wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 12:37 am BST

PDB ID	:	7Q7O / pdb_00007q7o
Title	:	Room temperature structure of the Rhodobacter Sphaeroides Photosynthetic Reaction Center F(M197)H mutant at atmospheric pressure after high helium gas pressure release
Authors	:	Lieske, J.; Guenther, S.; Saouane, S.; Selikhanov, G.K.; Gabdulkhakov, A.G.; Meents, A.
Deposited on	:	2021-11-09
Resolution	:	2.65 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:

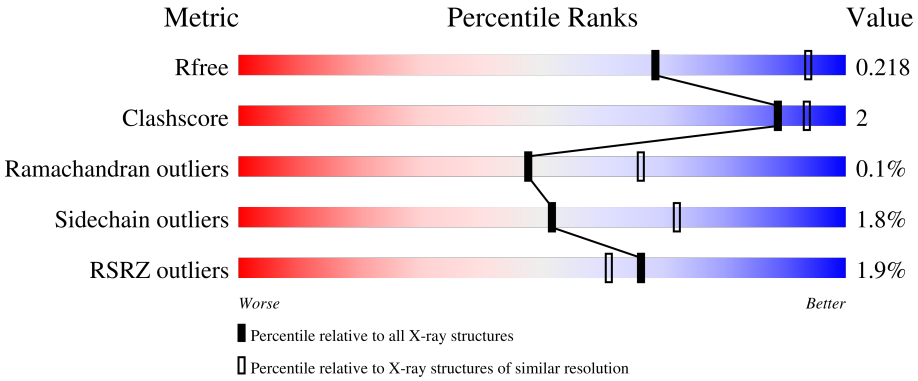
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	92% 7%
2	L	281	3% 96%
3	M	302	2% 95%

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
13	CIT	M	413	-	X	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 14659 atoms, of which 7294 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	4	0
			3726	1189	1870	318	339	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	2	0
			4447	1519	2200	357	363	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

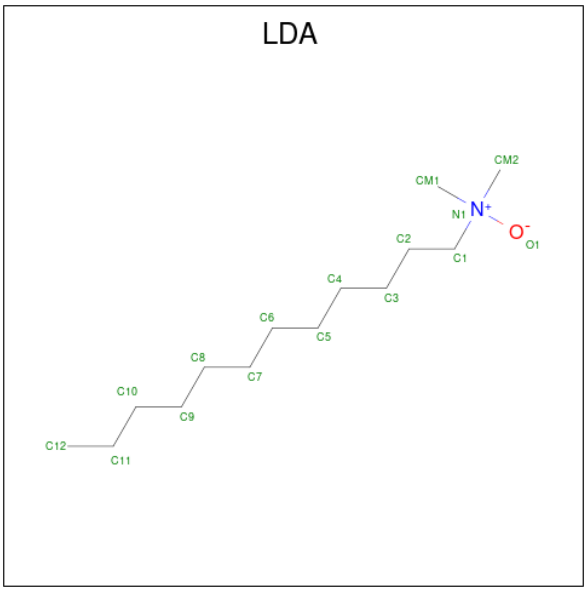
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	M	300	Total	C	H	N	O	S	0	5	0
			4775	1629	2340	398	398	10			

There are 2 discrepancies between the modelled and reference sequences:

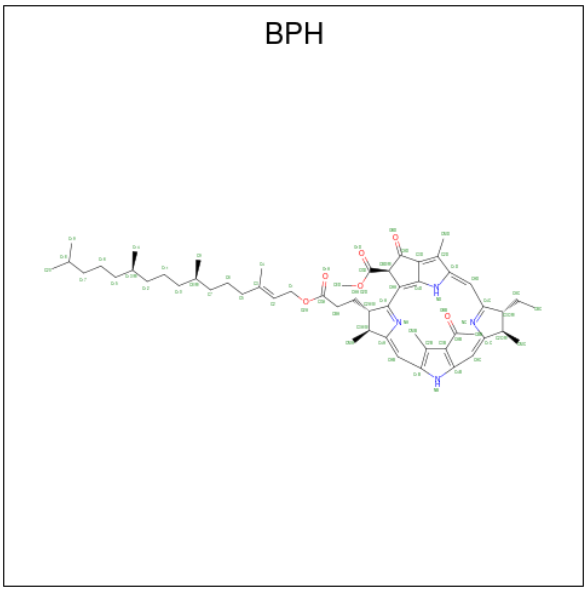
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP P0C0Y9
M	197	HIS	PHE	engineered mutation	UNP P0C0Y9

