



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2021 – 04:04 PM EST

PDB ID : 7M96  
Title : Bovine sigma-2 receptor bound to Z4857158944  
Authors : Alon, A.; Kruse, A.C.  
Deposited on : 2021-03-30  
Resolution : 2.41 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](mailto: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.

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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 : 2.24  
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) : 2.24

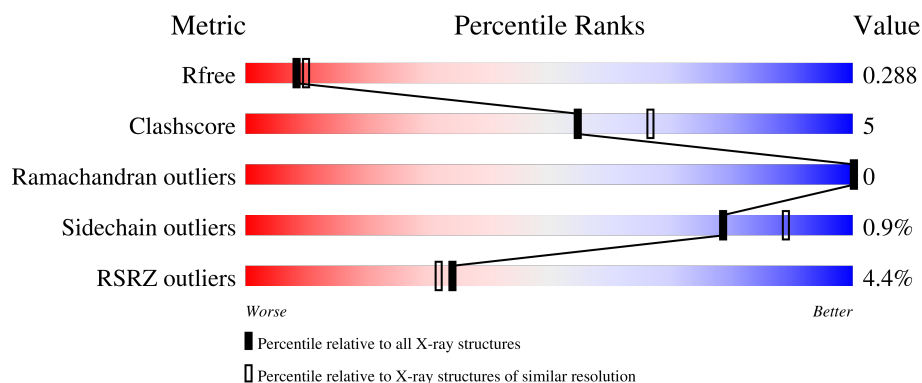
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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  $\geq 3$ , 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	174	<div> <div>3%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	B	174	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	C	174	<div> <div>2%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
1	D	174	<div> <div>6%</div> <div>81%</div> <div>14%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLC	D	204	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5725 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 Sigma intracellular receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1366	934	206	221	5			
1	B	166	Total	C	N	O	S	0	0	0
			1349	926	204	214	5			
1	C	163	Total	C	N	O	S	0	0	0
			1319	907	193	213	6			
1	D	165	Total	C	N	O	S	0	0	0
			1323	908	197	213	5			

There are 24 discrepancies between the modelled and reference sequences:

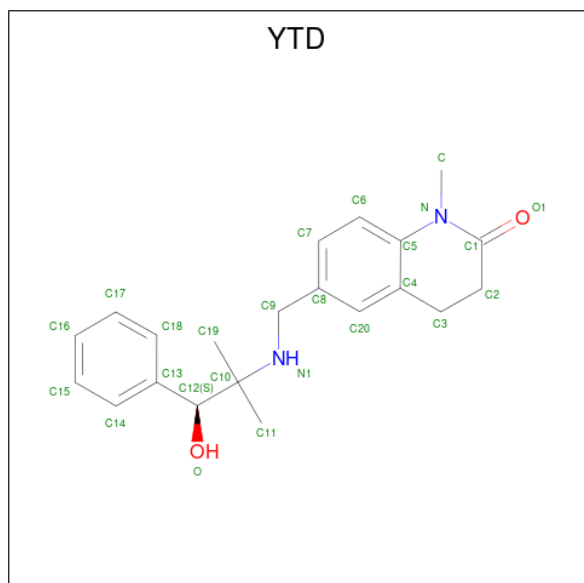
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q3MHW7
A	-4	PRO	-	expression tag	UNP Q3MHW7
A	-3	GLY	-	expression tag	UNP Q3MHW7
A	-2	GLY	-	expression tag	UNP Q3MHW7
A	-1	SER	-	expression tag	UNP Q3MHW7
A	0	SER	-	expression tag	UNP Q3MHW7
B	-5	GLY	-	expression tag	UNP Q3MHW7
B	-4	PRO	-	expression tag	UNP Q3MHW7
B	-3	GLY	-	expression tag	UNP Q3MHW7
B	-2	GLY	-	expression tag	UNP Q3MHW7
B	-1	SER	-	expression tag	UNP Q3MHW7
B	0	SER	-	expression tag	UNP Q3MHW7
C	-5	GLY	-	expression tag	UNP Q3MHW7
C	-4	PRO	-	expression tag	UNP Q3MHW7
C	-3	GLY	-	expression tag	UNP Q3MHW7
C	-2	GLY	-	expression tag	UNP Q3MHW7
C	-1	SER	-	expression tag	UNP Q3MHW7
C	0	SER	-	expression tag	UNP Q3MHW7
D	-5	GLY	-	expression tag	UNP Q3MHW7
D	-4	PRO	-	expression tag	UNP Q3MHW7
D	-3	GLY	-	expression tag	UNP Q3MHW7

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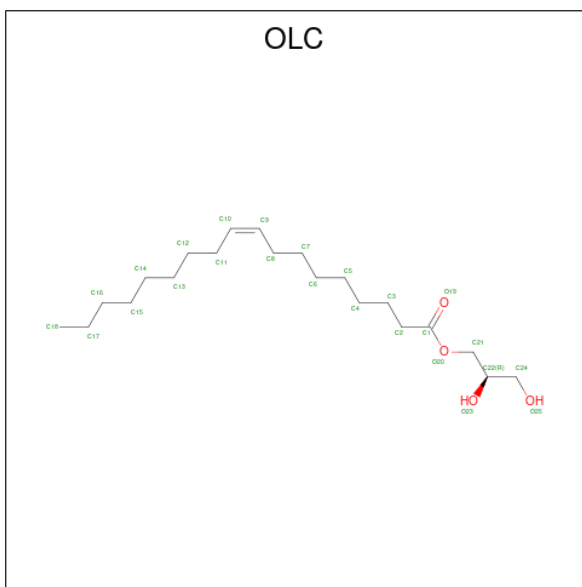
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q3MHW7
D	-1	SER	-	expression tag	UNP Q3MHW7
D	0	SER	-	expression tag	UNP Q3MHW7

- Molecule 2 is 6-({[(1S)-1-hydroxy-2-methyl-1-phenylpropan-2-yl]amino}methyl)-1-methyl-3,4-dihydroquinolin-2(1H)-one (three-letter code: YTD) (formula: C<sub>21</sub>H<sub>26</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	21	2	2		
2	B	1	Total	C	N	O	0	0
			25	21	2	2		
2	C	1	Total	C	N	O	0	0
			25	21	2	2		
2	D	1	Total	C	N	O	0	0
			25	21	2	2		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



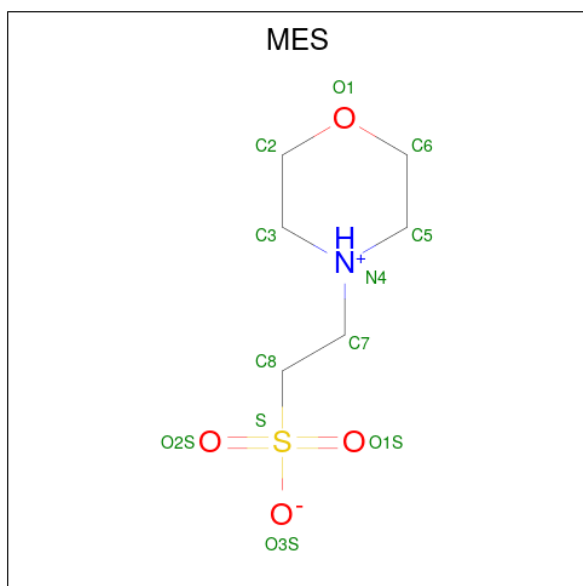
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 14 14	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 10 10	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 13 13	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 14 14	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 10 10	0	0
3	D	1	Total C 11 11	0	0
3	D	1	Total C 13 13	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 9 9	0	0
3	D	1	Total C 9 9	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 1 4 1	0	0
4	D	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0

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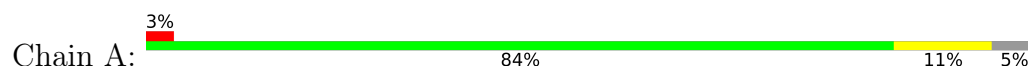
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total 11	O 11	0	0
5	C	7	Total 7	O 7	0	0
5	D	7	Total 7	O 7	0	0



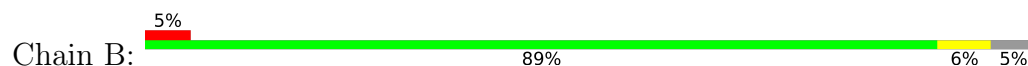
### 3 Residue-property plots [i](#)

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.

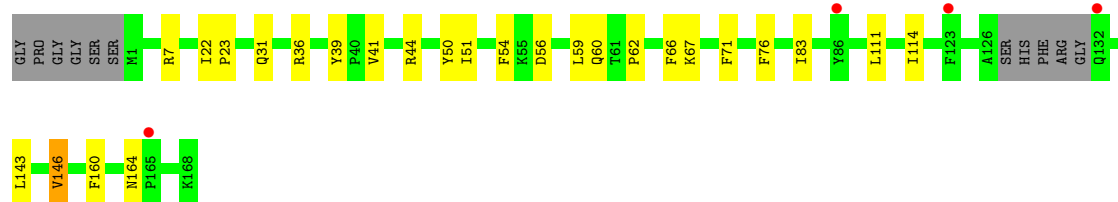
- Molecule 1: Sigma intracellular receptor 2



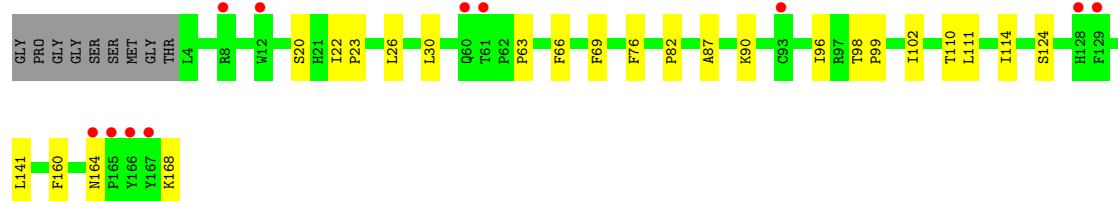
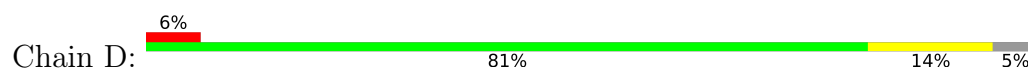
- Molecule 1: Sigma intracellular receptor 2



- Molecule 1: Sigma intracellular receptor 2



- Molecule 1: Sigma intracellular receptor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.70Å 55.35Å 92.95Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	40.19 – 2.41 47.52 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.9 (40.19-2.41) 98.0 (47.52-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.94 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.250 , 0.288 0.250 , 0.288	Depositor DCC
$R_{free}$ test set	1375 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2137e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, YTD, 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	0.26	0/1417	0.39	0/1937
1	B	0.26	0/1399	0.39	0/1914
1	C	0.25	0/1367	0.38	0/1872
1	D	0.25	0/1372	0.37	0/1879
All	All	0.26	0/5555	0.38	0/7602

