Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 10:09 PM JST

PDB ID	:	8JWY
Title	:	Crystal structure of A2AR-T4L in complex with 2-118
Authors	:	Weng, Y.; Chen, Y.; Xu, Y.; Song, G.
Deposited on	:	2023-06-29
Resolution	:	2.33 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:

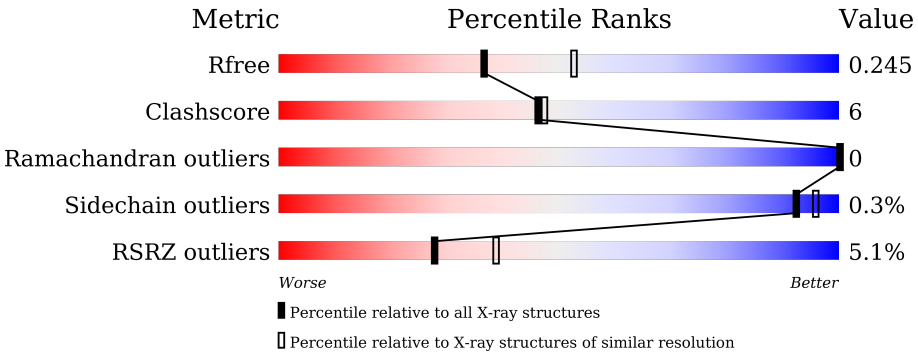
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	481	5% 81% 12% 7%

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
4	OLA	A	1222	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4119 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.

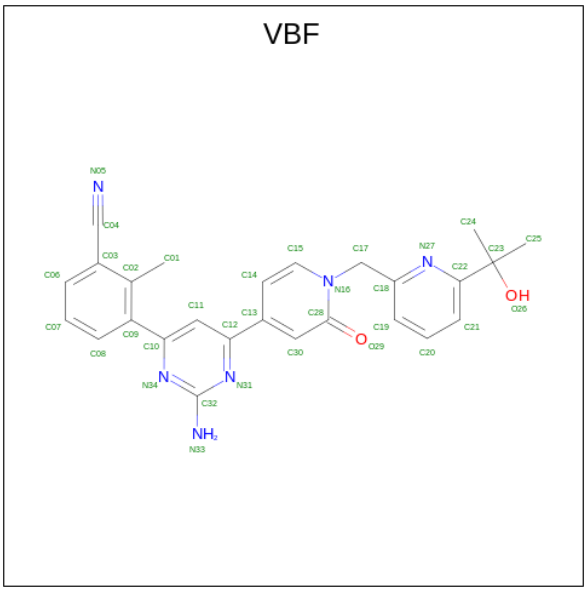
- Molecule 1 is a protein called Adenosine receptor A2a,Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3514	2283	605	602	24			

There are 21 discrepancies between the modelled and reference sequences:

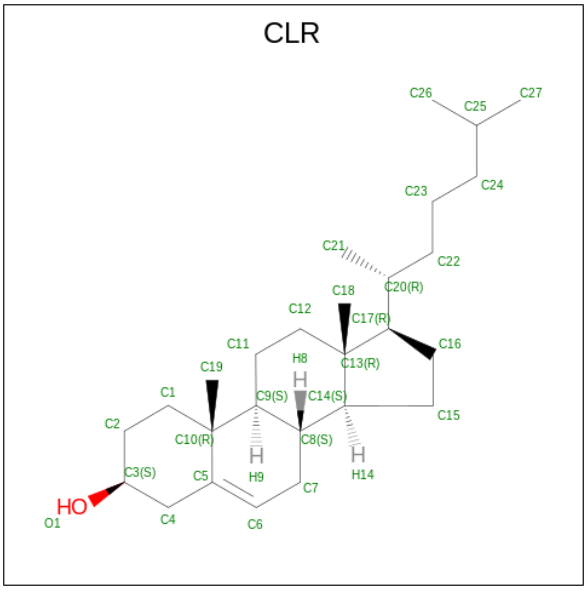
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP P29274
A	-6	TYR	-	expression tag	UNP P29274
A	-5	LYS	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	ASP	-	expression tag	UNP P29274
A	0	GLY	-	expression tag	UNP P29274
A	1	ALA	-	expression tag	UNP P29274
A	261	THR	CYS	engineered mutation	UNP D9IEF7
A	304	ALA	CYS	engineered mutation	UNP D9IEF7
A	464	HIS	-	expression tag	UNP P29274
A	465	HIS	-	expression tag	UNP P29274
A	466	HIS	-	expression tag	UNP P29274
A	467	HIS	-	expression tag	UNP P29274
A	468	HIS	-	expression tag	UNP P29274
A	469	HIS	-	expression tag	UNP P29274
A	470	HIS	-	expression tag	UNP P29274
A	471	HIS	-	expression tag	UNP P29274
A	472	HIS	-	expression tag	UNP P29274
A	473	HIS	-	expression tag	UNP P29274

- Molecule 2 is 3-[2-azanyl-6-[2-oxidanylidene-1-[[6-(2-oxidanylpropan-2-yl)pyridin-2-yl]methyl]pyridin-4-yl]pyrimidin-4-yl]-2-methyl-benzenecarbonitrile (three-letter code: VBF) (formula: $C_{26}H_{24}N_6O_2$) (labeled as "Ligand of Interest" by depositor).



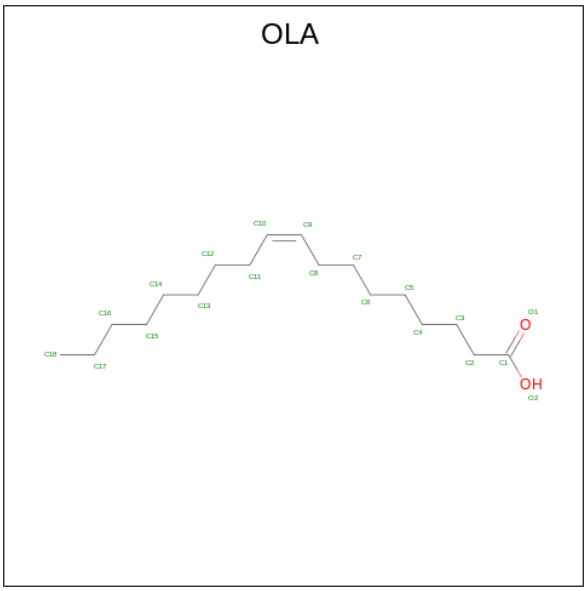
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 34 26 6 2	0	0

- 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 28 27 1	0	0

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 9 2	0	0
4	A	1	Total C O 15 13 2	0	0
4	A	1	Total C O 15 13 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 11 9 2	0	0
4	A	1	Total C O 15 13 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 14 12 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 15 13 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0

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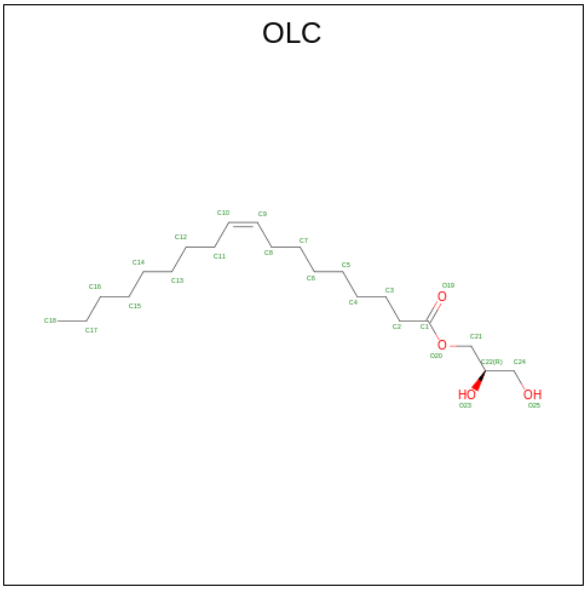
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 14 12 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 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
6	A	1	Total C O 25 21 4	0	0

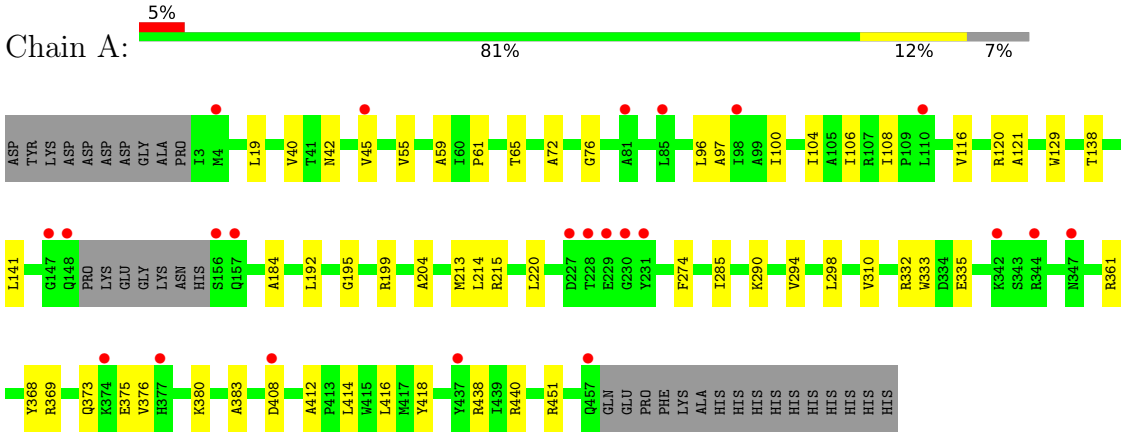
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	207	Total	O	0	0
			207	207		

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,Endolysin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.92Å 76.38Å 85.34Å 90.00° 101.97° 90.00°	Depositor
Resolution (Å)	24.90 – 2.33 24.90 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.90-2.33) 99.6 (24.90-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.33Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.245 0.206 , 0.245	Depositor DCC
R_{free} test set	1228 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4119	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% 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: NA, OLA, OLC, CLR, VBF

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	0.24	0/3589	0.46	0/4877

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3514	0	3595	39	0
2	A	34	0	0	0	0
3	A	28	0	46	0	0
4	A	310	0	474	24	0
5	A	1	0	0	0	0
6	A	25	0	40	2	0
7	A	207	0	0	1	0
All	All	4119	0	4155	51	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 6.

All (51) 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:1221:OLA:H183	4:A:1222:OLA:H9	1.68	0.75
1:A:65:THR:HG21	4:A:1206:OLA:H10	1.72	0.70
1:A:204:ALA:HB2	1:A:376:VAL:HG11	1.73	0.70
1:A:199:ARG:NH2	4:A:1208:OLA:O1	2.26	0.66
1:A:138:THR:HA	1:A:141:LEU:HD12	1.81	0.61
1:A:96:LEU:HD11	1:A:192:LEU:HD12	1.82	0.61
1:A:418:TYR:HB3	6:A:1219:OLC:H4	1.88	0.56
1:A:332:ARG:NH2	1:A:335:GLU:OE1	2.35	0.56
1:A:440:ARG:HG2	1:A:440:ARG:HH11	1.71	0.56
1:A:120:ARG:HD3	4:A:1220:OLA:H21	1.89	0.55
1:A:116:VAL:HG13	4:A:1220:OLA:H62	1.89	0.55
1:A:72:ALA:HB1	4:A:1206:OLA:H22	1.89	0.54
1:A:129:TRP:CE2	4:A:1204:OLA:H9	2.44	0.53
1:A:108:ILE:HG13	1:A:108:ILE:O	2.10	0.52
1:A:215:ARG:HD2	1:A:220:LEU:HD12	1.91	0.52
1:A:369:ARG:O	1:A:373:GLN:HG2	2.09	0.52
1:A:195:GLY:HA3	4:A:1208:OLA:H22	1.92	0.51
1:A:408:ASP:OD2	1:A:408:ASP:N	2.42	0.51
1:A:214:LEU:HD13	1:A:274:PHE:HZ	1.75	0.50
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.96	0.48
4:A:1220:OLA:H52	4:A:1220:OLA:H82	1.66	0.47
4:A:1205:OLA:H31	4:A:1212:OLA:H9	1.96	0.47
4:A:1210:OLA:H42	4:A:1210:OLA:H72	1.50	0.47
1:A:380:LYS:HE3	4:A:1218:OLA:H42	1.97	0.47
4:A:1212:OLA:H183	4:A:1212:OLA:H152	1.68	0.47
1:A:285:ILE:HD11	1:A:310:VAL:HG21	1.98	0.46
1:A:106:ILE:HG22	1:A:375:GLU:HB3	1.98	0.46
1:A:116:VAL:HG22	4:A:1220:OLA:H51	1.99	0.44
4:A:1214:OLA:H9	4:A:1214:OLA:H62	1.74	0.44
1:A:213:MET:HG3	1:A:368:TYR:CZ	2.52	0.44
1:A:412:ALA:HB1	1:A:416:LEU:HD23	1.99	0.44
1:A:451:ARG:NH1	7:A:1306:HOH:O	2.43	0.44
4:A:1206:OLA:H22	4:A:1206:OLA:H51	1.76	0.43
1:A:97:ALA:HA	4:A:1220:OLA:H10	2.00	0.43
4:A:1220:OLA:H122	4:A:1220:OLA:H151	1.55	0.43
1:A:290:LYS:HB3	1:A:290:LYS:HE2	1.68	0.43
1:A:76:GLY:HA2	4:A:1222:OLA:H52	2.01	0.43
1:A:100:ILE:O	1:A:104:ILE:HG12	2.19	0.43
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.87	0.42
4:A:1207:OLA:H22	4:A:1209:OLA:C1	2.50	0.42
1:A:61:PRO:O	1:A:65:THR:HG23	2.20	0.42
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1206:OLA:H71	4:A:1206:OLA:H42	1.55	0.42
1:A:333:TRP:HB3	1:A:361:ARG:HA	2.02	0.42
4:A:1207:OLA:H72	4:A:1207:OLA:H41	1.86	0.41
1:A:42:ASN:HA	1:A:45:VAL:HB	2.03	0.41
1:A:294:VAL:O	1:A:298:LEU:HG	2.20	0.41
6:A:1219:OLC:H5	6:A:1219:OLC:H2A	1.71	0.41
1:A:40:VAL:HG13	1:A:121:ALA:HB2	2.03	0.41
1:A:383:ALA:HB1	4:A:1218:OLA:C9	2.52	0.40
1:A:184:ALA:HB2	4:A:1209:OLA:H121	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	444/481 (92%)	437 (98%)	7 (2%)	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	373/404 (92%)	372 (100%)	1 (0%)	92 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	OLA	A	1215	-	14,14,19	0.90	1 (7%)	14,14,19	0.97	0
4	OLA	A	1208	-	10,10,19	0.61	0	10,10,19	1.22	2 (20%)
4	OLA	A	1217	-	19,19,19	0.79	1 (5%)	19,19,19	0.90	1 (5%)
4	OLA	A	1209	-	14,14,19	0.91	1 (7%)	14,14,19	1.01	1 (7%)
4	OLA	A	1221	-	19,19,19	0.78	1 (5%)	19,19,19	0.96	0
4	OLA	A	1222	-	13,13,19	0.95	1 (7%)	12,13,19	1.06	0
6	OLC	A	1219	-	24,24,24	0.98	1 (4%)	25,25,25	1.24	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OLA	A	1205	-	14,14,19	0.91	1 (7%)	14,14,19	1.00	1 (7%)
4	OLA	A	1212	-	19,19,19	0.77	1 (5%)	19,19,19	0.96	0
4	OLA	A	1214	-	19,19,19	0.78	1 (5%)	19,19,19	0.95	1 (5%)
4	OLA	A	1204	-	14,14,19	0.90	1 (7%)	14,14,19	1.06	1 (7%)
3	CLR	A	1202	-	31,31,31	0.38	0	48,48,48	0.67	0
4	OLA	A	1218	-	19,19,19	0.77	1 (5%)	19,19,19	1.03	2 (10%)
4	OLA	A	1206	-	19,19,19	0.78	1 (5%)	19,19,19	0.95	1 (5%)
4	OLA	A	1220	-	19,19,19	0.79	1 (5%)	19,19,19	0.92	1 (5%)
4	OLA	A	1216	-	19,19,19	0.79	1 (5%)	19,19,19	0.93	2 (10%)
2	VBF	A	1201	-	36,37,37	2.04	8 (22%)	45,54,54	2.42	11 (24%)
4	OLA	A	1203	-	10,10,19	0.63	0	10,10,19	1.21	2 (20%)
4	OLA	A	1210	-	19,19,19	0.78	1 (5%)	19,19,19	0.89	0
4	OLA	A	1207	-	19,19,19	0.80	1 (5%)	19,19,19	0.88	0
4	OLA	A	1213	-	13,13,19	0.95	1 (7%)	12,13,19	1.05	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	OLA	A	1215	-	-	8/12/12/17	-
4	OLA	A	1208	-	-	5/8/8/17	-
4	OLA	A	1217	-	-	11/17/17/17	-
4	OLA	A	1209	-	-	7/12/12/17	-
4	OLA	A	1221	-	-	8/17/17/17	-
4	OLA	A	1222	-	-	7/11/11/17	-
6	OLC	A	1219	-	-	9/24/24/24	-
4	OLA	A	1205	-	-	9/12/12/17	-
4	OLA	A	1212	-	-	8/17/17/17	-
4	OLA	A	1214	-	-	12/17/17/17	-
4	OLA	A	1204	-	-	6/12/12/17	-
3	CLR	A	1202	-	-	8/10/68/68	0/4/4/4
4	OLA	A	1218	-	-	6/17/17/17	-
4	OLA	A	1206	-	-	6/17/17/17	-
4	OLA	A	1220	-	-	14/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	1216	-	-	9/17/17/17	-
2	VBF	A	1201	-	-	0/19/20/20	0/4/4/4
4	OLA	A	1203	-	-	4/8/8/17	-
4	OLA	A	1210	-	-	8/17/17/17	-
4	OLA	A	1207	-	-	10/17/17/17	-
4	OLA	A	1213	-	-	7/11/11/17	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	VBF	C03-C04	5.99	1.53	1.44
2	A	1201	VBF	C32-N33	5.84	1.45	1.33
2	A	1201	VBF	C28-N16	-4.42	1.33	1.39
2	A	1201	VBF	C09-C10	-3.07	1.40	1.48
2	A	1201	VBF	C15-N16	-2.91	1.32	1.37
2	A	1201	VBF	O26-C23	-2.81	1.40	1.44
4	A	1205	OLA	C10-C9	2.73	1.47	1.31
4	A	1207	OLA	C10-C9	2.73	1.47	1.31
4	A	1213	OLA	C10-C9	2.72	1.47	1.31
4	A	1209	OLA	C10-C9	2.71	1.47	1.31
4	A	1214	OLA	C10-C9	2.71	1.47	1.31
4	A	1220	OLA	C10-C9	2.71	1.47	1.31
4	A	1204	OLA	C10-C9	2.71	1.47	1.31
4	A	1215	OLA	C10-C9	2.70	1.47	1.31
4	A	1217	OLA	C10-C9	2.70	1.47	1.31
4	A	1216	OLA	C10-C9	2.70	1.47	1.31
4	A	1221	OLA	C10-C9	2.70	1.47	1.31
4	A	1222	OLA	C10-C9	2.69	1.47	1.31
4	A	1206	OLA	C10-C9	2.69	1.47	1.31
4	A	1210	OLA	C10-C9	2.67	1.47	1.31
4	A	1212	OLA	C10-C9	2.67	1.47	1.31
4	A	1218	OLA	C10-C9	2.67	1.47	1.31
6	A	1219	OLC	O20-C1	2.59	1.40	1.33
2	A	1201	VBF	C12-C13	-2.13	1.39	1.47
2	A	1201	VBF	O29-C28	-2.04	1.19	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	VBF	C10-N34-C32	9.94	122.00	116.34
2	A	1201	VBF	C12-N31-C32	6.54	120.27	116.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	VBF	C18-C17-N16	-4.71	107.34	113.08
2	A	1201	VBF	C11-C10-N34	-4.05	117.53	122.35
6	A	1219	OLC	C8-C9-C10	3.64	152.66	124.73
2	A	1201	VBF	C30-C28-N16	2.80	119.85	116.28
2	A	1201	VBF	C13-C12-N31	2.68	120.61	116.66
6	A	1219	OLC	O20-C1-C2	2.66	120.27	111.91
2	A	1201	VBF	N34-C32-N31	-2.54	121.43	125.42
4	A	1218	OLA	C3-C2-C1	-2.37	108.49	114.47
2	A	1201	VBF	C01-C02-C09	2.36	125.04	120.93
2	A	1201	VBF	C13-C30-C28	-2.24	119.35	122.61
2	A	1201	VBF	C11-C12-N31	-2.15	119.51	123.40
4	A	1217	OLA	O2-C1-C2	2.13	120.89	114.03
4	A	1203	OLA	C3-C2-C1	-2.13	109.09	114.47
4	A	1208	OLA	O2-C1-C2	2.13	120.87	114.03
2	A	1201	VBF	O29-C28-C30	-2.11	120.33	125.72
4	A	1216	OLA	C3-C2-C1	-2.10	109.17	114.47
4	A	1208	OLA	C3-C2-C1	-2.09	109.21	114.47
4	A	1203	OLA	O2-C1-C2	2.07	120.67	114.03
4	A	1218	OLA	O2-C1-C2	2.07	120.67	114.03
4	A	1204	OLA	O2-C1-C2	2.04	120.59	114.03
4	A	1214	OLA	O2-C1-C2	2.03	120.54	114.03
4	A	1209	OLA	O2-C1-C2	2.02	120.53	114.03
4	A	1206	OLA	O2-C1-C2	2.02	120.52	114.03
4	A	1216	OLA	O2-C1-C2	2.02	120.51	114.03
4	A	1220	OLA	O2-C1-C2	2.02	120.50	114.03
4	A	1205	OLA	O2-C1-C2	2.00	120.46	114.03

