wwPDB X-ray Structure Validation Summary Report (i)

Aug 11, 2021 – 02:05 PM EDT

PDB ID	:	1LSH
Title	:	LIPID-PROTEIN INTERACTIONS IN LIPOVITELLIN
Authors	:	Thompson, J.R.; Banaszak, L.J.
Deposited on	:	2002-05-17
Resolution	:	1.90 Å(reported)

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

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

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

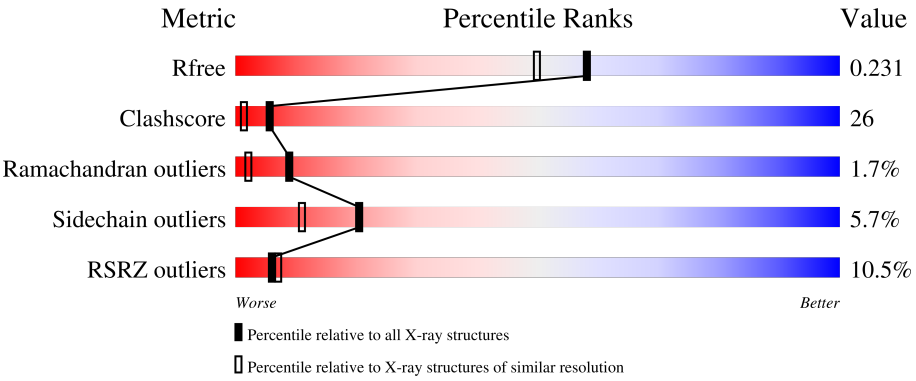
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	1056	7% 60% 26% · 10%
2	B	319	15% 26% 24% · · 45%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLD	A	2001[A]	X	-	-	-
3	PLD	A	2001[B]	X	-	-	-
3	PLD	A	2005[A]	X	-	-	-
3	PLD	A	2005[B]	X	-	-	-
3	PLD	A	2006	X	-	-	-
3	PLD	A	2007[A]	X	-	-	-
3	PLD	A	2007[B]	X	-	-	-
3	PLD	B	2003	-	X	-	-
4	UPL	A	2008	X	-	-	-
4	UPL	A	2009	X	-	-	-
4	UPL	A	2024	-	-	-	X
4	UPL	A	2047	-	-	-	X
4	UPL	A	2050	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10935 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 LIPOVITELLIN (LV-1N, LV-1C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	955	7781	4960	1362	1418	41	15	65	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLY	ALA	conflict	UNP Q91062
A	396	ALA	TYR	conflict	UNP Q91062
A	417	ASN	HIS	conflict	UNP Q91062
A	469	LYS	ASP	conflict	UNP Q91062
A	782	GLY	ARG	conflict	UNP Q91062
A	834	SER	HIS	conflict	UNP Q91062
A	?	-	GLN	deletion	UNP Q91062
A	1013	SER	HIS	conflict	UNP Q91062
A	1064	THR	GLN	conflict	UNP Q91062

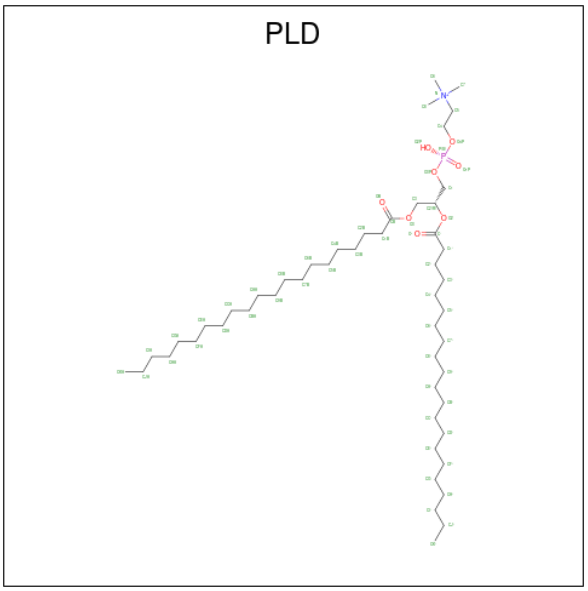
- Molecule 2 is a protein called LIPOVITELLIN (LV-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	174	1375	886	250	231	8	3	4	0

There are 2 discrepancies between the modelled and reference sequences:

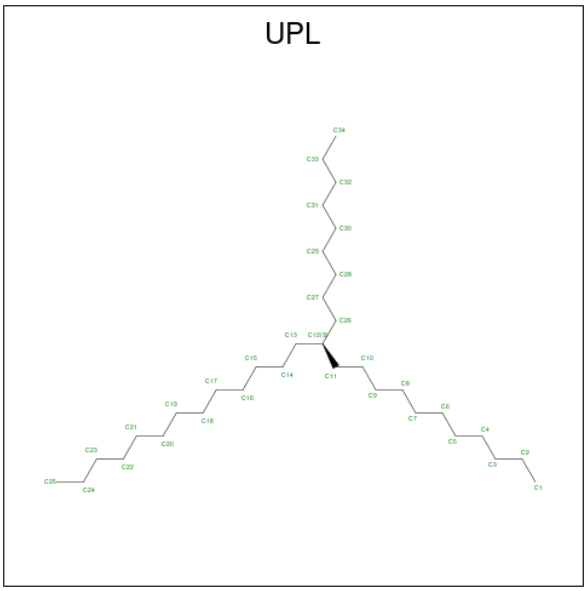
Chain	Residue	Modelled	Actual	Comment	Reference
B	1473	GLY	LYS	conflict	UNP Q91062
B	1489	ALA	LYS	conflict	UNP Q91062

- Molecule 3 is di-heneicosanoyl phosphatidyl choline (three-letter code: PLD) (formula: $C_{50}H_{101}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 57 47 1 8 1	0	1
3	A	1	Total C O P 35 26 8 1	0	0
3	A	1	Total C O P 34 25 8 1	0	0
3	A	1	Total C O P 53 44 8 1	0	1
3	A	1	Total C O P 34 25 8 1	0	0
3	A	1	Total C O P 40 31 8 1	0	1
3	B	1	Total C N O P 31 21 1 8 1	0	0

- Molecule 4 is UNKNOWN BRANCHED FRAGMENT OF PHOSPHOLIPID (three-letter code: UPL) (formula: $C_{34}H_{70}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 17 17	0	0
4	A	1	Total C 15 15	0	0
4	A	1	Total C 19 19	0	0
4	A	1	Total C 17 17	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 13 13	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 8 8	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 6 6	0	0
4	B	1	Total C 14 14	0	0
4	B	1	Total C 13 13	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 7 7	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 6 6	0	0

- Molecule 5 is water.

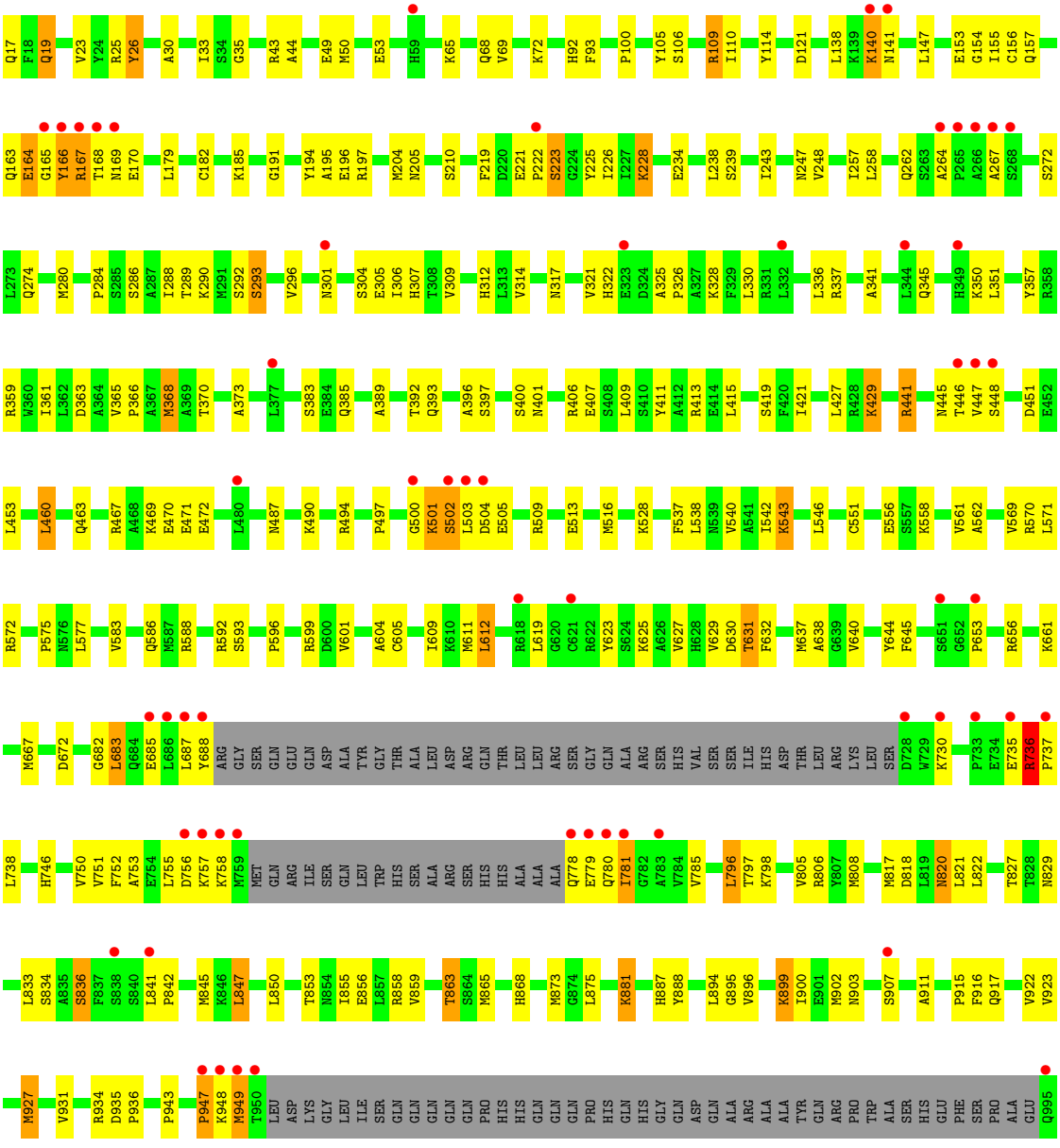
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1002	Total O 1002 1002	0	1
5	B	120	Total O 120 120	0	0

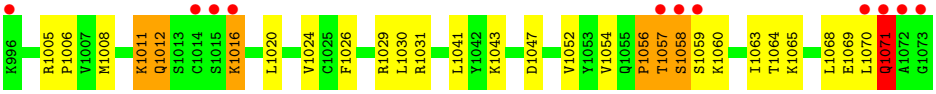
3 Residue-property plots (i)

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: LIPOVITELLIN (LV-1N, LV-1C)

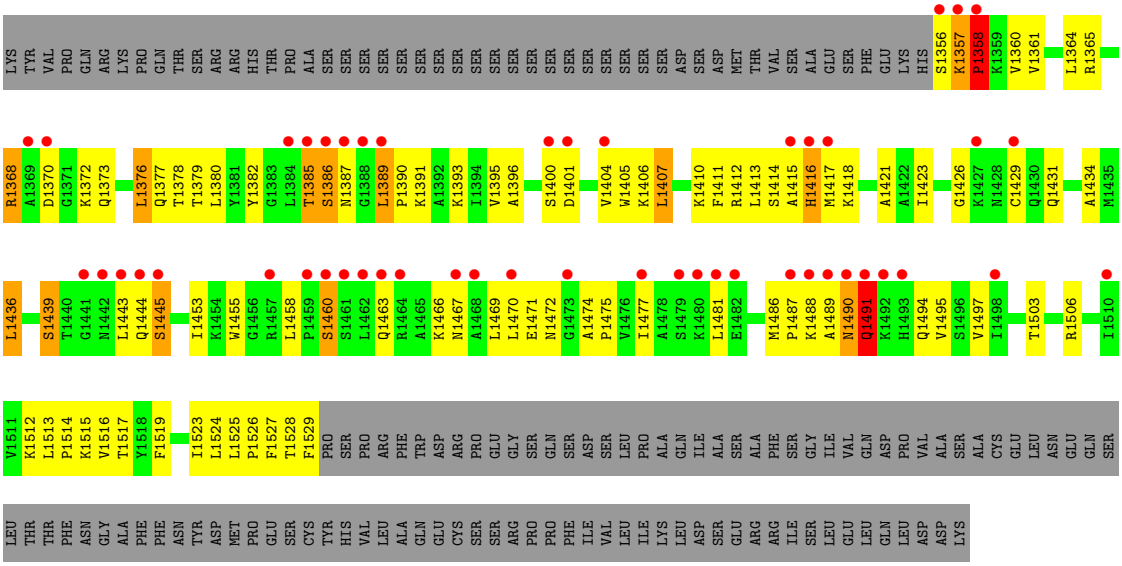
Chain A:





• Molecule 2: LIPOVITELLIN (LV-2)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.17Å 84.52Å 89.53Å 90.00° 100.39° 90.00°	Depositor
Resolution (Å)	21.60 – 1.90 21.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	74.3 (21.60-1.90) 74.4 (21.60-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.255 0.167 , 0.231	Depositor DCC
R_{free} test set	983 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 110.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10935	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: PCA, UPL, PLD

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	0.87	6/8093 (0.1%)	1.05	10/10921 (0.1%)
2	B	0.57	0/1412	0.91	1/1901 (0.1%)
All	All	0.83	6/9505 (0.1%)	1.03	11/12822 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	834[A]	SER	CB-OG	5.68	1.49	1.42
1	A	834[B]	SER	CB-OG	5.68	1.49	1.42
1	A	593	SER	CB-OG	5.66	1.49	1.42
1	A	196	GLU	CG-CD	5.25	1.59	1.51
1	A	26	TYR	CG-CD1	5.07	1.45	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	441	ARG	NE-CZ-NH1	-9.57	115.52	120.30
1	A	875	LEU	CA-CB-CG	-8.54	95.65	115.30
1	A	806	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	121	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	460	LEU	CA-CB-CG	5.89	128.86	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	SER	Mainchain
1	A	631	THR	Mainchain
1	A	796	LEU	Mainchain
1	A	820	ASN	Mainchain
1	A	863	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7781	0	8167	350	0
2	B	1375	0	1488	101	0
3	A	253	0	205	51	0
3	B	31	0	33	8	0
4	A	273	0	494	46	0
4	B	100	0	179	19	0
5	A	1002	0	0	64	0
5	B	120	0	0	11	0
All	All	10935	0	10566	518	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 26.

The worst 5 of 518 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LYS:HE3	1:A:543:LYS:H	1.09	1.11
3:A:2004:PLD:H2A2	3:A:2004:PLD:H32	1.35	1.05
1:A:1011:LYS:HD3	1:A:1012:GLN:H	1.25	1.01
3:A:2005[B]:PLD:H5'1	3:A:2007[B]:PLD:H8A1	1.46	0.97
1:A:588:ARG:HD2	1:A:609[A]:ILE:HD13	1.46	0.95

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	1012/1056 (96%)	959 (95%)	42 (4%)	11 (1%)	14 5
2	B	176/319 (55%)	153 (87%)	15 (8%)	8 (4%)	2 0
All	All	1188/1375 (86%)	1112 (94%)	57 (5%)	19 (2%)	9 2

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
1	A	1058	SER
2	B	1357	LYS
2	B	1385	THR
2	B	1386	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	881/900 (98%)	831 (94%)	50 (6%)	20 11
2	B	148/277 (53%)	137 (93%)	11 (7%)	13 6
All	All	1029/1177 (87%)	968 (94%)	61 (6%)	20 10

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	543	LYS

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Mol	Chain	Res	Type
2	B	1429	CYS
1	A	817	MET
2	B	1407	LEU
2	B	1491	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1463	GLN
2	B	1491	GLN
1	A	829	ASN
1	A	867	GLN
1	A	887	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PCA	A	17	1	7,8,9	2.11	1 (14%)	9,10,12	2.45	5 (55%)

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
1	PCA	A	17	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	PCA	CB-CG	-5.37	1.40	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	17	PCA	OE-CD-CG	-3.66	120.37	126.76
1	A	17	PCA	CB-CG-CD	-3.31	99.06	104.40
1	A	17	PCA	CA-N-CD	-3.05	103.15	113.58
1	A	17	PCA	CG-CD-N	2.96	116.06	108.39
1	A	17	PCA	CB-CA-C	-2.75	108.92	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

53 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	UPL	A	2015	-	12,12,33	0.41	0	11,11,33	0.51	0
4	UPL	B	2021	-	8,8,33	0.20	0	7,7,33	0.52	0
4	UPL	B	2043	-	4,4,33	0.24	0	3,3,33	0.41	0
4	UPL	A	2011	-	18,18,33	0.64	0	17,17,33	0.80	0
4	UPL	A	2012	-	16,16,33	0.37	0	15,15,33	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PLD	A	2001[A]	-	52,52,59	1.13	5 (9%)	58,60,67	2.14	12 (20%)
4	UPL	A	2039	-	4,4,33	0.53	0	3,3,33	0.31	0
4	UPL	A	2036	-	5,5,33	0.30	0	4,4,33	0.43	0
4	UPL	B	2045	-	4,4,33	0.36	0	3,3,33	0.61	0
3	PLD	A	2004	-	33,33,59	1.71	5 (15%)	37,38,67	2.12	13 (35%)
4	UPL	A	2024	-	5,5,33	0.42	0	4,4,33	0.58	0
4	UPL	B	2033	-	5,5,33	0.44	0	4,4,33	0.33	0
4	UPL	B	2046	-	4,4,33	0.38	0	3,3,33	0.36	0
4	UPL	A	2008	-	16,16,33	1.07	0	16,16,33	1.62	2 (12%)
4	UPL	A	2019	-	9,9,33	0.40	0	8,8,33	0.77	0
3	PLD	A	2006	-	33,33,59	1.18	4 (12%)	37,38,67	2.13	9 (24%)
4	UPL	A	2035	-	6,6,33	0.47	0	5,5,33	0.12	0
3	PLD	B	2003	-	30,30,59	1.23	4 (13%)	33,35,67	2.38	17 (51%)
4	UPL	A	2009	-	14,14,33	0.77	0	14,14,33	1.05	1 (7%)
4	UPL	B	2016	-	12,12,33	0.46	0	11,11,33	0.74	0
4	UPL	A	2020	-	5,5,33	0.49	0	4,4,33	0.27	0
3	PLD	A	2005[B]	-	45,45,59	1.27	3 (6%)	49,50,67	2.20	10 (20%)
3	PLD	A	2007[B]	-	36,36,59	8.85	7 (19%)	40,41,67	2.35	11 (27%)
4	UPL	B	2023	-	8,8,33	0.57	0	7,7,33	0.48	0
4	UPL	A	2048	-	9,9,33	0.65	0	8,8,33	0.83	0
4	UPL	B	2010	-	13,13,33	0.58	0	13,13,33	0.88	1 (7%)
4	UPL	B	2028	-	6,6,33	0.30	0	5,5,33	0.34	0
4	UPL	A	2014	-	15,15,33	0.57	0	14,14,33	1.77	2 (14%)
4	UPL	B	2031	-	6,6,33	0.42	0	5,5,33	0.61	0
4	UPL	A	2018	-	11,11,33	0.62	0	10,10,33	0.59	0
4	UPL	A	2026	-	7,7,33	0.92	0	6,6,33	0.61	0
4	UPL	A	2025	-	7,7,33	0.64	0	6,6,33	0.22	0
4	UPL	A	2013	-	15,15,33	0.56	0	14,14,33	0.75	0
3	PLD	A	2005[A]	-	45,45,59	1.29	3 (6%)	49,50,67	2.21	10 (20%)
4	UPL	A	2022	-	5,5,33	0.45	0	4,4,33	0.24	0
4	UPL	A	2029	-	8,8,33	0.50	0	7,7,33	0.72	0
4	UPL	A	2017	-	10,10,33	0.48	0	9,9,33	0.56	0
4	UPL	A	2042	-	4,4,33	0.53	0	3,3,33	0.28	0
3	PLD	A	2007[A]	-	36,36,59	1.55	5 (13%)	40,41,67	1.80	10 (25%)
4	UPL	B	2049	-	5,5,33	0.33	0	4,4,33	0.49	0
4	UPL	A	2030	-	6,6,33	0.75	0	5,5,33	0.85	0
4	UPL	A	2032	-	5,5,33	0.44	0	4,4,33	0.49	0
3	PLD	A	2001[B]	-	52,52,59	11.13	6 (11%)	58,60,67	2.97	14 (24%)
4	UPL	A	2050	-	5,5,33	0.33	0	4,4,33	0.47	0
4	UPL	A	2034	-	5,5,33	0.53	0	4,4,33	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	UPL	A	2047	-	4,4,33	0.30	0	3,3,33	0.39	0
4	UPL	A	2037	-	4,4,33	0.53	0	3,3,33	0.79	0
4	UPL	B	2027	-	6,6,33	0.38	0	5,5,33	0.55	0
3	PLD	A	2002	-	34,34,59	1.51	6 (17%)	38,39,67	1.84	9 (23%)
4	UPL	A	2040	-	4,4,33	0.78	0	3,3,33	0.69	0
4	UPL	B	2044	-	6,6,33	0.56	0	5,5,33	0.43	0
4	UPL	A	2038	-	5,5,33	0.49	0	4,4,33	0.59	0
4	UPL	A	2041	-	4,4,33	0.39	0	3,3,33	0.52	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	UPL	A	2015	-	-	7/10/10/33	-
4	UPL	B	2021	-	-	4/6/6/33	-
4	UPL	B	2043	-	-	1/2/2/33	-
4	UPL	A	2011	-	-	13/16/16/33	-
4	UPL	A	2012	-	-	8/14/14/33	-
3	PLD	A	2001[A]	-	1/1/5/5	20/56/56/63	-
4	UPL	A	2039	-	-	1/2/2/33	-
4	UPL	A	2036	-	-	2/3/3/33	-
4	UPL	B	2045	-	-	2/2/2/33	-
3	PLD	A	2004	-	-	17/35/35/63	-
4	UPL	A	2024	-	-	0/3/3/33	-
4	UPL	B	2033	-	-	2/3/3/33	-
4	UPL	B	2046	-	-	1/2/2/33	-
4	UPL	A	2008	-	1/1/1/1	8/16/16/33	-
4	UPL	A	2019	-	-	4/7/7/33	-
3	PLD	A	2006	-	1/1/4/5	22/35/35/63	-
4	UPL	A	2035	-	-	3/4/4/33	-
3	PLD	B	2003	-	-	19/34/34/63	-
4	UPL	A	2009	-	1/1/1/1	5/14/14/33	-
4	UPL	B	2016	-	-	5/10/10/33	-
4	UPL	A	2020	-	-	1/3/3/33	-
3	PLD	A	2005[B]	-	1/1/4/5	26/47/47/63	-
3	PLD	A	2007[B]	-	1/1/4/5	20/38/38/63	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UPL	B	2023	-	-	3/6/6/33	-
4	UPL	A	2048	-	-	4/7/7/33	-
4	UPL	B	2010	-	-	9/12/12/33	-
4	UPL	B	2028	-	-	2/4/4/33	-
4	UPL	A	2014	-	-	7/13/13/33	-
4	UPL	B	2031	-	-	2/4/4/33	-
4	UPL	A	2018	-	-	5/9/9/33	-
4	UPL	A	2026	-	-	2/5/5/33	-
4	UPL	A	2025	-	-	5/5/5/33	-
4	UPL	A	2013	-	-	8/13/13/33	-
3	PLD	A	2005[A]	-	1/1/4/5	27/47/47/63	-
4	UPL	A	2022	-	-	1/3/3/33	-
4	UPL	A	2029	-	-	3/6/6/33	-
4	UPL	A	2017	-	-	5/8/8/33	-
4	UPL	A	2042	-	-	2/2/2/33	-
3	PLD	A	2007[A]	-	1/1/4/5	21/38/38/63	-
4	UPL	B	2049	-	-	3/3/3/33	-
4	UPL	A	2030	-	-	2/4/4/33	-
4	UPL	A	2032	-	-	2/3/3/33	-
3	PLD	A	2001[B]	-	1/1/5/5	24/56/56/63	-
4	UPL	A	2050	-	-	3/3/3/33	-
4	UPL	A	2034	-	-	1/3/3/33	-
4	UPL	A	2047	-	-	2/2/2/33	-
4	UPL	A	2037	-	-	2/2/2/33	-
4	UPL	B	2027	-	-	3/4/4/33	-
3	PLD	A	2002	-	-	26/36/36/63	-
4	UPL	A	2040	-	-	0/2/2/33	-
4	UPL	B	2044	-	-	3/4/4/33	-
4	UPL	A	2038	-	-	2/3/3/33	-
4	UPL	A	2041	-	-	0/2/2/33	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001[B]	PLD	CG'-CF'	79.85	6.00	1.51
3	A	2007[B]	PLD	C9B-C8B	52.03	5.19	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2007[B]	PLD	C6B-C5B	5.75	1.83	1.51
3	A	2002	PLD	O3-CB	5.45	1.49	1.33
3	A	2007[A]	PLD	O3-CB	5.04	1.48	1.33

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001[B]	PLD	CG'-CF'-CE'	-15.01	38.20	114.42
3	A	2001[A]	PLD	C2-O2-C'	9.62	141.47	117.79
3	A	2001[B]	PLD	C2-O2-C'	9.62	141.47	117.79
3	A	2007[B]	PLD	C9B-C8B-C7B	-9.20	29.93	115.30
3	A	2005[A]	PLD	C2-O2-C'	8.57	138.89	117.79

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	2001[A]	PLD	C2
3	A	2001[B]	PLD	C2
3	A	2005[A]	PLD	C2
3	A	2005[B]	PLD	C2
3	A	2006	PLD	C2

5 of 370 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001[A]	PLD	C3-C2-O2-C'
3	A	2001[A]	PLD	C4-O4P-P-O2P
3	A	2001[B]	PLD	C3-C2-O2-C'
3	A	2001[B]	PLD	C4-O4P-P-O2P
3	A	2002	PLD	C3-C2-O2-C'

There are no ring outliers.

41 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2015	UPL	4	0
4	B	2021	UPL	4	0
4	A	2011	UPL	4	0
4	A	2012	UPL	3	0
3	A	2001[A]	PLD	4	0
4	A	2036	UPL	1	0

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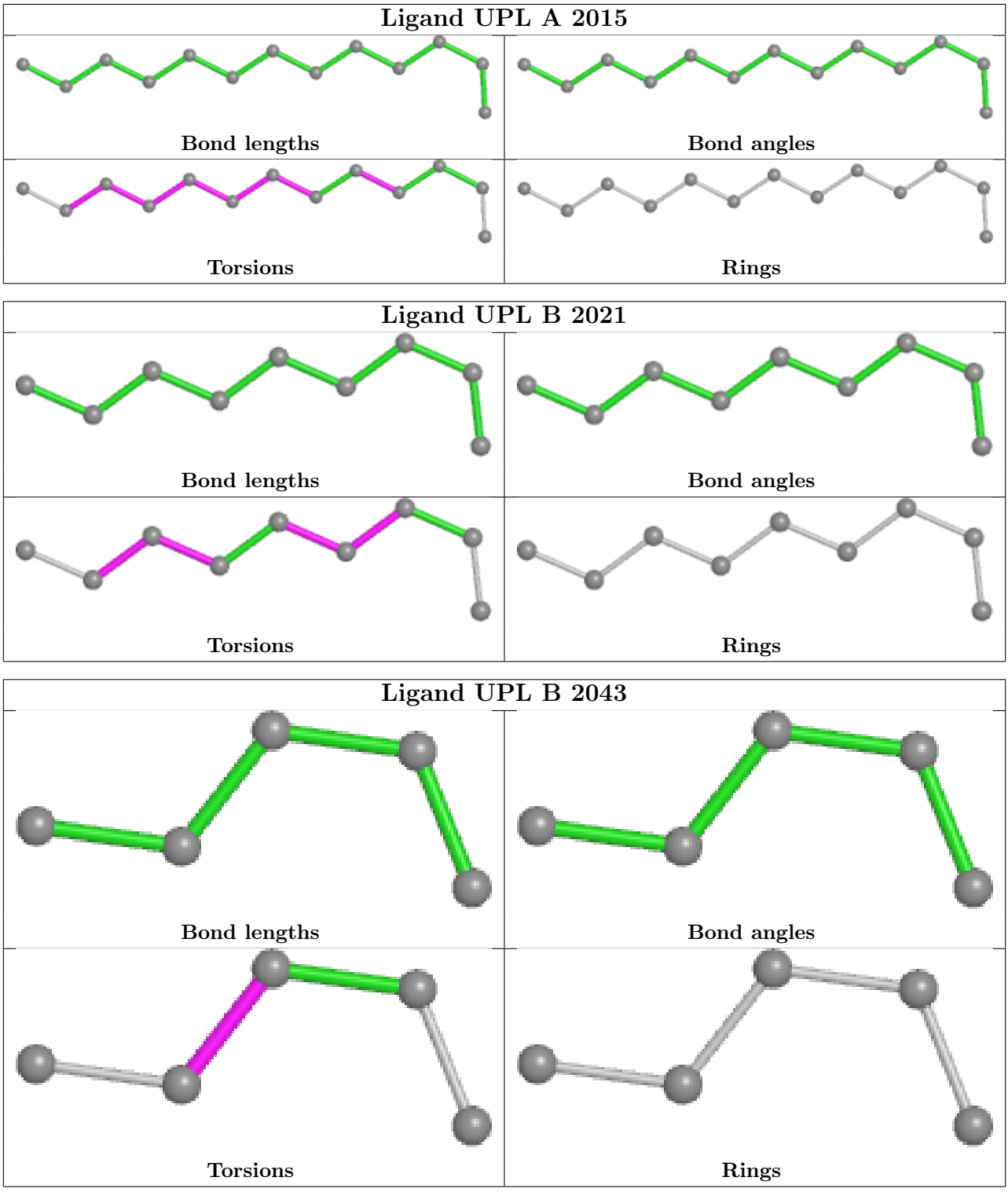
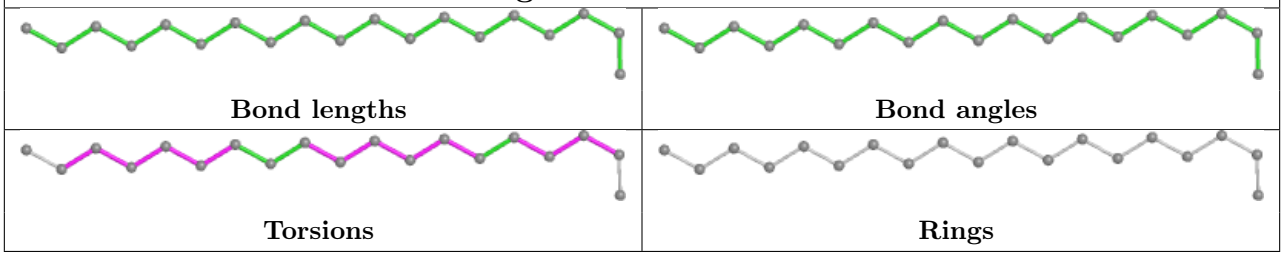
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2045	UPL	1	0
3	A	2004	PLD	13	0
4	A	2024	UPL	1	0
4	B	2033	UPL	1	0
4	B	2046	UPL	2	0
4	A	2008	UPL	3	0
4	A	2019	UPL	1	0
3	A	2006	PLD	9	0
3	B	2003	PLD	8	0
4	A	2009	UPL	7	0
4	B	2016	UPL	2	0
3	A	2005[B]	PLD	5	0
3	A	2007[B]	PLD	10	0
4	B	2023	UPL	2	0
4	A	2048	UPL	2	0
4	B	2010	UPL	6	0
4	B	2028	UPL	1	0
4	A	2014	UPL	2	0
4	A	2018	UPL	2	0
4	A	2026	UPL	3	0
4	A	2025	UPL	1	0
4	A	2013	UPL	7	0
4	A	2022	UPL	2	0
4	A	2029	UPL	1	0
4	A	2017	UPL	1	0
4	A	2042	UPL	1	0
4	B	2049	UPL	3	0
4	A	2030	UPL	1	0
4	A	2050	UPL	1	0
4	A	2034	UPL	1	0
4	A	2047	UPL	1	0
4	B	2027	UPL	2	0
3	A	2002	PLD	16	0
4	B	2044	UPL	1	0
4	A	2038	UPL	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

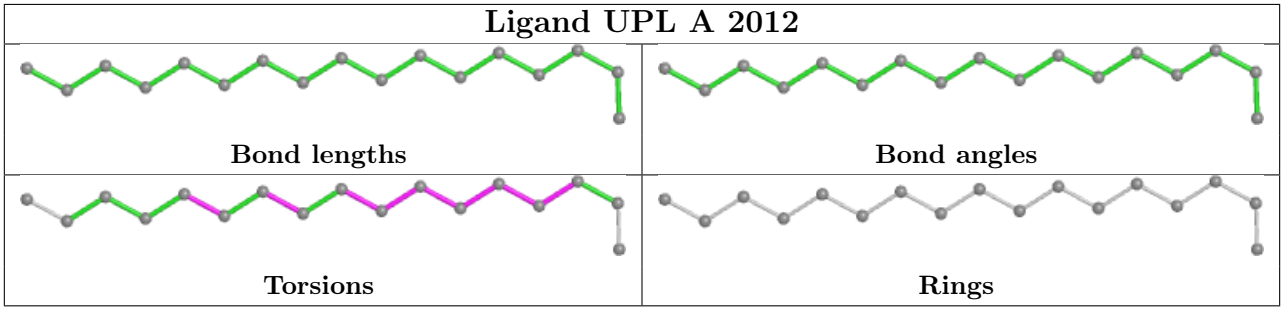
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



