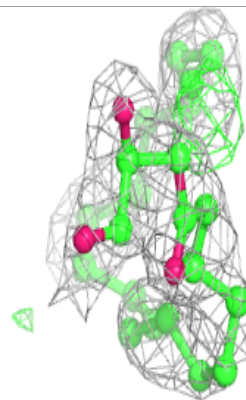
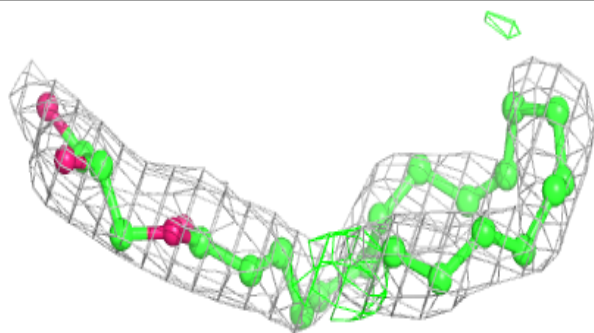
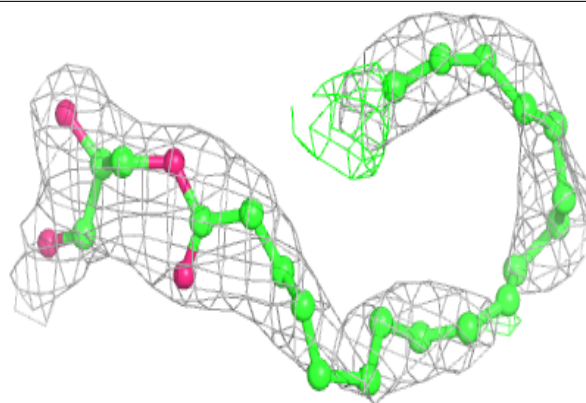
**Electron density around OLC A 403:**

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

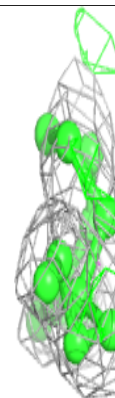
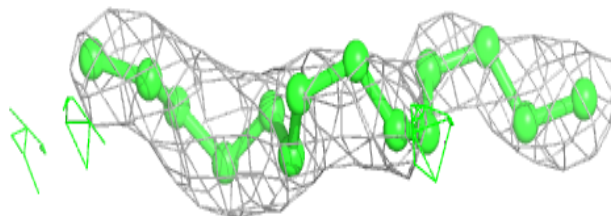
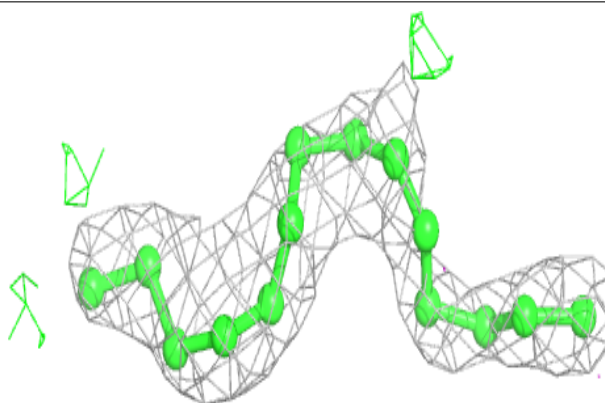


Electron density around OLC A 408:

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

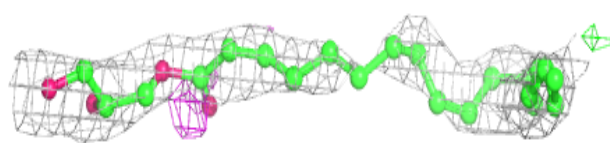
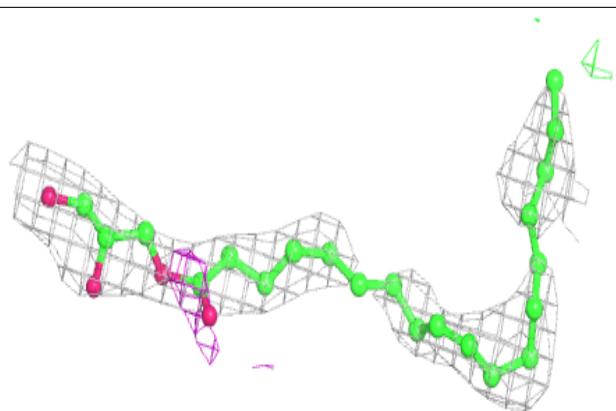
**Electron density around OLC A 412:**