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1204	OLA	C11-C10-C9-C8
4	A	1220	OLA	C11-C10-C9-C8
3	A	1202	CLR	C17-C20-C22-C23
4	A	1216	OLA	C4-C5-C6-C7
4	A	1207	OLA	C4-C5-C6-C7
3	A	1202	CLR	C21-C20-C22-C23
4	A	1210	OLA	C1-C2-C3-C4
4	A	1214	OLA	C1-C2-C3-C4
4	A	1215	OLA	C1-C2-C3-C4
4	A	1207	OLA	C11-C10-C9-C8
6	A	1219	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	A	1203	OLA	C1-C2-C3-C4
4	A	1205	OLA	C1-C2-C3-C4
4	A	1207	OLA	C1-C2-C3-C4
4	A	1208	OLA	C1-C2-C3-C4
4	A	1209	OLA	C1-C2-C3-C4
4	A	1217	OLA	C1-C2-C3-C4
4	A	1220	OLA	C1-C2-C3-C4
4	A	1221	OLA	C1-C2-C3-C4
4	A	1210	OLA	C4-C5-C6-C7
3	A	1202	CLR	C20-C22-C23-C24
4	A	1218	OLA	C1-C2-C3-C4
4	A	1210	OLA	C11-C12-C13-C14
4	A	1220	OLA	C12-C13-C14-C15
3	A	1202	CLR	C13-C17-C20-C22
4	A	1203	OLA	C4-C5-C6-C7
4	A	1205	OLA	C4-C5-C6-C7
4	A	1217	OLA	C13-C14-C15-C16
4	A	1207	OLA	C11-C12-C13-C14
4	A	1213	OLA	C3-C4-C5-C6
4	A	1216	OLA	C11-C12-C13-C14
4	A	1210	OLA	C3-C4-C5-C6
4	A	1222	OLA	C2-C3-C4-C5
6	A	1219	OLC	C6-C7-C8-C9
4	A	1208	OLA	C4-C5-C6-C7
4	A	1216	OLA	C13-C14-C15-C16
4	A	1220	OLA	C14-C15-C16-C17
4	A	1221	OLA	C11-C12-C13-C14
4	A	1218	OLA	C13-C14-C15-C16
4	A	1218	OLA	C4-C5-C6-C7
6	A	1219	OLC	C2-C1-O20-C21
4	A	1214	OLA	C14-C15-C16-C17
4	A	1221	OLA	C3-C4-C5-C6
4	A	1206	OLA	C11-C10-C9-C8
4	A	1212	OLA	C1-C2-C3-C4
4	A	1222	OLA	C4-C5-C6-C7
4	A	1217	OLA	C12-C13-C14-C15
4	A	1206	OLA	C3-C4-C5-C6
4	A	1214	OLA	C11-C12-C13-C14
4	A	1210	OLA	C14-C15-C16-C17
4	A	1218	OLA	C3-C4-C5-C6
4	A	1220	OLA	C11-C12-C13-C14
6	A	1219	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
3	A	1202	CLR	C16-C17-C20-C21
6	A	1219	OLC	C5-C6-C7-C8
4	A	1206	OLA	C4-C5-C6-C7
4	A	1222	OLA	C1-C2-C3-C4
4	A	1221	OLA	C2-C3-C4-C5
4	A	1220	OLA	C2-C3-C4-C5
4	A	1206	OLA	C5-C6-C7-C8
4	A	1216	OLA	C5-C6-C7-C8
4	A	1207	OLA	C2-C3-C4-C5
4	A	1217	OLA	C11-C12-C13-C14
4	A	1220	OLA	C6-C7-C8-C9
4	A	1212	OLA	C11-C12-C13-C14
3	A	1202	CLR	C16-C17-C20-C22
4	A	1204	OLA	C1-C2-C3-C4
4	A	1217	OLA	C2-C3-C4-C5
4	A	1216	OLA	C1-C2-C3-C4
3	A	1202	CLR	C13-C17-C20-C21
4	A	1218	OLA	C11-C12-C13-C14
4	A	1213	OLA	C5-C6-C7-C8
4	A	1205	OLA	C3-C4-C5-C6
4	A	1221	OLA	C12-C13-C14-C15
4	A	1205	OLA	C11-C10-C9-C8
4	A	1216	OLA	C11-C10-C9-C8
4	A	1210	OLA	C15-C16-C17-C18
4	A	1212	OLA	C14-C15-C16-C17
4	A	1214	OLA	C3-C4-C5-C6
4	A	1204	OLA	C4-C5-C6-C7
4	A	1218	OLA	C11-C10-C9-C8
4	A	1222	OLA	C11-C10-C9-C8
4	A	1207	OLA	C3-C4-C5-C6
4	A	1214	OLA	C5-C6-C7-C8
4	A	1212	OLA	C13-C14-C15-C16
6	A	1219	OLC	C3-C4-C5-C6
4	A	1212	OLA	C11-C10-C9-C8
4	A	1213	OLA	C11-C10-C9-C8
4	A	1215	OLA	C11-C10-C9-C8
4	A	1217	OLA	C11-C10-C9-C8
4	A	1216	OLA	C14-C15-C16-C17
4	A	1220	OLA	C13-C14-C15-C16
4	A	1214	OLA	C15-C16-C17-C18
4	A	1209	OLA	C11-C10-C9-C8
4	A	1221	OLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	A	1213	OLA	C9-C10-C11-C12
4	A	1221	OLA	C4-C5-C6-C7
3	A	1202	CLR	C22-C23-C24-C25
4	A	1210	OLA	C13-C14-C15-C16
6	A	1219	OLC	O20-C21-C22-C24
4	A	1215	OLA	C2-C3-C4-C5
4	A	1214	OLA	C10-C11-C12-C13
4	A	1212	OLA	C15-C16-C17-C18
4	A	1212	OLA	C4-C5-C6-C7
4	A	1214	OLA	C12-C13-C14-C15
4	A	1214	OLA	C13-C14-C15-C16
6	A	1219	OLC	C1-C2-C3-C4
4	A	1215	OLA	C3-C4-C5-C6
4	A	1209	OLA	C9-C10-C11-C12
4	A	1217	OLA	C9-C10-C11-C12
4	A	1210	OLA	C5-C6-C7-C8
4	A	1203	OLA	C3-C4-C5-C6
4	A	1220	OLA	O1-C1-C2-C3
4	A	1206	OLA	C11-C12-C13-C14
4	A	1217	OLA	C15-C16-C17-C18
4	A	1204	OLA	C5-C6-C7-C8
4	A	1213	OLA	O1-C1-C2-C3
4	A	1220	OLA	O2-C1-C2-C3
4	A	1209	OLA	C7-C8-C9-C10
4	A	1213	OLA	O2-C1-C2-C3
4	A	1207	OLA	O1-C1-C2-C3
4	A	1222	OLA	C7-C8-C9-C10
4	A	1207	OLA	O2-C1-C2-C3
4	A	1208	OLA	C2-C3-C4-C5
4	A	1205	OLA	C7-C8-C9-C10
4	A	1206	OLA	C9-C10-C11-C12
4	A	1220	OLA	C7-C8-C9-C10
4	A	1208	OLA	O2-C1-C2-C3
4	A	1220	OLA	C3-C4-C5-C6
4	A	1222	OLA	O2-C1-C2-C3
4	A	1207	OLA	C7-C8-C9-C10
4	A	1204	OLA	C10-C11-C12-C13
4	A	1205	OLA	C10-C11-C12-C13
4	A	1205	OLA	O2-C1-C2-C3
4	A	1215	OLA	O2-C1-C2-C3
4	A	1220	OLA	C5-C6-C7-C8
4	A	1207	OLA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	1213	OLA	C7-C8-C9-C10
4	A	1215	OLA	C9-C10-C11-C12
4	A	1221	OLA	C7-C8-C9-C10
4	A	1209	OLA	O2-C1-C2-C3
4	A	1203	OLA	C5-C6-C7-C8
4	A	1209	OLA	C4-C5-C6-C7
4	A	1205	OLA	O1-C1-C2-C3
4	A	1208	OLA	O1-C1-C2-C3
4	A	1222	OLA	O1-C1-C2-C3
4	A	1215	OLA	O1-C1-C2-C3
4	A	1204	OLA	C9-C10-C11-C12
4	A	1217	OLA	C7-C8-C9-C10
4	A	1217	OLA	O2-C1-C2-C3
4	A	1214	OLA	C7-C8-C9-C10
4	A	1216	OLA	C7-C8-C9-C10
4	A	1212	OLA	C5-C6-C7-C8
4	A	1220	OLA	C9-C10-C11-C12
4	A	1214	OLA	O2-C1-C2-C3
4	A	1209	OLA	O1-C1-C2-C3
4	A	1205	OLA	C9-C10-C11-C12
4	A	1214	OLA	O1-C1-C2-C3
4	A	1217	OLA	O1-C1-C2-C3
6	A	1219	OLC	O20-C21-C22-O23
4	A	1215	OLA	C4-C5-C6-C7
4	A	1216	OLA	O1-C1-C2-C3

There are no ring outliers.

