Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 10:35 PM EDT

PDB ID	:	8E7Z
Title	:	RsTSPO mutant -A138F
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Deposited on	:	2022-08-25
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 (i) symbol.

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

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

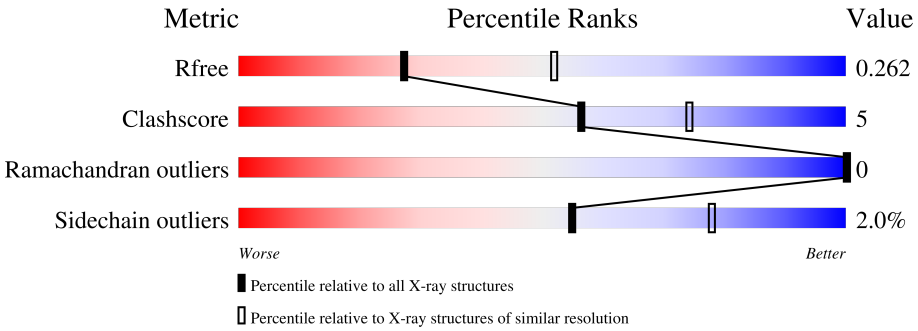
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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)

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%

Mol	Chain	Length	Quality of chain
1	A	158	87% 11% ••
1	B	158	88% 10% •
1	C	158	82% 13% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3981 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.

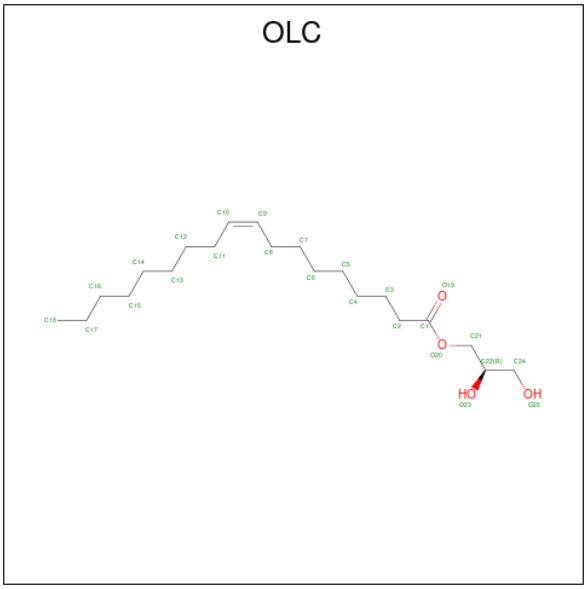
- Molecule 1 is a protein called Tryptophan-rich sensory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1243	840	194	198	11			
1	B	155	Total	C	N	O	S	0	0	0
			1231	833	194	194	10			
1	C	149	Total	C	N	O	S	5	0	0
			1165	791	178	186	10			

There are 3 discrepancies between the modelled and reference sequences:

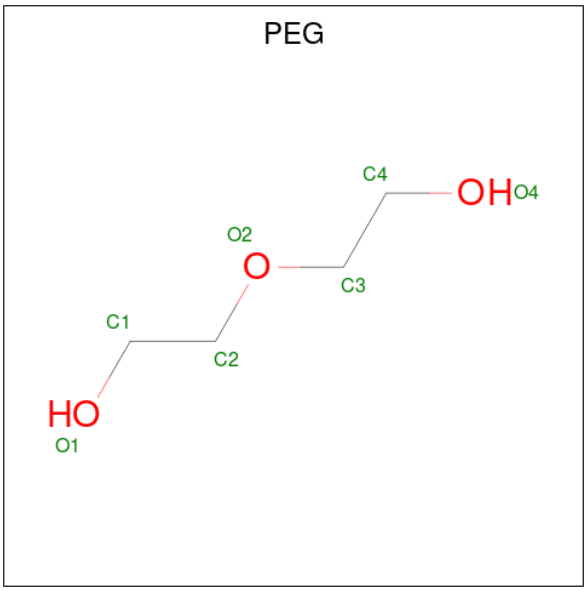
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	PHE	ALA	engineered mutation	UNP Q9RFC8
B	138	PHE	ALA	engineered mutation	UNP Q9RFC8
C	138	PHE	ALA	engineered mutation	UNP Q9RFC8

- 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 O 25 21 4	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C O 17 13 4	0	0
2	A	1	Total C 15 15	0	0
2	A	1	Total C O 18 14 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 12 8 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	C	1	Total C 17 17	0	0
2	C	1	Total C O 24 21 3	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

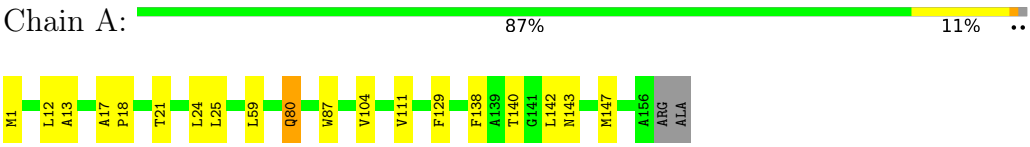
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	0	0
4	B	12	Total O 12 12	0	0
4	C	17	Total O 17 17	0	0

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. 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. 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.

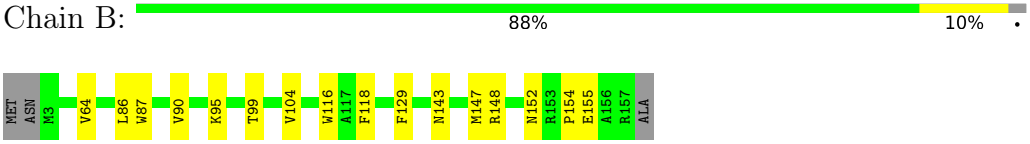
• Molecule 1: Tryptophan-rich sensory protein

Chain A:



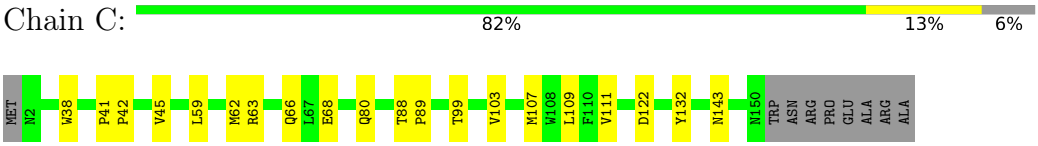
• Molecule 1: Tryptophan-rich sensory protein

Chain B:



• Molecule 1: Tryptophan-rich sensory protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	58.55Å 99.53Å 95.48Å 90.00° 100.12° 90.00°	Depositor
Resolution (Å)	47.13 – 2.60 47.13 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.13-2.60) 72.0 (47.13-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.31 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.204 , 0.263 0.204 , 0.262	Depositor DCC
R_{free} test set	1819 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.1	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	3981	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, PEG

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	0/1293	0.40	0/1778
1	B	0.28	0/1281	0.40	0/1763
1	C	0.27	0/1212	0.41	0/1670
All	All	0.27	0/3786	0.40	0/5211

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	1243	0	1202	14	0
1	B	1231	0	1184	13	0
1	C	1165	0	1106	12	0
2	A	112	0	167	7	0
2	B	87	0	133	6	0
2	C	91	0	149	1	0
3	C	7	0	10	1	0
4	A	16	0	0	1	0
4	B	12	0	0	0	0
4	C	17	0	0	0	0
All	All	3981	0	3951	39	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 5.

All (39) 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:C:88:THR:HG23	1:C:89:PRO:HD3	1.69	0.74
1:B:148:ARG:HG2	2:B:202:OLC:H24A	1.71	0.70
2:A:206:OLC:H10	2:B:204:OLC:H12	1.72	0.70
1:A:24:LEU:HD11	1:B:99:THR:HG21	1.76	0.68
1:A:12:LEU:HG	2:A:206:OLC:H4A	1.76	0.66
1:C:80:GLN:NE2	1:C:132:TYR:OH	2.28	0.66
1:C:109:LEU:HD21	2:C:204:OLC:H8	1.79	0.64
1:A:138:PHE:HD1	2:A:202:OLC:H18A	1.62	0.64
1:B:116:TRP:HD1	2:B:201:OLC:H3A	1.68	0.59
1:B:154:PRO:HD2	1:B:155:GLU:OE1	2.04	0.57
1:A:140:THR:HG21	2:A:204:OLC:H6	1.87	0.56
1:B:116:TRP:CD1	2:B:201:OLC:H3A	2.45	0.51
1:B:87:TRP:CD1	1:B:104:VAL:HB	2.45	0.50
2:A:201:OLC:H18A	2:A:205:OLC:H12	1.94	0.49
1:C:107:MET:O	1:C:111:VAL:HG23	2.13	0.49
1:B:147:MET:HE2	2:B:202:OLC:H2	1.94	0.48
1:C:99:THR:O	1:C:103:VAL:HG23	2.12	0.48
1:A:25:LEU:O	1:C:38:TRP:NE1	2.47	0.48
1:B:152:ASN:H	1:B:152:ASN:HD22	1.61	0.47
1:A:1:MET:N	4:A:302:HOH:O	2.37	0.47
1:A:80:GLN:HG3	1:A:111:VAL:HG22	1.97	0.47
1:A:59:LEU:HD13	2:A:201:OLC:H4A	1.97	0.46
1:A:87:TRP:CD1	1:A:104:VAL:HB	2.49	0.46
1:C:41:PRO:HB2	1:C:45:VAL:HG11	1.98	0.46
1:A:138:PHE:CZ	1:A:142:LEU:HD11	2.51	0.45
1:B:155:GLU:H	1:B:155:GLU:CD	2.20	0.45
1:C:42:PRO:O	1:C:45:VAL:HG12	2.17	0.45
2:A:203:OLC:H4A	2:A:205:OLC:H6A	1.99	0.44
1:A:18:PRO:O	1:A:21:THR:OG1	2.28	0.44
1:A:13:ALA:HB1	2:B:204:OLC:H12A	2.00	0.43
1:C:62:MET:O	1:C:66:GLN:HG3	2.19	0.43
1:A:17:ALA:HA	1:B:86:LEU:HD22	2.01	0.43
1:C:88:THR:CG2	1:C:89:PRO:HD3	2.45	0.43
1:B:64:VAL:HG21	1:B:118:PHE:CD1	2.53	0.43
1:B:95:LYS:O	1:B:155:GLU:HB3	2.20	0.41
1:C:63:ARG:NH1	1:C:122:ASP:OD2	2.54	0.41
1:B:86:LEU:O	1:B:90:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HD21	3:C:201:PEG:H22	2.02	0.41
1:A:147:MET:HE2	1:A:147:MET:HB2	1.86	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	154/158 (98%)	154 (100%)	0	0	100	100
1	B	153/158 (97%)	151 (99%)	2 (1%)	0	100	100
1	C	147/158 (93%)	146 (99%)	1 (1%)	0	100	100
All	All	454/474 (96%)	451 (99%)	3 (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	119/124 (96%)	116 (98%)	3 (2%)	47	73
1	B	116/124 (94%)	114 (98%)	2 (2%)	60	81
1	C	108/124 (87%)	106 (98%)	2 (2%)	57	79
All	All	343/372 (92%)	336 (98%)	7 (2%)	55	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	129	PHE
1	A	143	ASN
1	B	129	PHE
1	B	143	ASN
1	C	68	GLU
1	C	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	ASN
1	C	80	GLN