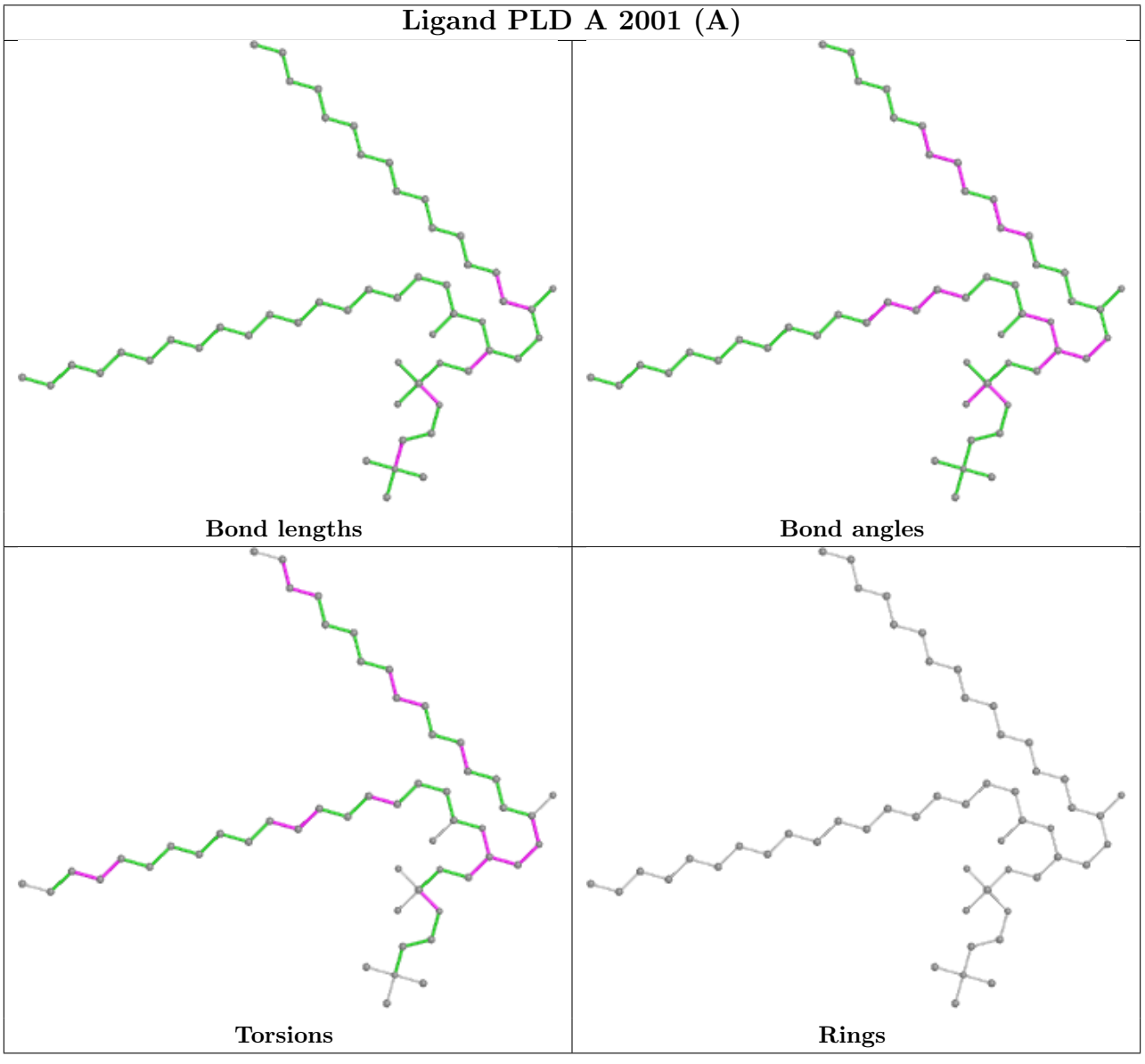
Ligand UPL A 2011



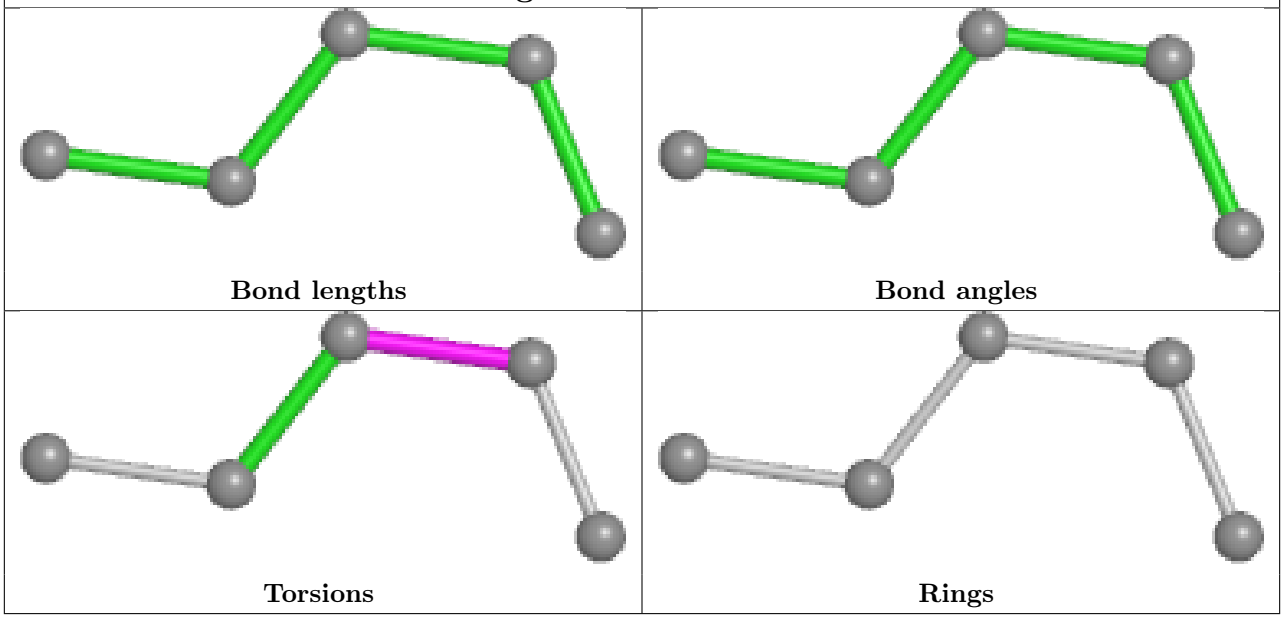
Ligand UPL A 2012



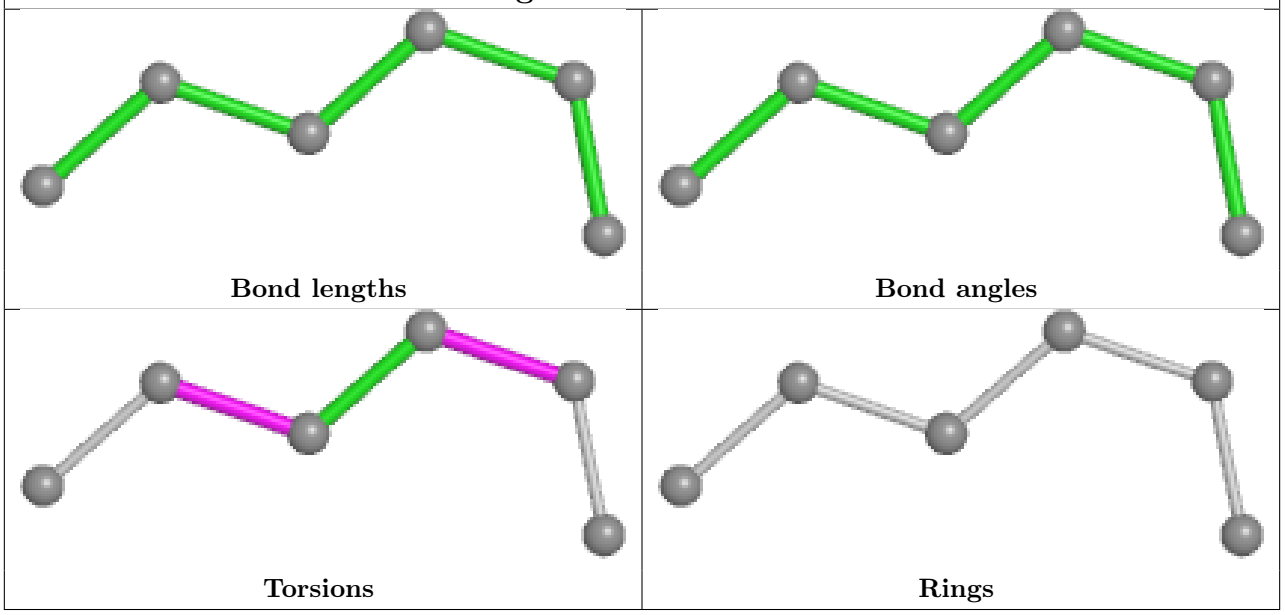
Ligand PLD A 2001 (A)