14 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1208	OLA	2	0
4	A	1209	OLA	2	0
4	A	1221	OLA	1	0
4	A	1222	OLA	2	0
6	A	1219	OLC	2	0
4	A	1205	OLA	1	0
4	A	1212	OLA	2	0
4	A	1214	OLA	1	0
4	A	1204	OLA	1	0
4	A	1218	OLA	2	0
4	A	1206	OLA	4	0
4	A	1220	OLA	6	0

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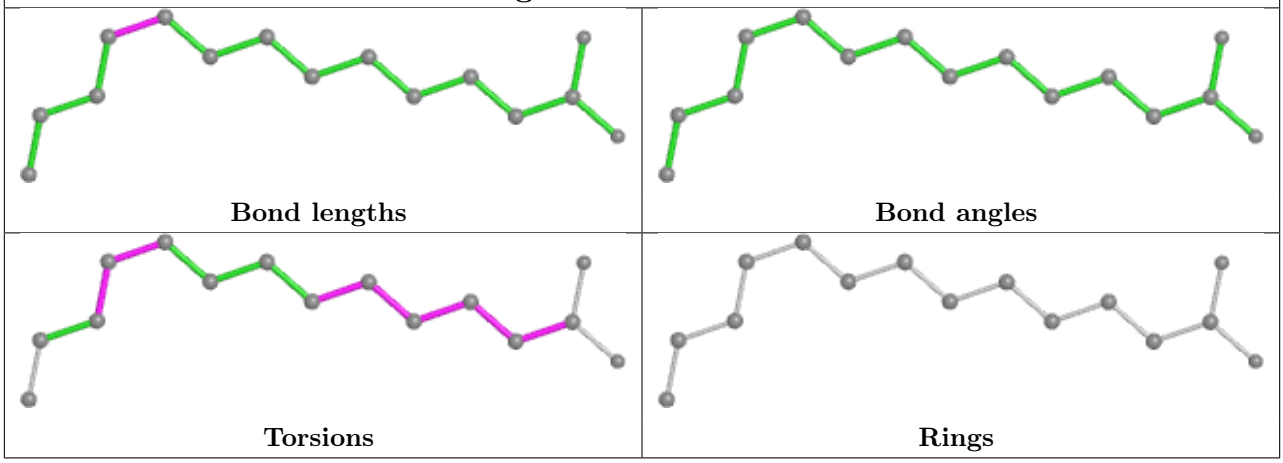
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1210	OLA	1	0
4	A	1207	OLA	2	0

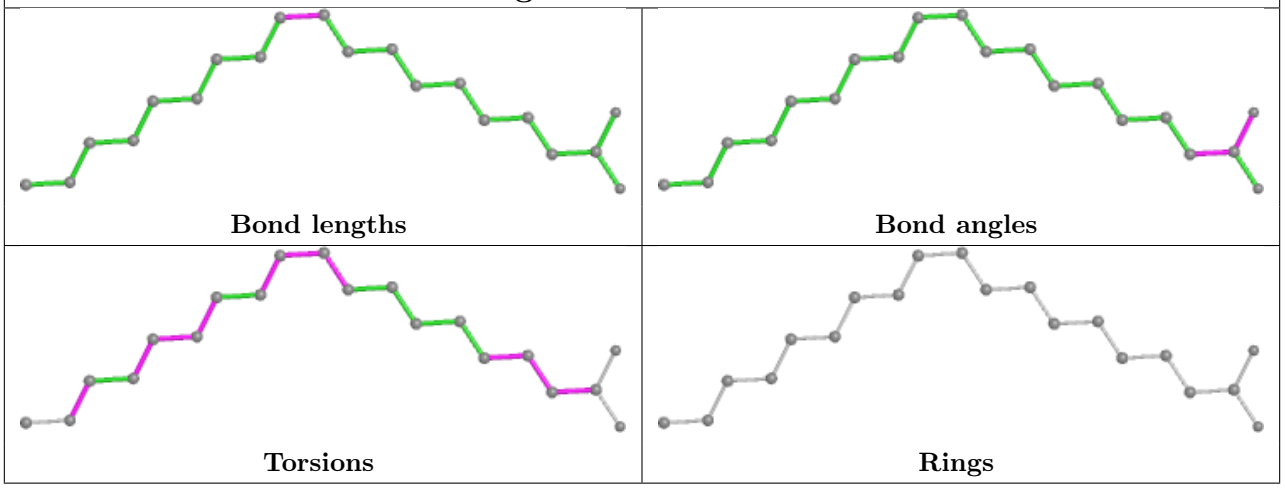
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 OLA A 1215

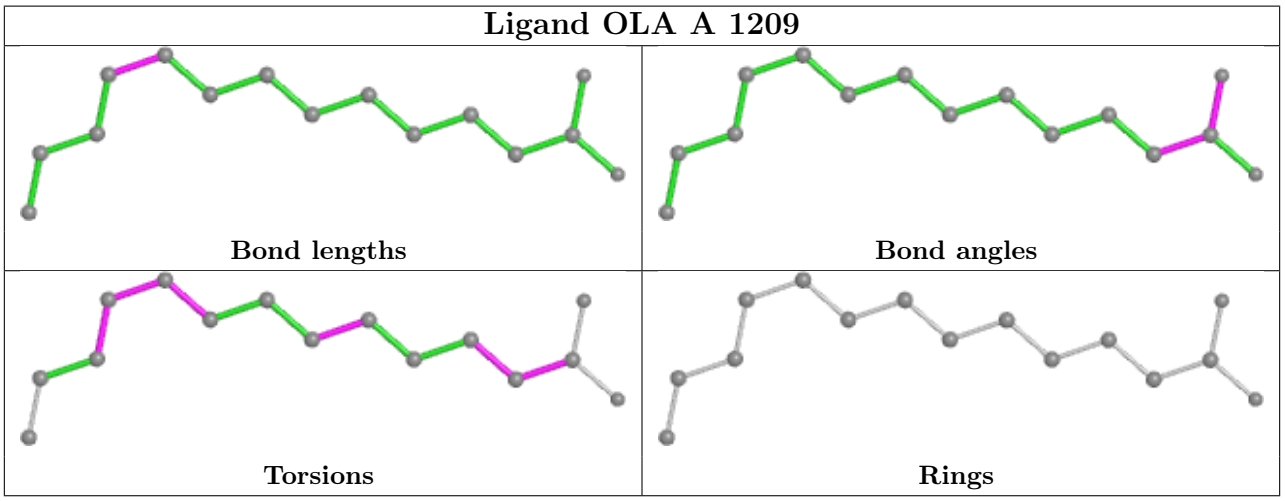


Ligand OLA A 1208

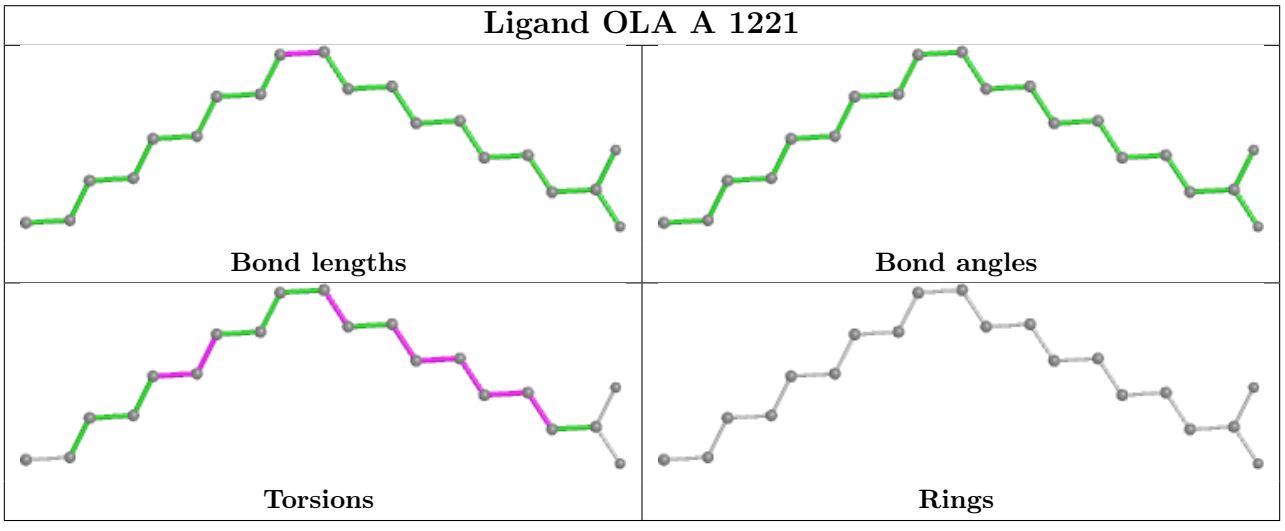
Ligand OLA A 1217



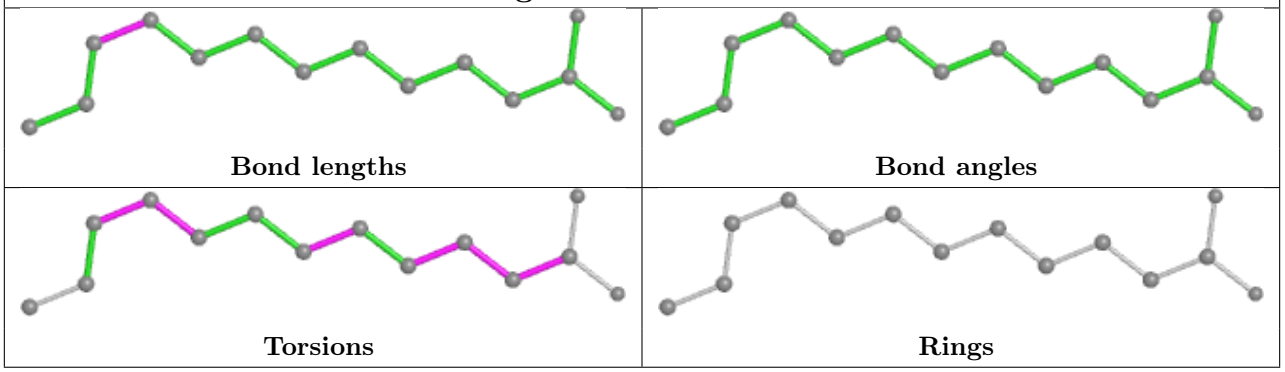
Ligand OLA A 1209



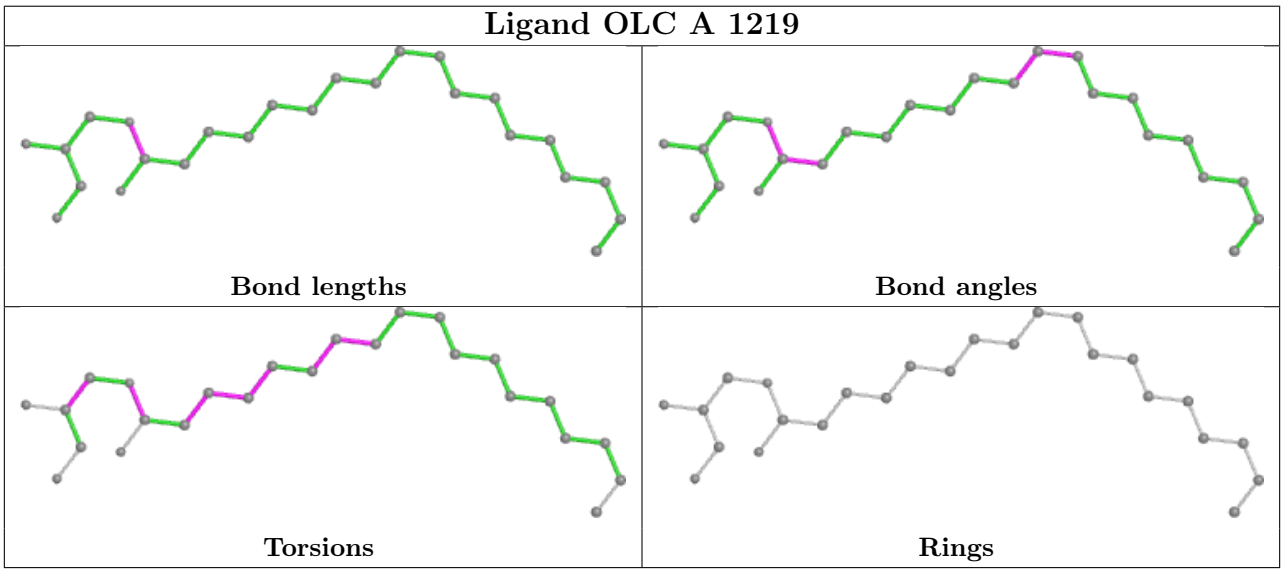
Ligand OLA A 1221



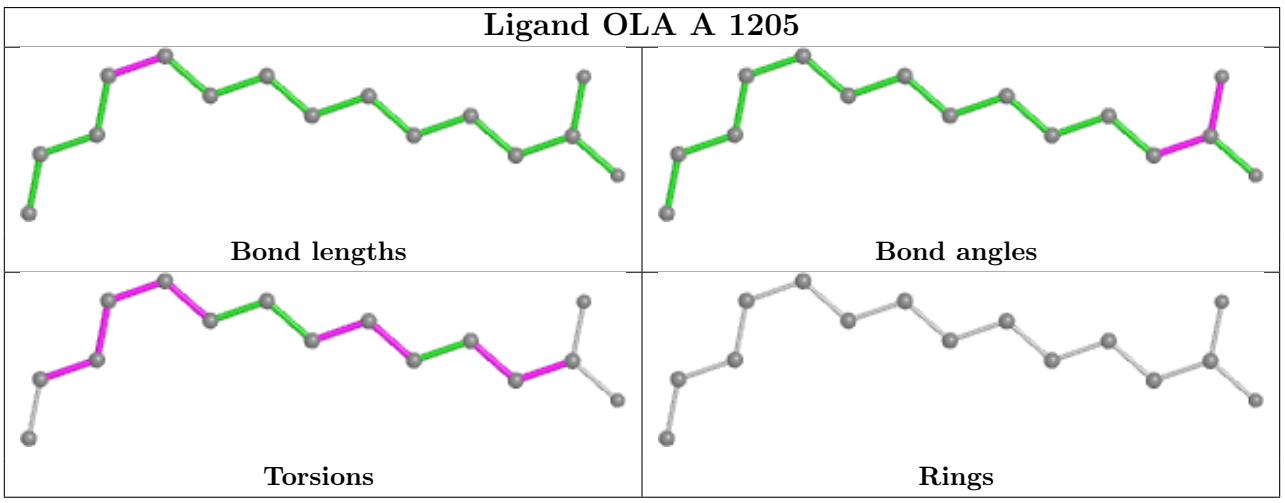
Ligand OLA A 1222



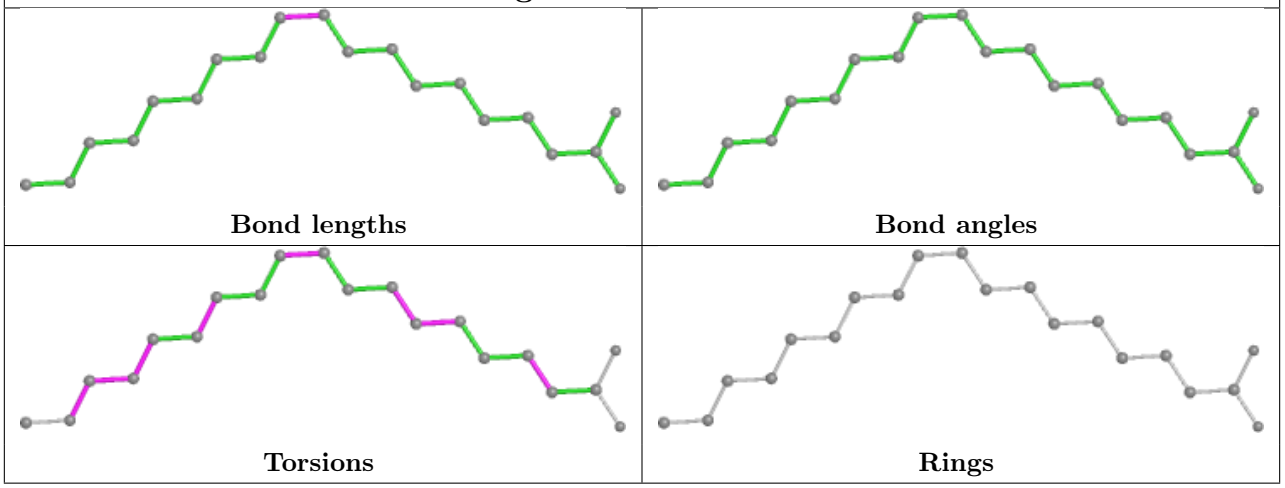
Ligand OLC A 1219



Ligand OLA A 1205



Ligand OLA A 1212



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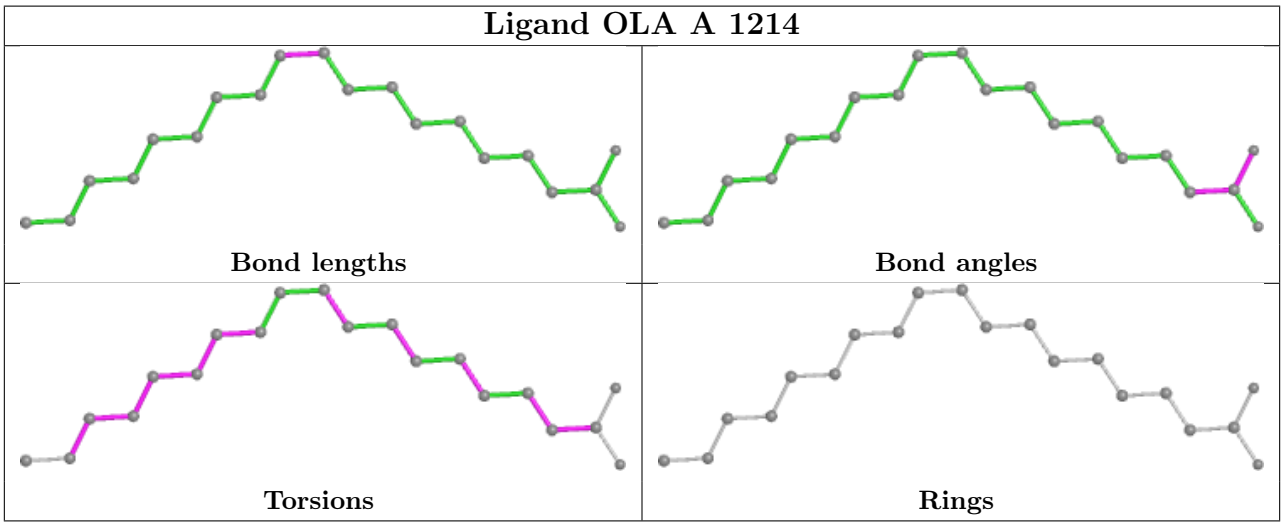