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)

15 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	201	-	24,24,24	0.70	1 (4%)	25,25,25	0.99	1 (4%)
2	OLC	B	202	-	24,24,24	0.69	1 (4%)	25,25,25	0.96	1 (4%)
2	OLC	A	203	-	11,11,24	0.26	0	9,10,25	0.76	0
2	OLC	B	201	-	24,24,24	0.68	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	C	202	-	16,16,24	0.21	0	15,15,25	0.77	0
2	OLC	C	205	-	24,24,24	0.68	1 (4%)	25,25,25	1.00	1 (4%)
3	PEG	C	201	-	6,6,6	0.13	0	5,5,5	0.08	0
2	OLC	B	204	-	24,24,24	0.68	1 (4%)	25,25,25	0.92	1 (4%)
2	OLC	C	203	-	23,23,24	0.66	1 (4%)	23,23,25	1.11	2 (8%)
2	OLC	A	202	-	24,24,24	0.70	1 (4%)	25,25,25	0.90	1 (4%)
2	OLC	B	203	-	11,11,24	1.00	1 (9%)	12,12,25	1.07	1 (8%)
2	OLC	A	206	-	17,17,24	0.81	1 (5%)	18,18,25	1.09	1 (5%)
2	OLC	C	204	-	24,24,24	0.70	1 (4%)	25,25,25	0.91	1 (4%)
2	OLC	A	205	-	14,14,24	0.23	0	13,13,25	0.73	0
2	OLC	A	204	-	16,16,24	0.86	1 (6%)	17,17,25	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	201	-	-	9/24/24/24	-
2	OLC	B	202	-	-	9/24/24/24	-
2	OLC	A	203	-	-	4/9/9/24	-
2	OLC	B	201	-	-	12/24/24/24	-
2	OLC	C	202	-	-	9/14/14/24	-
2	OLC	C	205	-	-	13/24/24/24	-
3	PEG	C	201	-	-	0/4/4/4	-
2	OLC	B	204	-	-	9/24/24/24	-
2	OLC	C	203	-	-	5/22/22/24	-
2	OLC	A	202	-	-	11/24/24/24	-
2	OLC	B	203	-	-	0/11/11/24	-
2	OLC	A	206	-	-	7/17/17/24	-
2	OLC	C	204	-	-	13/24/24/24	-
2	OLC	A	205	-	-	4/12/12/24	-
2	OLC	A	204	-	-	5/16/16/24	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	204	OLC	O20-C1	2.78	1.41	1.33
2	A	202	OLC	O20-C1	2.74	1.41	1.33
2	B	203	OLC	O20-C1	2.68	1.41	1.33
2	A	204	OLC	O20-C1	2.66	1.41	1.33
2	A	201	OLC	O20-C1	2.65	1.41	1.33
2	A	206	OLC	O20-C1	2.64	1.41	1.33
2	C	203	OLC	O20-C1	2.64	1.41	1.33
2	B	201	OLC	O20-C1	2.63	1.41	1.33
2	C	205	OLC	O20-C1	2.63	1.41	1.33
2	B	202	OLC	O20-C1	2.61	1.41	1.33
2	B	204	OLC	O20-C1	2.57	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	205	OLC	O20-C1-C2	2.85	120.86	111.91
2	A	201	OLC	O20-C1-C2	2.78	120.62	111.91
2	B	202	OLC	O20-C1-C2	2.72	120.44	111.91
2	C	203	OLC	O20-C1-C2	2.71	120.42	111.91
2	A	204	OLC	O20-C1-C2	2.64	120.20	111.91
2	B	203	OLC	O20-C1-C2	2.63	120.16	111.91
2	C	204	OLC	O20-C1-C2	2.61	120.11	111.91
2	A	206	OLC	O20-C1-C2	2.58	120.02	111.91
2	A	202	OLC	O20-C1-C2	2.51	119.78	111.91
2	B	204	OLC	O20-C1-C2	2.34	119.26	111.91
2	B	201	OLC	O20-C1-C2	2.30	119.14	111.91
2	C	203	OLC	C21-C22-C24	-2.09	109.40	113.95

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	202	OLC	O20-C21-C22-O23
2	B	201	OLC	O20-C21-C22-O23
2	B	202	OLC	C21-C22-C24-O25
2	B	204	OLC	O19-C1-O20-C21
2	C	205	OLC	C21-C22-C24-O25
2	A	206	OLC	O19-C1-O20-C21
2	B	204	OLC	C2-C1-O20-C21
2	A	206	OLC	C2-C1-O20-C21
2	B	201	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	B	202	OLC	C2-C1-O20-C21
2	A	201	OLC	O20-C21-C22-C24
2	B	201	OLC	C1-C2-C3-C4
2	B	204	OLC	C1-C2-C3-C4
2	A	201	OLC	O20-C21-C22-O23
2	A	204	OLC	O20-C21-C22-O23
2	C	204	OLC	C1-C2-C3-C4
2	B	201	OLC	O19-C1-O20-C21
2	B	202	OLC	O23-C22-C24-O25
2	A	201	OLC	C1-C2-C3-C4
2	A	202	OLC	C1-C2-C3-C4
2	A	206	OLC	C1-C2-C3-C4
2	B	202	OLC	O19-C1-O20-C21
2	C	204	OLC	O20-C21-C22-O23
2	A	205	OLC	C6-C7-C8-C9
2	B	204	OLC	C4-C5-C6-C7
2	C	204	OLC	C14-C15-C16-C17
2	C	204	OLC	C2-C1-O20-C21
2	B	201	OLC	O20-C21-C22-C24
2	C	204	OLC	O20-C21-C22-C24
2	C	202	OLC	C5-C6-C7-C8
2	A	202	OLC	C2-C3-C4-C5
2	B	201	OLC	C4-C5-C6-C7
2	C	204	OLC	C5-C6-C7-C8
2	C	203	OLC	C1-C2-C3-C4
2	C	205	OLC	C12-C13-C14-C15
2	A	202	OLC	C3-C4-C5-C6
2	C	204	OLC	C13-C14-C15-C16
2	C	205	OLC	C2-C3-C4-C5
2	A	201	OLC	C21-C22-C24-O25
2	C	205	OLC	C1-C2-C3-C4
2	A	206	OLC	C4-C5-C6-C7
2	C	204	OLC	C11-C12-C13-C14
2	A	204	OLC	C4-C5-C6-C7
2	B	201	OLC	C3-C4-C5-C6
2	A	206	OLC	C2-C3-C4-C5
2	A	201	OLC	O23-C22-C24-O25
2	A	202	OLC	C12-C13-C14-C15
2	B	204	OLC	C2-C3-C4-C5
2	B	204	OLC	C10-C11-C12-C13
2	B	202	OLC	C13-C14-C15-C16
2	C	204	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	A	201	OLC	C2-C1-O20-C21
2	A	203	OLC	C9-C10-C11-C12
2	A	205	OLC	C10-C11-C12-C13
2	B	204	OLC	C3-C4-C5-C6
2	C	205	OLC	C14-C15-C16-C17
2	B	202	OLC	C5-C6-C7-C8
2	B	201	OLC	C2-C3-C4-C5
2	A	206	OLC	C6-C7-C8-C9
2	B	204	OLC	C13-C14-C15-C16
2	A	201	OLC	O19-C1-O20-C21
2	C	202	OLC	C4-C5-C6-C7
2	A	202	OLC	C6-C7-C8-C9
2	A	202	OLC	C11-C12-C13-C14
2	A	206	OLC	C5-C6-C7-C8
2	C	205	OLC	O23-C22-C24-O25
2	A	202	OLC	O20-C21-C22-C24
2	C	204	OLC	C12-C13-C14-C15
2	B	201	OLC	C13-C14-C15-C16
2	C	202	OLC	C13-C14-C15-C16
2	B	202	OLC	C1-C2-C3-C4
2	A	205	OLC	C5-C6-C7-C8
2	C	205	OLC	C13-C14-C15-C16
2	A	203	OLC	C1-C2-C3-C4
2	C	203	OLC	C2-C3-C4-C5
2	C	205	OLC	C5-C6-C7-C8
2	C	205	OLC	C2-C1-O20-C21
2	C	205	OLC	C6-C7-C8-C9
2	C	205	OLC	O19-C1-O20-C21
2	A	202	OLC	C13-C14-C15-C16
2	A	204	OLC	C6-C7-C8-C9
2	A	201	OLC	C15-C16-C17-C18
2	A	205	OLC	C1-C2-C3-C4
2	C	204	OLC	C9-C10-C11-C12
2	B	202	OLC	C9-C10-C11-C12
2	C	203	OLC	O20-C21-C22-C24
2	C	202	OLC	C10-C11-C12-C13
2	C	202	OLC	C15-C16-C17-C18
2	B	201	OLC	C6-C7-C8-C9
2	A	204	OLC	O20-C21-C22-C24
2	A	203	OLC	C5-C6-C7-C8
2	C	202	OLC	C9-C10-C11-C12
2	B	204	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	203	OLC	C7-C8-C9-C10
2	C	203	OLC	C5-C6-C7-C8
2	C	204	OLC	C3-C4-C5-C6
2	C	205	OLC	C9-C10-C11-C12
2	C	202	OLC	C2-C3-C4-C5
2	B	201	OLC	O20-C1-C2-C3
2	A	201	OLC	C9-C10-C11-C12
2	A	202	OLC	C7-C8-C9-C10
2	C	204	OLC	C6-C7-C8-C9
2	C	203	OLC	C9-C10-C11-C12
2	C	205	OLC	C7-C8-C9-C10
2	B	202	OLC	C7-C8-C9-C10
2	B	201	OLC	O19-C1-C2-C3
2	C	202	OLC	C7-C8-C9-C10
2	C	202	OLC	C14-C15-C16-C17
2	A	204	OLC	C2-C3-C4-C5
2	A	202	OLC	C14-C15-C16-C17

There are no ring outliers.

