Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 12:23 AM JST

PDB ID	:	8GNE
Title	:	Crystal structure of human adenosine A2A receptor in complex with an insurmountable inverse agonist, KW-6356.
Authors	:	Suzuki, M.; Saito, J.; Miyagi, H.; Yasunaga, M.
Deposited on	:	2022-08-23
Resolution	:	2.30 Å(reported)

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

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

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

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

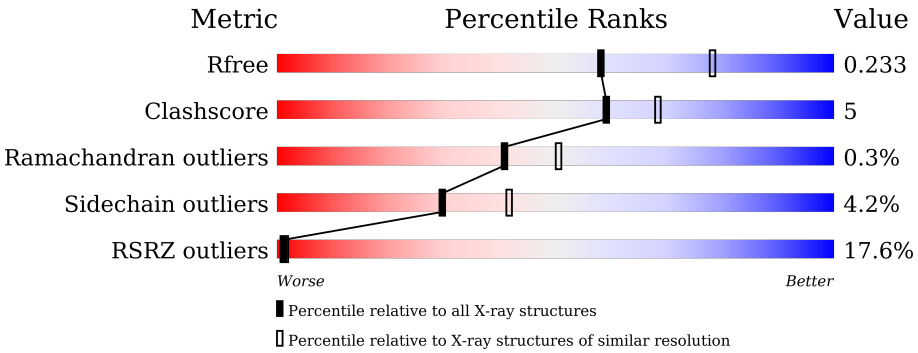
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	431	16% 80% 10% • 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3585 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 Adenosine receptor A2a,Soluble cytochrome b562.

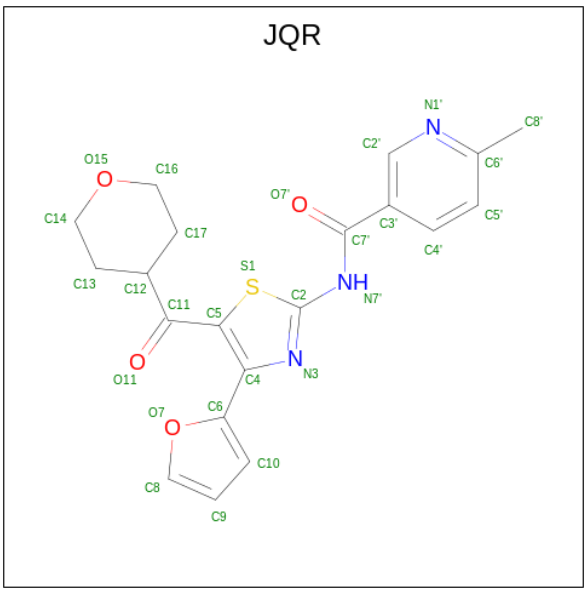
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	3026	1976	509	520	21	0	2	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	ASP	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	LYS	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	154	GLN	ASN	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

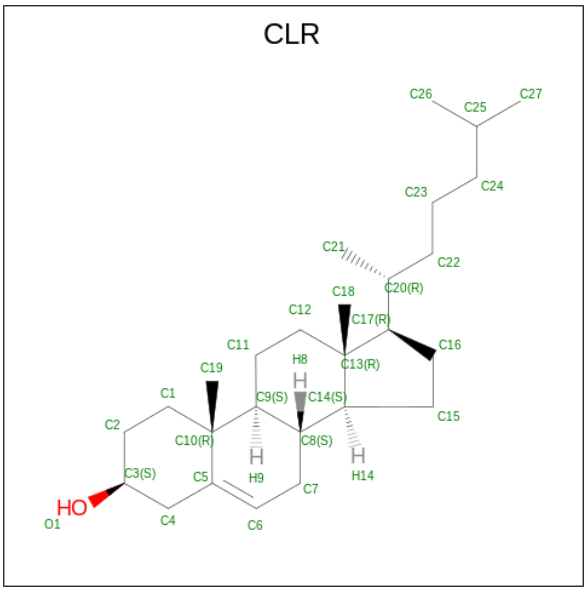
- Molecule 2 is {N}-[4-(furan-2-yl)-5-(oxan-4-ylcarbonyl)-1,3-thiazol-2-yl]-6-methyl-pyridine-3-carboxamide (three-letter code: JQR) (formula: $C_{20}H_{19}N_3O_4S$) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	20	3	4	1		

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		

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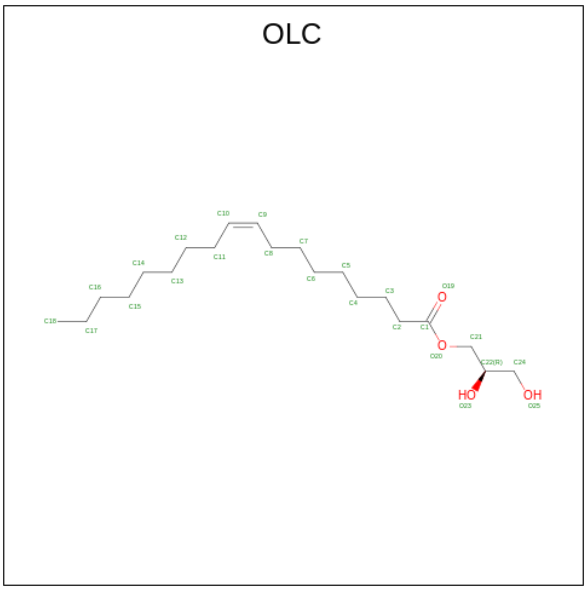
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 27 1	0	0

- Molecule 4 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
4	A	1	Total C O 16 12 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 21 17 4	0	0
4	A	1	Total C O 21 17 4	0	0
4	A	1	Total C O 19 15 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 19 15 4	0	0
4	A	1	Total C O 19 15 4	0	0
4	A	1	Total C O 19 15 4	0	0
4	A	1	Total C O 19 15 4	0	0

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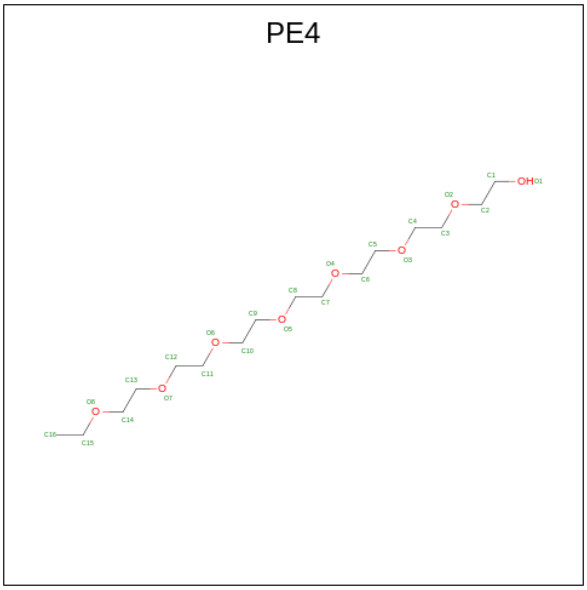
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 12 4	0	0
4	A	1	Total C O 21 17 4	0	0
4	A	1	Total C O 22 18 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 14 10 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 21 17 4	0	0

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 7 4	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0

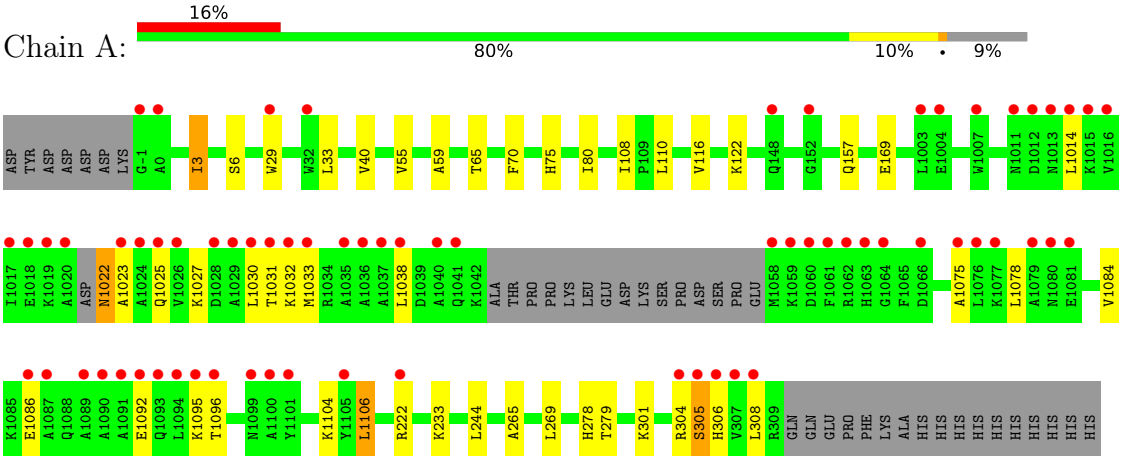
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	63	Total O 63 63	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: Adenosine receptor A2a,Soluble cytochrome b562



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.35Å 180.51Å 141.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 2.30 47.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.17-2.30) 99.4 (47.08-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.190 , 0.235 0.198 , 0.233	Depositor DCC
R_{free} test set	1119 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3585	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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: JQR, NA, CLR, OLC, PE4

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	0.79	2/3093 (0.1%)	0.89	0/4209

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	GLU	CD-OE1	6.52	1.32	1.25
1	A	169	GLU	CD-OE2	5.16	1.31	1.25

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	3026	0	3079	32	0
2	A	28	0	0	1	0
3	A	84	0	138	2	0
4	A	372	0	531	6	0
5	A	11	0	13	0	0
6	A	1	0	0	0	0
7	A	63	0	0	2	0
All	All	3585	0	3761	34	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 (34) 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)
4:A:1211:OLC:O23	7:A:1301:HOH:O	1.87	0.93
1:A:304:ARG:O	1:A:308:LEU:HB3	1.81	0.81
1:A:110[B]:LEU:HD23	1:A:110[B]:LEU:H	1.49	0.76
1:A:80:ILE:HD11	3:A:1203:CLR:H182	1.72	0.70
1:A:1022:ASN:HD22	1:A:1023:ALA:H	1.39	0.70
1:A:278:HIS:NE2	7:A:1302:HOH:O	2.27	0.67
1:A:1023:ALA:HB2	1:A:1084:VAL:HG22	1.76	0.66
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.32	0.59
1:A:80:ILE:HD11	3:A:1203:CLR:C18	2.33	0.58
1:A:1078:LEU:HD13	1:A:1086:GLU:HB3	1.84	0.57
1:A:1023:ALA:HB2	1:A:1084:VAL:CG2	2.33	0.57
1:A:1027:LYS:O	1:A:1031:THR:HG23	2.05	0.56
2:A:1201:JQR:O7'	2:A:1201:JQR:S1	2.63	0.56
1:A:75:HIS:HB2	4:A:1213:OLC:H24	1.92	0.52
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.92	0.51
1:A:1106:LEU:HD11	1:A:222:ARG:NH2	2.27	0.49
1:A:108:ILE:HG13	1:A:108:ILE:O	2.12	0.48
1:A:3:ILE:HA	1:A:6:SER:HB3	1.95	0.48
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.95	0.47
1:A:122:LYS:HB3	1:A:122:LYS:HE2	1.62	0.46
1:A:65:THR:HG22	1:A:70:PHE:CE1	2.51	0.46
1:A:3:ILE:O	1:A:3:ILE:HG12	2.17	0.45
1:A:33:LEU:HD21	4:A:1222:OLC:C21	2.47	0.44
1:A:1014:LEU:HD12	1:A:1095:LYS:HE3	1.99	0.43
1:A:1030:LEU:HD11	1:A:1075:ALA:HB1	2.01	0.43
1:A:29:TRP:CE2	4:A:1222:OLC:H3A	2.54	0.43
1:A:157:GLN:HE21	1:A:157:GLN:HB3	1.68	0.42
1:A:33:LEU:HD21	4:A:1222:OLC:H21	1.99	0.42
1:A:75:HIS:HB2	4:A:1213:OLC:C24	2.50	0.42
1:A:265:ALA:HB1	1:A:269:LEU:HD23	2.01	0.42
1:A:1014:LEU:CD2	1:A:1033:MET:HE1	2.50	0.42
1:A:1022:ASN:HD22	1:A:1023:ALA:N	2.10	0.42
1:A:305:SER:HB2	1:A:306:HIS:CD2	2.55	0.41
1:A:1014:LEU:CD2	1:A:1033:MET:CE	3.00	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	387/431 (90%)	374 (97%)	12 (3%)	1 (0%)	41 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	SER

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	315/360 (88%)	302 (96%)	13 (4%)	30 43

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	1022	ASN
1	A	1025	GLN
1	A	1032	LYS
1	A	1038	LEU
1	A	1092	GLU
1	A	1096	THR
1	A	1104	LYS
1	A	1106	LEU
1	A	233	LYS

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Mol	Chain	Res	Type
1	A	244	LEU
1	A	279	THR
1	A	301	LYS