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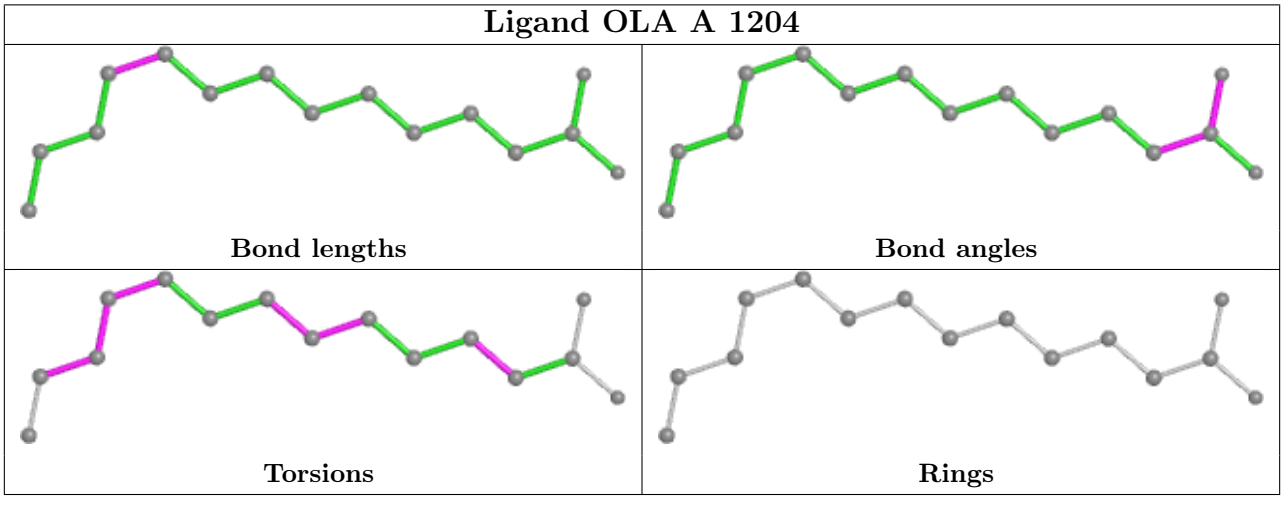
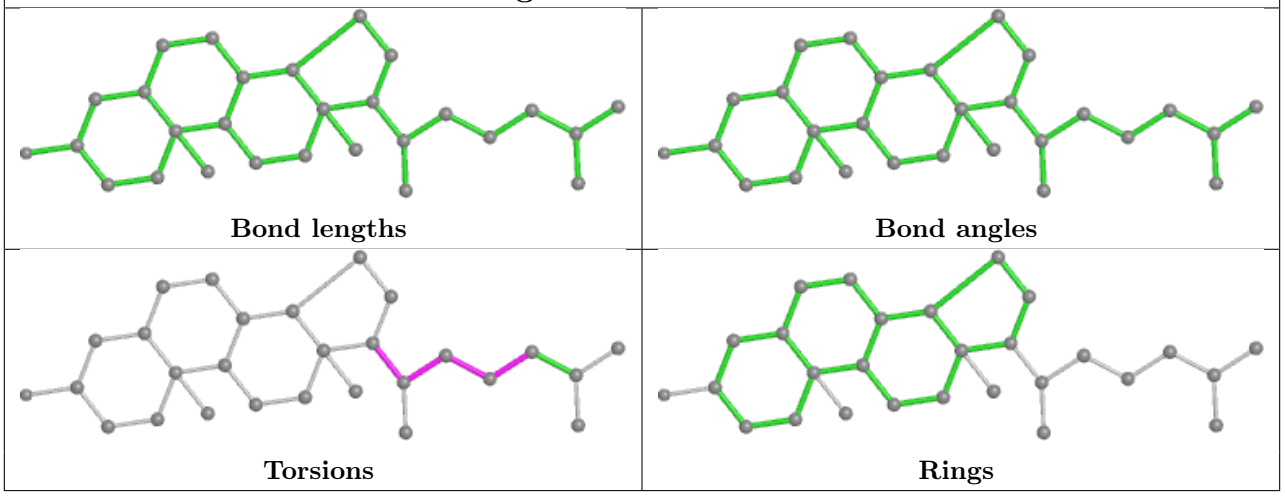
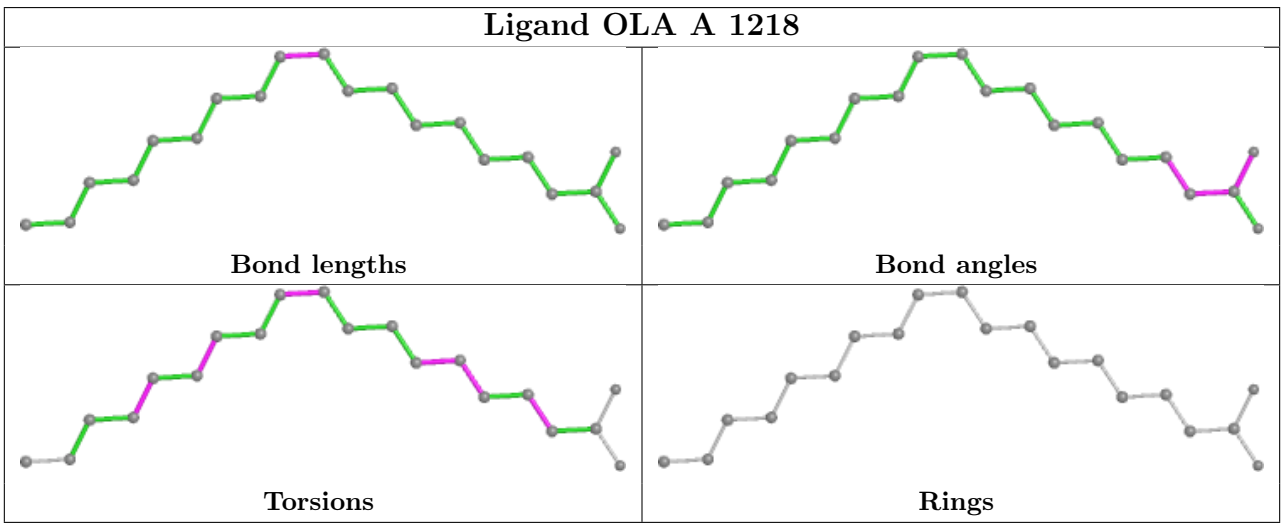