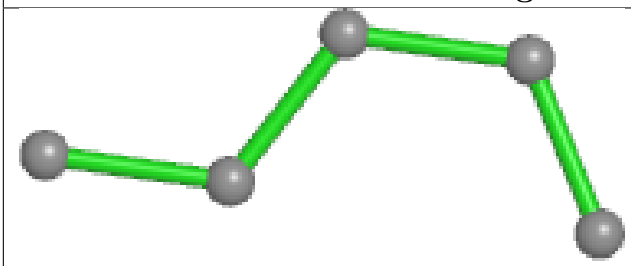
Ligand UPL A 2039



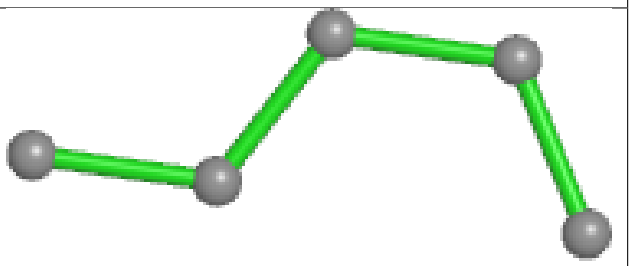
Ligand UPL A 2036



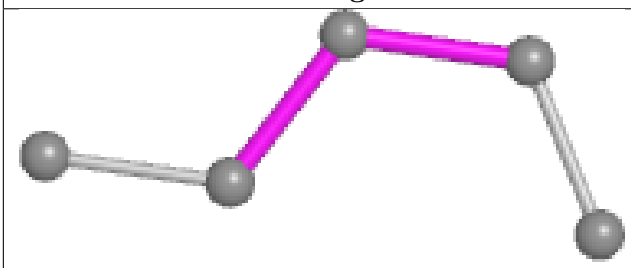
Ligand UPL B 2045



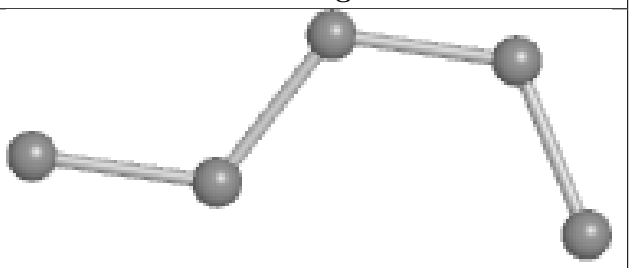
Bond lengths



Bond angles

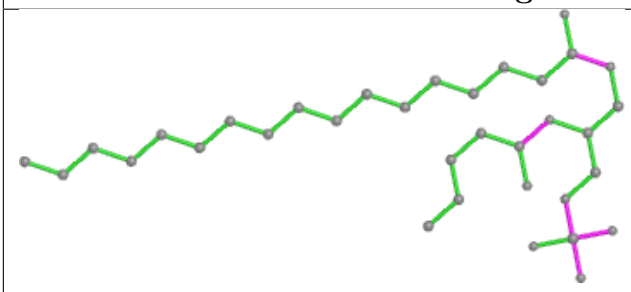


Torsions

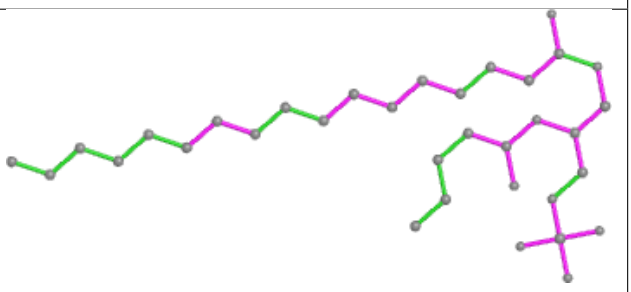


Rings

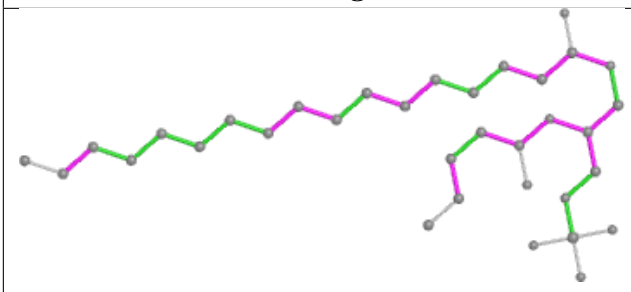
Ligand PLD A 2004



Bond lengths



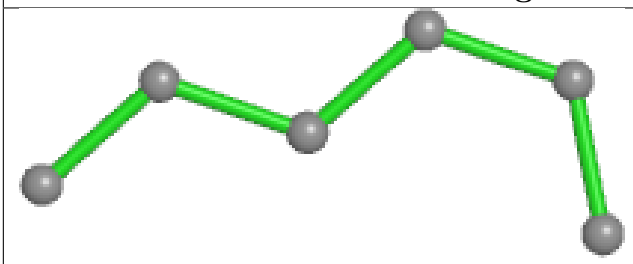
Bond angles



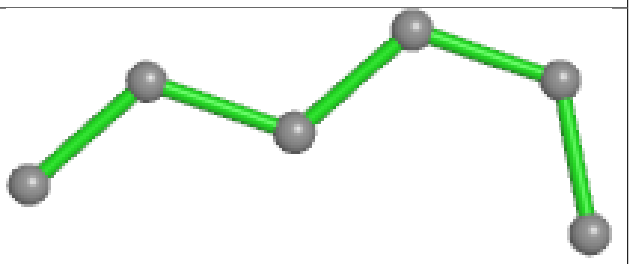
Torsions

Rings

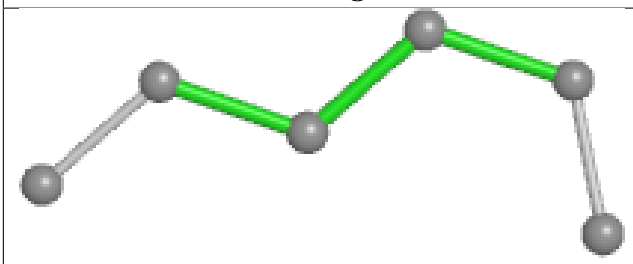
Ligand UPL A 2024



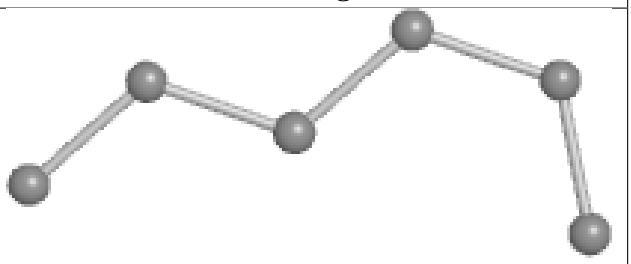
Bond lengths



Bond angles

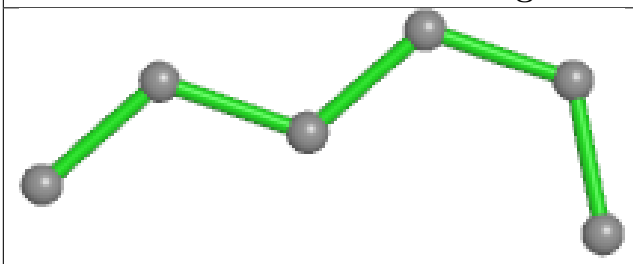


Torsions

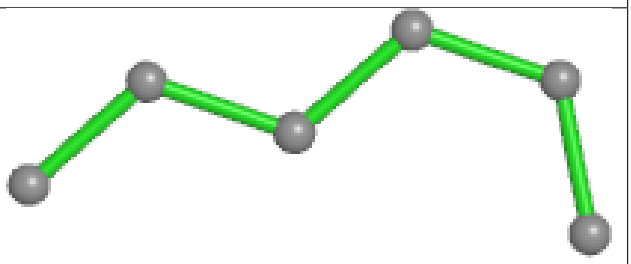


Rings

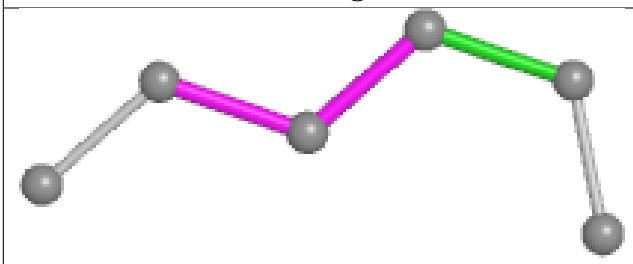
Ligand UPL B 2033



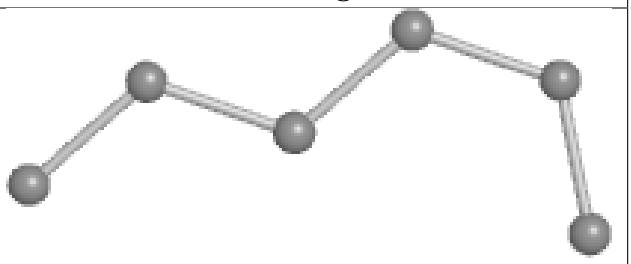
Bond lengths



Bond angles

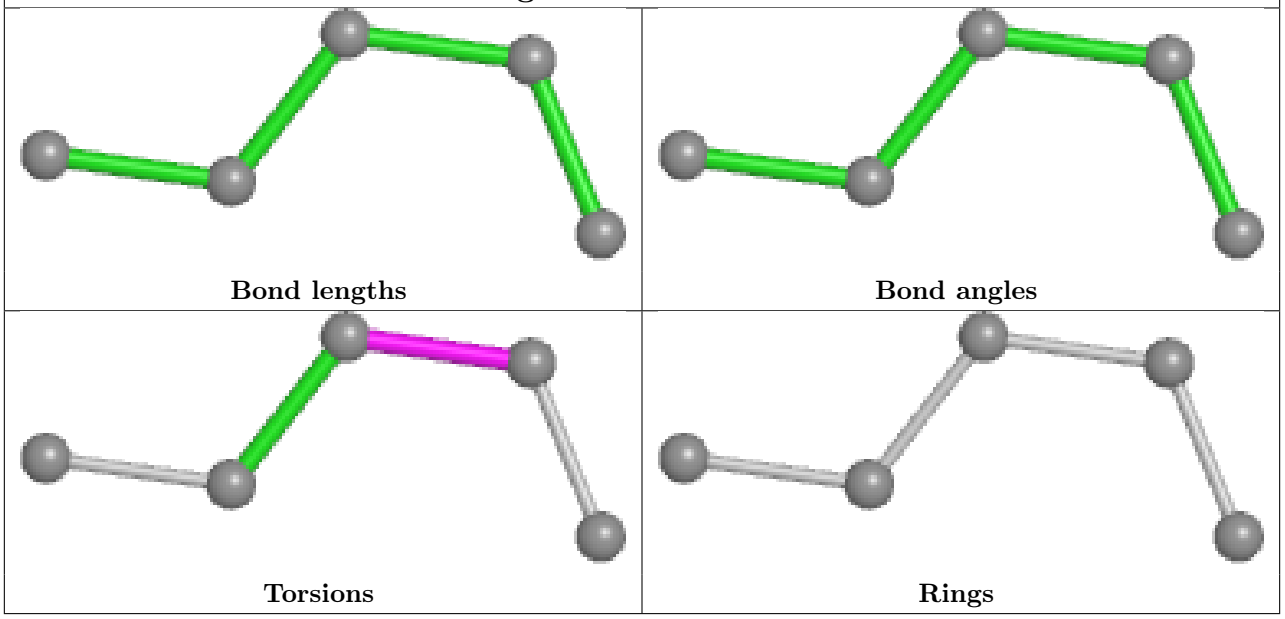


Torsions

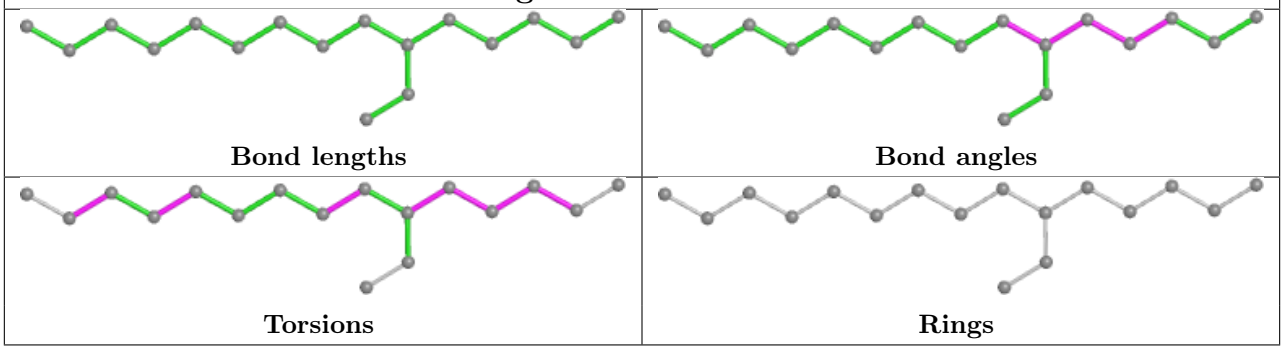


Rings

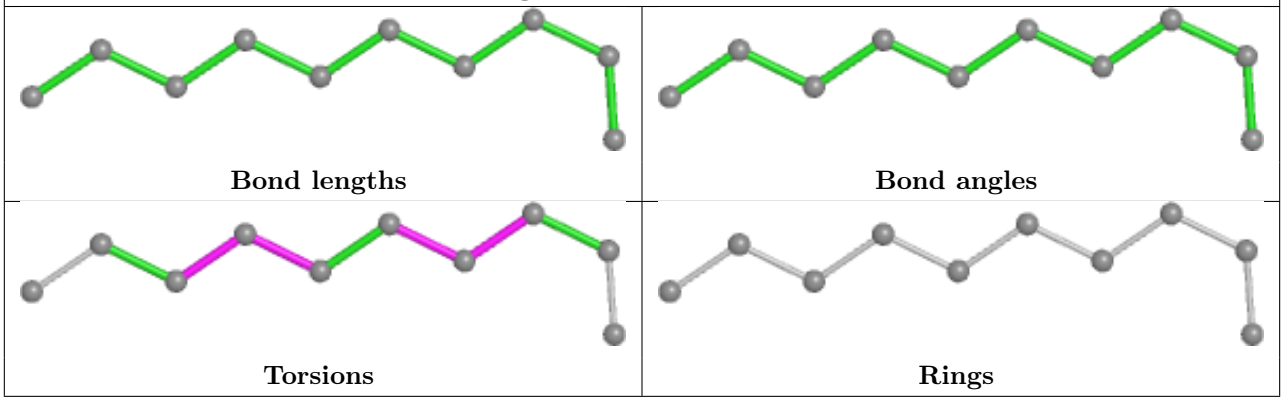
Ligand UPL B 2046



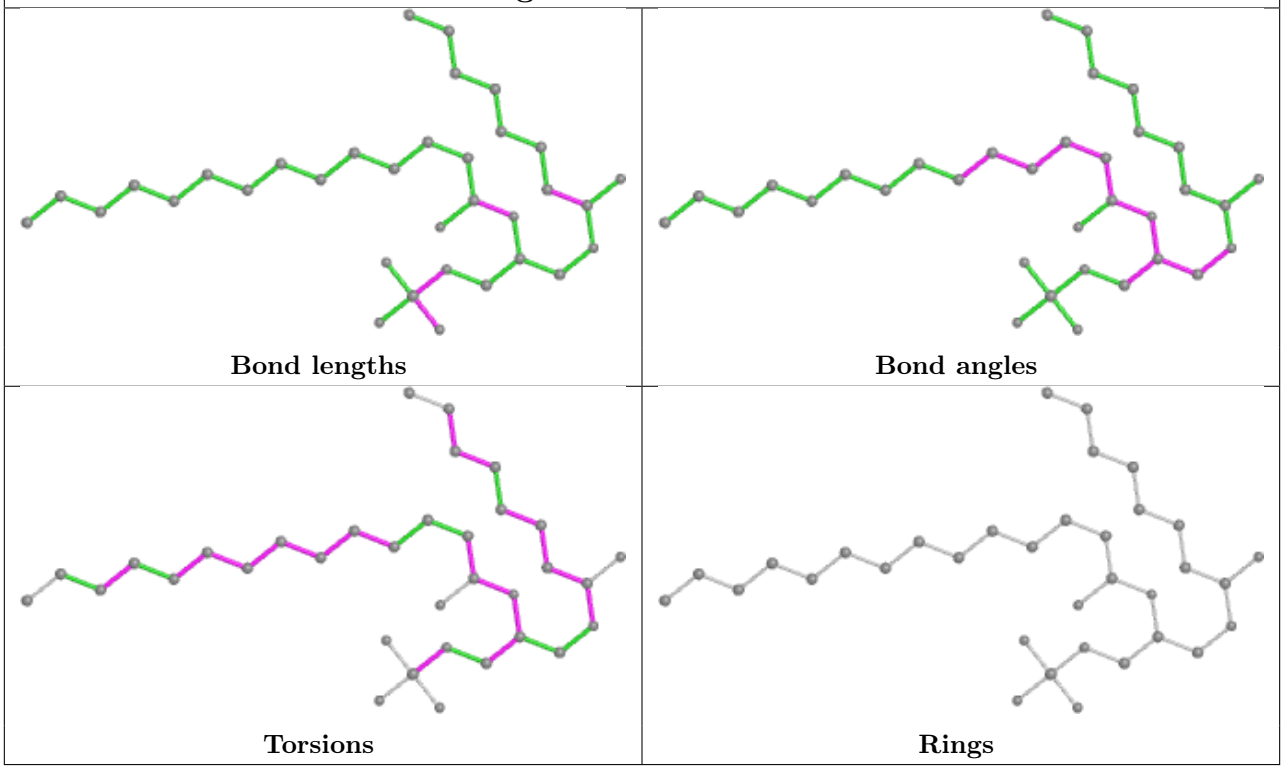
Ligand UPL A 2008



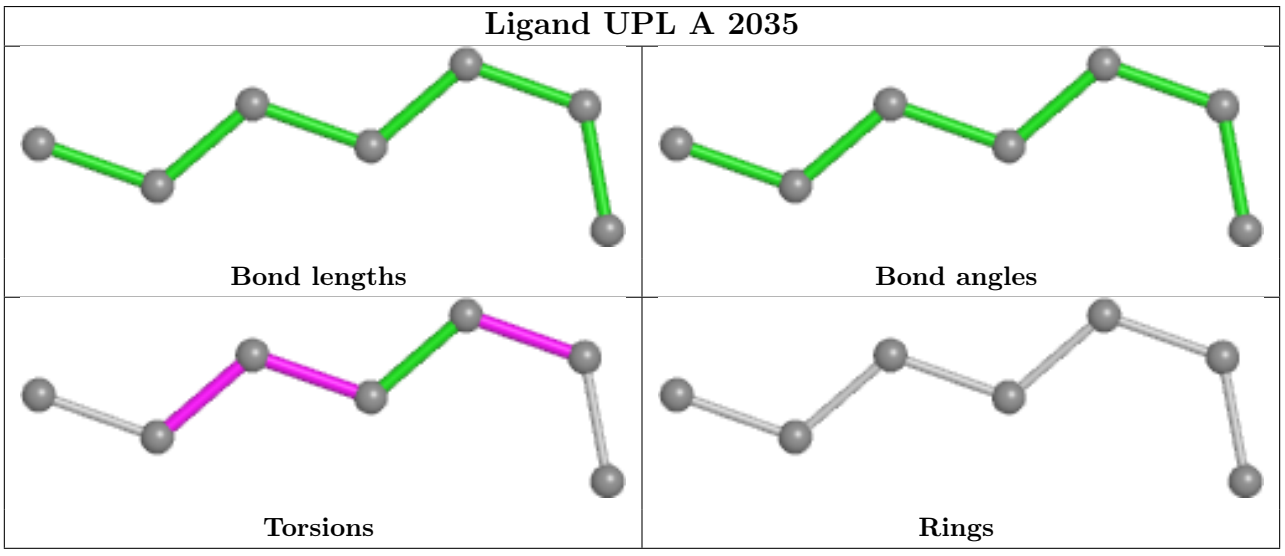
Ligand UPL A 2019



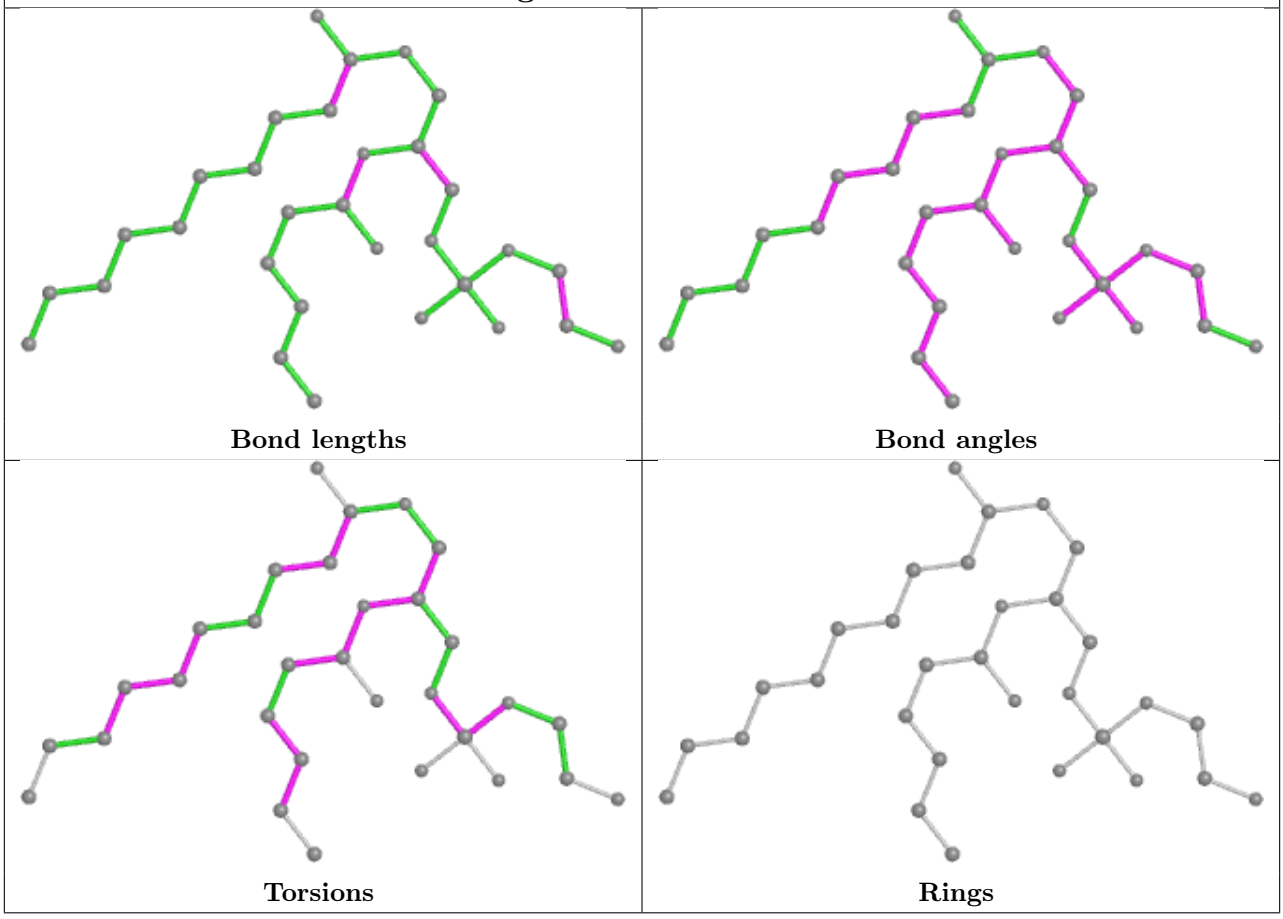
Ligand PLD A 2006



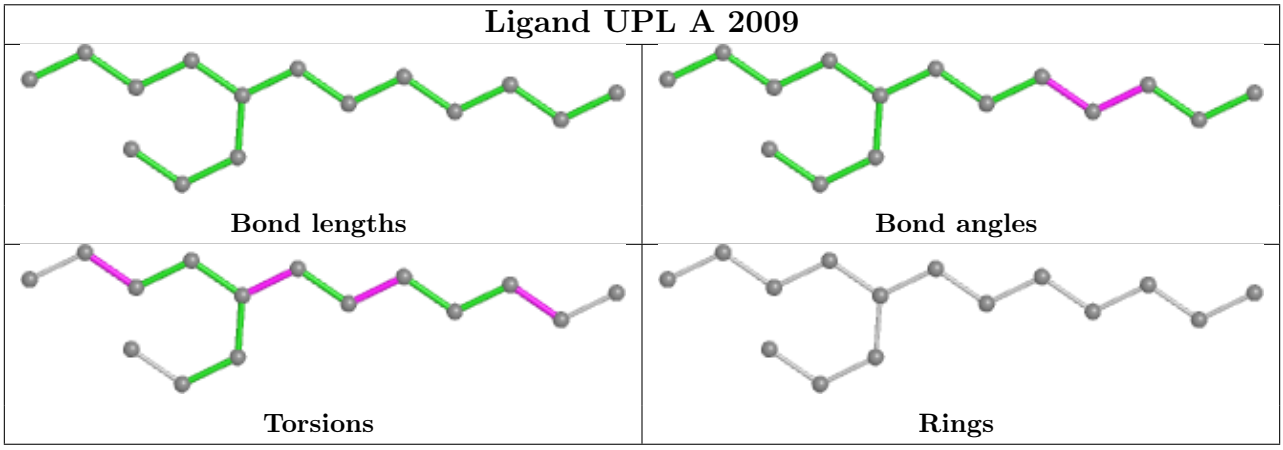
Ligand UPL A 2035



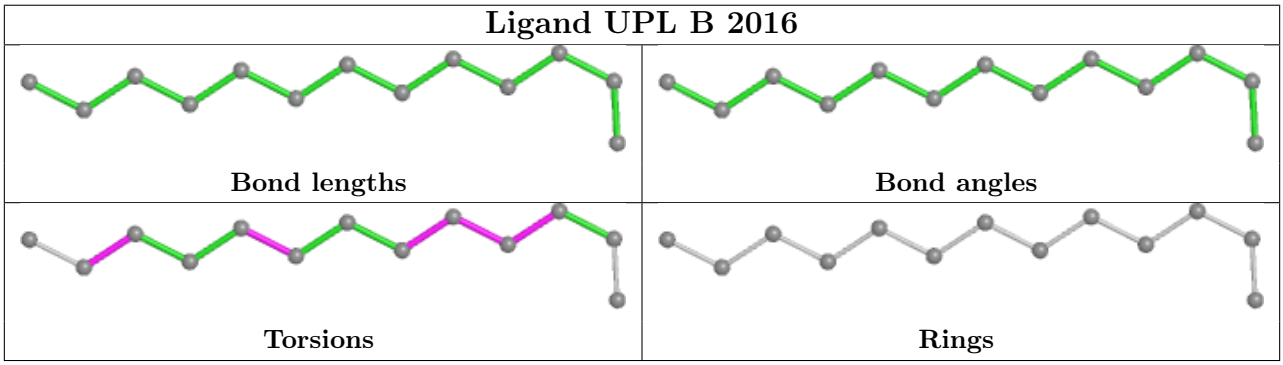
Ligand PLD B 2003



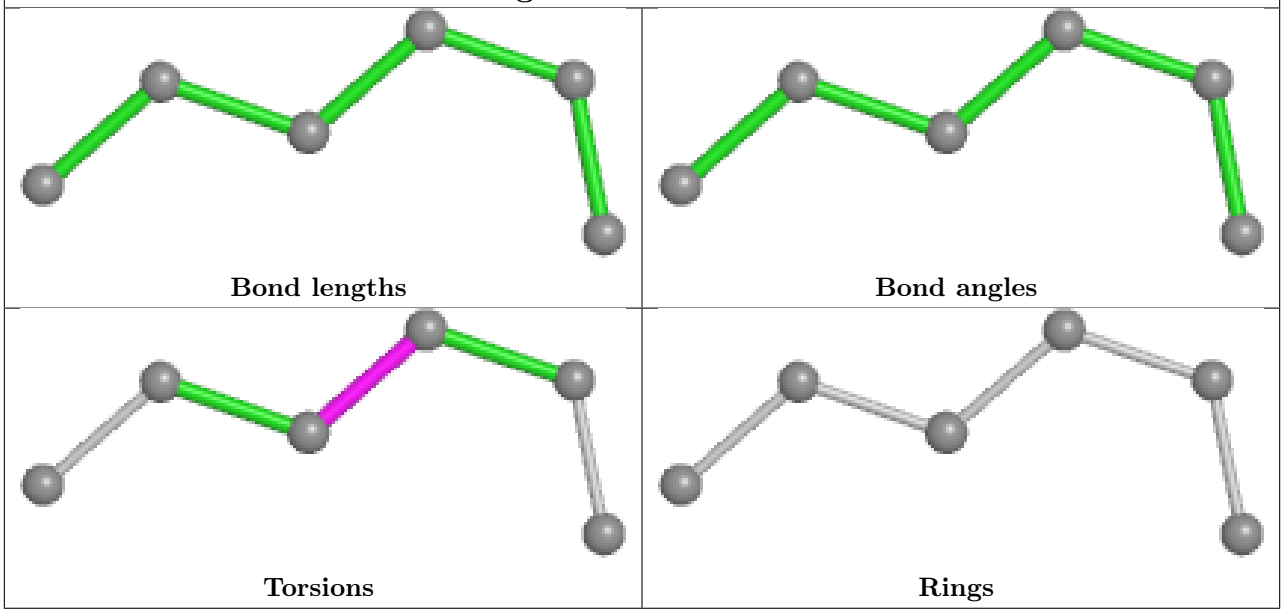
Ligand UPL A 2009



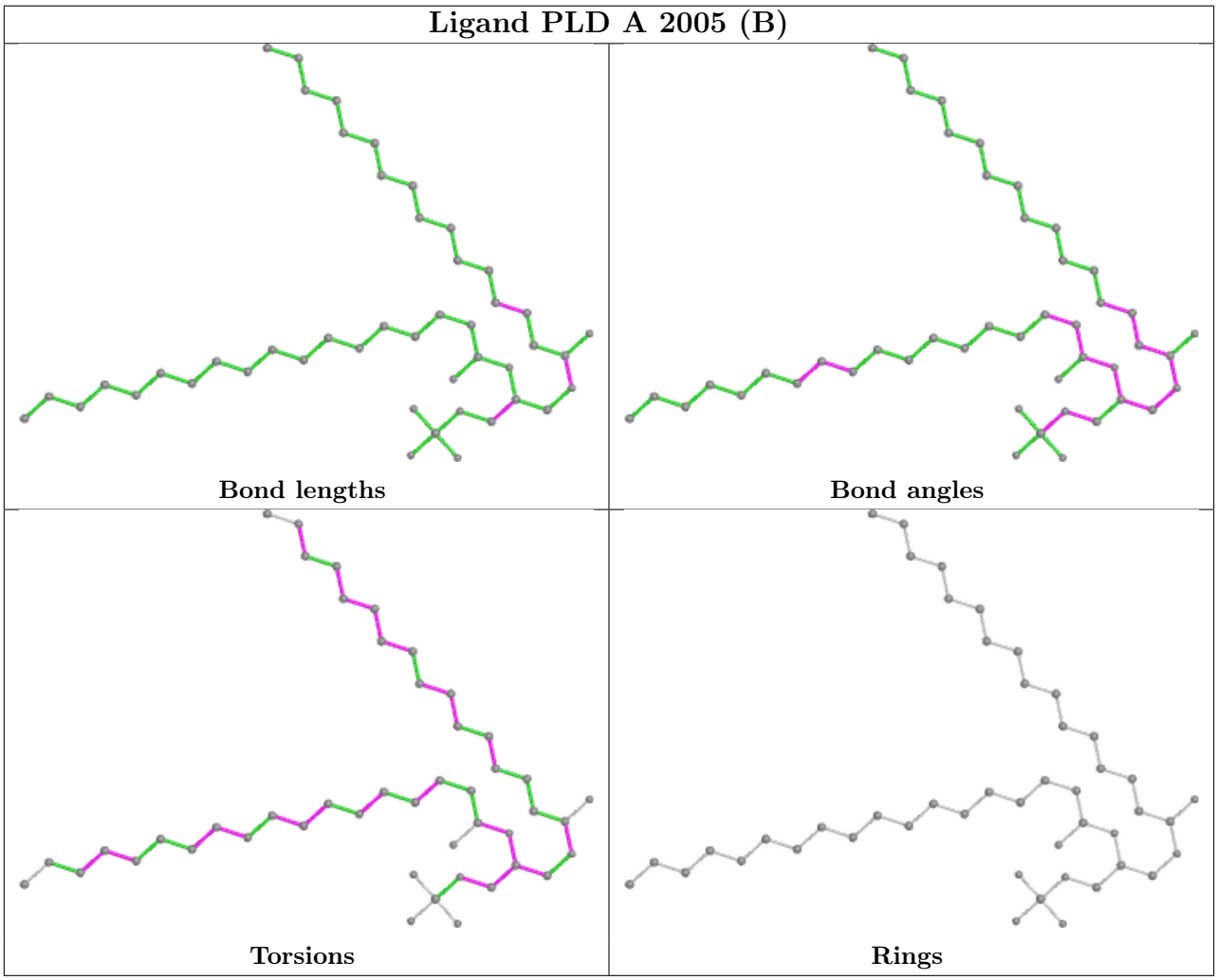
Ligand UPL B 2016



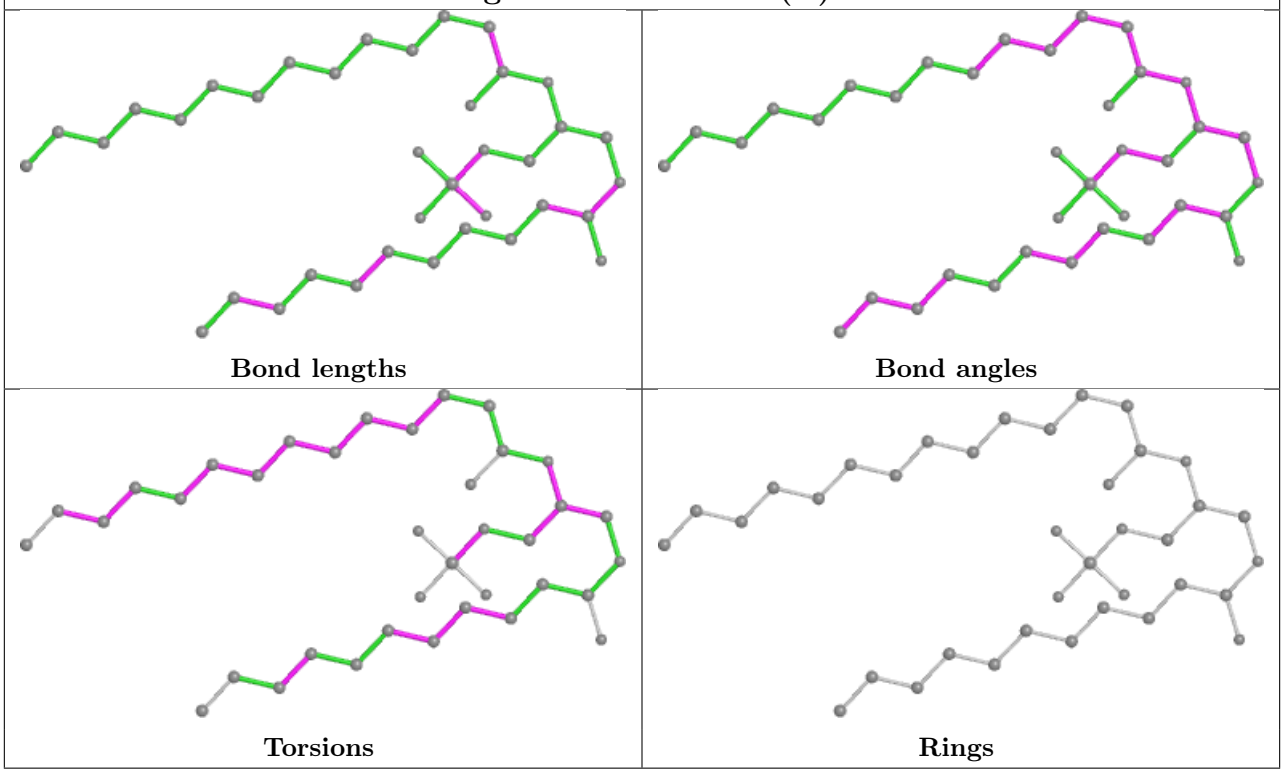
Ligand UPL A 2020



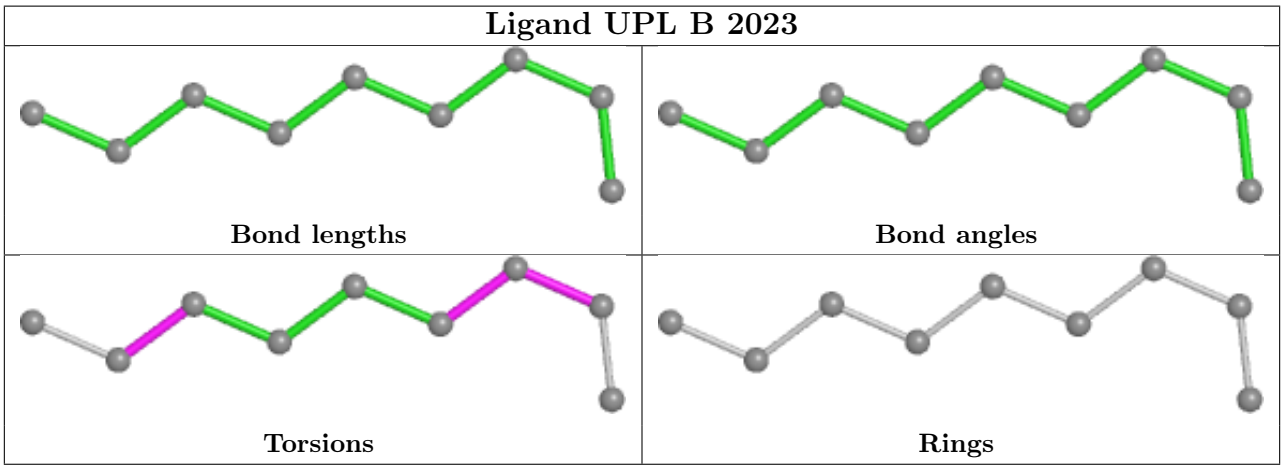
Ligand PLD A 2005 (B)



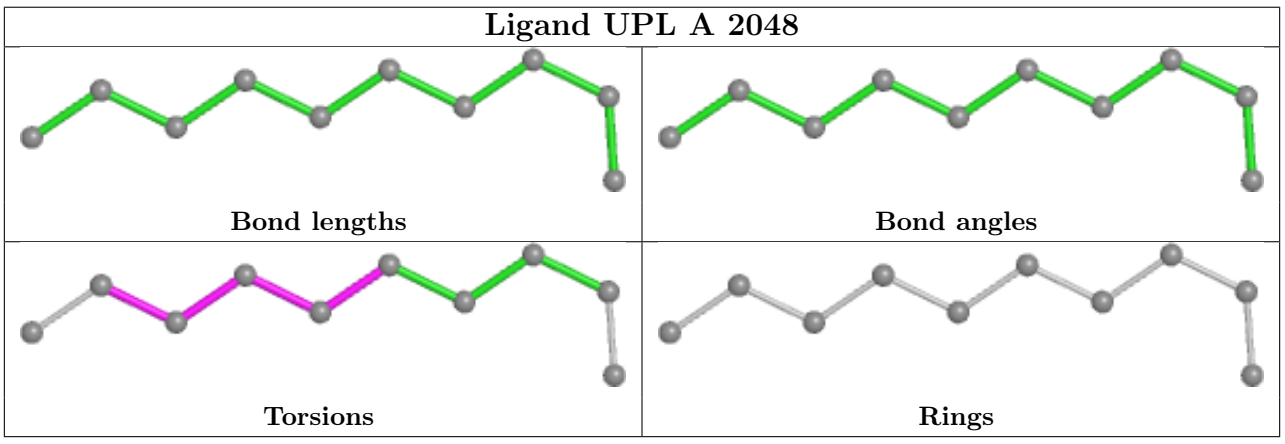
Ligand PLD A 2007 (B)



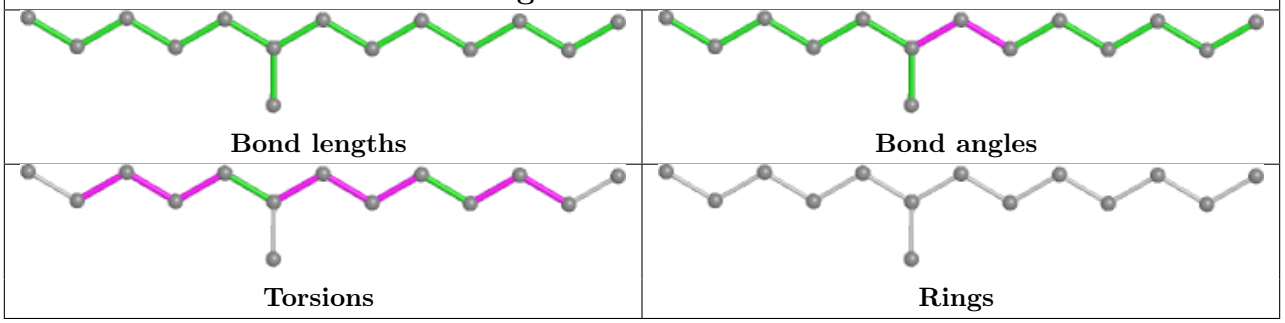
Ligand UPL B 2023



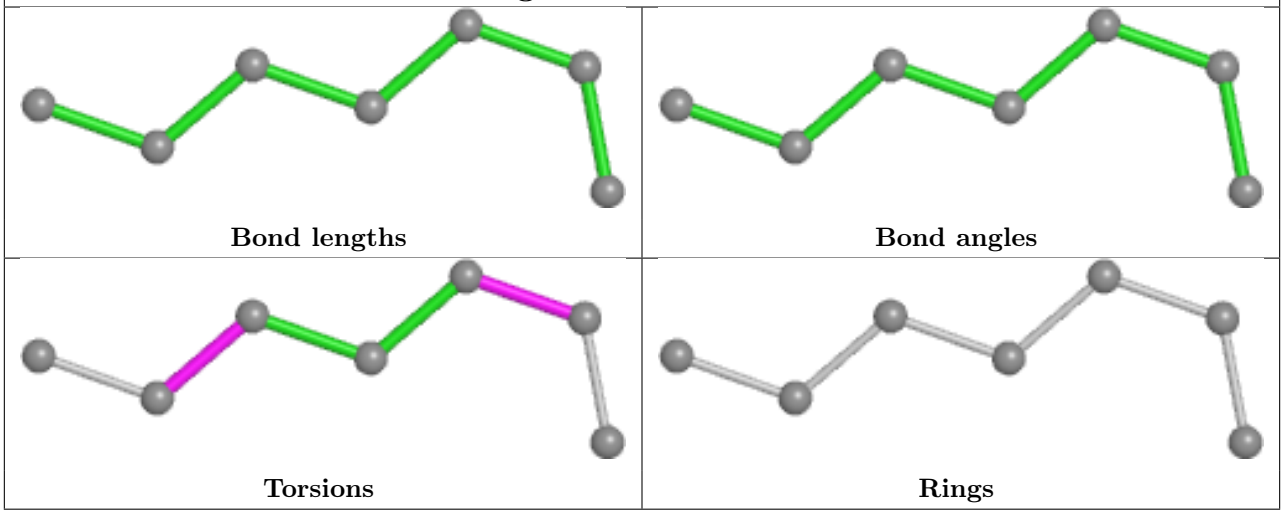
Ligand UPL A 2048



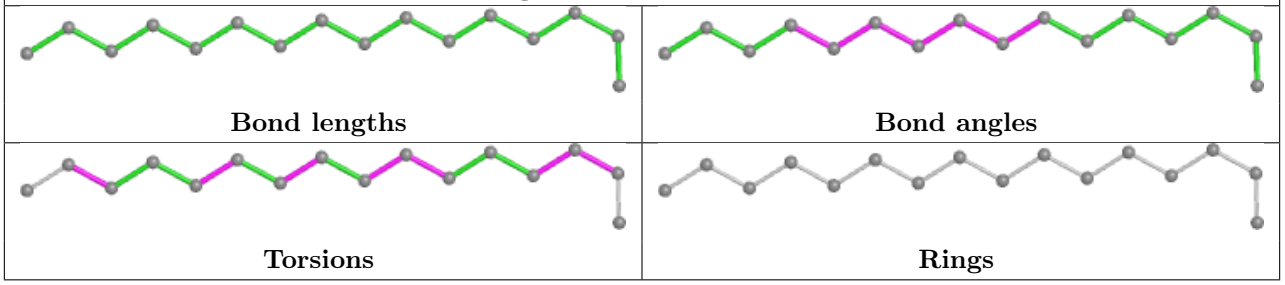
Ligand UPL B 2010



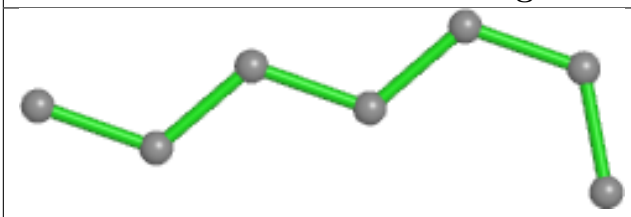
Ligand UPL B 2028



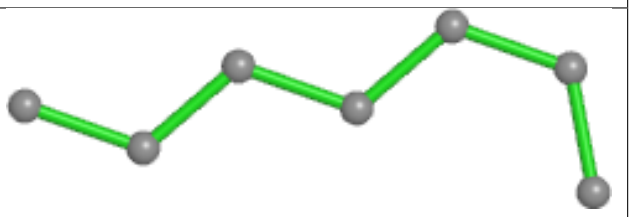
Ligand UPL A 2014



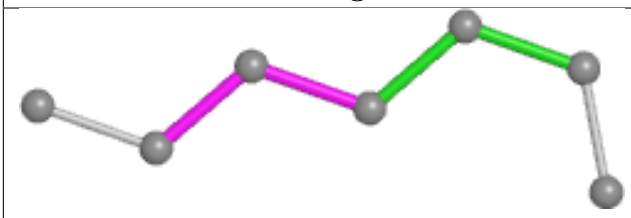
Ligand UPL B 2031



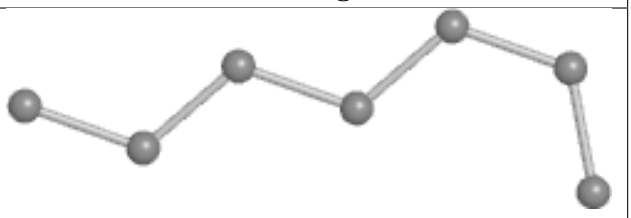
Bond lengths



Bond angles

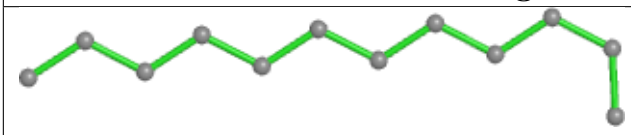


Torsions

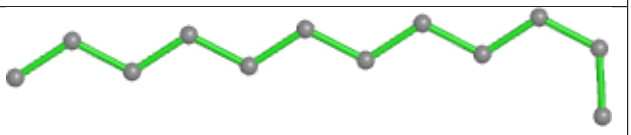


Rings

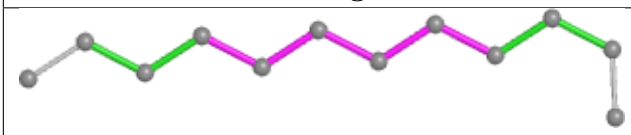
Ligand UPL A 2018



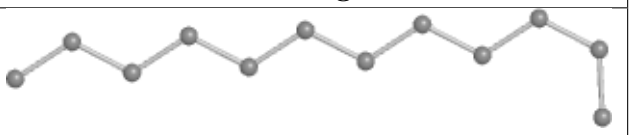
Bond lengths



Bond angles

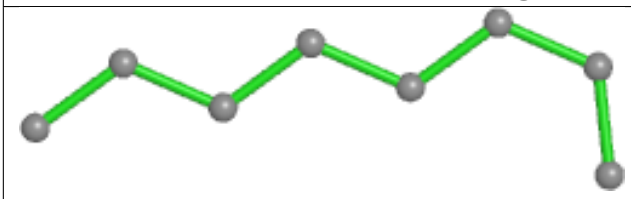


Torsions

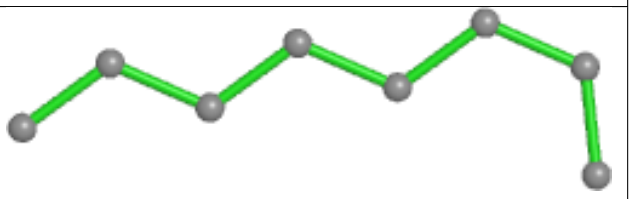


Rings

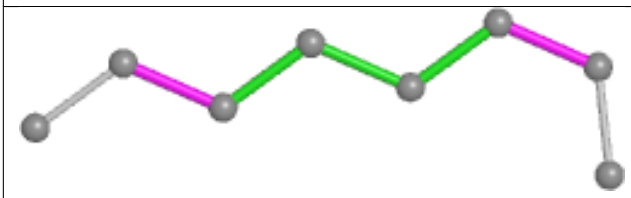
Ligand UPL A 2026



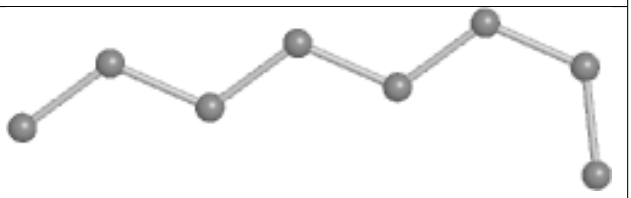
Bond lengths



Bond angles

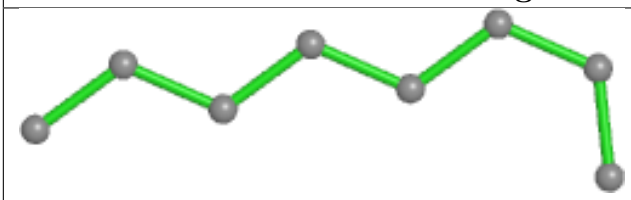


Torsions

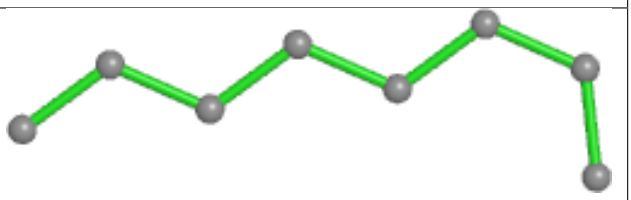


Rings

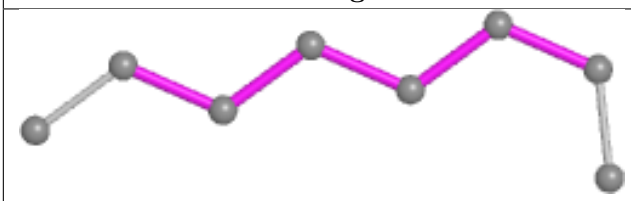
Ligand UPL A 2025



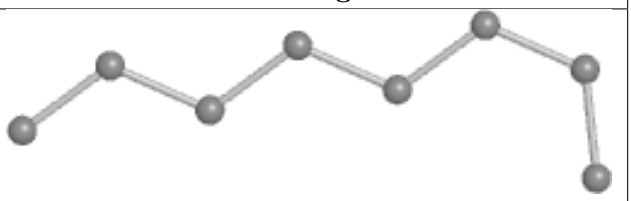
Bond lengths



Bond angles

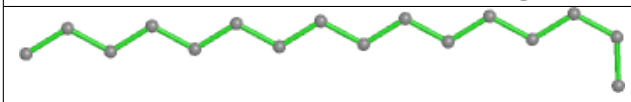


Torsions

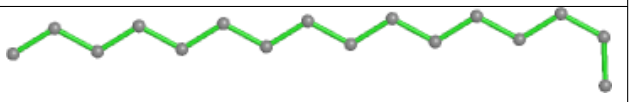


Rings

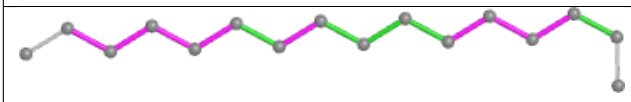
Ligand UPL A 2013



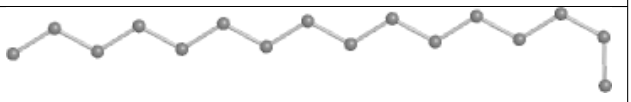
Bond lengths



Bond angles

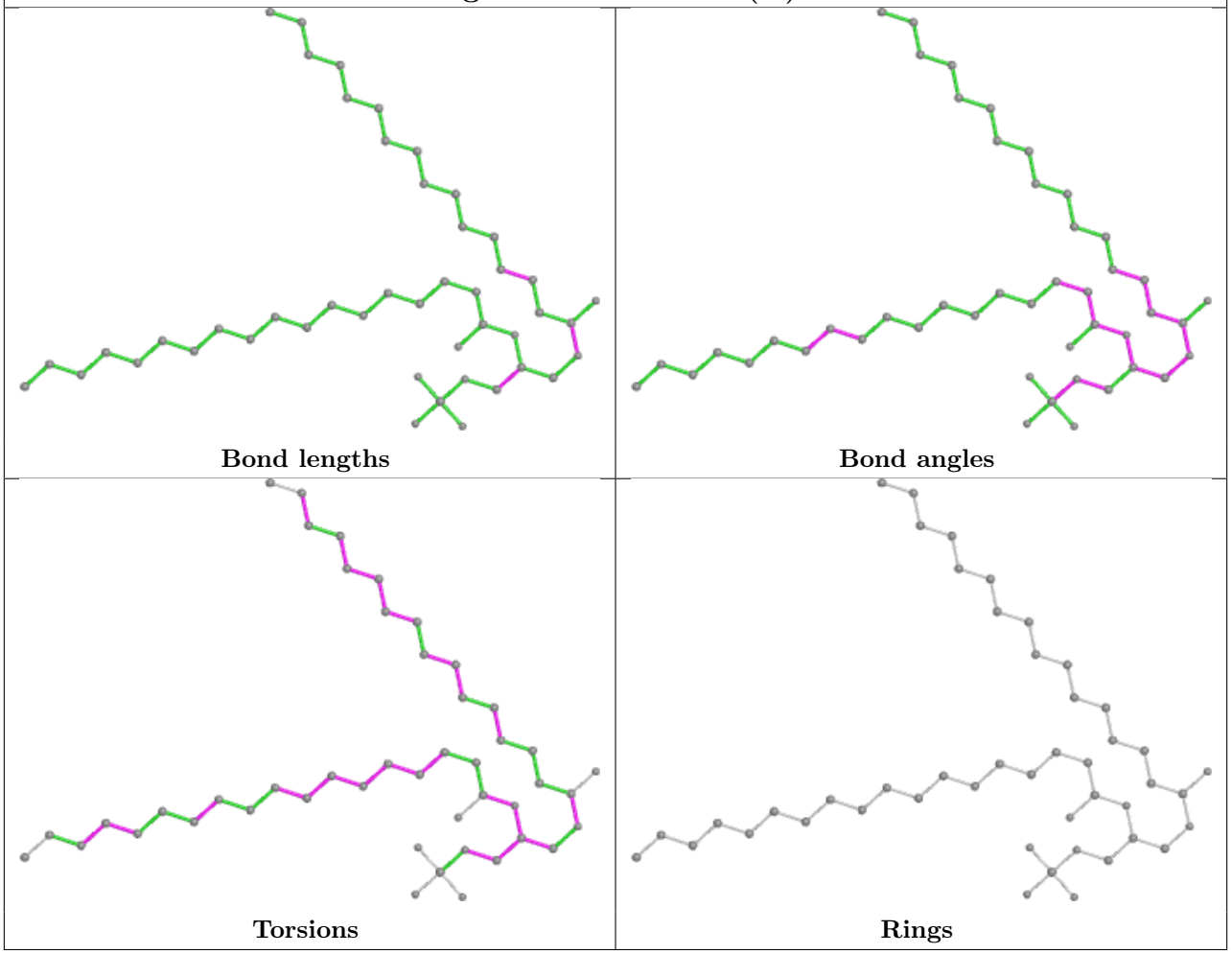


Torsions

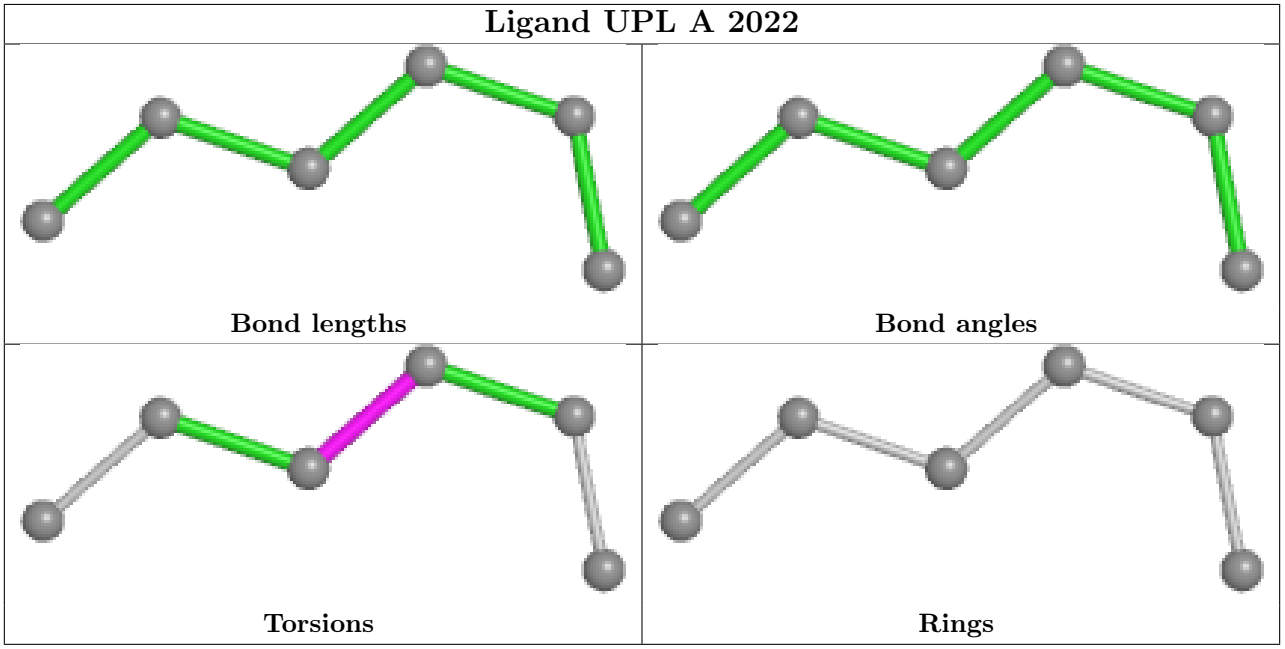


Rings

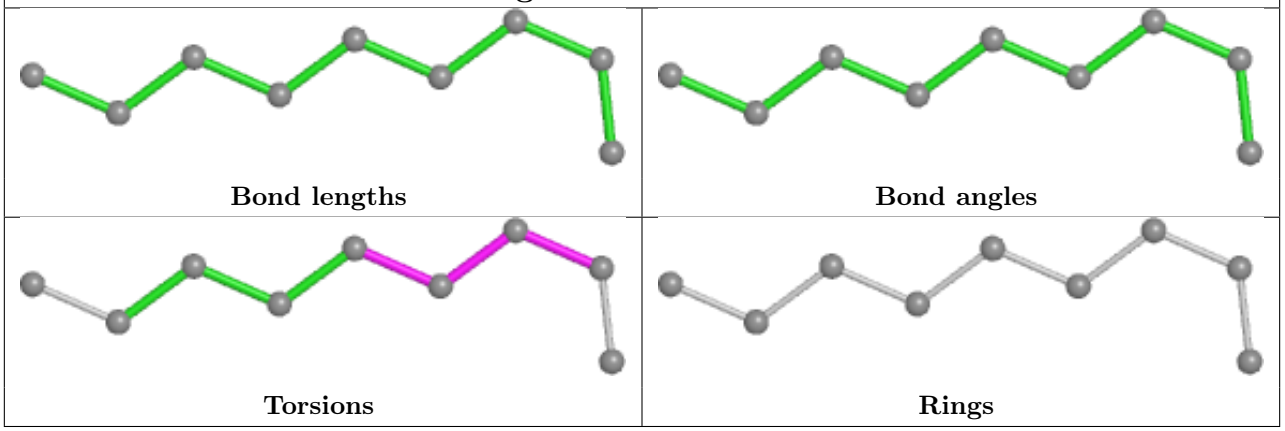
Ligand PLD A 2005 (A)



