wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2022 – 06:18 pm GMT

PDB ID	:	7Q7M
Title	:	Room temperature structure of the Rhodobacter Sphaeroides Photosynthetic Reaction Center F(M197)H mutant at 100 MPa helium gas pressure in a sapphire capillary
Authors	:	Lieske, J.; Guenther, S.; Saouane, S.; Selikhanov, G.K.; Gabdulkhakov, A.G.; Meents, A.
Deposited on	:	2021-11-09
Resolution	:	2.55 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

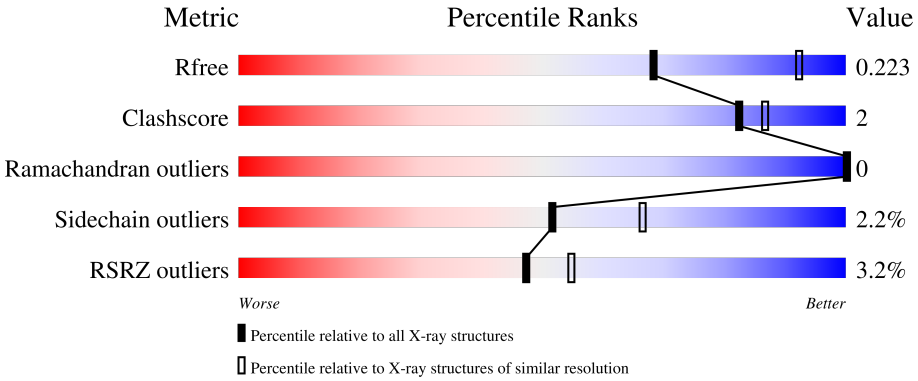
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	H	241	3% 94% 6%
2	L	281	4% 96%
3	M	302	2% 93% 6%

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	LDA	L	307	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 14861 atoms, of which 7386 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 Reaction center protein H chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	240	Total	C	H	N	O	S	0	6	0
			3770	1202	1894	322	342	10			

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	281	Total	C	H	N	O	S	0	3	0
			4467	1528	2209	358	364	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	engineered mutation	UNP P0C0Y8

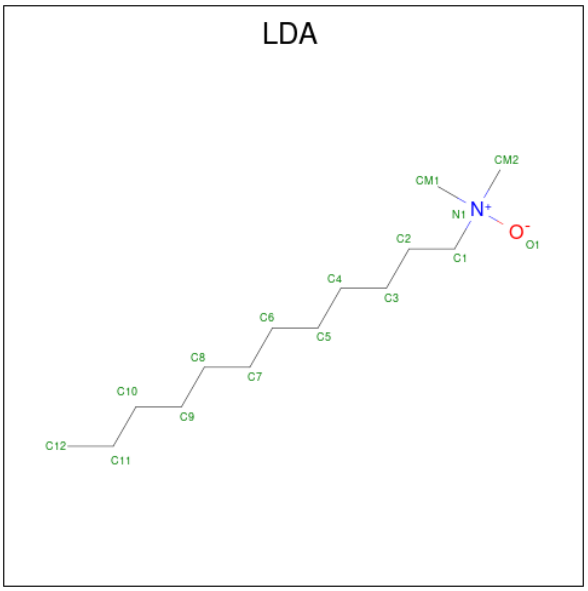
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	M	300	Total	C	H	N	O	S	0	6	0
			4799	1635	2353	402	399	10			

There are 2 discrepancies between the modelled and reference sequences:

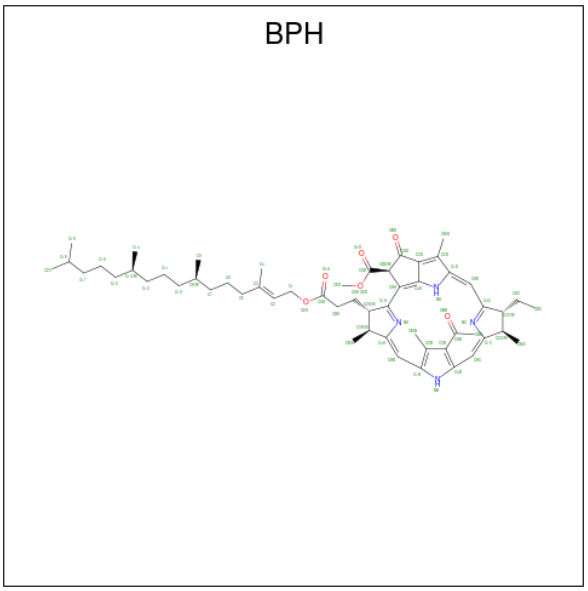
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP P0C0Y9
M	197	HIS	PHE	engineered mutation	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$) (labeled as "Ligand of Interest" by depositor).



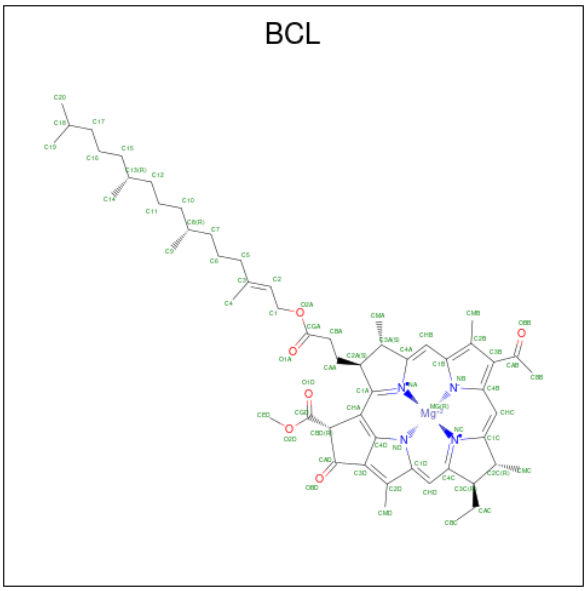
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	H	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	H	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	L	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	L	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	L	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	M	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	M	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	M	1	Total	C	H	N	O	0	0
			47	14	31	1	1		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	H	N	O	0	0
			141	55	76	4	6		
5	M	1	Total	C	H	N	O	0	0
			95	40	45	4	6		

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	L	1	Total	C	H	Mg	N	O	0	0
			140	55	74	1	4	6		

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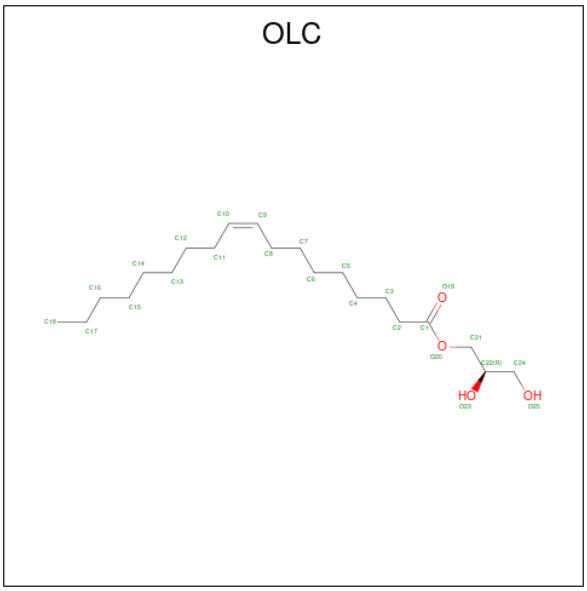
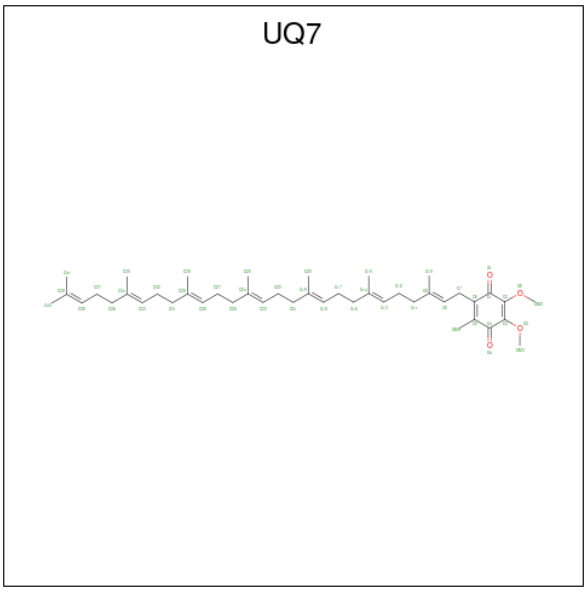
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	L	1	Total	C	H	Mg	N	O	0	0
			140	55	74	1	4	6		
6	M	1	Total	C	H	Mg	N	O	0	0
			140	55	74	1	4	6		
6	M	1	Total	C	H	Mg	N	O	0	0
			97	41	45	1	4	6		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	H	O	0	1
			130	42	80	8		
7	M	1	Total	C	H	O	0	1
			65	21	40	4		

- Molecule 8 is UBIQUINONE-7 (three-letter code: UQ7) (formula: $C_{44}H_{66}O_4$) (labeled as "Ligand of Interest" by depositor).

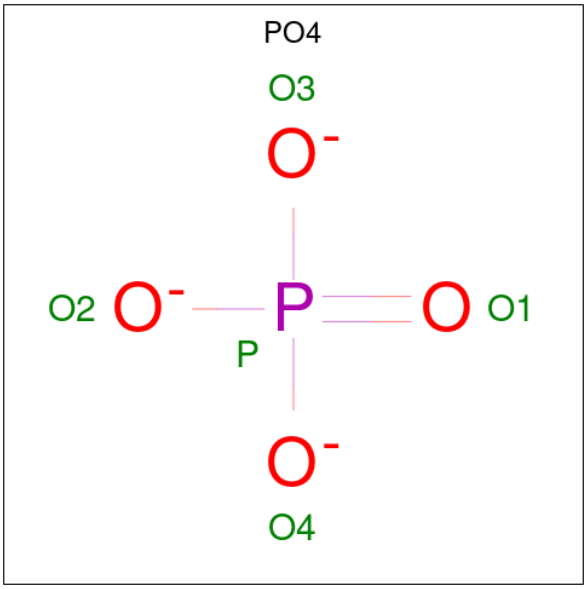


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	M	1	113	44	65	4	0	0

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

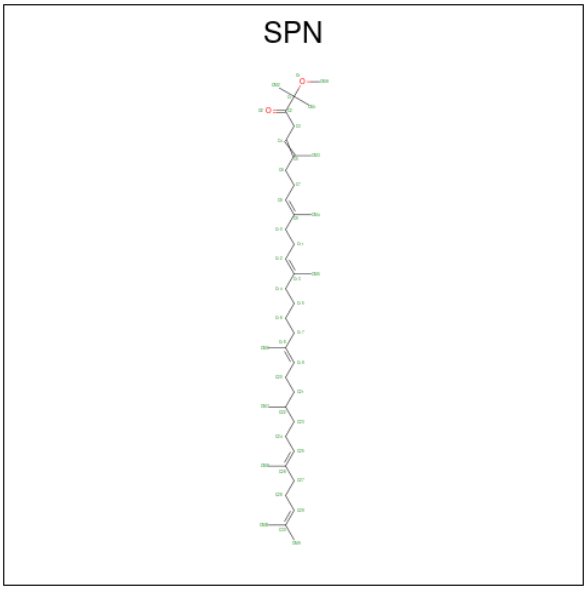
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
9	M	1	1	1	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



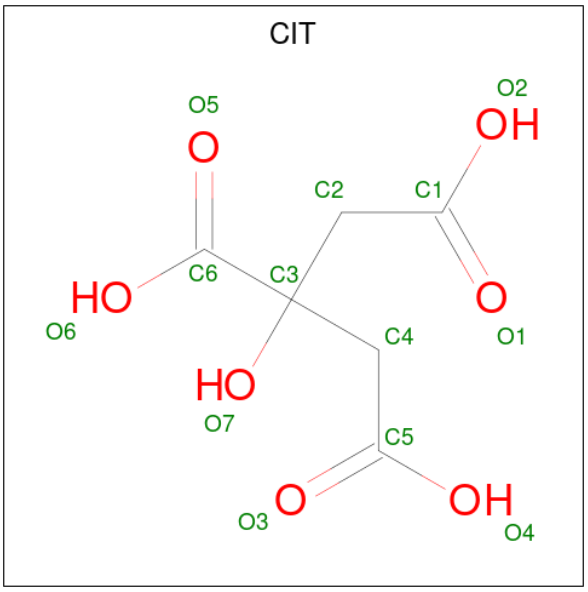
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total O P 5 4 1	0	0
10	M	1	Total O P 5 4 1	0	0

- Molecule 11 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C H O 113 41 70 2	0	1

- Molecule 12 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C H O 21 6 8 7	0	0

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total Cl 1 1	0	0

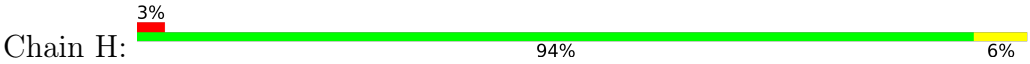
- Molecule 14 is water.

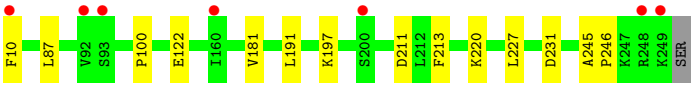
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	H	87	Total O 88 88	0	1
14	L	50	Total O 50 50	0	0
14	M	57	Total O 57 57	0	0

3 Residue-property plots (i)

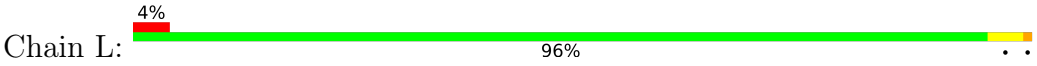
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reaction center protein H chain

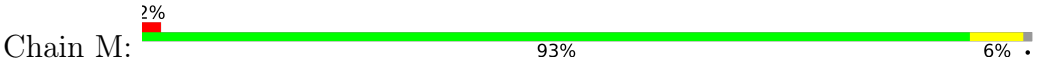


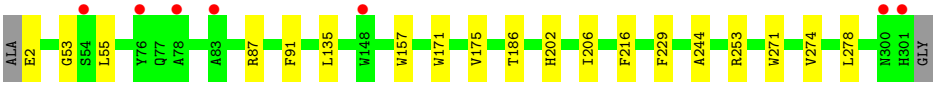


• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.21Å 102.21Å 237.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.95 – 2.55 46.95 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.95-2.55) 89.1 (46.95-2.55)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.85 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.13-2998_9999	Depositor
R, R_{free}	0.183 , 0.223 0.183 , 0.223	Depositor DCC
R_{free} test set	1686 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14861	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: FE, LDA, OLC, CIT, UQ7, BCL, SPN, BPH, PO4, CL

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	H	0.26	0/1936	0.44	0/2630
2	L	0.25	0/2355	0.39	0/3224
3	M	0.25	0/2553	0.39	0/3486
All	All	0.25	0/6844	0.41	0/9340

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	H	1876	1894	1885	7	0
2	L	2258	2209	2202	5	0
3	M	2446	2353	2338	13	0
4	H	48	93	93	1	0
4	L	48	93	93	0	0
4	M	48	93	93	2	0
5	L	65	76	76	0	0
5	M	50	45	43	3	0
6	L	132	148	148	4	0
6	M	118	119	117	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	50	80	80	0	0
7	M	25	40	40	0	0
8	M	48	65	66	0	0
9	M	1	0	0	0	0
10	M	10	0	0	0	0
11	M	43	70	70	3	0
12	M	13	8	5	2	0
13	M	1	0	0	0	0
14	H	88	0	0	0	0
14	L	50	0	0	0	0
14	M	57	0	0	0	0
All	All	7475	7386	7349	36	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 2.