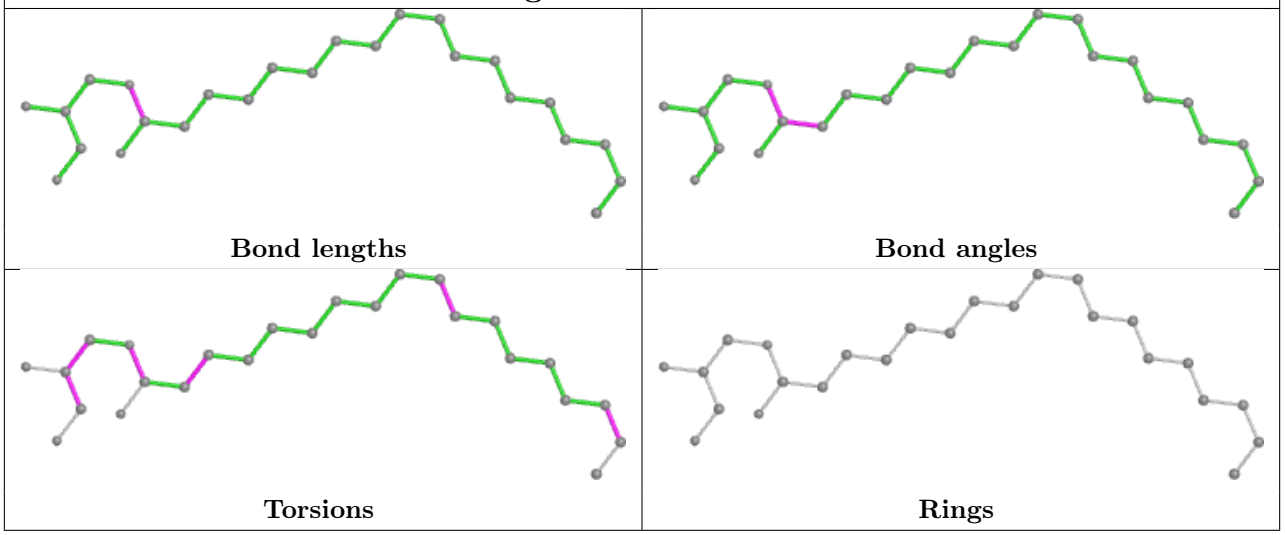
11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	OLC	2	0
2	B	202	OLC	2	0
2	A	203	OLC	1	0
2	B	201	OLC	2	0
3	C	201	PEG	1	0
2	B	204	OLC	2	0
2	A	202	OLC	1	0
2	A	206	OLC	2	0
2	C	204	OLC	1	0
2	A	205	OLC	2	0
2	A	204	OLC	1	0

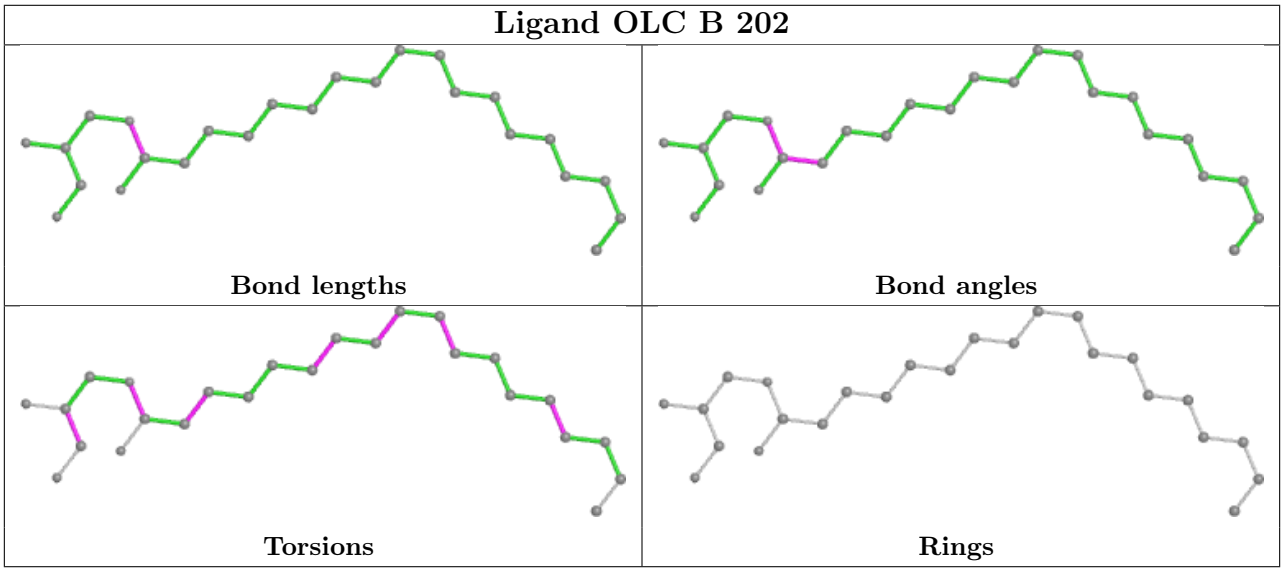
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