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 [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	1366	0	1356	14	0
1	B	1349	0	1334	7	0
1	C	1319	0	1298	18	0
1	D	1323	0	1288	17	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	1	0
2	D	25	0	0	0	0
3	A	73	0	107	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	93	2	0
3	C	30	0	47	3	0
3	D	48	0	71	5	0
4	A	12	0	12	2	0
4	D	12	0	12	1	0
5	A	12	0	0	0	0
5	B	11	0	0	0	0
5	C	7	0	0	0	0
5	D	7	0	0	0	0
All	All	5725	0	5618	59	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 (59) 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:51:ILE:HD13	1:C:60:GLN:HB2	1.66	0.77
1:A:7:ARG:NH2	4:A:208:MES:O1S	2.18	0.77
1:A:7:ARG:NH2	4:A:208:MES:S	2.62	0.72
1:D:111:LEU:HD23	1:D:114:ILE:HD12	1.74	0.69
1:A:97:ARG:HA	1:A:161:MET:HE2	1.81	0.62
1:D:82:PRO:HB3	3:D:203:OLC:H18B	1.83	0.60
1:A:111:LEU:HD23	1:A:114:ILE:HD12	1.84	0.58
1:A:83:ILE:HD13	1:D:141:LEU:HD21	1.87	0.57
1:C:56:ASP:HA	1:C:143:LEU:HD21	1.88	0.54
1:A:22:ILE:HB	1:A:23:PRO:HD3	1.89	0.54
1:A:56:ASP:HA	1:A:143:LEU:HD21	1.89	0.53
1:B:63:PRO:HD2	1:B:66:PHE:HB3	1.90	0.53
1:C:111:LEU:HD23	1:C:114:ILE:HD12	1.90	0.53
1:C:71:PHE:CD2	3:C:204:OLC:H9	2.44	0.53
3:A:206:OLC:H14A	1:D:141:LEU:HG	1.91	0.53
1:B:111:LEU:HD23	1:B:114:ILE:HD12	1.92	0.51
1:C:146:VAL:HG13	2:C:201:YTD:O	2.10	0.51
1:C:22:ILE:HB	1:C:23:PRO:HD3	1.91	0.51
1:D:102:ILE:HG22	3:D:202:OLC:H8A	1.95	0.49
1:D:164:ASN:O	1:D:168:LYS:N	2.45	0.49
1:D:160:PHE:O	1:D:164:ASN:HB2	2.13	0.48
1:D:22:ILE:HB	1:D:23:PRO:HD3	1.97	0.47
3:A:209:OLC:H11A	1:B:67:LYS:HB3	1.97	0.47
1:D:63:PRO:HD2	1:D:66:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HD11	3:B:202:OLC:H16	1.98	0.46
3:A:202:OLC:H17A	3:A:204:OLC:H11	1.98	0.46
1:D:87:ALA:HB3	1:D:96:ILE:HD12	1.97	0.46
1:C:62:PRO:HB2	1:C:67:LYS:HG3	1.97	0.46
1:B:148:ILE:HG22	1:B:149:PRO:HD3	1.97	0.46
1:C:76:PHE:HB3	3:C:203:OLC:H8A	1.97	0.46
1:C:60:GLN:O	1:C:62:PRO:HD3	2.17	0.45
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.83	0.45
1:C:83:ILE:HD12	3:C:202:OLC:H13	1.98	0.45
4:D:207:MES:H82	4:D:207:MES:H51	1.75	0.45
1:D:69:PHE:CD2	1:D:110:THR:HG23	2.52	0.45
3:A:203:OLC:H7	3:A:203:OLC:H10	1.78	0.44
1:C:41:VAL:HG22	1:C:44:ARG:HH11	1.81	0.44
1:A:54:PHE:HB3	1:A:143:LEU:HD13	2.00	0.43
1:C:50:TYR:CD1	1:C:54:PHE:HD2	2.36	0.43
1:A:86:TYR:CD1	3:A:207:OLC:H9	2.54	0.42
1:C:62:PRO:HB3	1:C:66:PHE:HD2	1.84	0.42
1:A:153:ILE:HB	1:A:154:PRO:HD3	2.02	0.42
1:A:25:THR:HA	1:A:29:ASP:HB2	2.00	0.42
1:C:31:GLN:HG2	1:C:39:TYR:CZ	2.54	0.42
1:C:7:ARG:HG3	1:C:160:PHE:HZ	1.85	0.41
1:D:20:SER:O	1:D:23:PRO:HD2	2.20	0.41
1:A:51:ILE:HD13	1:A:60:GLN:HB2	2.01	0.41
1:D:90:LYS:HB2	3:D:203:OLC:H8	2.02	0.41
1:B:111:LEU:HD11	1:B:150:TYR:HB2	2.02	0.41
1:C:160:PHE:O	1:C:164:ASN:HB2	2.20	0.41
1:D:26:LEU:HD23	1:D:30:LEU:HD12	2.02	0.40
1:A:7:ARG:HG3	1:A:160:PHE:HZ	1.84	0.40
1:C:36:ARG:HB3	1:C:44:ARG:HH21	1.86	0.40
1:D:160:PHE:CD1	3:D:205:OLC:H8	2.57	0.40
1:D:98:THR:HB	1:D:99:PRO:HD3	2.04	0.40
1:A:86:TYR:HD1	3:A:207:OLC:H9	1.86	0.40
3:B:206:OLC:H9	3:B:206:OLC:H6	1.61	0.40
1:C:59:LEU:HD23	1:C:59:LEU:HA	1.95	0.40
1:D:76:PHE:HB3	3:D:202:OLC:H7A	2.04	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	164/174 (94%)	161 (98%)	3 (2%)	0	100	100
1	B	164/174 (94%)	159 (97%)	5 (3%)	0	100	100
1	C	159/174 (91%)	154 (97%)	5 (3%)	0	100	100
1	D	163/174 (94%)	157 (96%)	6 (4%)	0	100	100
All	All	650/696 (93%)	631 (97%)	19 (3%)	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	144/155 (93%)	143 (99%)	1 (1%)	84	92
1	B	138/155 (89%)	136 (99%)	2 (1%)	67	81
1	C	135/155 (87%)	134 (99%)	1 (1%)	84	92
1	D	133/155 (86%)	132 (99%)	1 (1%)	81	91
All	All	550/620 (89%)	545 (99%)	5 (1%)	78	89

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

Mol	Chain	Res	Type
1	A	141	LEU
1	B	21	HIS

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Mol	Chain	Res	Type
1	B	31	GLN
1	C	146	VAL
1	D	124	SER

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

26 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	$\# Z  > 2$
3	OLC	D	205	-	8,8,24	0.43	0	7,7,25	0.87	0
3	OLC	A	205	-	9,9,24	0.35	0	8,8,25	0.67	0
3	OLC	A	206	-	8,8,24	0.40	0	6,7,25	0.70	0
3	OLC	D	203	-	12,12,24	0.36	0	11,11,25	0.70	0
3	OLC	B	204	-	12,12,24	0.35	0	11,11,25	0.71	0
3	OLC	C	203	-	11,11,24	0.34	0	10,10,25	0.67	0
3	OLC	D	202	-	10,10,24	0.39	0	8,9,25	0.73	0
3	OLC	B	205	-	10,10,24	0.35	0	9,9,25	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	YTD	B	201	-	26,27,27	0.13	0	33,39,39	0.68	1 (3%)
3	OLC	B	203	-	9,9,24	0.42	0	8,8,25	0.89	0
3	OLC	D	206	-	8,8,24	0.41	0	6,7,25	0.68	0
3	OLC	A	203	-	11,11,24	0.36	0	10,10,25	0.68	0
4	MES	D	207	-	12,12,12	2.31	1 (8%)	14,16,16	2.07	5 (35%)
3	OLC	A	207	-	8,8,24	0.41	0	6,7,25	0.66	0
2	YTD	D	201	-	26,27,27	0.16	0	33,39,39	0.44	0
2	YTD	A	201	-	26,27,27	0.13	0	33,39,39	0.67	1 (3%)
3	OLC	B	206	-	13,13,24	0.34	0	12,12,25	0.75	0
3	OLC	C	204	-	9,9,24	0.37	0	8,8,25	0.64	0
3	OLC	A	202	-	13,13,24	0.34	0	12,12,25	0.73	0
4	MES	A	208	-	12,12,12	2.27	1 (8%)	14,16,16	1.69	3 (21%)
3	OLC	A	204	-	8,8,24	0.39	0	6,7,25	0.76	0
3	OLC	C	202	-	7,7,24	0.31	0	6,6,25	0.71	0
3	OLC	B	202	-	7,7,24	0.31	0	6,6,25	0.71	0
3	OLC	D	204	-	5,5,24	0.33	0	4,4,25	0.53	0
2	YTD	C	201	-	26,27,27	0.13	0	33,39,39	0.54	1 (3%)
3	OLC	A	209	-	9,9,24	0.37	0	8,8,25	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	D	205	-	-	3/6/6/24	-
3	OLC	A	205	-	-	2/7/7/24	-
3	OLC	A	206	-	-	2/6/6/24	-
3	OLC	D	203	-	-	1/10/10/24	-
3	OLC	B	204	-	-	4/10/10/24	-
3	OLC	C	203	-	-	2/9/9/24	-
3	OLC	D	202	-	-	3/8/8/24	-
3	OLC	B	205	-	-	1/8/8/24	-
2	YTD	B	201	-	-	7/15/29/29	0/3/3/3
3	OLC	B	203	-	-	2/7/7/24	-
3	OLC	D	206	-	-	2/6/6/24	-
3	OLC	A	203	-	-	3/9/9/24	-
4	MES	D	207	-	-	3/6/14/14	0/1/1/1
3	OLC	A	207	-	-	4/6/6/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YTD	D	201	-	-	7/15/29/29	0/3/3/3
2	YTD	A	201	-	-	7/15/29/29	0/3/3/3
3	OLC	B	206	-	-	6/11/11/24	-
3	OLC	C	204	-	-	2/7/7/24	-
3	OLC	A	202	-	-	1/11/11/24	-
4	MES	A	208	-	-	3/6/14/14	0/1/1/1
3	OLC	A	204	-	-	2/6/6/24	-
3	OLC	C	202	-	-	0/5/5/24	-
3	OLC	B	202	-	-	0/5/5/24	-
3	OLC	D	204	-	-	0/3/3/24	-
2	YTD	C	201	-	-	6/15/29/29	0/3/3/3
3	OLC	A	209	-	-	1/7/7/24	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	207	MES	C8-S	-7.74	1.66	1.77
4	A	208	MES	C8-S	-7.58	1.66	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	208	MES	C5-N4-C3	3.88	117.57	108.83
4	D	207	MES	C5-N4-C3	3.57	116.86	108.83
4	D	207	MES	C6-C5-N4	-3.25	105.18	110.10
4	D	207	MES	O1S-S-C8	3.23	110.81	106.92
2	B	201	YTD	C9-N1-C10	3.18	119.83	115.84
2	A	201	YTD	C9-N1-C10	3.10	119.73	115.84
4	D	207	MES	C7-N4-C5	3.04	119.01	111.23
4	A	208	MES	O3S-S-C8	2.74	110.21	105.77
4	D	207	MES	O1-C6-C5	-2.74	105.77	111.80
2	C	201	YTD	C9-N1-C10	2.16	118.54	115.84
4	A	208	MES	O1-C6-C5	-2.05	107.29	111.80

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	YTD	C11-C10-C12-C13
2	A	201	YTD	C19-C10-C12-O

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Mol	Chain	Res	Type	Atoms
2	A	201	YTD	C19-C10-C12-C13
2	A	201	YTD	C11-C10-N1-C9
2	A	201	YTD	C12-C10-N1-C9
2	A	201	YTD	C19-C10-N1-C9
2	B	201	YTD	C11-C10-C12-O
2	B	201	YTD	C11-C10-C12-C13
2	B	201	YTD	C19-C10-C12-O
2	B	201	YTD	C19-C10-C12-C13
2	B	201	YTD	C11-C10-N1-C9
2	B	201	YTD	C12-C10-N1-C9
2	B	201	YTD	C19-C10-N1-C9
2	C	201	YTD	C11-C10-C12-O
2	C	201	YTD	C11-C10-C12-C13
2	C	201	YTD	C19-C10-C12-O
2	C	201	YTD	C19-C10-C12-C13
2	C	201	YTD	C8-C9-N1-C10
2	D	201	YTD	C11-C10-C12-C13
2	D	201	YTD	C19-C10-C12-O
2	D	201	YTD	C19-C10-C12-C13
2	D	201	YTD	C11-C10-N1-C9
2	D	201	YTD	C12-C10-N1-C9
3	A	204	OLC	C7-C8-C9-C10
3	D	206	OLC	C7-C8-C9-C10
4	A	208	MES	N4-C7-C8-S
4	D	207	MES	C7-C8-S-O1S
2	D	201	YTD	C19-C10-N1-C9
4	D	207	MES	C7-C8-S-O3S
3	A	206	OLC	C7-C8-C9-C10
3	A	205	OLC	C7-C8-C9-C10
3	B	203	OLC	C3-C4-C5-C6
3	B	204	OLC	C10-C11-C12-C13
4	A	208	MES	C8-C7-N4-C3
4	A	208	MES	C8-C7-N4-C5
3	D	205	OLC	C4-C5-C6-C7
3	B	205	OLC	C7-C8-C9-C10
3	A	207	OLC	C7-C8-C9-C10
3	D	202	OLC	C9-C10-C11-C12
3	B	206	OLC	C15-C16-C17-C18
3	D	205	OLC	C6-C7-C8-C9
3	B	206	OLC	C6-C7-C8-C9
2	A	201	YTD	C11-C10-C12-O
2	D	201	YTD	C11-C10-C12-O

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Mol	Chain	Res	Type	Atoms
3	A	203	OLC	C7-C8-C9-C10
3	B	204	OLC	C9-C10-C11-C12
4	D	207	MES	C7-C8-S-O2S
3	B	204	OLC	C7-C8-C9-C10
3	D	203	OLC	C7-C8-C9-C10
3	C	204	OLC	C9-C10-C11-C12
3	B	206	OLC	C14-C15-C16-C17
3	D	206	OLC	C9-C10-C11-C12
3	A	203	OLC	C10-C11-C12-C13
3	C	203	OLC	C10-C11-C12-C13
3	A	207	OLC	C10-C11-C12-C13
3	B	206	OLC	C12-C13-C14-C15
3	A	206	OLC	C9-C10-C11-C12
3	A	205	OLC	C9-C10-C11-C12
3	A	202	OLC	C9-C10-C11-C12
3	A	207	OLC	C12-C13-C14-C15
3	A	209	OLC	C7-C8-C9-C10
3	B	203	OLC	C7-C8-C9-C10
3	B	206	OLC	C9-C10-C11-C12
3	C	204	OLC	C7-C8-C9-C10
3	D	202	OLC	C7-C8-C9-C10
3	D	205	OLC	C7-C8-C9-C10
3	D	202	OLC	C3-C4-C5-C6
3	B	206	OLC	C7-C8-C9-C10
3	A	203	OLC	C9-C10-C11-C12
3	A	204	OLC	C9-C10-C11-C12
3	A	207	OLC	C9-C10-C11-C12
2	C	201	YTD	O-C12-C13-C18
3	B	204	OLC	C12-C13-C14-C15
3	C	203	OLC	C2-C3-C4-C5

There are no ring outliers.