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

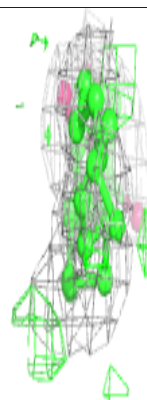
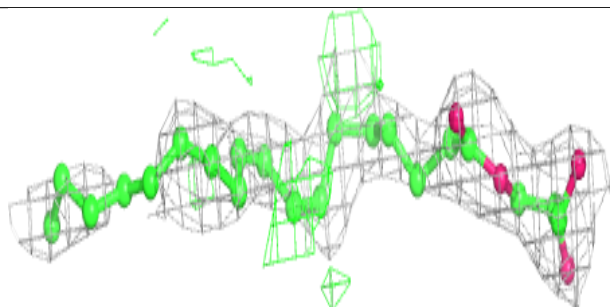
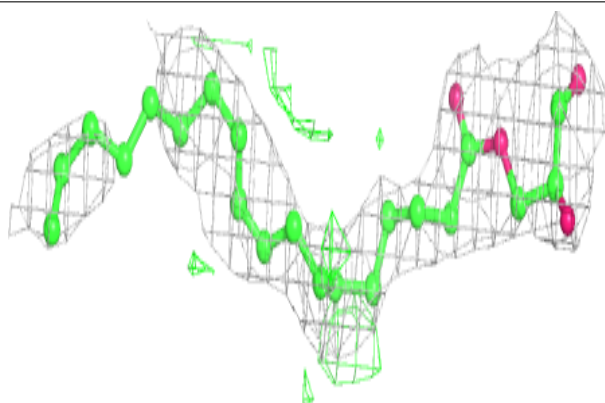


Electron density around OLC A 404:

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

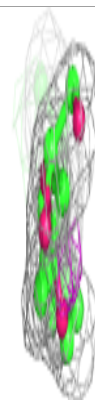
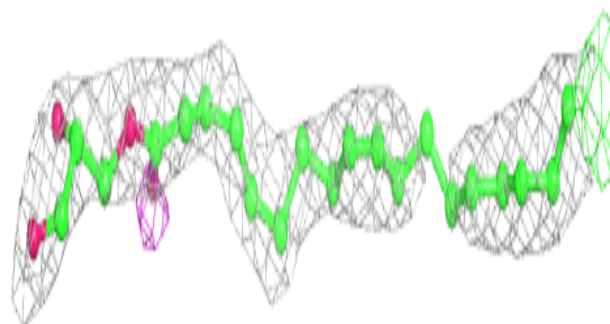
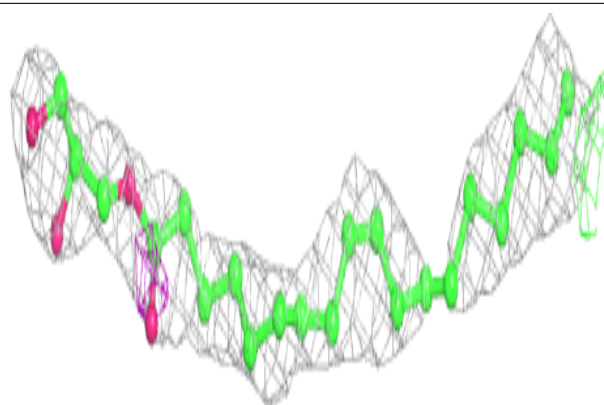
**Electron density around OLC A 411:**