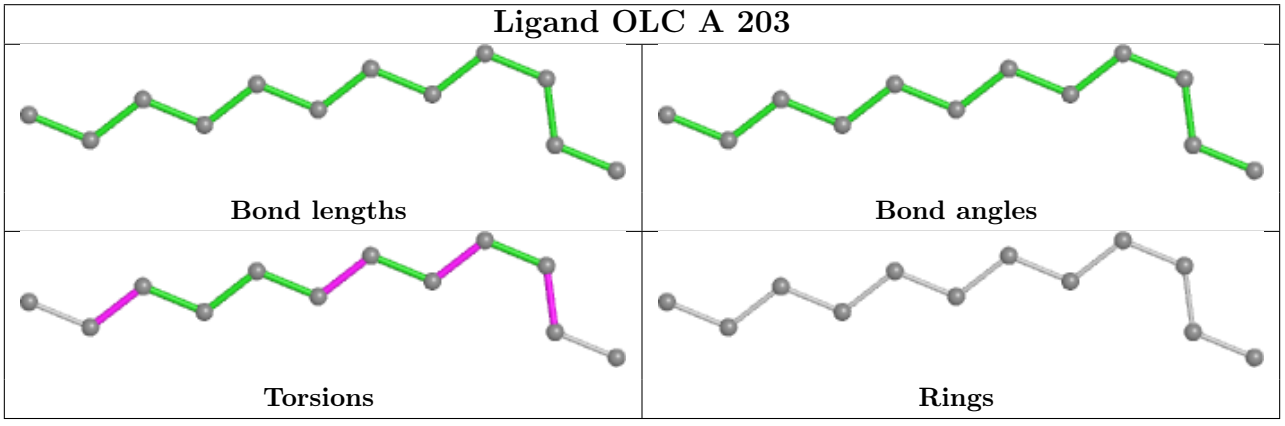
Ligand OLC A 201



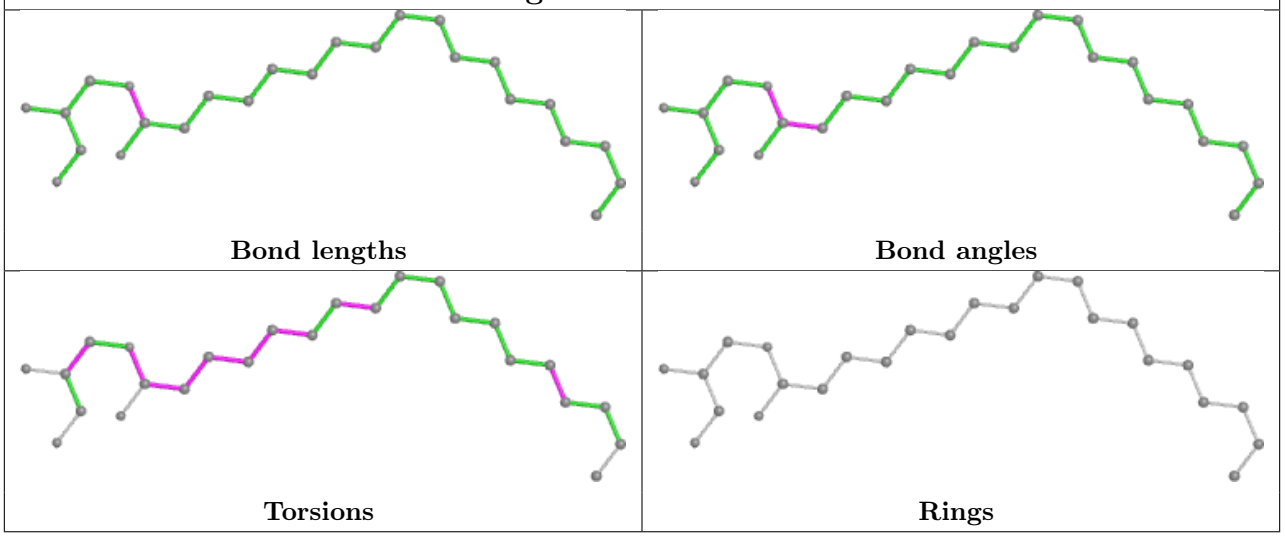
Ligand OLC B 202



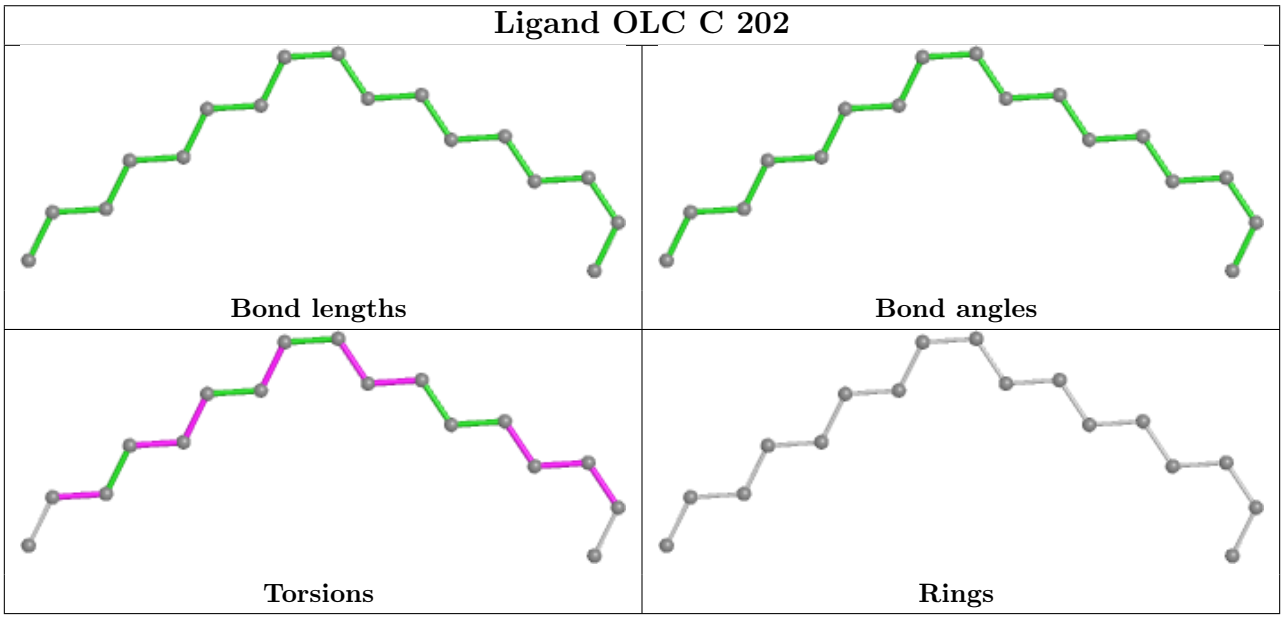
Ligand OLC A 203



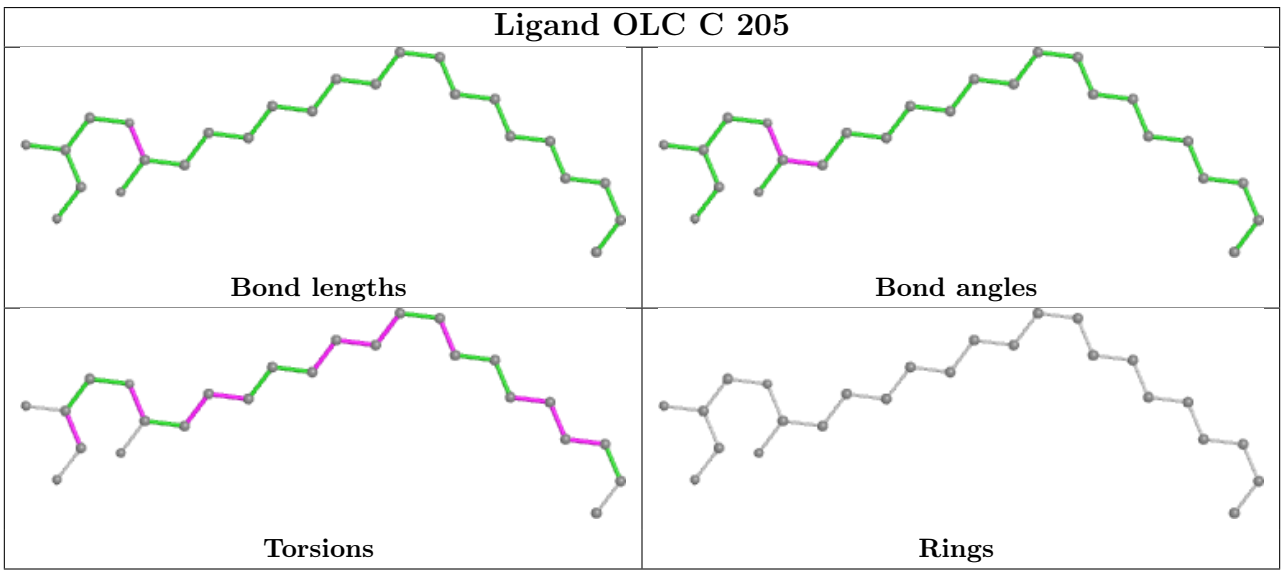
Ligand OLC B 201



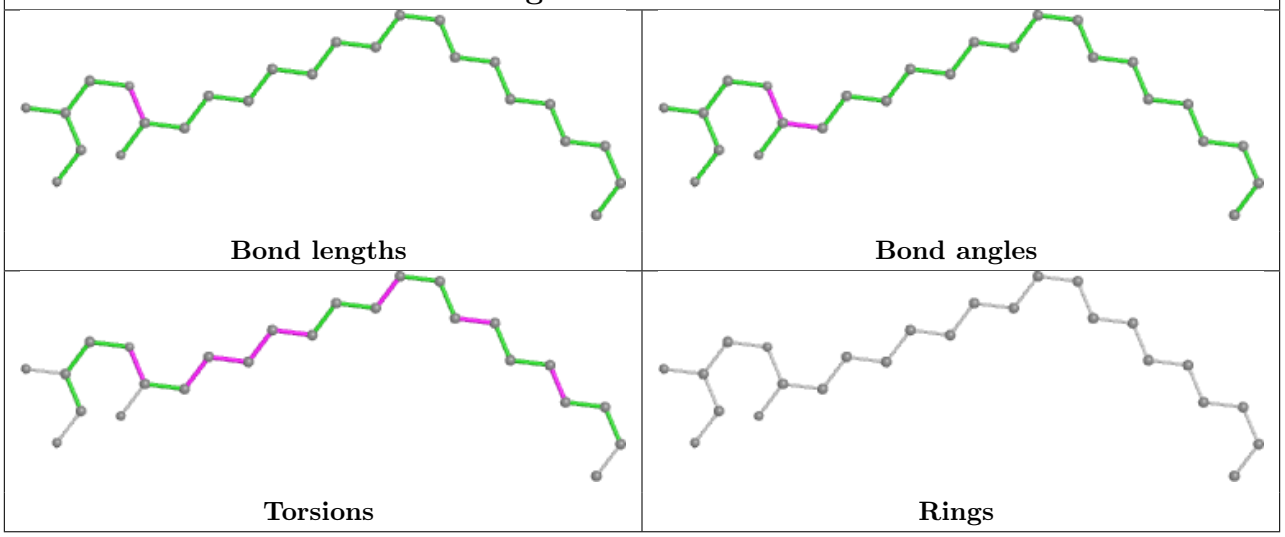
Ligand OLC C 202



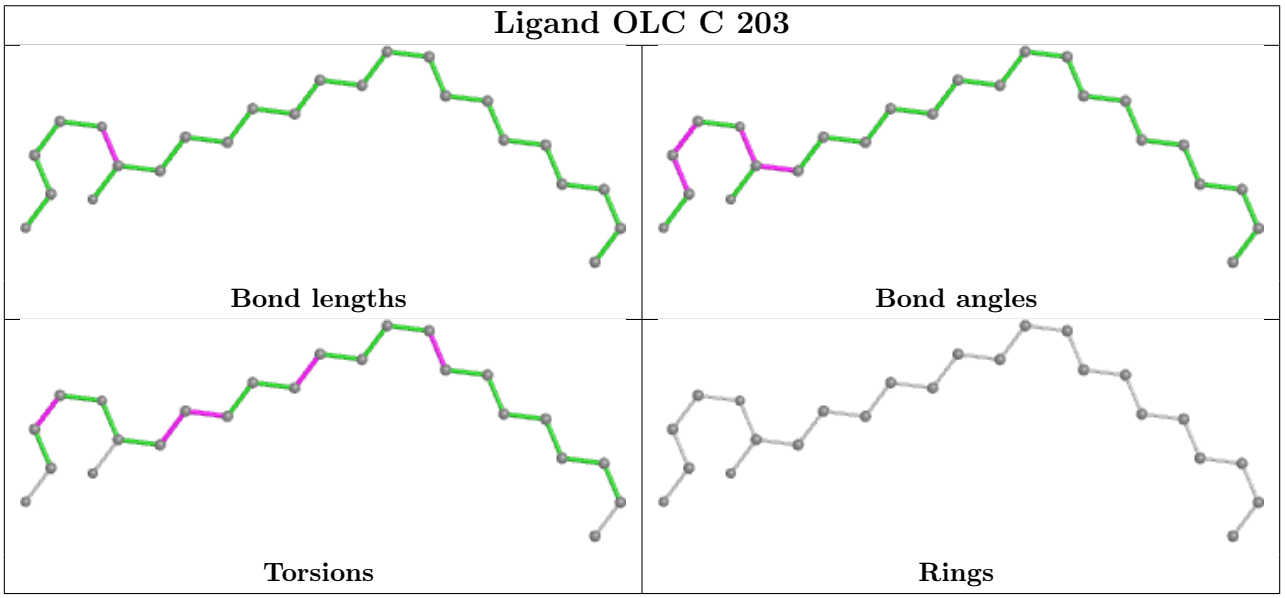
Ligand OLC C 205



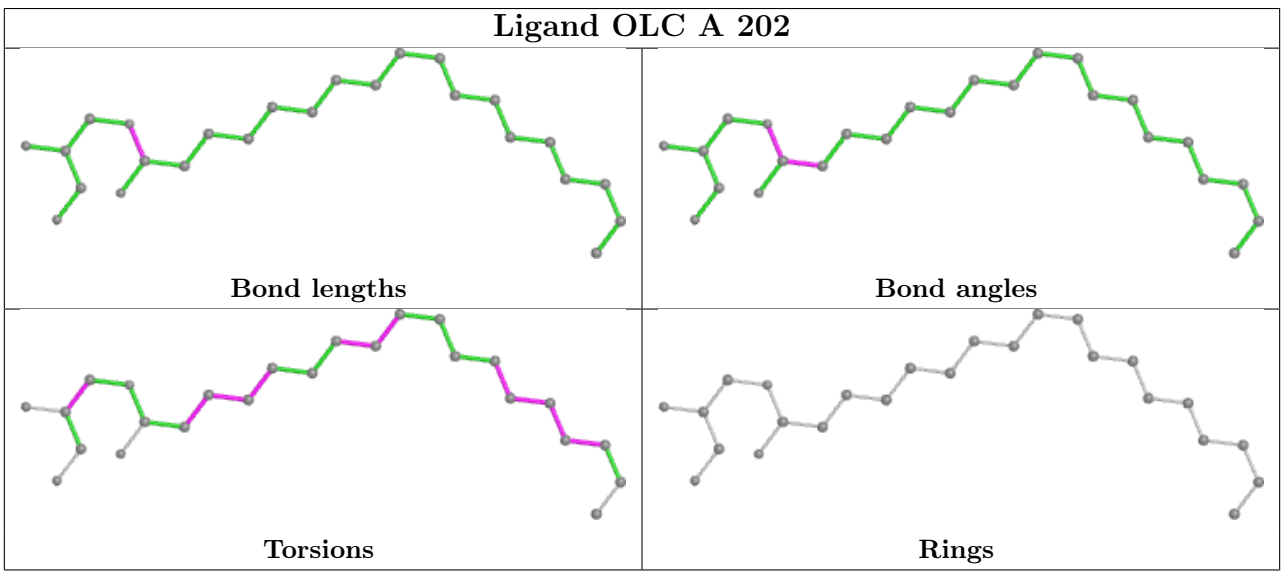