17 monomers are involved in 20 short contacts:

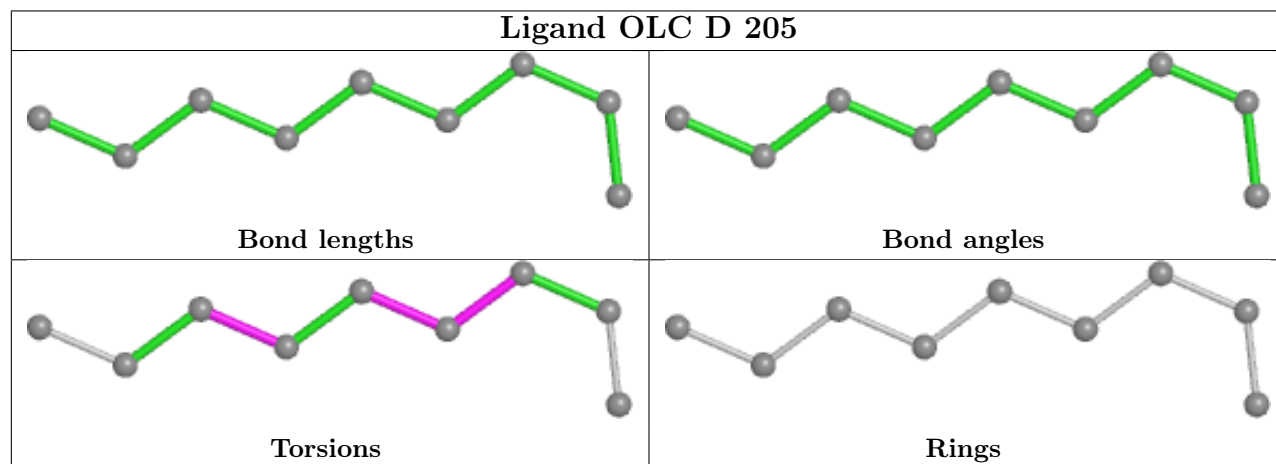
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	205	OLC	1	0
3	A	206	OLC	1	0
3	D	203	OLC	2	0
3	C	203	OLC	1	0
3	D	202	OLC	2	0
3	A	203	OLC	1	0
4	D	207	MES	1	0

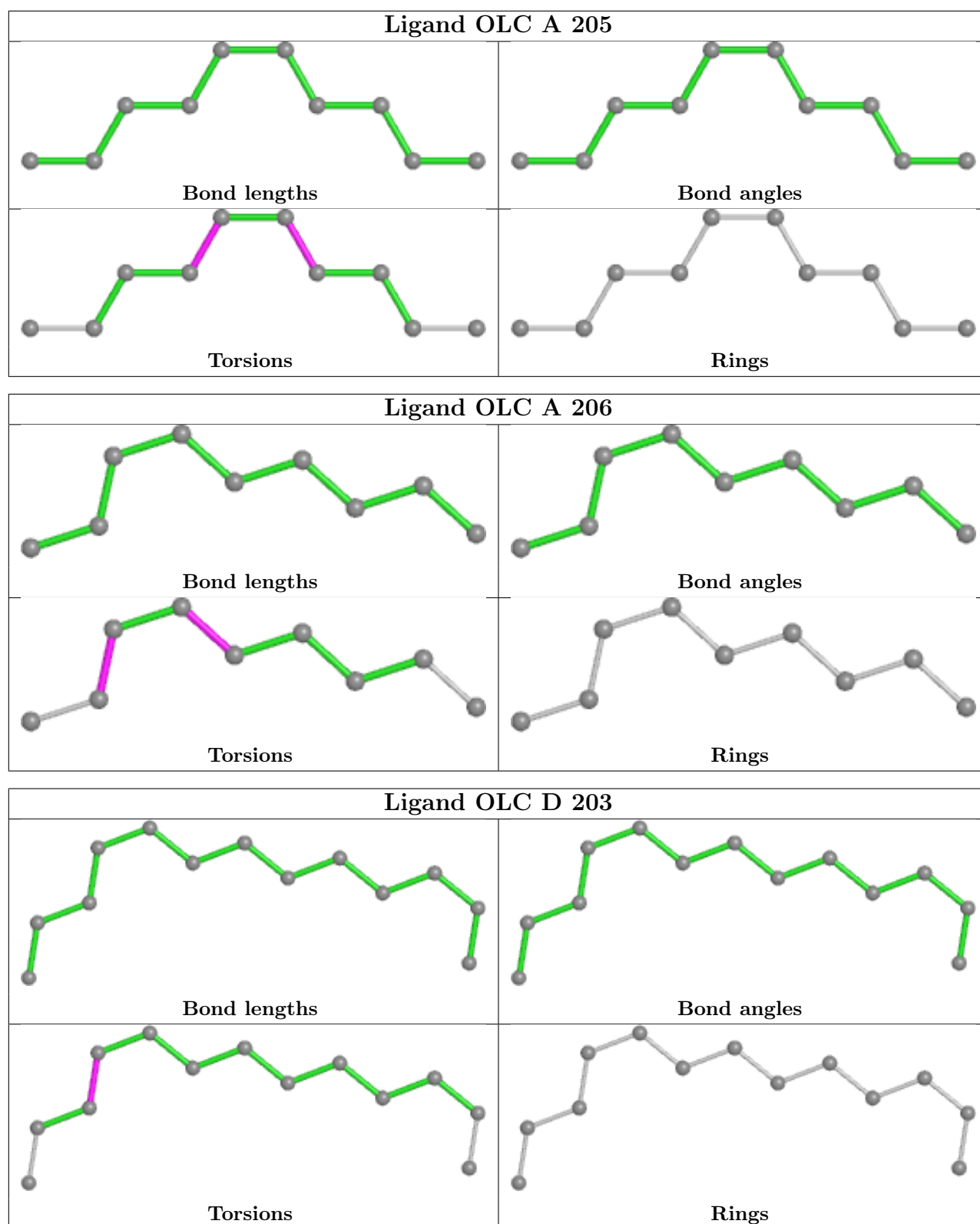
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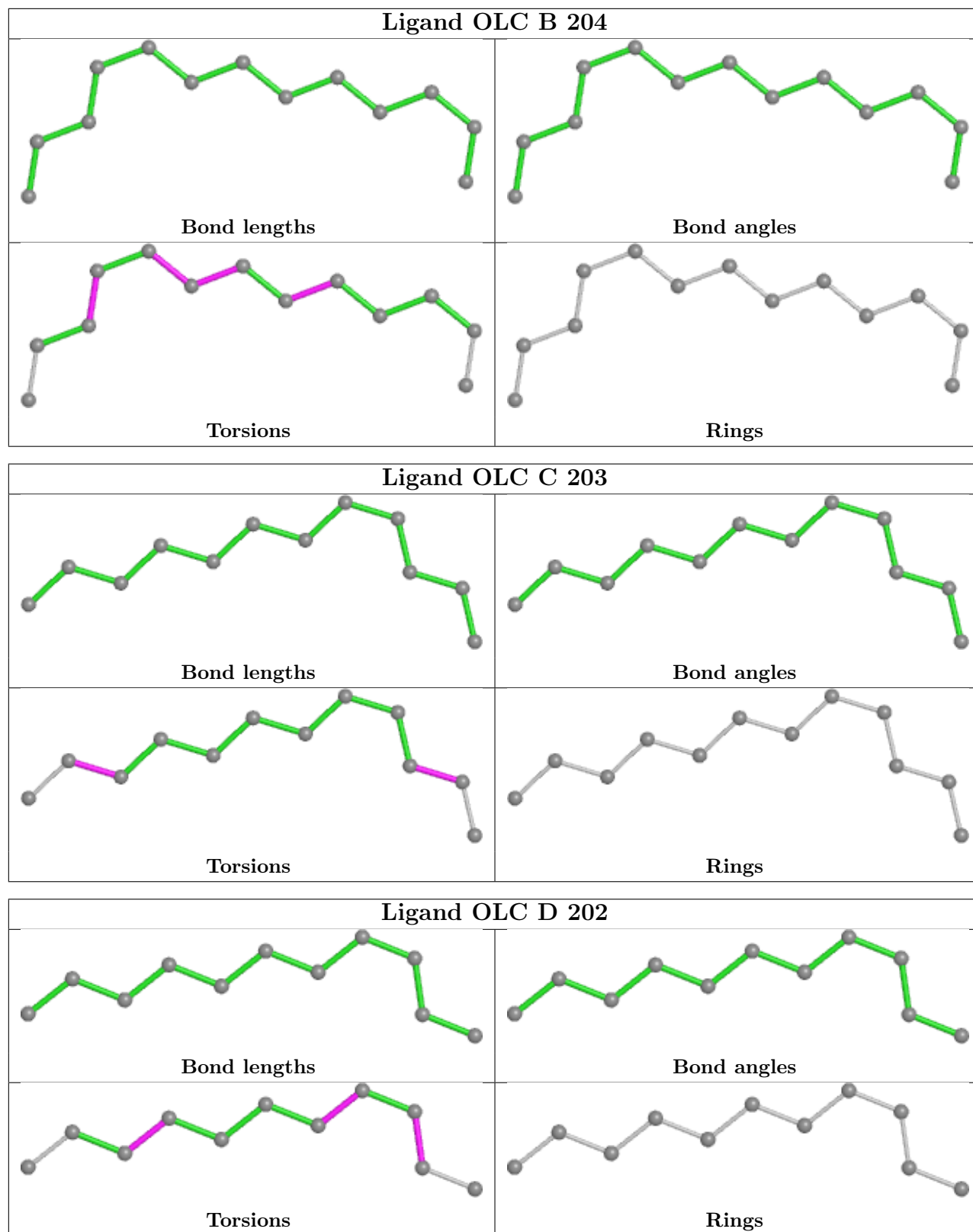
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	207	OLC	2	0
3	B	206	OLC	1	0
3	C	204	OLC	1	0
3	A	202	OLC	1	0
4	A	208	MES	2	0
3	A	204	OLC	1	0
3	C	202	OLC	1	0
3	B	202	OLC	1	0
2	C	201	YTD	1	0
3	A	209	OLC	1	0

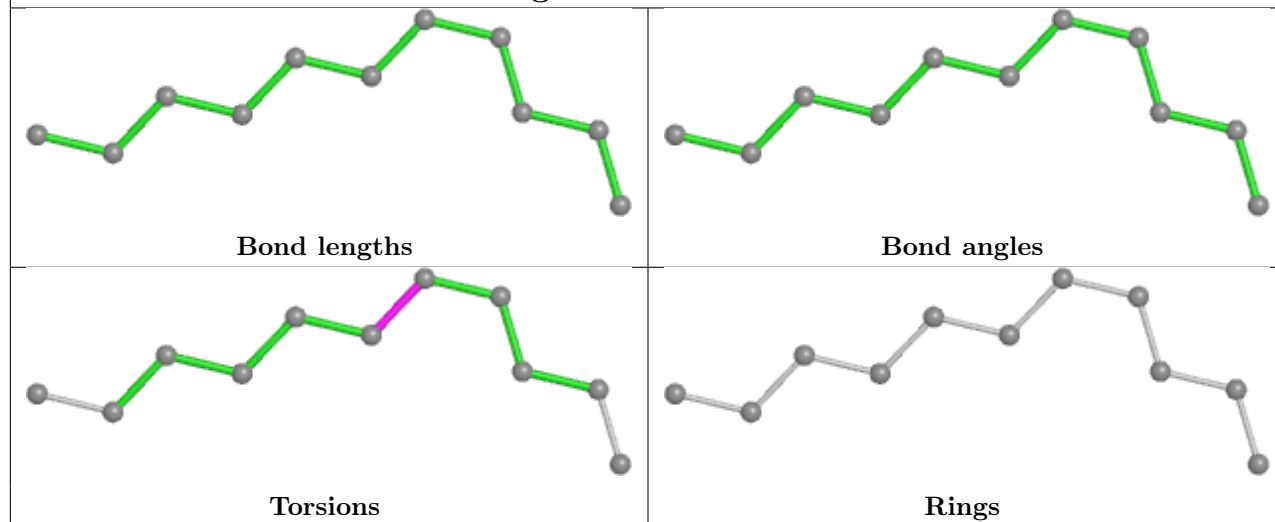
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