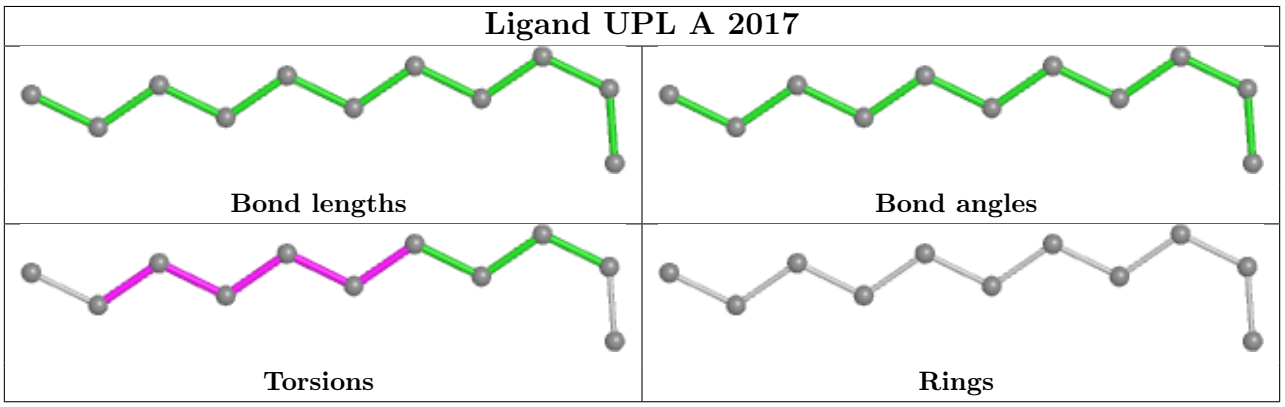
Ligand UPL A 2022



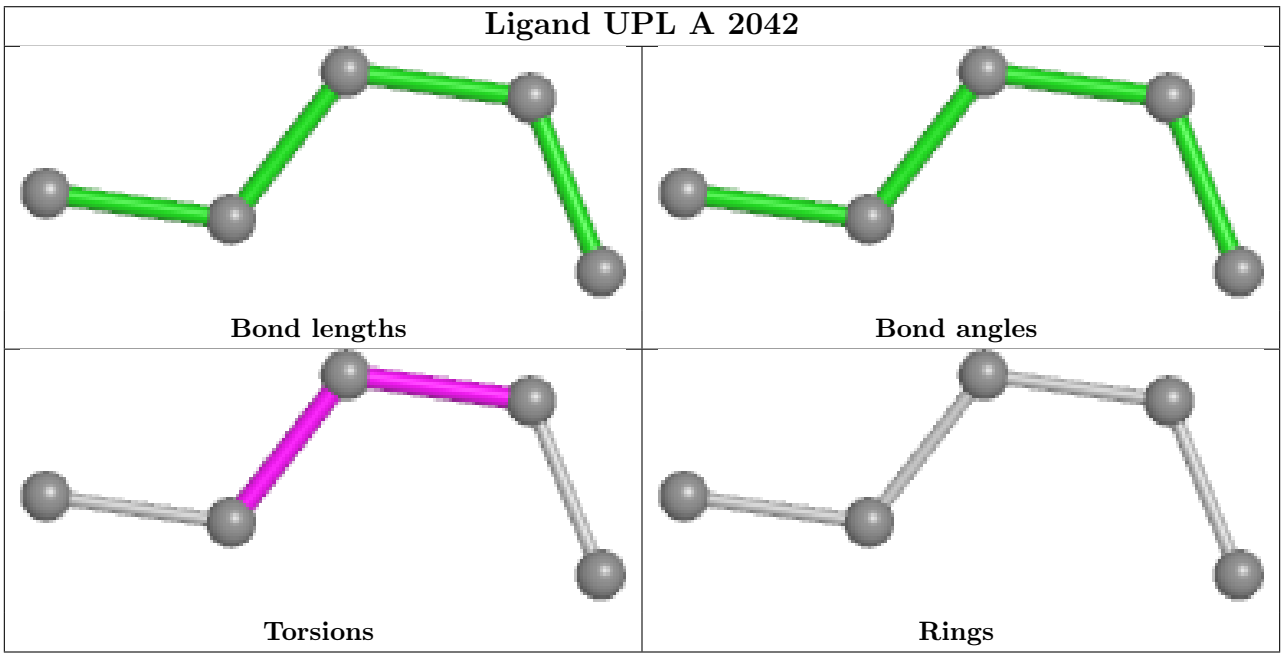
Ligand UPL A 2029



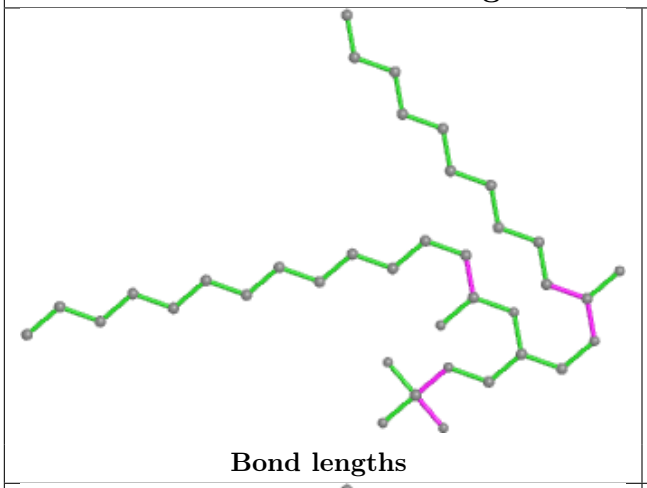
Ligand UPL A 2017



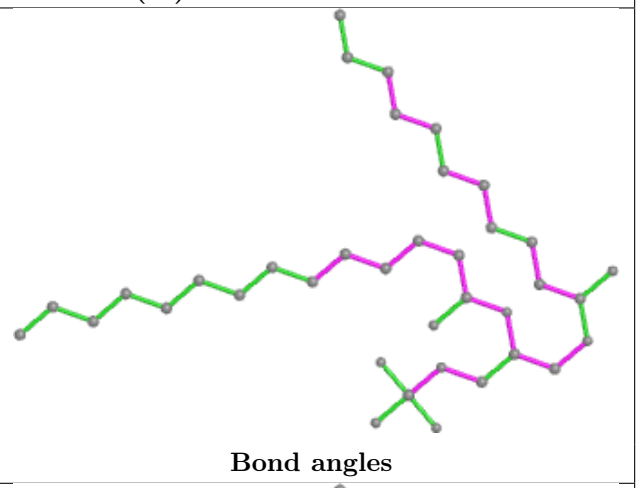
Ligand UPL A 2042



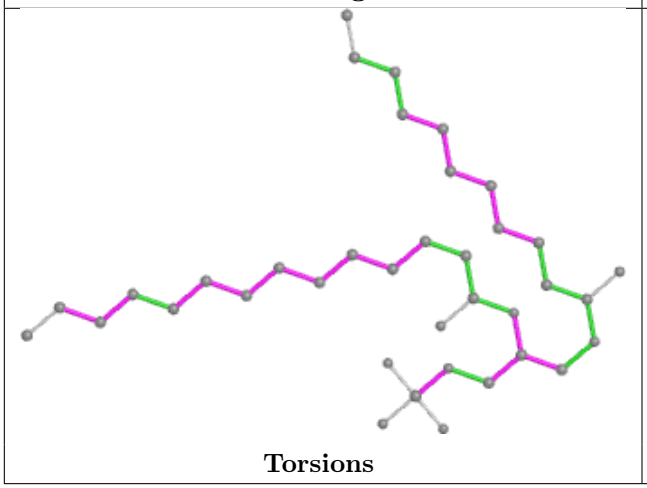
Ligand PLD A 2007 (A)



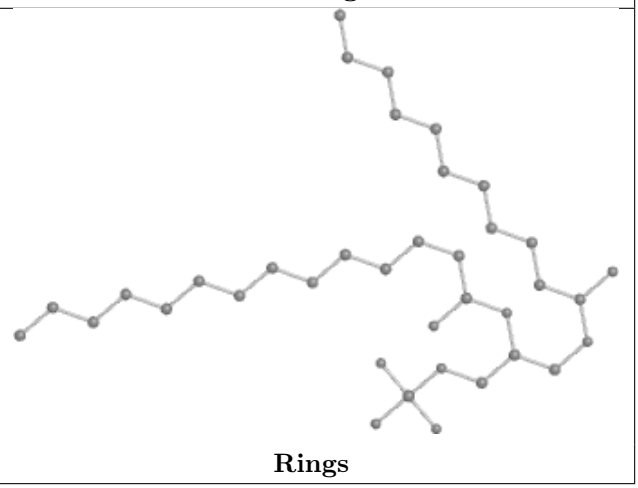
Bond lengths



Bond angles

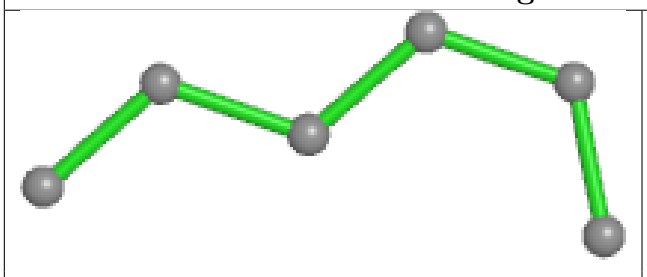


Torsions

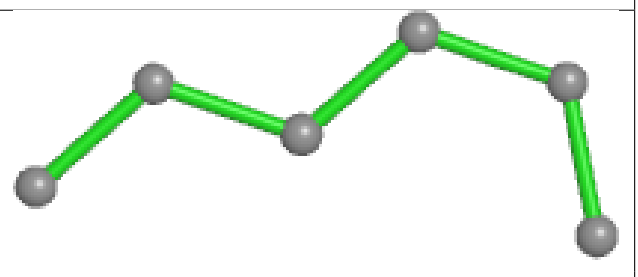


Rings

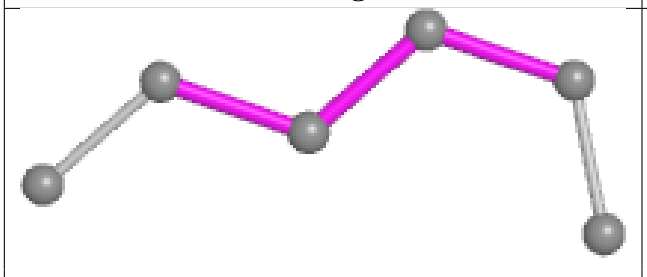
Ligand UPL B 2049



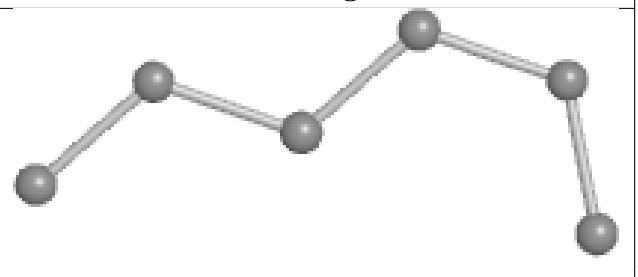
Bond lengths



Bond angles

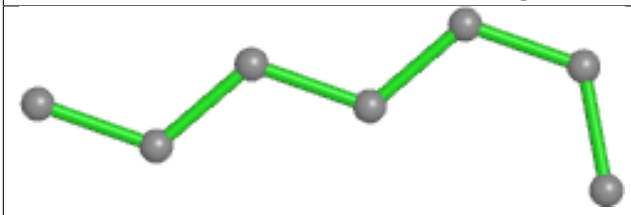


Torsions

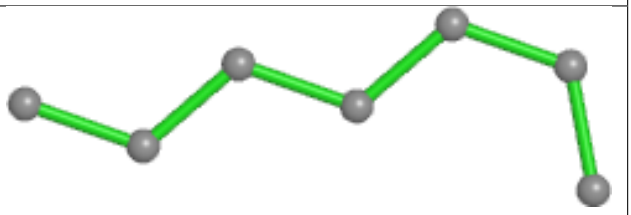


Rings

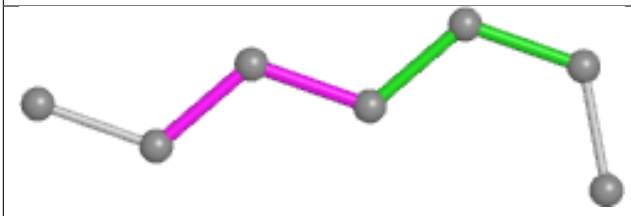
Ligand UPL A 2030



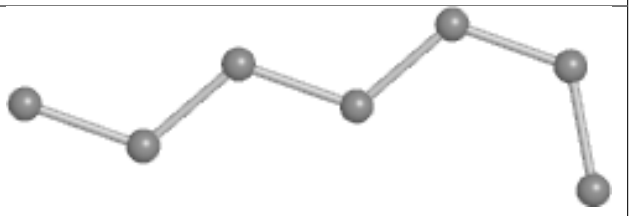
Bond lengths



Bond angles

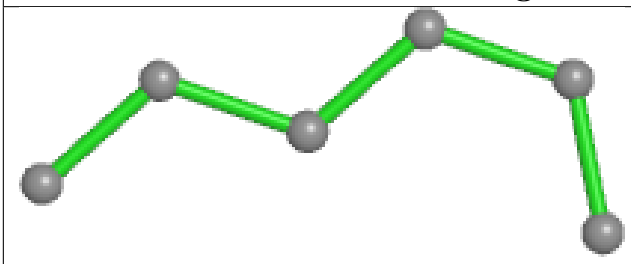


Torsions

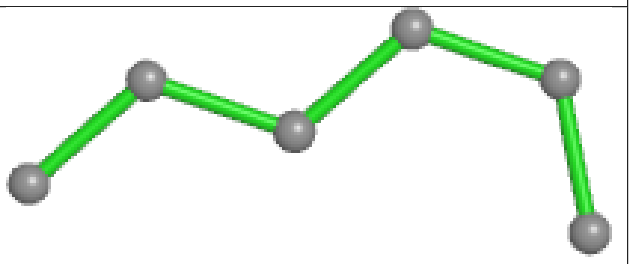


Rings

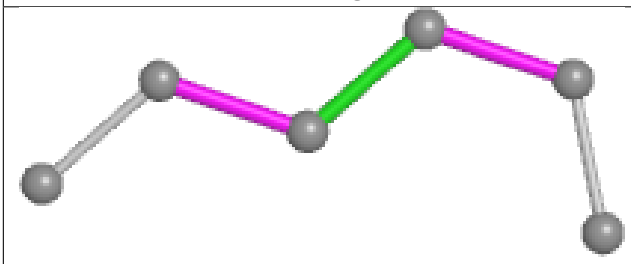
Ligand UPL A 2032



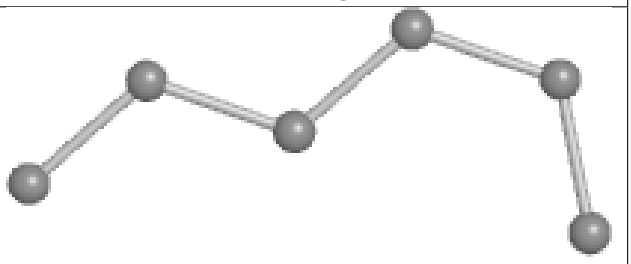
Bond lengths



Bond angles

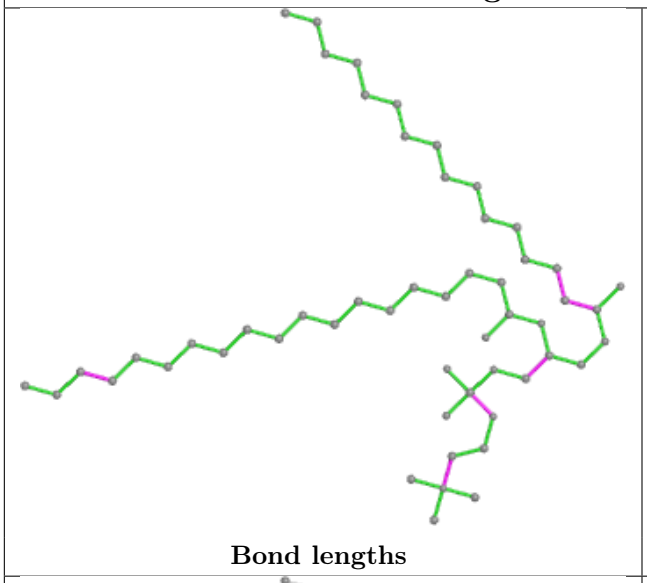


Torsions

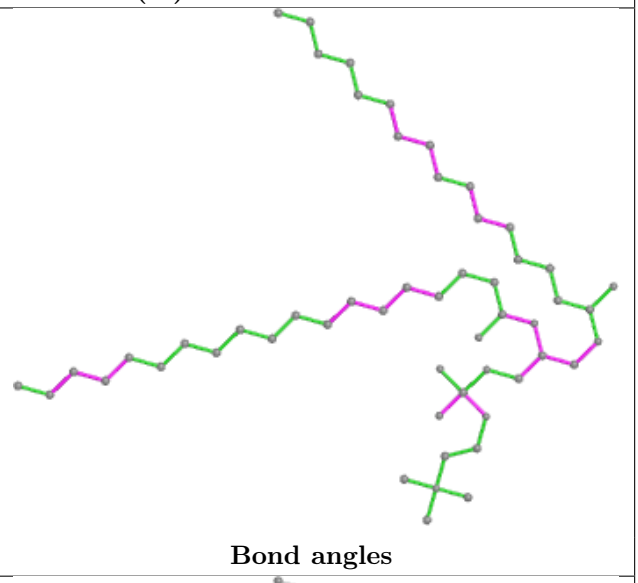


Rings

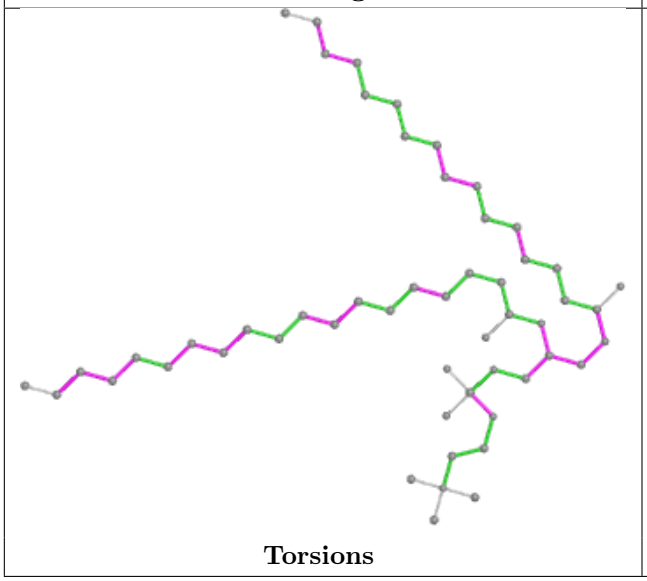
Ligand PLD A 2001 (B)



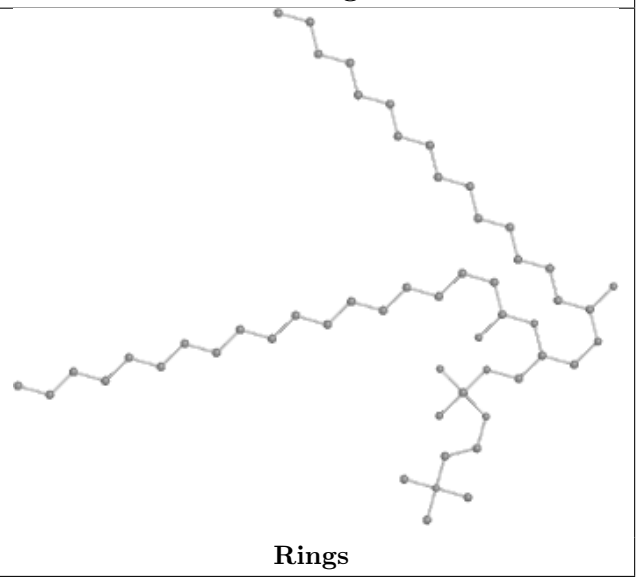
Bond lengths



Bond angles

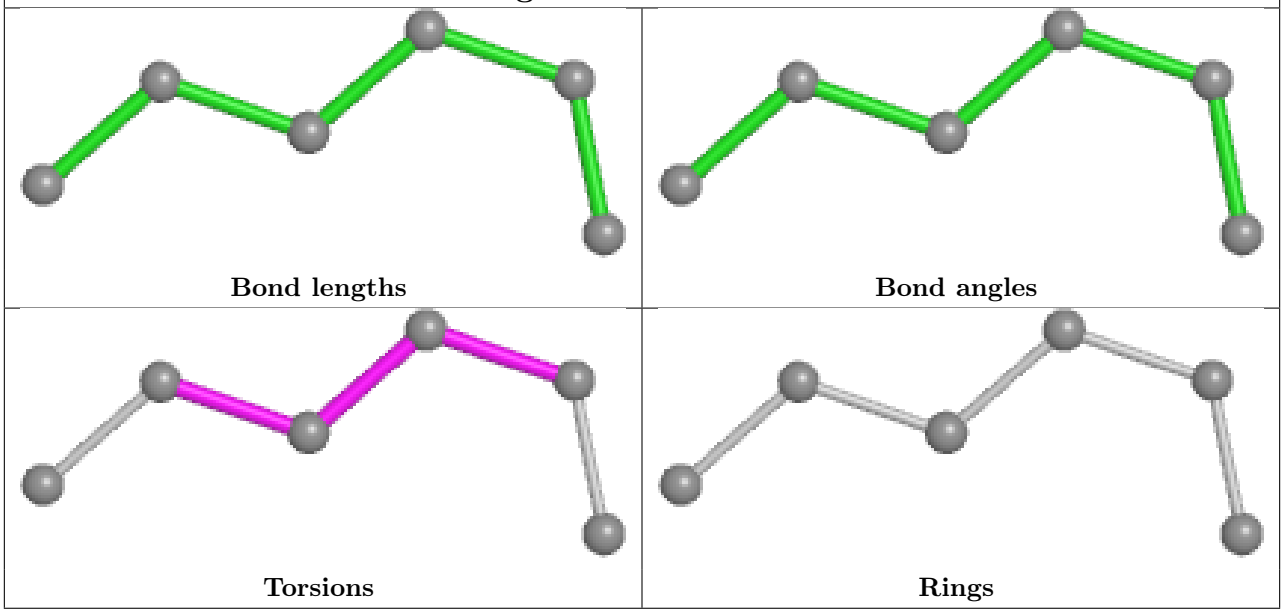


Torsions

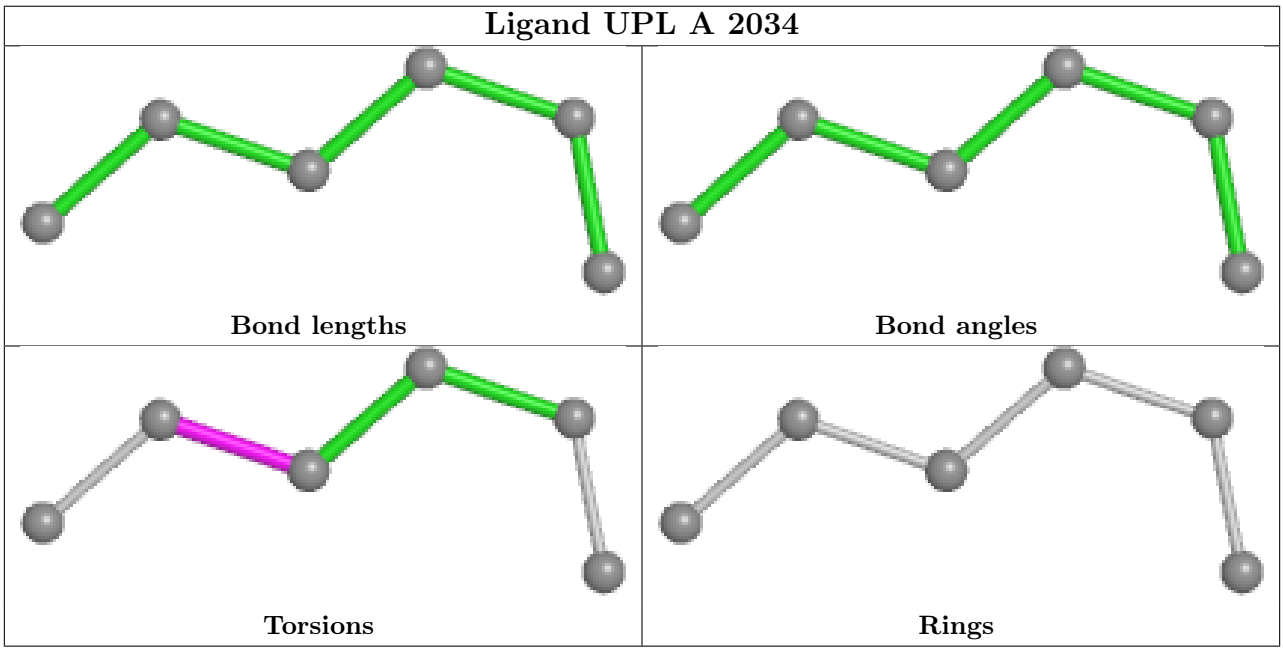


Rings

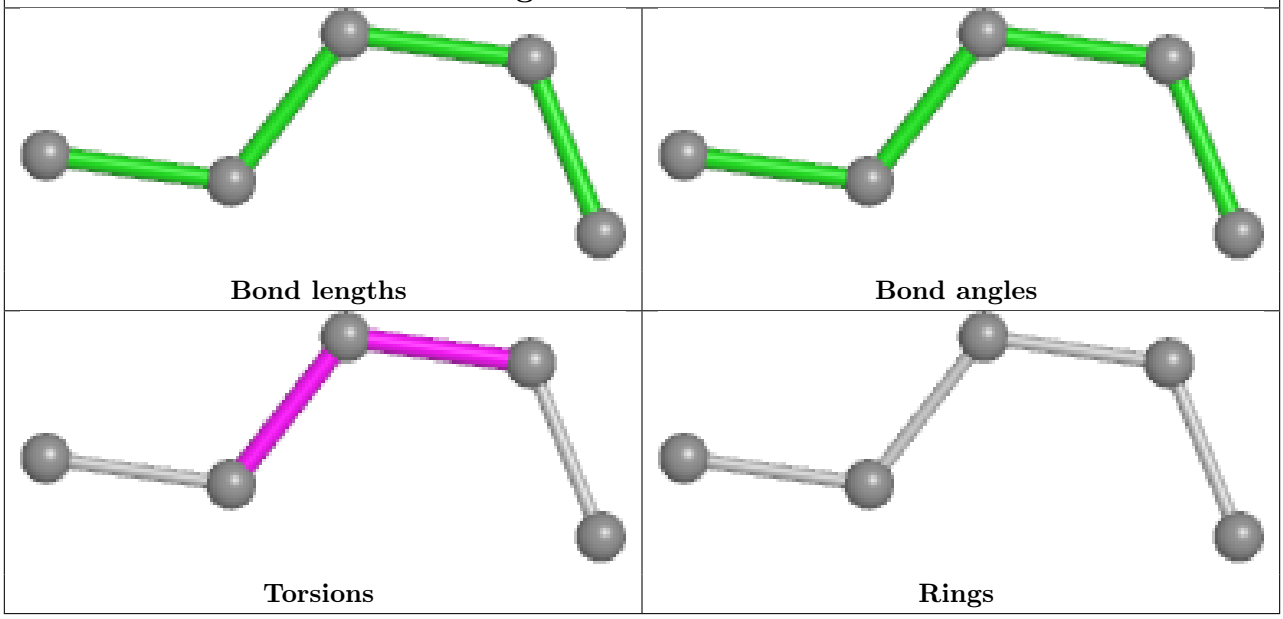
Ligand UPL A 2050



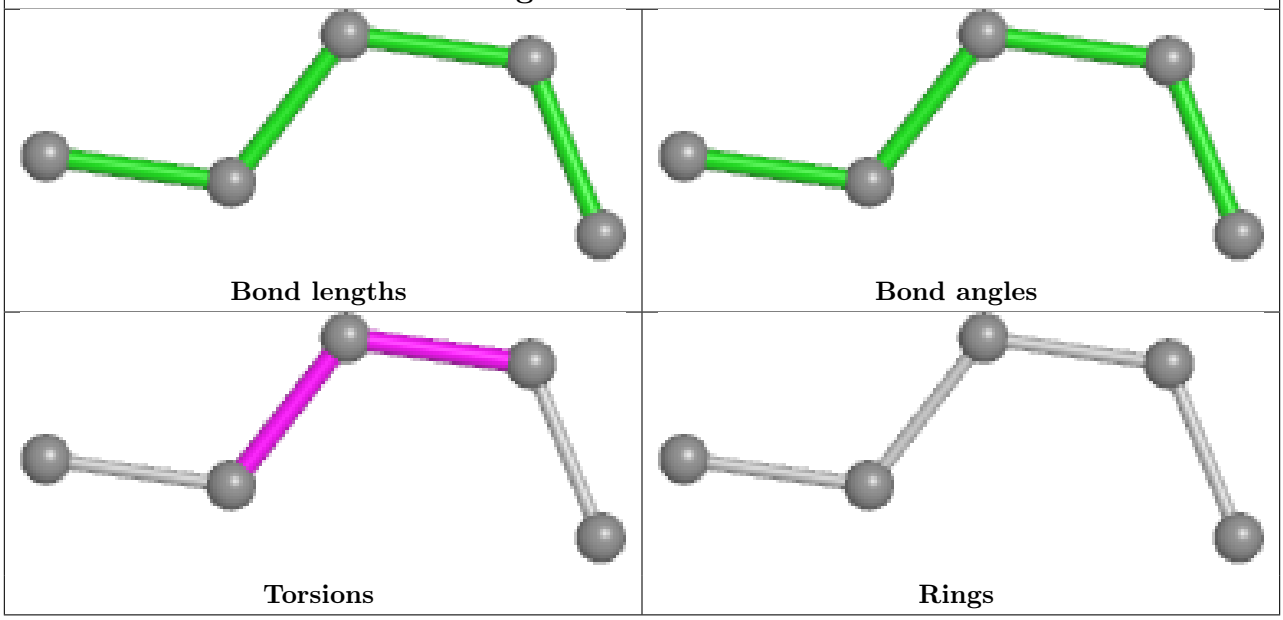
Ligand UPL A 2034



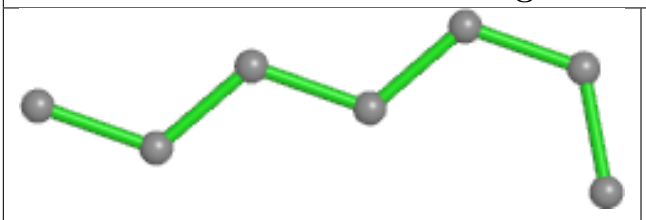
Ligand UPL A 2047



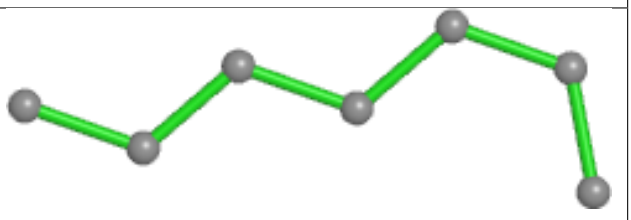
Ligand UPL A 2037



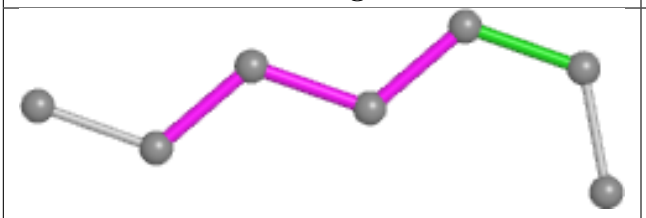
Ligand UPL B 2027



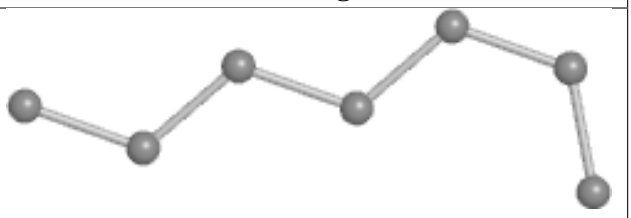
Bond lengths



Bond angles

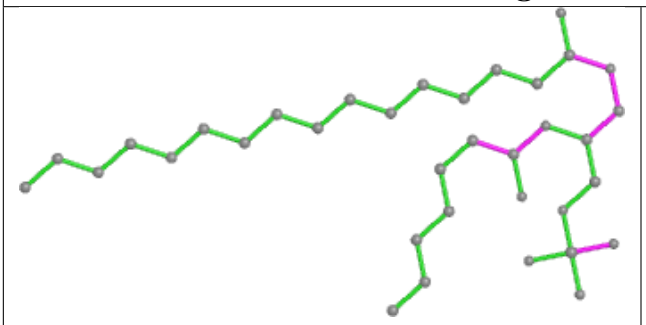


Torsions

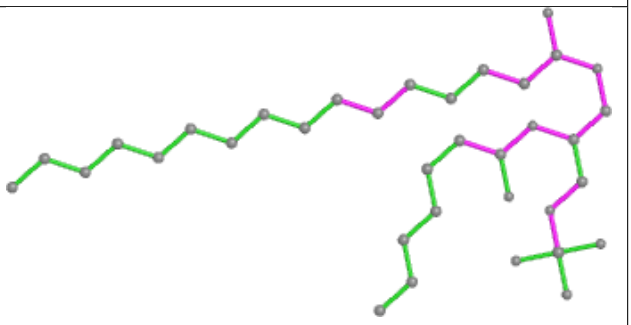


Rings

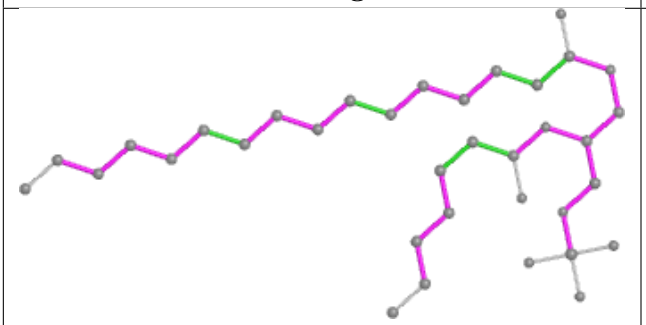
Ligand PLD A 2002



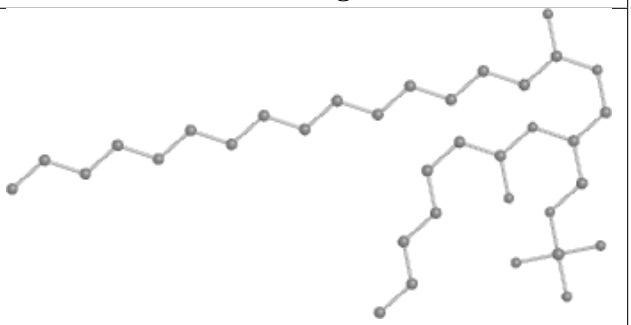
Bond lengths



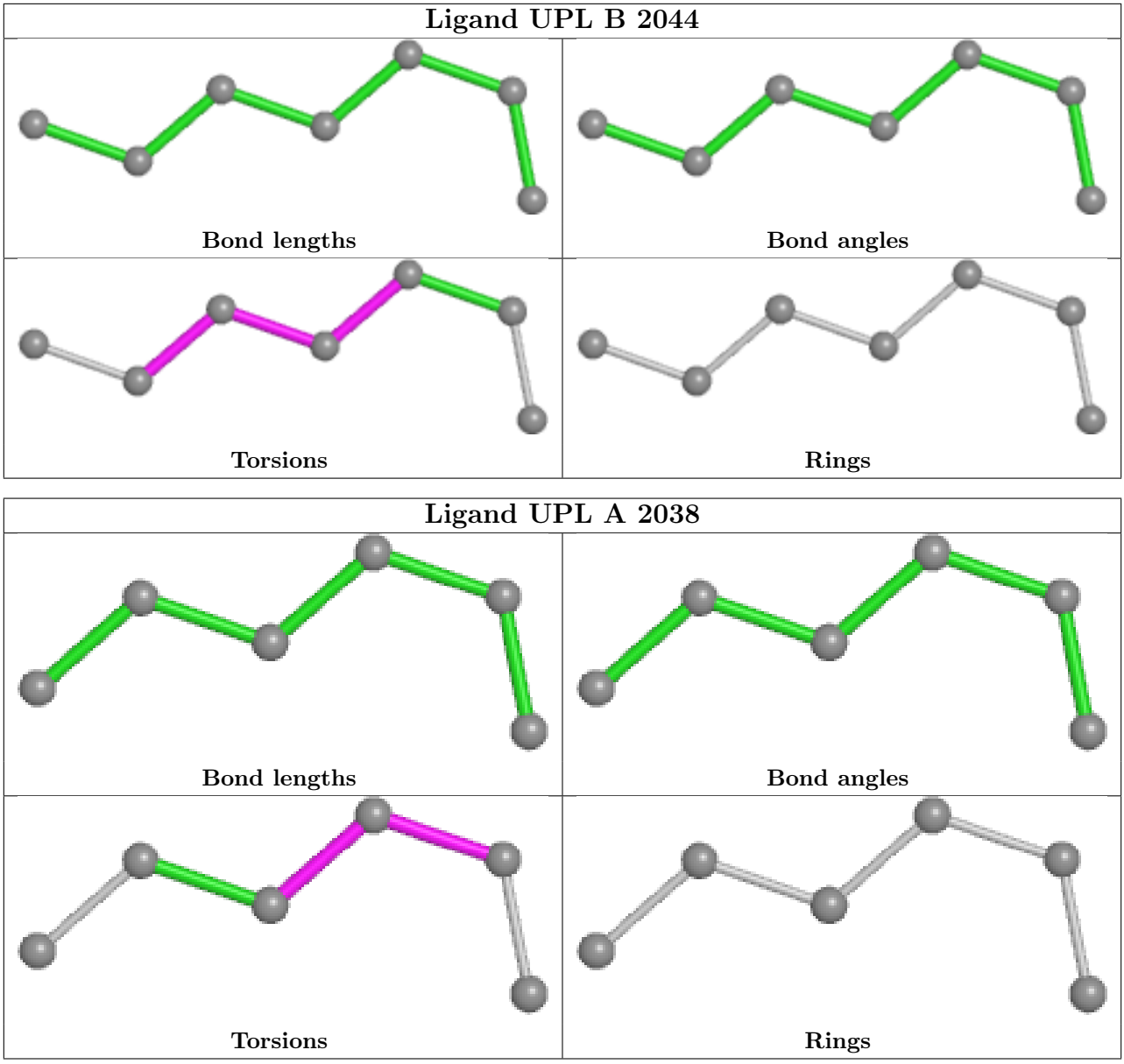
Bond angles



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	954/1056 (90%)	0.21	69 (7%) 15 17	19, 35, 77, 100	3 (0%)
2	B	174/319 (54%)	1.24	49 (28%) 0 0	36, 67, 96, 100	1 (0%)
All	All	1128/1375 (82%)	0.37	118 (10%) 6 7	19, 39, 86, 100	4 (0%)