Ligand OLC B 204



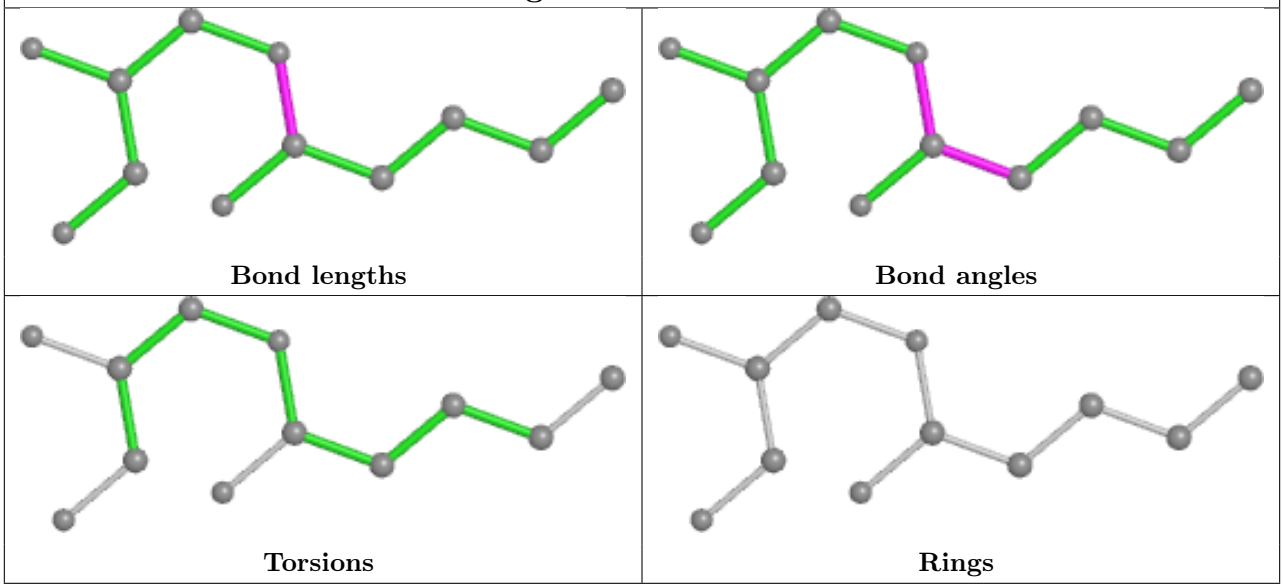
Ligand OLC C 203



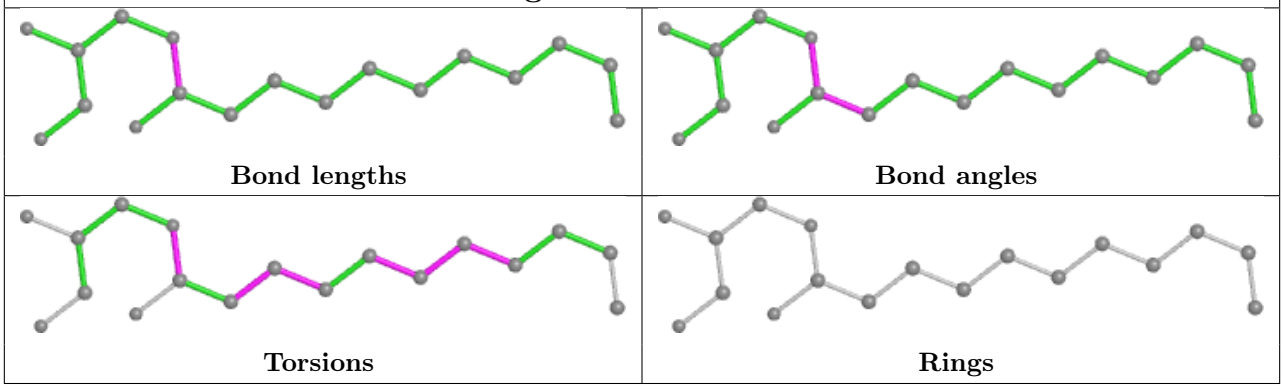
Ligand OLC A 202



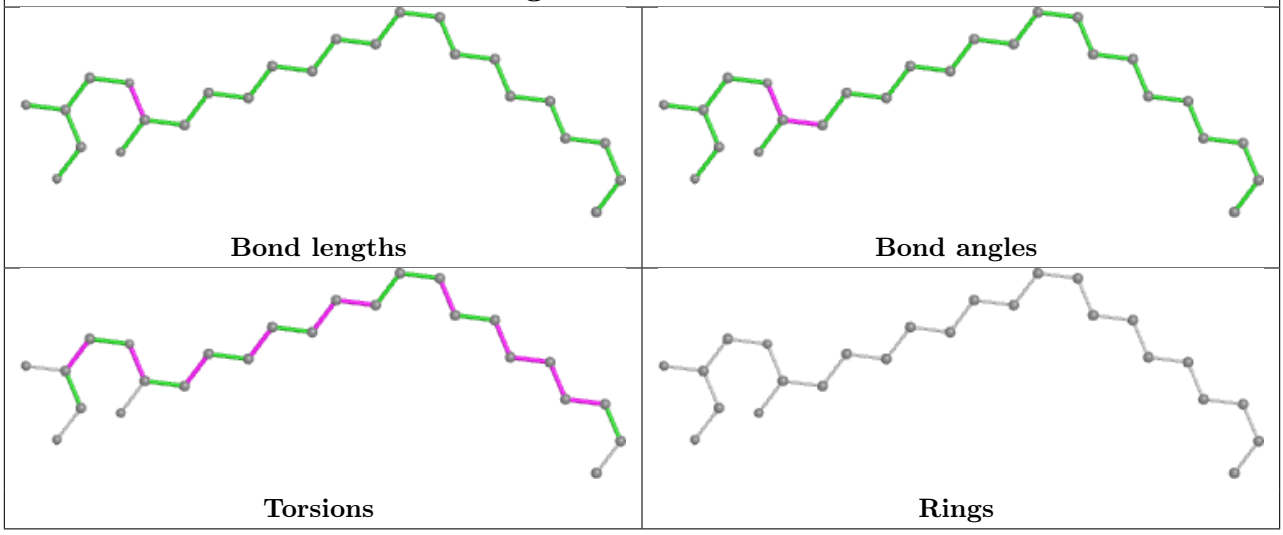
Ligand OLC B 203

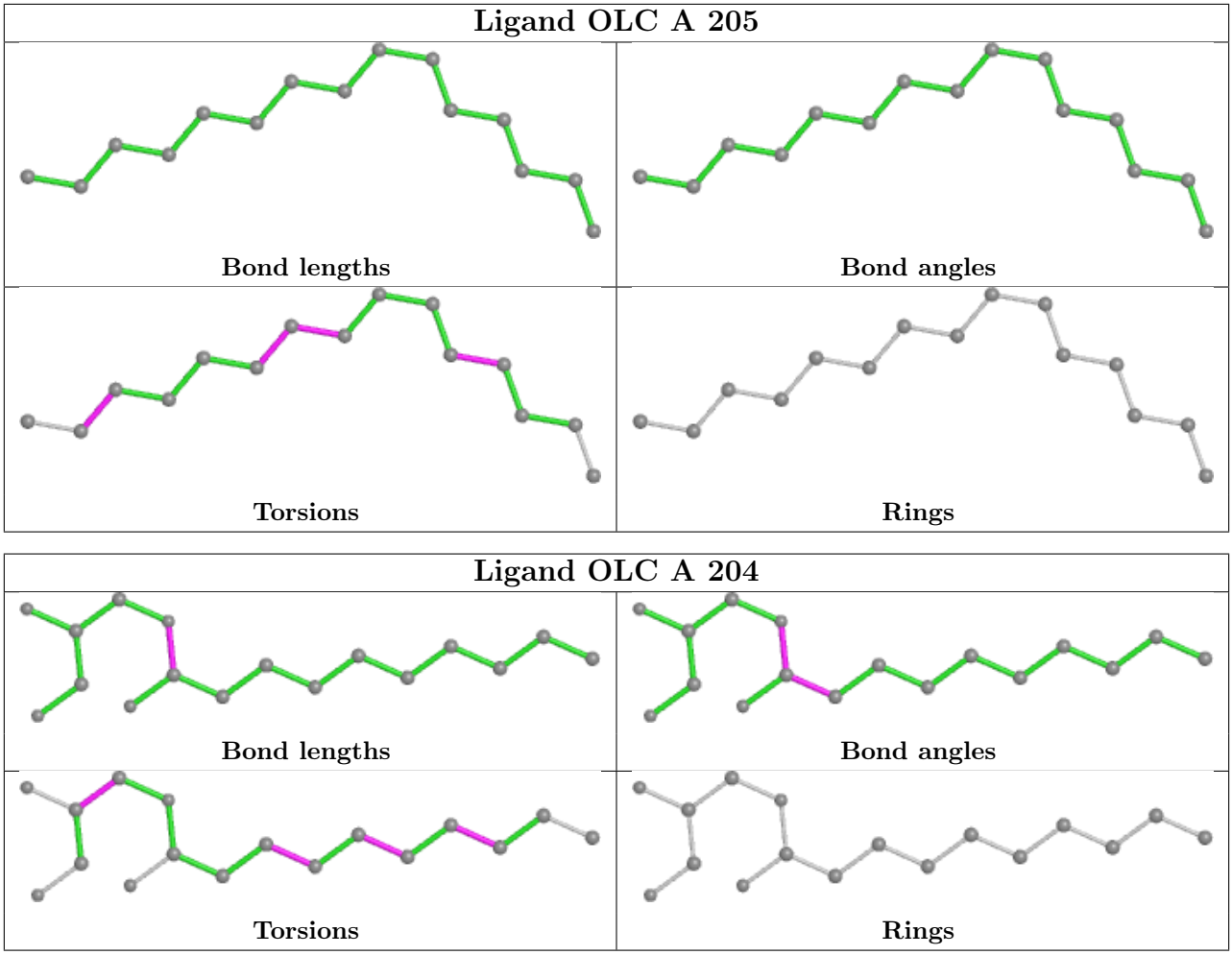


Ligand OLC A 206



Ligand OLC C 204





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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