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



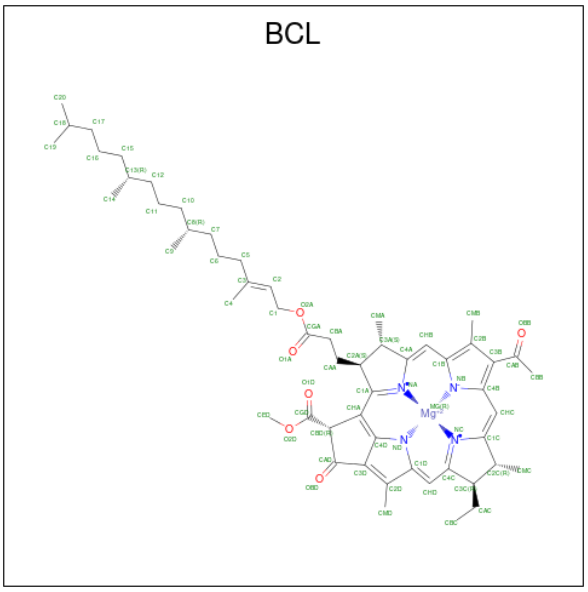
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	H	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	H	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	L	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	L	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	L	1	Total	C	H	N	O	0	0
			47	14	31	1	1		
4	M	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 (CCD ID: 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 (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



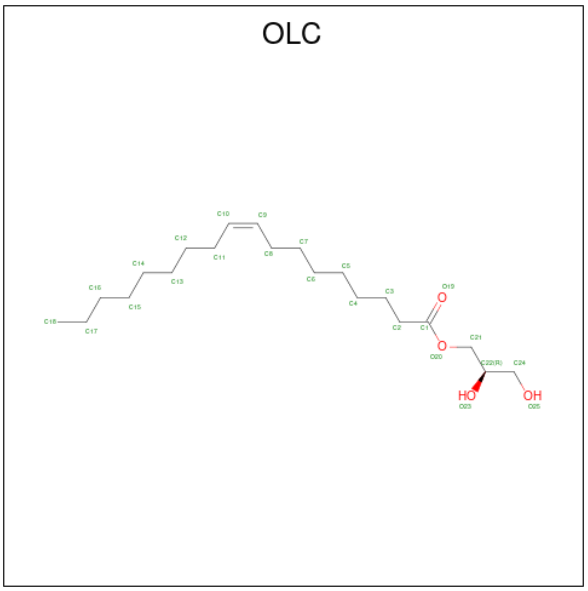
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	L	1	Total	C	H	Mg	N	O	0	0
			140	55	74	1	4	6		

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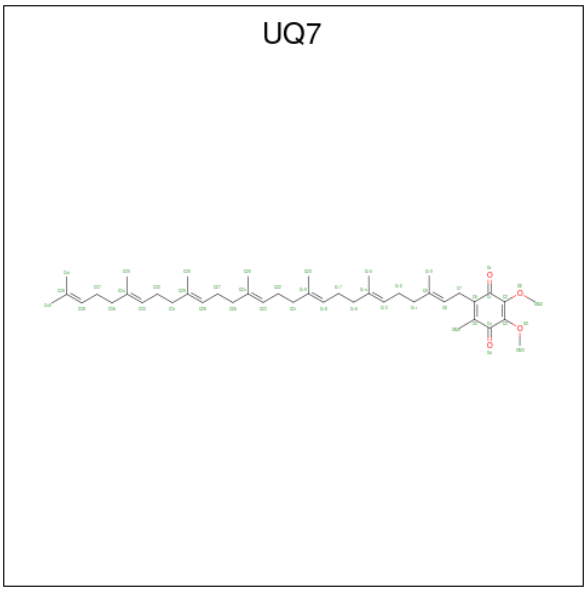
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	L	1	Total	C	H	Mg	N	O	0	0
			140	55	74	1	4	6		
6	M	1	Total	C	H	Mg	N	O	0	0
			139	55	73	1	4	6		
6	M	1	Total	C	H	Mg	N	O	0	0
			94	40	43	1	4	6		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: 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	0
			65	21	40	4		
7	M	1	Total	C	H	O	0	1
			65	21	40	4		