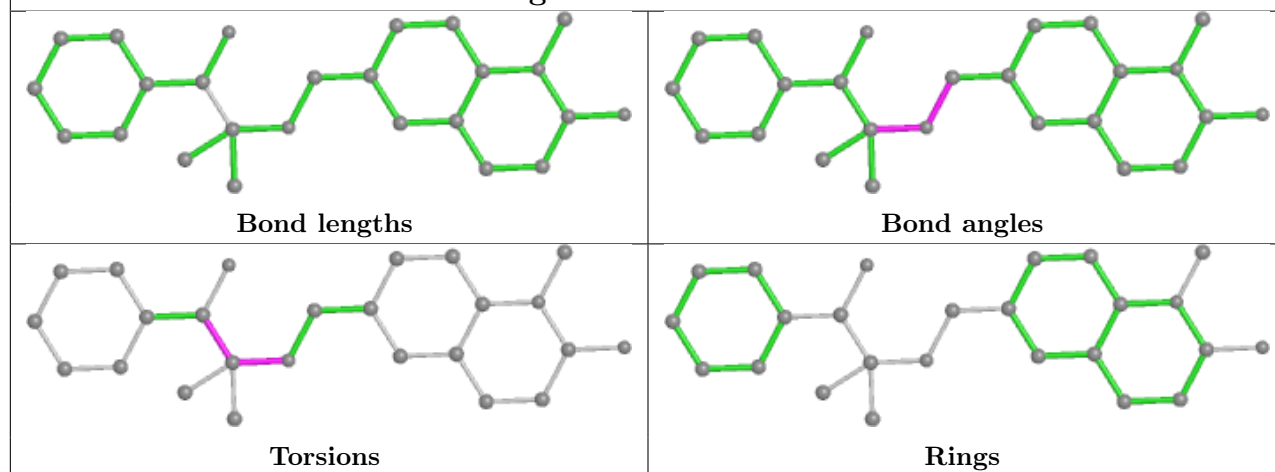




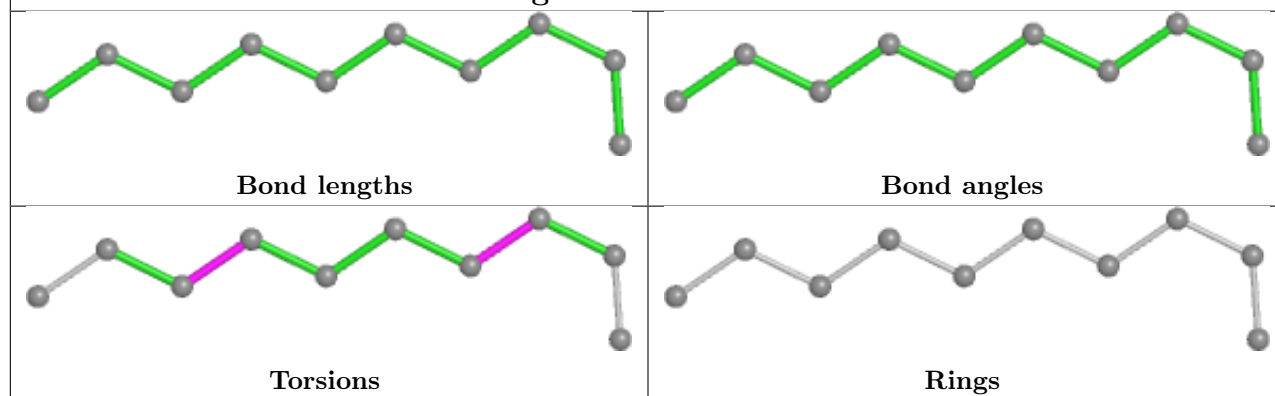
## Ligand OLC B 205

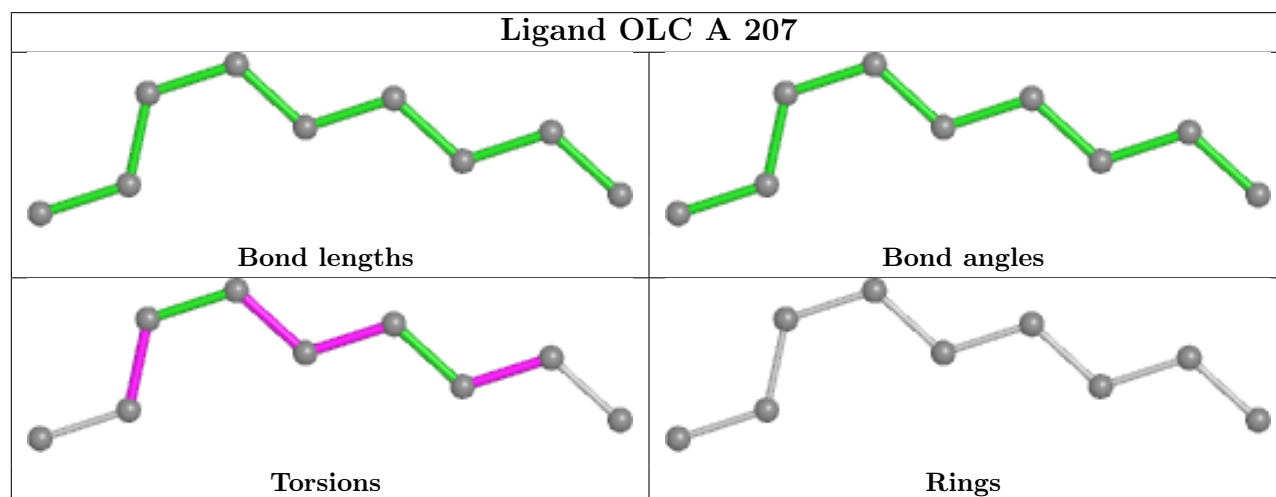
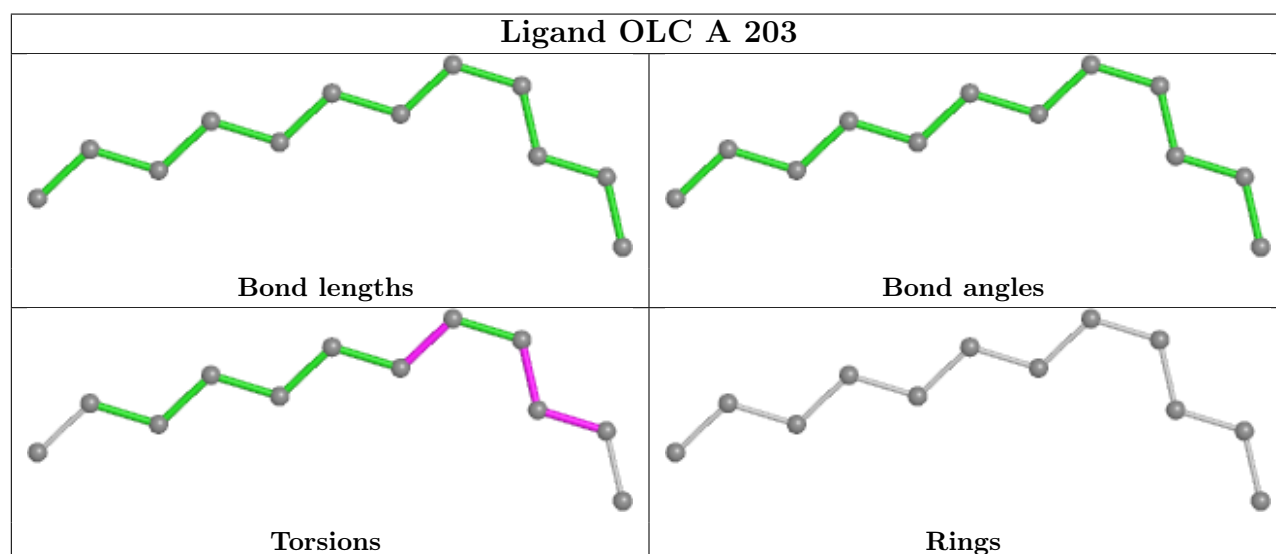
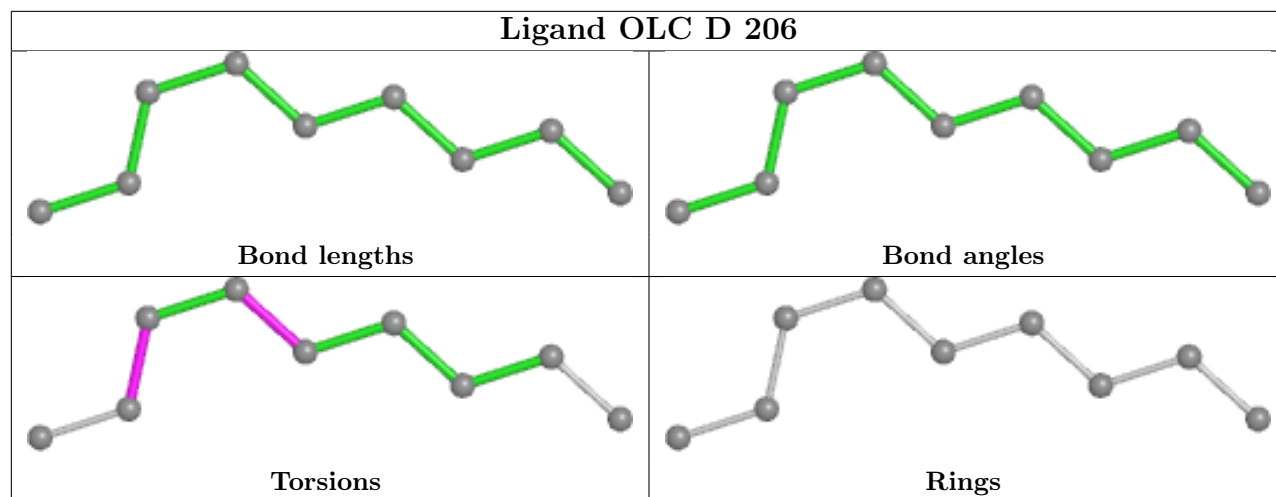


## Ligand YTD B 201

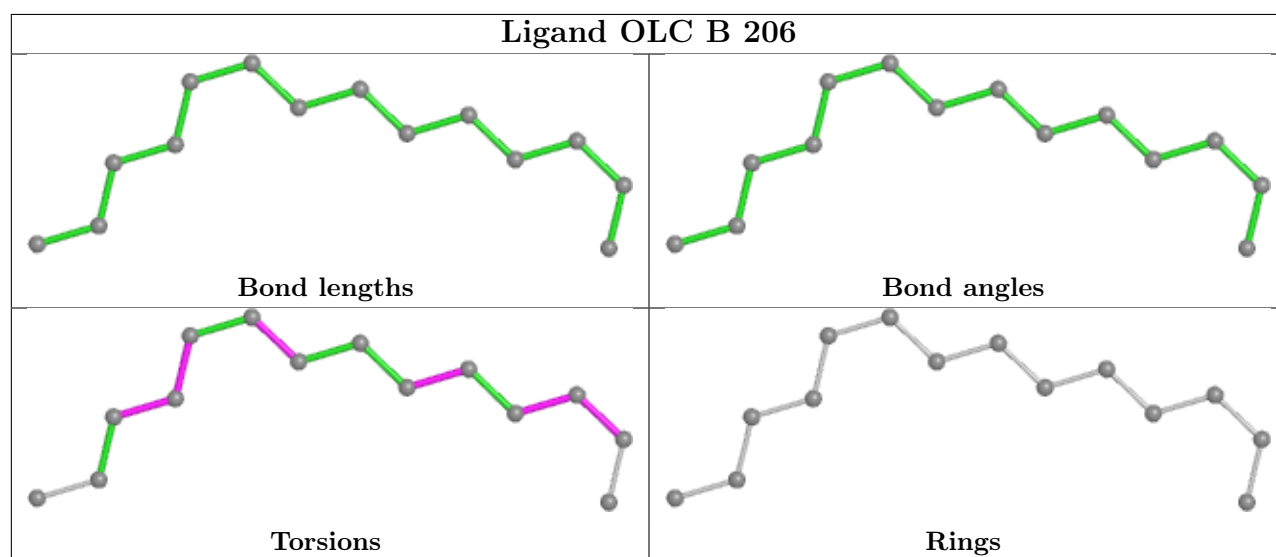
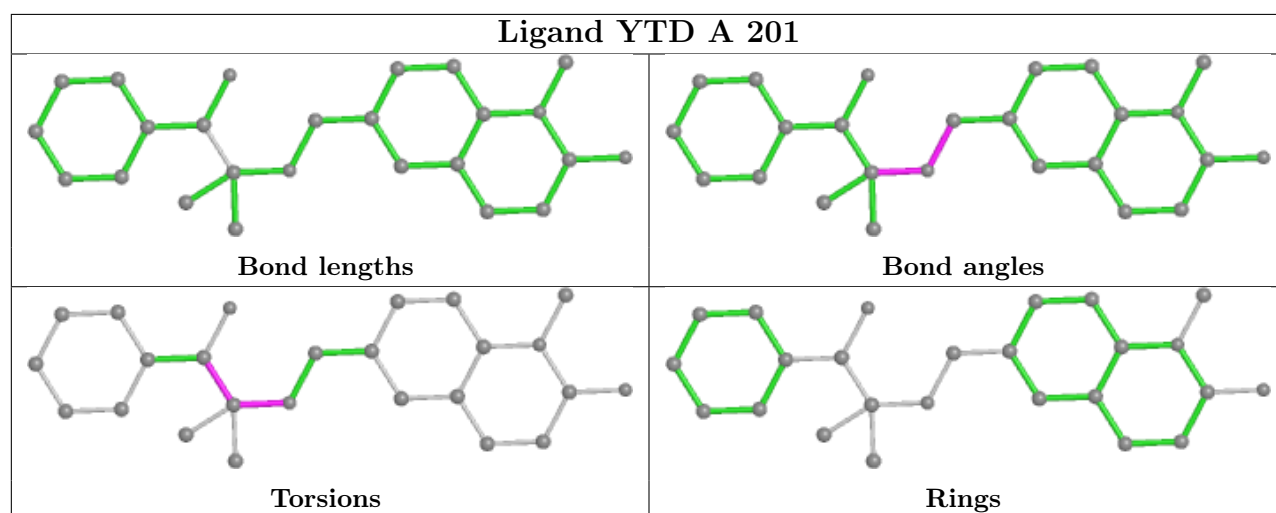
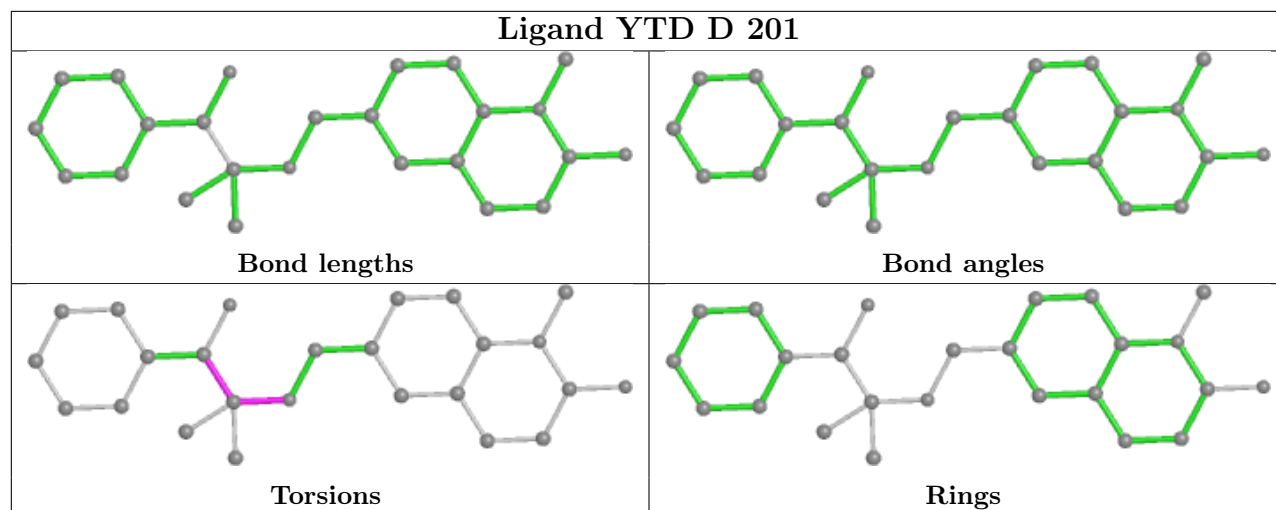