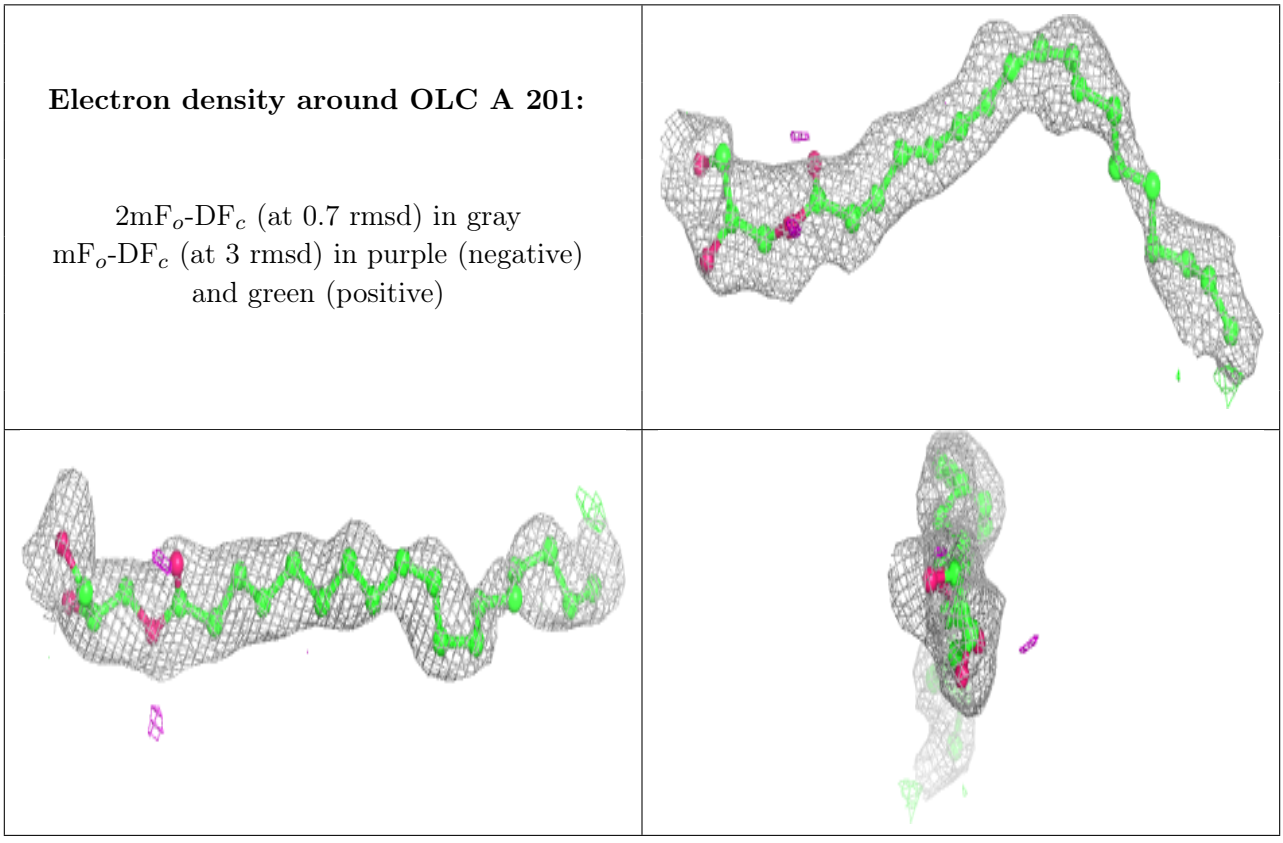
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

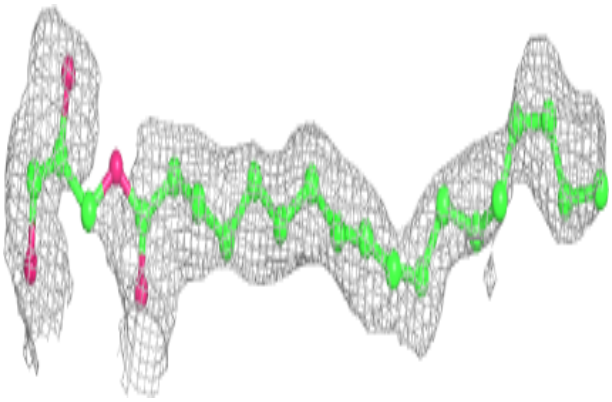
Electron density around OLC A 201:

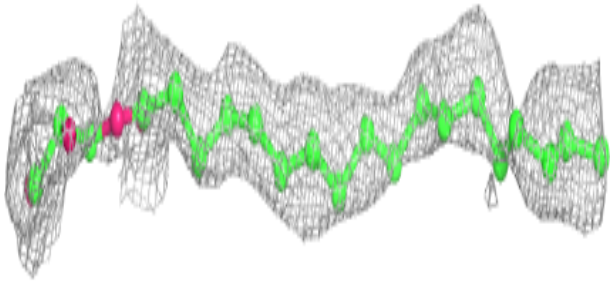
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

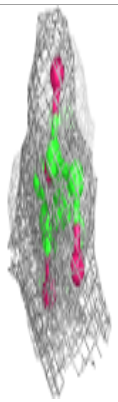


Electron density around OLC A 202:

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

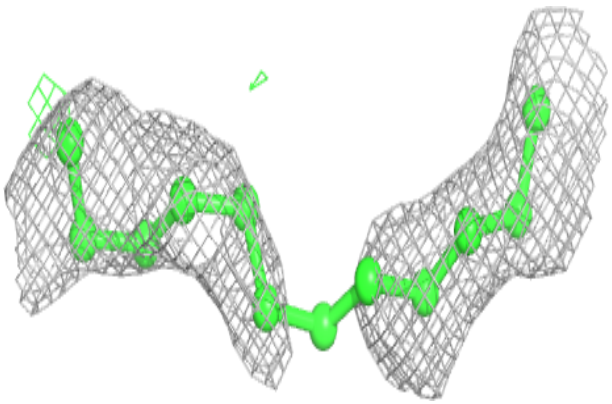


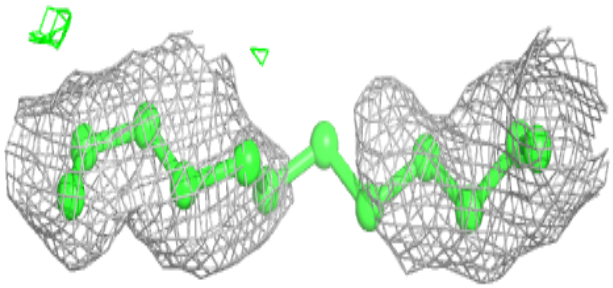


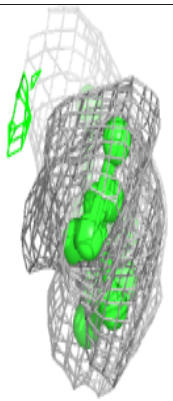


Electron density around OLC A 203:

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

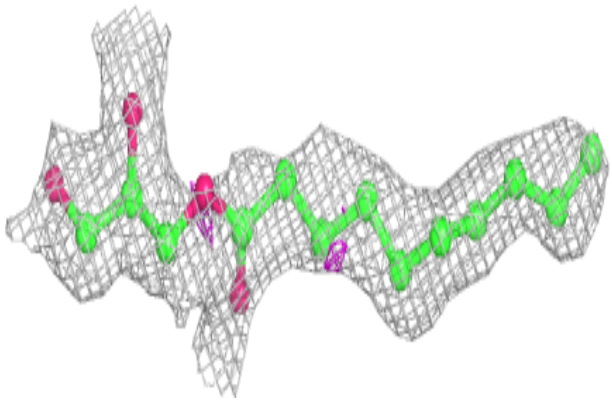


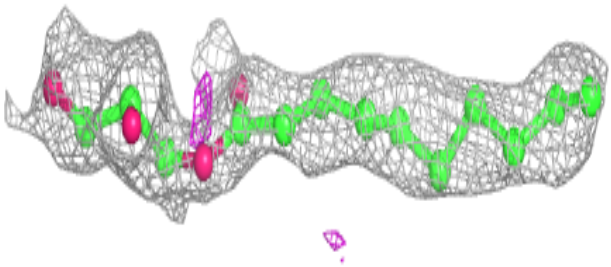


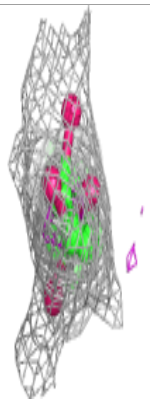


Electron density around OLC A 204:

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

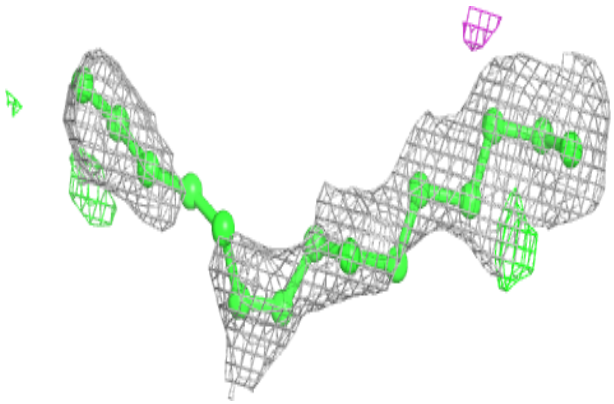


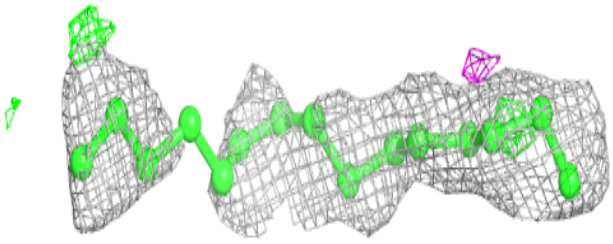


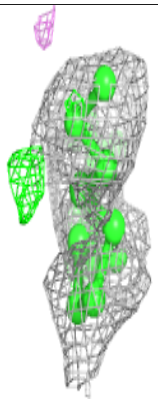


Electron density around OLC A 205:

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

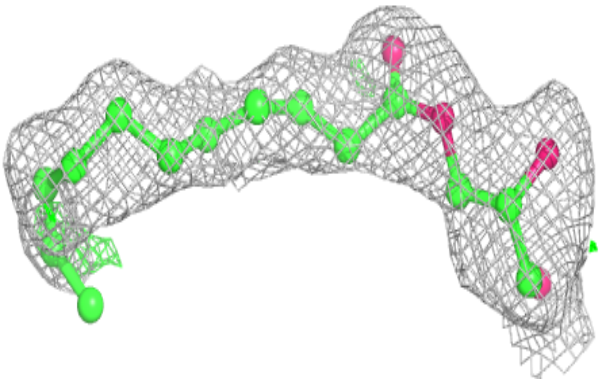


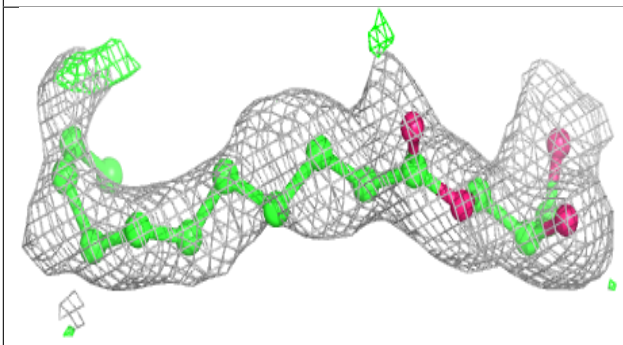


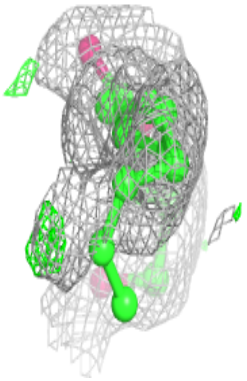


Electron density around OLC A 206:

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

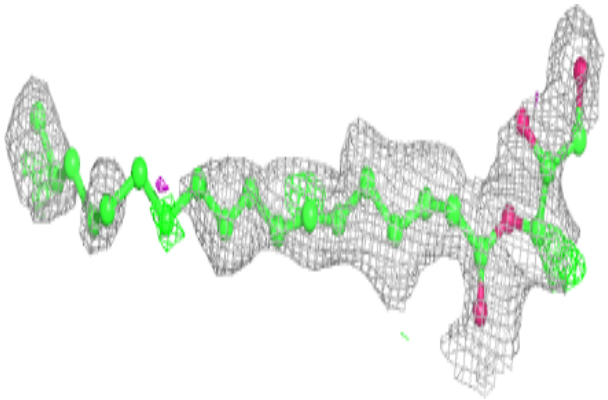


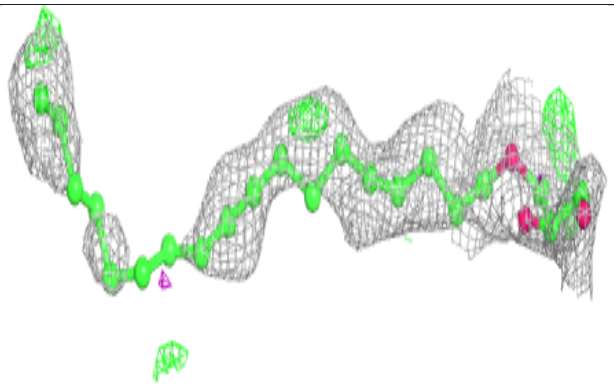


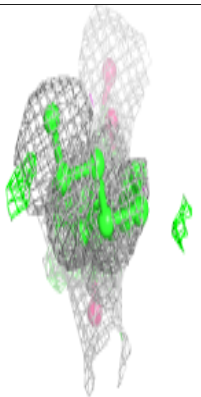


Electron density around OLC B 201:

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

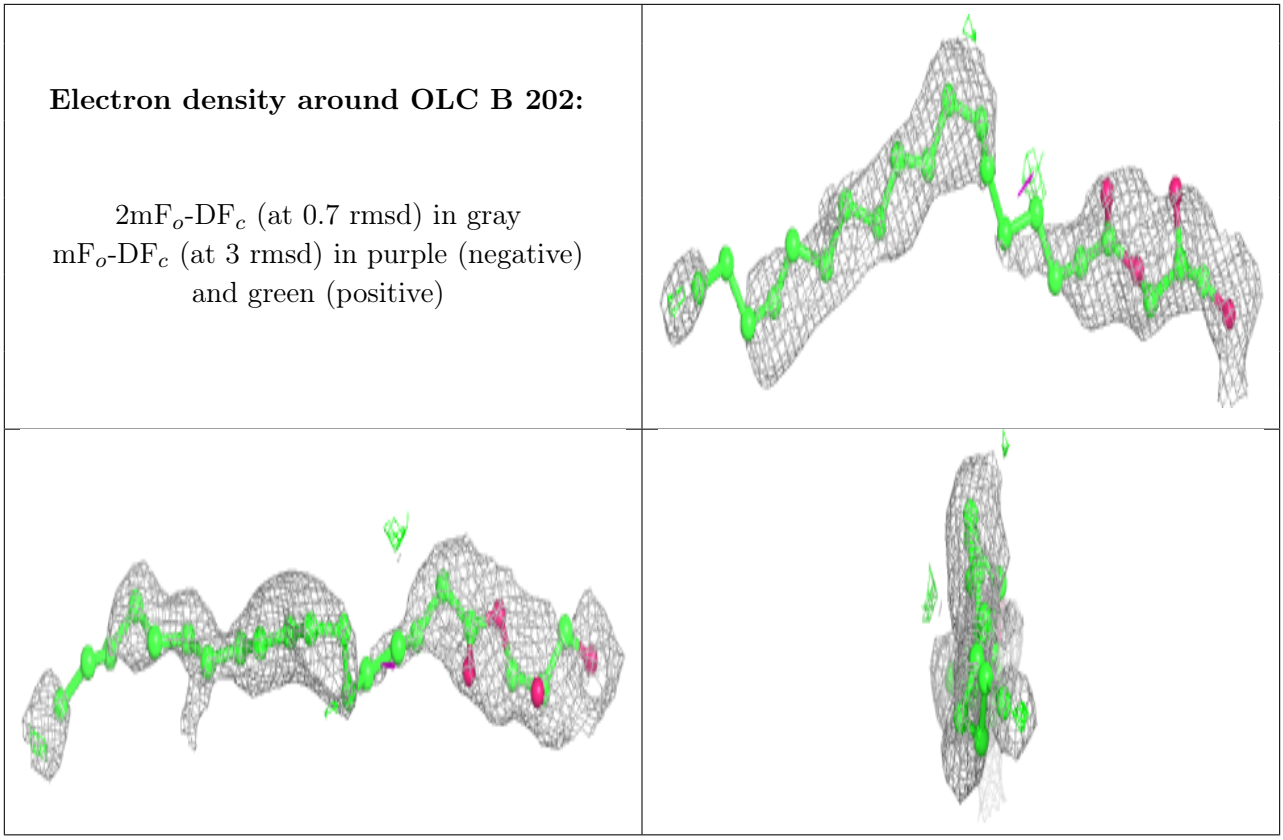






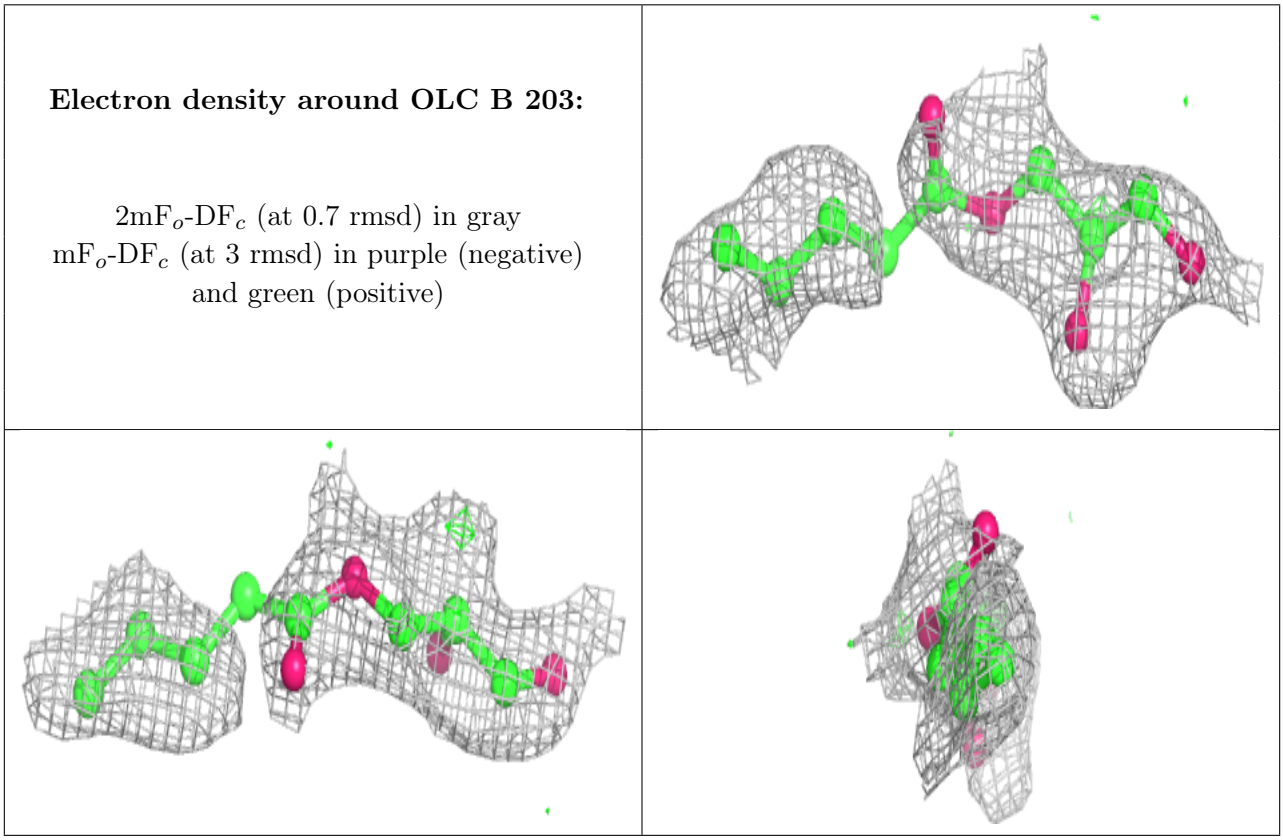
Electron density around OLC B 202:

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



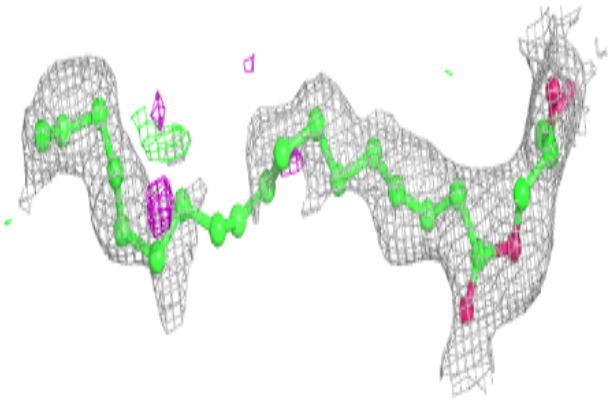
Electron density around OLC B 203:

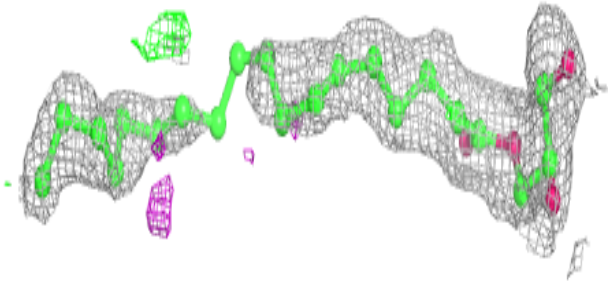
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

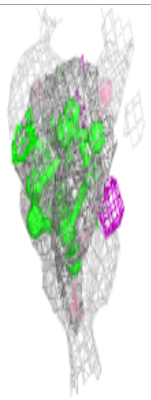


Electron density around OLC B 204:

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

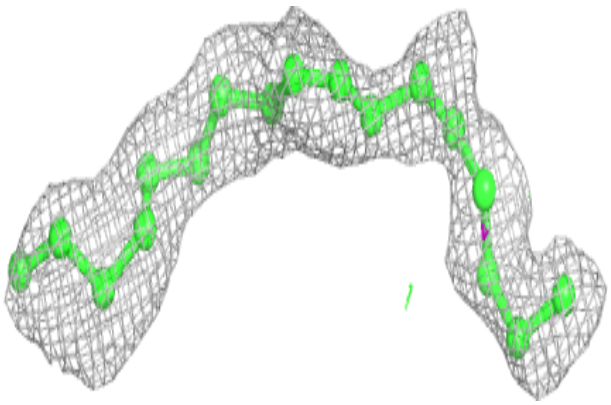


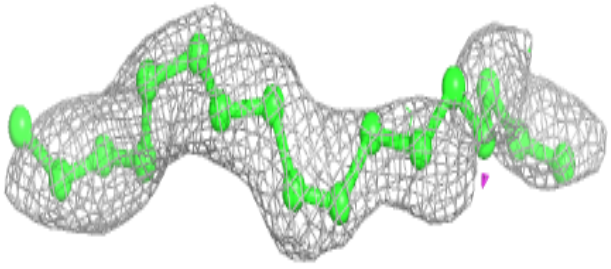


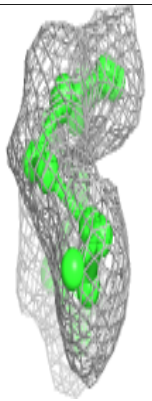


Electron density around OLC C 202:

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

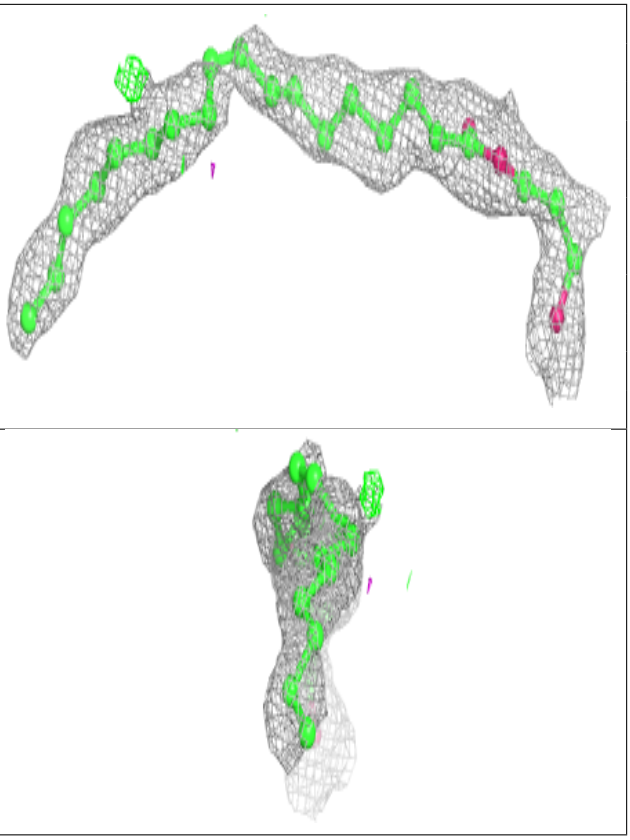






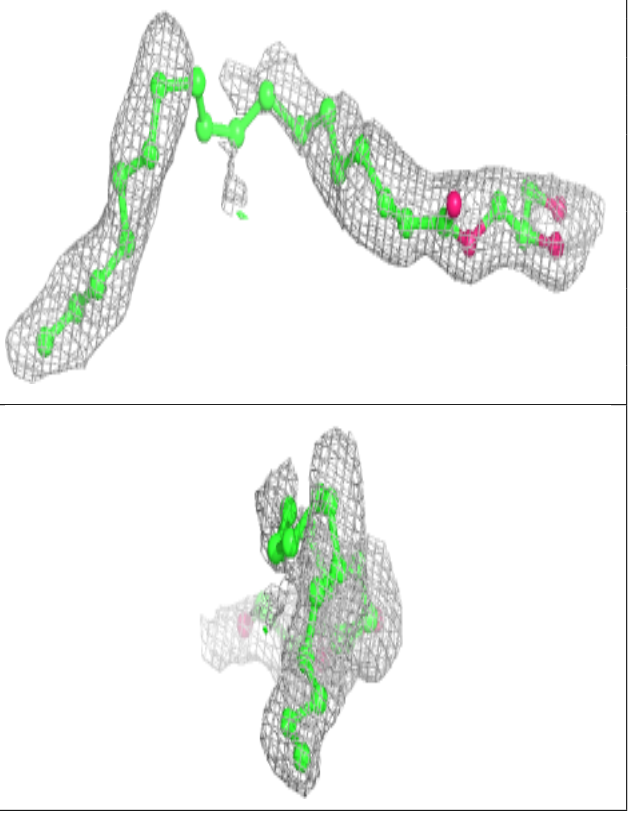
Electron density around OLC C 203:

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



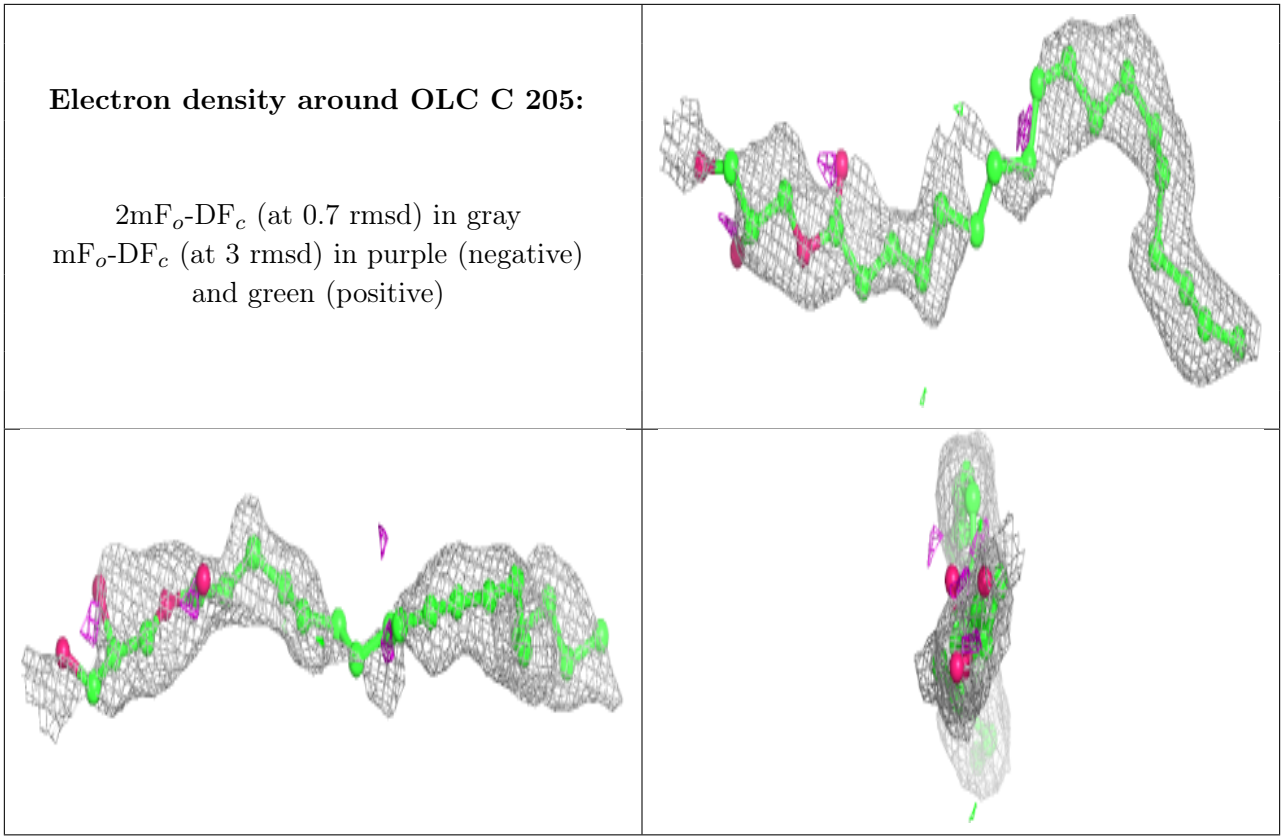
Electron density around OLC C 204:

$2mF_o$-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 C 205:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.