The worst 5 of 36 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:H:181:VAL:HG21	1:H:191:LEU:HD12	1.74	0.68
4:M:411:LDA:HM21	4:M:411:LDA:H32	1.74	0.67
6:L:302:BCL:HMB1	6:L:302:BCL:HBB2	1.79	0.64
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.84	0.60
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.37	0.60

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	H	244/241 (101%)	239 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	282/281 (100%)	275 (98%)	7 (2%)	0	100	100
3	M	304/302 (101%)	298 (98%)	6 (2%)	0	100	100
All	All	830/824 (101%)	812 (98%)	18 (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	H	201/196 (103%)	197 (98%)	4 (2%)	55	70
2	L	223/220 (101%)	216 (97%)	7 (3%)	40	54
3	M	241/236 (102%)	237 (98%)	4 (2%)	60	75
All	All	665/652 (102%)	650 (98%)	15 (2%)	52	65

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	247	CYS
3	M	253[A]	ARG
2	L	265	TRP
3	M	253[B]	ARG
3	M	2	GLU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	OLC	L	304[A]	-	24,24,24	0.21	0	25,25,25	0.20	0
7	OLC	M	409[B]	-	24,24,24	0.17	0	25,25,25	0.18	0
6	BCL	M	403	-	44,60,74	1.38	4 (9%)	52,98,115	1.43	11 (21%)
7	OLC	L	304[B]	-	24,24,24	0.22	0	25,25,25	0.23	0
4	LDA	H	303	-	12,15,15	0.36	0	14,17,17	0.59	0
8	UQ7	M	401	-	48,48,48	0.22	0	58,61,61	0.42	0
4	LDA	L	305	-	12,15,15	0.35	0	14,17,17	0.35	0
6	BCL	L	303	-	58,74,74	1.27	5 (8%)	69,115,115	1.21	8 (11%)
4	LDA	L	306	-	12,15,15	0.34	0	14,17,17	0.46	0
11	SPN	M	410[A]	-	40,42,42	0.16	0	50,52,52	0.60	2 (4%)
4	LDA	H	302	-	12,15,15	0.37	0	14,17,17	0.99	2 (14%)
5	BPH	L	301	-	51,70,70	0.50	0	52,101,101	0.84	3 (5%)
4	LDA	M	411	-	12,15,15	0.35	0	14,17,17	0.34	0
6	BCL	L	302	-	58,74,74	1.22	5 (8%)	69,115,115	1.16	7 (10%)
10	PO4	M	408	-	4,4,4	0.90	0	6,6,6	0.45	0
4	LDA	M	406	-	12,15,15	0.35	0	14,17,17	0.67	0
5	BPH	M	404	-	36,55,70	0.85	1 (2%)	34,83,101	1.21	4 (11%)
4	LDA	H	301	-	12,15,15	0.35	0	14,17,17	0.22	0
10	PO4	M	412	-	4,4,4	0.91	0	6,6,6	0.42	0
4	LDA	L	307	-	12,15,15	0.34	0	14,17,17	0.57	0
6	BCL	M	402	-	58,74,74	1.22	5 (8%)	69,115,115	1.33	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LDA	M	407	-	12,15,15	0.34	0	14,17,17	0.24	0
12	CIT	M	413	-	12,12,12	0.20	0	17,17,17	0.65	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	L	304[A]	-	-	18/24/24/24	-
7	OLC	M	409[B]	-	-	8/24/24/24	-
6	BCL	M	403	-	-	4/21/121/137	-
7	OLC	L	304[B]	-	-	14/24/24/24	-
4	LDA	H	303	-	-	10/13/13/13	-
8	UQ7	M	401	-	-	4/45/69/69	0/1/1/1
4	LDA	L	305	-	-	6/13/13/13	-
6	BCL	L	303	-	-	2/37/137/137	-
4	LDA	L	306	-	-	8/13/13/13	-
11	SPN	M	410[A]	-	-	22/50/51/51	-
4	LDA	H	302	-	-	10/13/13/13	-
5	BPH	L	301	-	-	9/37/105/105	0/5/6/6
4	LDA	M	411	-	-	6/13/13/13	-
6	BCL	L	302	-	-	4/37/137/137	-
4	LDA	M	406	-	-	5/13/13/13	-
5	BPH	M	404	-	-	4/19/87/105	0/5/6/6
4	LDA	H	301	-	-	4/13/13/13	-
4	LDA	L	307	-	-	7/13/13/13	-
6	BCL	M	402	-	-	13/37/137/137	-
4	LDA	M	407	-	-	6/13/13/13	-
12	CIT	M	413	-	-	5/16/16/16	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	302	BCL	C1B-NB	5.24	1.39	1.35
6	L	303	BCL	C1B-NB	5.22	1.39	1.35
6	M	403	BCL	C1B-NB	5.20	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	402	BCL	C1B-NB	4.96	1.39	1.35
6	M	402	BCL	MG-NA	4.71	2.17	2.06

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	402	BCL	C4A-NA-C1A	4.21	108.60	106.71
6	M	402	BCL	CAD-C3D-C4D	-3.97	106.26	108.47
6	L	303	BCL	CAD-C3D-C4D	-3.65	106.44	108.47
6	M	402	BCL	CMB-C2B-C1B	-3.40	123.23	128.46
6	L	302	BCL	OBD-CAD-CBD	-3.37	121.08	125.89

There are no chirality outliers.

5 of 169 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	302	LDA	C2-C1-N1-CM1
4	H	302	LDA	N1-C1-C2-C3
4	H	303	LDA	C2-C1-N1-O1
4	H	303	LDA	C2-C1-N1-CM1
4	H	303	LDA	N1-C1-C2-C3

There are no ring outliers.

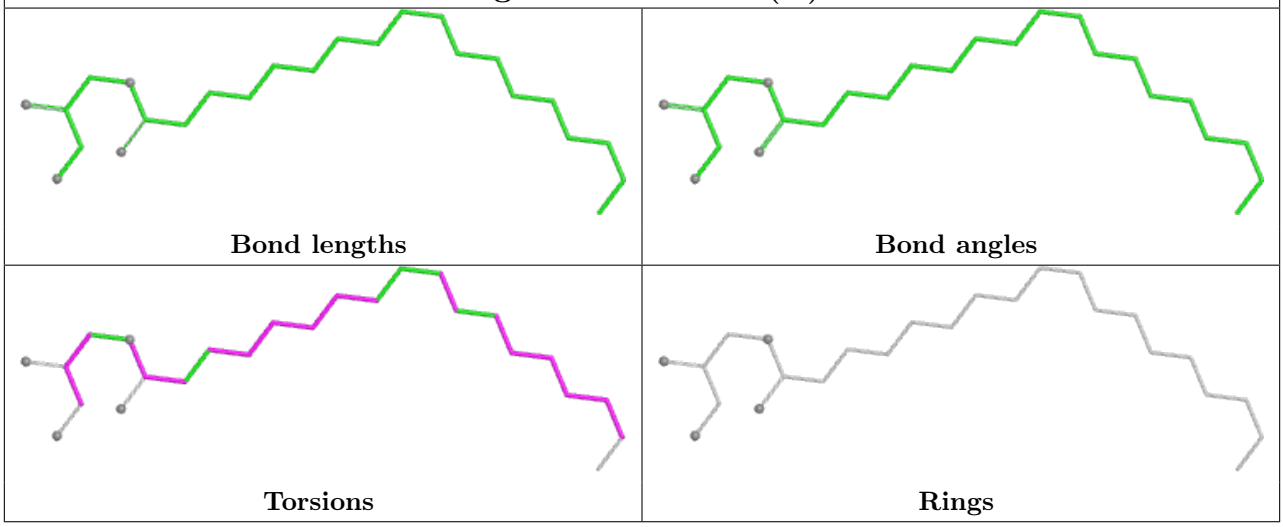
9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	403	BCL	4	0
4	H	303	LDA	1	0
6	L	303	BCL	2	0
11	M	410[A]	SPN	3	0
4	M	411	LDA	2	0
6	L	302	BCL	2	0
5	M	404	BPH	3	0
6	M	402	BCL	2	0
12	M	413	CIT	2	0

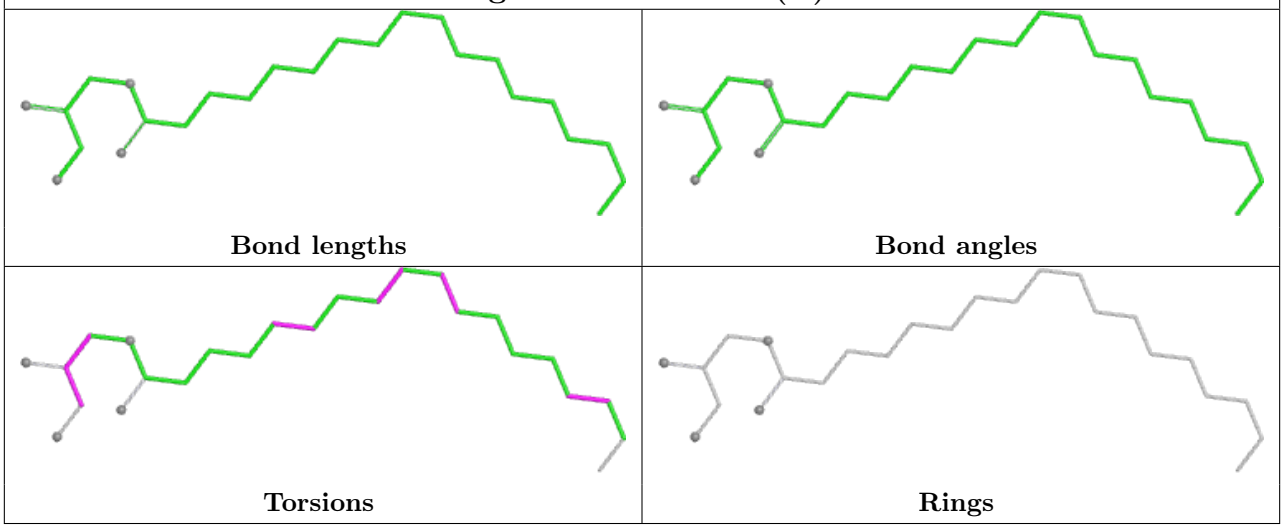
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

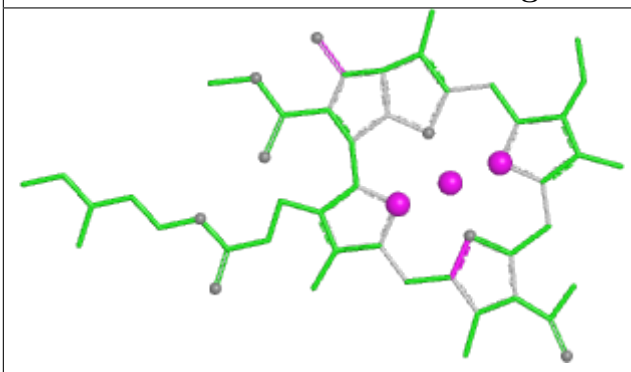
Ligand OLC L 304 (A)



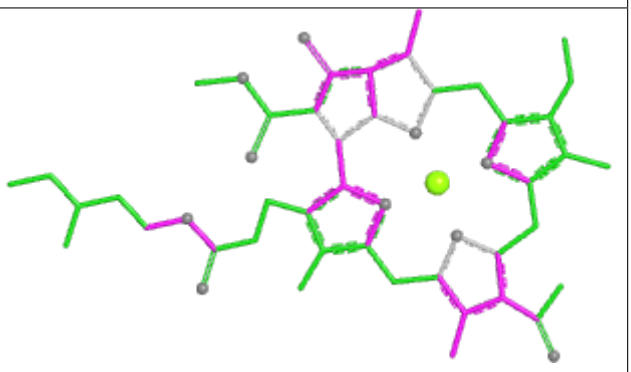
Ligand OLC M 409 (B)



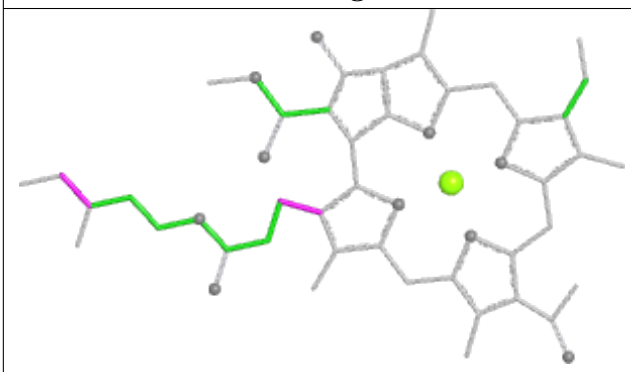
Ligand BCL M 403



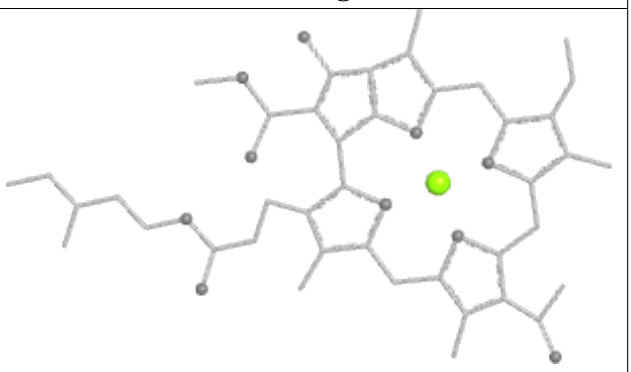
Bond lengths



Bond angles

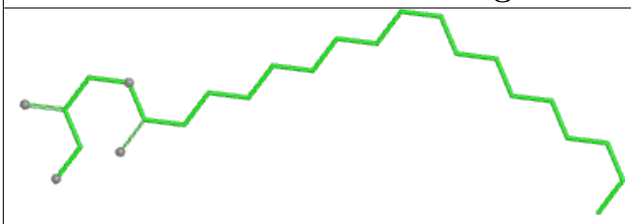


Torsions



Rings

Ligand OLC L 304 (B)



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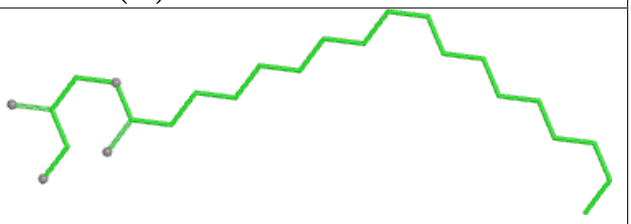

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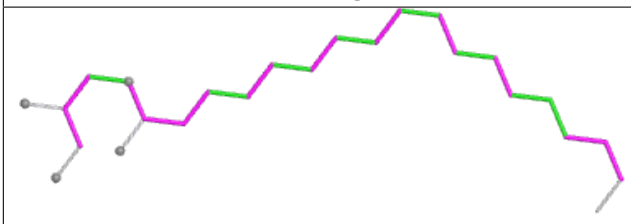
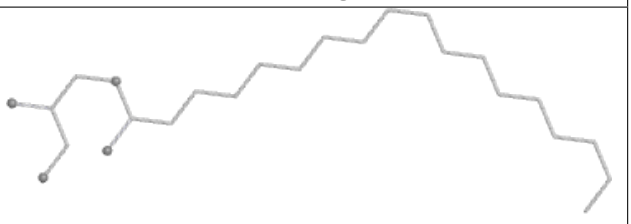
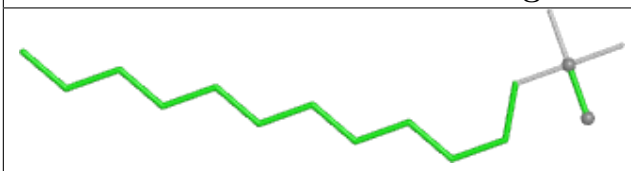
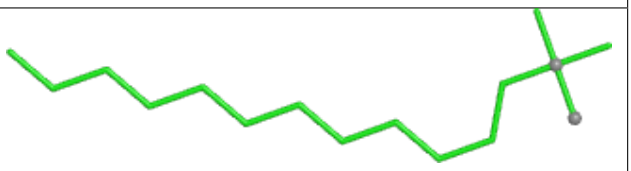
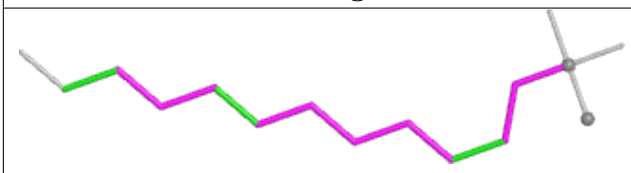
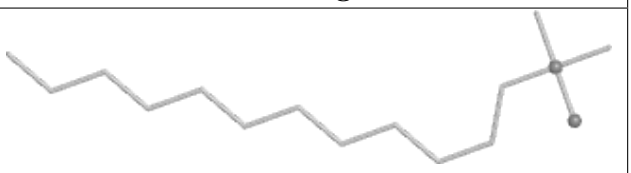