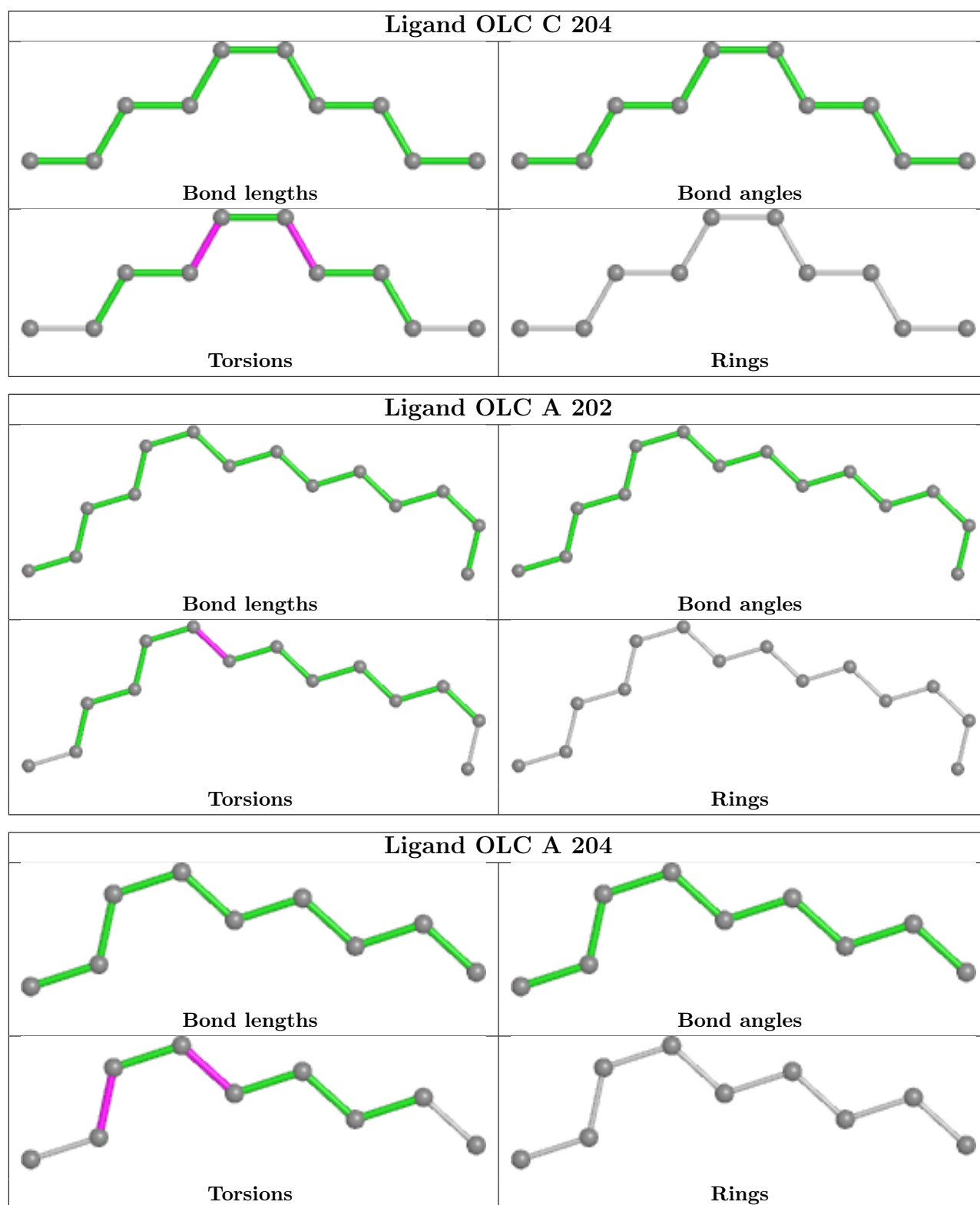
## Ligand OLC B 203

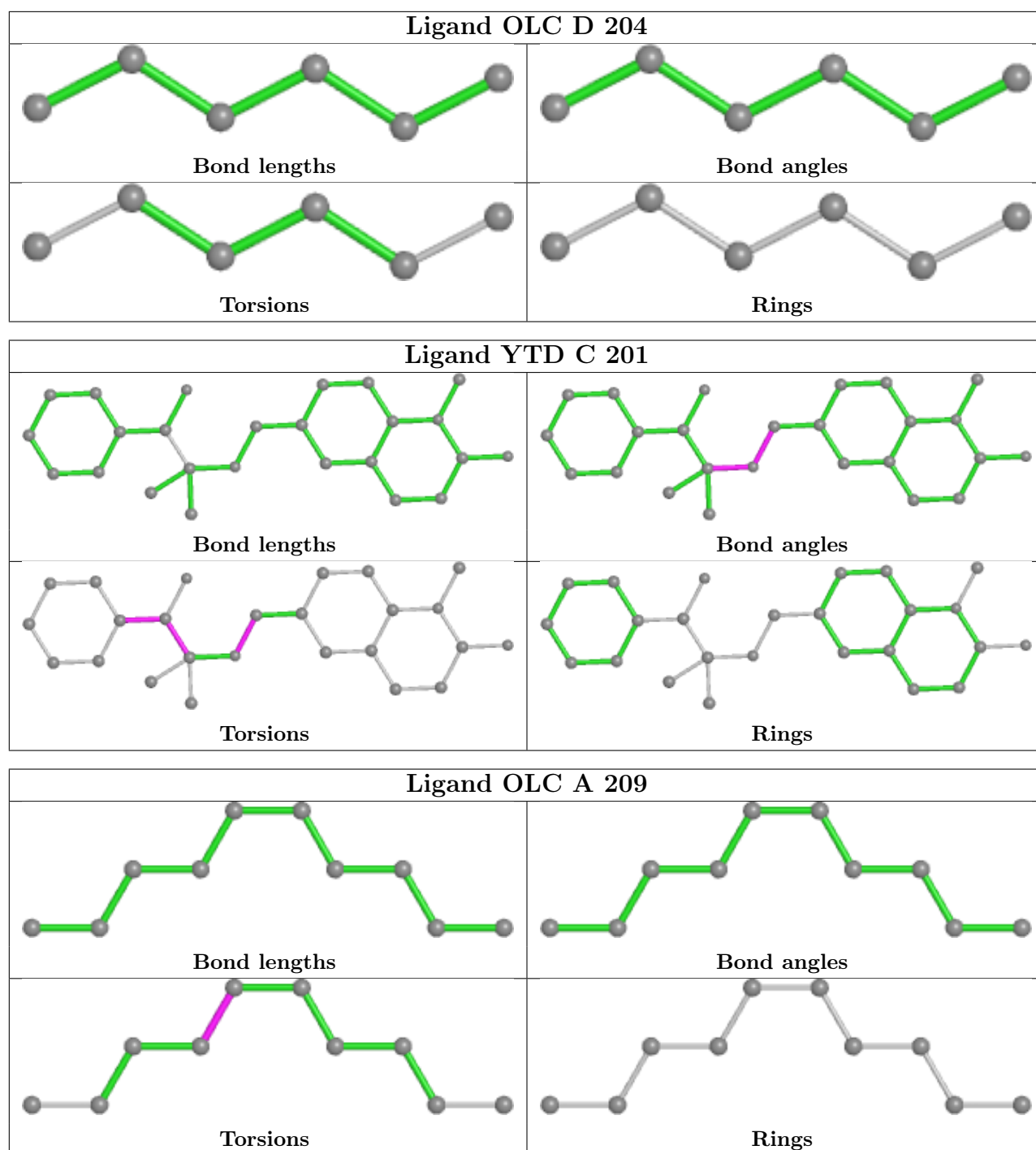












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	166/174 (95%)	0.16	5 (3%) 50 48	40, 53, 71, 91	0
1	B	166/174 (95%)	0.27	9 (5%) 25 23	39, 56, 86, 128	0
1	C	163/174 (93%)	0.17	4 (2%) 57 54	41, 57, 81, 108	0
1	D	165/174 (94%)	0.22	11 (6%) 17 15	42, 55, 89, 129	0
All	All	660/696 (94%)	0.20	29 (4%) 34 32	39, 55, 81, 129	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	GLY	6.5
1	D	165	PRO	5.3
1	B	126	ALA	4.4
1	D	12	TRP	4.1
1	A	126	ALA	3.7
1	C	86	TYR	3.4
1	D	166	TYR	3.2
1	B	167	TYR	3.1
1	A	124	SER	3.0
1	A	125	LYS	2.8
1	B	51	ILE	2.6
1	D	167	TYR	2.5
1	D	93	CYS	2.5
1	D	61	THR	2.5
1	B	92	GLY	2.5
1	B	129	PHE	2.4
1	B	130	ARG	2.4
1	D	128	HIS	2.4
1	C	132	GLN	2.4
1	A	41	VAL	2.4
1	D	8	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	124	SER	2.2
1	A	127	SER	2.1
1	D	129	PHE	2.1
1	C	165	PRO	2.1
1	B	45	ASN	2.0
1	C	123	PHE	2.0
1	D	60	GLN	2.0
1	D	164	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