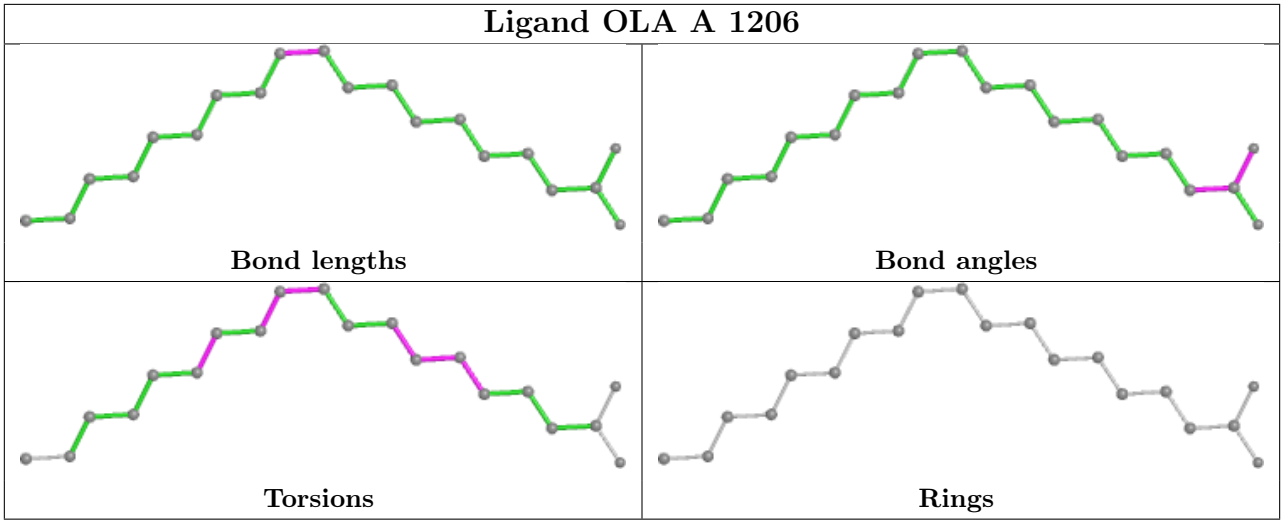
Ligand CLR A 1202



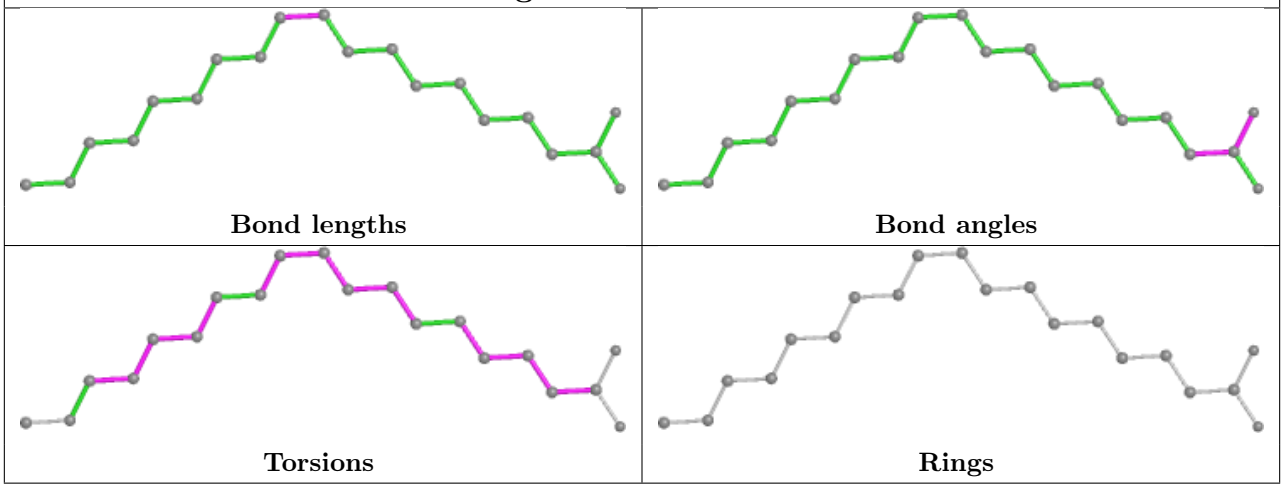
Ligand OLA A 1218



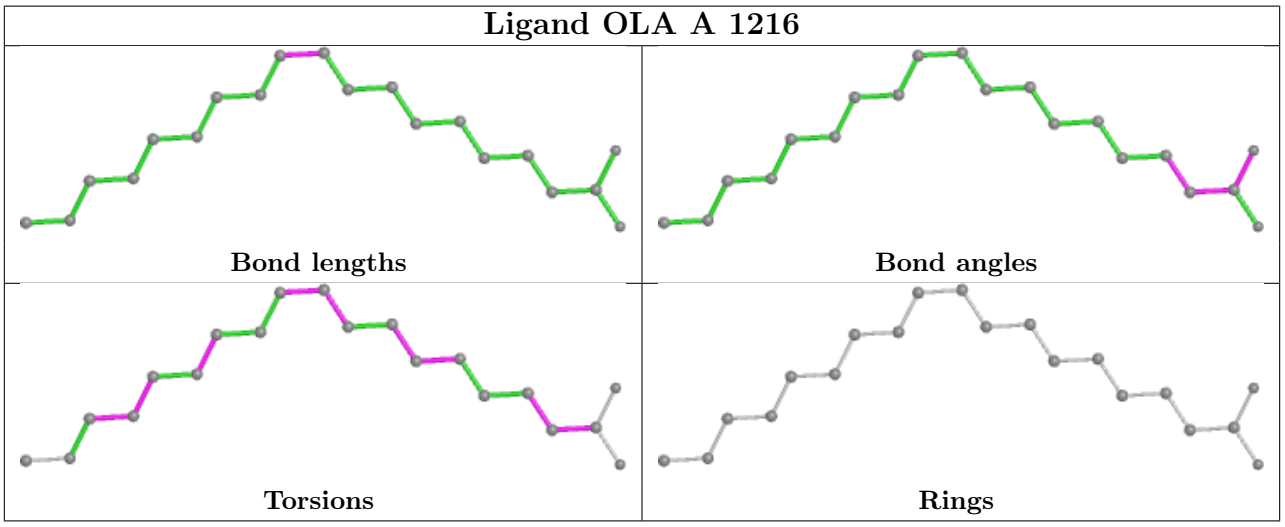
Ligand OLA A 1206



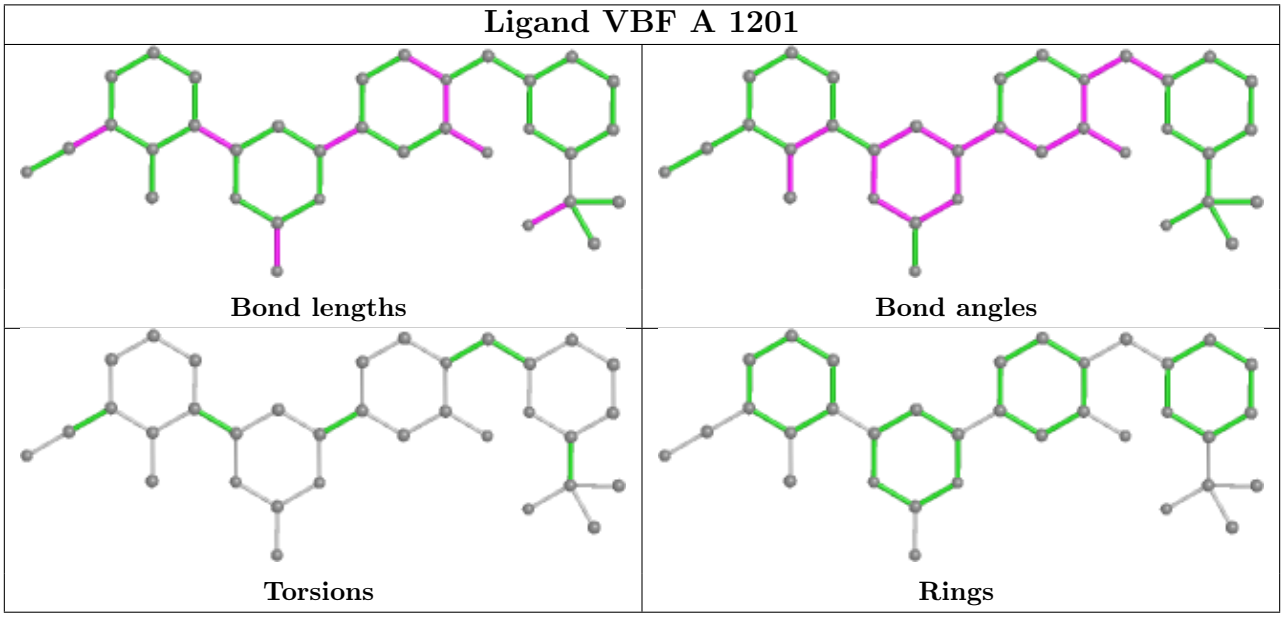
Ligand OLA A 1220



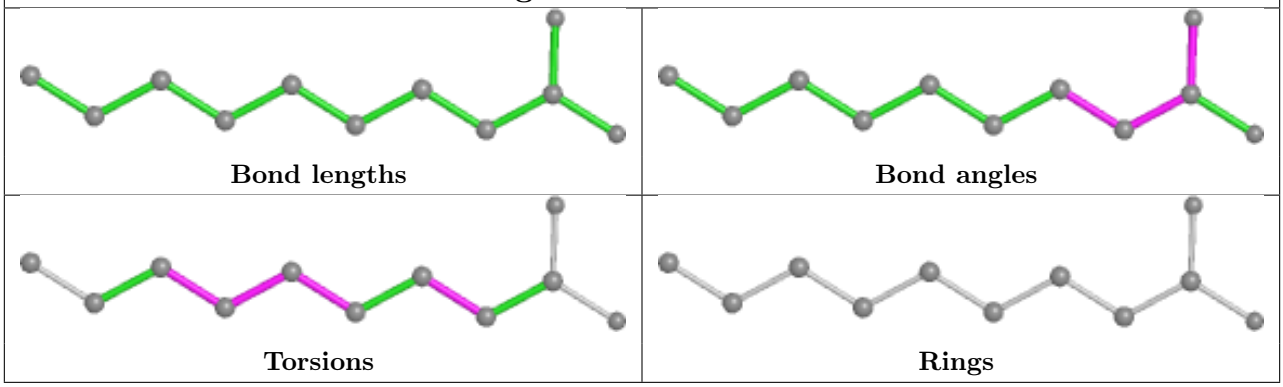
Ligand OLA A 1216



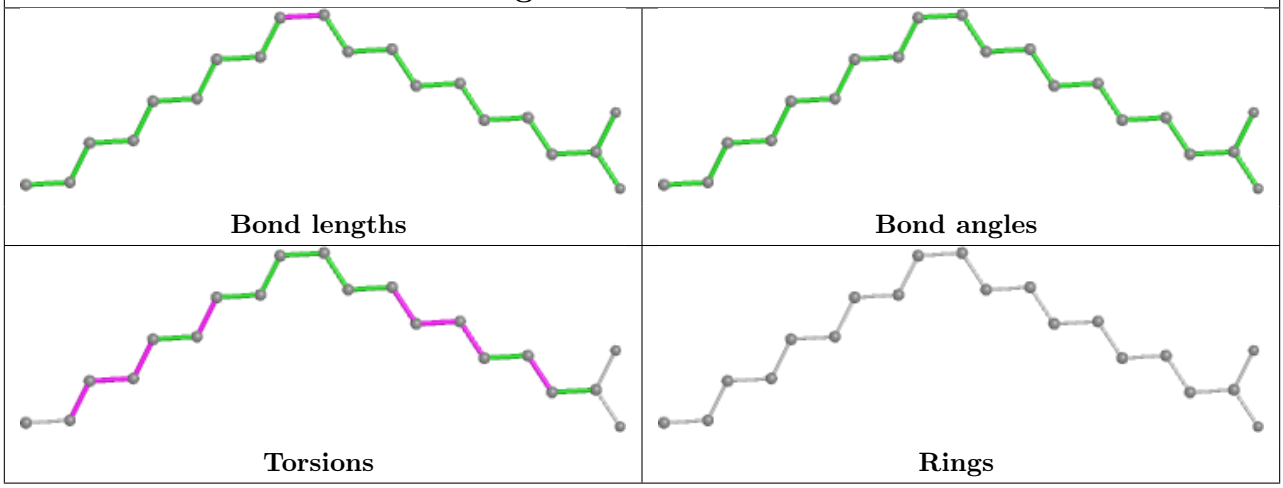
Ligand VBF A 1201



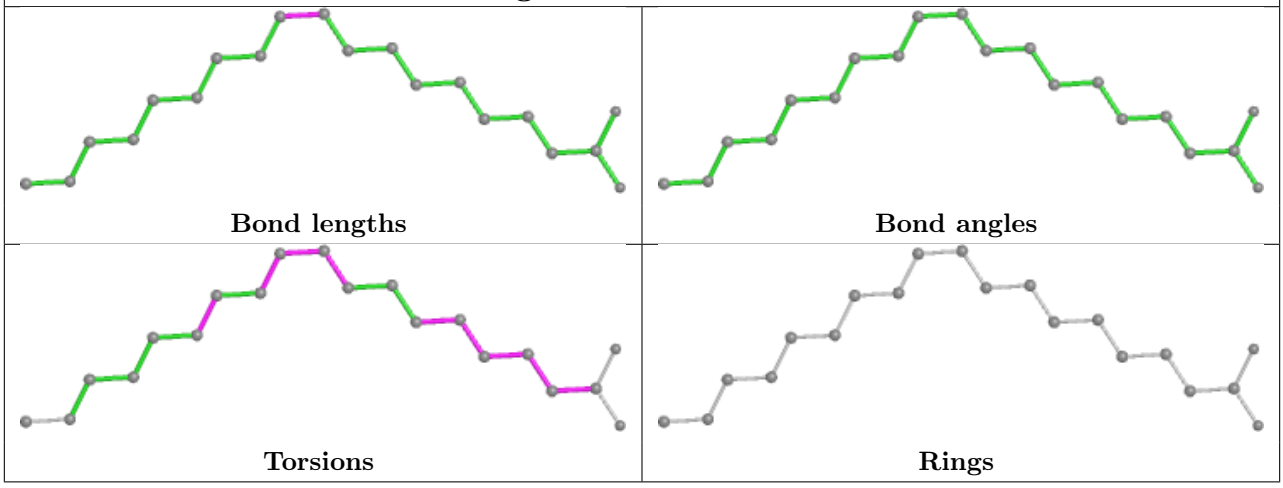
Ligand OLA A 1203

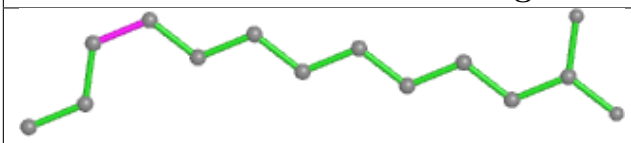
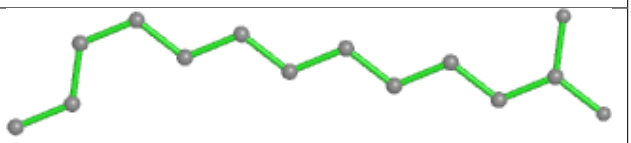
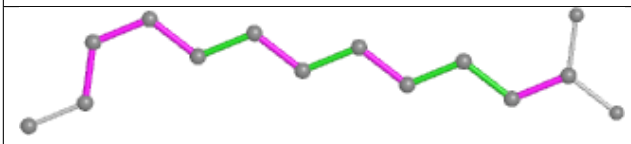
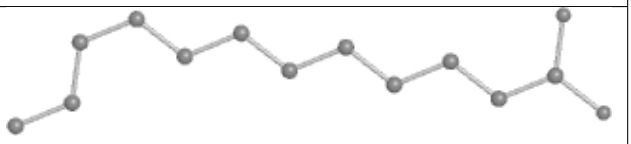


Ligand OLA A 1210



Ligand OLA A 1207



Ligand OLA A 1213	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	448/481 (93%)	0.19	23 (5%) 28 39	22, 35, 60, 83	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	SER	5.2
1	A	147	GLY	4.8
1	A	457	GLN	4.8
1	A	229	GLU	4.4
1	A	228	THR	4.1
1	A	231	TYR	4.1
1	A	148	GLN	3.6
1	A	437	TYR	3.4
1	A	4	MET	3.2
1	A	344	ARG	3.1
1	A	98	ILE	3.0
1	A	230	GLY	2.8
1	A	157	GLN	2.6
1	A	227	ASP	2.5
1	A	110	LEU	2.5
1	A	81	ALA	2.5
1	A	374	LYS	2.3
1	A	342	LYS	2.2
1	A	45	VAL	2.2
1	A	347	ASN	2.2
1	A	85	LEU	2.1
1	A	408	ASP	2.1
1	A	377	HIS	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)

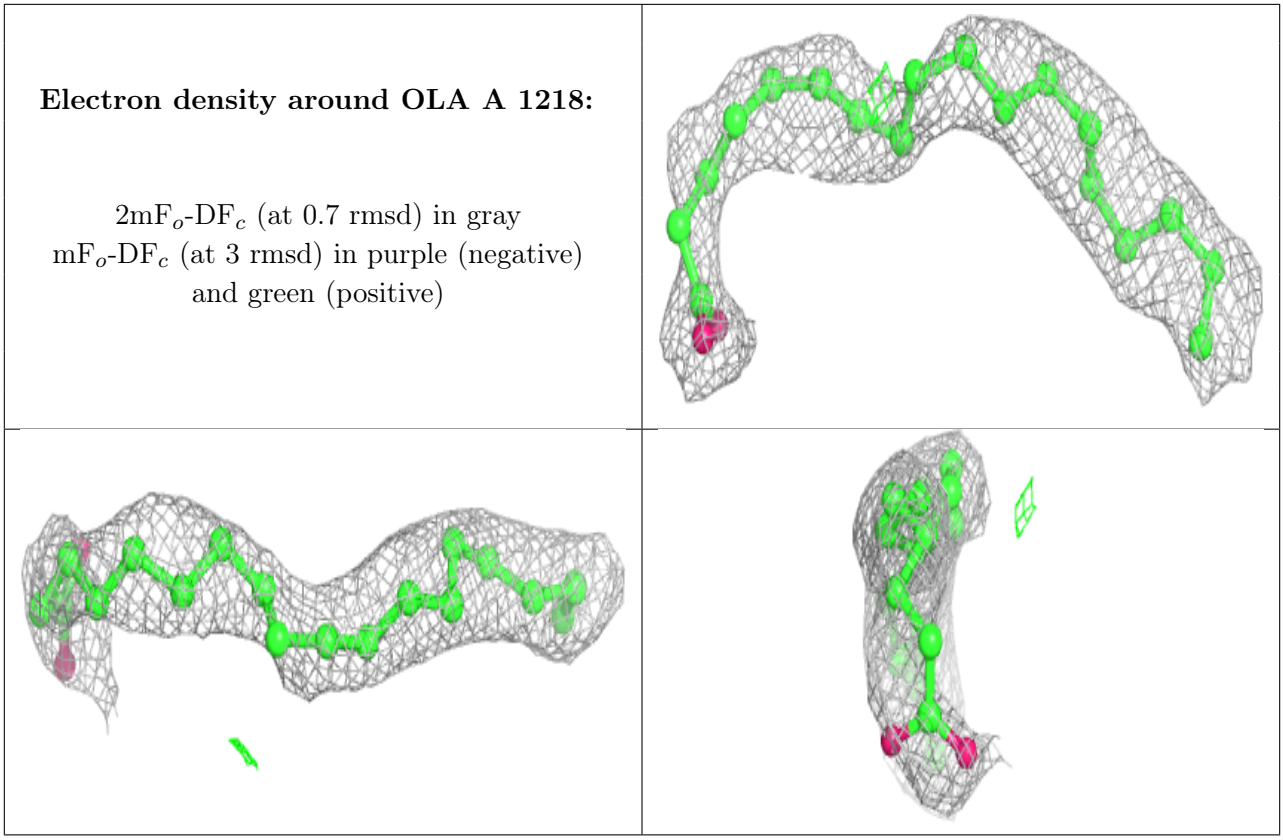
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	OLA	A	1218	20/20	0.72	0.22	35,50,83,84	0
4	OLA	A	1217	20/20	0.75	0.34	43,53,65,67	0
4	OLA	A	1216	20/20	0.76	0.32	43,55,79,82	0
4	OLA	A	1213	14/20	0.77	0.40	61,68,86,94	0
4	OLA	A	1220	20/20	0.77	0.25	34,44,60,67	0
4	OLA	A	1222	14/20	0.77	0.46	52,59,77,84	0
6	OLC	A	1219	25/25	0.77	0.31	41,55,66,70	0
4	OLA	A	1215	15/20	0.81	0.35	39,46,62,62	0
4	OLA	A	1210	20/20	0.82	0.23	35,43,56,59	0
3	CLR	A	1202	28/28	0.82	0.20	41,53,59,61	0
4	OLA	A	1206	20/20	0.82	0.21	33,43,58,69	0
4	OLA	A	1207	20/20	0.84	0.31	36,51,69,78	0
4	OLA	A	1204	15/20	0.84	0.22	39,46,52,53	0
4	OLA	A	1209	15/20	0.85	0.26	40,48,54,55	0
4	OLA	A	1221	20/20	0.85	0.31	42,48,56,71	0
4	OLA	A	1214	20/20	0.86	0.18	34,41,64,69	0
4	OLA	A	1212	20/20	0.88	0.23	41,46,65,68	0
4	OLA	A	1205	15/20	0.89	0.17	30,41,55,60	0
4	OLA	A	1208	11/20	0.89	0.15	35,39,52,57	0
4	OLA	A	1203	11/20	0.89	0.21	39,42,51,57	0
2	VBF	A	1201	34/34	0.94	0.18	22,28,31,35	0
5	NA	A	1211	1/1	0.98	0.09	31,31,31,31	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.

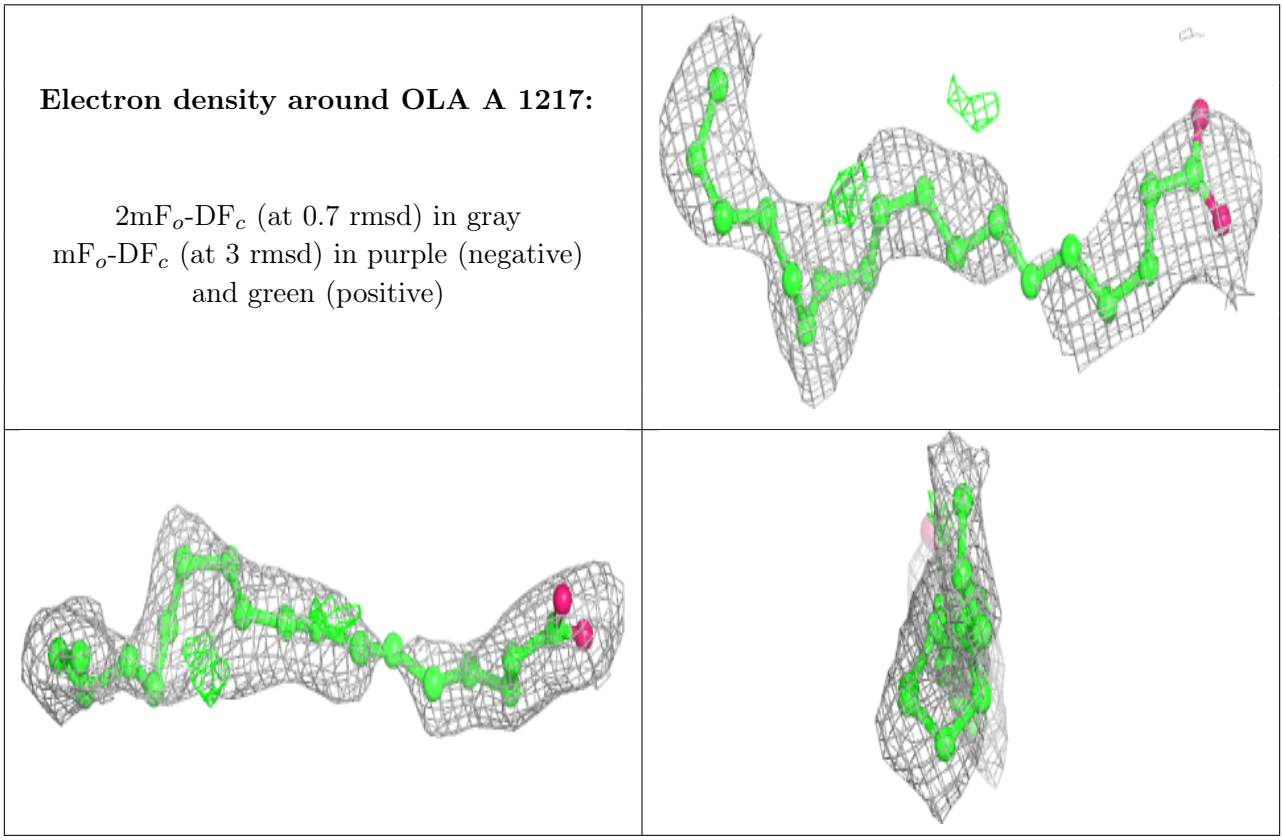
Electron density around OLA A 1218:

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



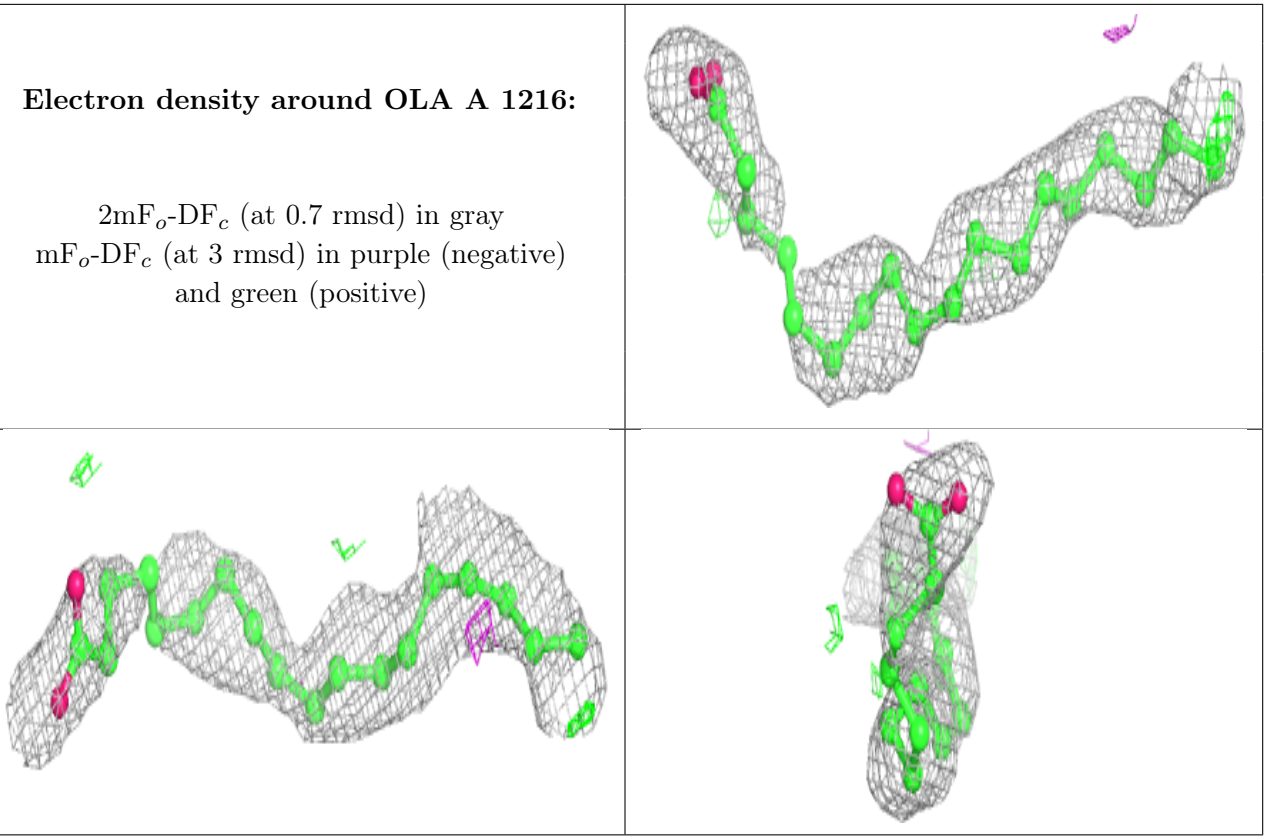
Electron density around OLA A 1217:

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



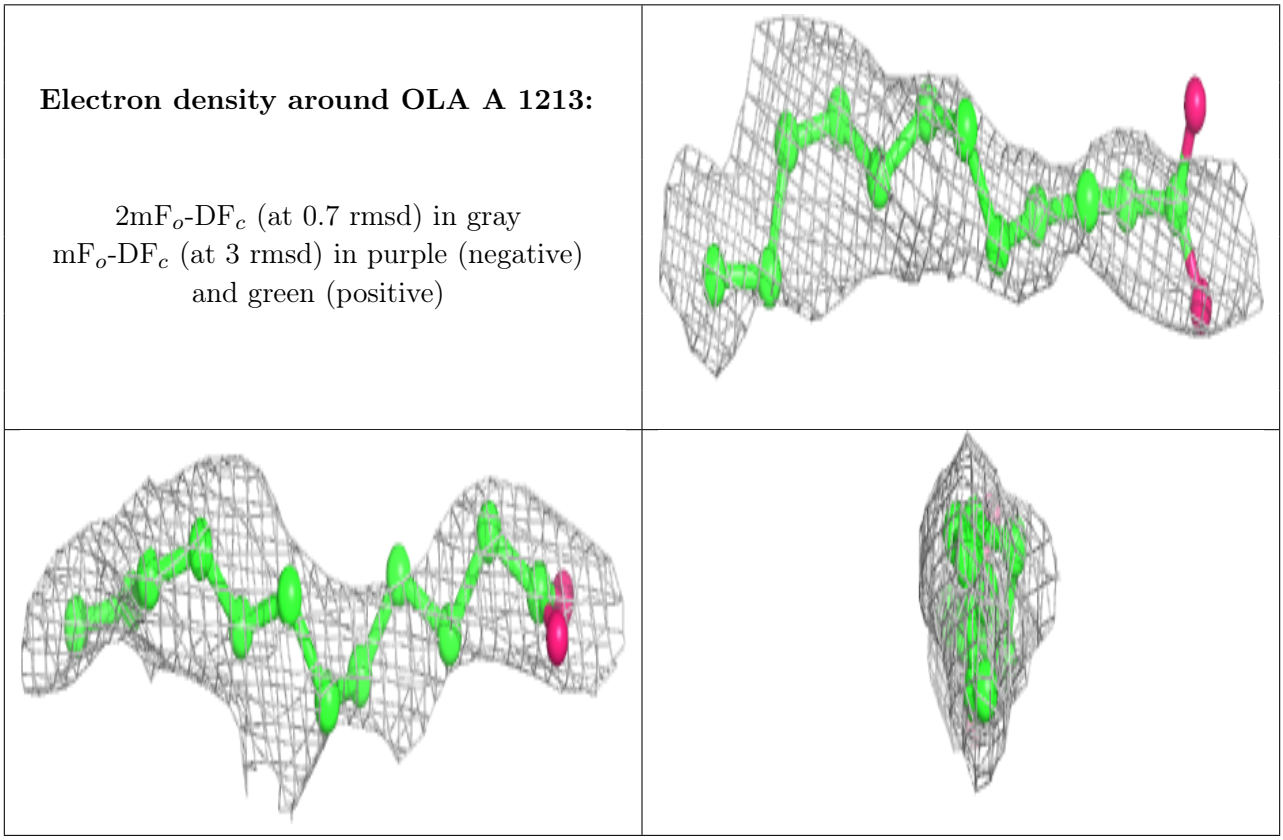
Electron density around OLA A 1216:

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



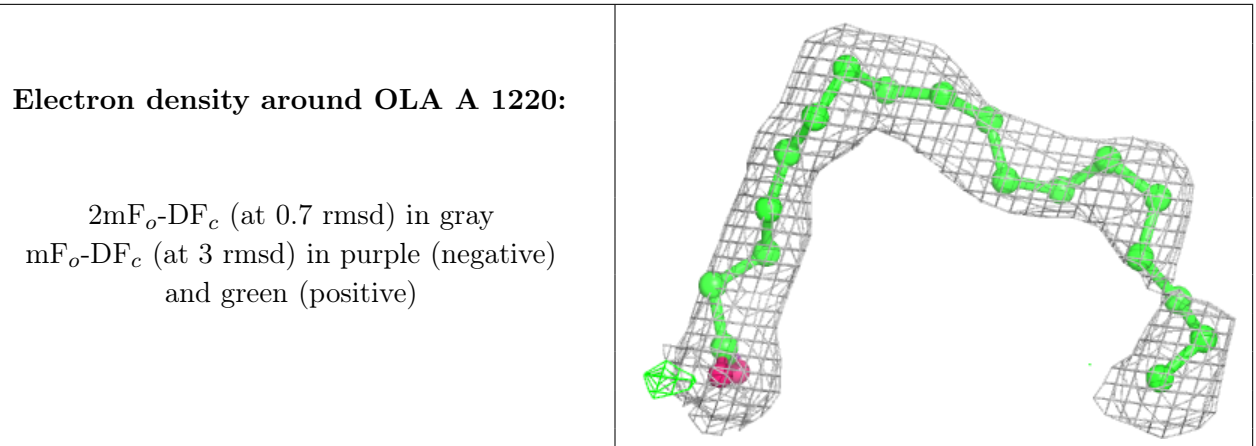
Electron density around OLA A 1213:

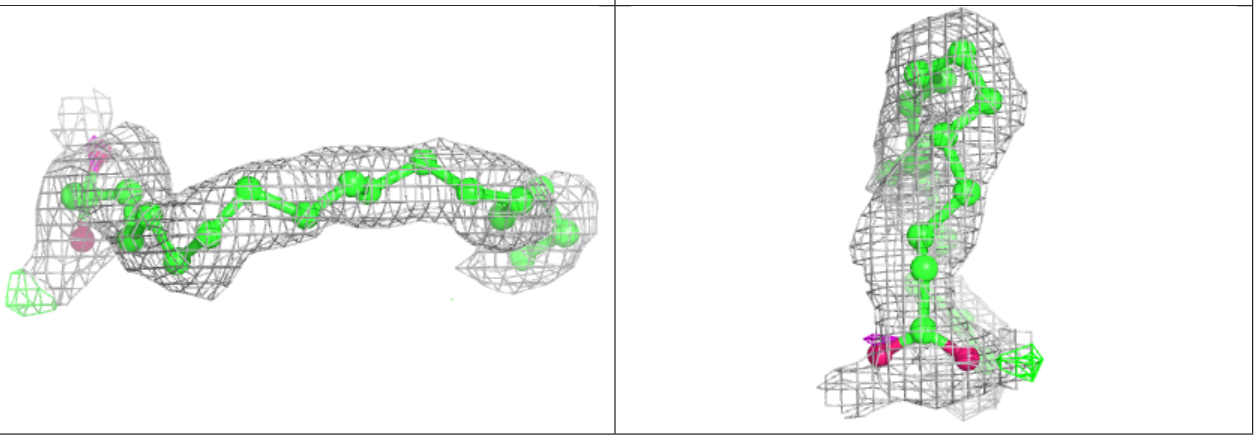
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA A 1220:

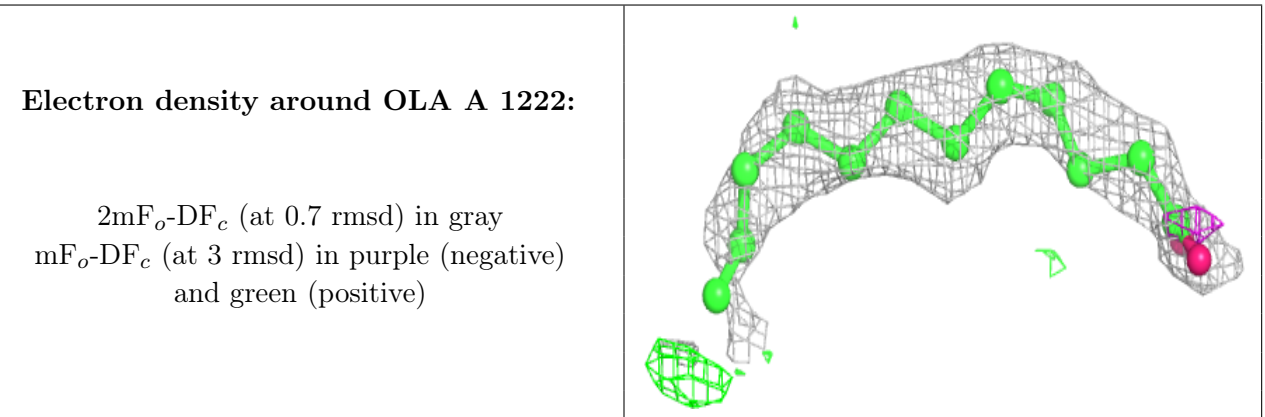
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

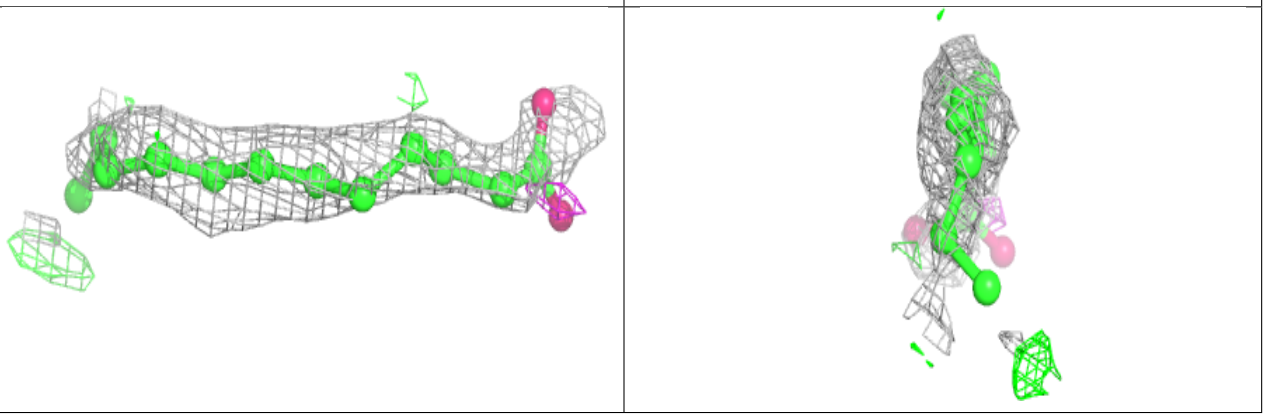




Electron density around OLA A 1222:

$2mF_o$-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 1219:

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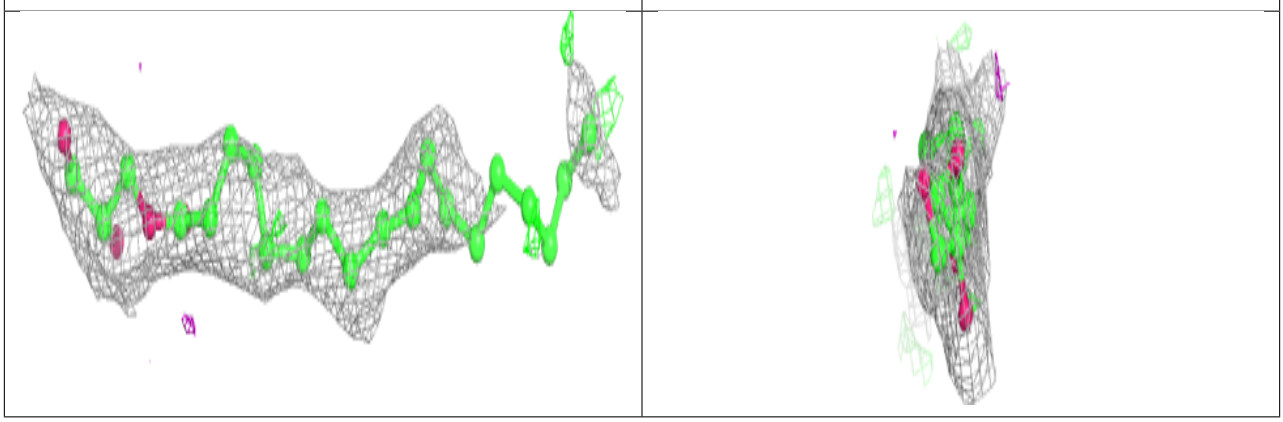
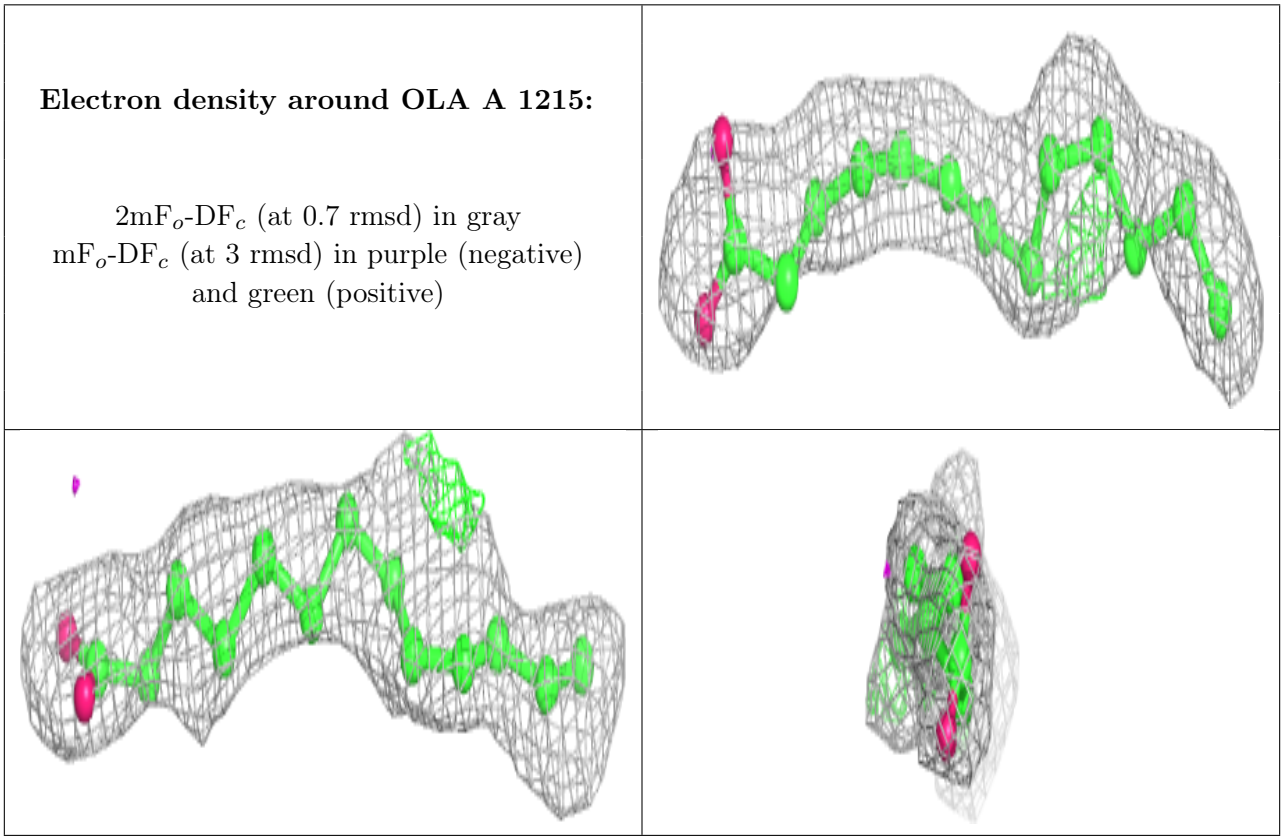
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