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

Mol	Chain	Res	Type
1	A	157	GLN
1	A	1022	ASN
1	A	306	HIS

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)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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	$\#\|Z\| > 2$
4	OLC	A	1216	-	20,20,24	1.06	1 (5%)	21,21,25	0.86	2 (9%)
4	OLC	A	1212	-	18,18,24	1.12	1 (5%)	18,19,25	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OLC	A	1207	-	20,20,24	1.14	1 (5%)	21,21,25	0.83	1 (4%)
4	OLC	A	1220	-	24,24,24	0.97	1 (4%)	25,25,25	1.03	2 (8%)
4	OLC	A	1219	-	13,13,24	1.33	1 (7%)	14,14,25	1.47	2 (14%)
4	OLC	A	1218	-	24,24,24	1.18	1 (4%)	25,25,25	0.86	2 (8%)
4	OLC	A	1217	-	21,21,24	1.06	1 (4%)	22,22,25	0.67	1 (4%)
4	OLC	A	1209	-	18,18,24	1.16	1 (5%)	18,19,25	1.11	2 (11%)
4	OLC	A	1222	-	20,20,24	1.10	1 (5%)	21,21,25	0.88	1 (4%)
3	CLR	A	1204	-	31,31,31	0.29	0	48,48,48	0.45	0
4	OLC	A	1208	-	20,20,24	1.01	1 (5%)	21,21,25	0.83	2 (9%)
4	OLC	A	1221	-	24,24,24	0.85	1 (4%)	25,25,25	0.90	2 (8%)
5	PE4	A	1223	-	10,10,23	0.33	0	9,9,22	0.18	0
4	OLC	A	1210	-	24,24,24	1.06	1 (4%)	25,25,25	0.92	1 (4%)
2	JQR	A	1201	-	22,31,31	1.12	2 (9%)	26,43,43	1.56	6 (23%)
4	OLC	A	1213	-	18,18,24	1.22	1 (5%)	18,19,25	1.09	2 (11%)
4	OLC	A	1215	-	15,15,24	1.27	1 (6%)	16,16,25	0.99	1 (6%)
4	OLC	A	1205	-	15,15,24	0.97	1 (6%)	16,16,25	1.17	2 (12%)
4	OLC	A	1206	-	24,24,24	1.03	1 (4%)	25,25,25	1.24	3 (12%)
3	CLR	A	1202	-	31,31,31	0.35	0	48,48,48	0.45	0
4	OLC	A	1214	-	18,18,24	1.21	1 (5%)	18,19,25	1.05	1 (5%)
4	OLC	A	1211	-	18,18,24	1.39	1 (5%)	18,19,25	1.27	2 (11%)
3	CLR	A	1203	-	31,31,31	0.33	0	48,48,48	0.50	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
4	OLC	A	1216	-	-	6/20/20/24	-
4	OLC	A	1212	-	-	8/18/18/24	-
4	OLC	A	1207	-	-	4/20/20/24	-
4	OLC	A	1220	-	-	8/24/24/24	-
4	OLC	A	1219	-	-	3/13/13/24	-
4	OLC	A	1218	-	-	9/24/24/24	-
4	OLC	A	1217	-	-	8/21/21/24	-
4	OLC	A	1209	-	-	8/18/18/24	-
4	OLC	A	1222	-	-	9/20/20/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	A	1204	-	-	4/10/68/68	0/4/4/4
4	OLC	A	1208	-	-	10/20/20/24	-
4	OLC	A	1221	-	-	5/24/24/24	-
5	PE4	A	1223	-	-	4/8/8/21	-
4	OLC	A	1210	-	-	10/24/24/24	-
2	JQR	A	1201	-	-	1/10/28/28	0/4/4/4
4	OLC	A	1213	-	-	11/18/18/24	-
4	OLC	A	1215	-	-	9/15/15/24	-
4	OLC	A	1205	-	-	7/15/15/24	-
4	OLC	A	1206	-	-	8/24/24/24	-
3	CLR	A	1202	-	-	3/10/68/68	0/4/4/4
4	OLC	A	1214	-	-	9/18/18/24	-
4	OLC	A	1211	-	-	8/18/18/24	-
3	CLR	A	1203	-	-	0/10/68/68	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1218	OLC	O20-C1	5.30	1.48	1.33
4	A	1211	OLC	O20-C1	5.25	1.48	1.33
4	A	1210	OLC	O20-C1	4.90	1.47	1.33
4	A	1207	OLC	O20-C1	4.88	1.47	1.33
4	A	1213	OLC	O20-C1	4.79	1.47	1.33
4	A	1214	OLC	O20-C1	4.75	1.47	1.33
4	A	1206	OLC	O20-C1	4.66	1.47	1.33
4	A	1222	OLC	O20-C1	4.63	1.46	1.33
4	A	1215	OLC	O20-C1	4.60	1.46	1.33
4	A	1209	OLC	O20-C1	4.59	1.46	1.33
4	A	1217	OLC	O20-C1	4.55	1.46	1.33
4	A	1216	OLC	O20-C1	4.51	1.46	1.33
4	A	1212	OLC	O20-C1	4.49	1.46	1.33
4	A	1220	OLC	O20-C1	4.44	1.46	1.33
4	A	1219	OLC	O20-C1	4.42	1.46	1.33
4	A	1208	OLC	O20-C1	4.27	1.45	1.33
4	A	1221	OLC	O20-C1	3.92	1.44	1.33
4	A	1205	OLC	O20-C1	3.46	1.43	1.33
2	A	1201	JQR	O7'-C7'	-2.07	1.19	1.23
2	A	1201	JQR	C17-C12	2.02	1.58	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	JQR	O7'-C7'-C3'	-4.23	113.39	120.94
4	A	1206	OLC	O20-C1-C2	4.13	124.88	111.91
4	A	1219	OLC	O20-C1-C2	4.01	124.50	111.91
4	A	1220	OLC	O20-C1-C2	3.55	123.06	111.91
4	A	1211	OLC	O20-C1-C2	3.42	122.64	111.91
4	A	1209	OLC	O20-C1-C2	3.33	122.36	111.91
4	A	1212	OLC	O20-C1-C2	3.17	121.86	111.91
2	A	1201	JQR	C3'-C7'-N7'	3.16	122.88	115.92
4	A	1214	OLC	O20-C1-C2	3.14	121.77	111.91
4	A	1206	OLC	O20-C1-O19	-2.99	116.03	123.59
4	A	1205	OLC	O20-C1-C2	2.94	121.13	111.91
4	A	1221	OLC	O20-C1-C2	2.79	120.67	111.91
4	A	1210	OLC	O20-C1-C2	2.78	120.63	111.91
4	A	1205	OLC	O20-C1-O19	-2.70	116.78	123.59
4	A	1216	OLC	O20-C1-C2	2.58	120.02	111.91
4	A	1213	OLC	O20-C1-C2	2.56	119.95	111.91
4	A	1208	OLC	O20-C1-C2	2.56	119.95	111.91
4	A	1219	OLC	O20-C1-O19	-2.55	117.15	123.59
4	A	1218	OLC	O20-C1-C2	2.54	119.87	111.91
4	A	1215	OLC	O20-C1-C2	2.53	119.84	111.91
4	A	1207	OLC	O20-C1-C2	2.41	119.47	111.91
4	A	1206	OLC	O20-C21-C22	2.38	117.28	105.77
4	A	1220	OLC	O20-C1-O19	-2.36	117.64	123.59
4	A	1211	OLC	O20-C21-C22	2.34	117.09	105.77
4	A	1222	OLC	C21-O20-C1	2.31	125.67	117.12
2	A	1201	JQR	C10-C9-C8	-2.29	104.77	112.92
2	A	1201	JQR	C17-C12-C11	2.16	114.85	110.49
4	A	1209	OLC	O20-C1-O19	-2.14	118.20	123.59
4	A	1221	OLC	O20-C1-O19	-2.11	118.26	123.59
4	A	1208	OLC	O20-C1-O19	-2.10	118.29	123.59
4	A	1213	OLC	O20-C21-C22	2.09	115.88	105.77
4	A	1217	OLC	O20-C1-C2	2.08	118.45	111.91
4	A	1216	OLC	O20-C1-O19	-2.07	118.38	123.59
2	A	1201	JQR	C2'-N1'-C6'	2.05	119.82	117.45
4	A	1218	OLC	C21-O20-C1	2.04	124.68	117.12
2	A	1201	JQR	O11-C11-C5	2.04	122.87	119.98

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1205	OLC	O20-C21-C22-O23
4	A	1209	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
4	A	1209	OLC	O20-C21-C22-O23
4	A	1211	OLC	C9-C10-C11-C12
4	A	1211	OLC	C21-C22-C24-O25
4	A	1212	OLC	C21-C22-C24-O25
4	A	1213	OLC	C21-C22-C24-O25
4	A	1213	OLC	O20-C21-C22-C24
4	A	1213	OLC	O20-C21-C22-O23
4	A	1214	OLC	C9-C10-C11-C12
4	A	1214	OLC	C21-C22-C24-O25
4	A	1214	OLC	O20-C21-C22-C24
4	A	1215	OLC	C21-C22-C24-O25
4	A	1218	OLC	C21-C22-C24-O25
4	A	1222	OLC	C21-C22-C24-O25
4	A	1222	OLC	O23-C22-C24-O25
4	A	1219	OLC	O19-C1-O20-C21
4	A	1219	OLC	C2-C1-O20-C21
4	A	1211	OLC	O20-C21-C22-O23
4	A	1214	OLC	O20-C21-C22-O23
4	A	1220	OLC	O20-C21-C22-O23
4	A	1210	OLC	C2-C1-O20-C21
5	A	1223	PE4	O3-C5-C6-O4
4	A	1206	OLC	C2-C1-O20-C21
4	A	1208	OLC	C2-C1-O20-C21
4	A	1212	OLC	C2-C1-O20-C21
4	A	1217	OLC	C2-C1-O20-C21
4	A	1211	OLC	O20-C21-C22-C24
4	A	1212	OLC	O19-C1-O20-C21
4	A	1209	OLC	O23-C22-C24-O25
4	A	1214	OLC	O23-C22-C24-O25
4	A	1208	OLC	O19-C1-O20-C21
3	A	1204	CLR	C17-C20-C22-C23
5	A	1223	PE4	O1-C1-C2-O2
4	A	1210	OLC	O19-C1-O20-C21
4	A	1217	OLC	O19-C1-O20-C21
4	A	1206	OLC	O19-C1-O20-C21
3	A	1204	CLR	C21-C20-C22-C23
4	A	1215	OLC	O20-C21-C22-O23
4	A	1221	OLC	O20-C21-C22-O23
4	A	1205	OLC	C2-C1-O20-C21
4	A	1206	OLC	C13-C14-C15-C16
4	A	1214	OLC	C5-C6-C7-C8
4	A	1216	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	A	1215	OLC	O20-C21-C22-C24
4	A	1210	OLC	C14-C15-C16-C17
4	A	1211	OLC	C2-C3-C4-C5
4	A	1220	OLC	C4-C5-C6-C7
4	A	1213	OLC	C3-C4-C5-C6
4	A	1206	OLC	C12-C13-C14-C15
4	A	1217	OLC	C4-C5-C6-C7
4	A	1220	OLC	C13-C14-C15-C16
4	A	1205	OLC	C21-C22-C24-O25
4	A	1209	OLC	C21-C22-C24-O25
4	A	1208	OLC	O20-C21-C22-O23
4	A	1210	OLC	C12-C13-C14-C15
4	A	1222	OLC	C2-C3-C4-C5
4	A	1208	OLC	C4-C5-C6-C7
4	A	1218	OLC	C13-C14-C15-C16
4	A	1220	OLC	C5-C6-C7-C8
3	A	1202	CLR	C22-C23-C24-C25
4	A	1206	OLC	C11-C12-C13-C14
4	A	1211	OLC	C5-C6-C7-C8
4	A	1218	OLC	C5-C6-C7-C8
4	A	1218	OLC	C10-C11-C12-C13
3	A	1204	CLR	C22-C23-C24-C25
4	A	1205	OLC	O19-C1-O20-C21
4	A	1213	OLC	C2-C1-O20-C21
4	A	1213	OLC	O19-C1-O20-C21
4	A	1208	OLC	C10-C11-C12-C13
4	A	1210	OLC	C6-C7-C8-C9
4	A	1216	OLC	C6-C7-C8-C9
4	A	1208	OLC	O20-C21-C22-C24
4	A	1216	OLC	C2-C1-O20-C21
4	A	1214	OLC	C1-C2-C3-C4
4	A	1210	OLC	C2-C3-C4-C5
4	A	1207	OLC	C2-C3-C4-C5
4	A	1214	OLC	C2-C1-O20-C21
4	A	1217	OLC	C11-C12-C13-C14
4	A	1220	OLC	C11-C12-C13-C14
4	A	1211	OLC	O23-C22-C24-O25
4	A	1215	OLC	O23-C22-C24-O25
4	A	1218	OLC	O23-C22-C24-O25
4	A	1217	OLC	C6-C7-C8-C9
4	A	1216	OLC	O19-C1-O20-C21
4	A	1218	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	A	1215	OLC	C3-C4-C5-C6
4	A	1221	OLC	C4-C5-C6-C7
4	A	1214	OLC	O19-C1-O20-C21
4	A	1215	OLC	C2-C1-O20-C21
4	A	1213	OLC	C5-C6-C7-C8
4	A	1210	OLC	C3-C4-C5-C6
4	A	1212	OLC	C3-C4-C5-C6
5	A	1223	PE4	C5-C6-O4-C7
4	A	1220	OLC	C15-C16-C17-C18
4	A	1217	OLC	C12-C13-C14-C15
4	A	1208	OLC	C5-C6-C7-C8
4	A	1208	OLC	C3-C4-C5-C6
4	A	1209	OLC	C9-C10-C11-C12
4	A	1213	OLC	C9-C10-C11-C12
4	A	1215	OLC	O19-C1-O20-C21
4	A	1210	OLC	C4-C5-C6-C7
4	A	1207	OLC	C10-C11-C12-C13
4	A	1209	OLC	C3-C4-C5-C6
4	A	1205	OLC	O23-C22-C24-O25
4	A	1213	OLC	O23-C22-C24-O25
4	A	1222	OLC	C5-C6-C7-C8
4	A	1215	OLC	C5-C6-C7-C8
4	A	1205	OLC	O20-C21-C22-C24
4	A	1213	OLC	C1-C2-C3-C4
4	A	1209	OLC	C6-C7-C8-C9
4	A	1218	OLC	C11-C12-C13-C14
4	A	1216	OLC	C5-C6-C7-C8
4	A	1219	OLC	C4-C5-C6-C7
5	A	1223	PE4	C1-C2-O2-C3
4	A	1216	OLC	C11-C12-C13-C14
4	A	1212	OLC	O23-C22-C24-O25
4	A	1206	OLC	C14-C15-C16-C17
4	A	1212	OLC	C2-C3-C4-C5
4	A	1207	OLC	C3-C4-C5-C6
3	A	1202	CLR	C17-C20-C22-C23
4	A	1209	OLC	C2-C3-C4-C5
4	A	1220	OLC	O20-C21-C22-C24
4	A	1221	OLC	O20-C21-C22-C24
3	A	1202	CLR	C20-C22-C23-C24
4	A	1206	OLC	C4-C5-C6-C7
4	A	1222	OLC	C4-C5-C6-C7
4	A	1222	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
4	A	1217	OLC	C5-C6-C7-C8
4	A	1221	OLC	C10-C11-C12-C13
4	A	1205	OLC	C6-C7-C8-C9
4	A	1212	OLC	C6-C7-C8-C9
4	A	1208	OLC	C9-C10-C11-C12
4	A	1221	OLC	C9-C10-C11-C12
4	A	1222	OLC	C9-C10-C11-C12
4	A	1210	OLC	C9-C10-C11-C12
4	A	1212	OLC	C7-C8-C9-C10
4	A	1206	OLC	C9-C10-C11-C12
4	A	1207	OLC	C7-C8-C9-C10
4	A	1208	OLC	C7-C8-C9-C10
4	A	1210	OLC	C7-C8-C9-C10
4	A	1218	OLC	C7-C8-C9-C10
4	A	1220	OLC	C7-C8-C9-C10
3	A	1204	CLR	C23-C24-C25-C26
4	A	1222	OLC	O20-C1-C2-C3
4	A	1213	OLC	C7-C8-C9-C10
2	A	1201	JQR	O11-C11-C12-C13
4	A	1217	OLC	C9-C10-C11-C12
4	A	1218	OLC	C15-C16-C17-C18
4	A	1215	OLC	C6-C7-C8-C9
4	A	1222	OLC	O19-C1-C2-C3
4	A	1211	OLC	C7-C8-C9-C10

There are no ring outliers.

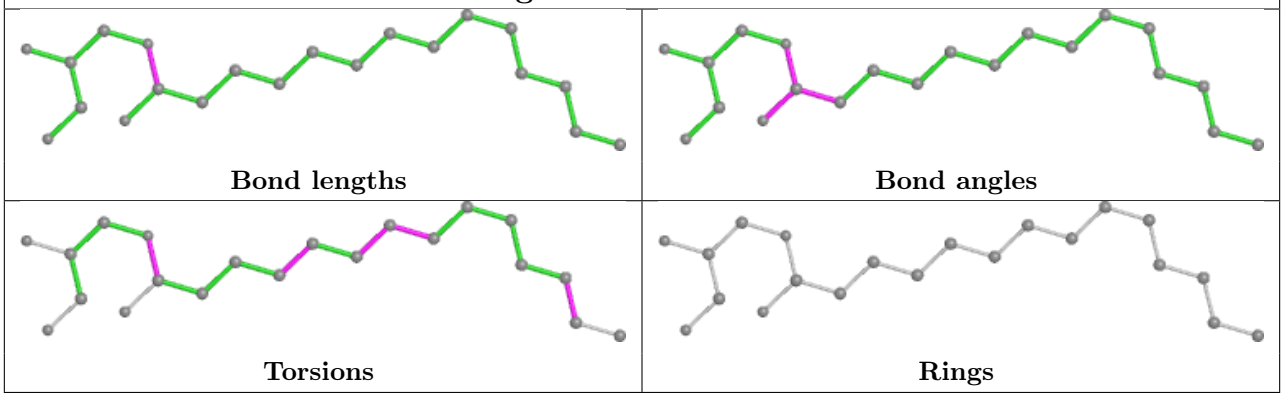
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1222	OLC	3	0
2	A	1201	JQR	1	0
4	A	1213	OLC	2	0
4	A	1211	OLC	1	0
3	A	1203	CLR	2	0

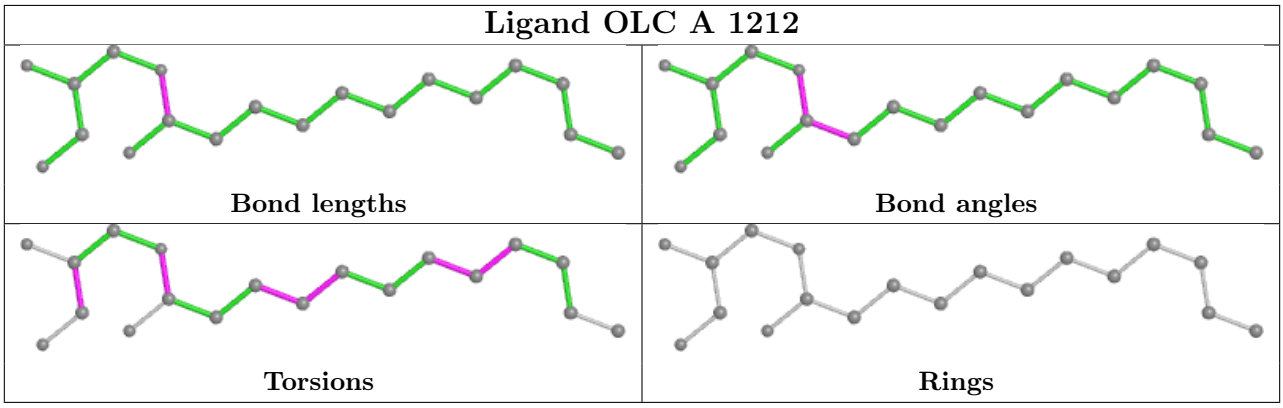
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