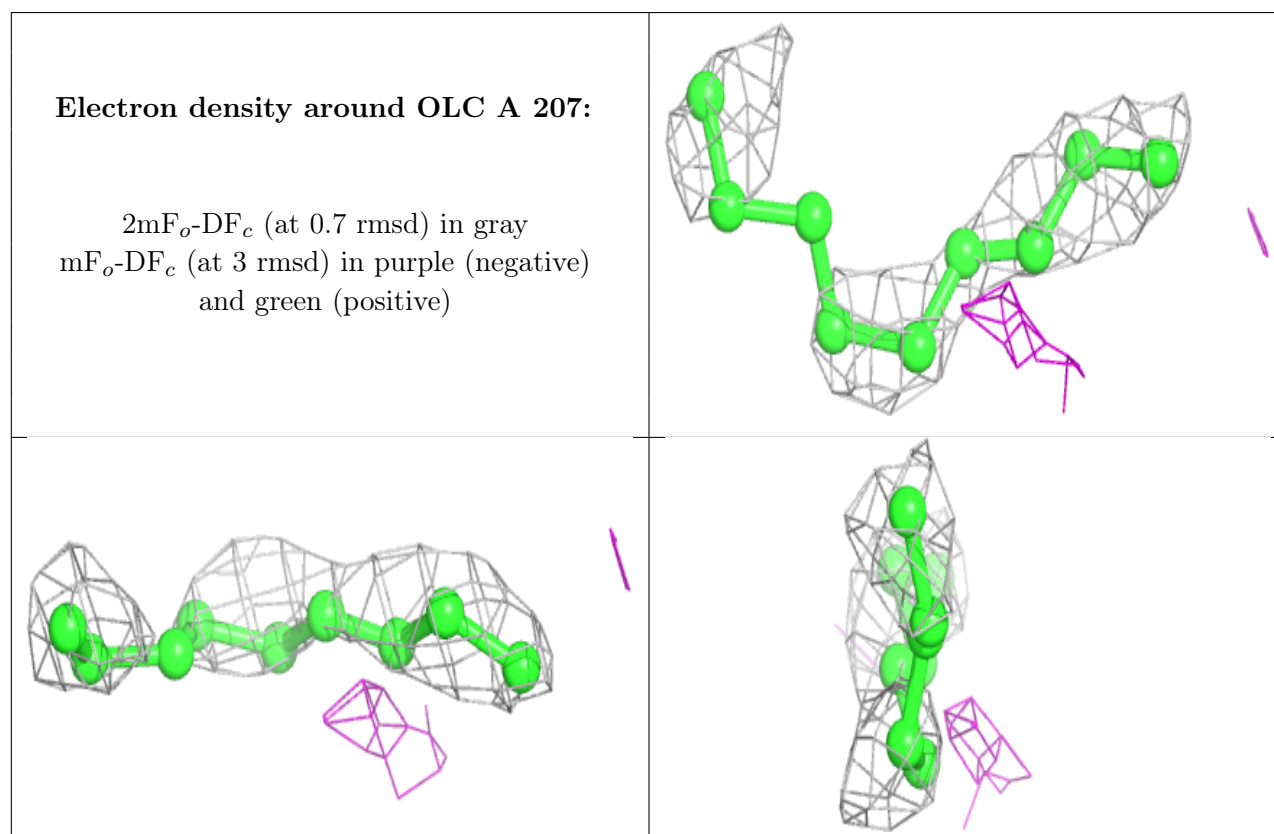
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	OLC	B	202	8/25	0.47	0.38	44,62,70,72	0
3	OLC	A	207	9/25	0.55	0.38	48,59,67,70	0
3	OLC	D	204	6/25	0.55	0.50	60,63,66,74	0
3	OLC	C	204	10/25	0.57	0.32	51,54,66,69	0
4	MES	A	208	12/12	0.64	0.27	58,72,82,82	0
3	OLC	D	203	13/25	0.67	0.29	58,66,73,76	0
4	MES	D	207	12/12	0.69	0.24	66,81,94,95	0
3	OLC	B	206	14/25	0.70	0.23	58,68,70,70	0
3	OLC	D	205	9/25	0.75	0.21	54,61,64,65	0
3	OLC	D	206	9/25	0.76	0.23	59,66,73,77	0
3	OLC	C	202	8/25	0.77	0.21	61,64,66,67	0
3	OLC	B	204	13/25	0.79	0.23	51,61,68,68	0
3	OLC	A	209	10/25	0.79	0.38	58,63,69,69	0
2	YTD	C	201	25/25	0.80	0.25	56,69,83,85	0
3	OLC	A	205	10/25	0.81	0.26	56,67,72,72	0

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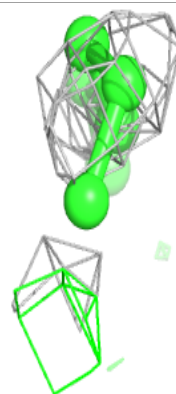
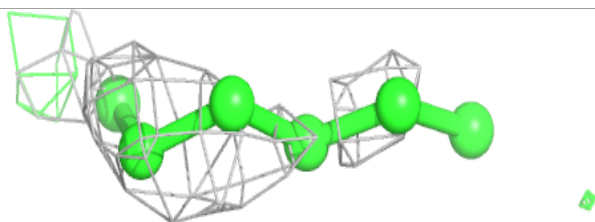
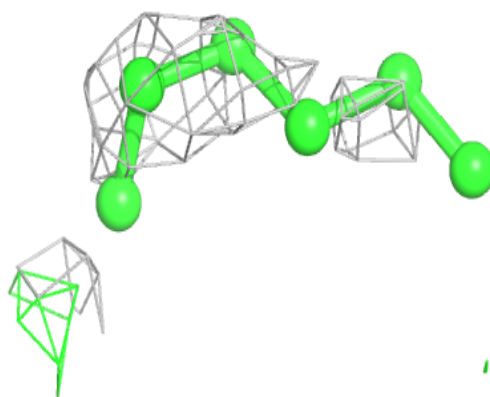
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OLC	A	203	12/25	0.81	0.21	59,64,68,69	0
3	OLC	A	204	9/25	0.82	0.22	52,60,63,66	0
3	OLC	C	203	12/25	0.84	0.23	36,45,54,60	0
3	OLC	A	206	9/25	0.84	0.17	56,62,69,70	0
3	OLC	B	203	10/25	0.85	0.16	48,56,66,71	0
3	OLC	A	202	14/25	0.85	0.21	45,54,61,63	0
2	YTD	B	201	25/25	0.88	0.17	50,60,79,87	0
2	YTD	D	201	25/25	0.88	0.25	50,60,83,86	0
2	YTD	A	201	25/25	0.89	0.25	47,58,75,76	0
3	OLC	B	205	11/25	0.89	0.22	40,44,55,58	0
3	OLC	D	202	11/25	0.93	0.18	41,51,57,58	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.

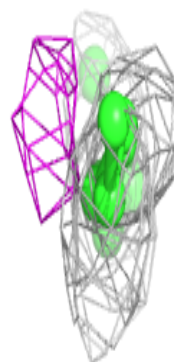
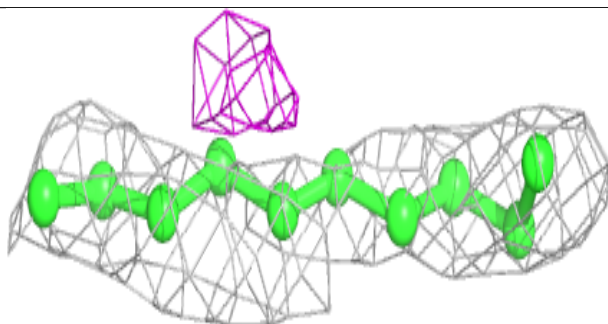
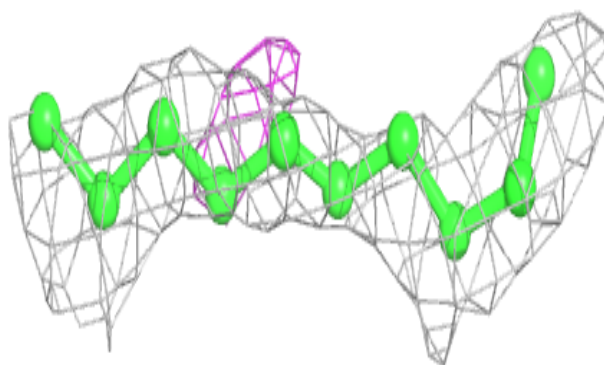


**Electron density around OLC D 204:**

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

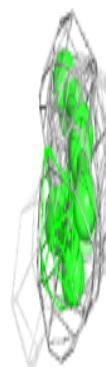
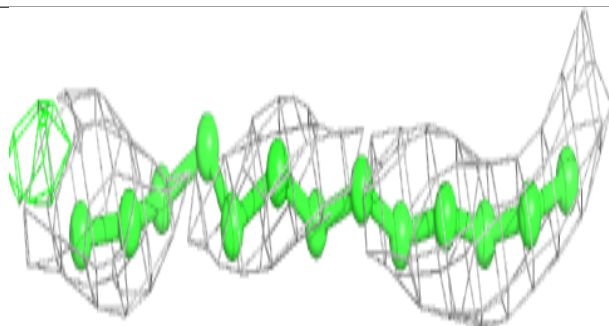
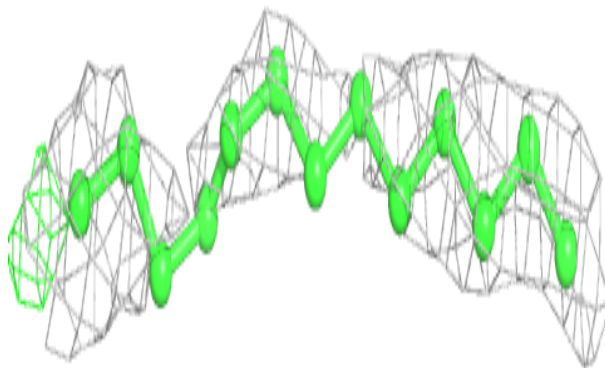
**Electron density around OLC C 204:**

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

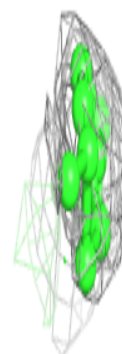
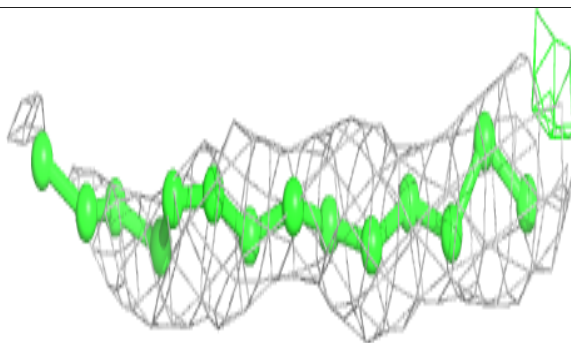
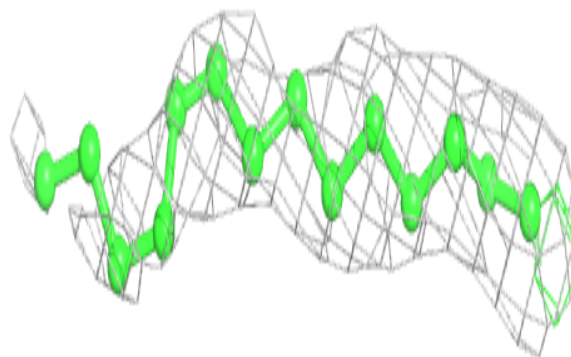


**Electron density around OLC D 203:**

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

**Electron density around OLC B 206:**

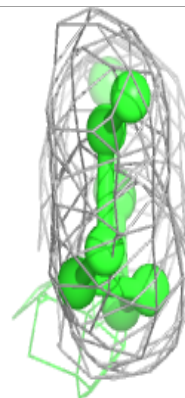
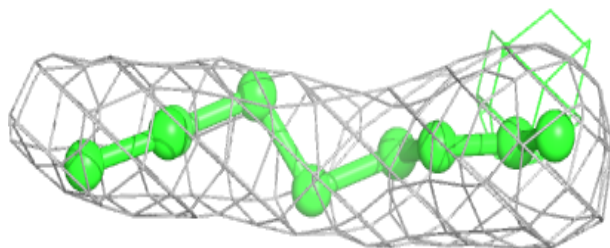
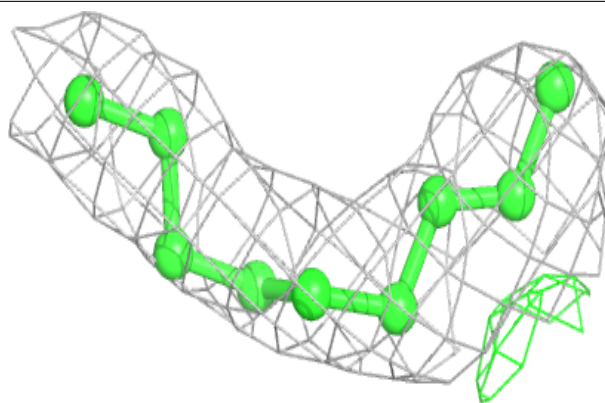
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



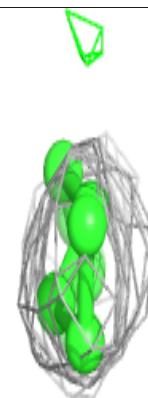
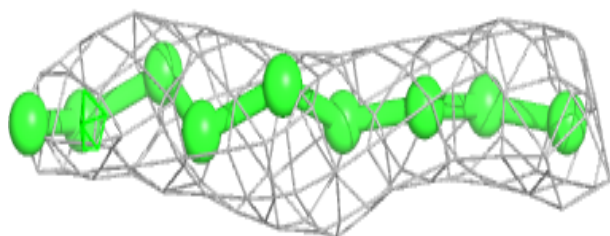
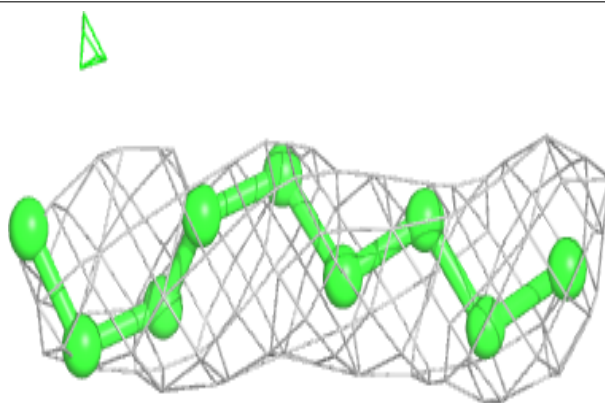