Torsions



Rings

Ligand LDA H 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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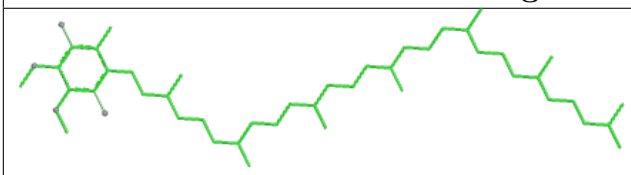
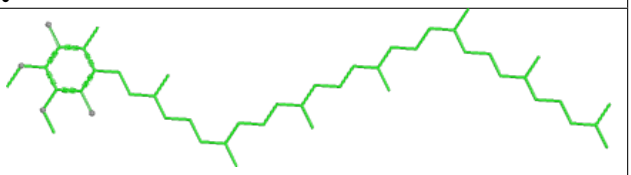
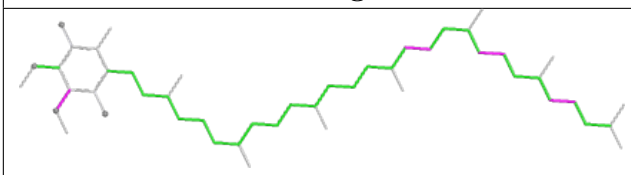
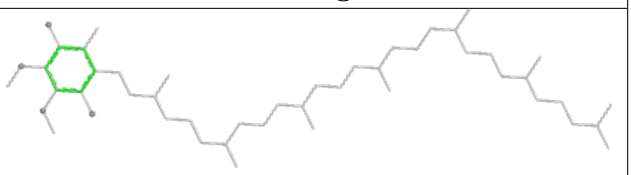
 Bond lengths	 Bond angles
 Torsions	 Rings

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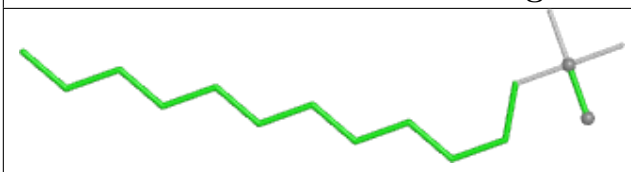
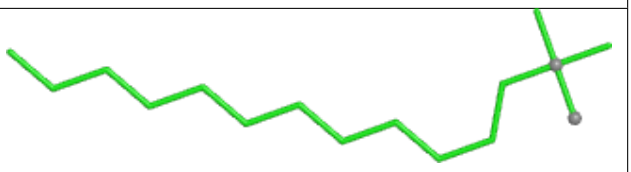
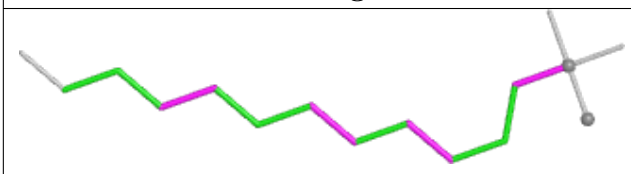
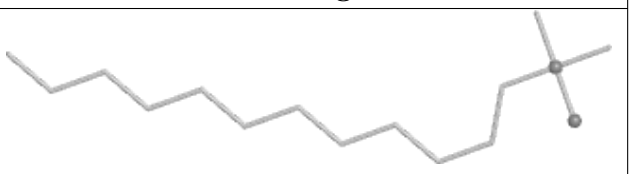
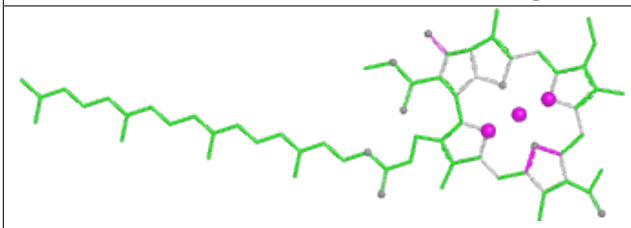
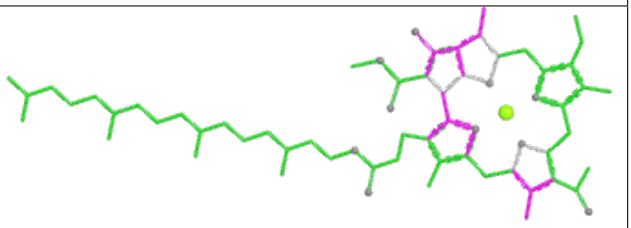
 Bond lengths	 Bond angles
 Torsions	 Rings

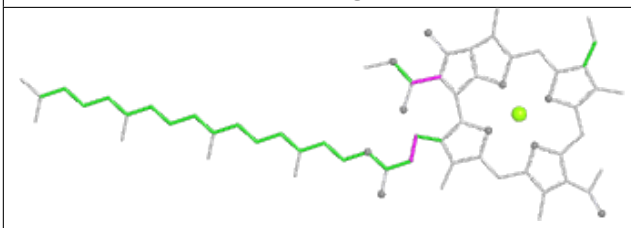
Ligand BCL L 303



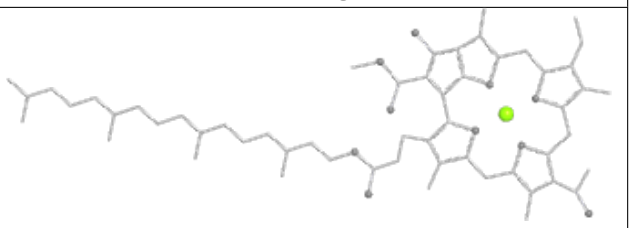
Bond lengths



Bond angles

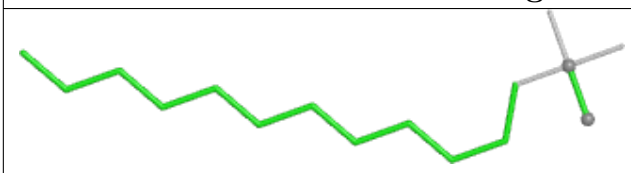


Torsions

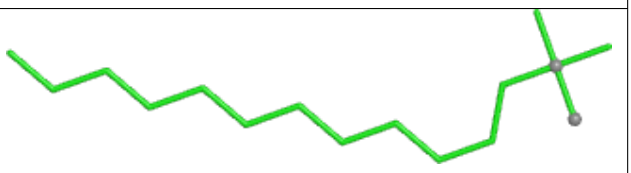


Rings

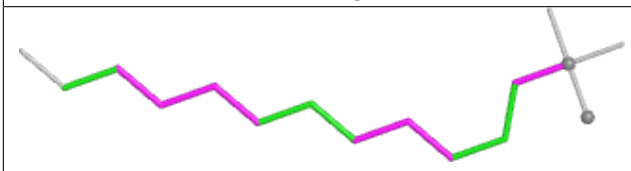
Ligand LDA L 306



Bond lengths



Bond angles



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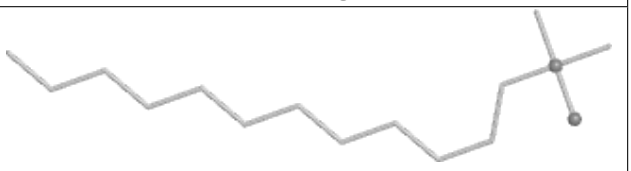
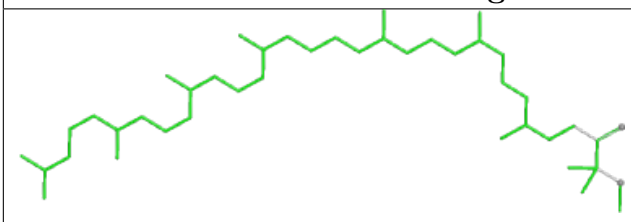
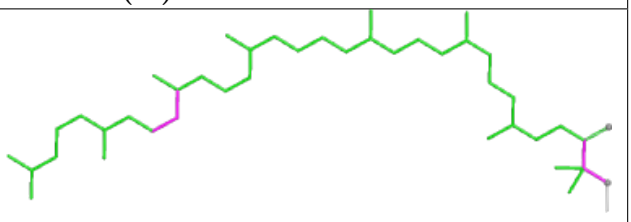


Rings

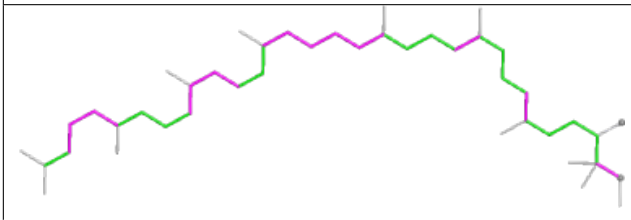
Ligand SPN M 410 (A)



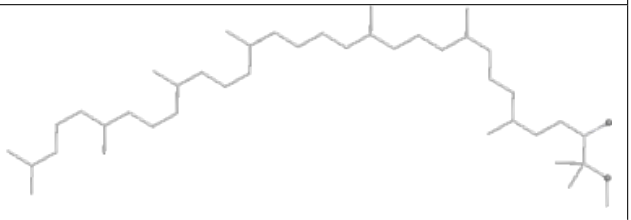
Bond lengths



Bond angles

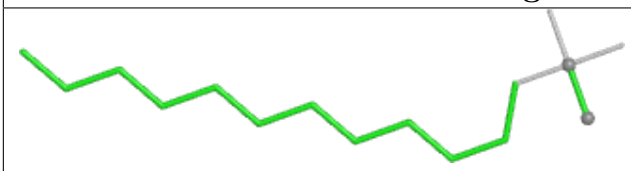


Torsions

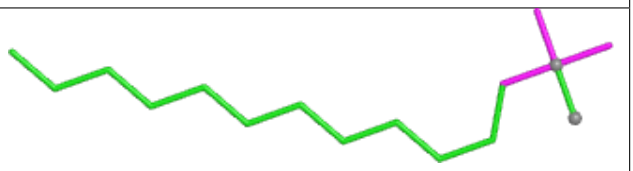


Rings

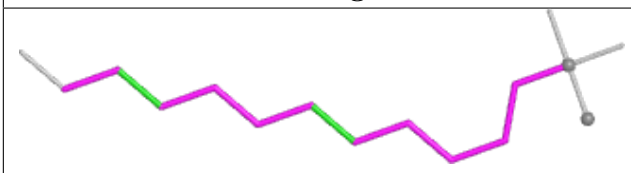
Ligand LDA H 302



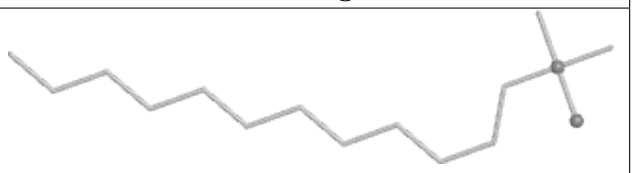
Bond lengths



Bond angles



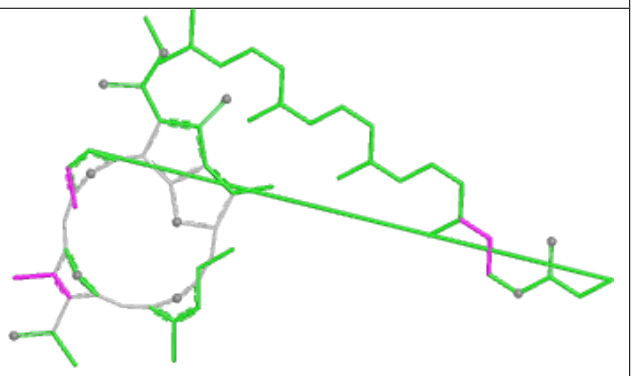
Torsions



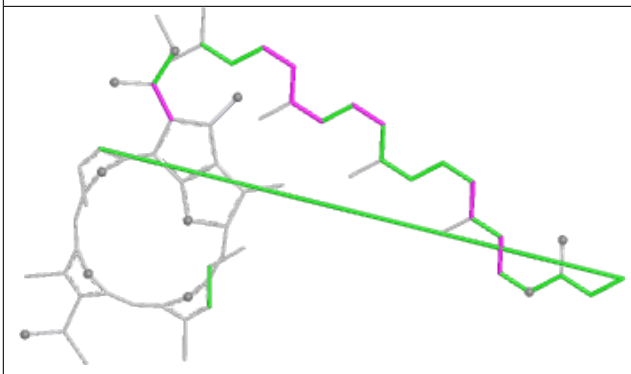
Rings

Ligand BPH L 301

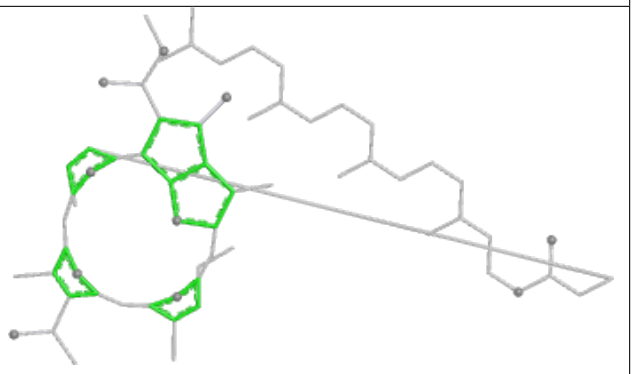
Bond lengths



Bond angles

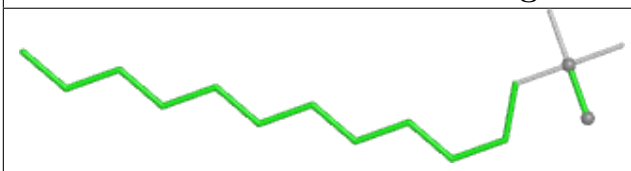


Torsions

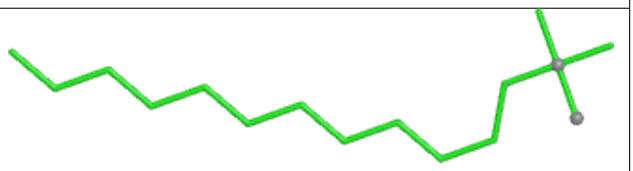


Rings

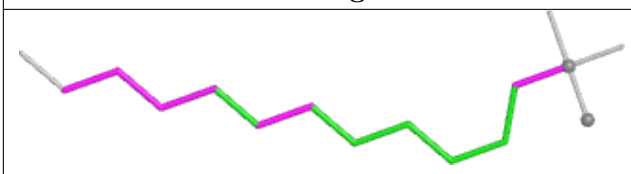
Ligand LDA M 411



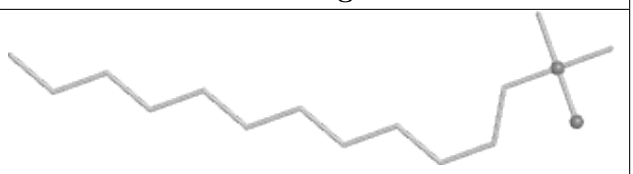
Bond lengths



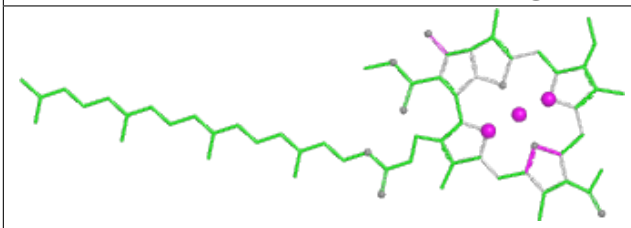
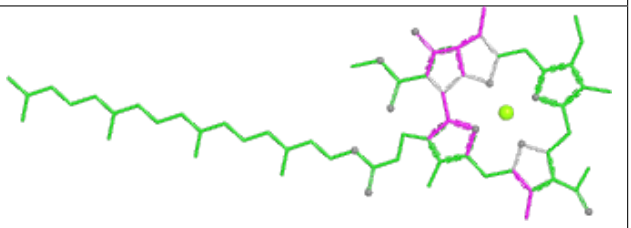
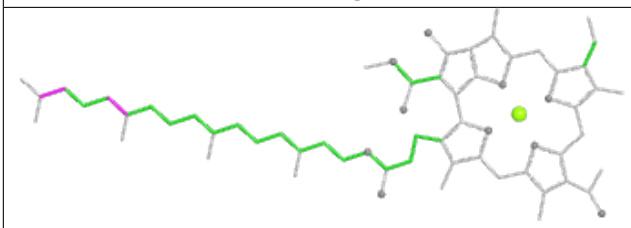
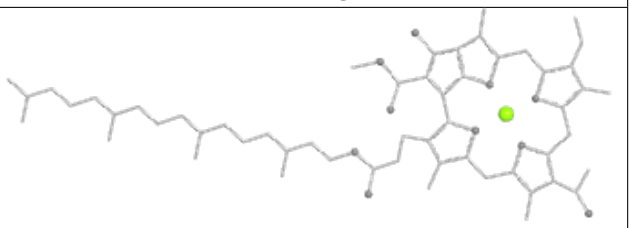
Bond angles