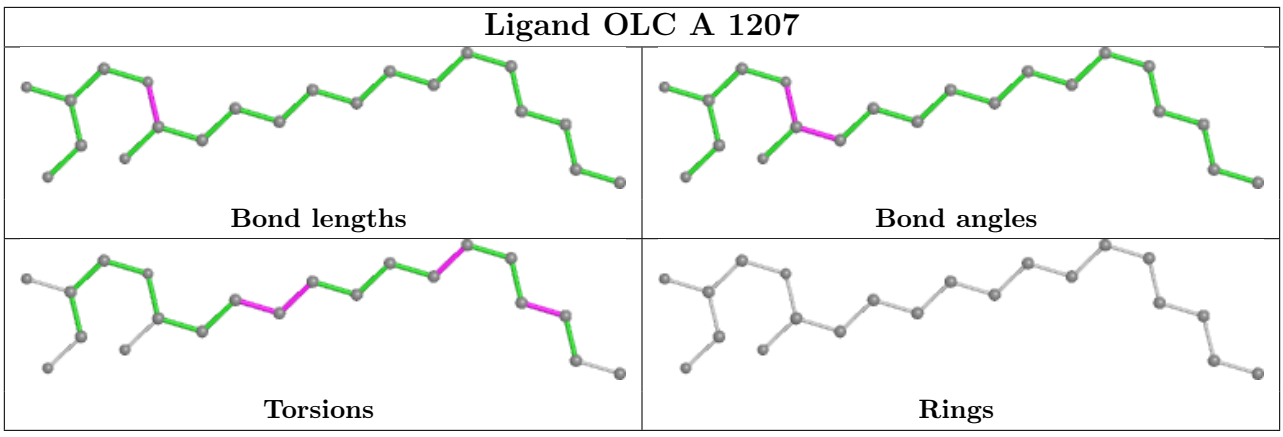
Ligand OLC A 1216



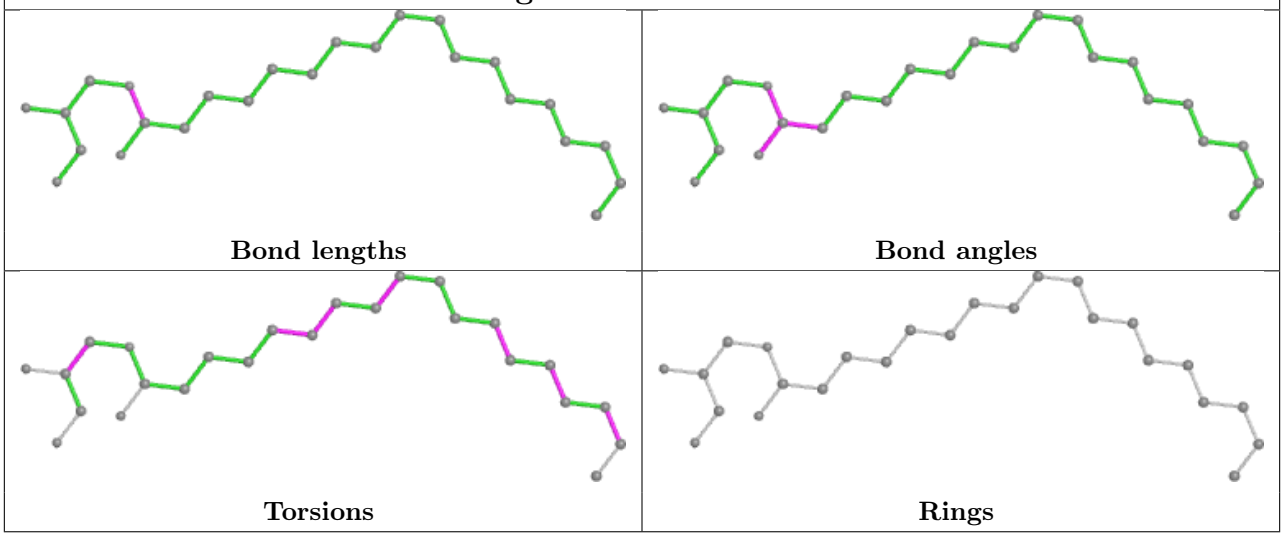
Ligand OLC A 1212



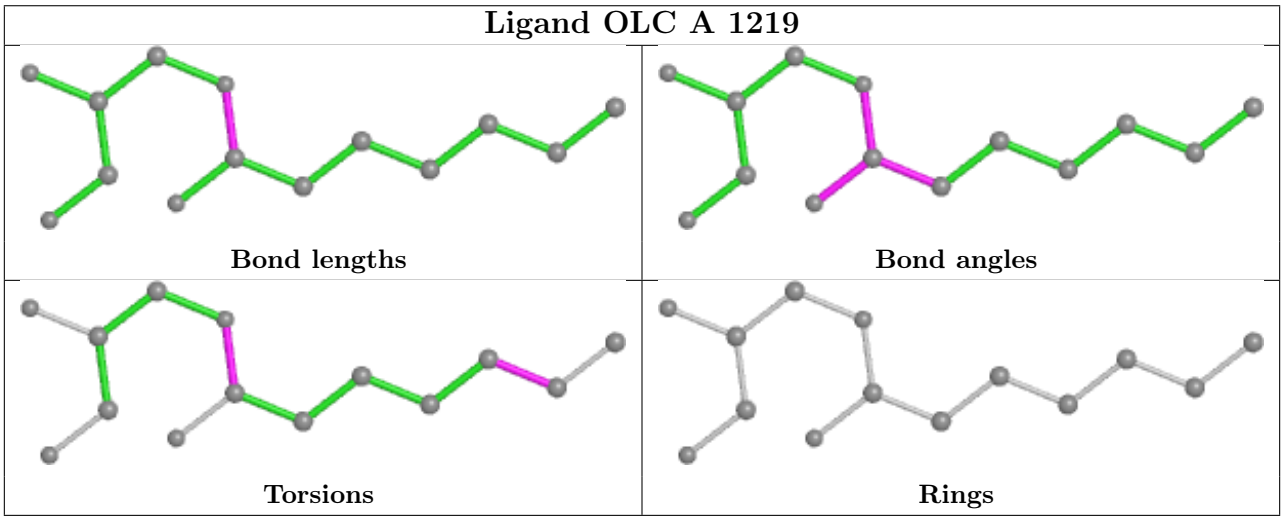
Ligand OLC A 1207



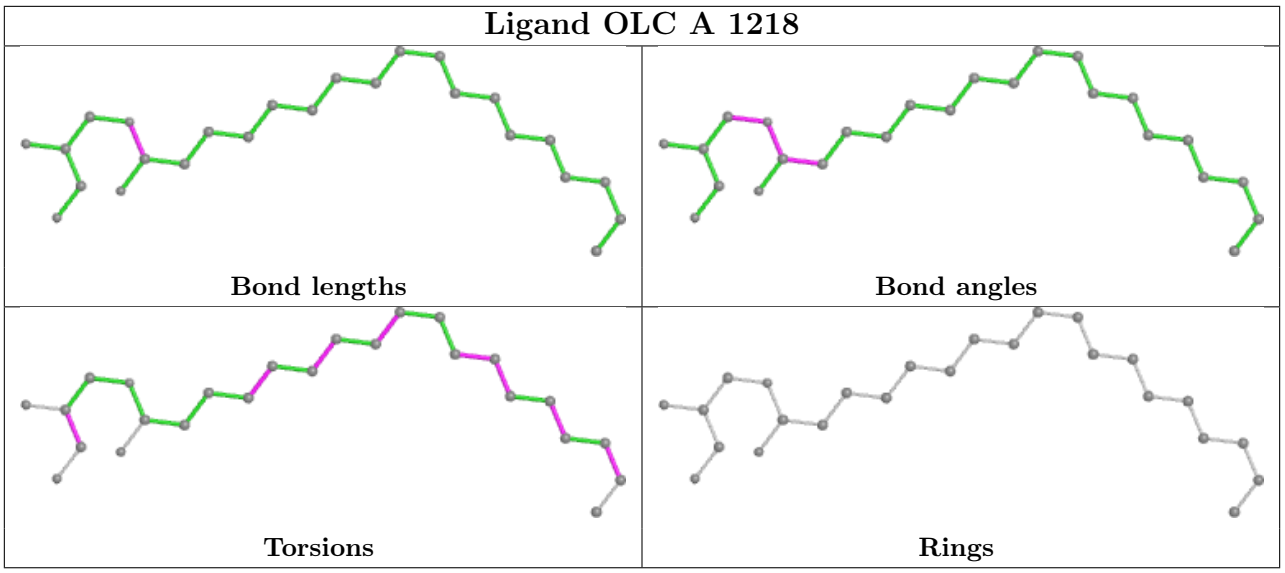
Ligand OLC A 1220



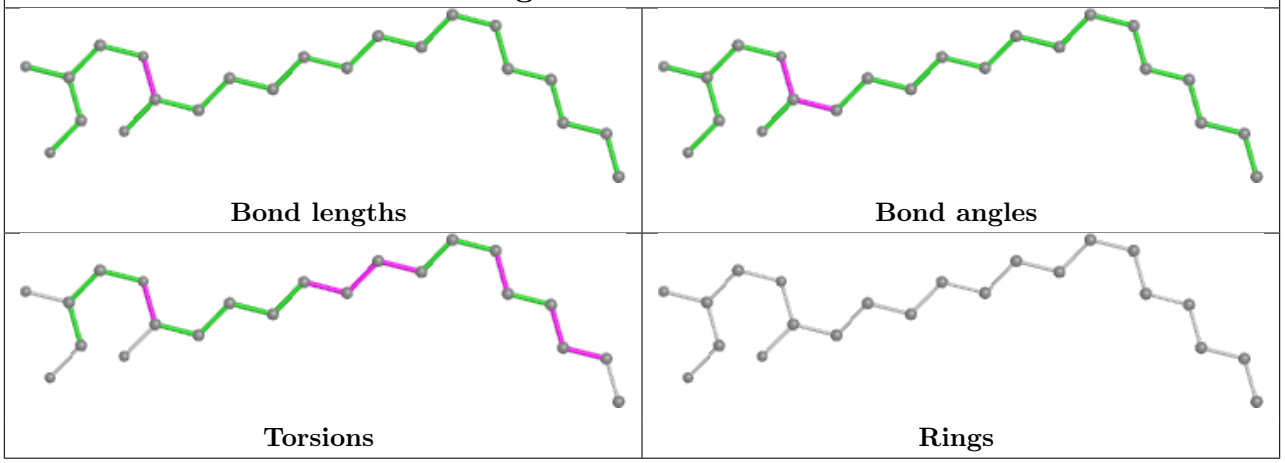
Ligand OLC A 1219



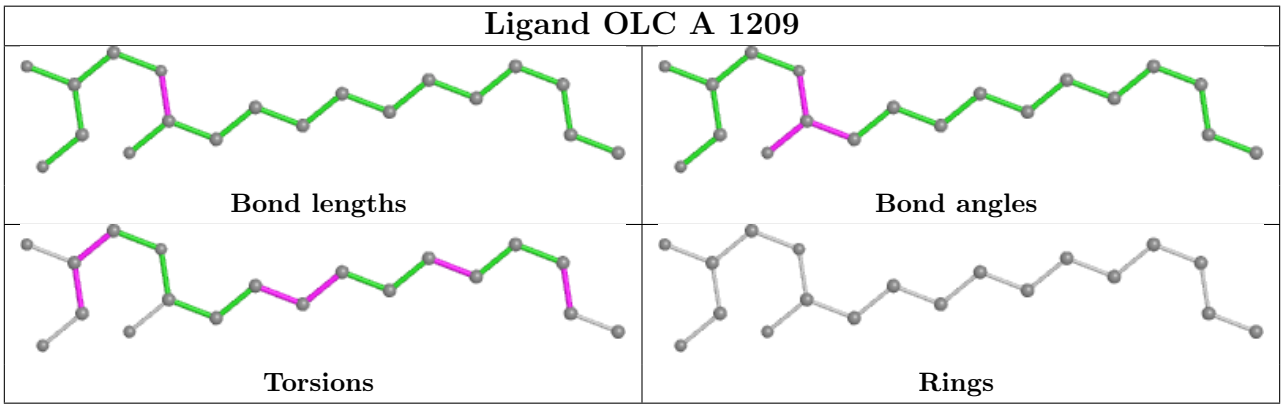
Ligand OLC A 1218



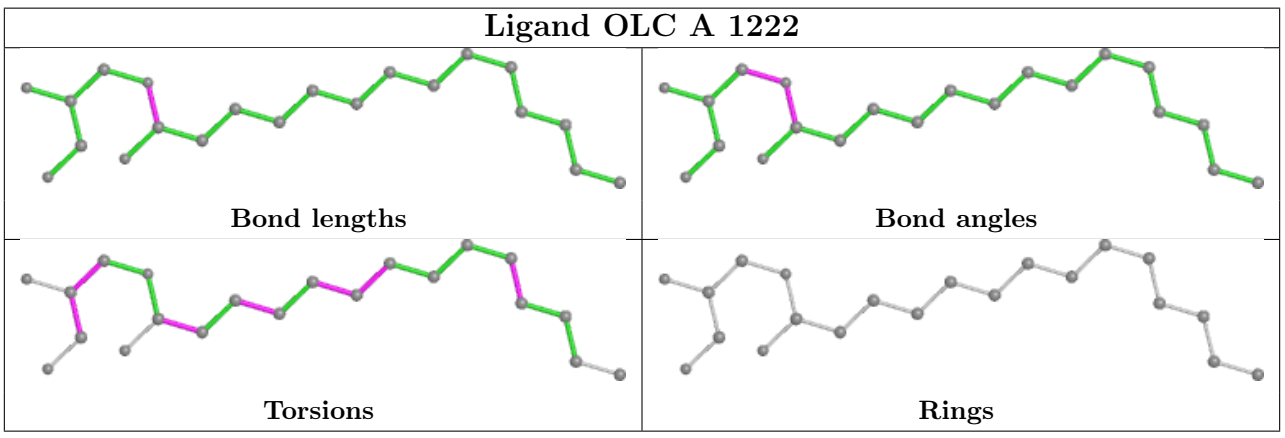
Ligand OLC A 1217



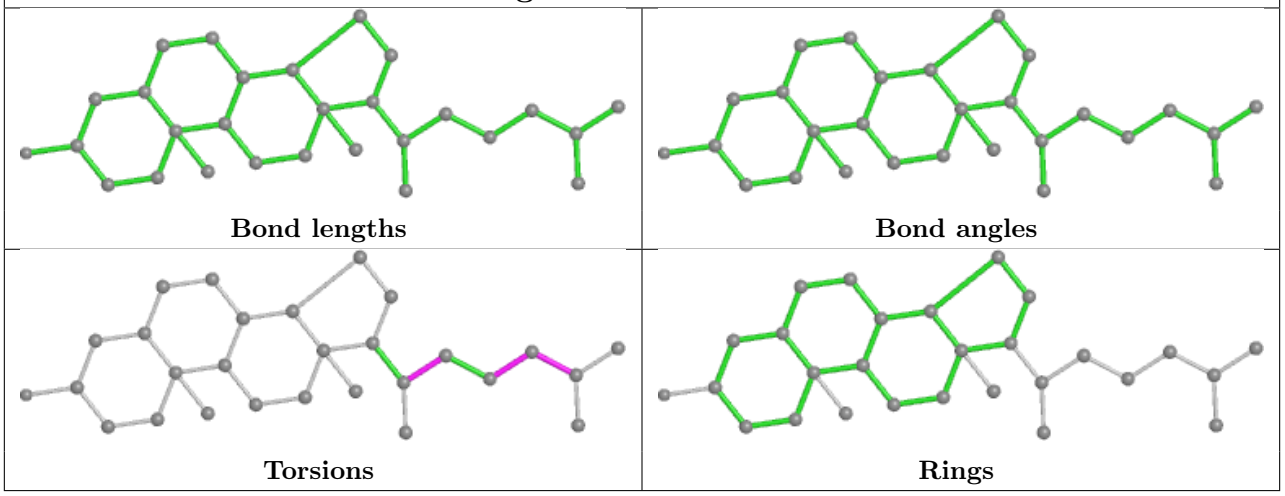
Ligand OLC A 1209



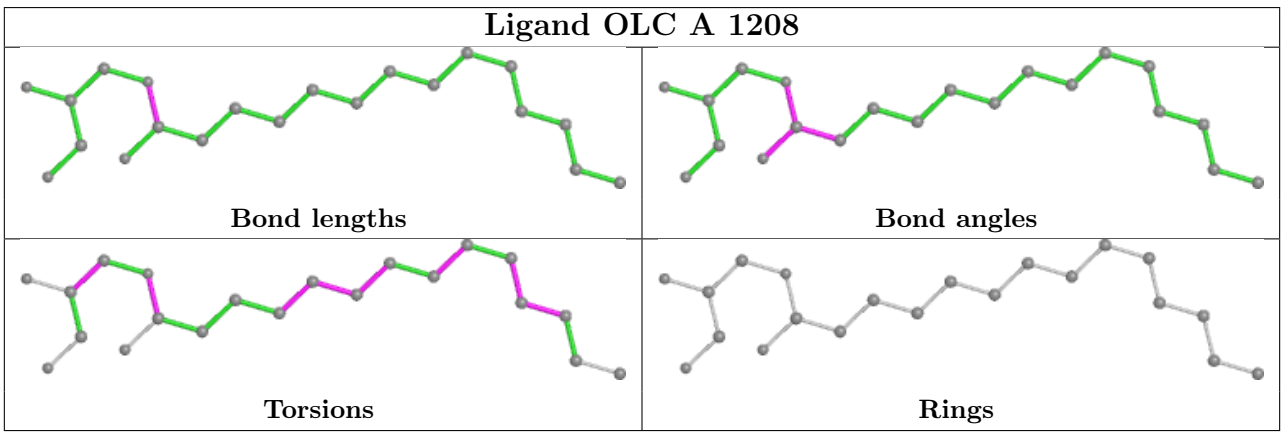
Ligand OLC A 1222



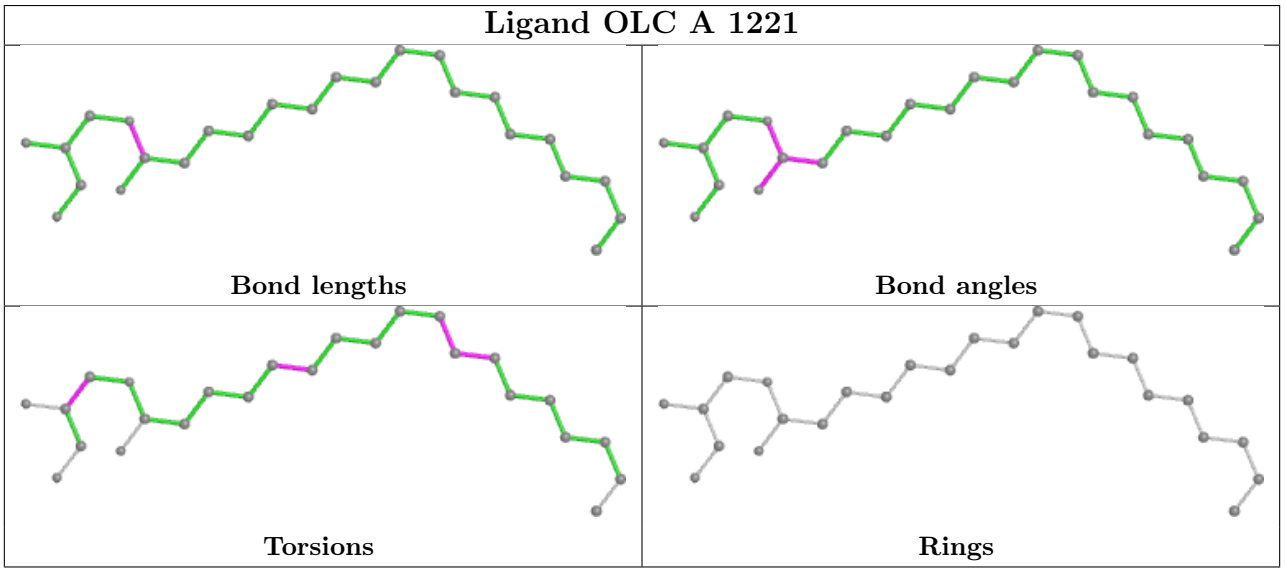
Ligand CLR A 1204



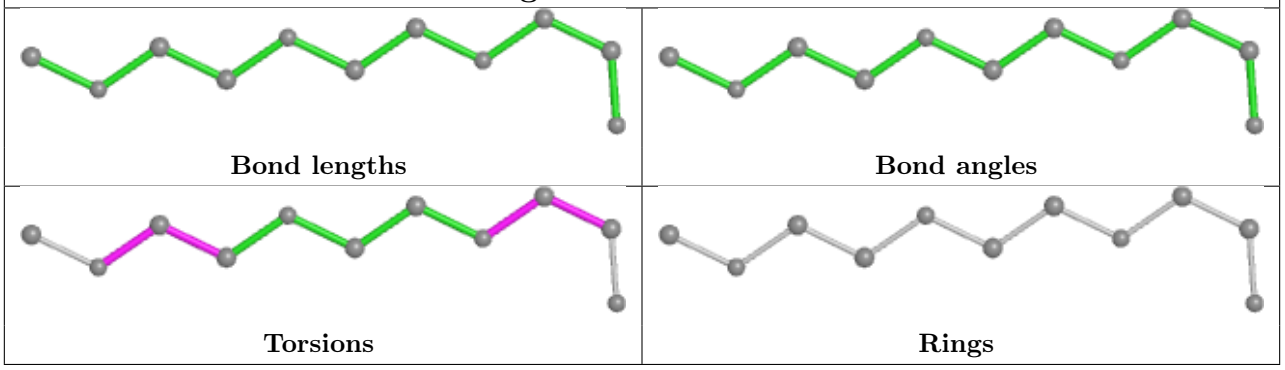
Ligand OLC A 1208



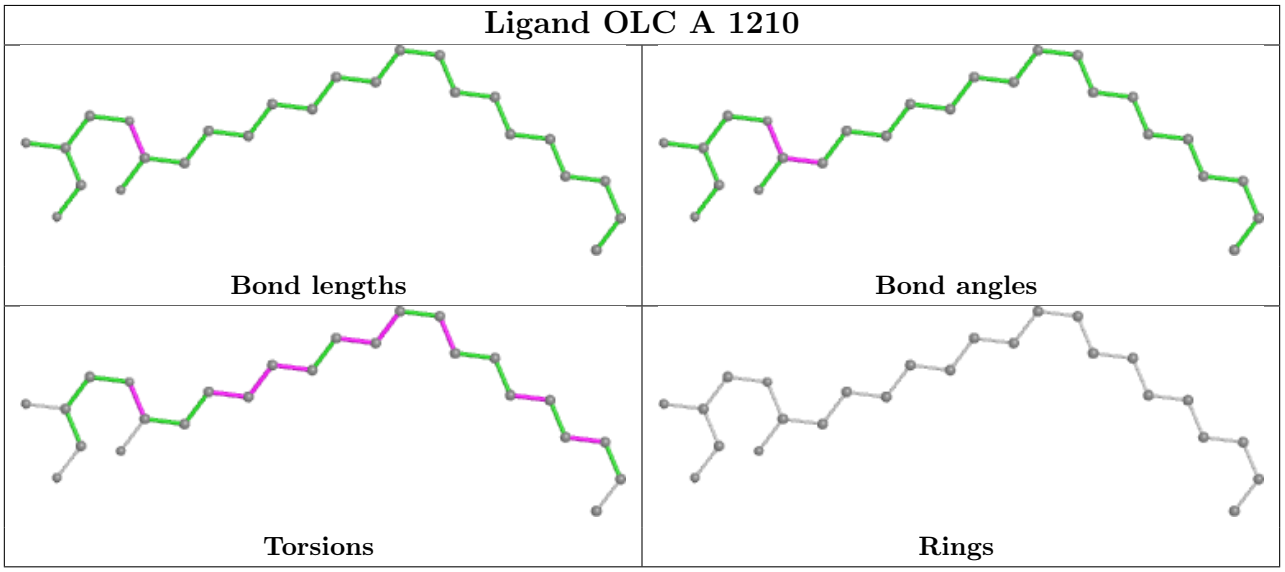
Ligand OLC A 1221



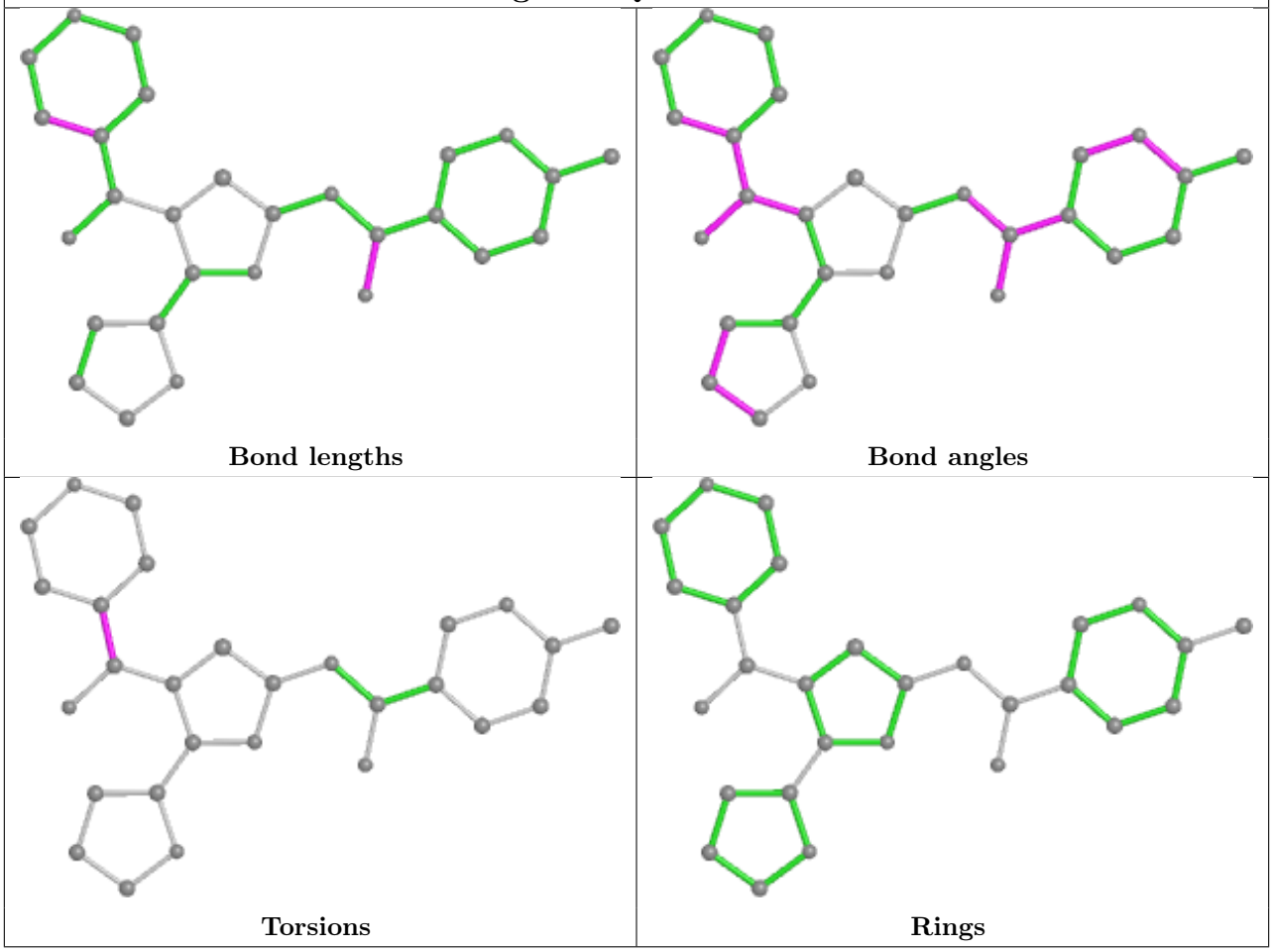
Ligand PE4 A 1223



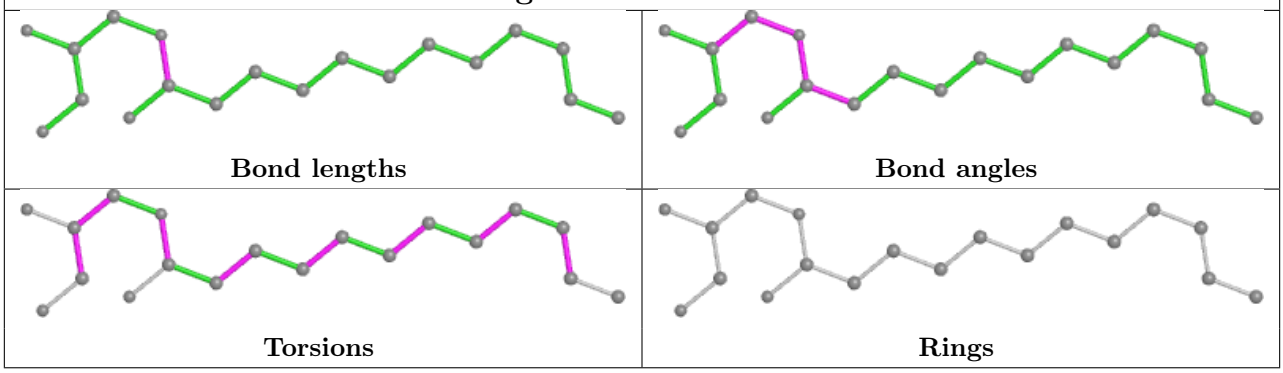
Ligand OLC A 1210



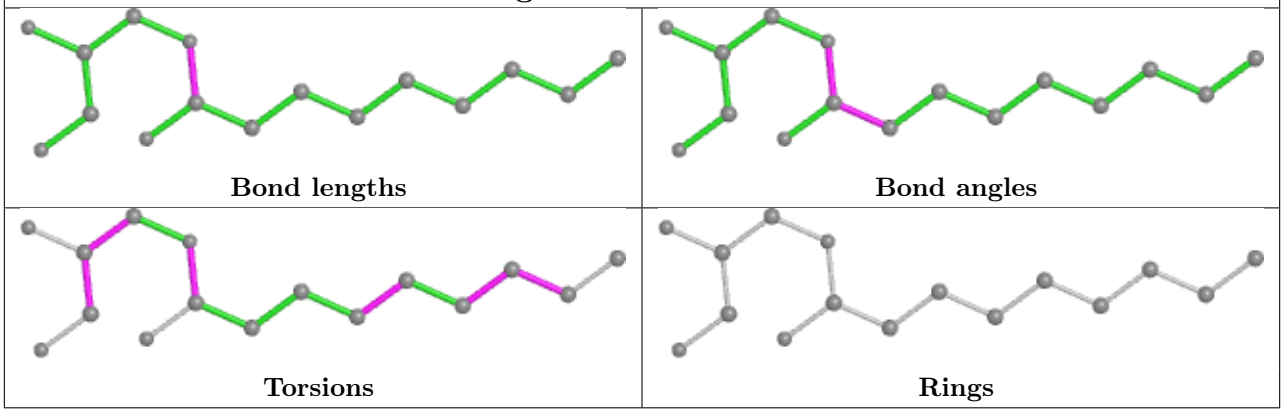
Ligand JQR A 1201



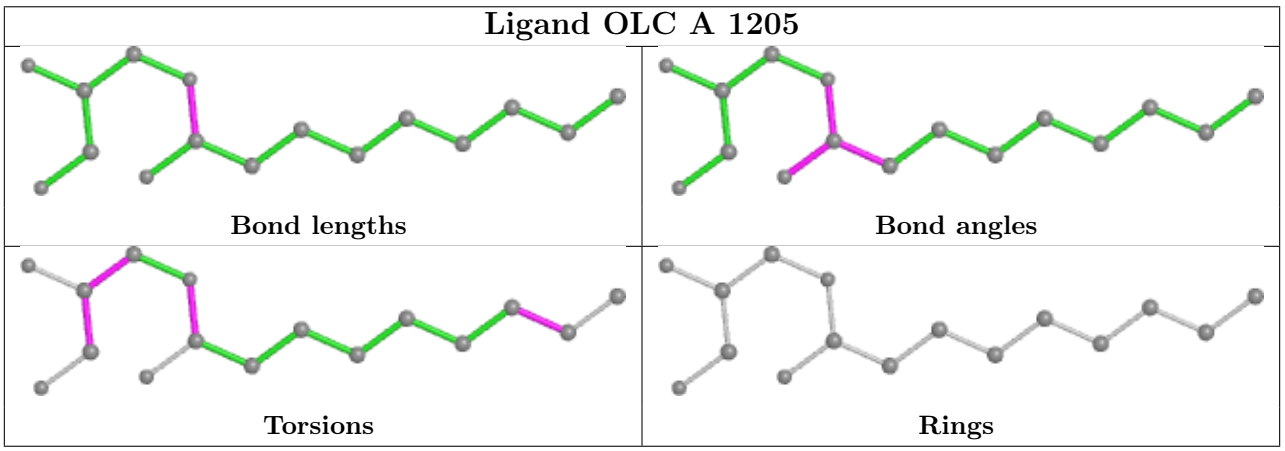
Ligand OLC A 1213



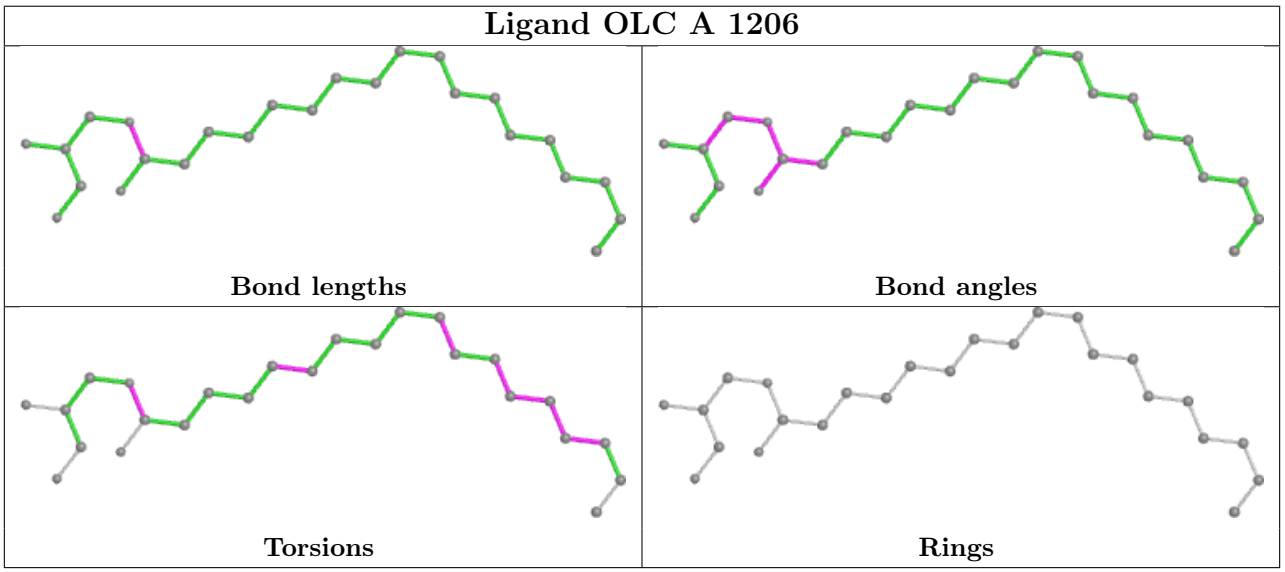
Ligand OLC A 1215

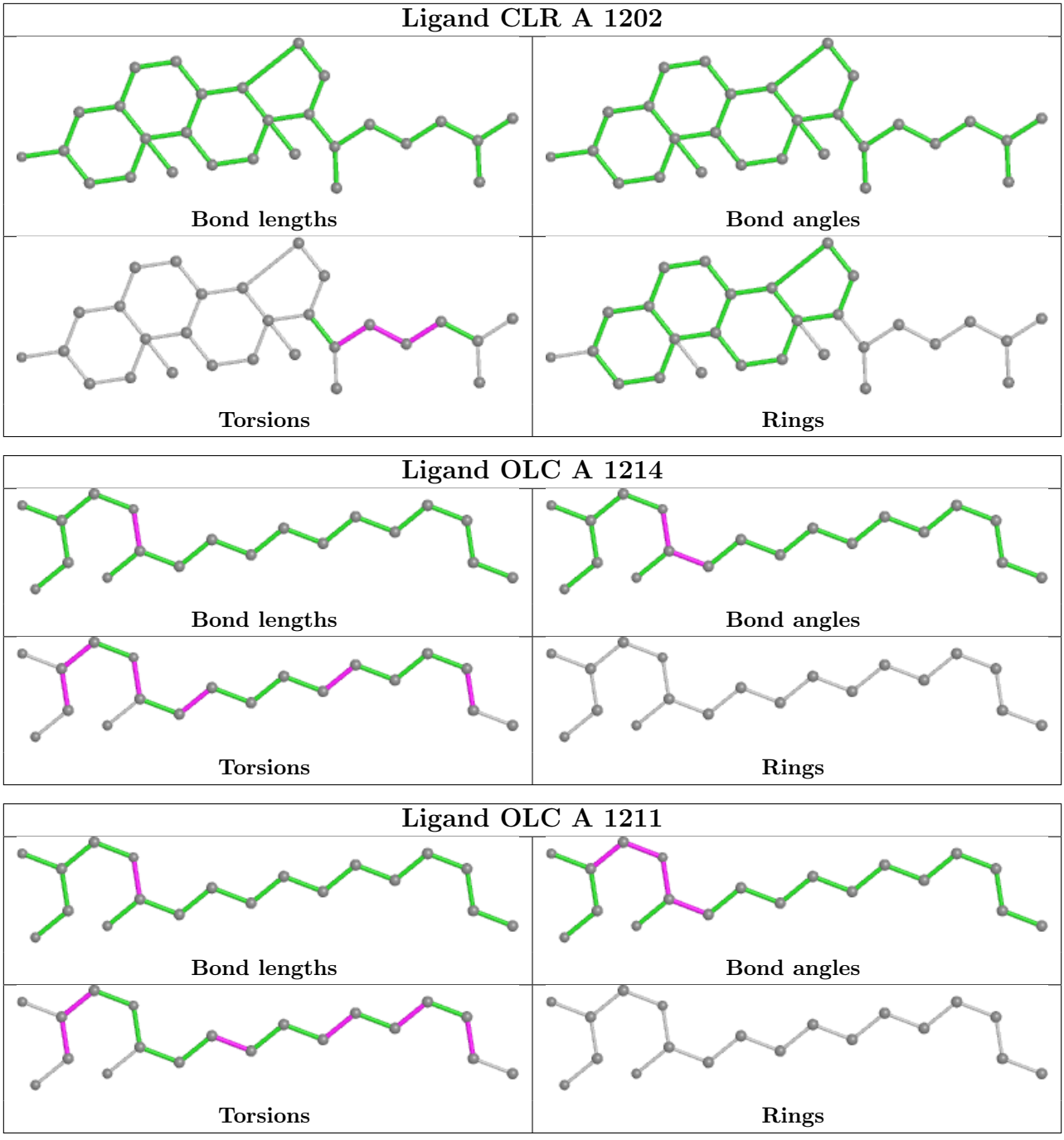


Ligand OLC A 1205



Ligand OLC A 1206





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	391/431 (90%)	0.84	69 (17%) 1 1	24, 43, 96, 120	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1020	ALA	8.7