**Electron density around OLC D 205:**

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

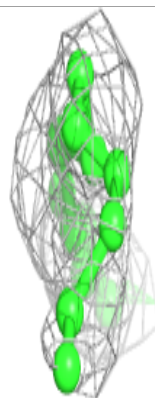
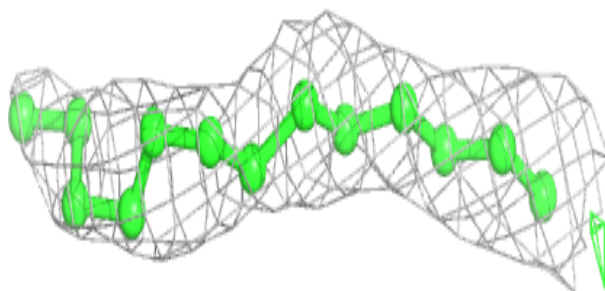
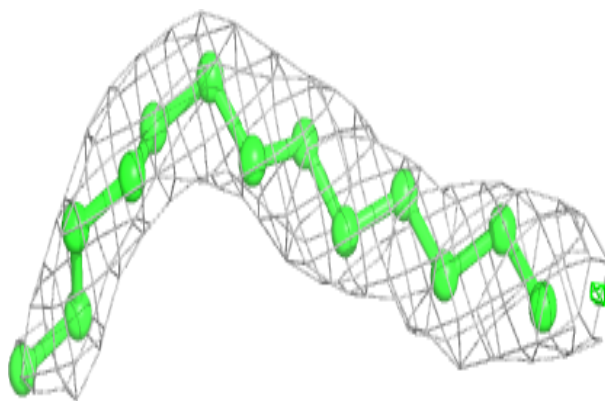
**Electron density around OLC D 206:**

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

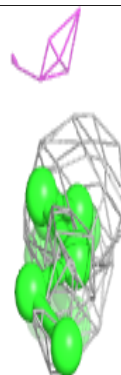
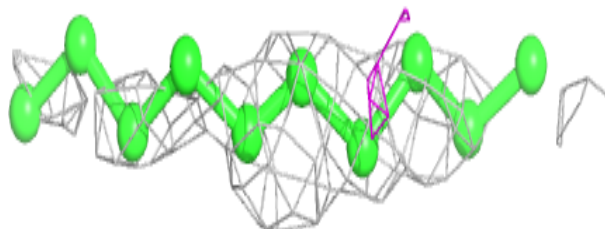
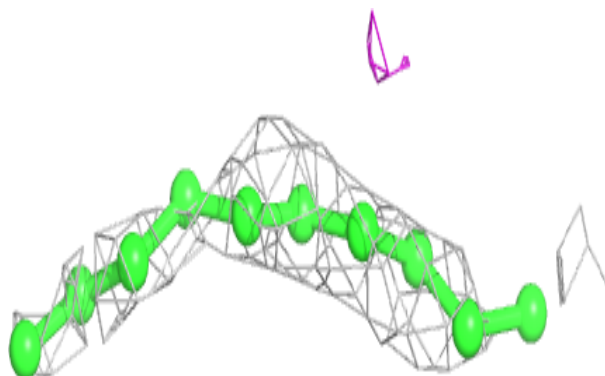


**Electron density around OLC B 204:**

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

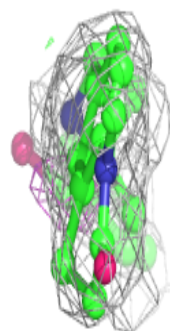
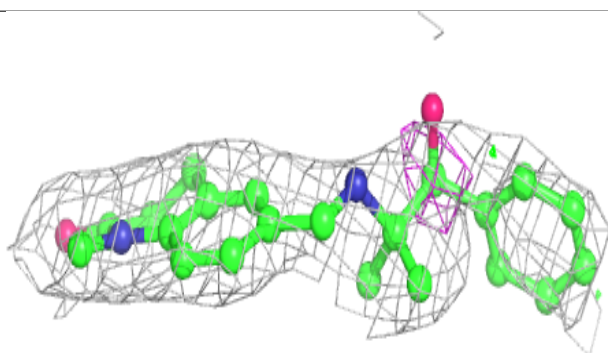
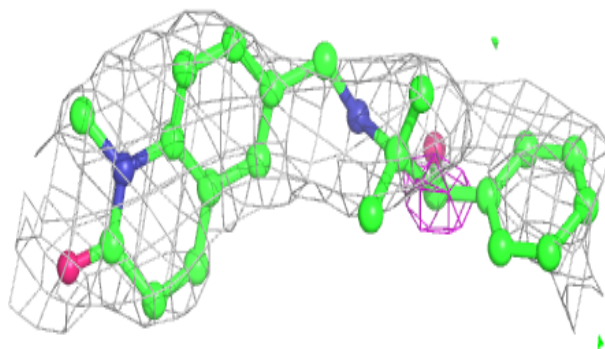
**Electron density around OLC A 209:**

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

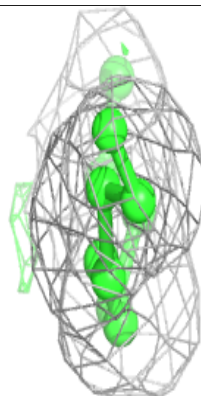
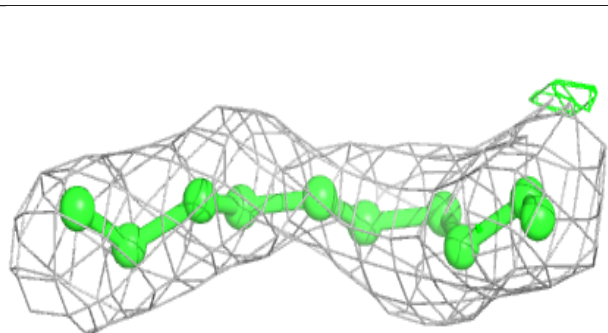
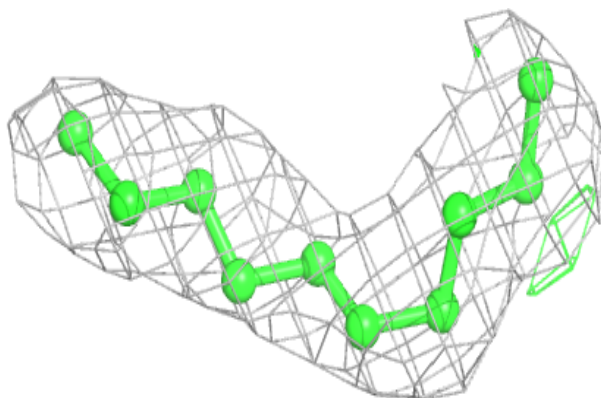


**Electron density around YTD C 201:**

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

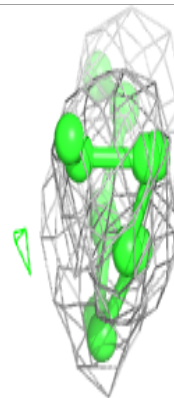
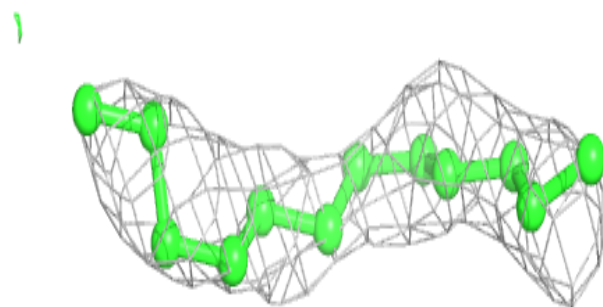
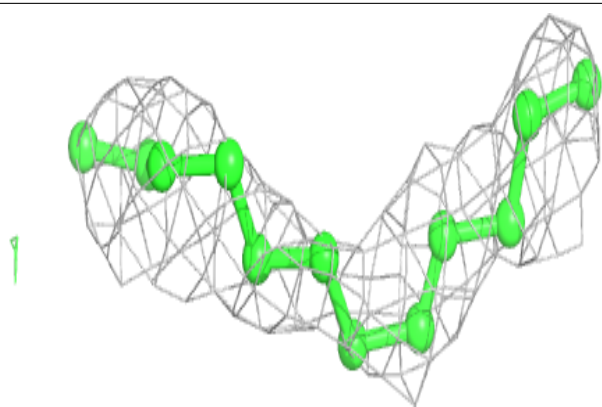
**Electron density around OLC A 205:**

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

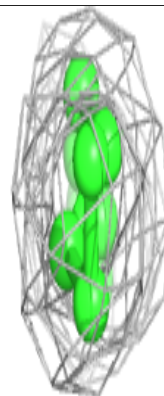
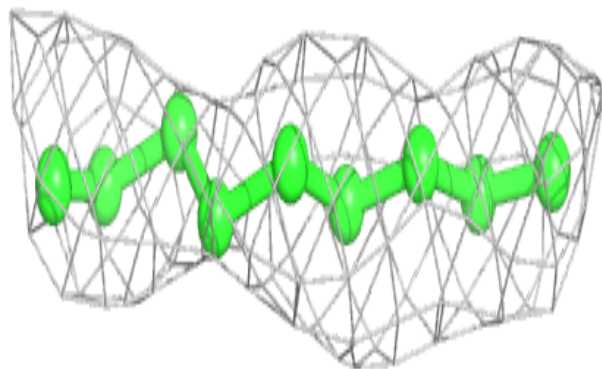
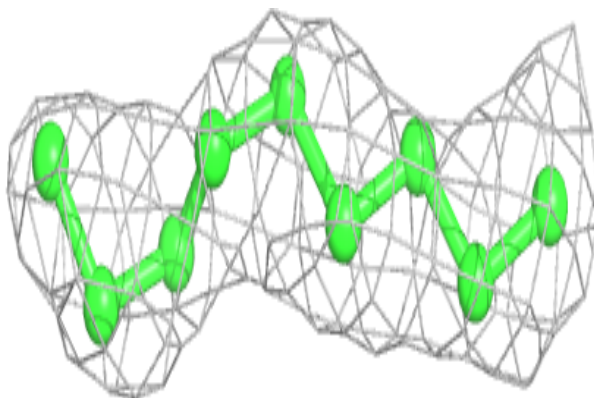


**Electron density around OLC A 203:**

$2mF_o-DF_c$  (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:**

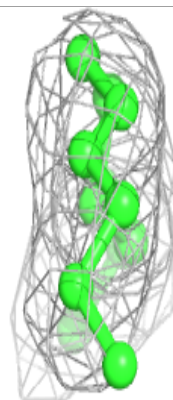
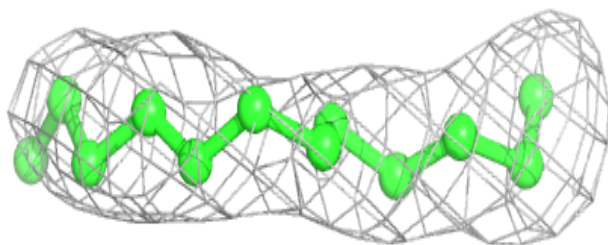
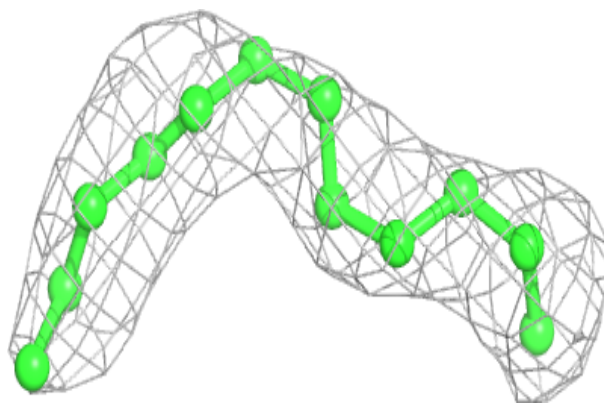
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



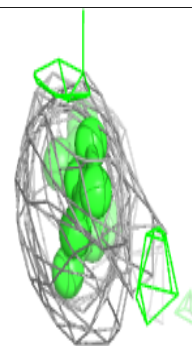
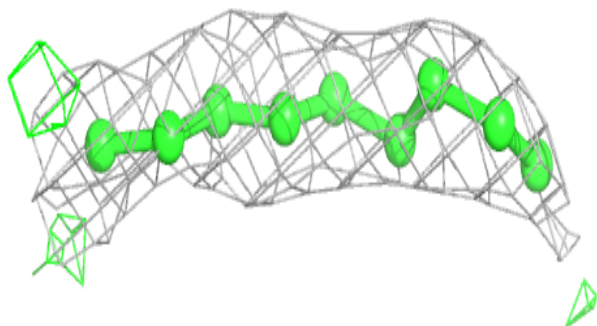
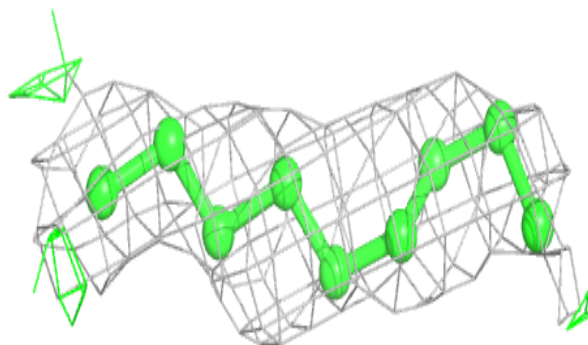