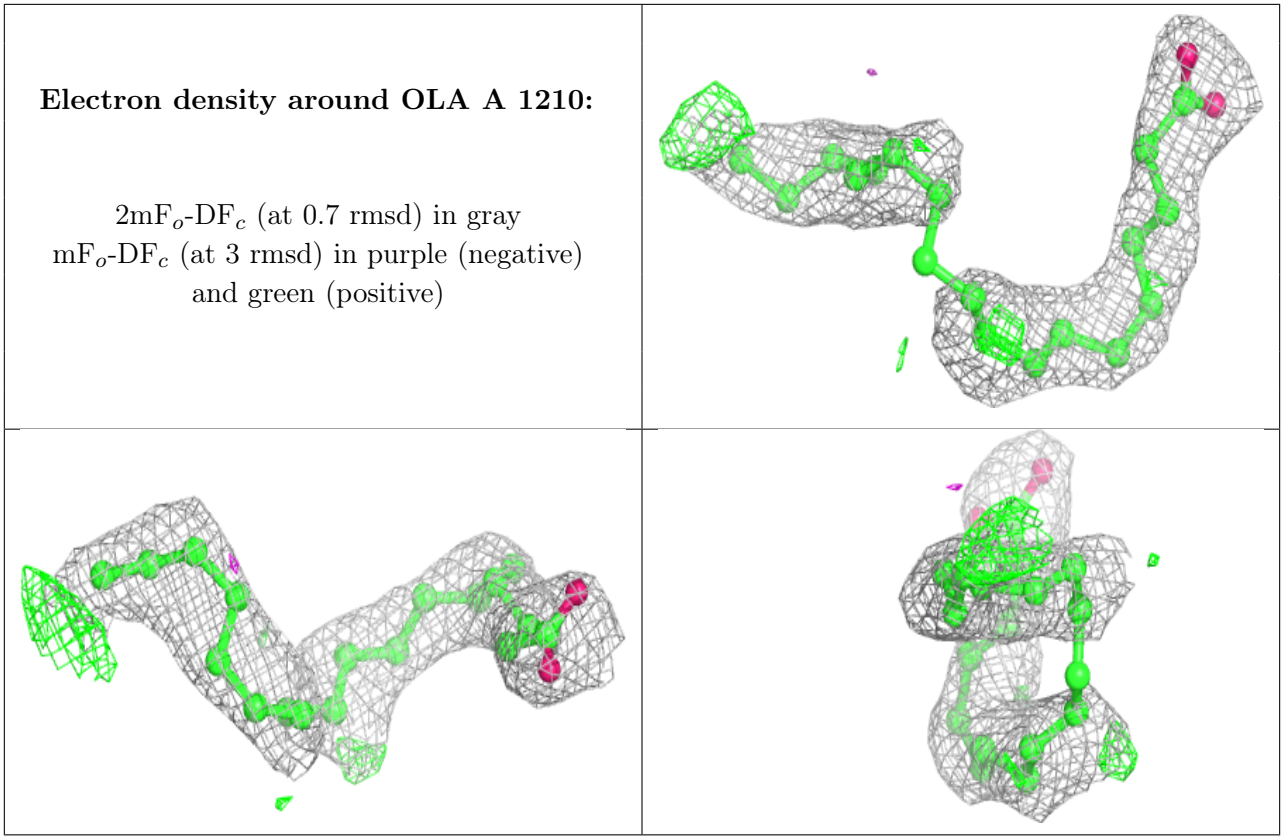
Electron density around OLA A 1215:

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



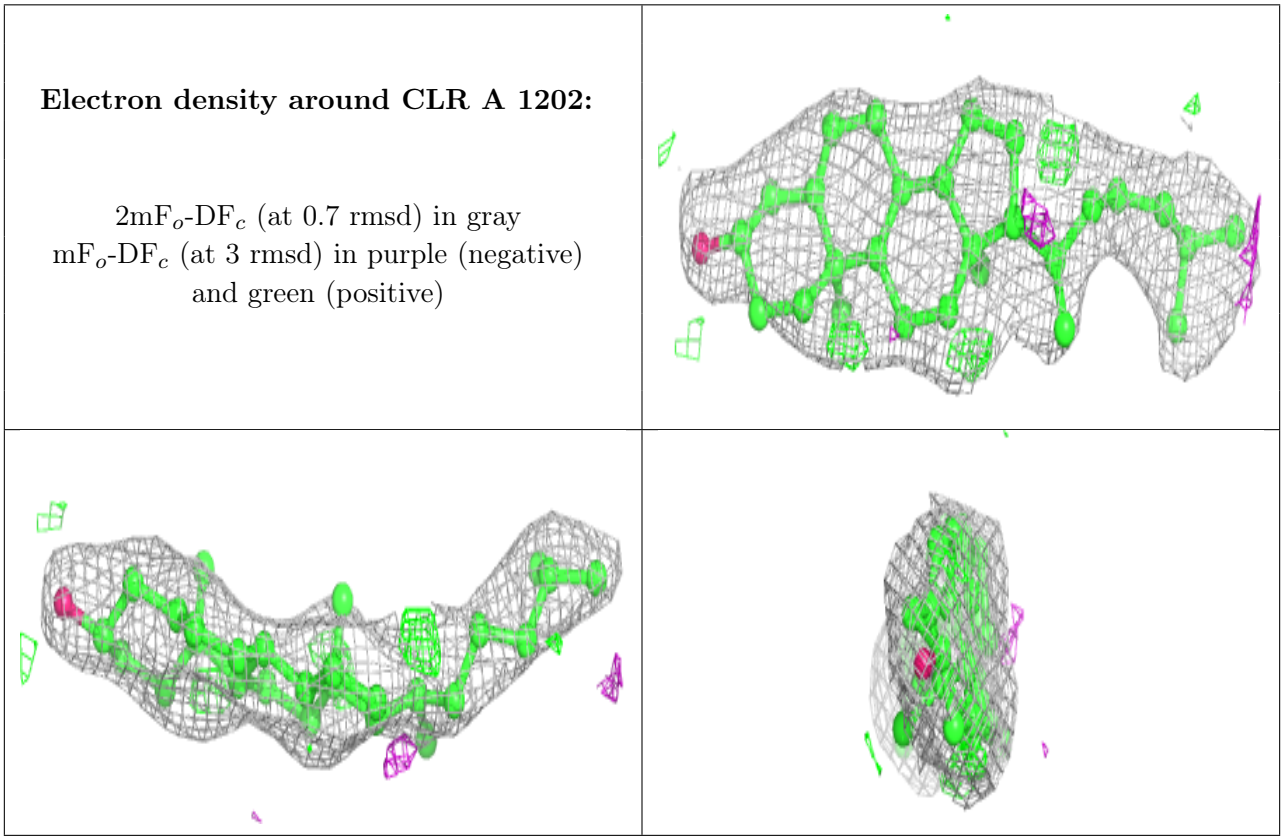
Electron density around OLA A 1210:

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



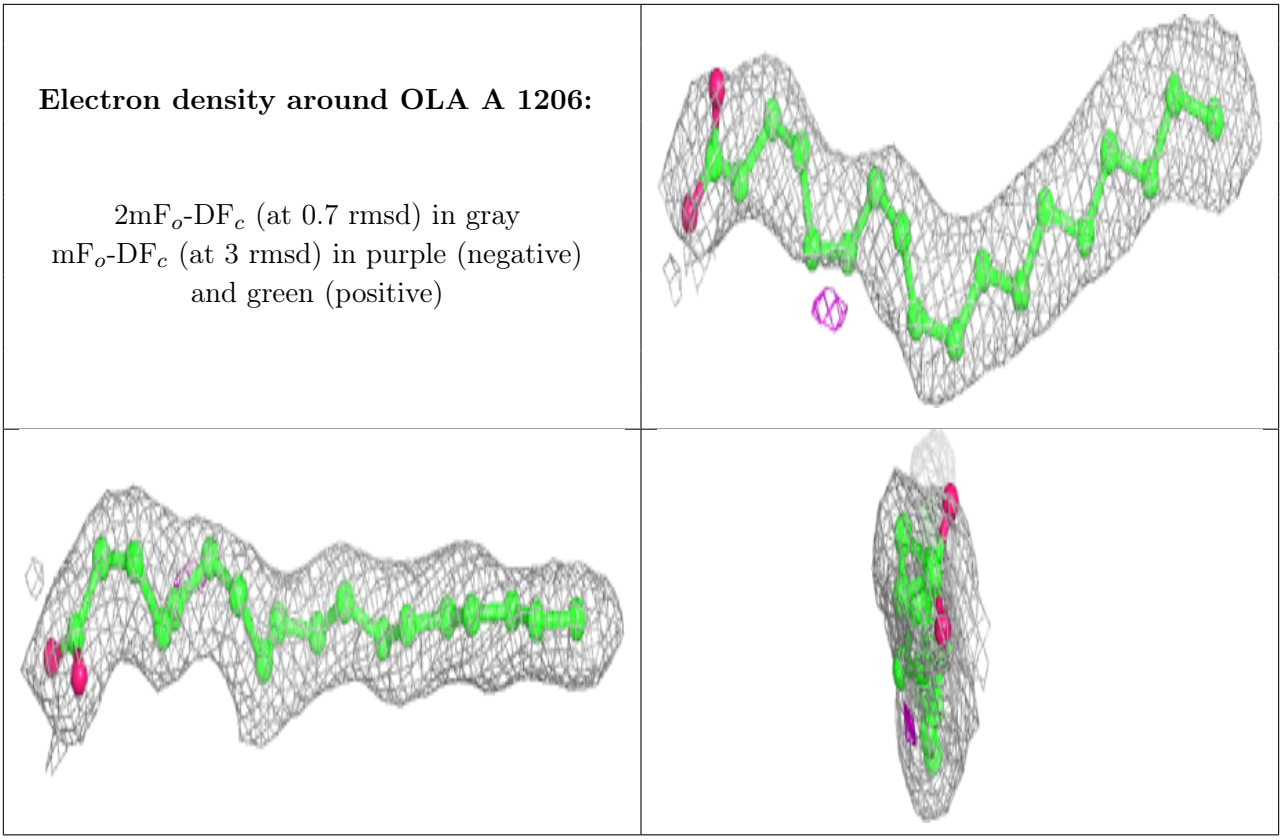
Electron density around CLR A 1202:

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



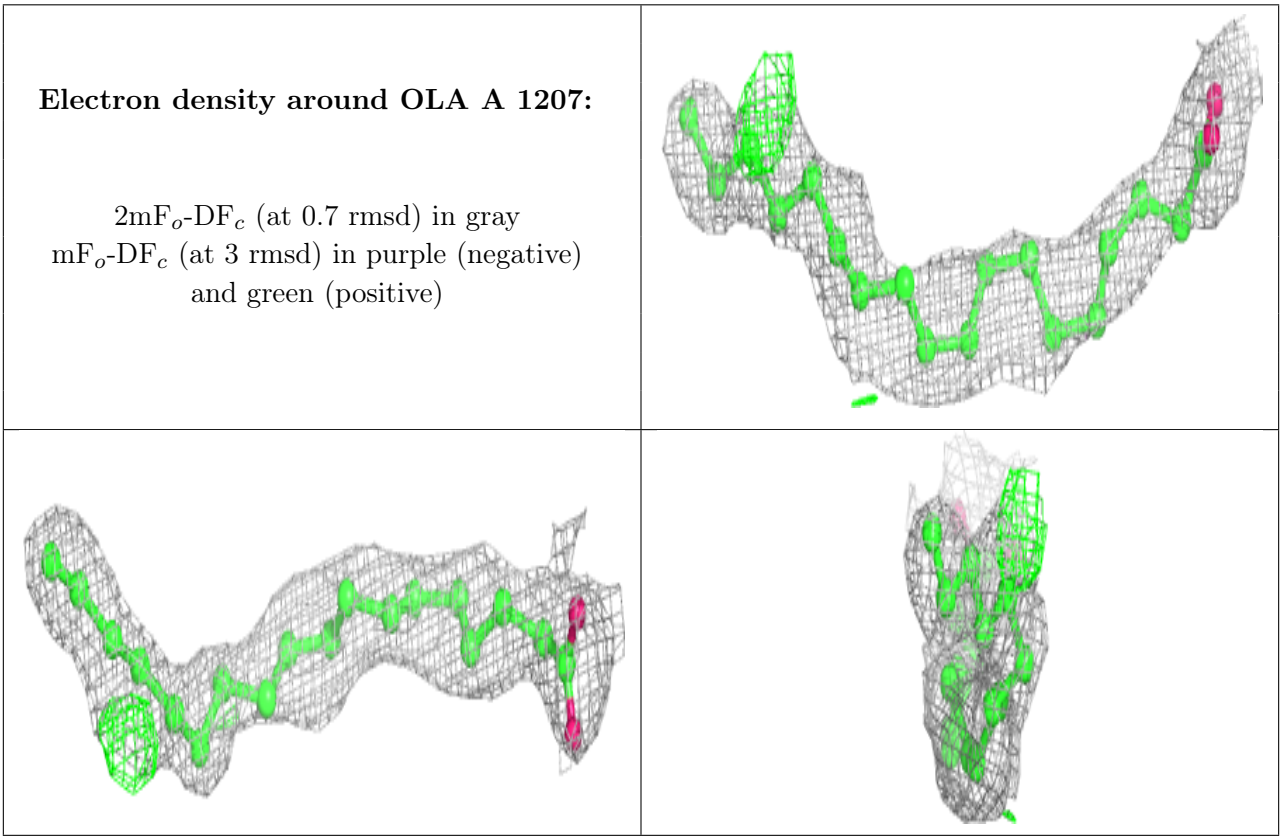
Electron density around OLA A 1206:

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



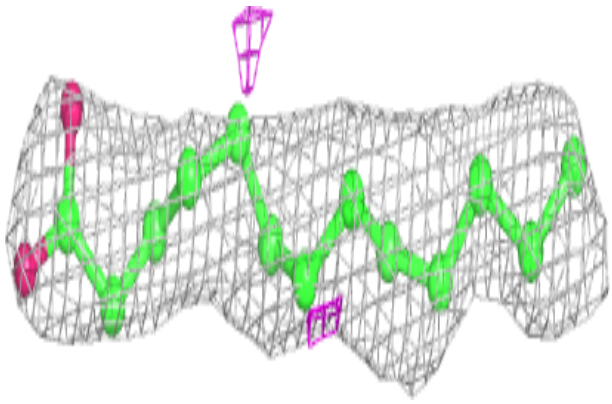
Electron density around OLA A 1207:

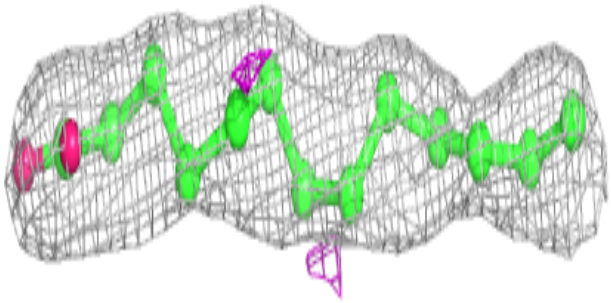
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

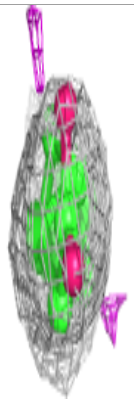


Electron density around OLA A 1204:

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

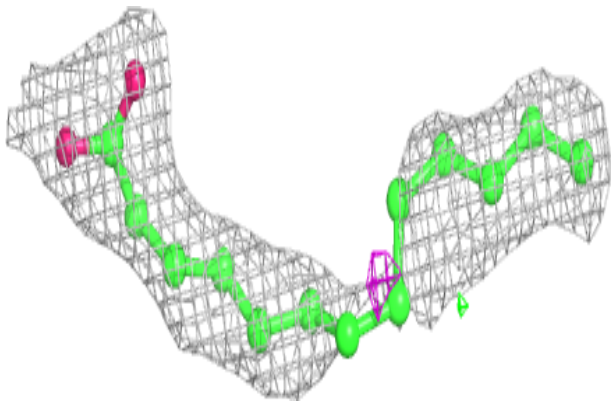


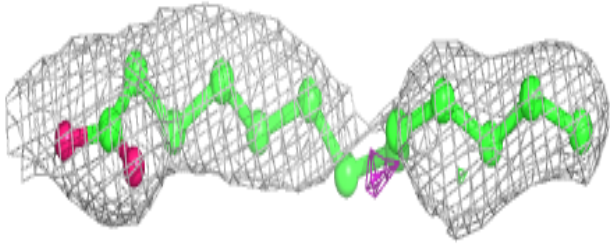


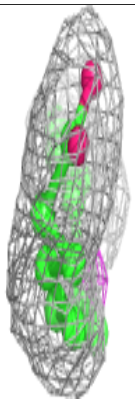


Electron density around OLA A 1209:

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

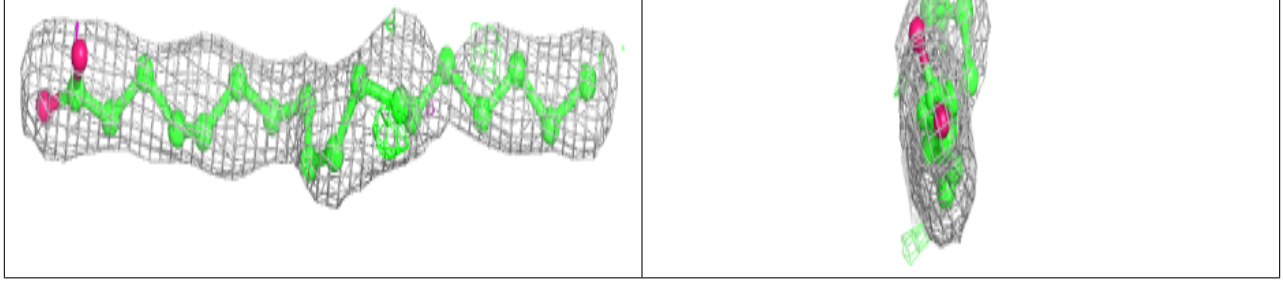






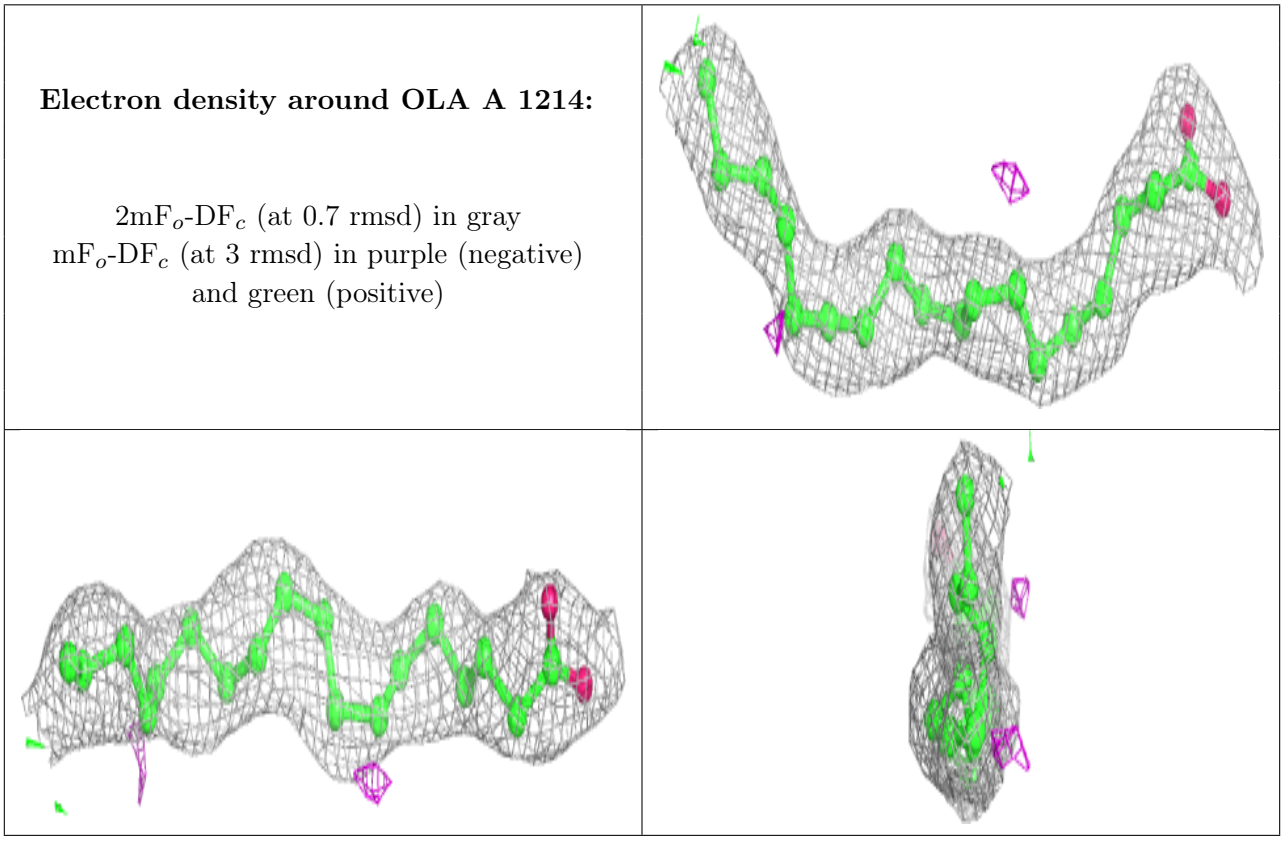
Electron density around OLA A 1221:

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



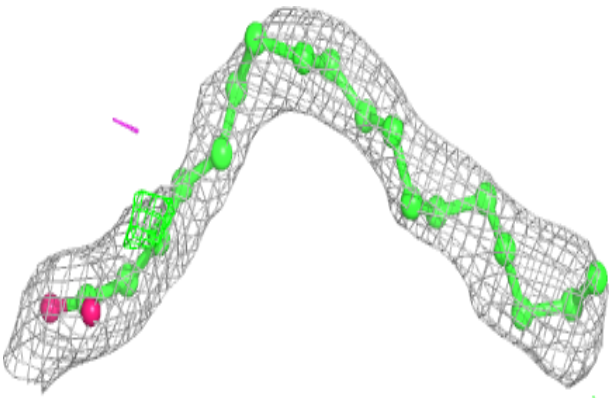
Electron density around OLA A 1214:

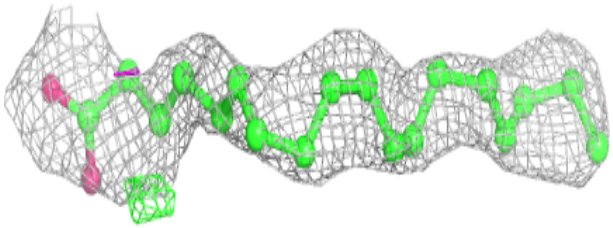
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

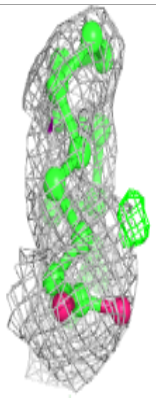


Electron density around OLA A 1212:

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

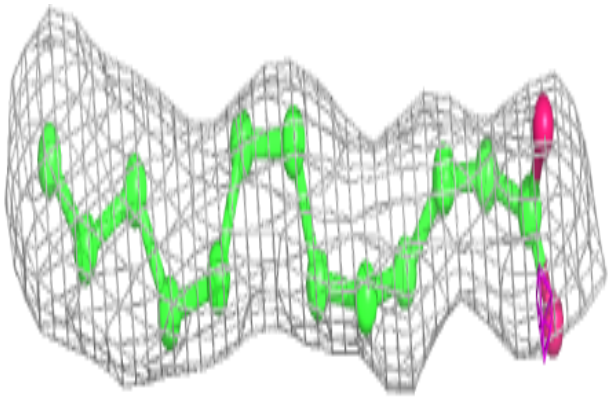


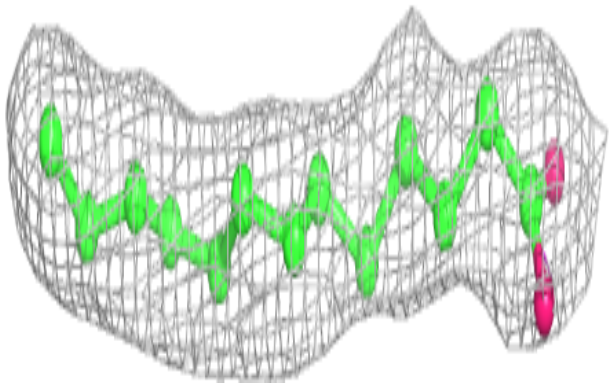


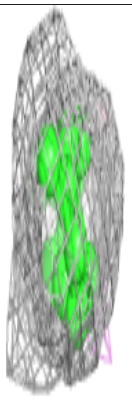


Electron density around OLA A 1205:

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

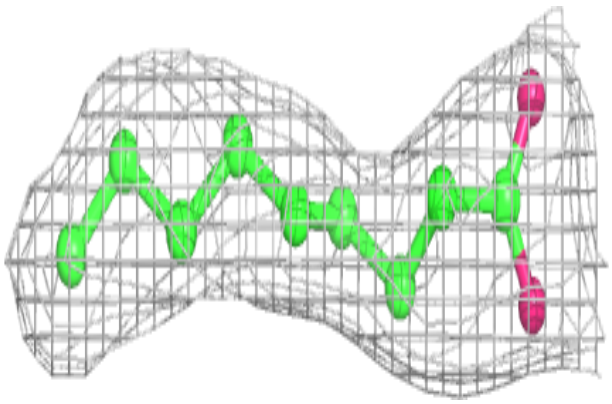


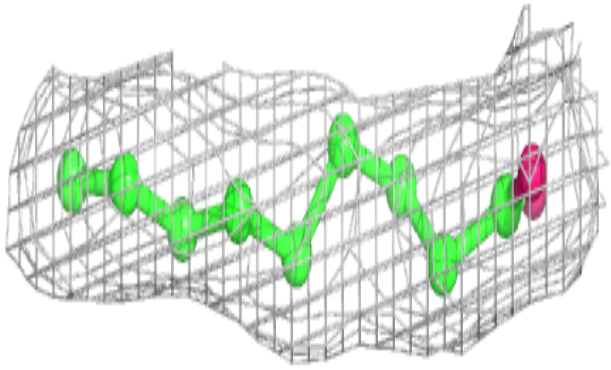


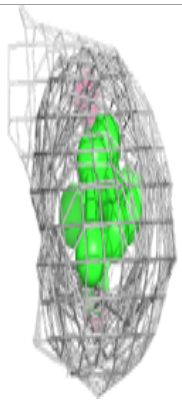


Electron density around OLA A 1208:

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

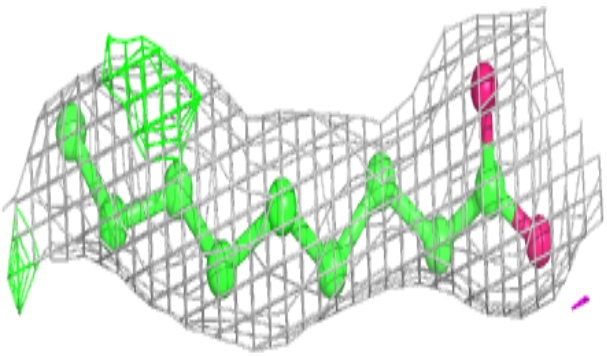


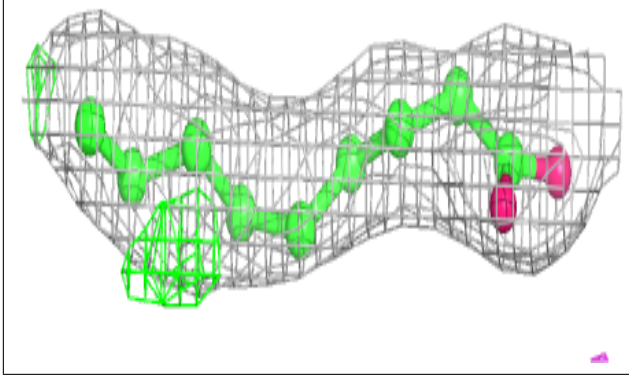


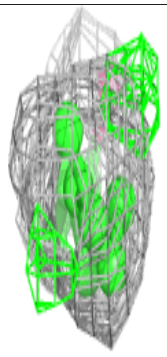


Electron density around OLA A 1203:

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

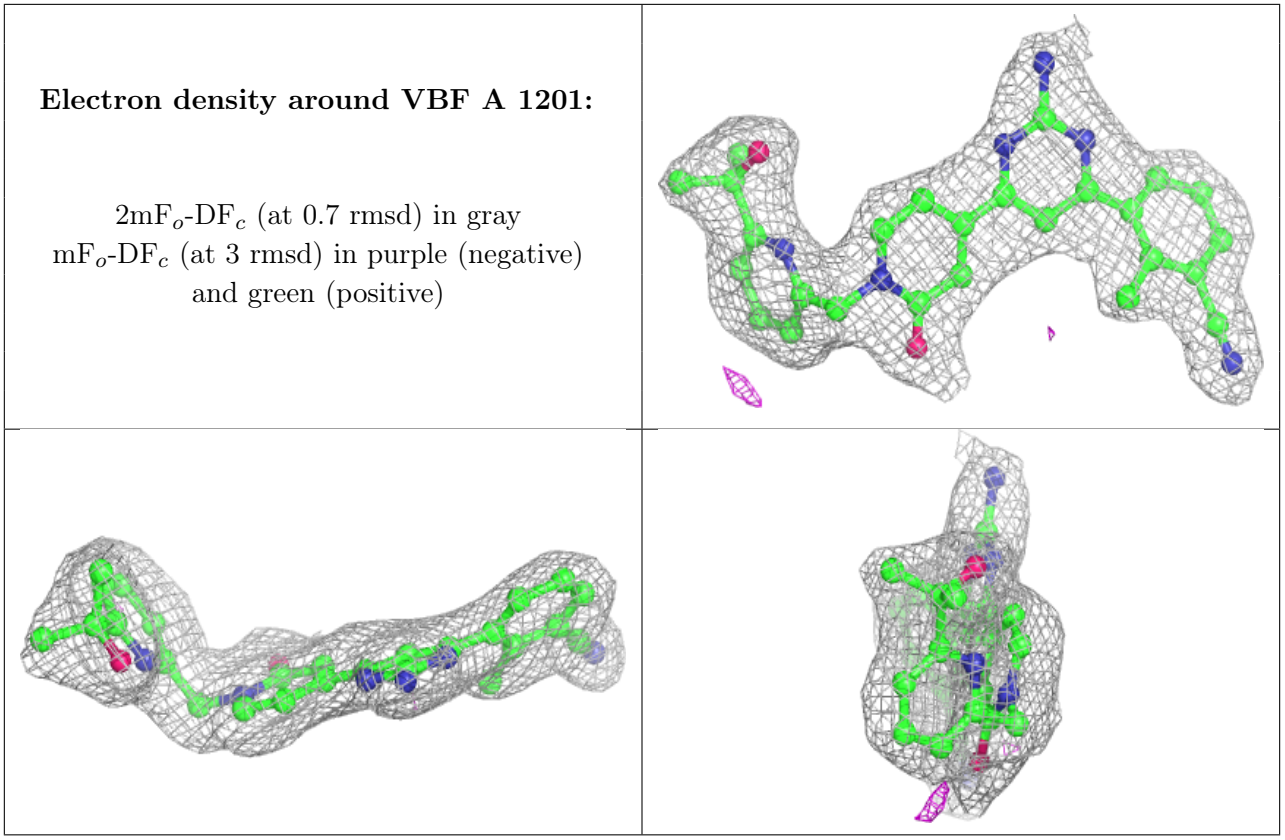






Electron density around VBF A 1201:

$2mF_o$-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

There are no such residues in this entry.