1	A	1060	ASP	7.0
1	A	1090	ALA	6.8
1	A	1028	ASP	6.4
1	A	1061	PHE	6.3
1	A	1063	HIS	5.6
1	A	1059	LYS	5.6
1	A	1105	TYR	5.2
1	A	1030	LEU	5.2
1	A	1033	MET	5.2
1	A	1023	ALA	5.1
1	A	1029	ALA	5.0
1	A	1026	VAL	4.8
1	A	306	HIS	4.8
1	A	1101	TYR	4.8
1	A	1017	ILE	4.5
1	A	1024	ALA	4.4
1	A	1058	MET	4.3
1	A	1080	ASN	4.2
1	A	1095	LYS	4.2
1	A	308	LEU	4.0
1	A	1013	ASN	3.9
1	A	1037	ALA	3.8
1	A	1016	VAL	3.7
1	A	1092	GLU	3.6
1	A	1094	LEU	3.4
1	A	1019	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1089	ALA	3.4
1	A	1093	GLN	3.3
1	A	1099	ASN	3.2
1	A	1087	ALA	3.2
1	A	1012	ASP	3.2
1	A	1091	ALA	3.1
1	A	1015	LYS	3.1
1	A	1032	LYS	3.1
1	A	1066	ASP	3.1
1	A	1011	ASN	3.1
1	A	0	ALA	3.0
1	A	1062	ARG	3.0
1	A	-1	GLY	3.0
1	A	1040	ALA	2.9
1	A	1007	TRP	2.9
1	A	1100	ALA	2.8
1	A	1018	GLU	2.8
1	A	1075	ALA	2.7
1	A	152	GLY	2.6
1	A	1038	LEU	2.6
1	A	1041	GLN	2.6
1	A	1036	ALA	2.6
1	A	222	ARG	2.5
1	A	304	ARG	2.5
1	A	305	SER	2.4
1	A	1004	GLU	2.4
1	A	1035	ALA	2.4
1	A	1096	THR	2.4
1	A	1077	LYS	2.3
1	A	1031	THR	2.3
1	A	307	VAL	2.3
1	A	148	GLN	2.3
1	A	29	TRP	2.2
1	A	1003	LEU	2.2
1	A	1064	GLY	2.2
1	A	1076	LEU	2.2
1	A	1079	ALA	2.2
1	A	1086	GLU	2.1
1	A	1081	GLU	2.1
1	A	1014	LEU	2.1
1	A	32	TRP	2.0