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

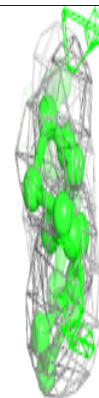
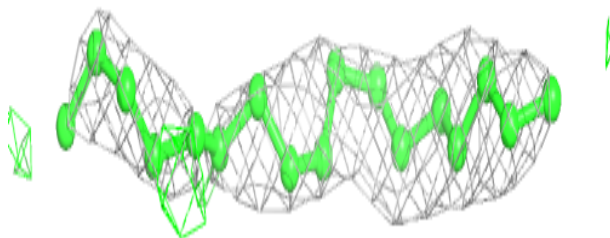
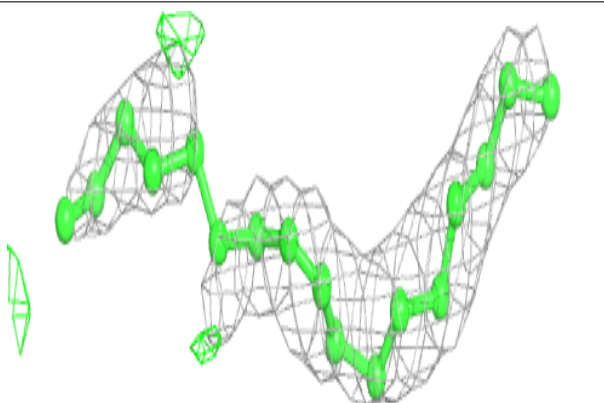


Electron density around OLB A 405:

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

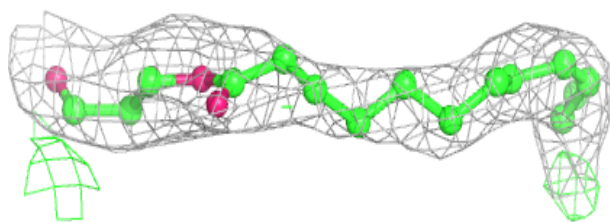
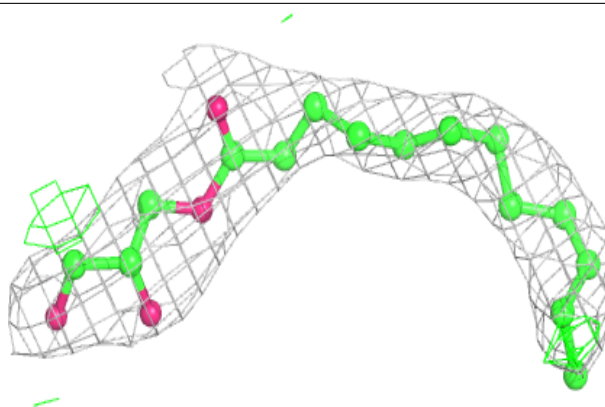
**Electron density around OLC A 407:**

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

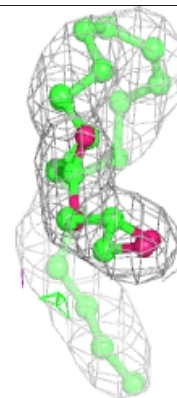
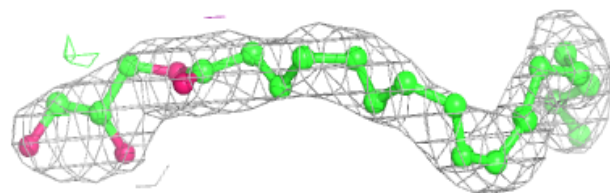
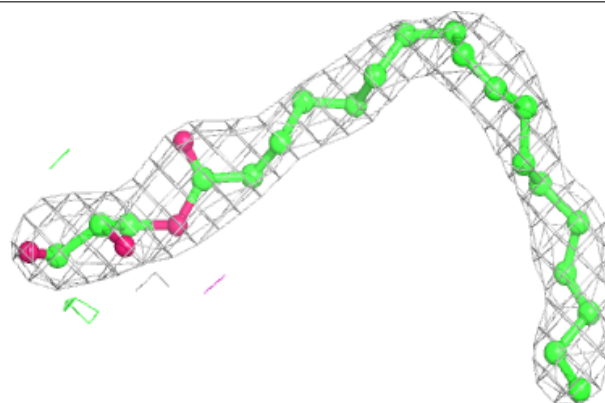


Electron density around OLC A 402:

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

**Electron density around OLC A 409:**

$2mF_o-DF_c$ (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.