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	LEU	8.6
1	A	266	ALA	7.6
2	B	1460	SER	7.3
1	A	447	VAL	6.8
2	B	1370	ASP	6.7

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

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
1	PCA	A	17	8/9	0.97	0.08	35,44,51,58	0

6.3 Carbohydrates

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	UPL	B	2016	13/34	0.35	0.35	71,86,91,95	0
4	UPL	A	2029	9/34	0.44	0.26	89,91,96,97	0
3	PLD	A	2006	34/60	0.44	0.33	62,88,99,100	0
4	UPL	A	2012	17/34	0.55	0.22	68,77,89,90	0
4	UPL	A	2038	6/34	0.59	0.19	81,85,87,92	0
4	UPL	A	2048	10/34	0.60	0.28	77,82,87,89	0
4	UPL	A	2008	17/34	0.62	0.28	86,91,100,100	0
4	UPL	B	2044	7/34	0.64	0.22	75,81,82,82	0
4	UPL	A	2018	12/34	0.68	0.14	60,73,81,82	0
4	UPL	B	2027	7/34	0.68	0.21	81,85,89,90	0
4	UPL	B	2031	7/34	0.68	0.21	81,82,85,85	0
4	UPL	A	2050	6/34	0.68	0.49	88,89,91,91	0
4	UPL	A	2030	7/34	0.69	0.20	37,58,72,73	0
4	UPL	A	2040	5/34	0.70	0.21	56,58,71,71	0
4	UPL	A	2024	6/34	0.71	0.43	75,89,95,95	0
4	UPL	A	2041	5/34	0.73	0.28	87,90,95,96	0
4	UPL	A	2009	15/34	0.74	0.18	55,68,78,85	0
4	UPL	A	2020	6/34	0.74	0.30	70,77,80,82	0
3	PLD	A	2007[B]	37/60	0.75	0.17	51,92,100,100	3
4	UPL	A	2019	10/34	0.75	0.23	66,75,81,86	0
3	PLD	A	2007[A]	37/60	0.75	0.17	51,92,100,100	3
4	UPL	B	2028	7/34	0.76	0.30	87,92,93,93	0
3	PLD	A	2005[B]	46/60	0.76	0.23	31,85,99,100	7
3	PLD	A	2005[A]	46/60	0.76	0.23	31,85,99,100	7
3	PLD	A	2002	35/60	0.77	0.20	49,79,90,94	0
4	UPL	A	2025	8/34	0.77	0.14	73,77,79,84	0
4	UPL	A	2026	8/34	0.77	0.27	43,71,84,85	0
4	UPL	A	2035	7/34	0.79	0.15	55,78,94,95	0
4	UPL	B	2021	9/34	0.79	0.18	63,75,79,82	0
4	UPL	A	2047	5/34	0.79	0.41	84,90,94,95	0
4	UPL	A	2015	13/34	0.81	0.15	75,80,89,92	0
3	PLD	B	2003	31/60	0.82	0.17	63,84,90,93	2
4	UPL	A	2039	5/34	0.82	0.15	58,62,73,78	0
4	UPL	A	2042	5/34	0.82	0.35	68,81,83,84	0
4	UPL	A	2036	6/34	0.83	0.15	87,89,90,91	0
4	UPL	B	2033	6/34	0.83	0.15	78,83,87,89	0
4	UPL	A	2037	5/34	0.83	0.14	52,60,62,69	0

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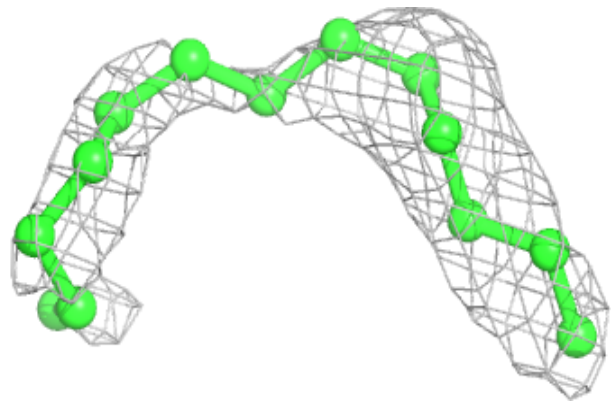
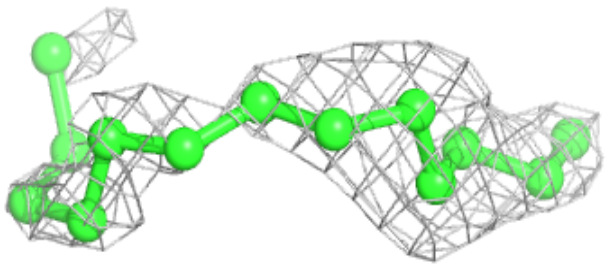
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UPL	A	2011	19/34	0.84	0.13	41,68,85,87	0
4	UPL	B	2023	9/34	0.85	0.18	52,68,71,72	0
4	UPL	A	2013	16/34	0.85	0.15	75,85,90,91	0
4	UPL	A	2032	6/34	0.86	0.26	77,82,88,91	0
4	UPL	B	2010	14/34	0.86	0.14	62,78,81,85	0
4	UPL	A	2022	6/34	0.87	0.12	87,88,94,94	0
4	UPL	B	2046	5/34	0.88	0.14	75,80,82,84	0
4	UPL	A	2017	11/34	0.89	0.12	44,67,94,97	0
4	UPL	B	2045	5/34	0.90	0.33	73,78,84,85	0
4	UPL	A	2034	6/34	0.90	0.09	59,62,65,65	0
4	UPL	A	2014	16/34	0.92	0.28	36,46,57,60	0
4	UPL	B	2049	6/34	0.92	0.12	90,92,100,100	0
3	PLD	A	2001[B]	53/60	0.93	0.19	24,43,74,83	4
3	PLD	A	2001[A]	53/60	0.93	0.19	27,44,74,83	4
3	PLD	A	2004	34/60	0.93	0.12	53,69,86,87	0
4	UPL	B	2043	5/34	0.94	0.20	78,81,82,84	0

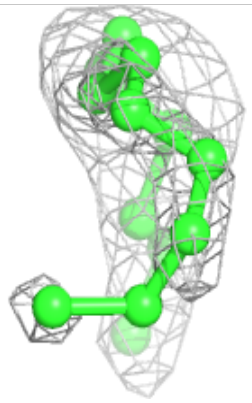
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UPL B 2016:

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

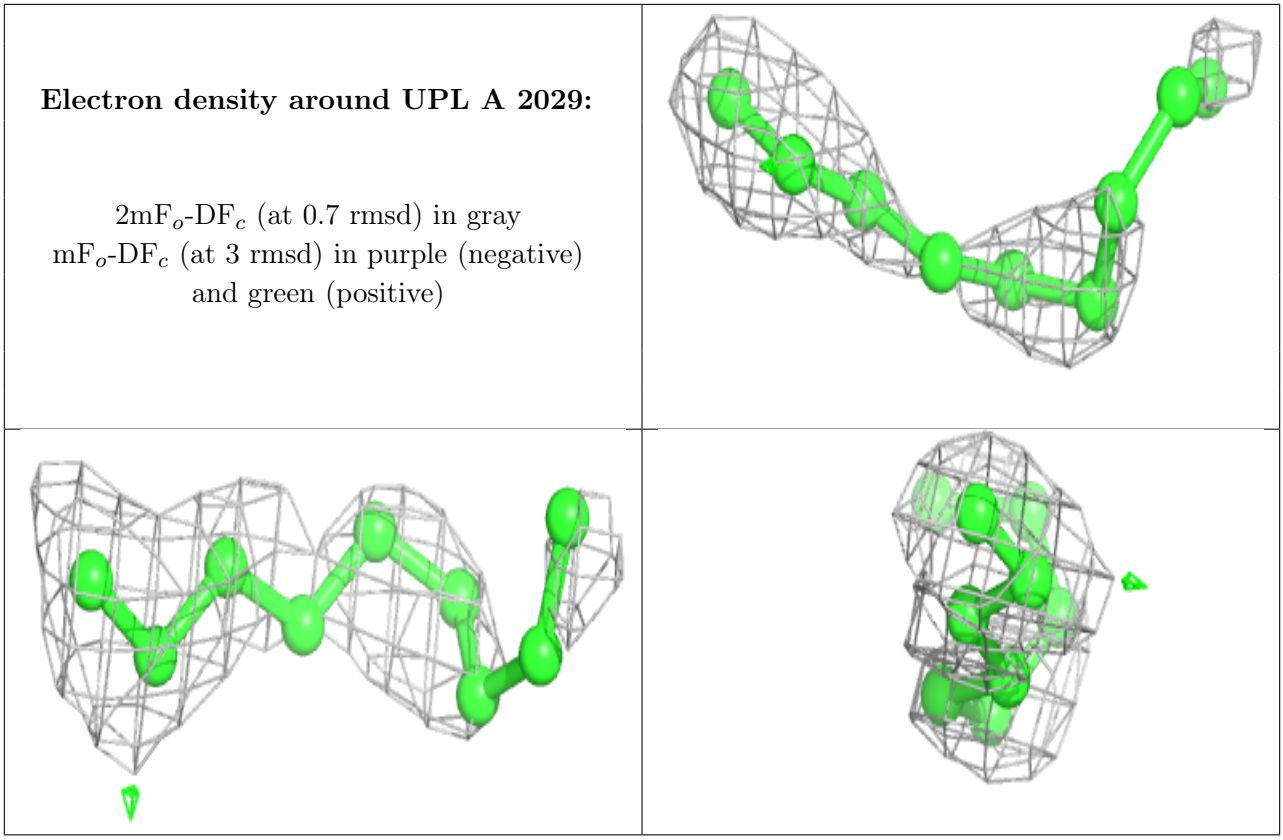






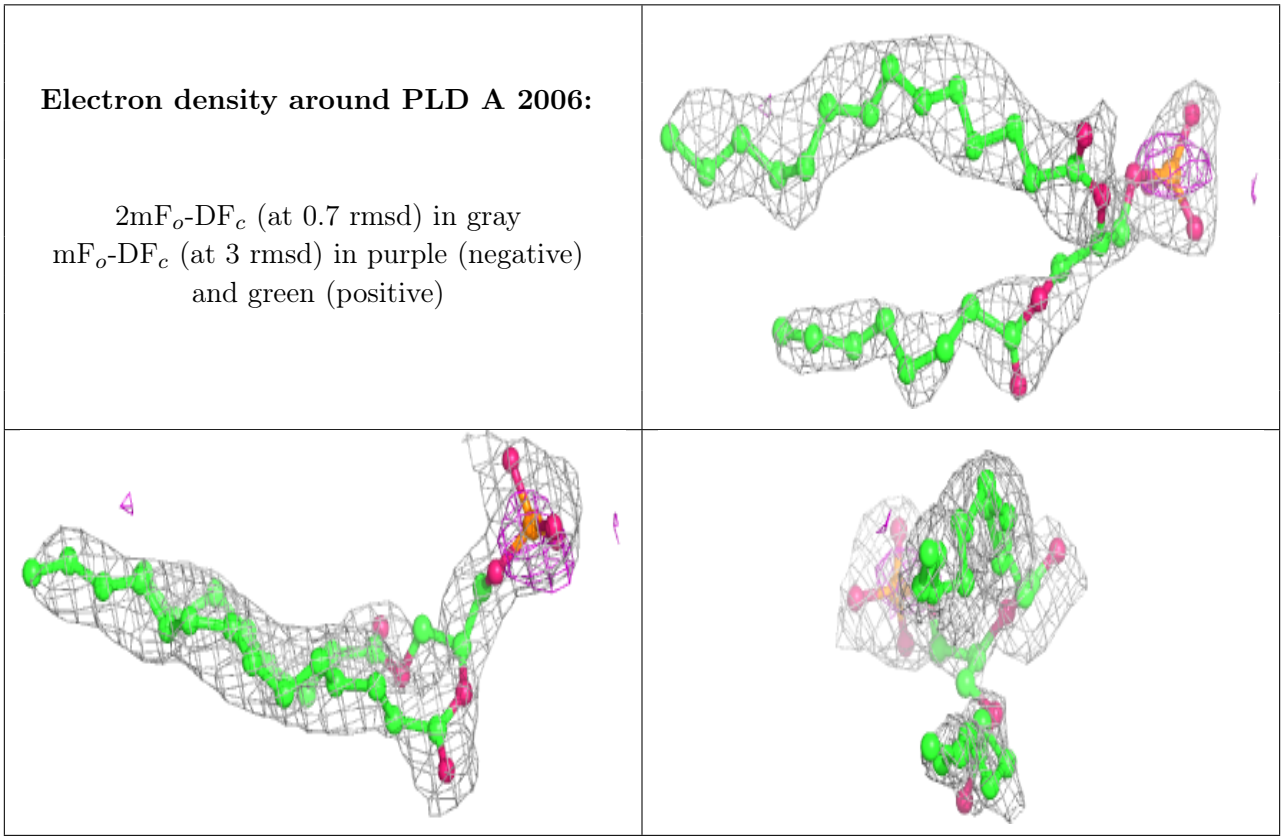
Electron density around UPL A 2029:

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



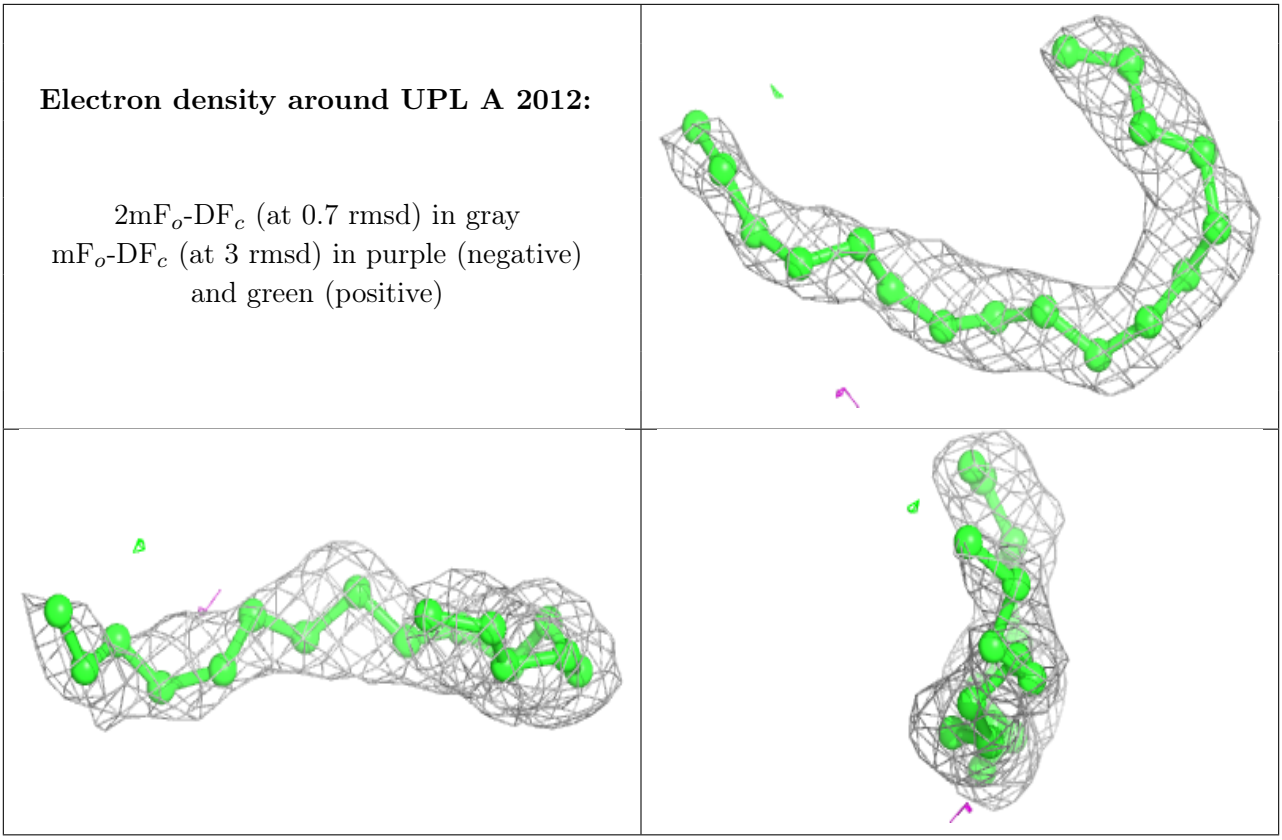
Electron density around PLD A 2006:

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



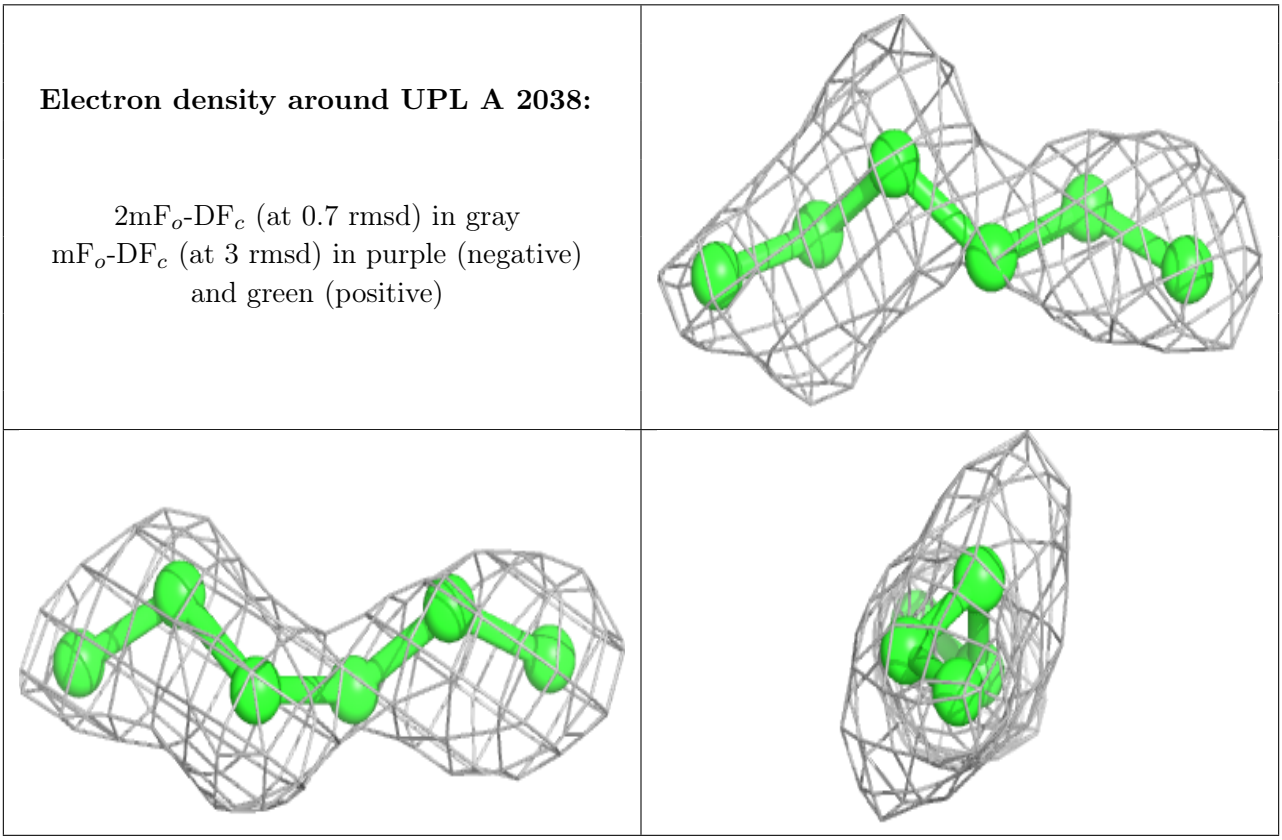
Electron density around UPL A 2012:

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



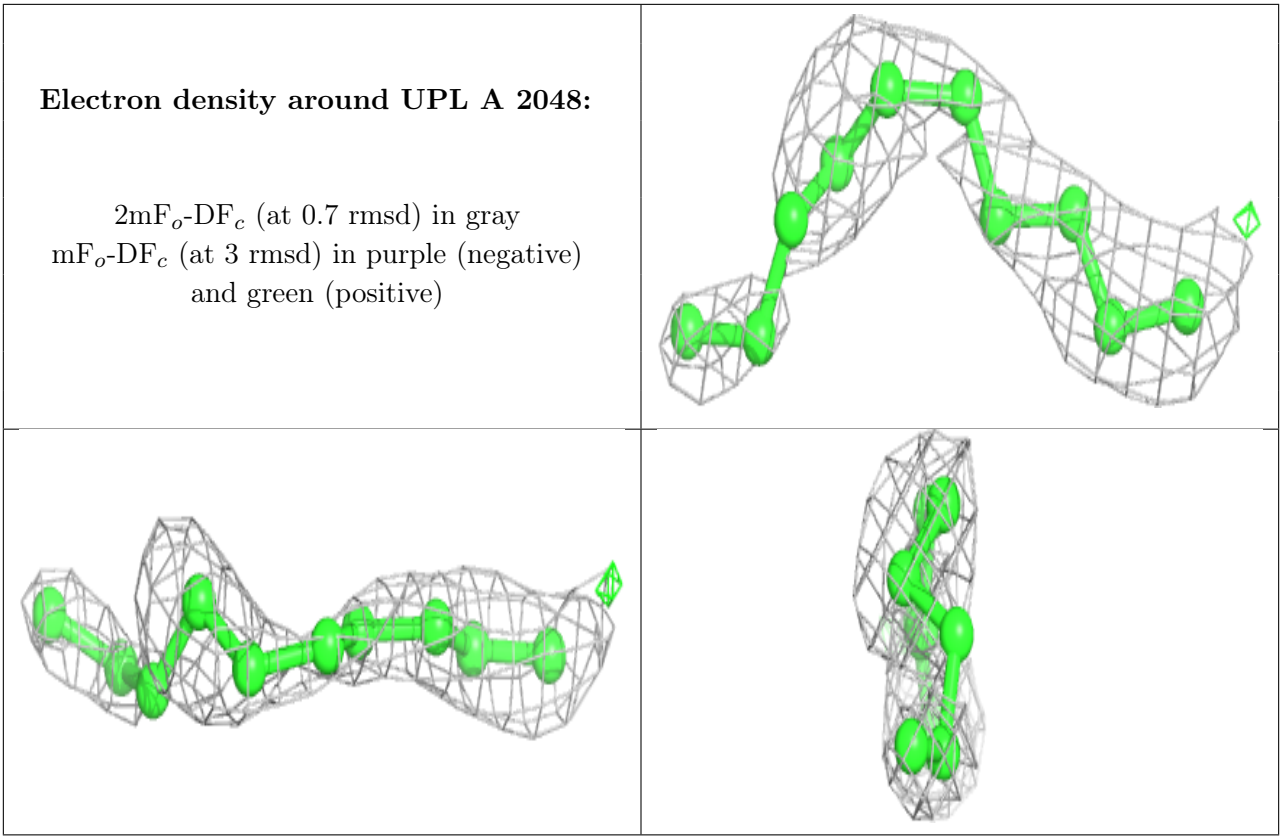
Electron density around UPL A 2038:

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



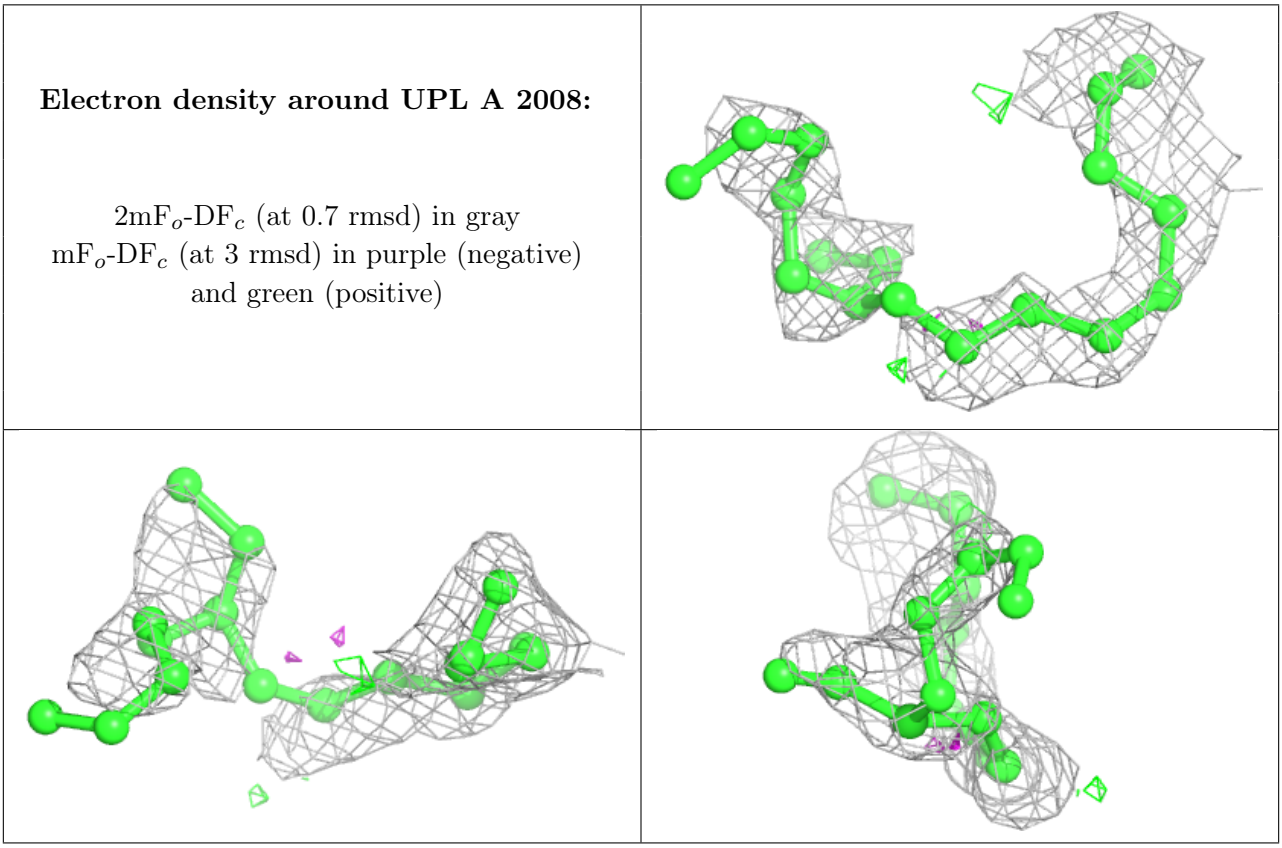
Electron density around UPL A 2048:

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



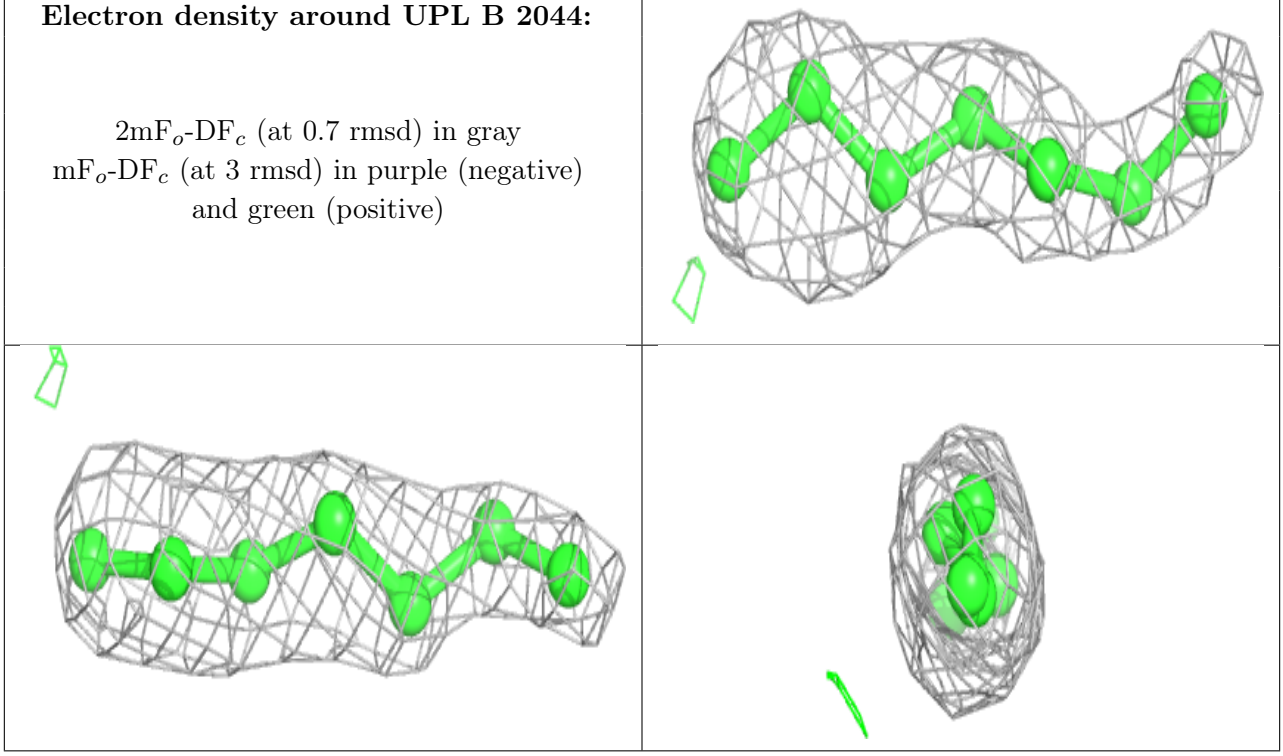
Electron density around UPL A 2008:

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



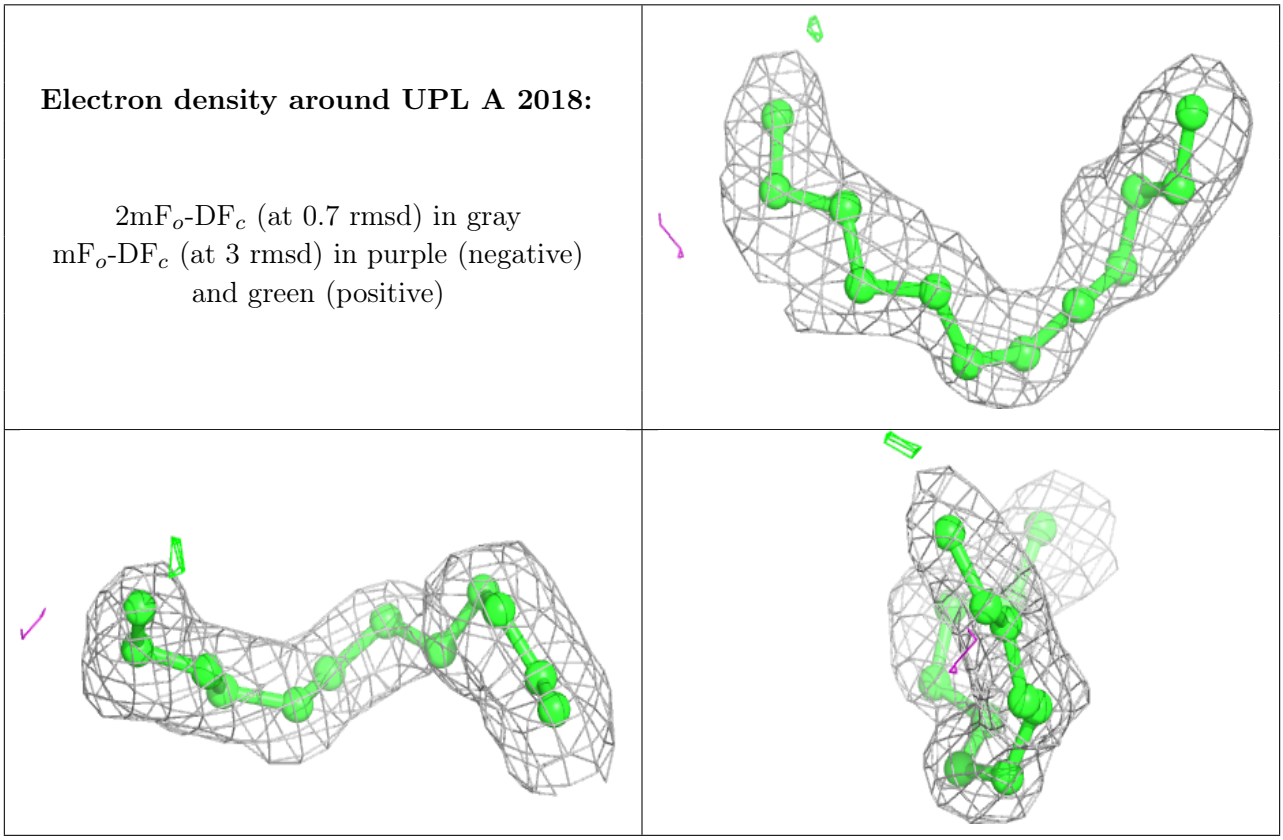
Electron density around UPL B 2044:

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



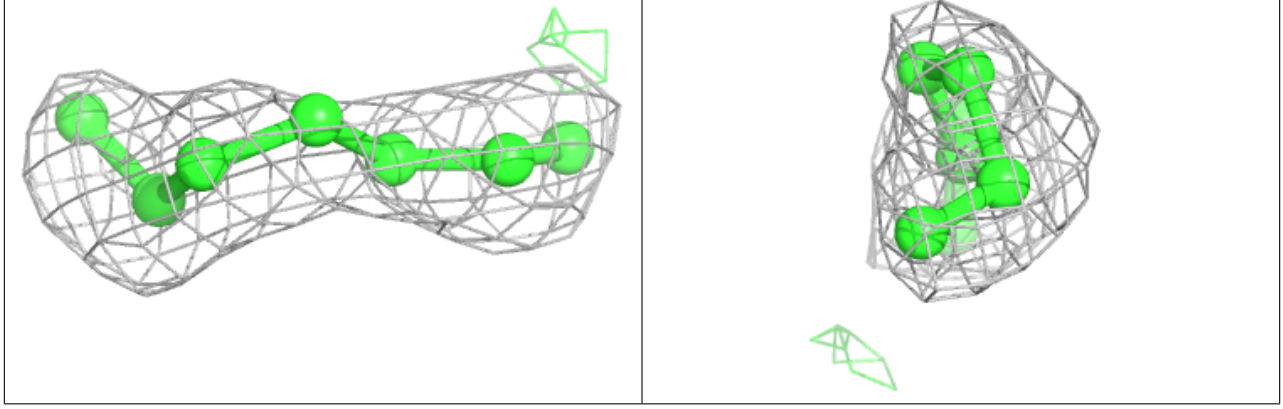
Electron density around UPL A 2018:

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



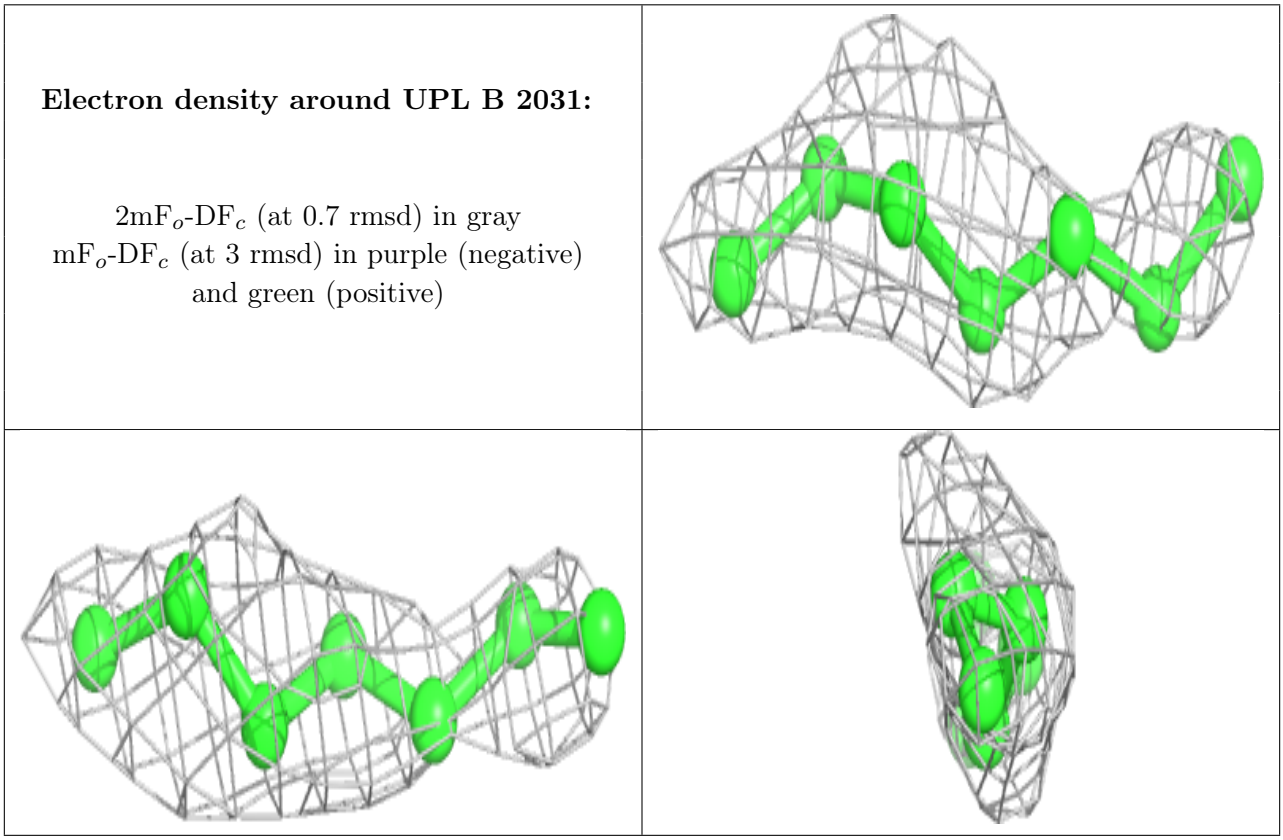
Electron density around UPL B 2027:

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



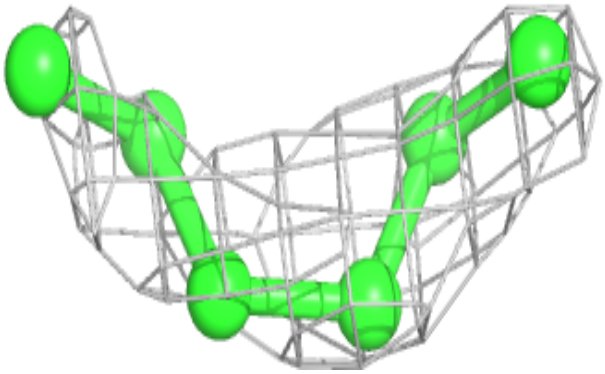
Electron density around UPL B 2031:

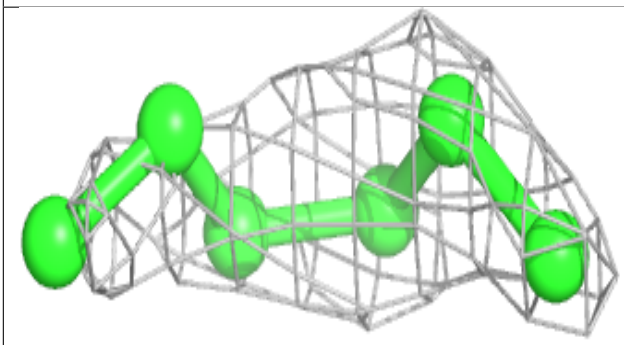
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

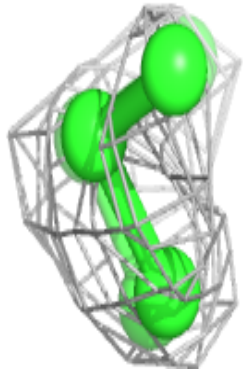


Electron density around UPL A 2050:

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

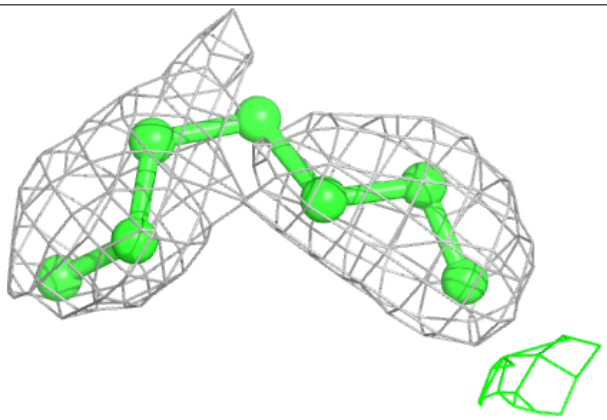


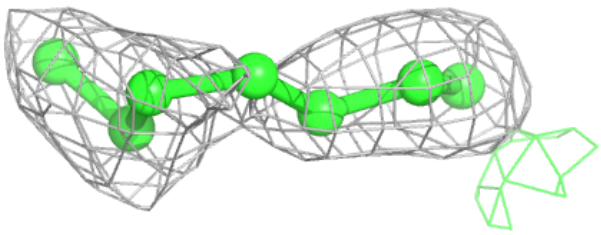


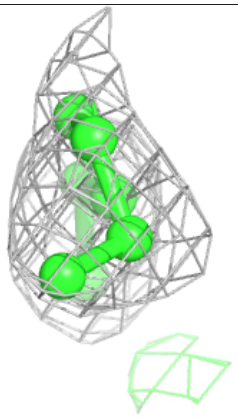


Electron density around UPL A 2030:

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

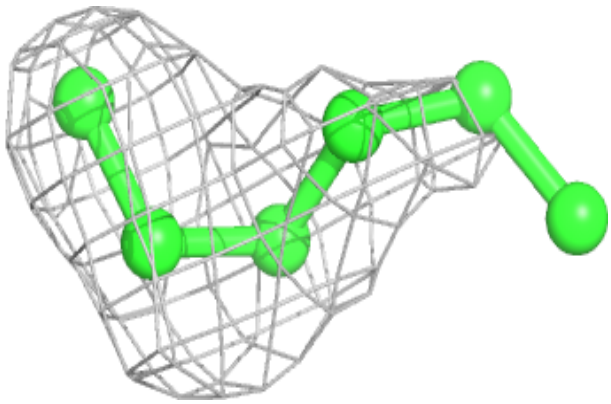


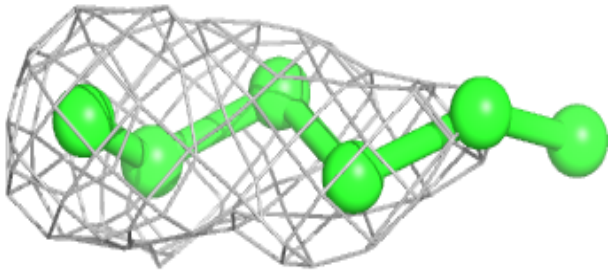


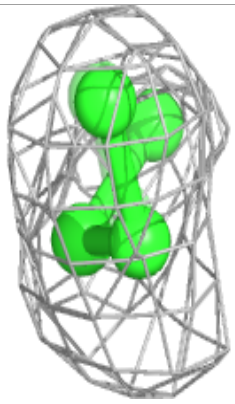


Electron density around UPL A 2024:

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

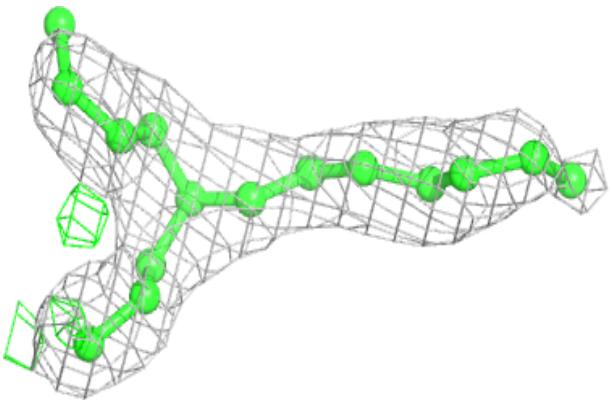


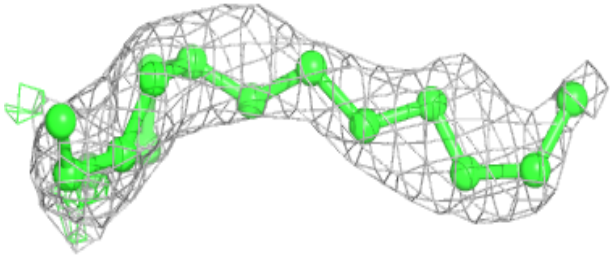


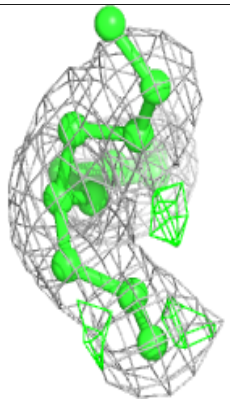


Electron density around UPL A 2009:

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

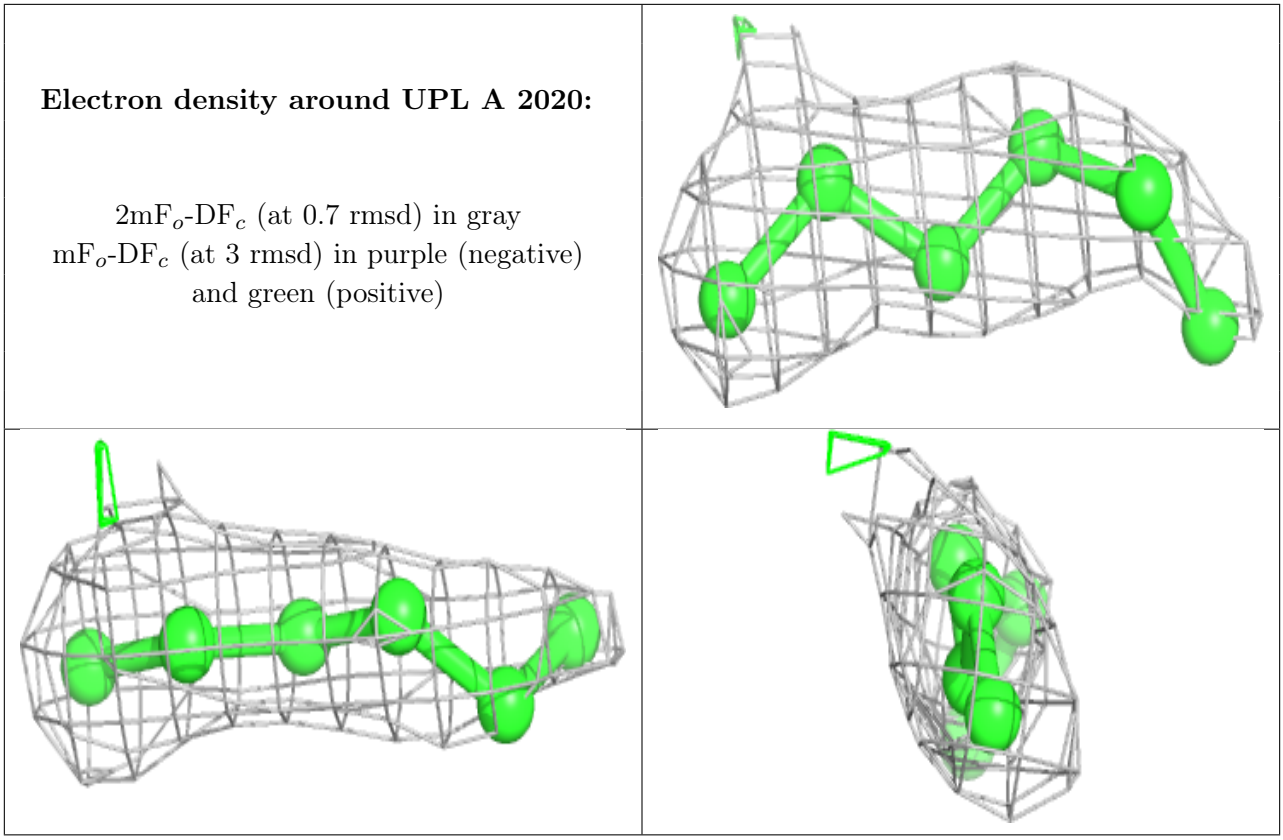






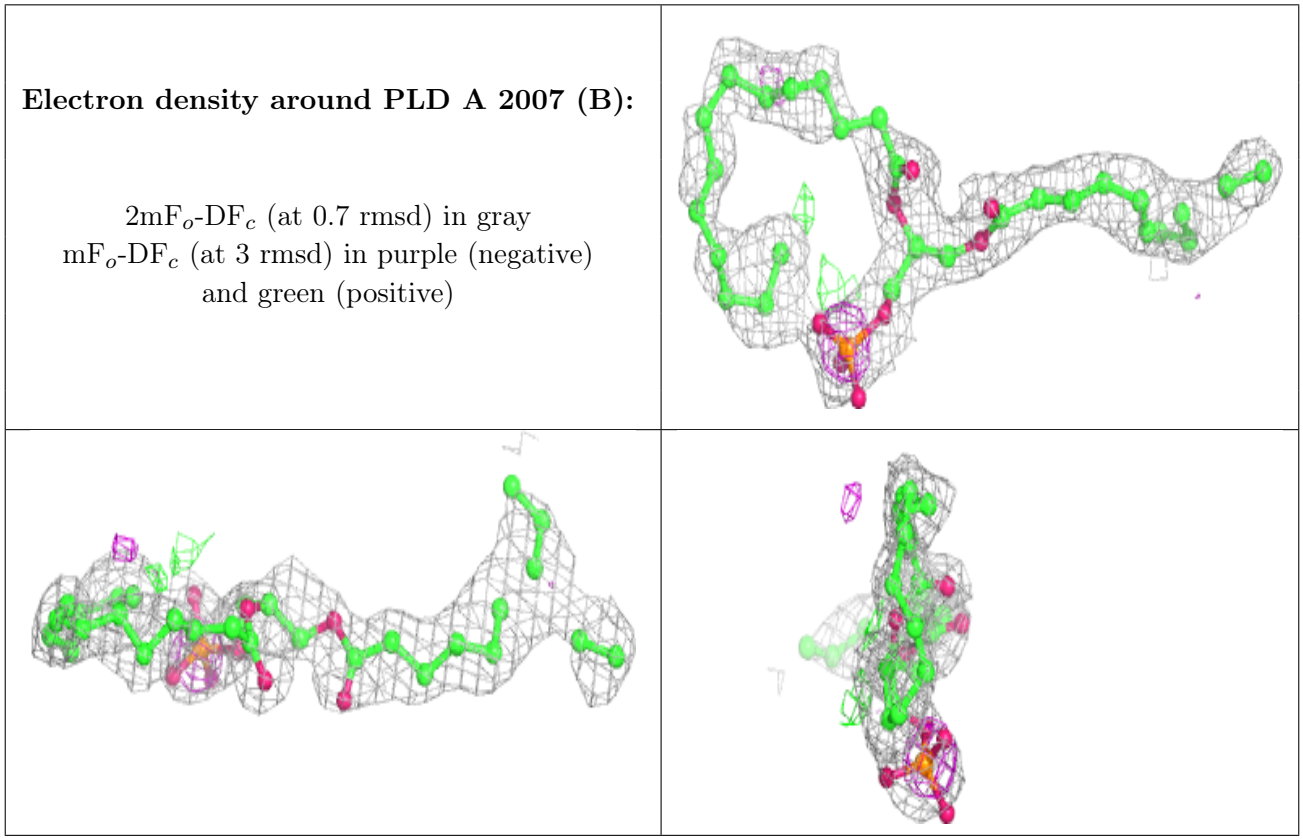
Electron density around UPL A 2020:

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



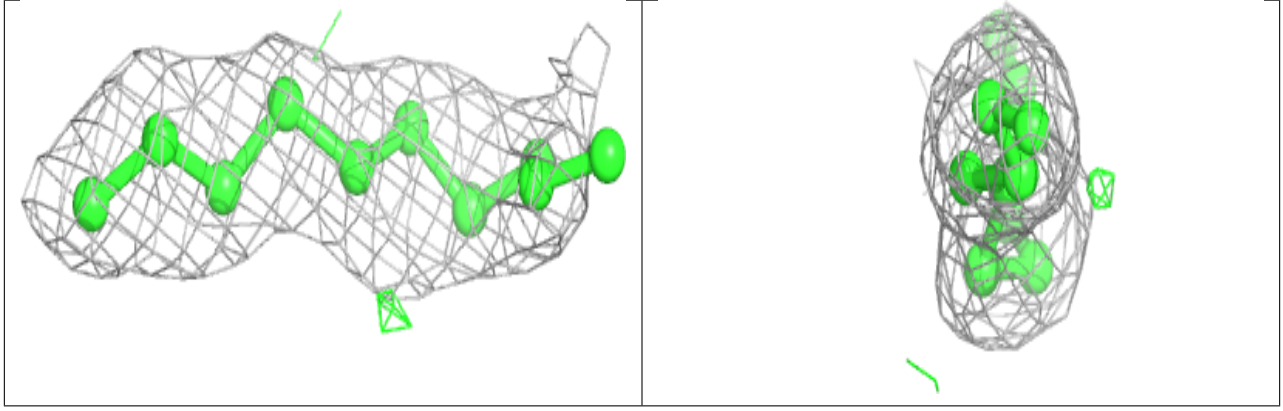
Electron density around PLD A 2007 (B):

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



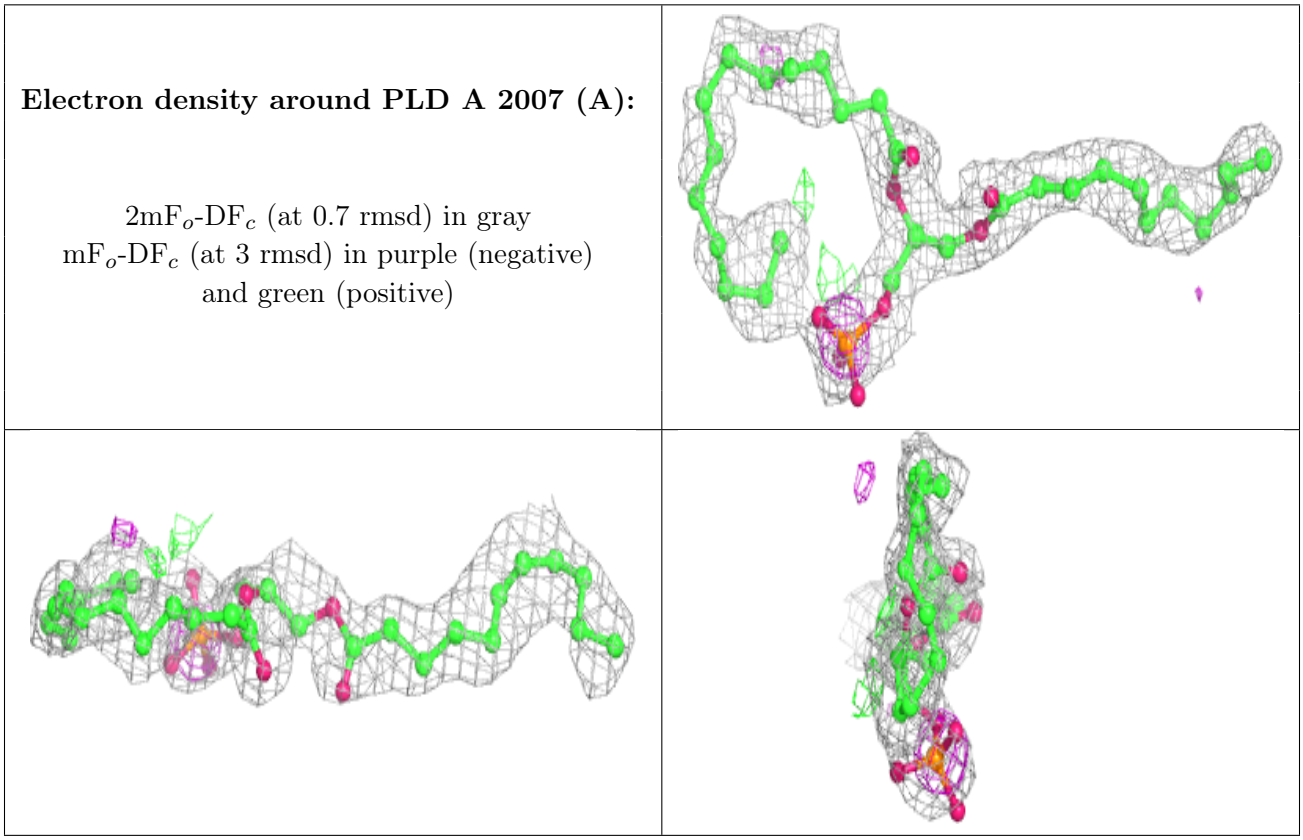
Electron density around UPL A 2019:

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



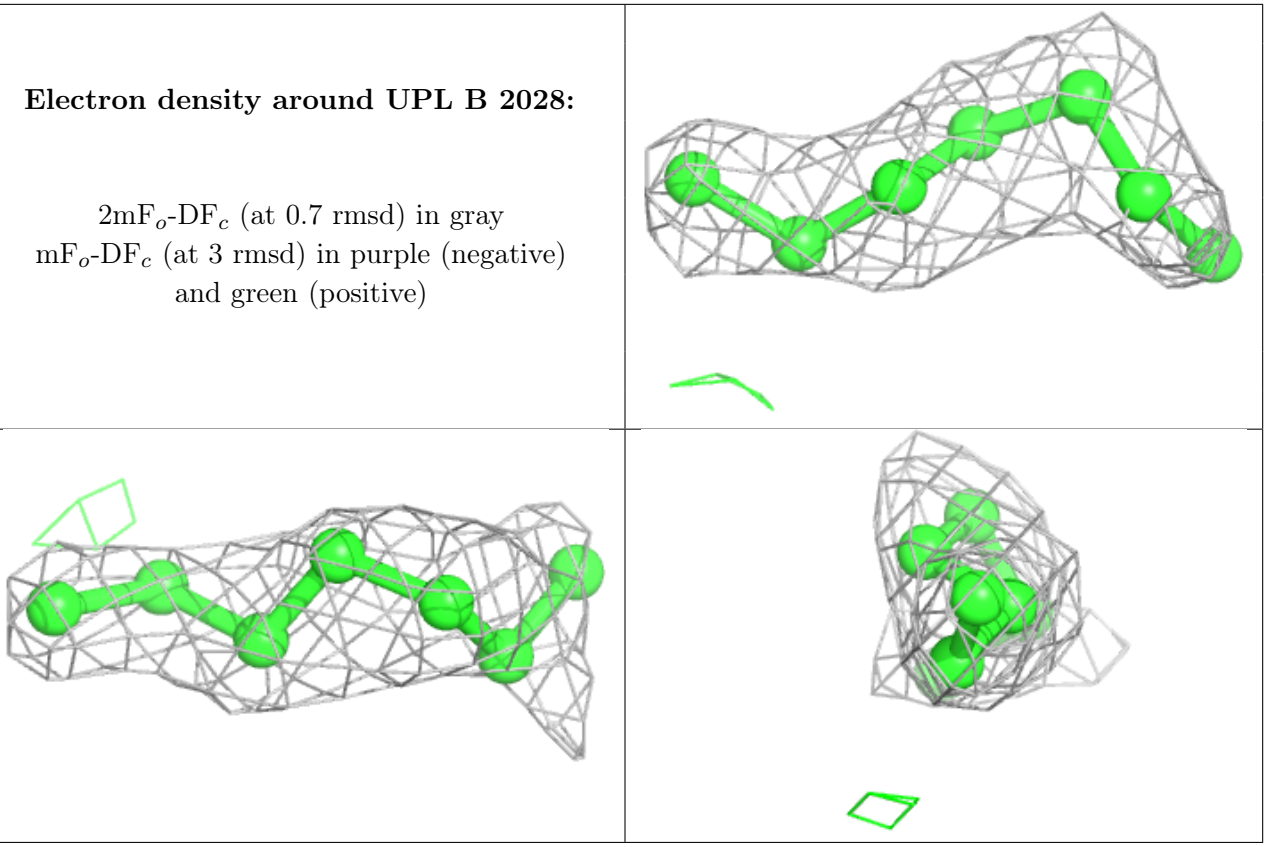
Electron density around PLD A 2007 (A):

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



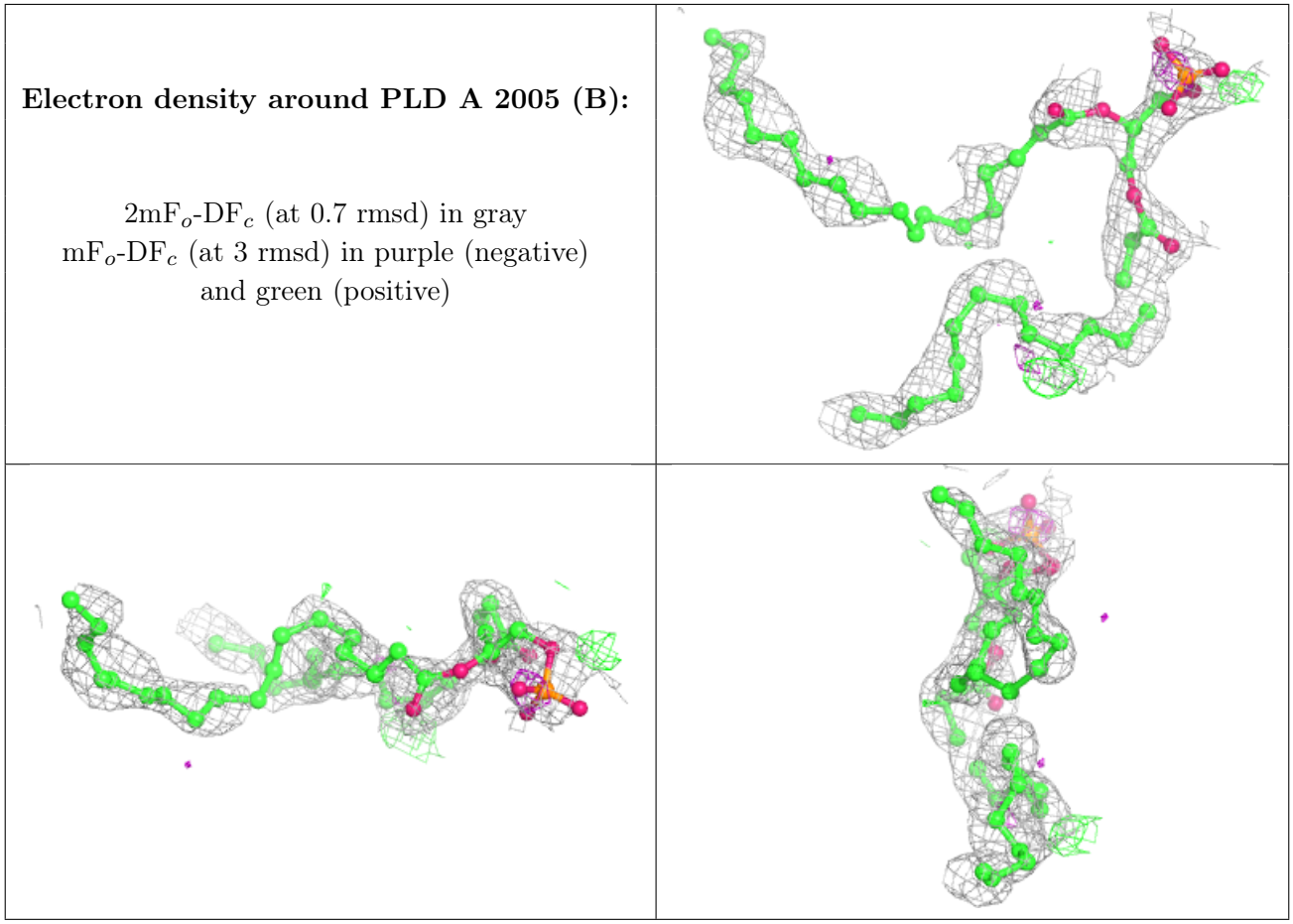
Electron density around UPL B 2028:

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



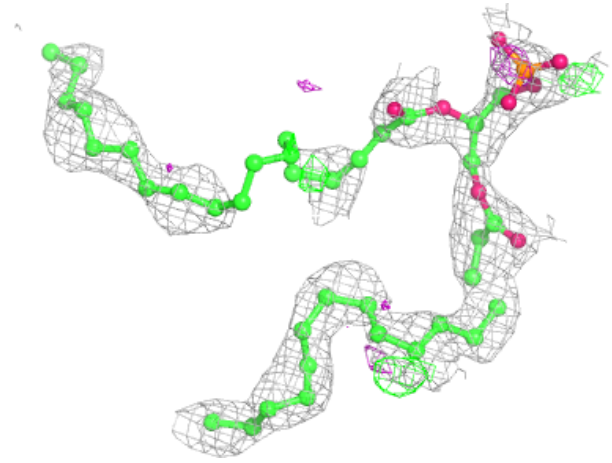
Electron density around PLD A 2005 (B):

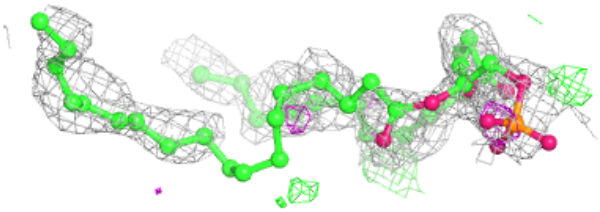
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

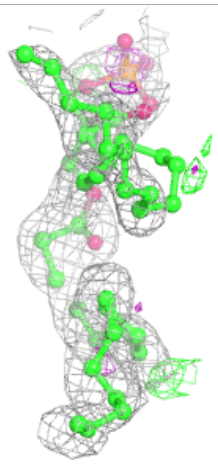


Electron density around PLD A 2005 (A):