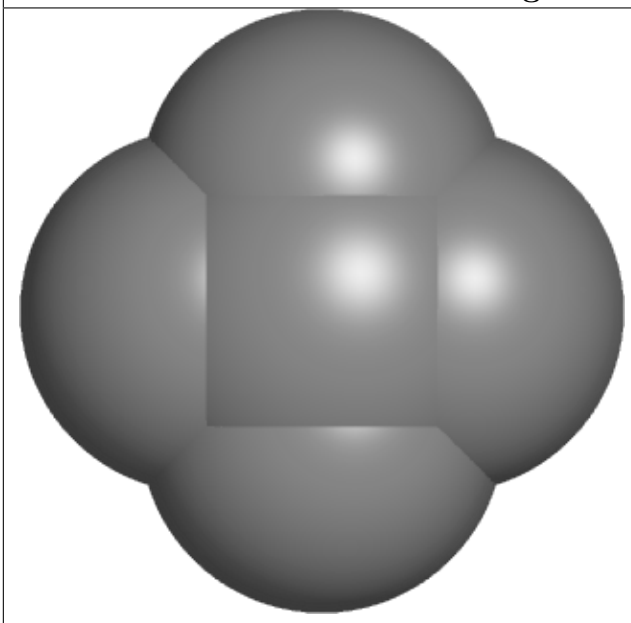
Torsions



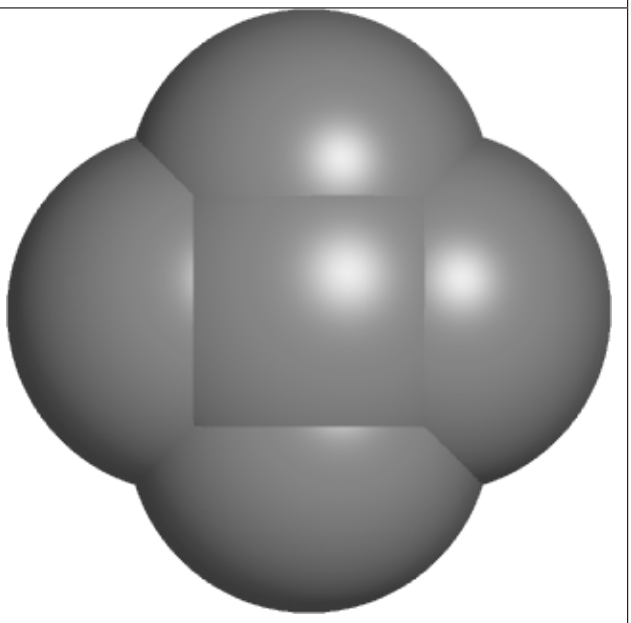
Rings

Ligand BCL L 302	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

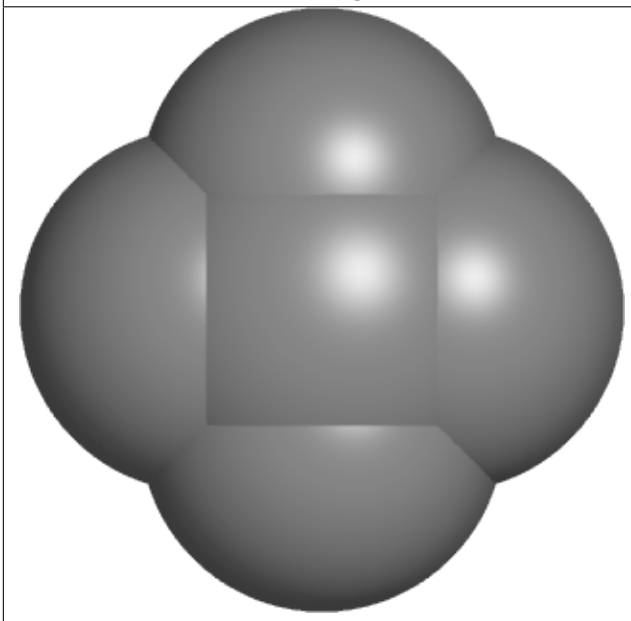
Ligand PO4 M 408



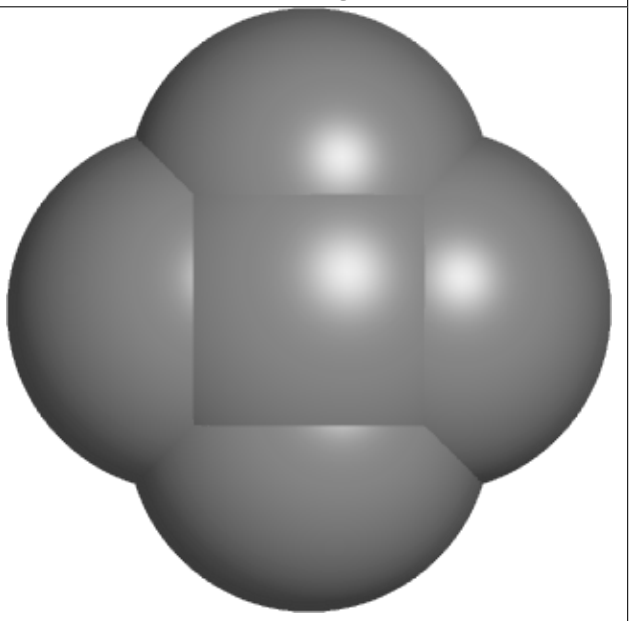
Bond lengths



Bond angles

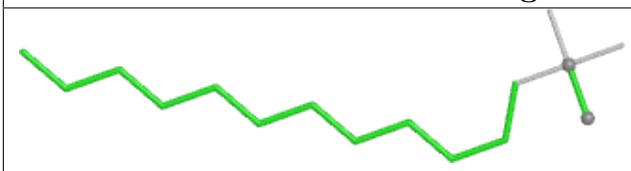


Torsions

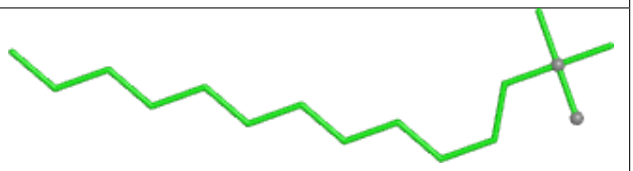


Rings

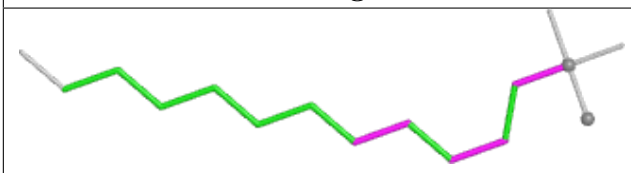
Ligand LDA M 406



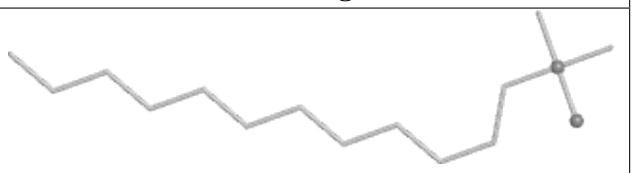
Bond lengths



Bond angles

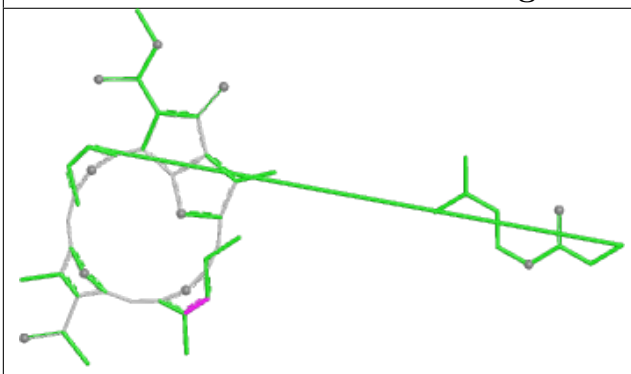


Torsions

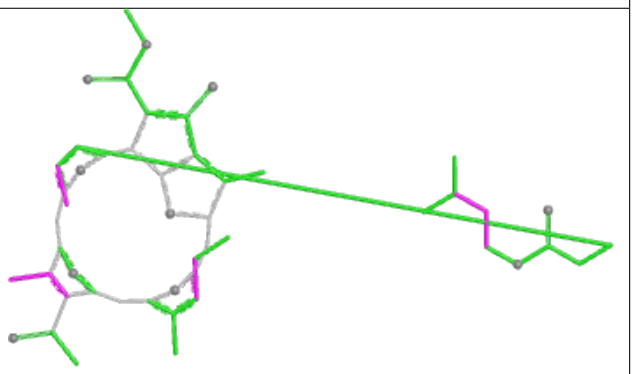


Rings

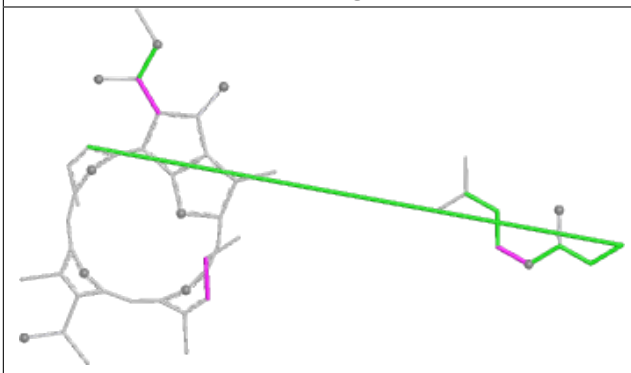
Ligand BPH M 404



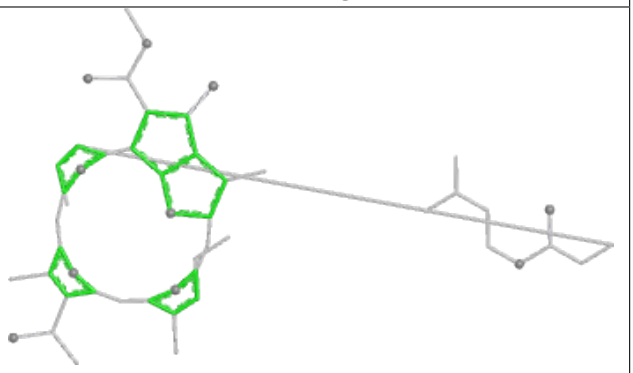
Bond lengths



Bond angles

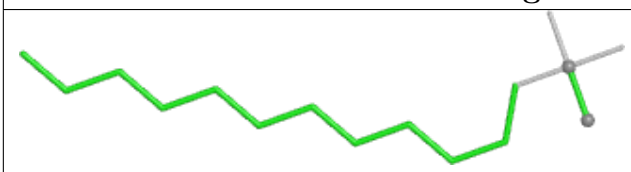


Torsions

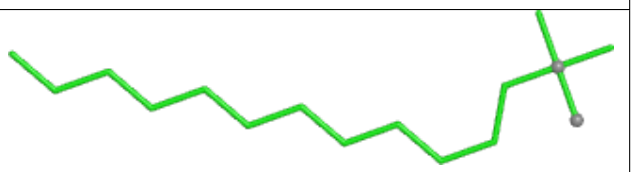


Rings

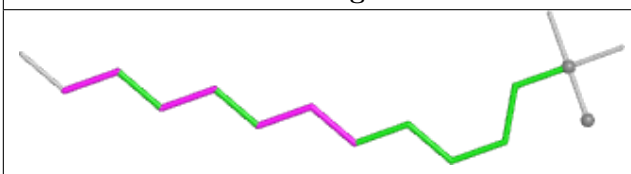
Ligand LDA H 301



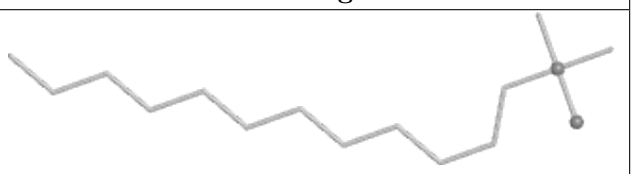
Bond lengths



Bond angles

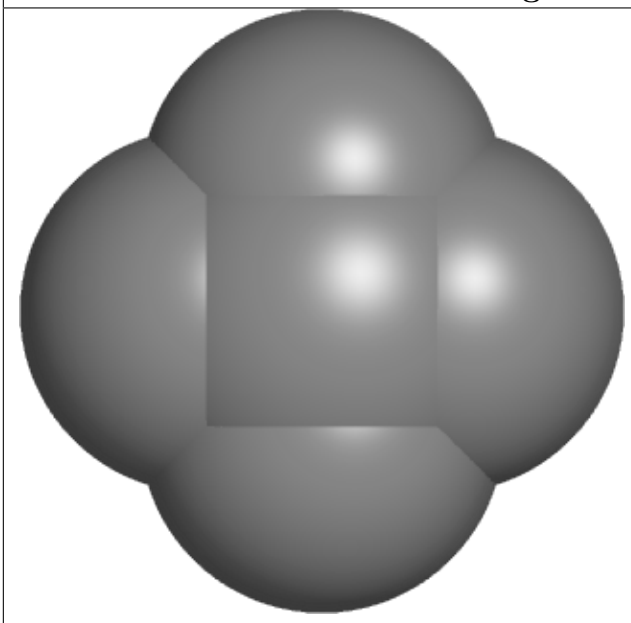


Torsions

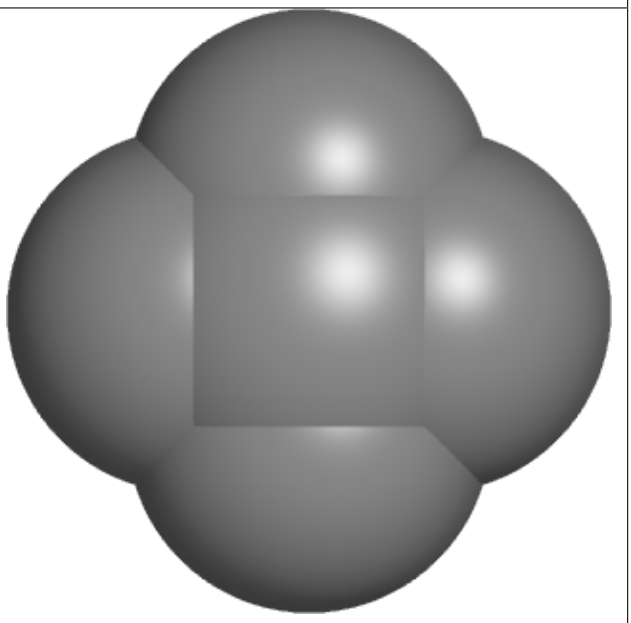


Rings

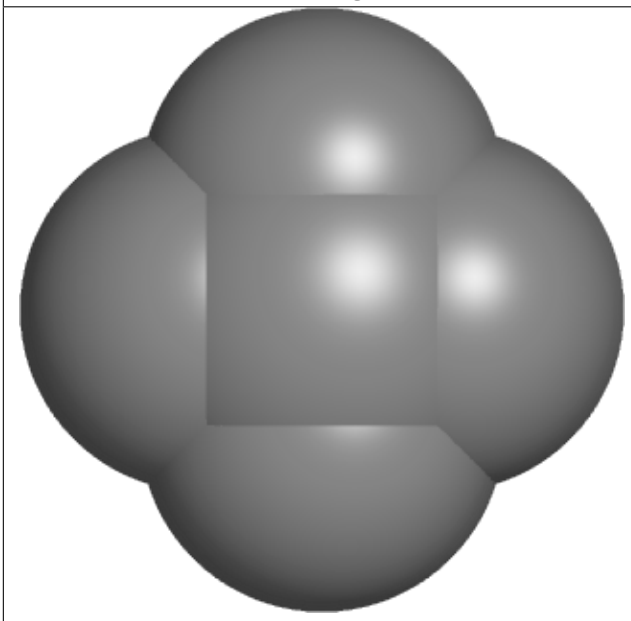
Ligand PO4 M 412



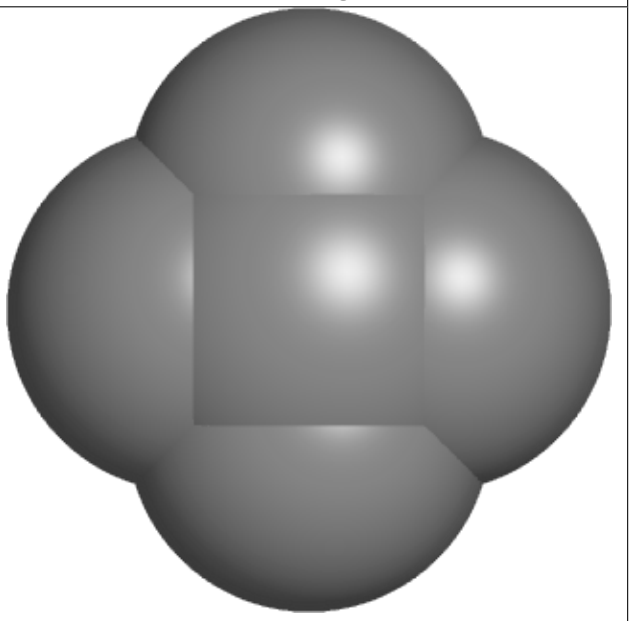
Bond lengths



Bond angles

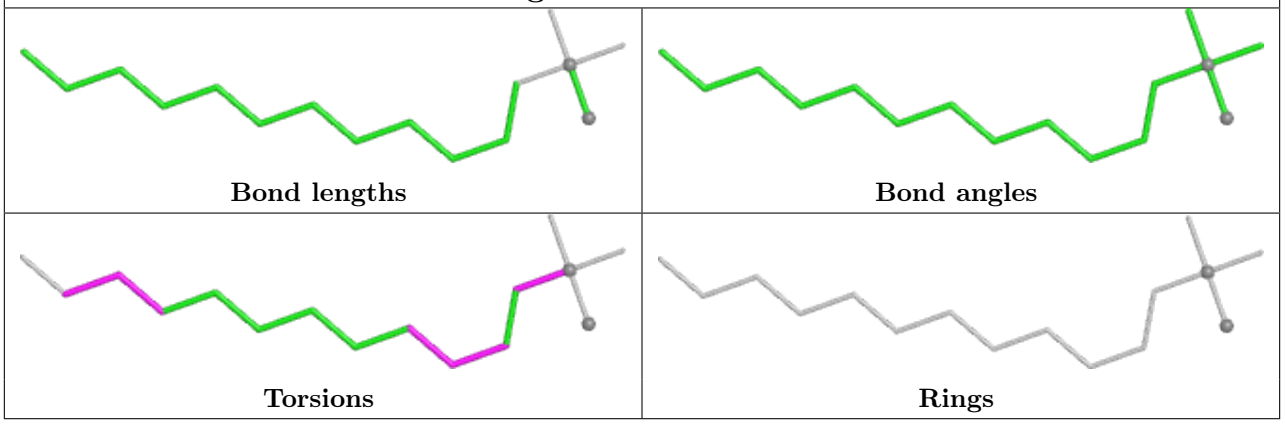


Torsions

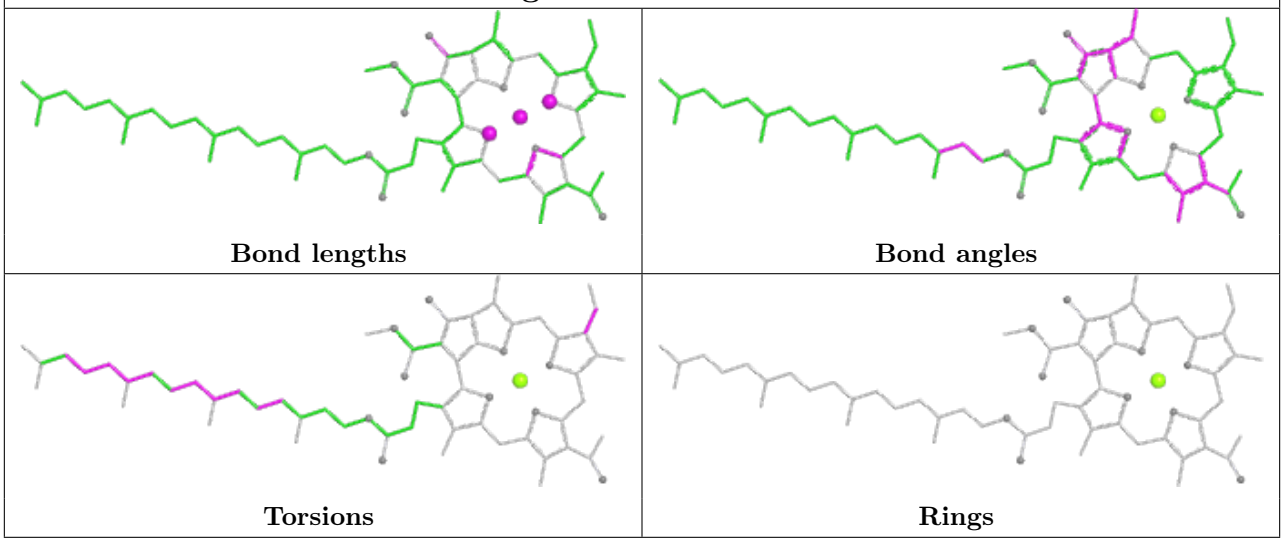


Rings

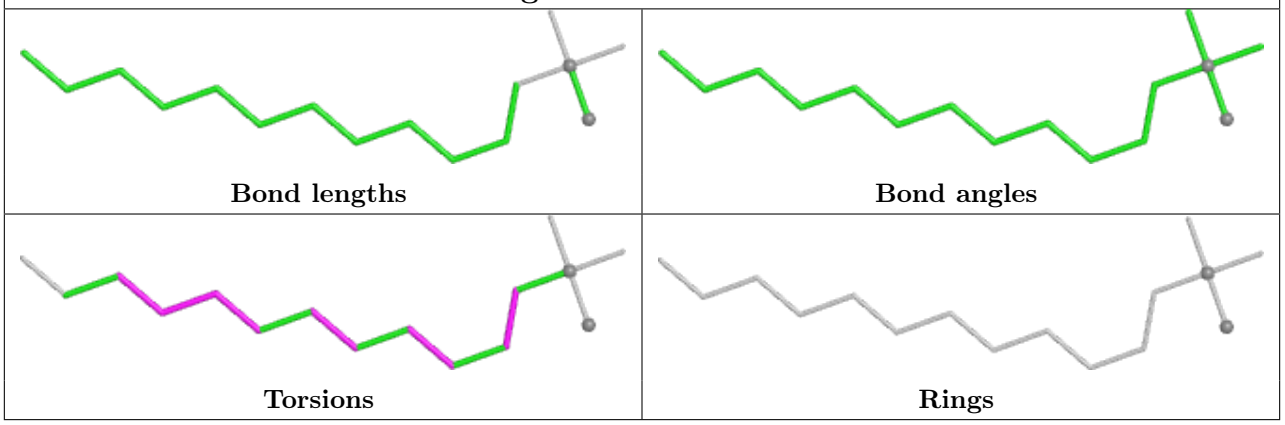
Ligand LDA L 307



Ligand BCL M 402



Ligand LDA M 407



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	H	240/241 (99%)	-0.09	7 (2%) 51 59	24, 40, 69, 147	0
2	L	281/281 (100%)	-0.10	12 (4%) 35 42	22, 39, 95, 118	0
3	M	300/302 (99%)	-0.10	7 (2%) 60 67	21, 38, 69, 92	0
All	All	821/824 (99%)	-0.09	26 (3%) 47 55	21, 39, 76, 147	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	277	GLY	6.3