1	A	1025	GLN	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

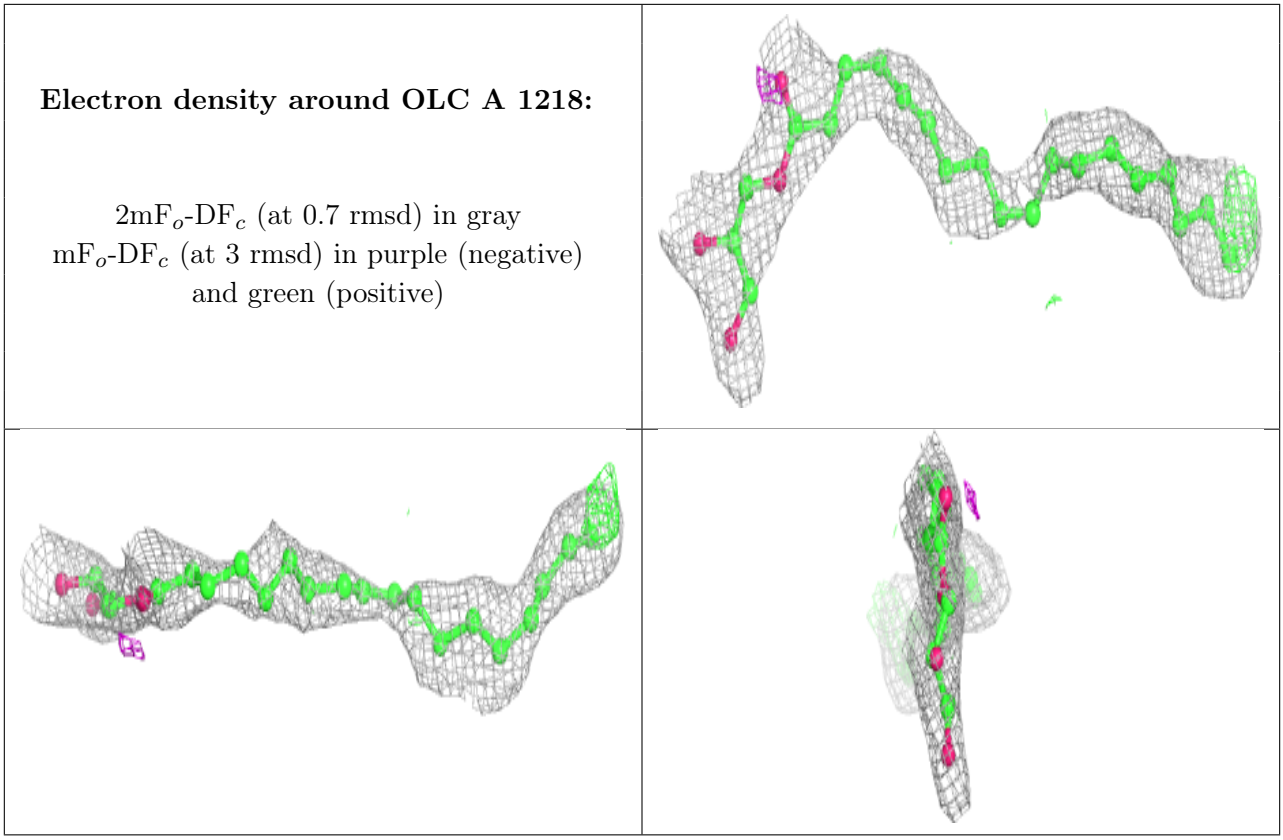
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLC	A	1218	25/25	0.50	0.31	62,72,80,80	0
4	OLC	A	1210	25/25	0.53	0.32	87,96,108,112	0
4	OLC	A	1217	22/25	0.62	0.31	66,80,92,95	0
4	OLC	A	1216	21/25	0.64	0.33	66,73,89,91	0
4	OLC	A	1213	19/25	0.65	0.33	70,79,101,102	0
4	OLC	A	1211	19/25	0.66	0.29	48,67,78,83	0
4	OLC	A	1206	25/25	0.68	0.27	56,74,83,86	0
4	OLC	A	1222	21/25	0.70	0.34	81,94,100,103	0
4	OLC	A	1215	16/25	0.75	0.21	76,92,99,102	0
4	OLC	A	1207	21/25	0.76	0.22	54,61,97,104	0
4	OLC	A	1219	14/25	0.77	0.27	57,63,75,75	0
4	OLC	A	1214	19/25	0.78	0.26	55,69,87,90	0
4	OLC	A	1208	21/25	0.79	0.21	71,75,89,91	0
4	OLC	A	1220	25/25	0.80	0.23	53,76,93,98	0
6	NA	A	1224	1/1	0.81	0.16	59,59,59,59	0
4	OLC	A	1212	19/25	0.83	0.25	63,73,100,102	0
4	OLC	A	1209	19/25	0.84	0.19	64,69,84,84	0
4	OLC	A	1221	25/25	0.86	0.25	45,66,89,93	0
5	PE4	A	1223	11/24	0.87	0.23	58,67,75,77	0
3	CLR	A	1203	28/28	0.88	0.17	37,42,73,79	0
4	OLC	A	1205	16/25	0.91	0.22	47,55,74,75	0
3	CLR	A	1204	28/28	0.93	0.17	50,57,81,86	0
3	CLR	A	1202	28/28	0.94	0.15	36,40,55,58	0
2	JQR	A	1201	28/28	0.97	0.15	29,33,44,51	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.