**Electron density around OLC C 203:**

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

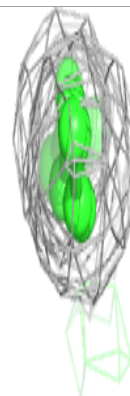
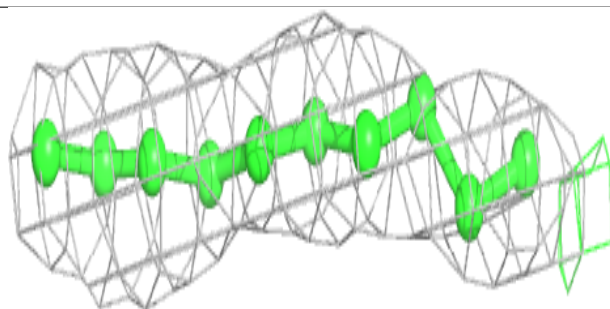
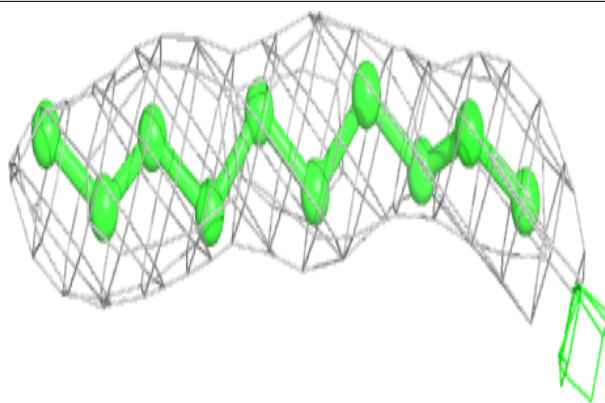
**Electron density around OLC A 206:**

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

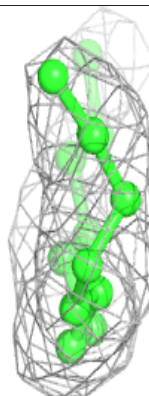
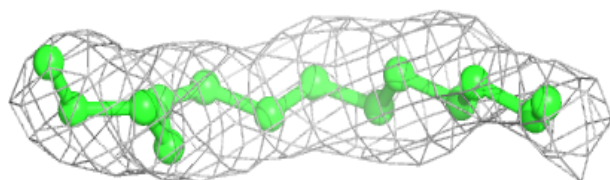
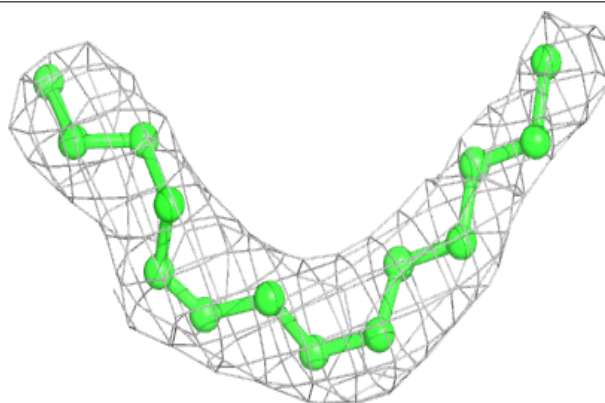


**Electron density around OLC B 203:**

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

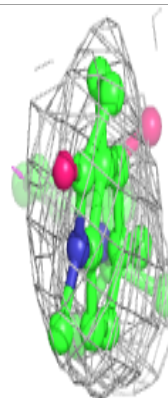
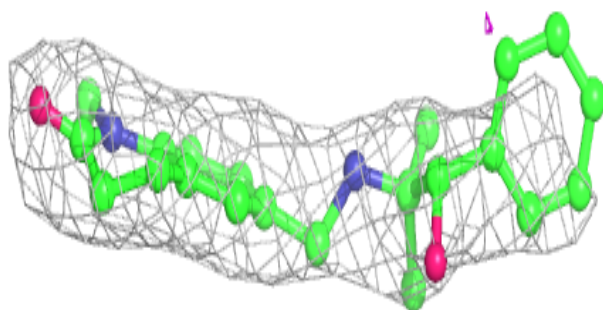
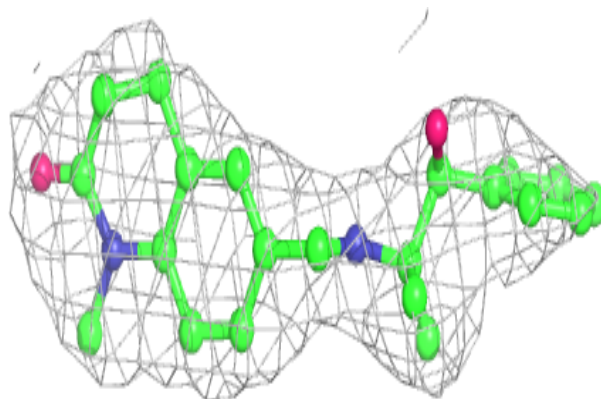
**Electron density around OLC A 202:**

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

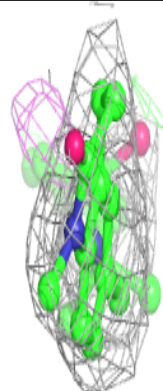
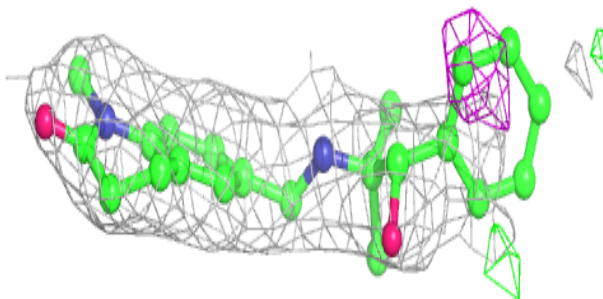
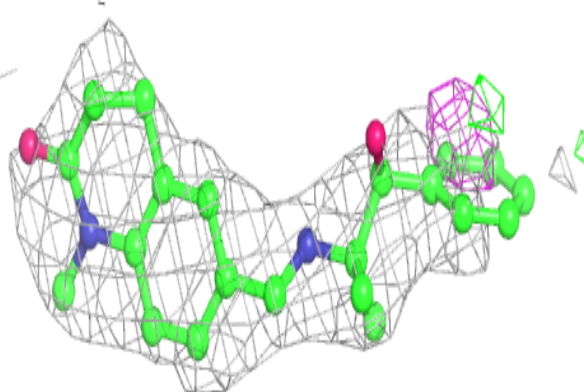


**Electron density around YTD B 201:**

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

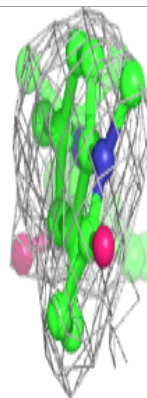
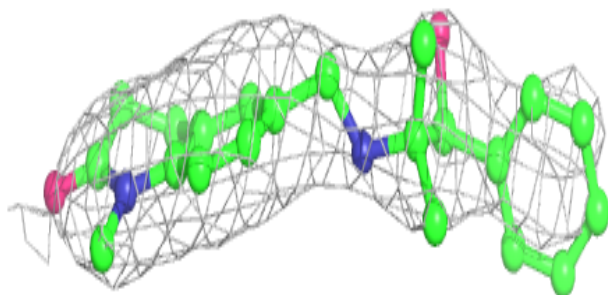
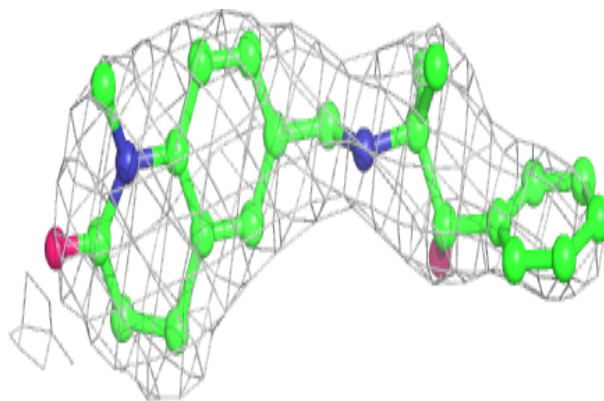
**Electron density around YTD D 201:**

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

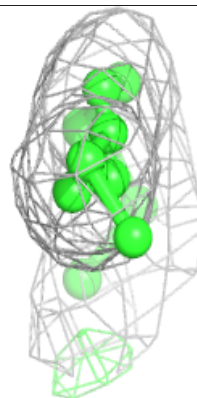
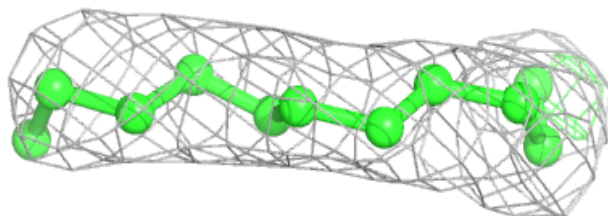
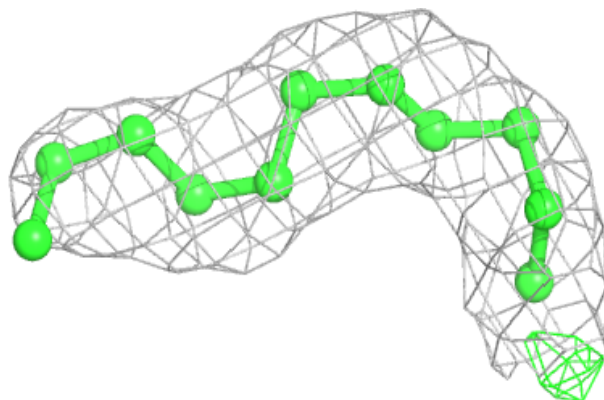


**Electron density around YTD A 201:**

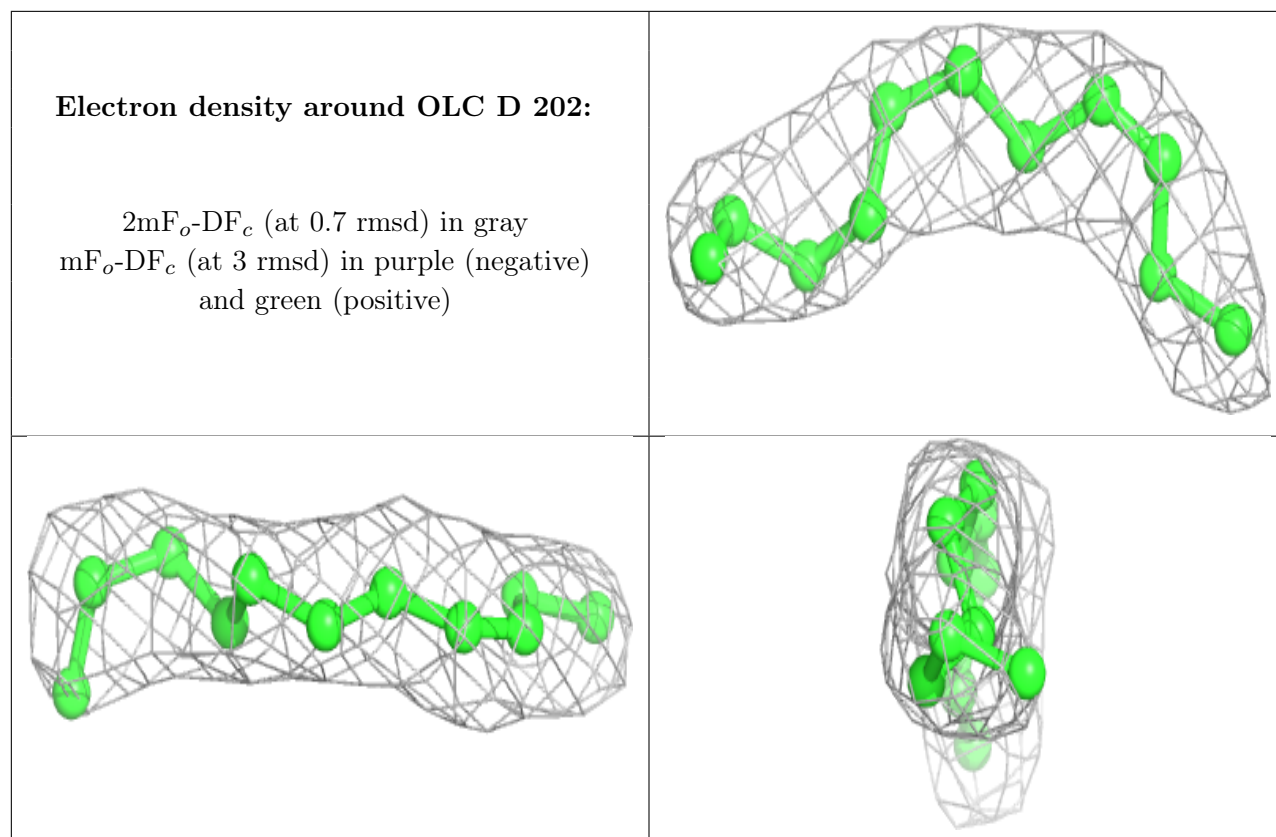
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around OLC B 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](#)

There are no such residues in this entry.