2	L	270	PRO	6.0
2	L	59	TRP	4.4
3	M	301	HIS	4.3
3	M	300	ASN	3.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

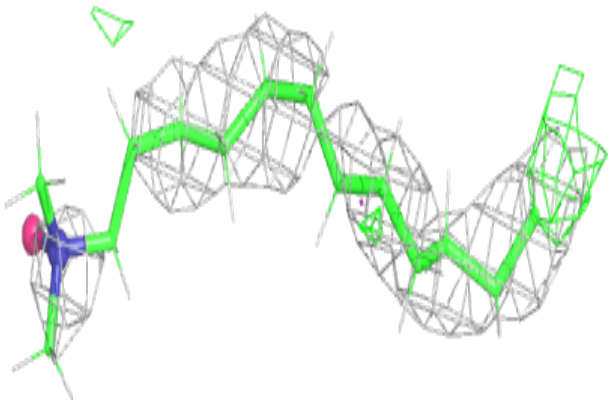
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

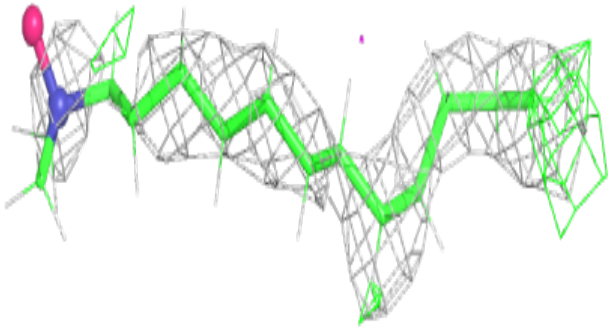
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LDA	L	307	16/16	0.54	0.46	84,103,137,137	0
4	LDA	M	406	16/16	0.72	0.31	61,84,124,127	0
4	LDA	H	302	16/16	0.73	0.31	79,96,105,107	0
7	OLC	M	409[B]	25/25	0.74	0.28	55,72,87,89	65
12	CIT	M	413	13/13	0.74	0.29	147,153,183,186	0
4	LDA	L	305	16/16	0.77	0.29	66,84,125,125	0
4	LDA	L	306	16/16	0.78	0.30	65,84,111,112	0
11	SPN	M	410[A]	43/43	0.79	0.32	52,71,87,88	113
4	LDA	M	411	16/16	0.80	0.23	69,100,147,148	0
10	PO4	M	412	5/5	0.80	0.22	136,136,136,136	0
7	OLC	L	304[A]	25/25	0.81	0.35	47,66,84,85	65
7	OLC	L	304[B]	25/25	0.81	0.35	47,67,84,85	65
4	LDA	H	303	16/16	0.82	0.29	75,97,120,120	0
4	LDA	M	407	16/16	0.88	0.24	45,66,83,85	0
4	LDA	H	301	16/16	0.89	0.21	50,77,126,129	0
8	UQ7	M	401	48/48	0.92	0.24	27,61,107,112	0
10	PO4	M	408	5/5	0.94	0.18	60,61,65,69	0
6	BCL	M	403	52/66	0.95	0.13	26,36,57,62	0
5	BPH	L	301	65/65	0.96	0.16	19,36,56,61	0
6	BCL	L	303	66/66	0.96	0.14	24,36,99,119	0
6	BCL	M	402	66/66	0.96	0.14	29,39,84,87	0
6	BCL	L	302	66/66	0.97	0.16	25,39,80,82	0
5	BPH	M	404	50/65	0.97	0.13	24,36,65,76	0
13	CL	M	414	1/1	0.97	0.09	44,44,44,44	0
9	FE	M	405	1/1	0.98	0.23	36,36,36,36	0

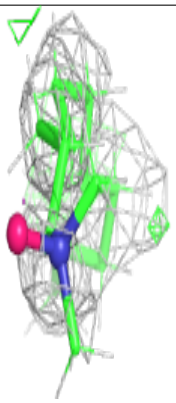
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LDA L 307:

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

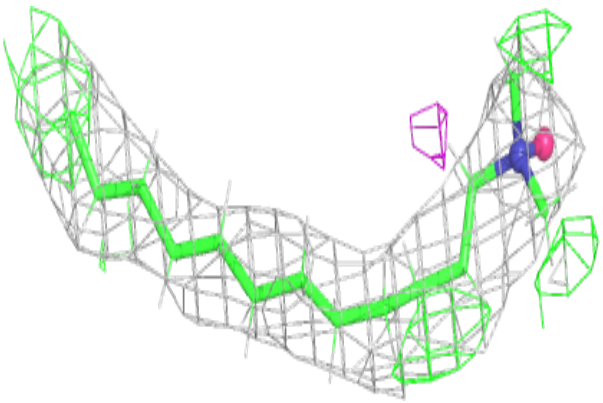


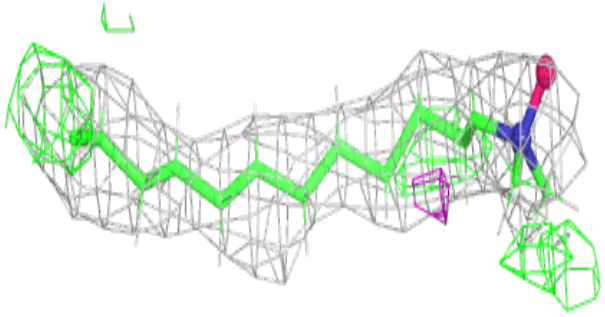


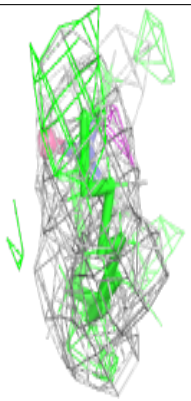


Electron density around LDA M 406:

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

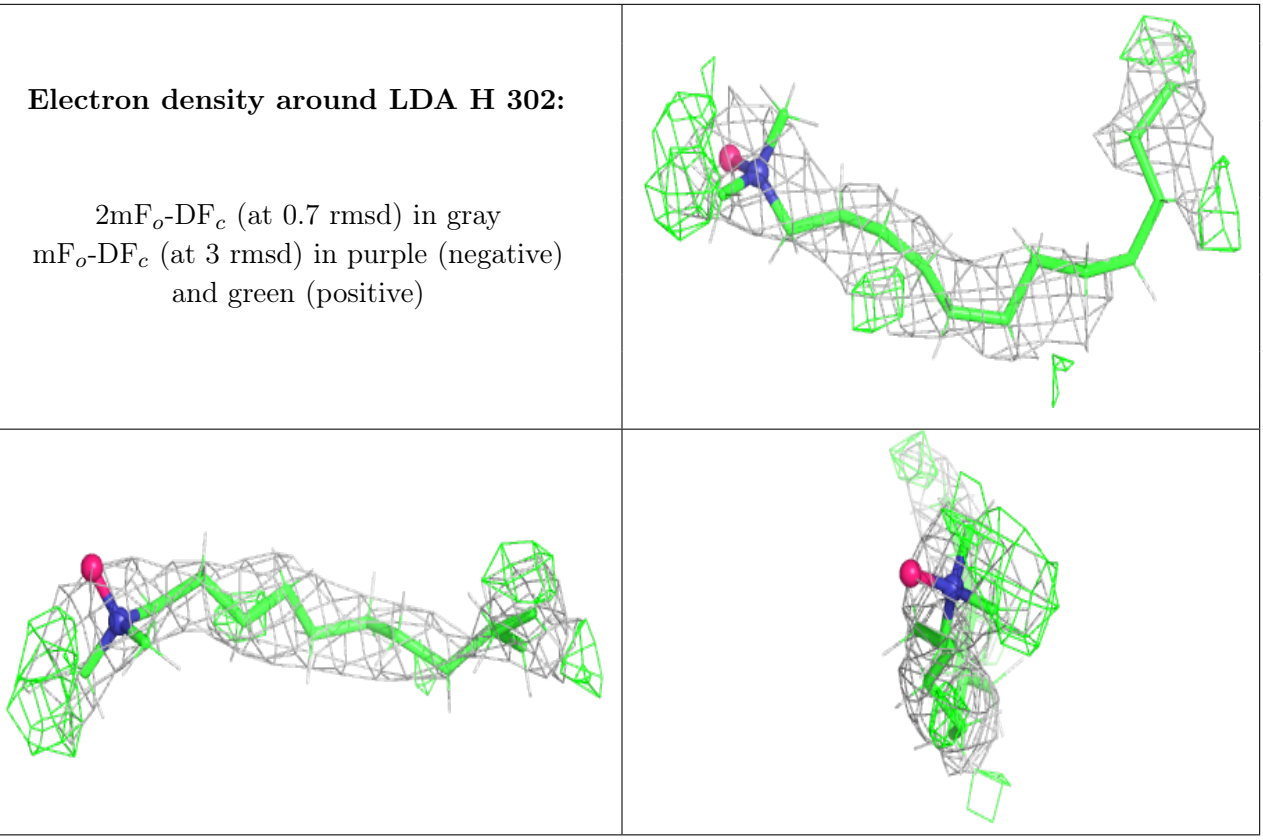






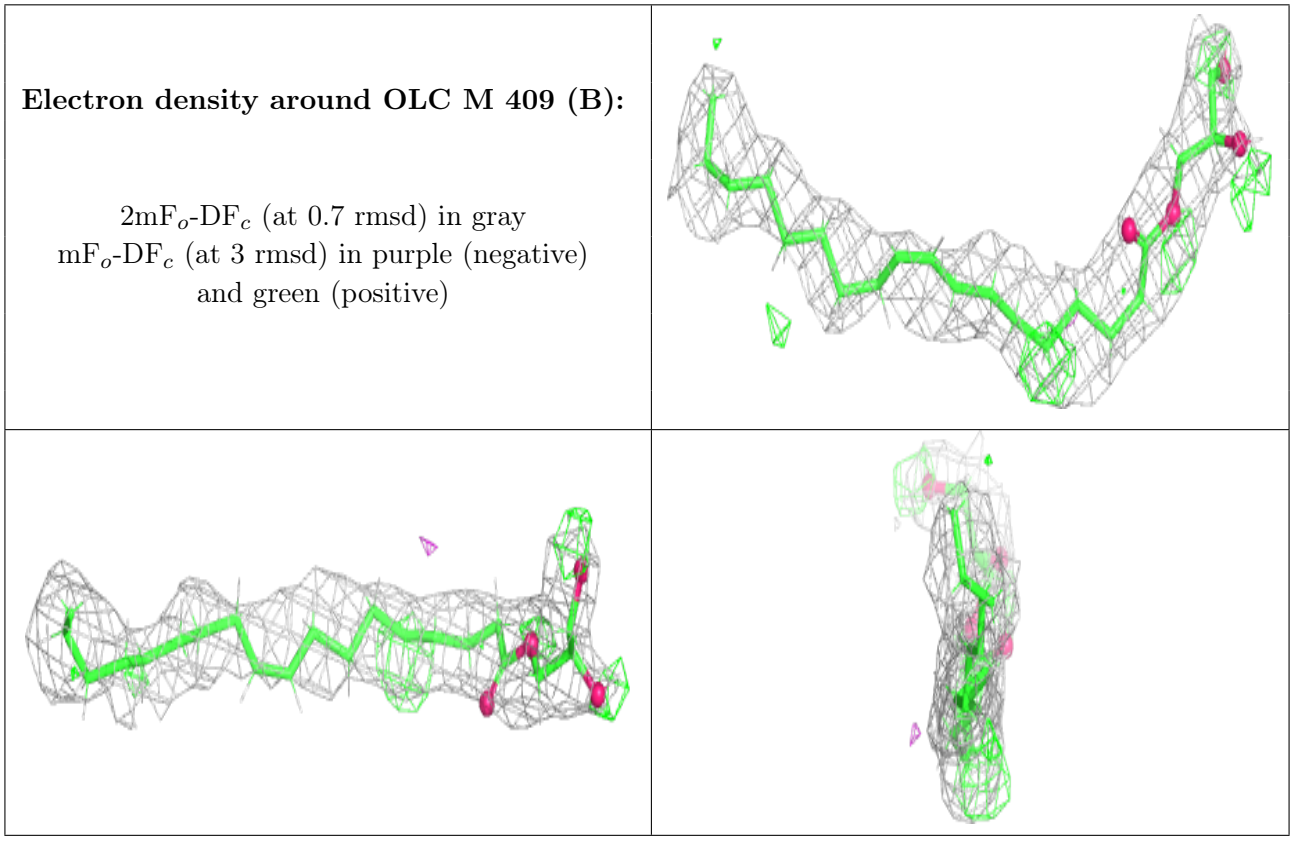
Electron density around LDA H 302:

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



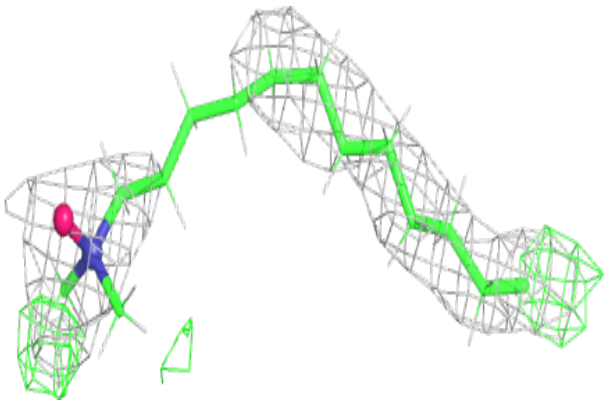
Electron density around OLC M 409 (B):

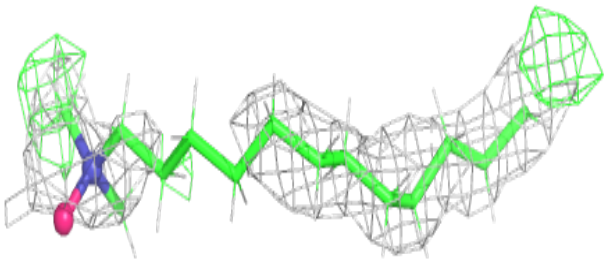
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

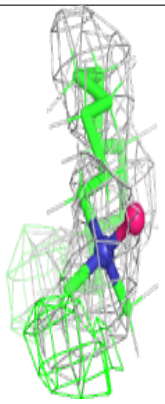


Electron density around LDA L 305:

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

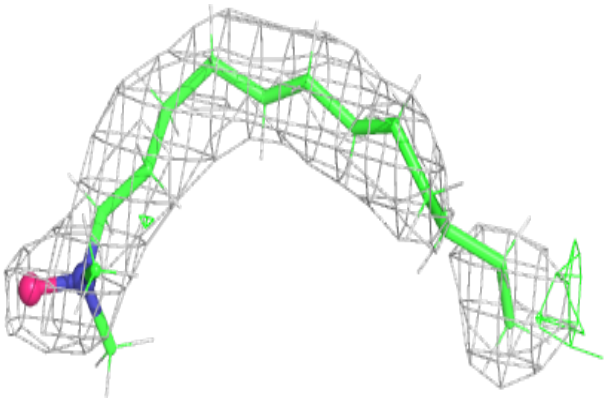


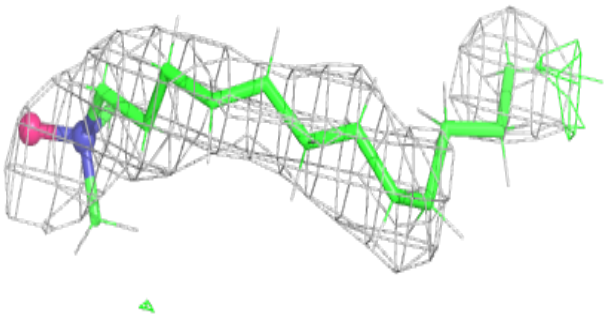


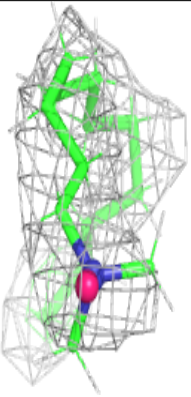


Electron density around LDA L 306:

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

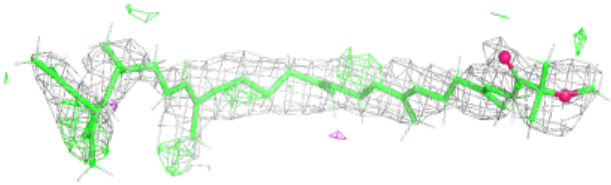


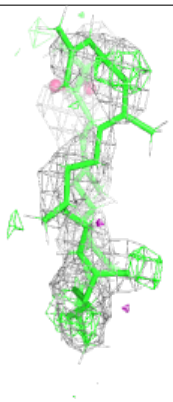




Electron density around SPN M 410 (A):

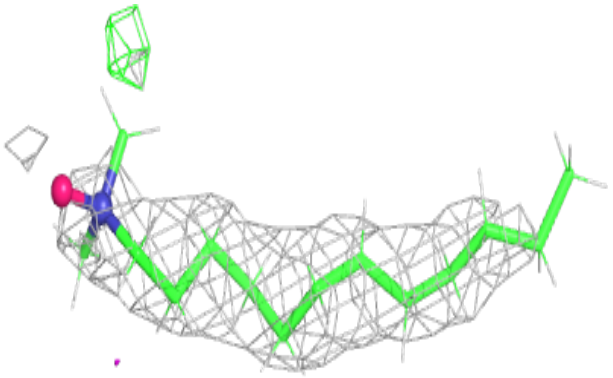
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

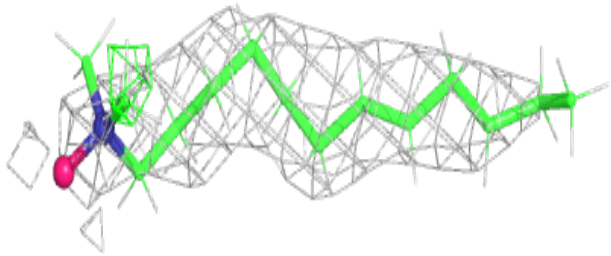


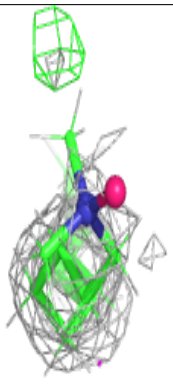


Electron density around LDA M 411:

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

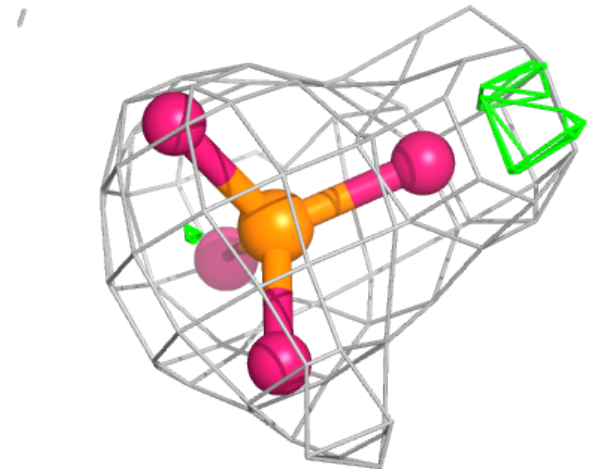


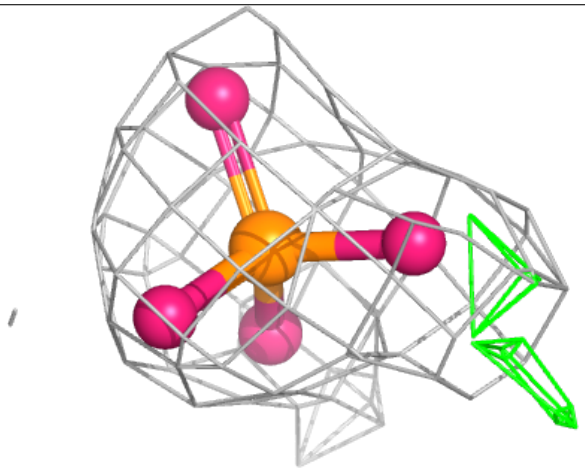


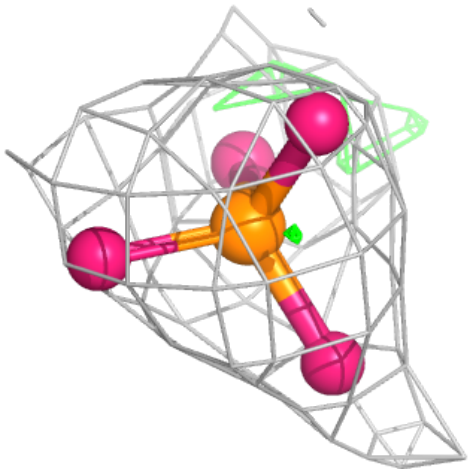


Electron density around PO4 M 412:

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

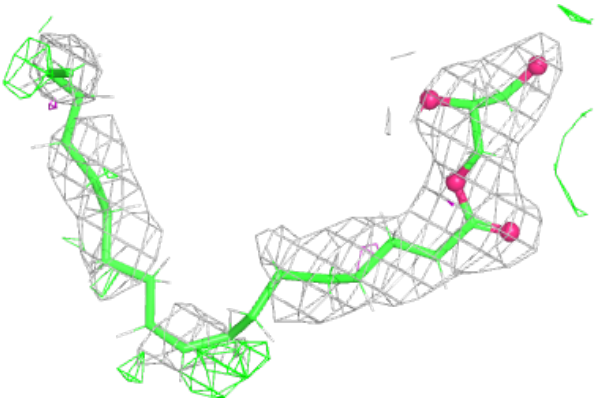


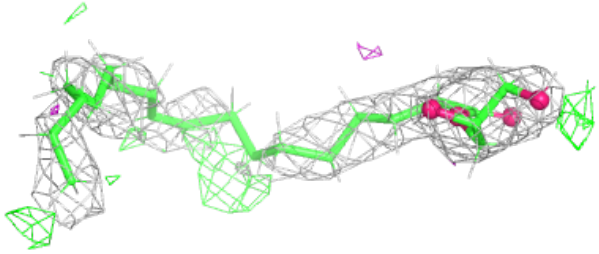




Electron density around OLC L 304 (A):

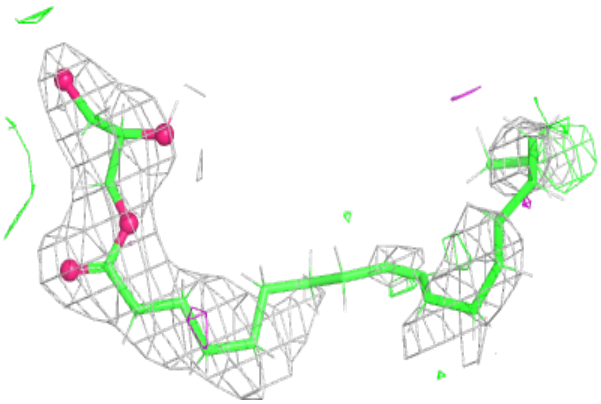
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

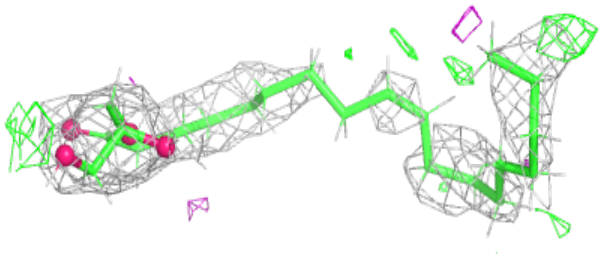


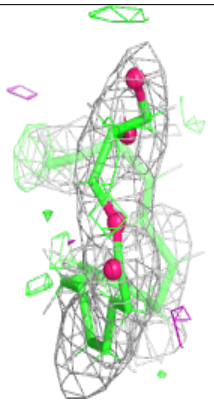


Electron density around OLC L 304 (B):