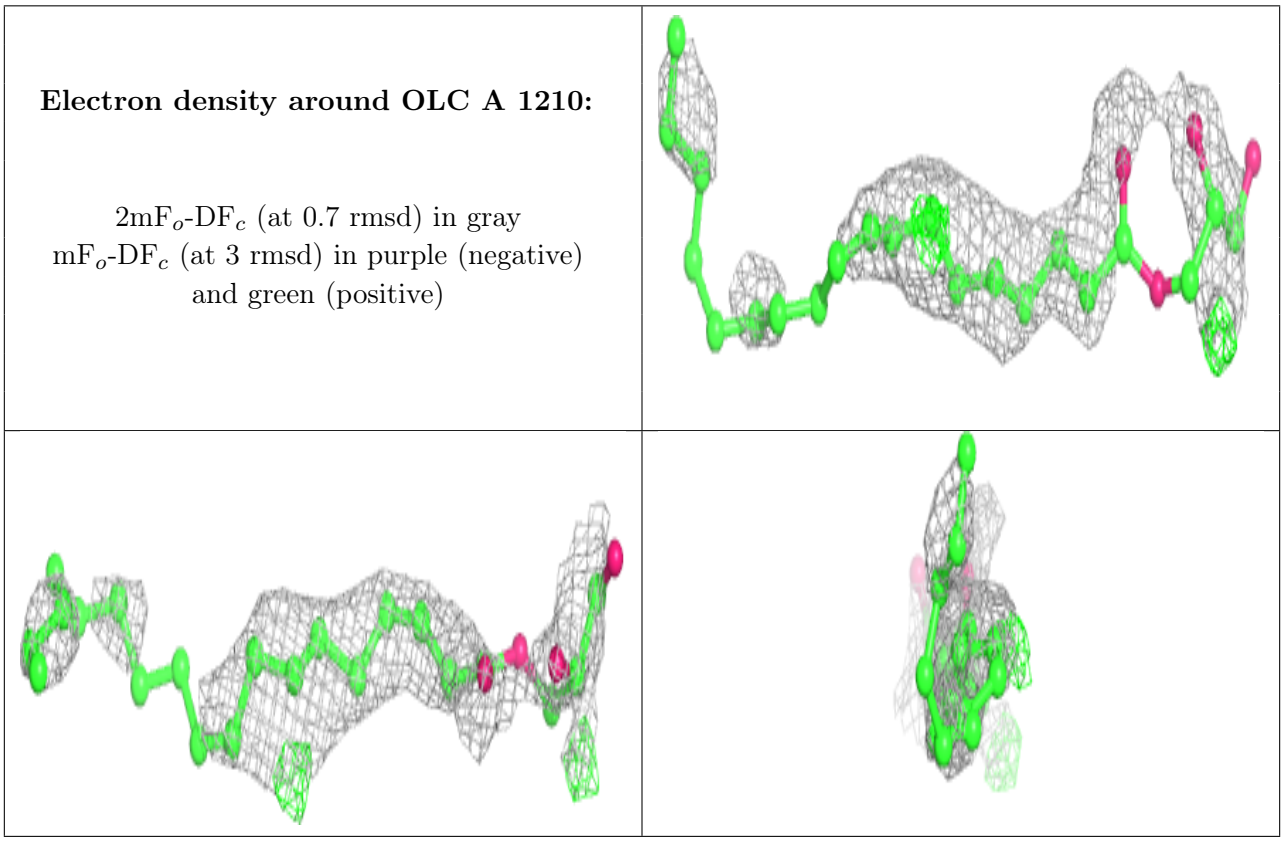
Electron density around OLC A 1218:

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



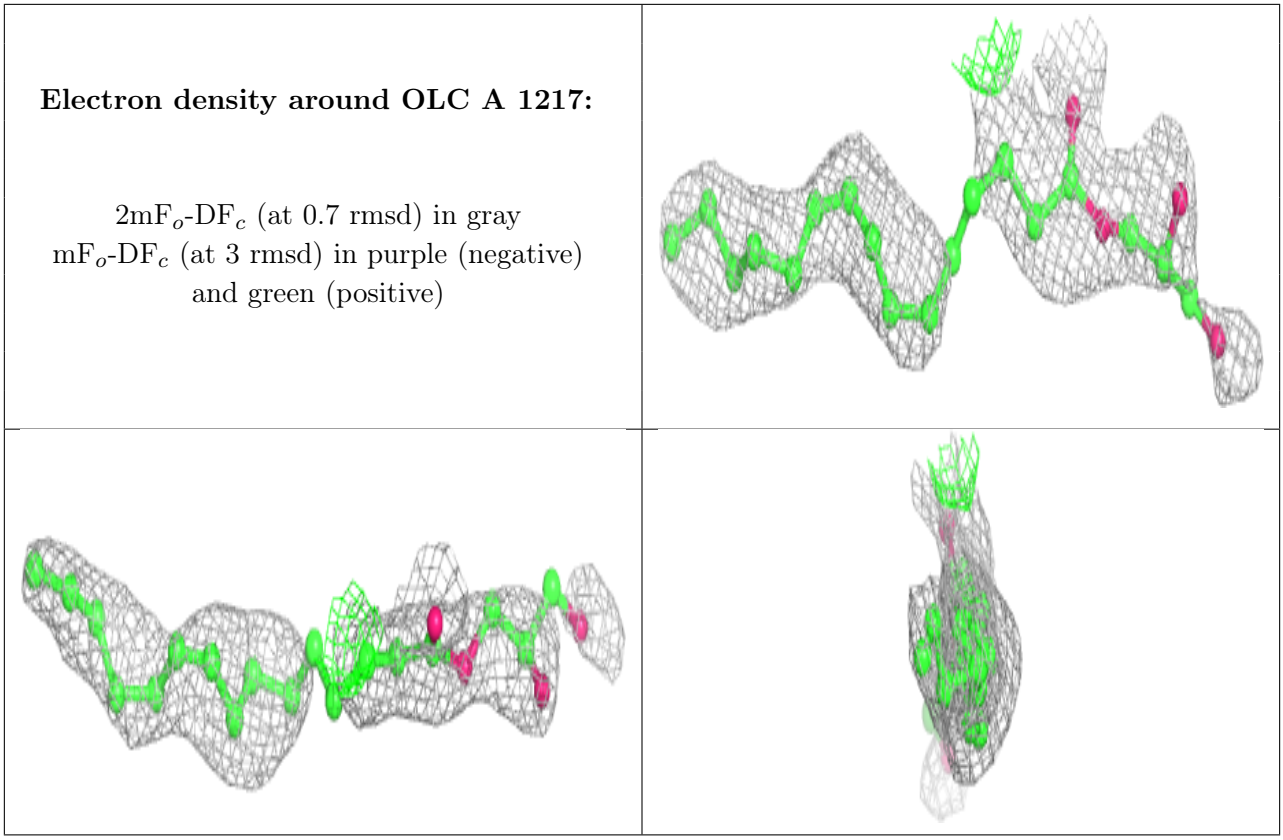
Electron density around OLC A 1210:

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



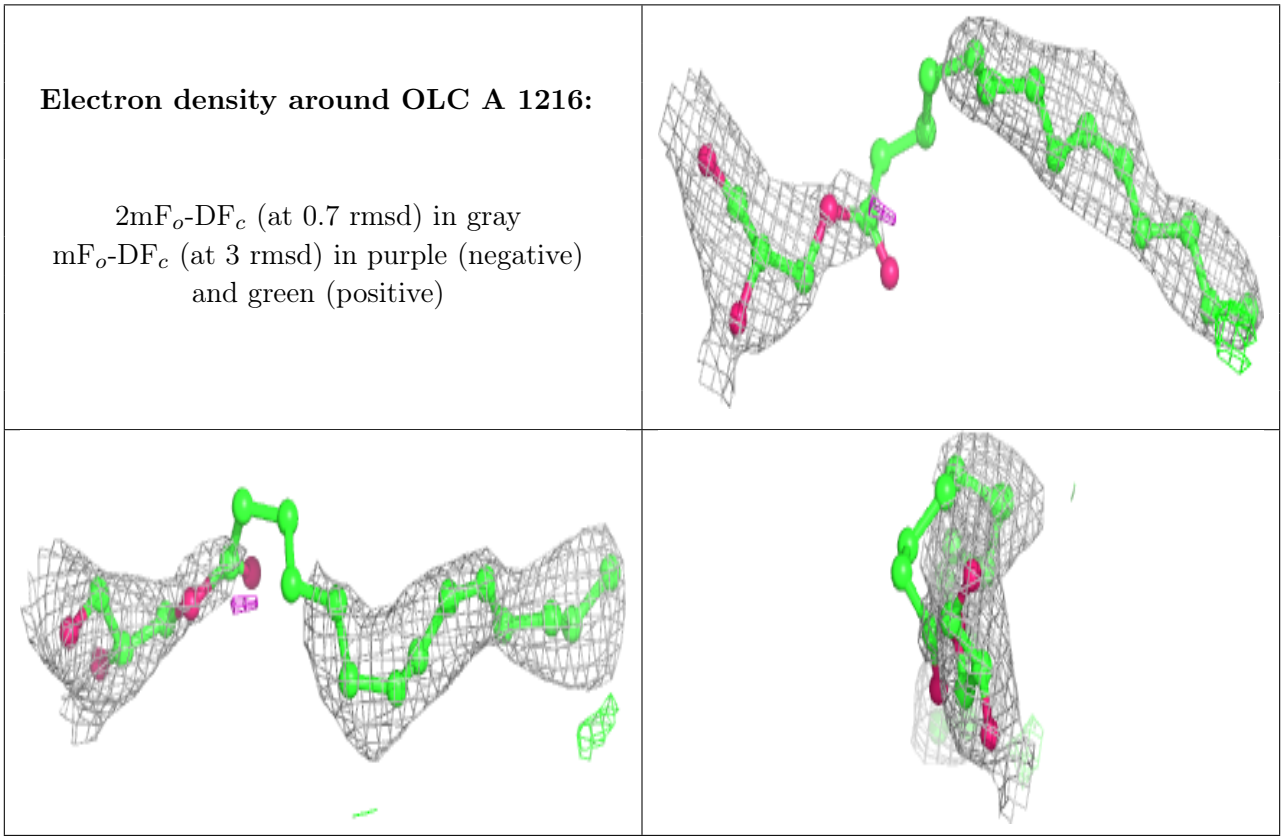
Electron density around OLC A 1217:

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



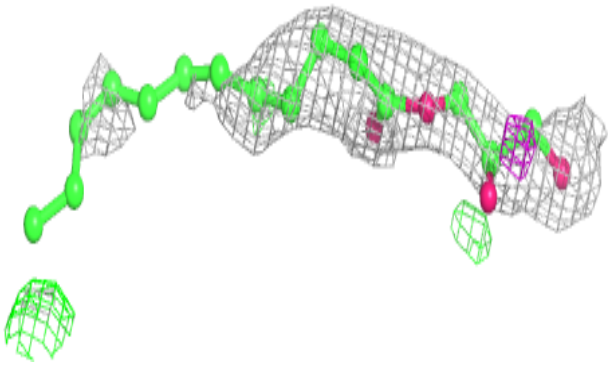
Electron density around OLC A 1216:

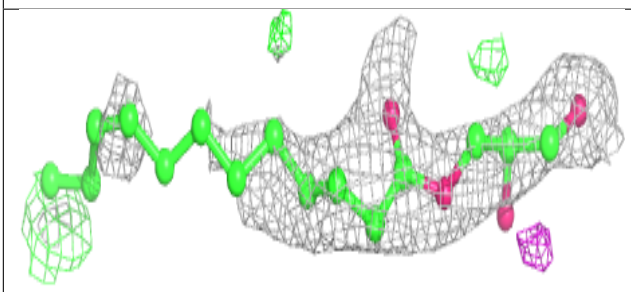
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

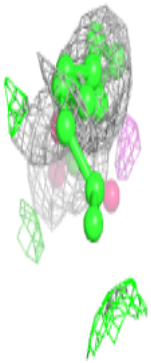


Electron density around OLC A 1213:

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

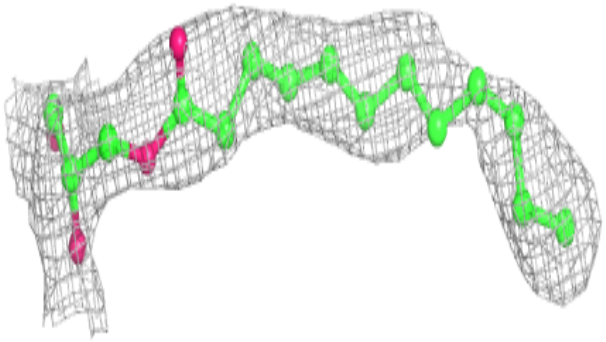


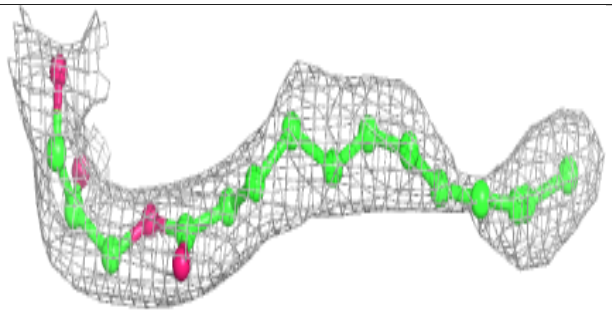


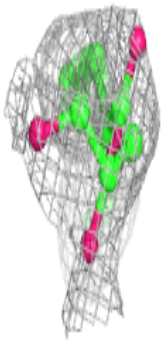


Electron density around OLC A 1211:

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

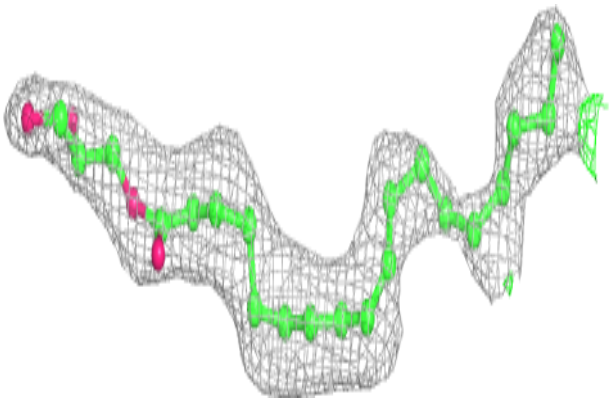


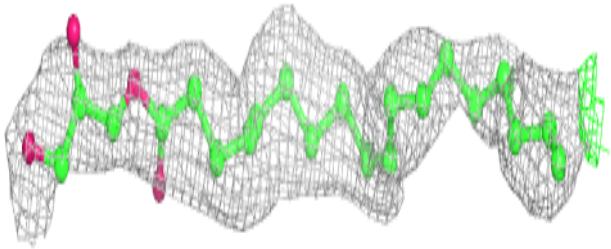


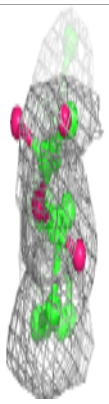


Electron density around OLC A 1206:

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

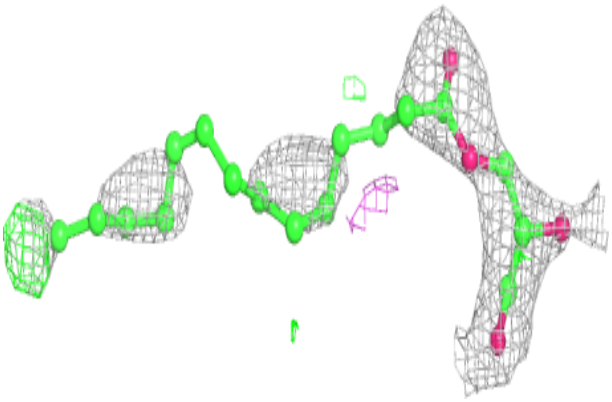


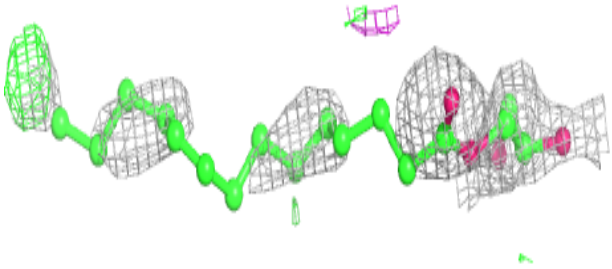


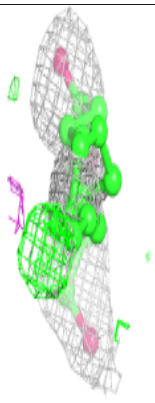


Electron density around OLC A 1222:

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

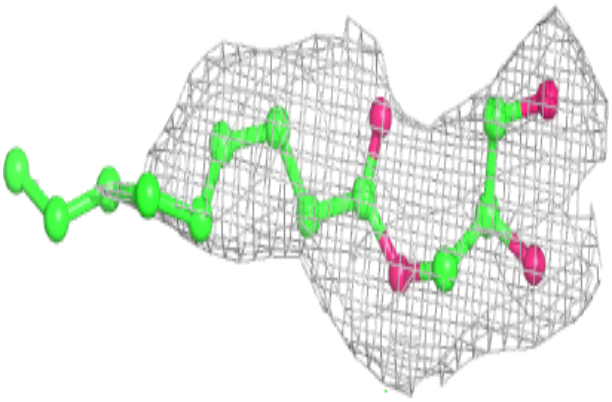


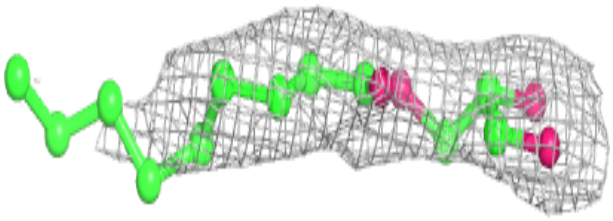


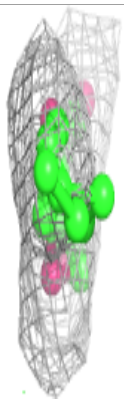


Electron density around OLC A 1215:

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

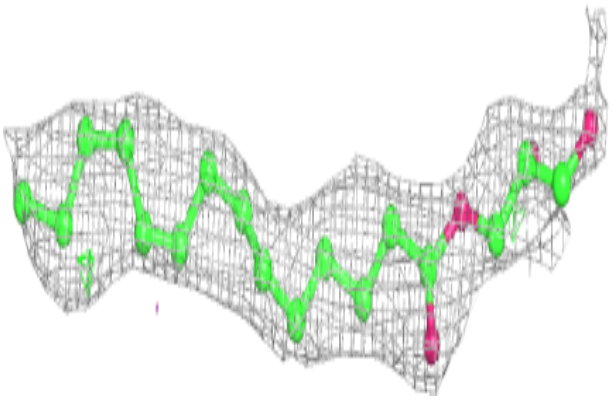


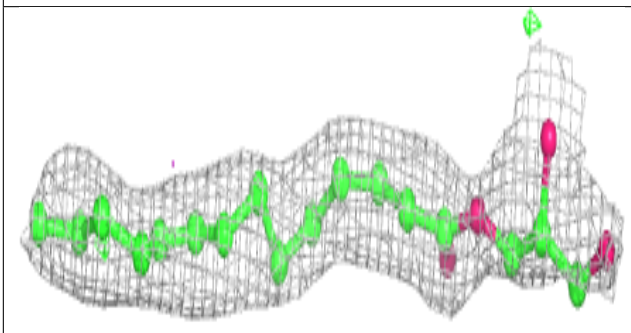


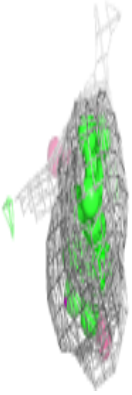


Electron density around OLC A 1207:

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

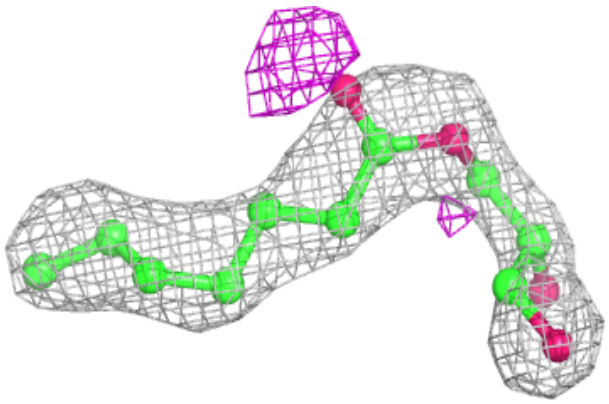


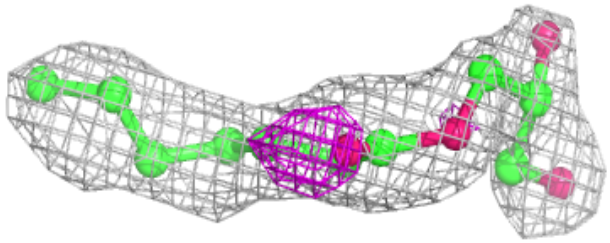


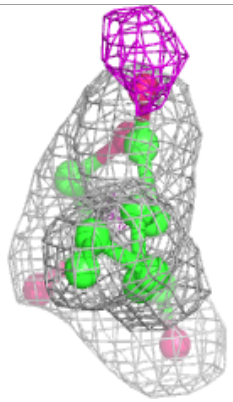


Electron density around OLC A 1219:

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

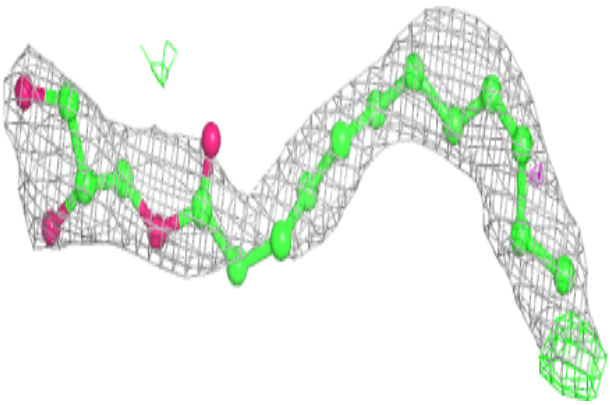


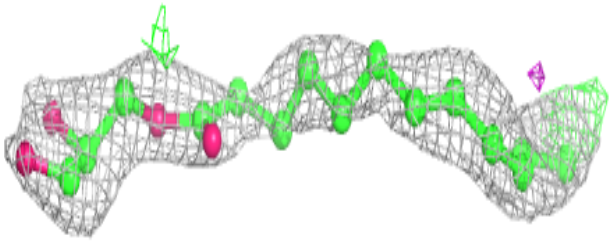


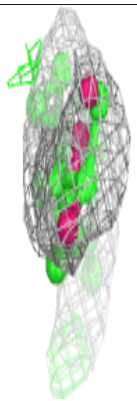


Electron density around OLC A 1214:

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

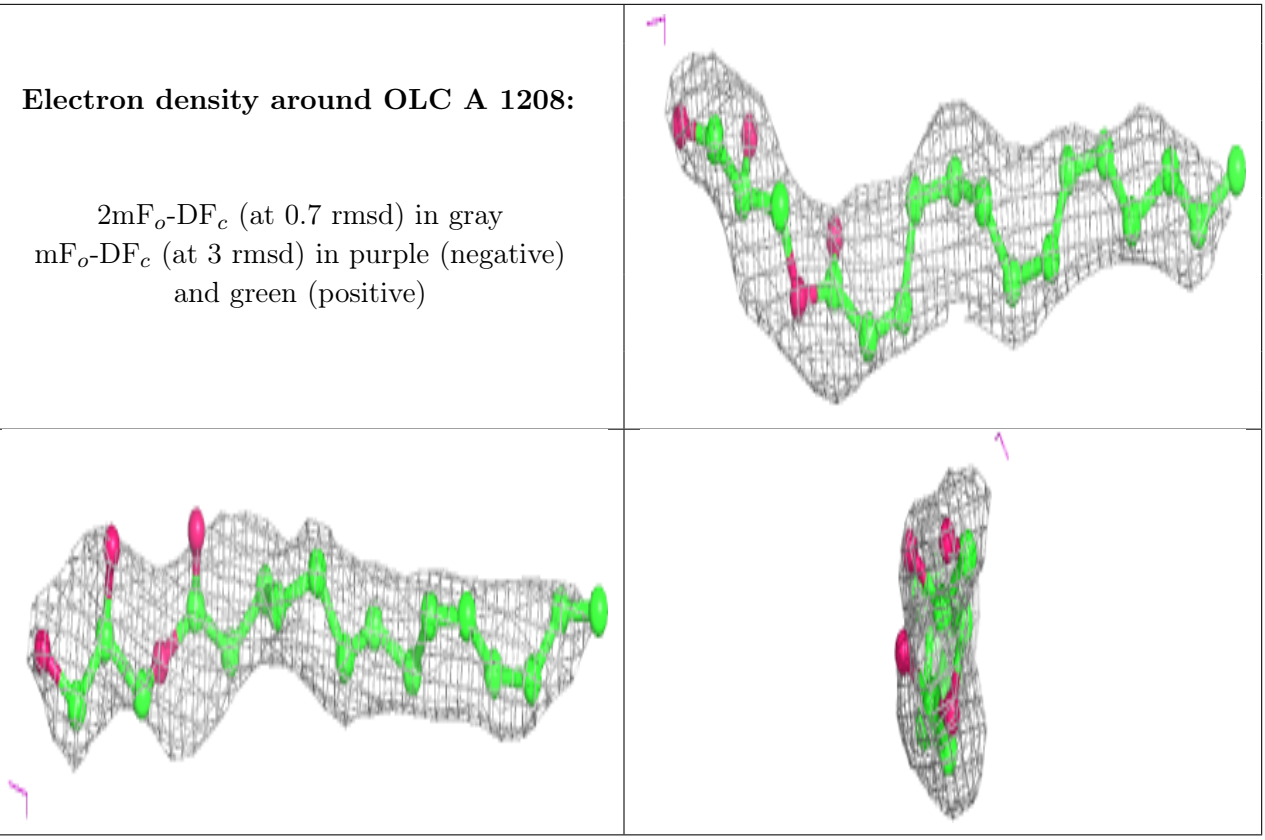






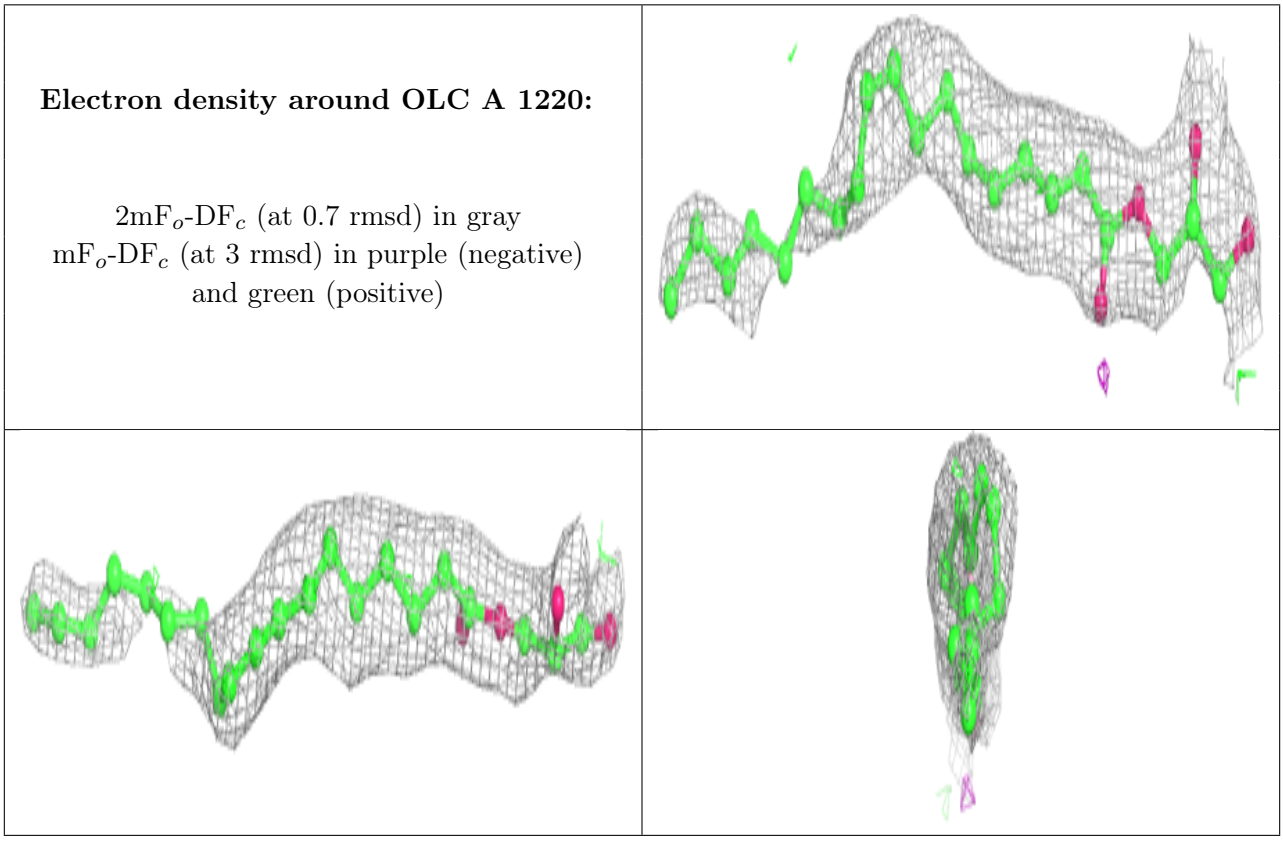
Electron density around OLC A 1208:

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



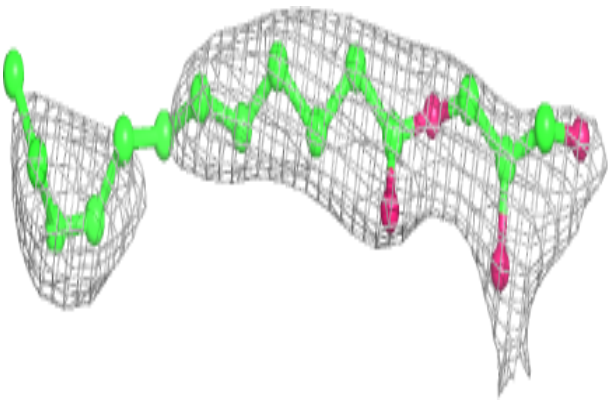
Electron density around OLC A 1220:

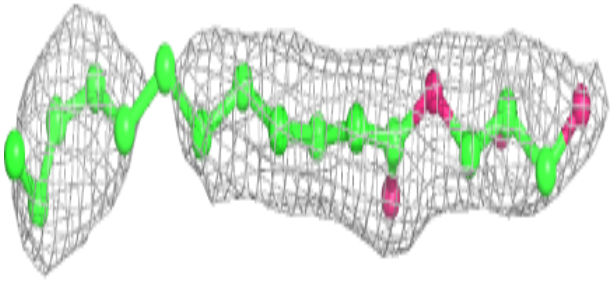
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

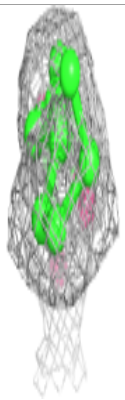


Electron density around OLC A 1212:

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

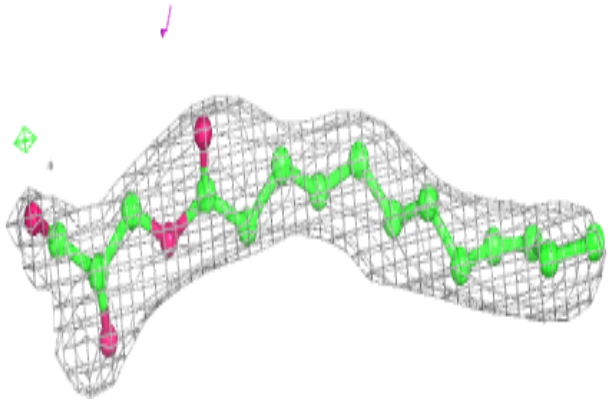


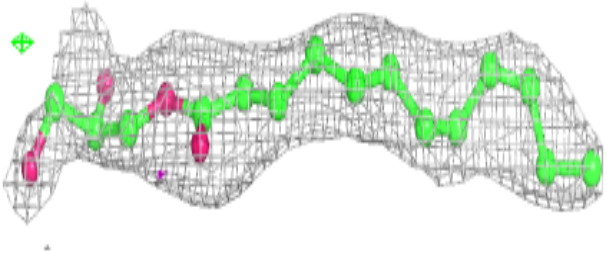


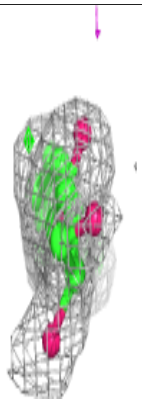


Electron density around OLC A 1209:

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

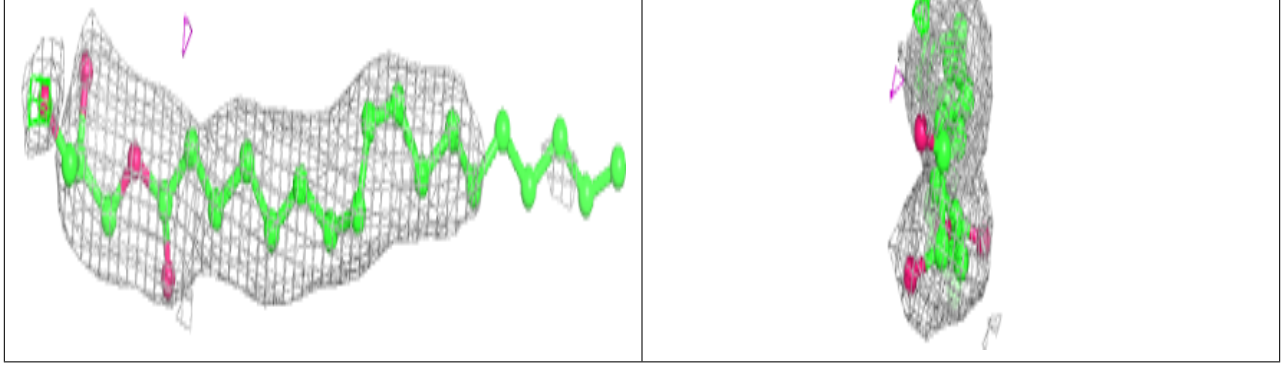






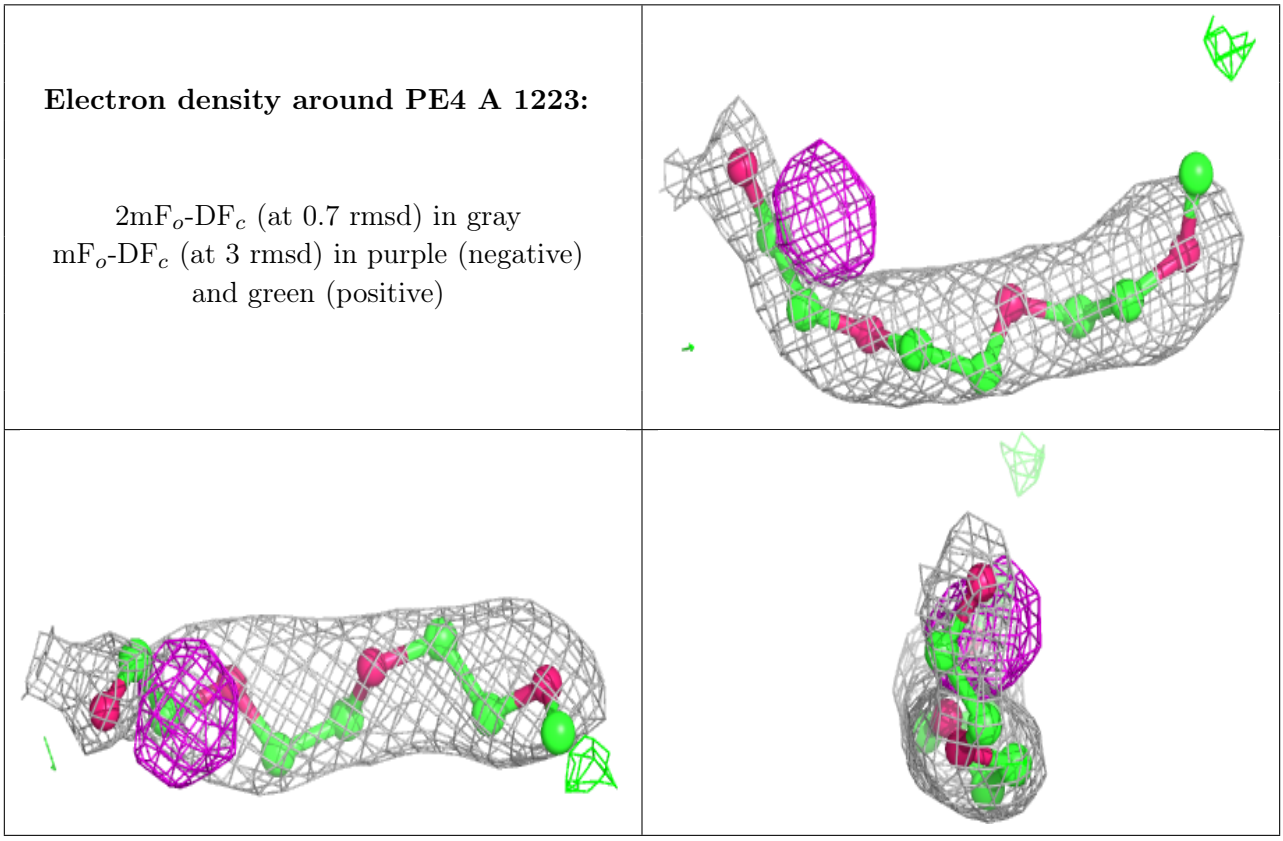
Electron density around OLC A 1221:

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



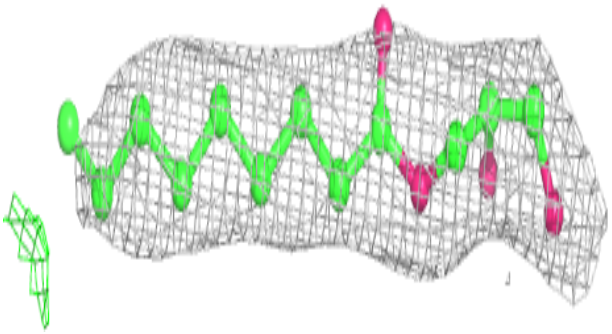
Electron density around PE4 A 1223:

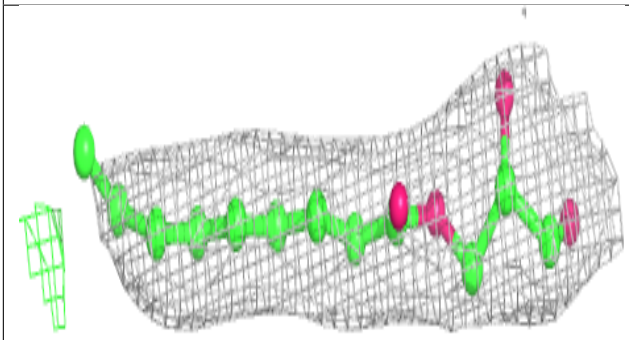
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

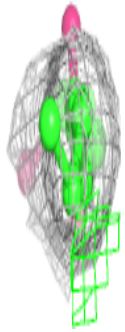


Electron density around OLC A 1205:

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

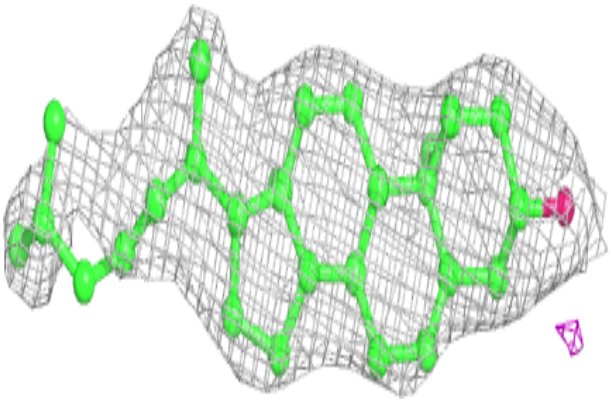


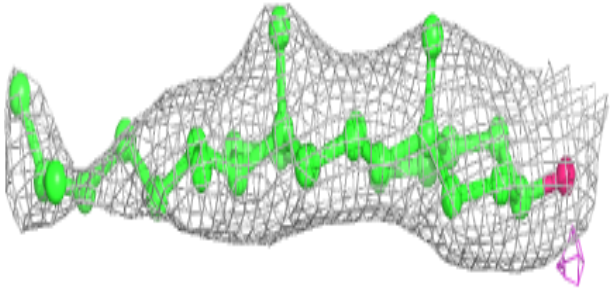


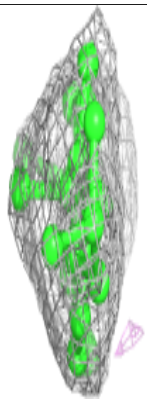


Electron density around CLR A 1204:

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

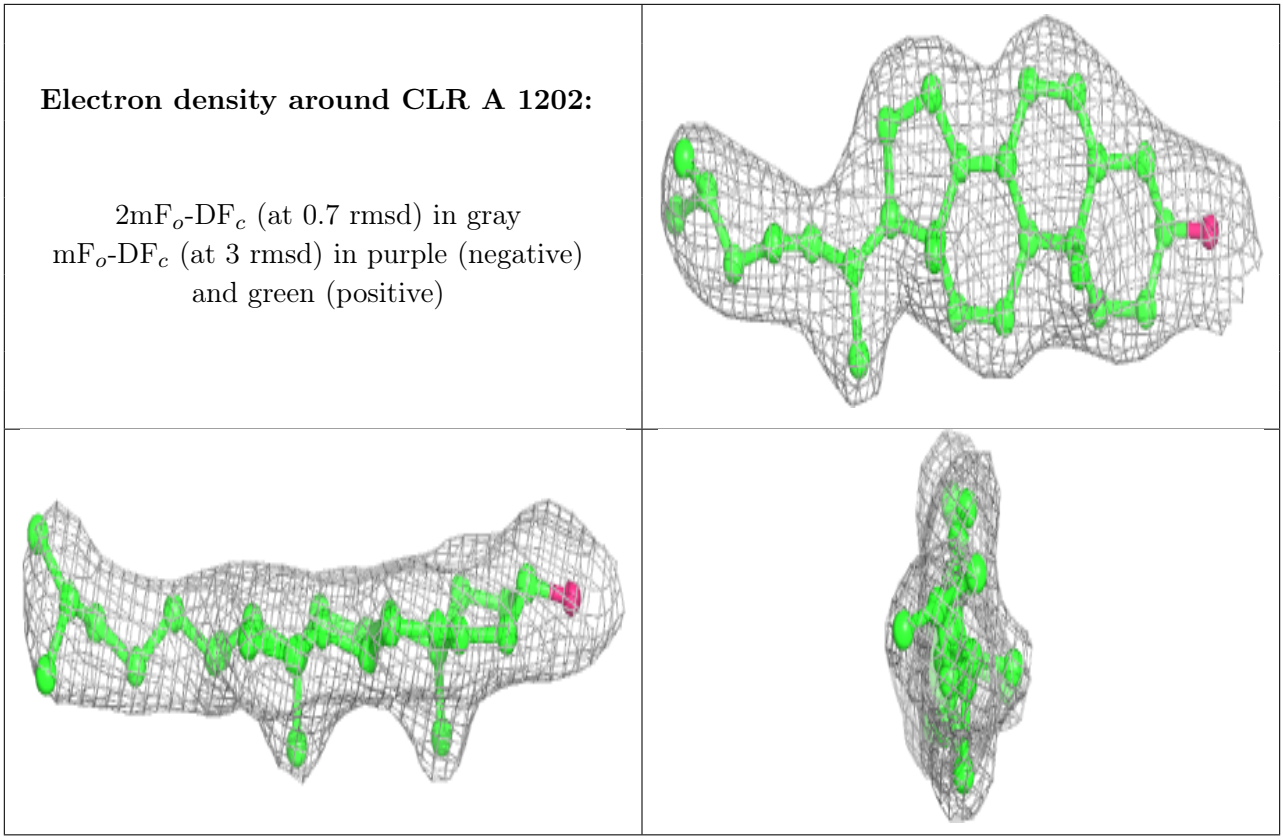






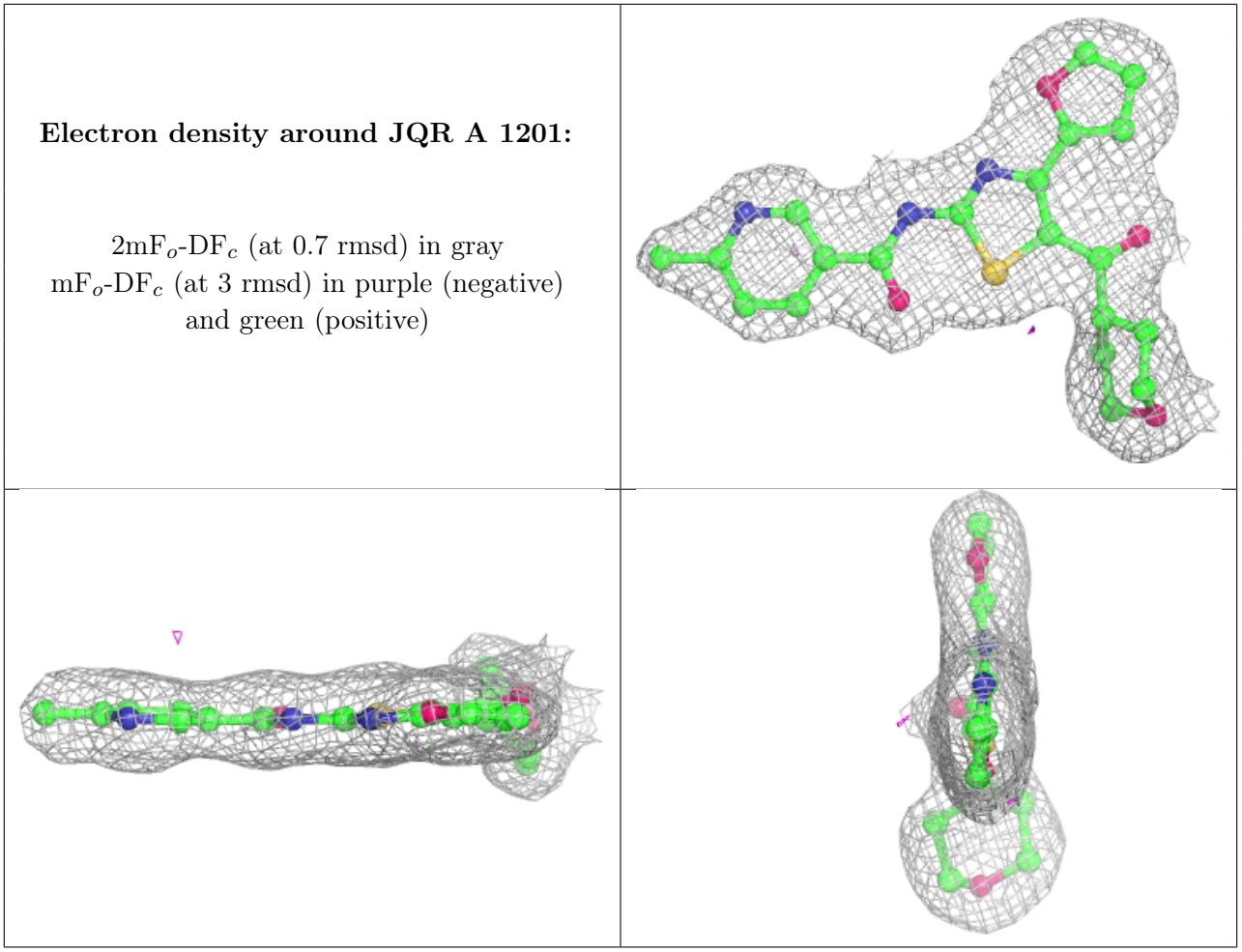
Electron density around CLR A 1202:

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



Electron density around JQR A 1201:

$2mF_o$-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.