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

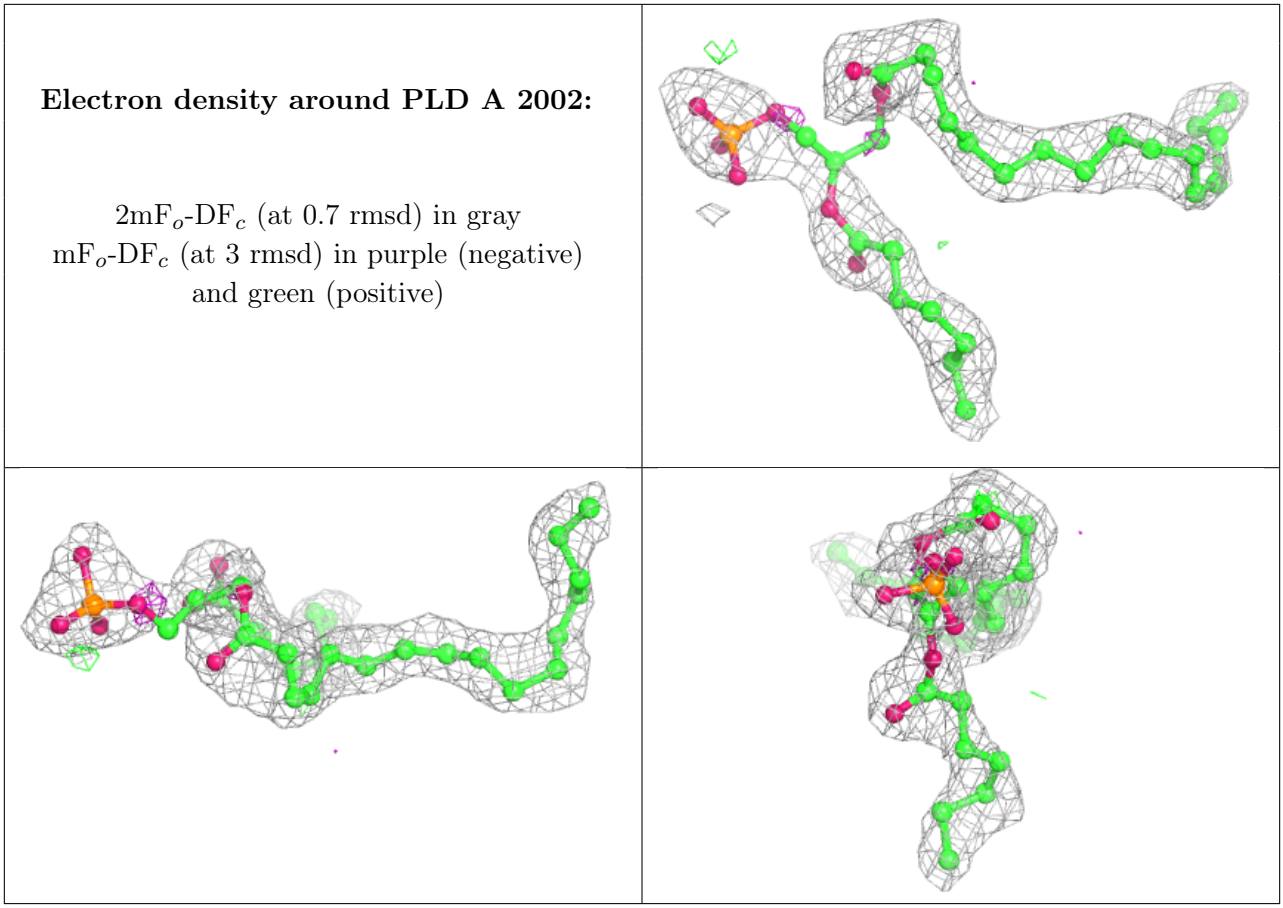






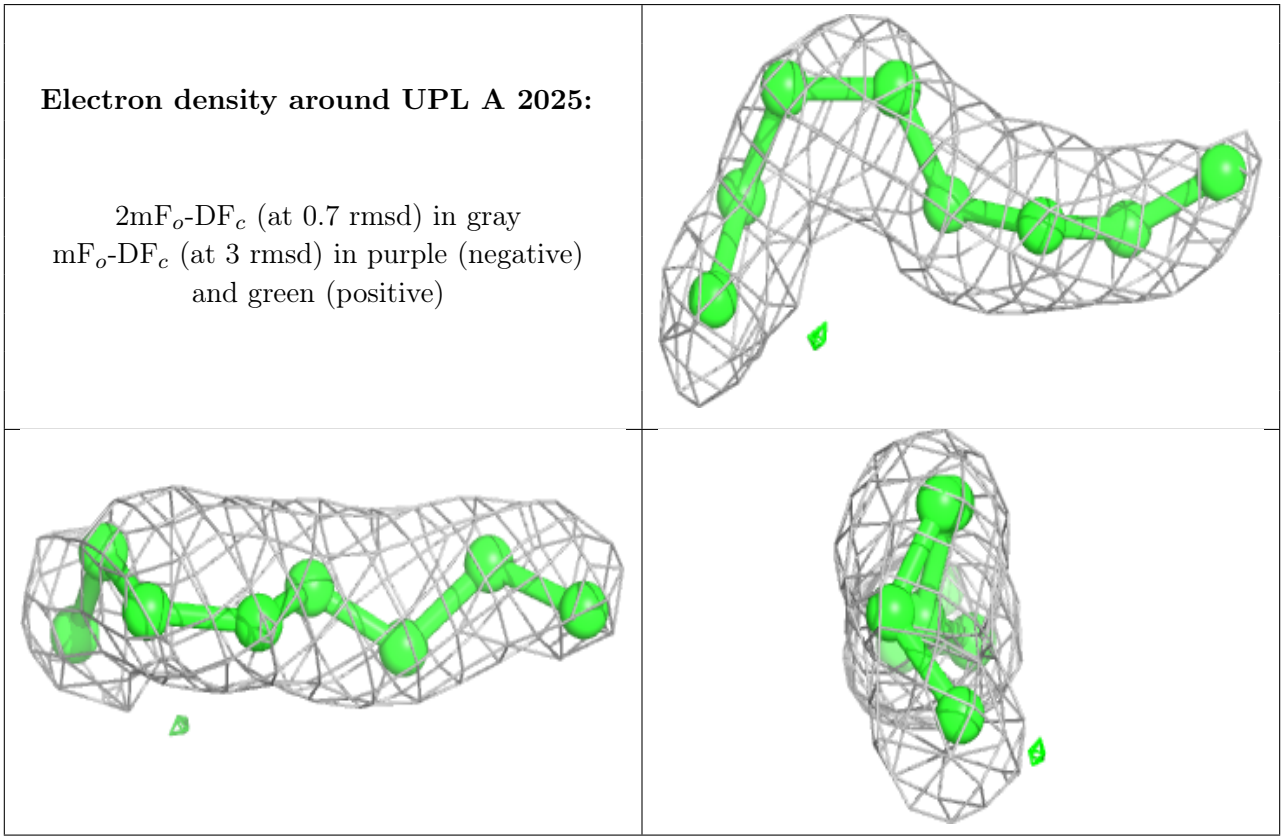
Electron density around PLD A 2002:

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



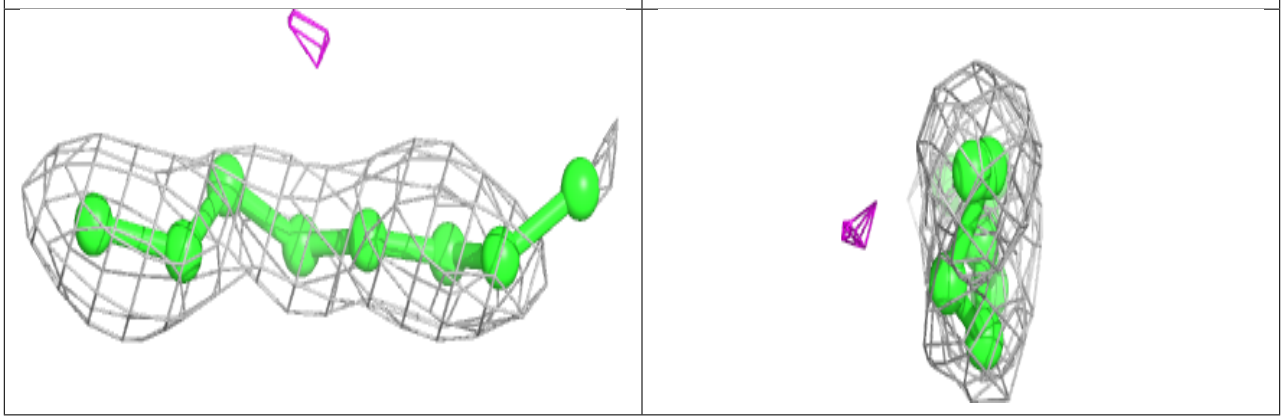
Electron density around UPL A 2025:

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



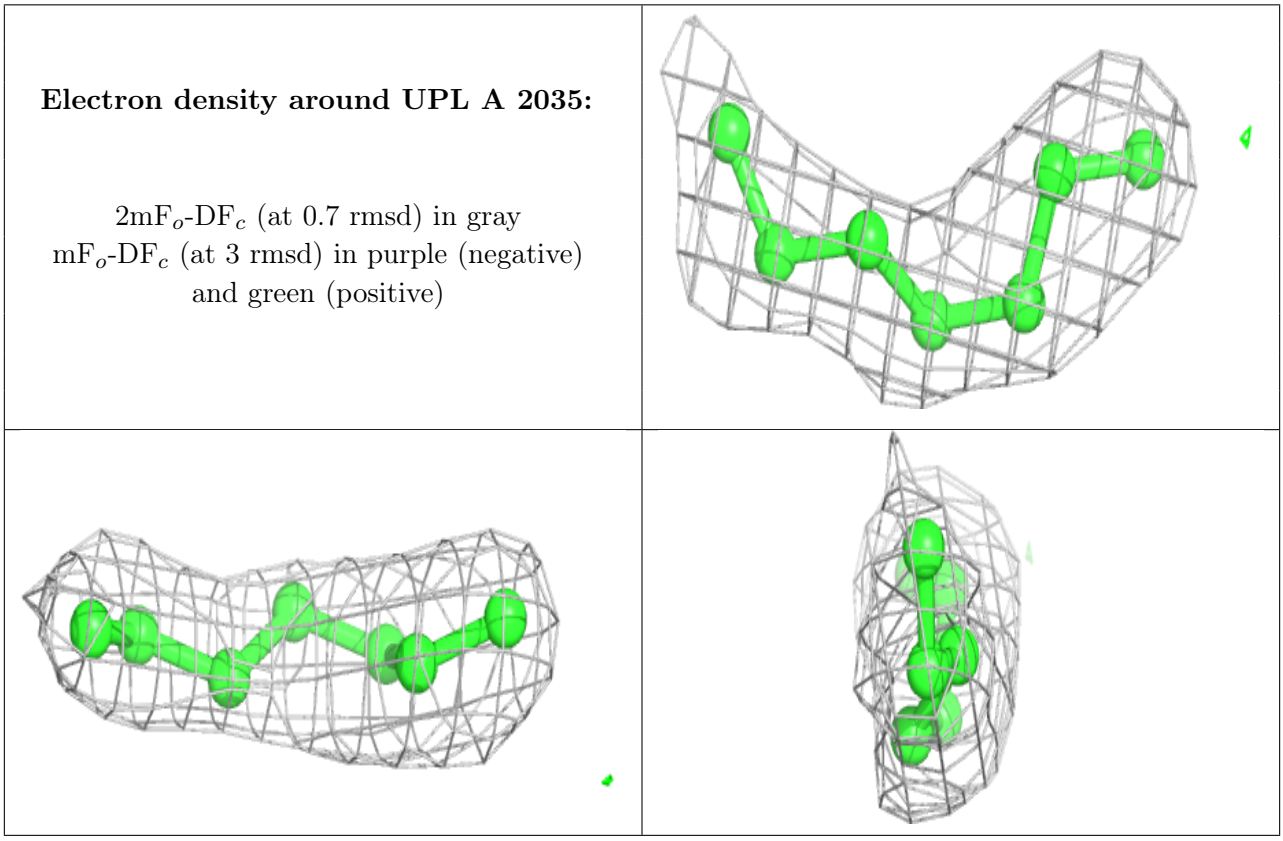
Electron density around UPL A 2026:

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



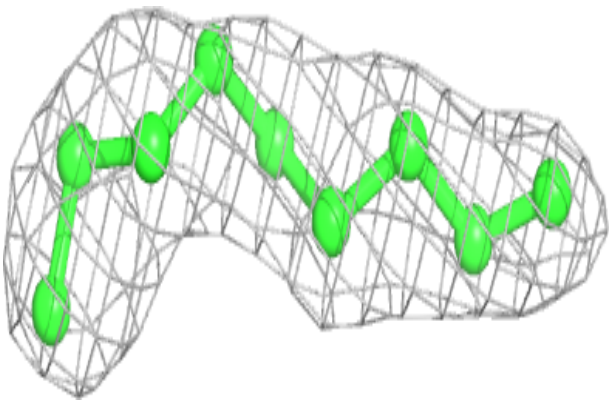
Electron density around UPL A 2035:

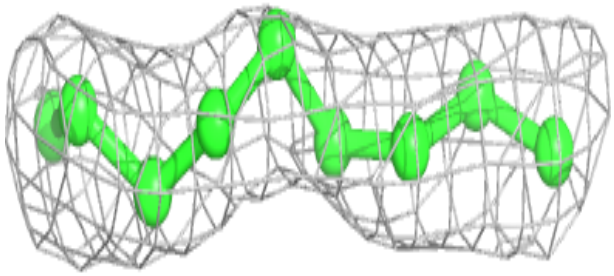
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

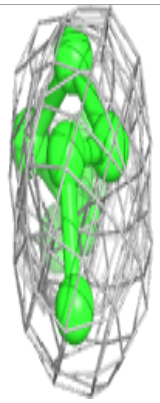


Electron density around UPL B 2021:

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

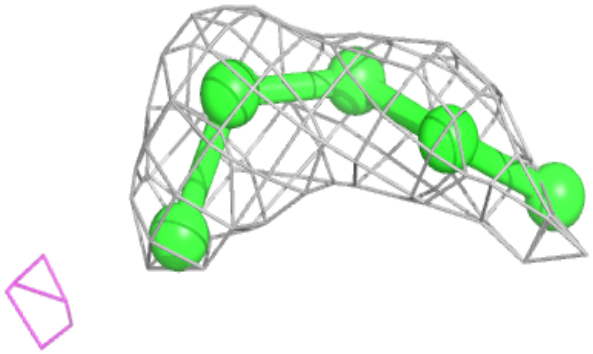


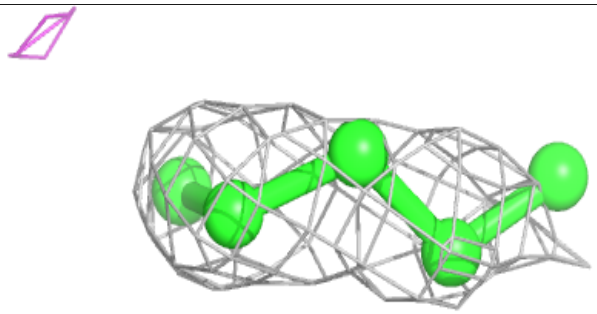


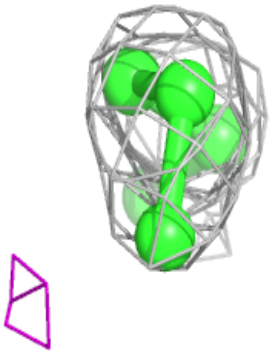


Electron density around UPL A 2047:

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

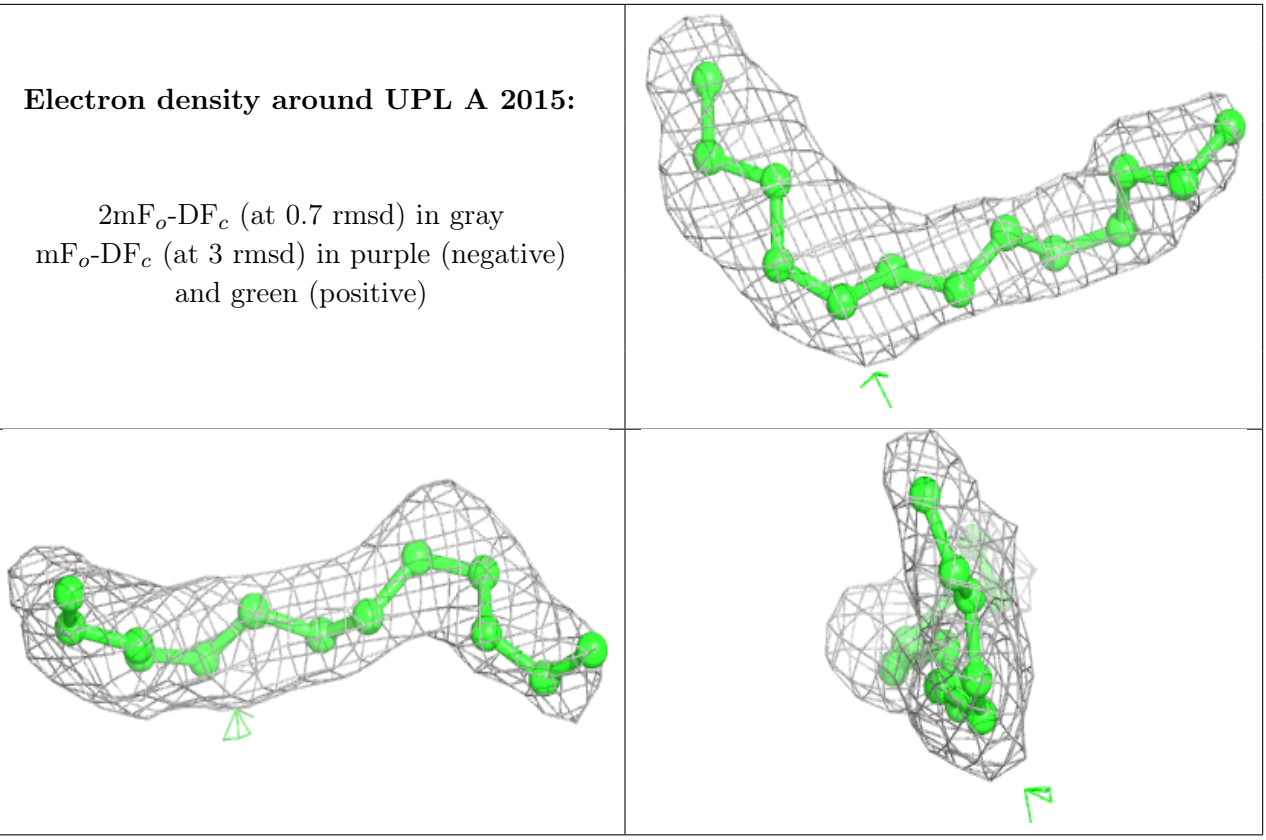






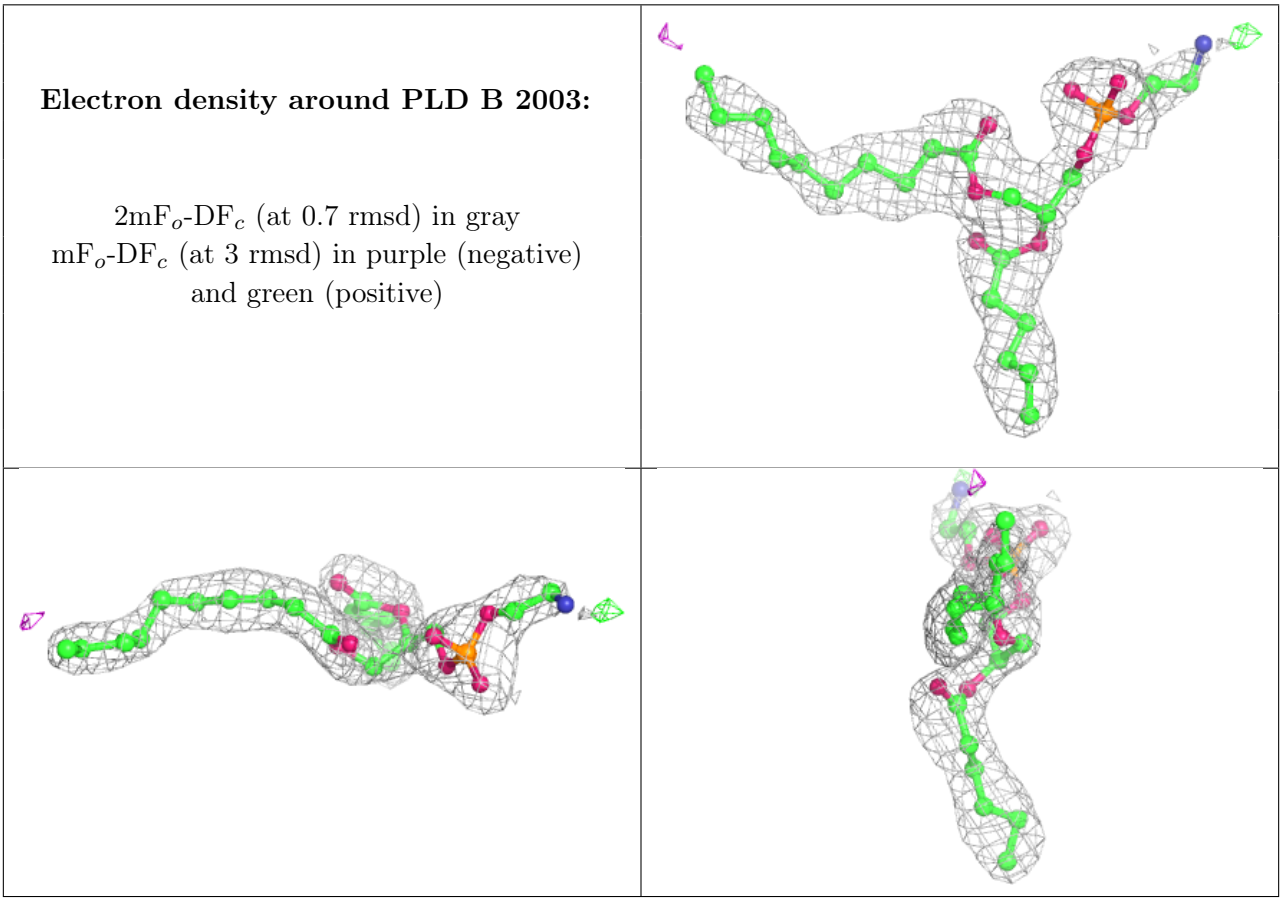
Electron density around UPL A 2015:

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



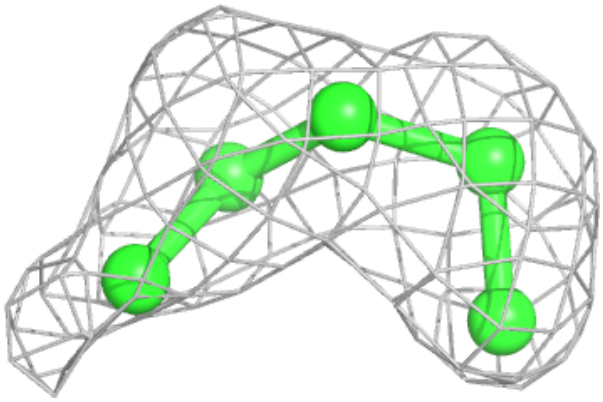
Electron density around PLD B 2003:

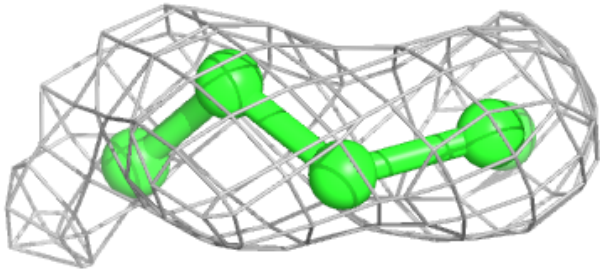
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

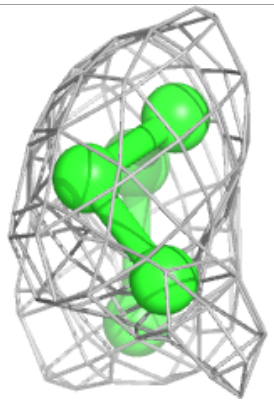


Electron density around UPL A 2039:

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

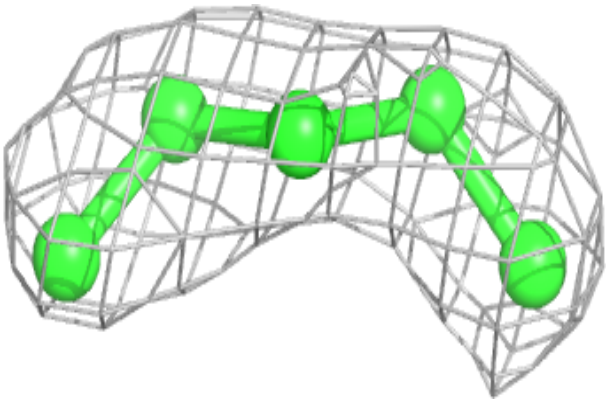


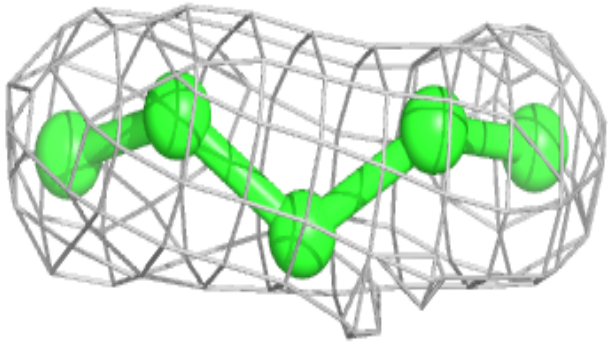


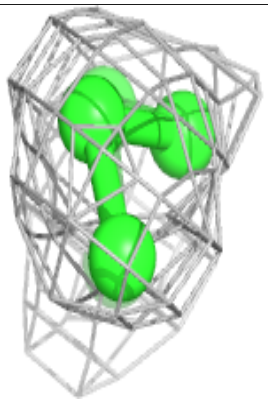


Electron density around UPL A 2042:

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

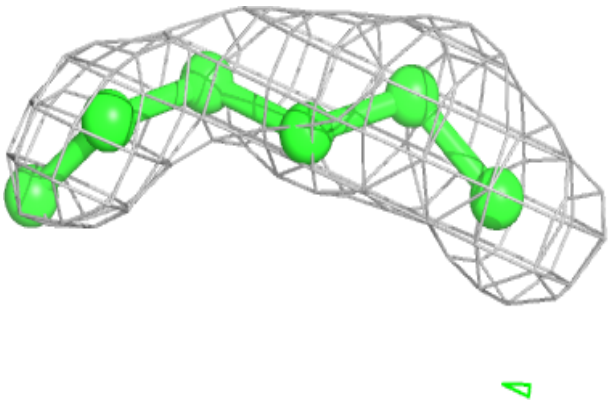


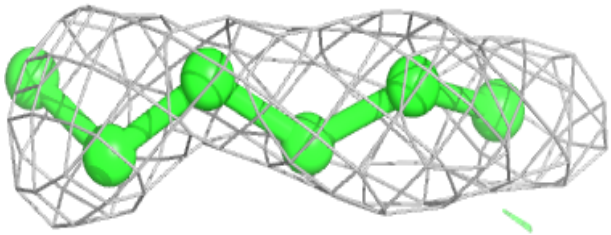


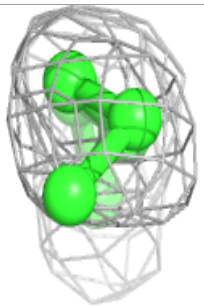


Electron density around UPL A 2036:

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

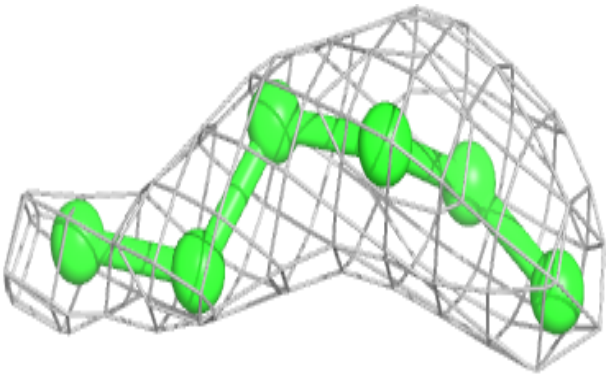


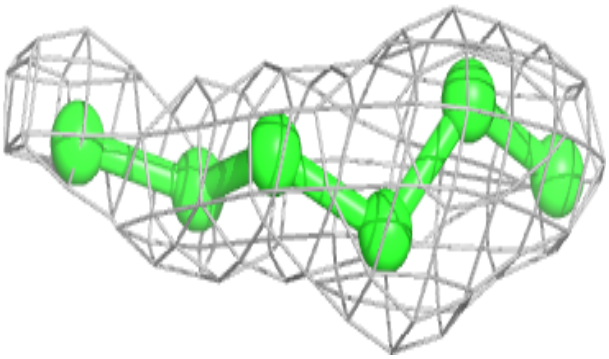


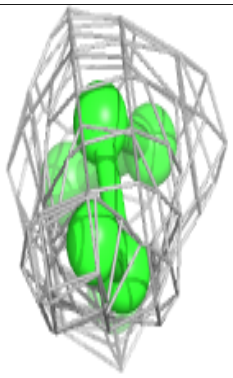


Electron density around UPL B 2033:

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

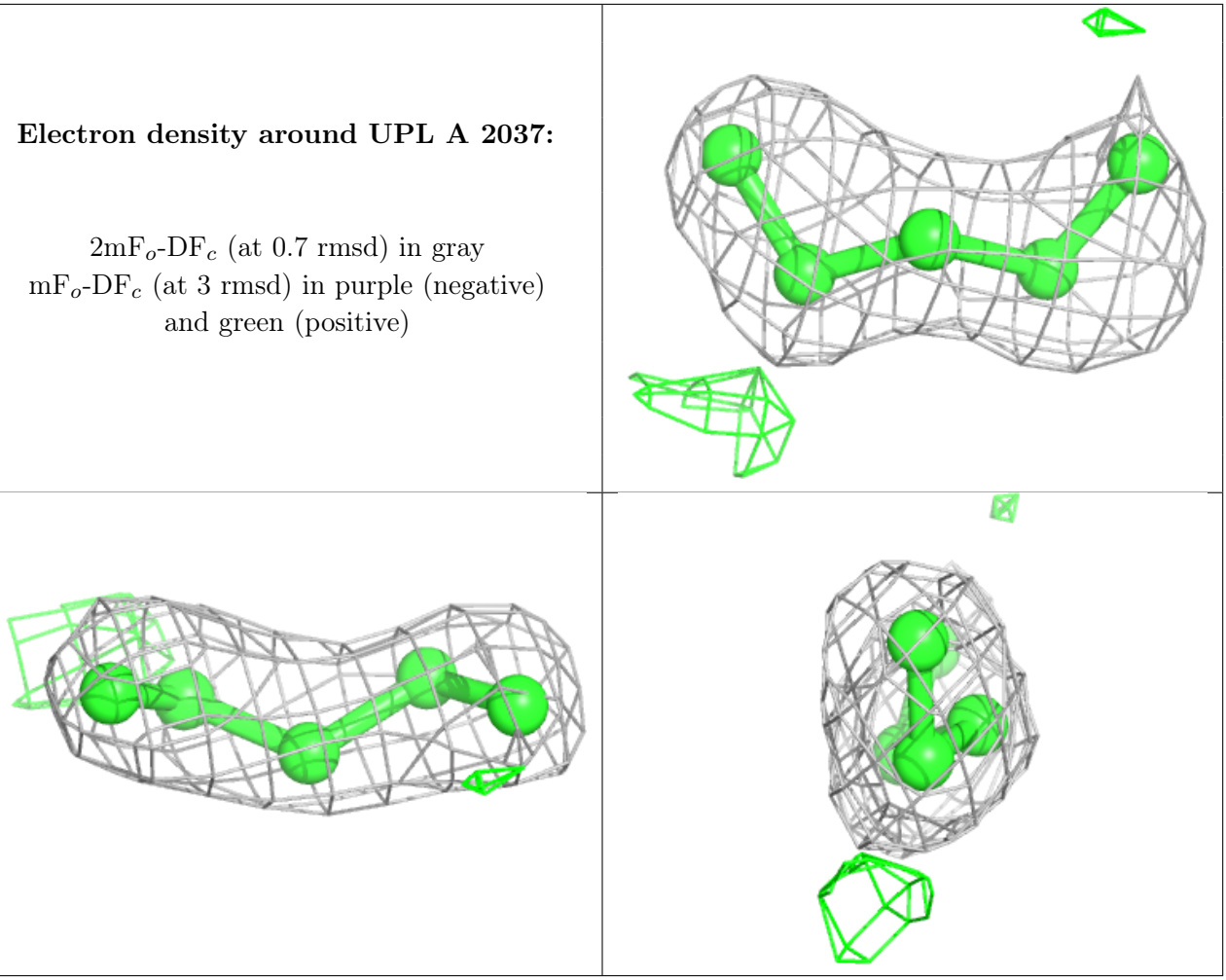






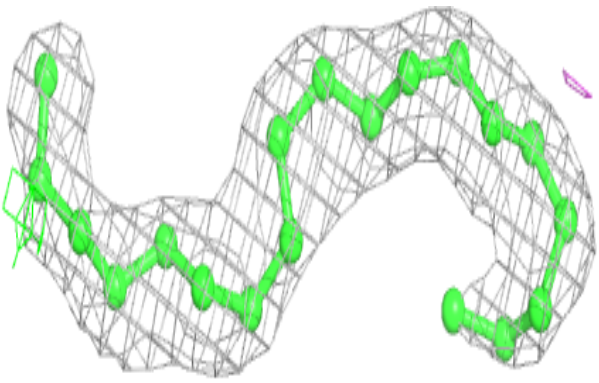
Electron density around UPL A 2037:

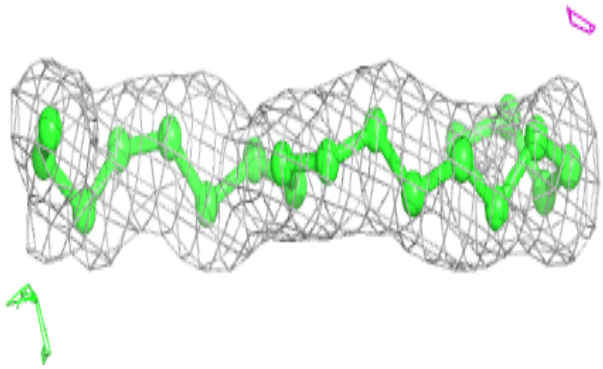
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

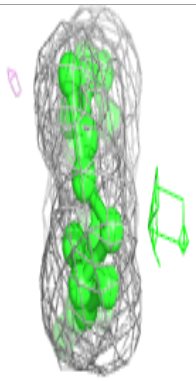


Electron density around UPL A 2011:

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

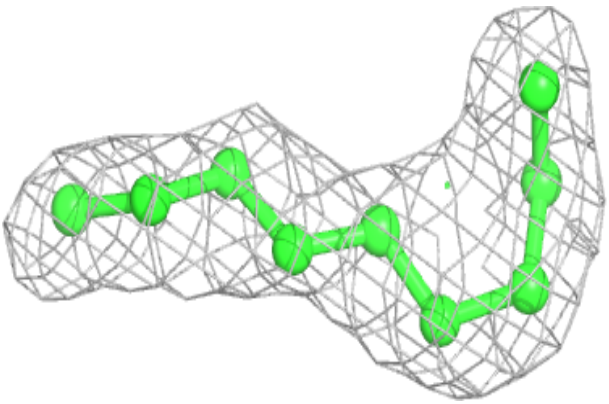


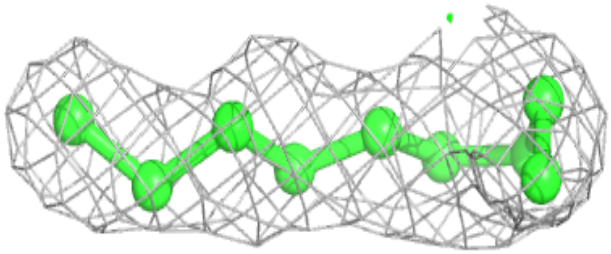


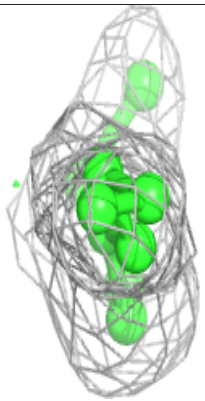


Electron density around UPL B 2023:

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

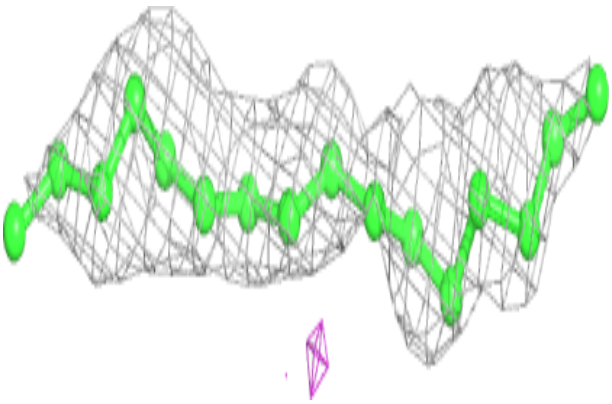


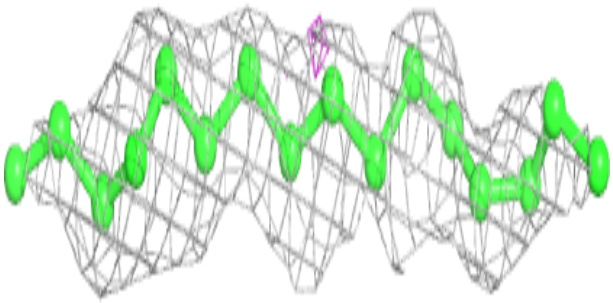


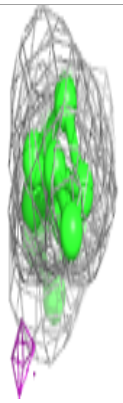


Electron density around UPL A 2013:

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

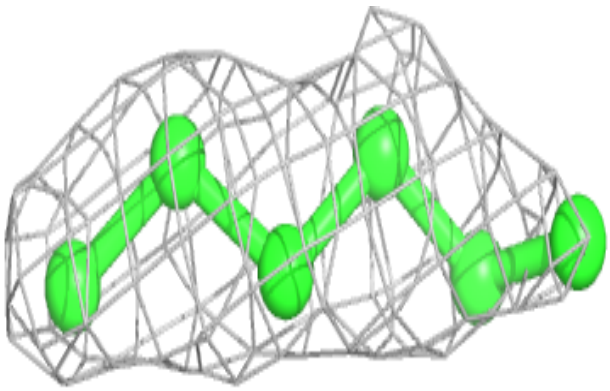


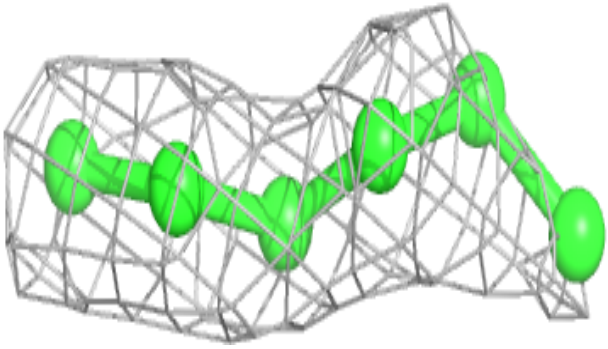


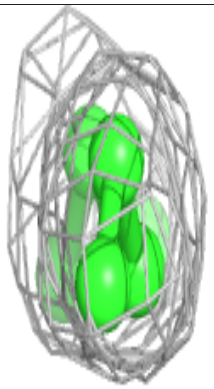


Electron density around UPL A 2032:

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

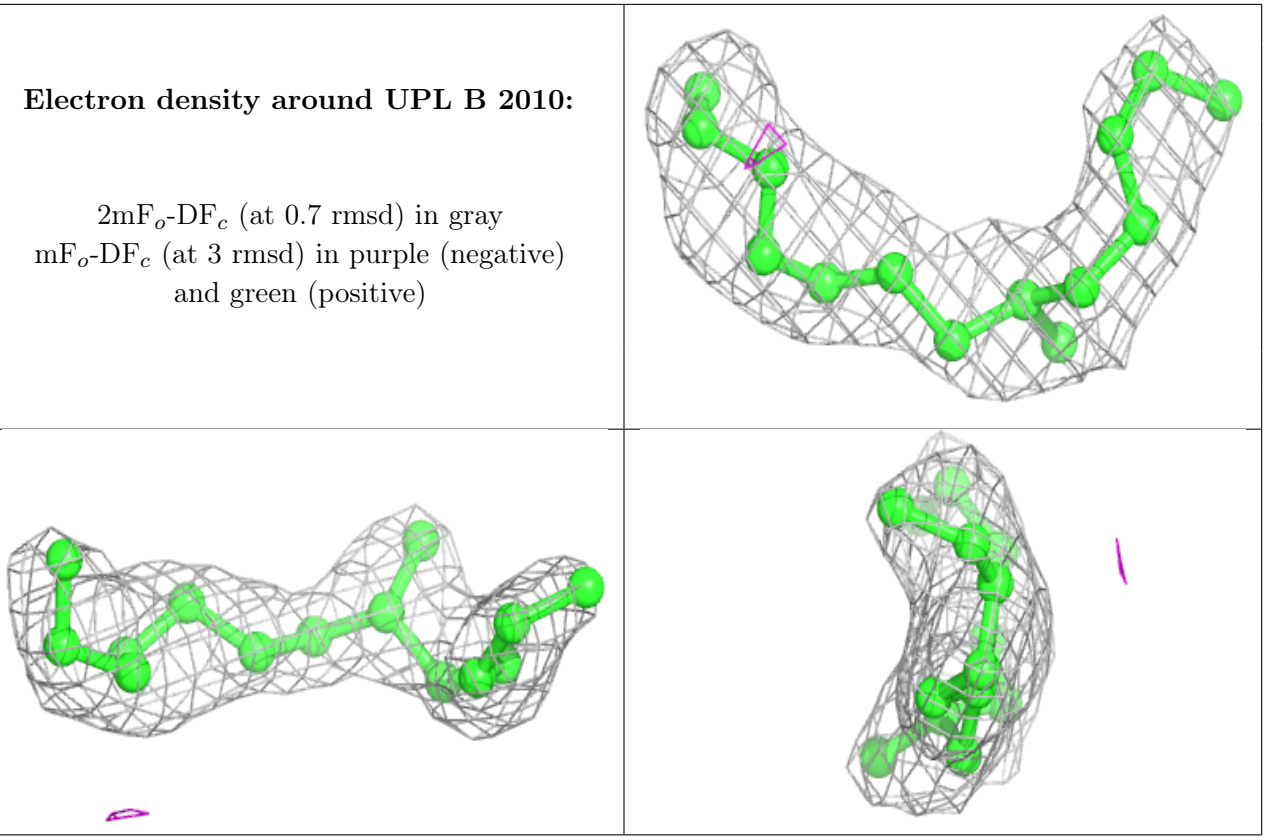






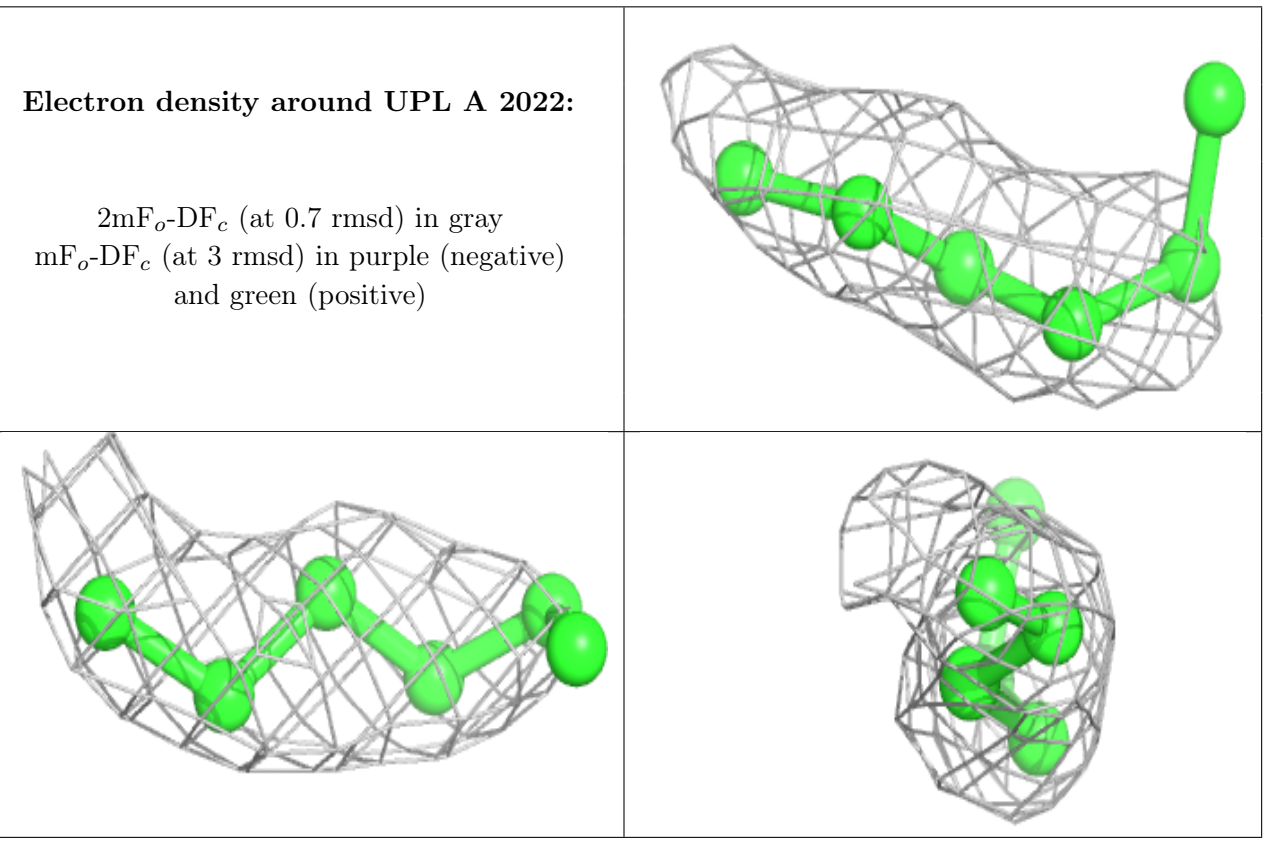
Electron density around UPL B 2010:

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



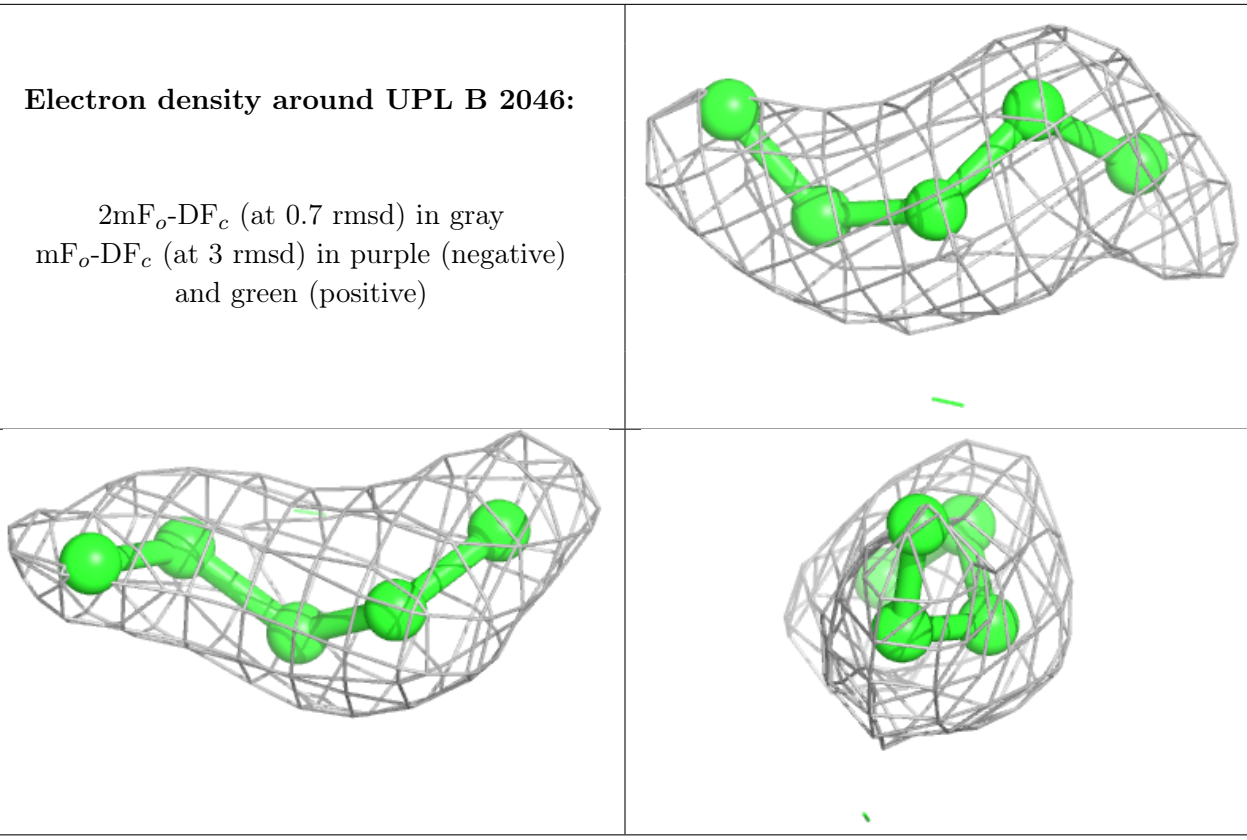
Electron density around UPL A 2022:

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



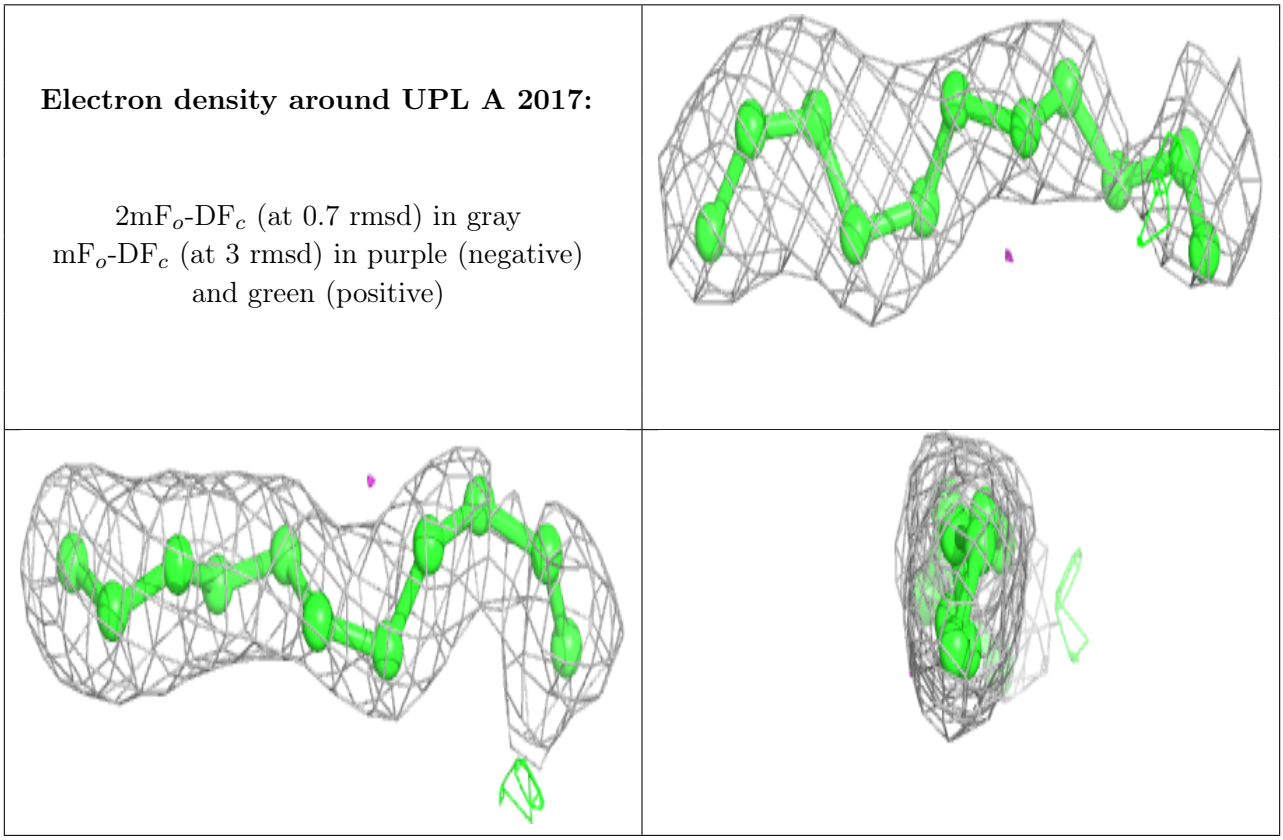
Electron density around UPL B 2046:

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



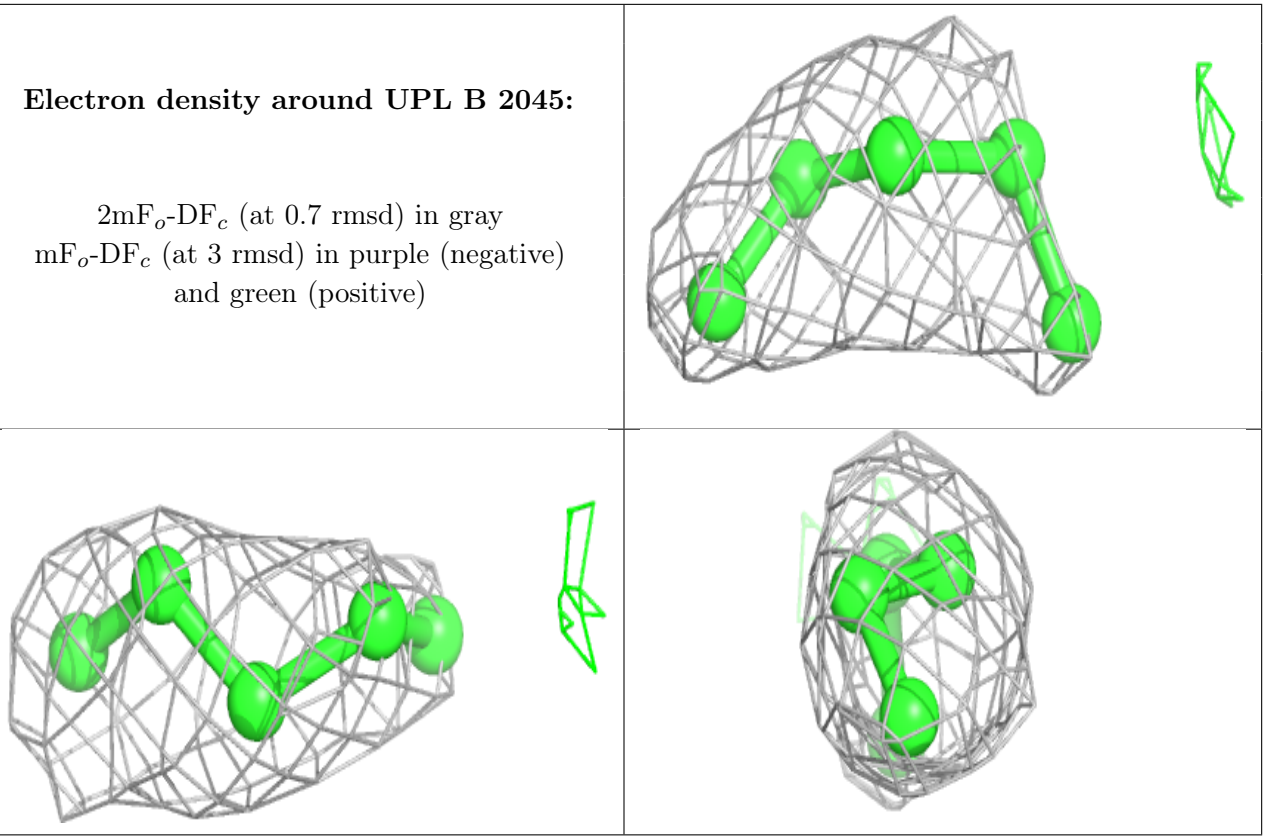
Electron density around UPL A 2017:

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



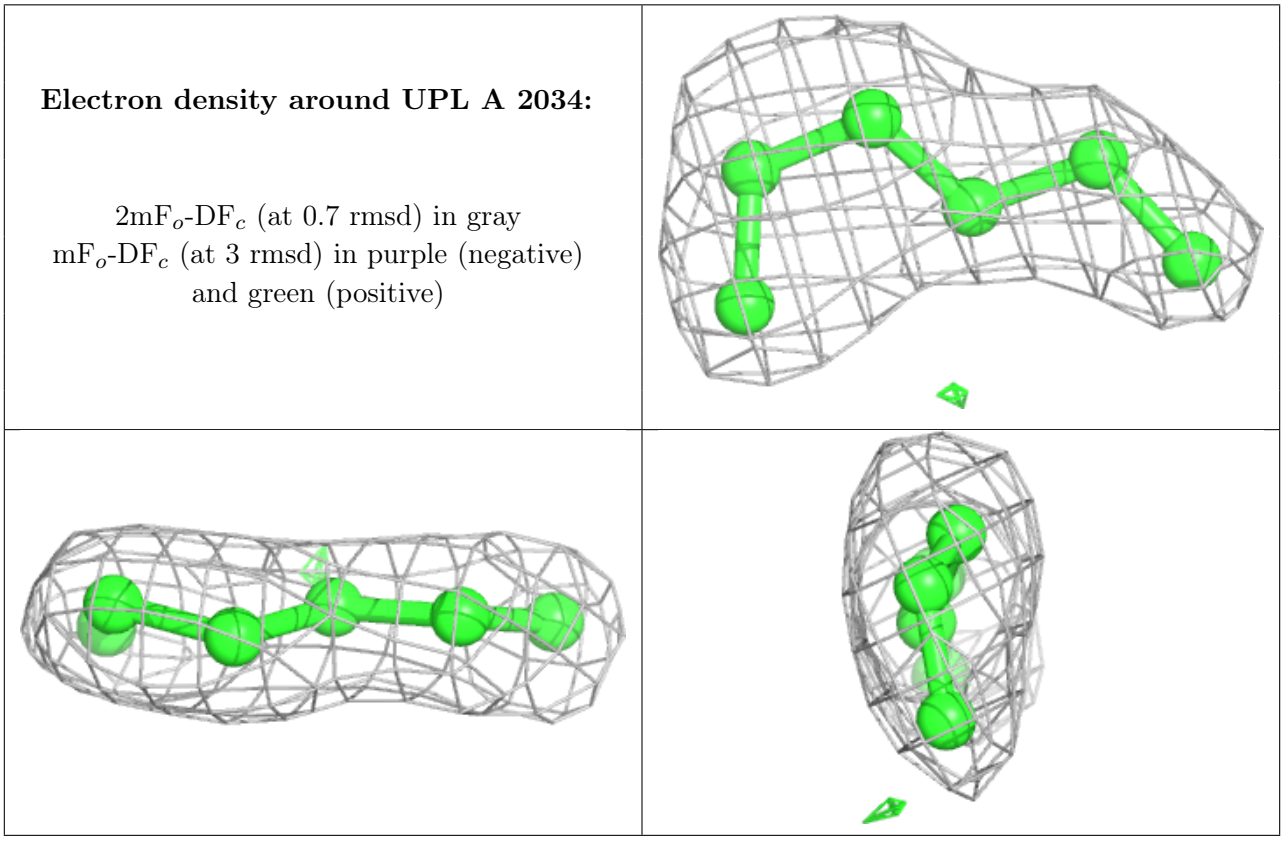
Electron density around UPL B 2045:

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



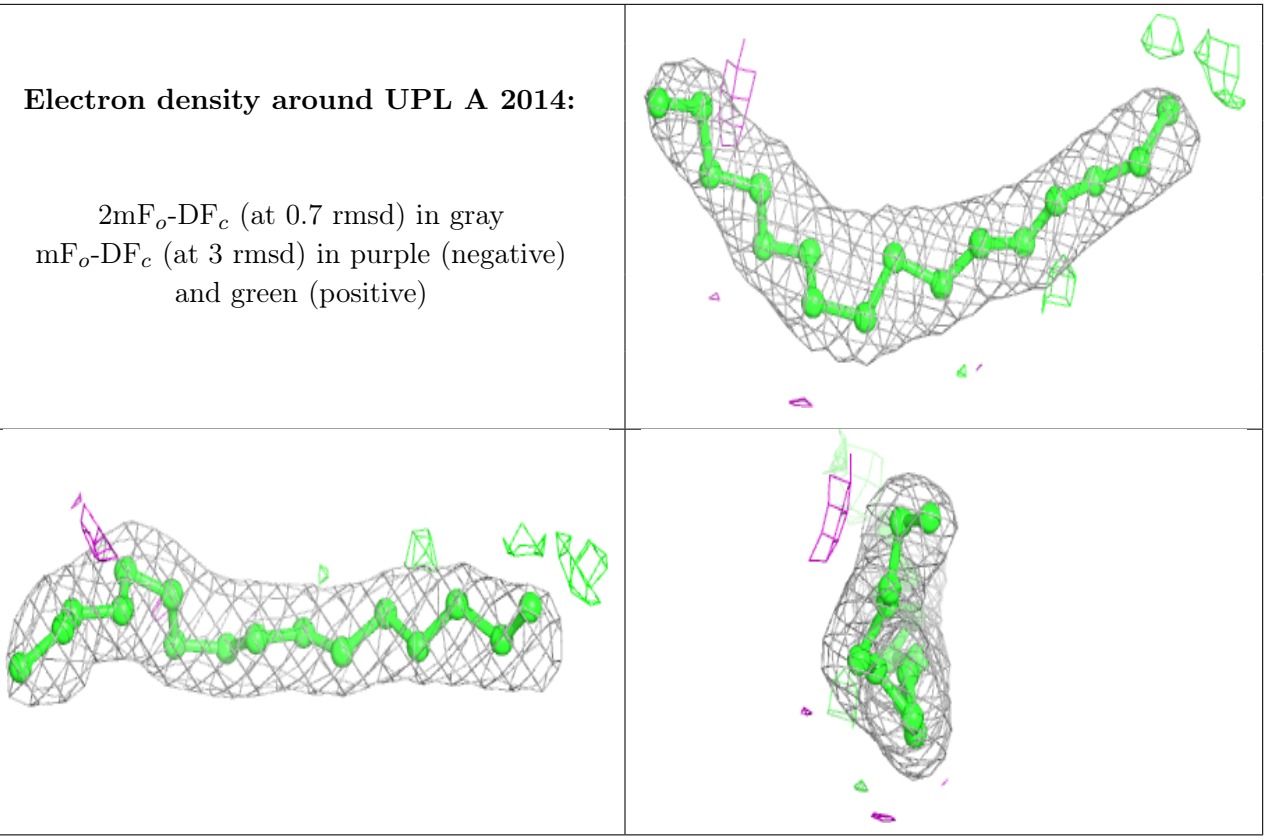
Electron density around UPL A 2034:

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



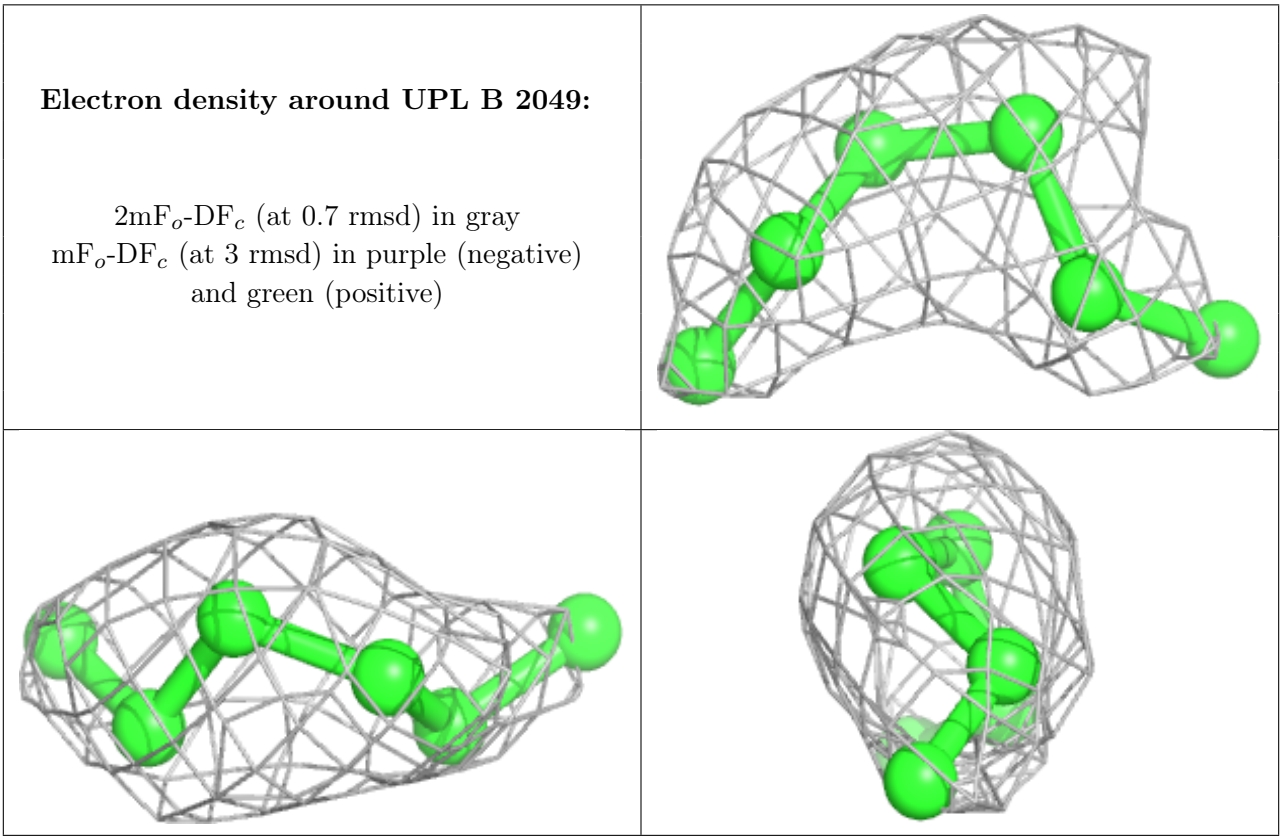
Electron density around UPL A 2014:

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



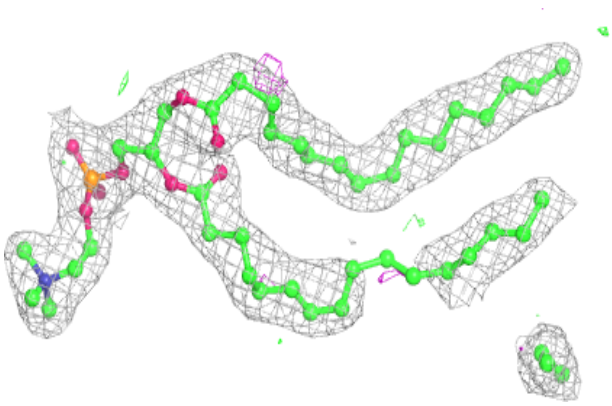
Electron density around UPL B 2049:

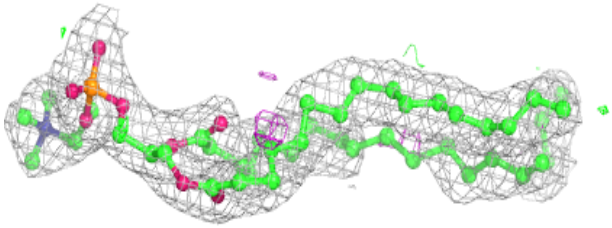
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

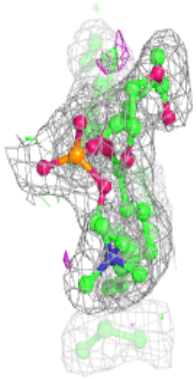


Electron density around PLD A 2001 (B):

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

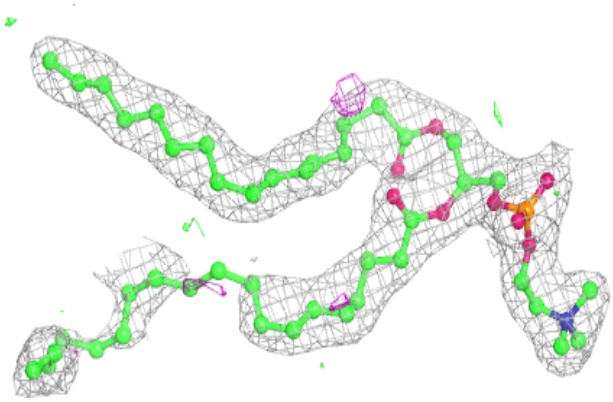


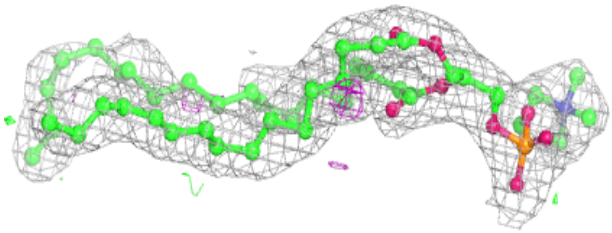


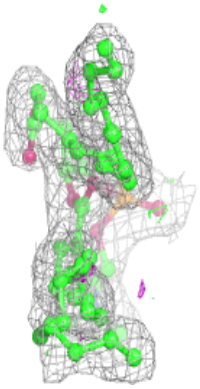


Electron density around PLD A 2001 (A):

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

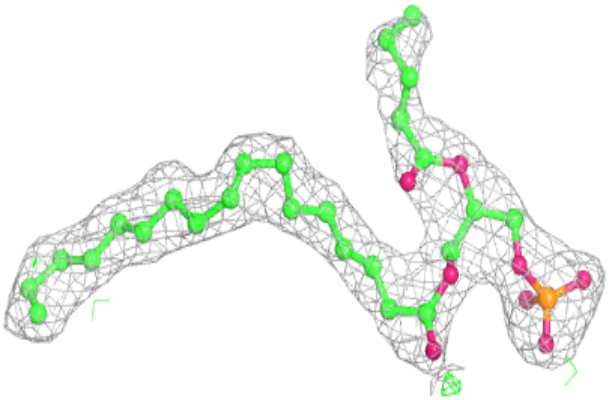


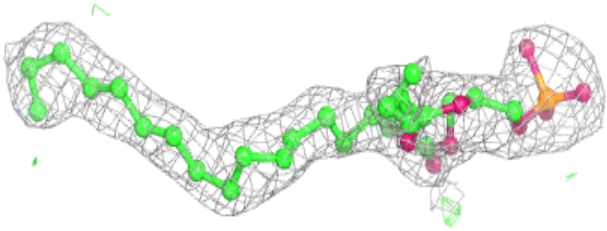


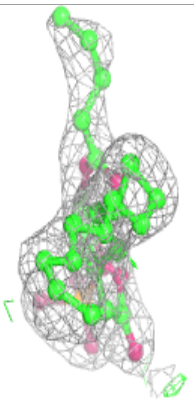


Electron density around PLD A 2004:

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

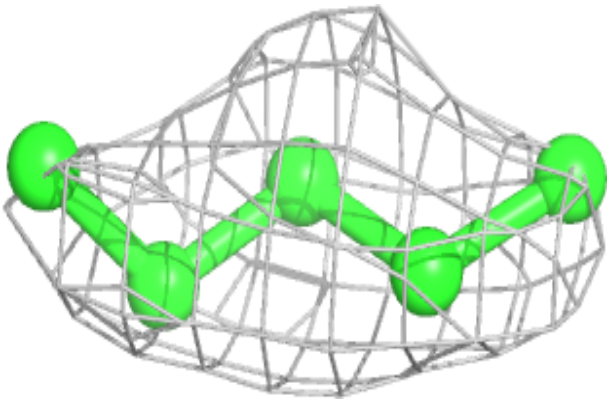


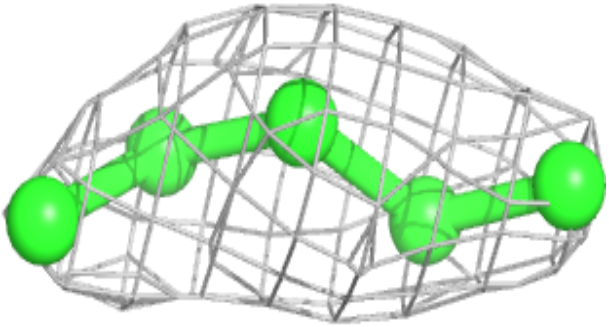




Electron density around UPL B 2043:

$2mF_o$-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.