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

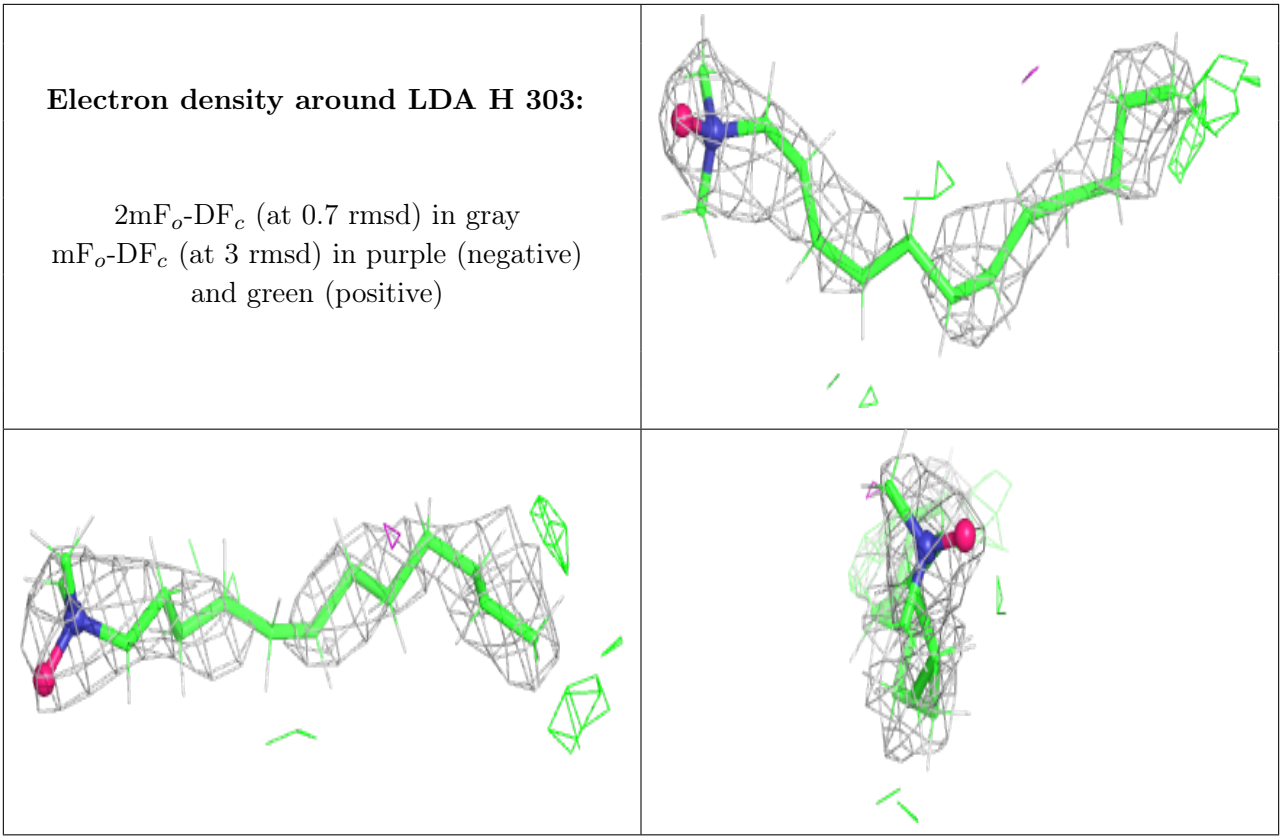






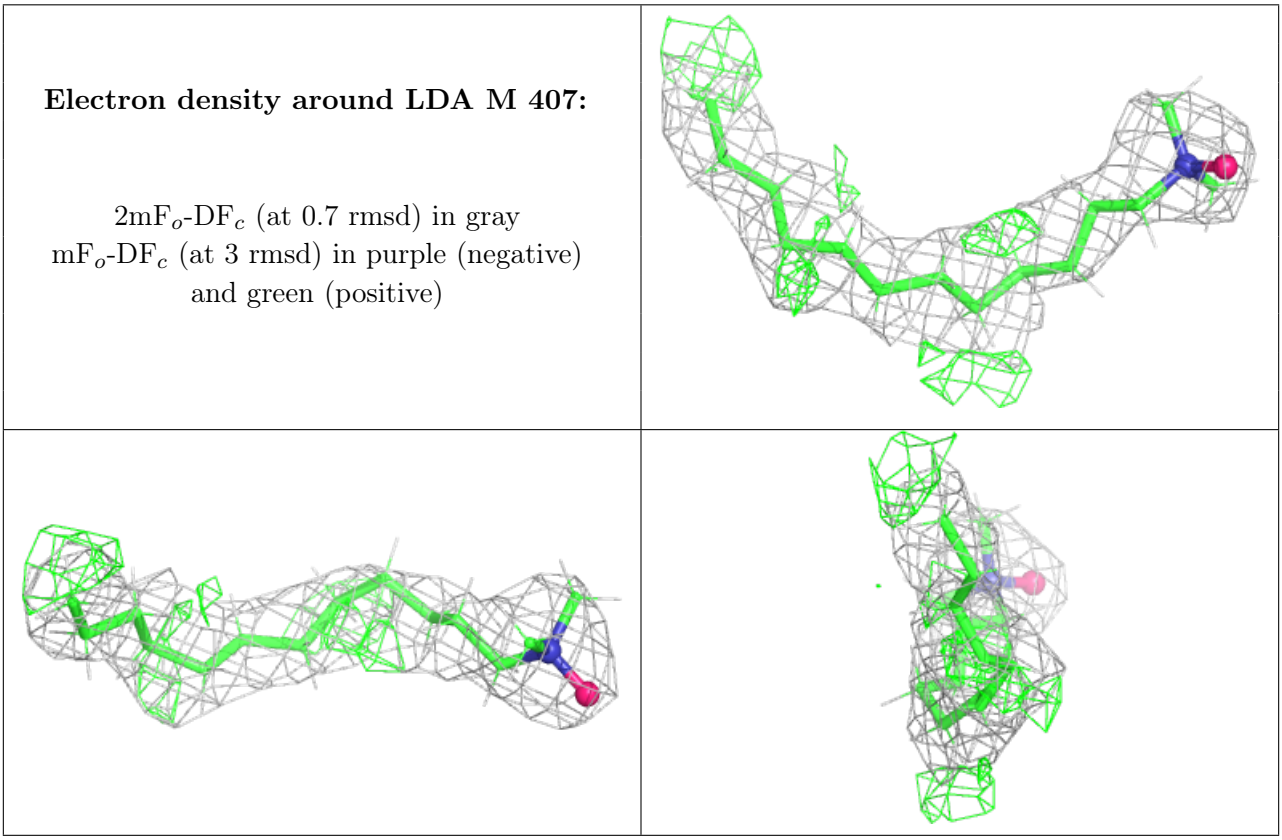
Electron density around LDA H 303:

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



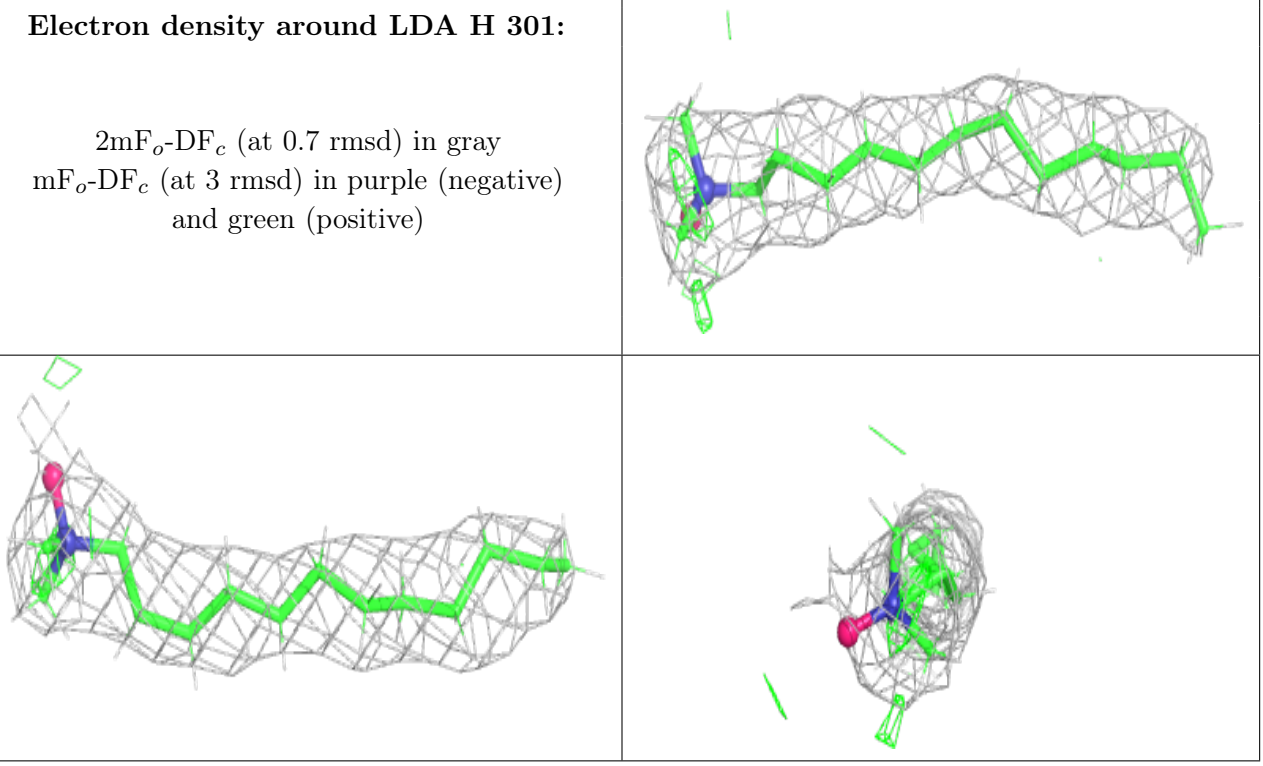
Electron density around LDA M 407:

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



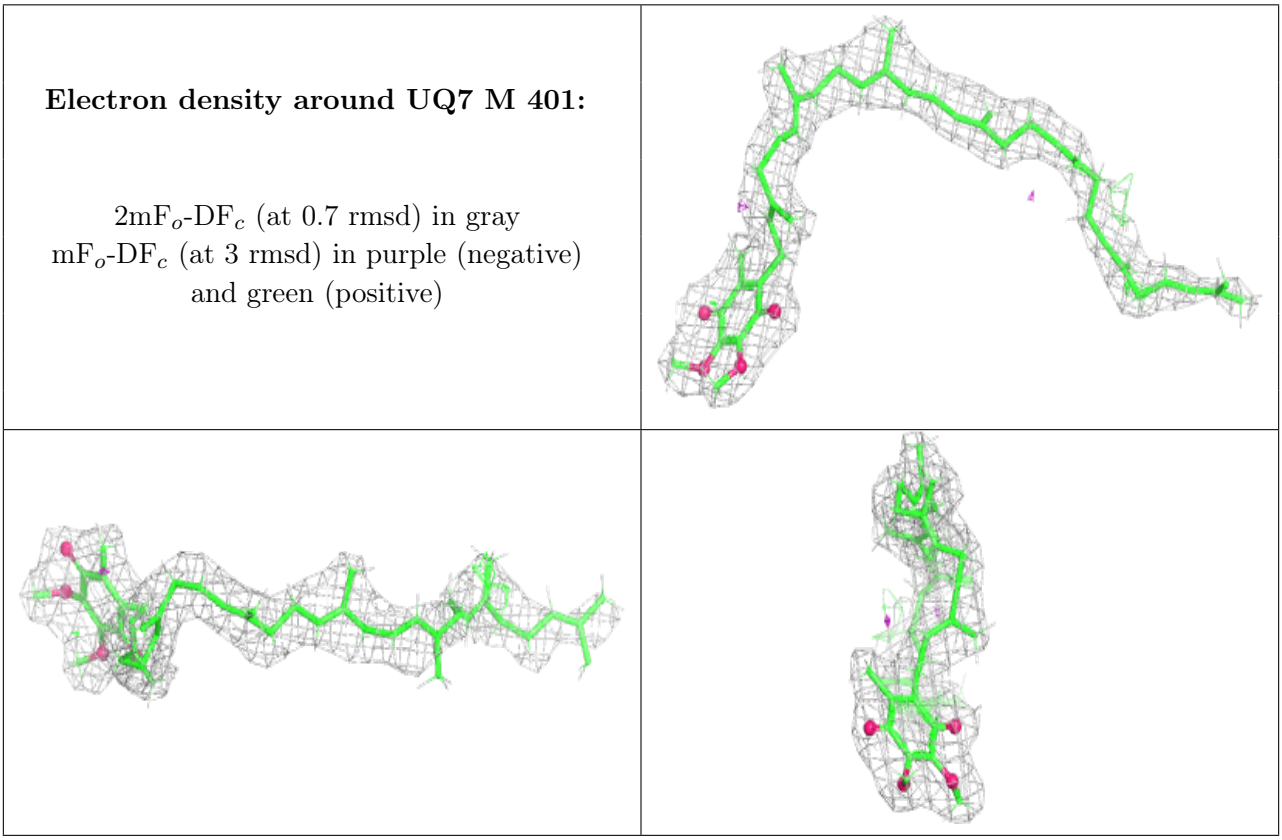
Electron density around LDA H 301:

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



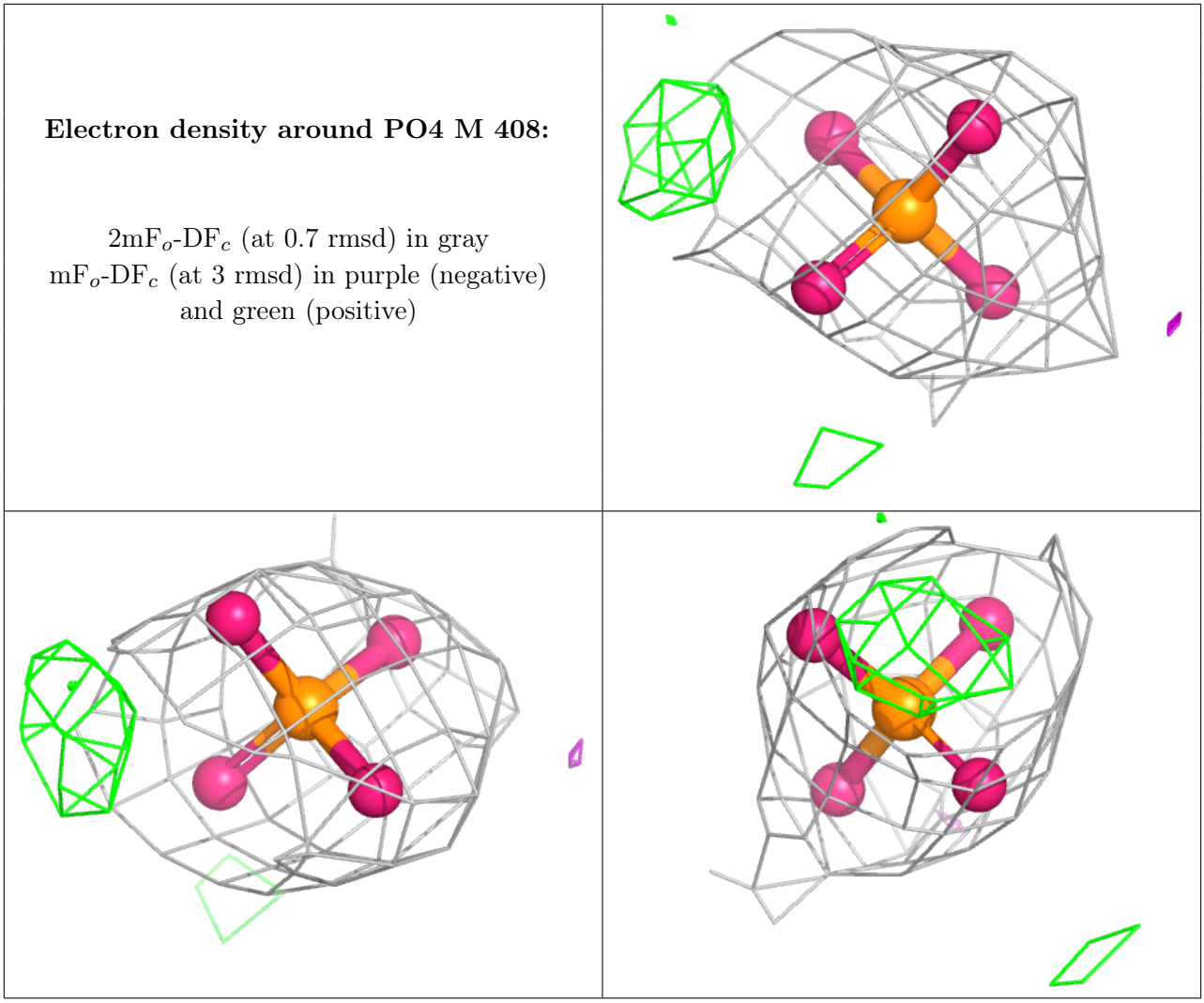
Electron density around UQ7 M 401:

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



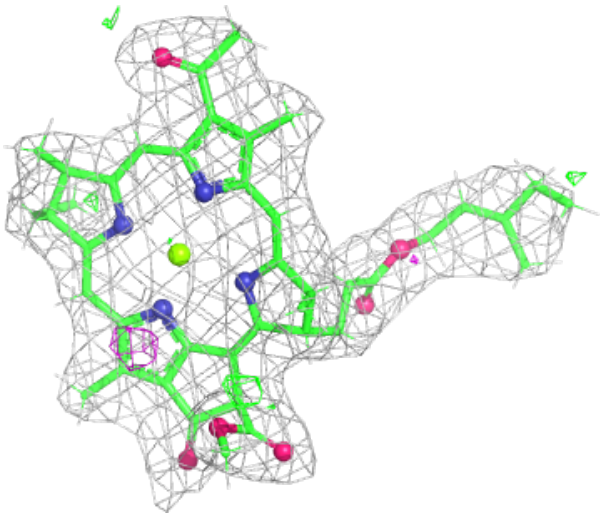
Electron density around PO4 M 408:

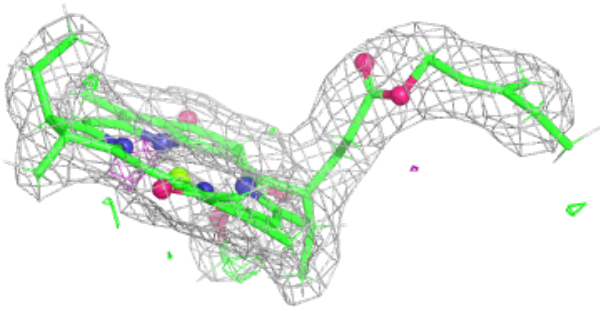
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

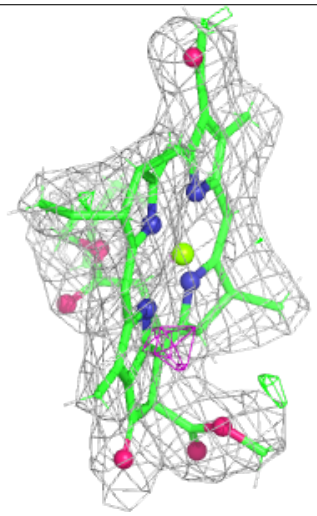


Electron density around BCL M 403:

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

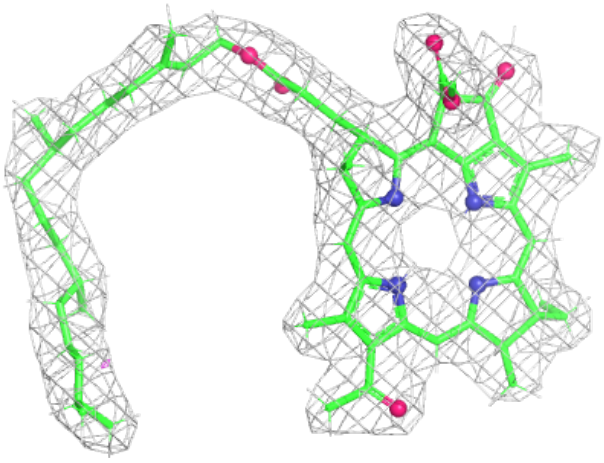


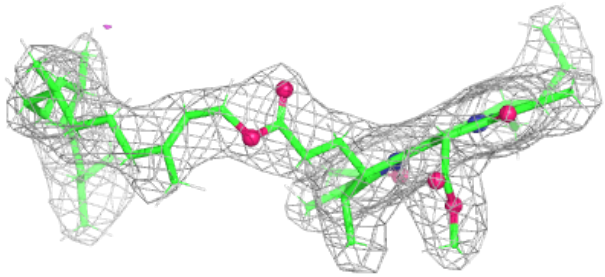




Electron density around BPH L 301:

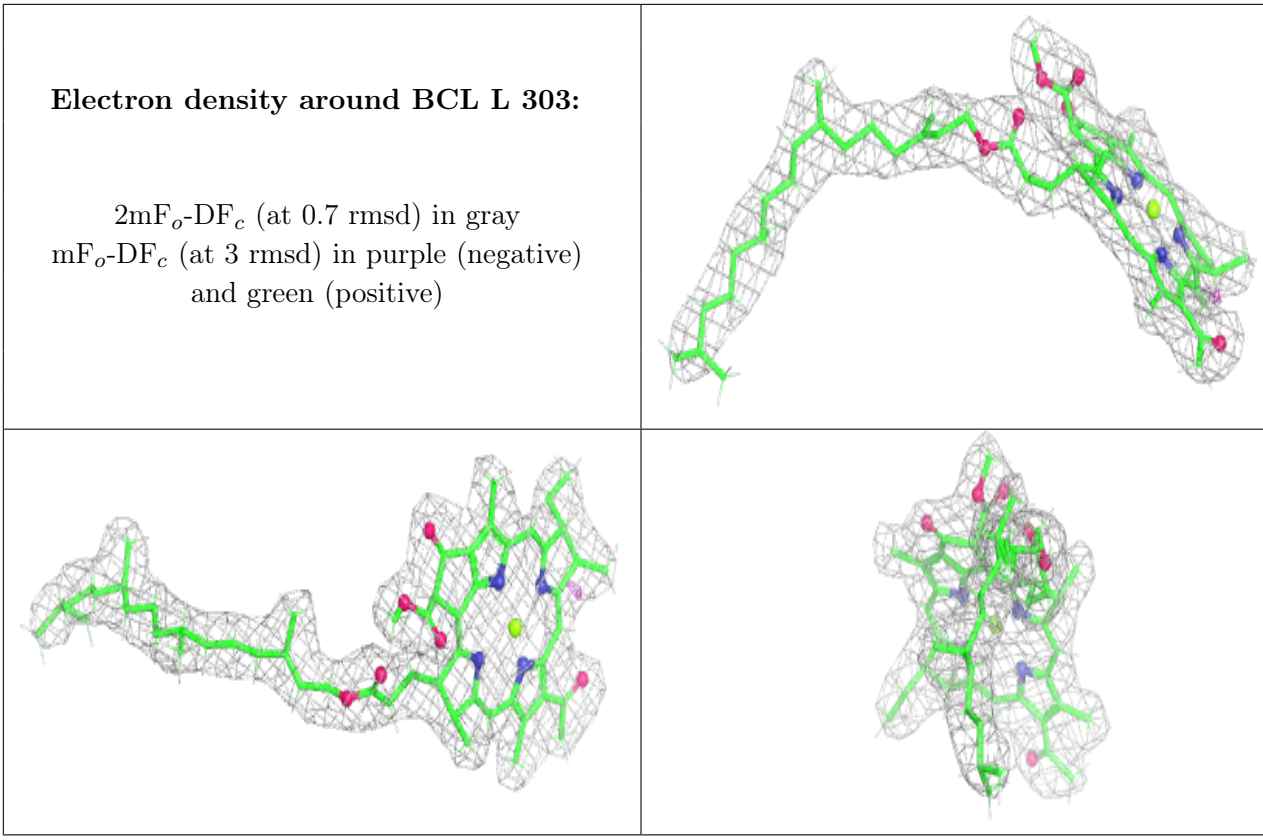
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





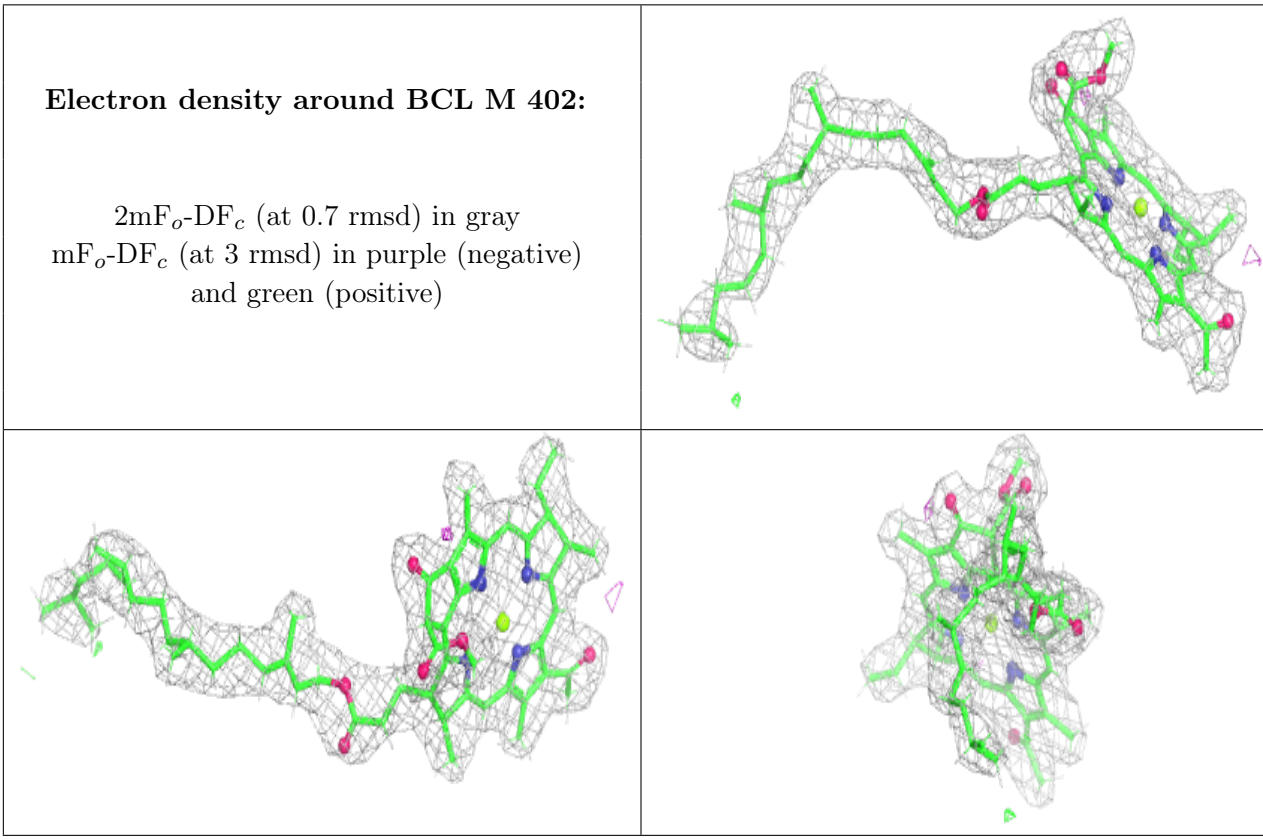
Electron density around BCL L 303:

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



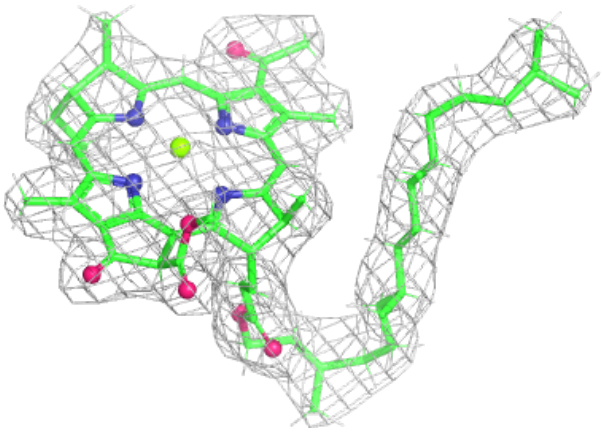
Electron density around BCL M 402:

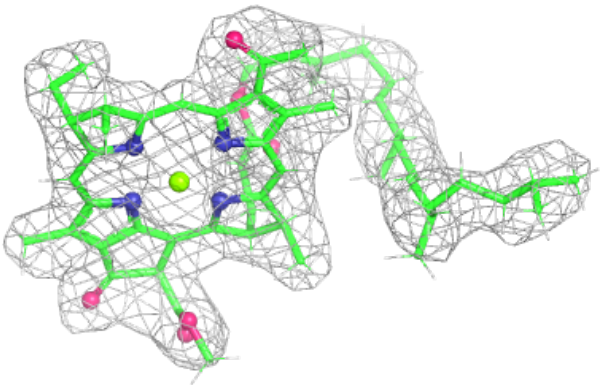
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

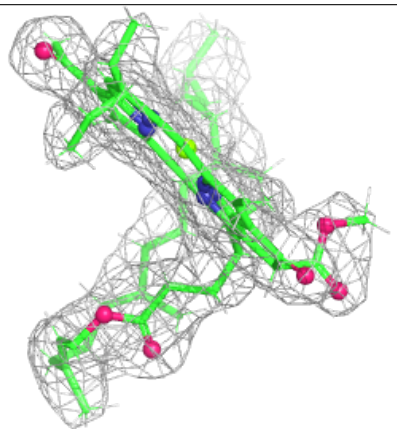


Electron density around BCL L 302:

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

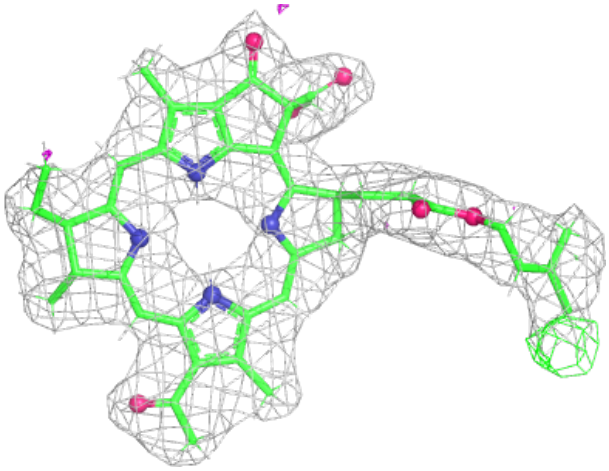


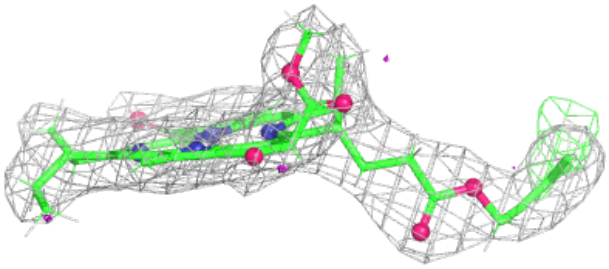


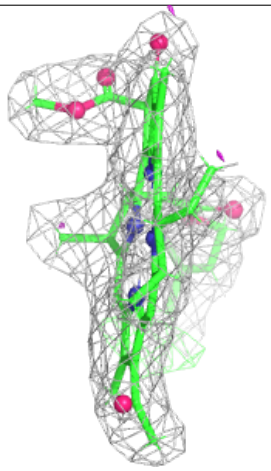


Electron density around BPH M 404:

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

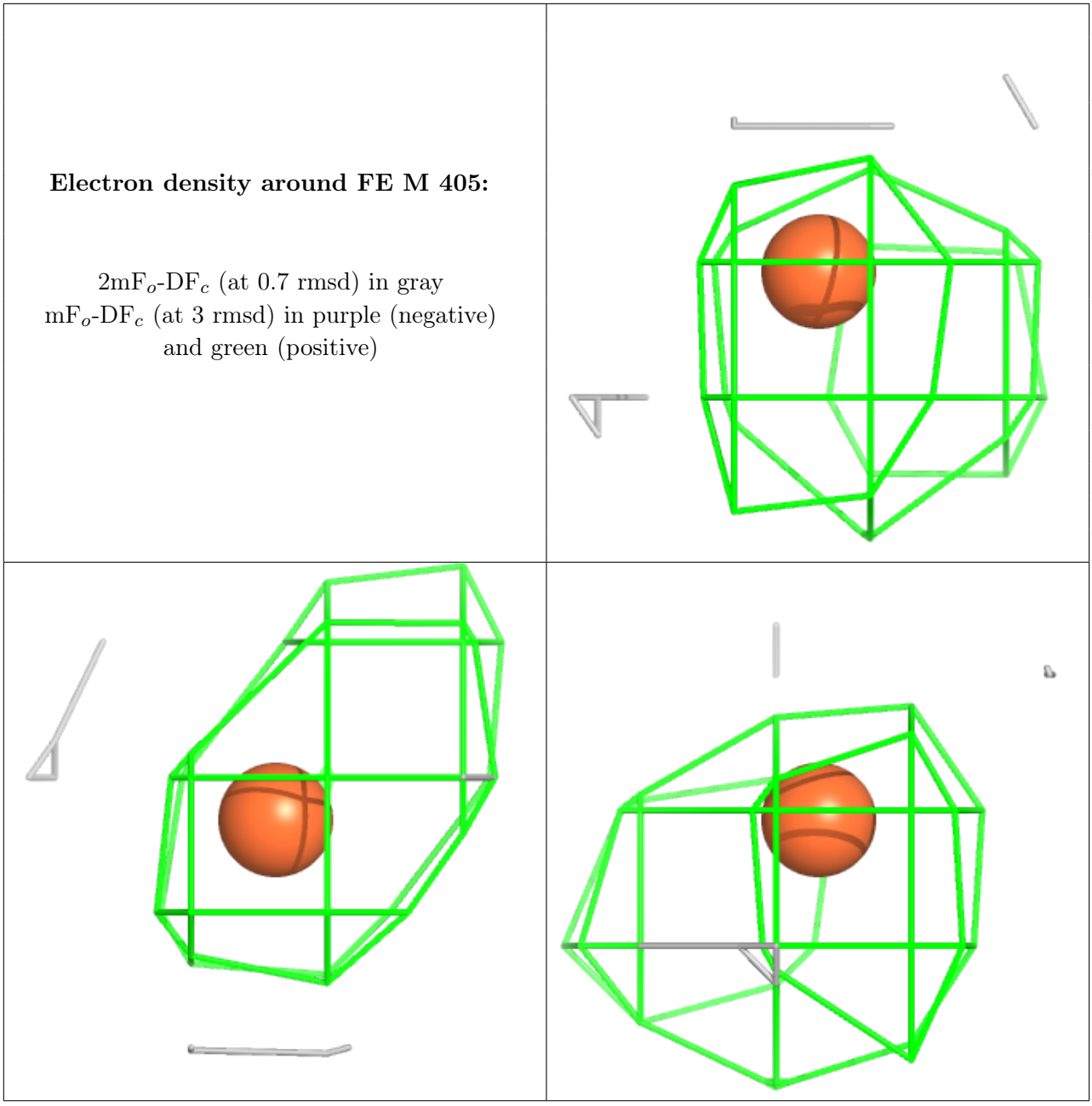






Electron density around FE M 405:

$2mF_o$-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.