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

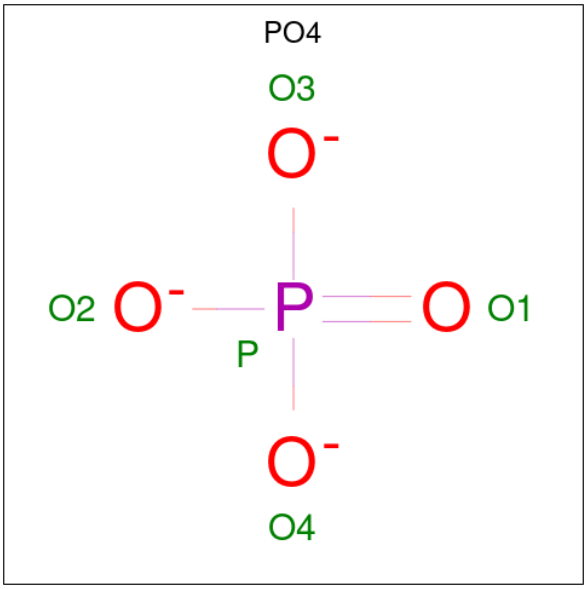


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	M	1	113	44	65	4	0	0

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

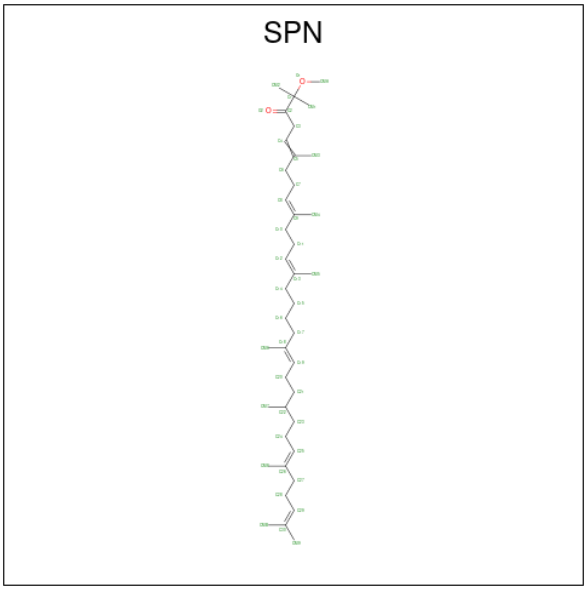
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
9	M	1	1	1	0	0

- Molecule 10 is PHOSPHATE ION (CCD ID: 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 (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).

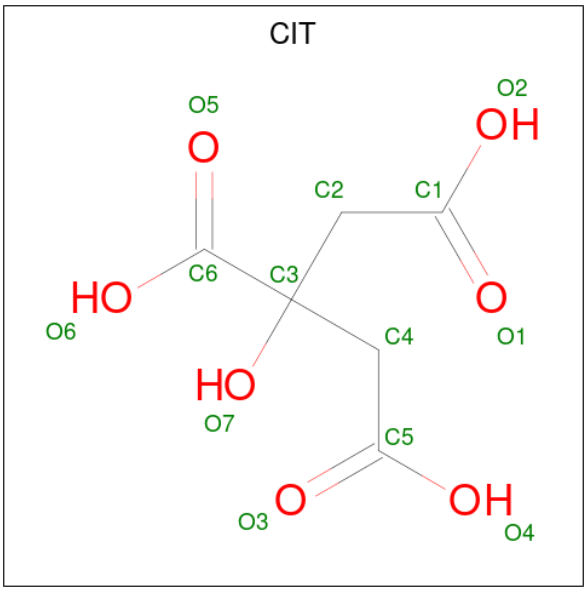


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C H O 113 41 70 2	0	1

- Molecule 12 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 13 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C H O 18 6 5 7	0	0

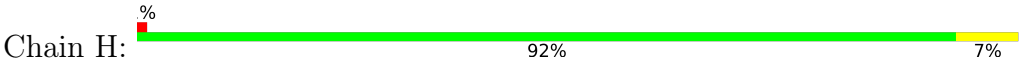
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	H	66	Total O 67 67	0	1
14	L	40	Total O 40 40	0	0
14	M	46	Total O 46 46	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.

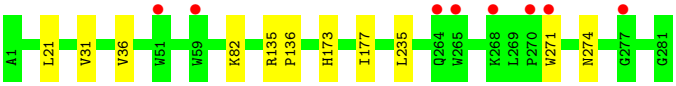
• Molecule 1: Reaction center protein H chain





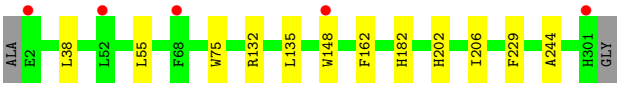
• Molecule 2: Reaction center protein L chain





• 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	102.52Å 102.52Å 237.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.07 – 2.65 47.07 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.07-2.65) 89.6 (47.07-2.65)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.13-2998_9999	Depositor
R, R_{free}	0.176 , 0.215 0.181 , 0.218	Depositor DCC
R_{free} test set	1515 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 64.9	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	14659	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: PO4, OLC, FE, UQ7, LDA, SPN, CL, BPH, BCL, CIT

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	0.14	0/1919	0.28	0/2608
2	L	0.13	0/2343	0.27	0/3208
3	M	0.13	0/2542	0.28	0/3472
All	All	0.13	0/6804	0.28	0/9288

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	1856	1870	1864	8	0
2	L	2247	2200	2194	3	0
3	M	2435	2340	2326	7	0
4	H	48	93	93	2	0
4	L	48	93	93	1	0
4	M	48	93	93	1	0
5	L	65	76	76	1	0
5	M	50	45	43	2	0
6	L	132	148	148	2	0
6	M	117	116	115	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	25	40	40	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	1	0	0	1	0
13	M	13	5	5	0	0
14	H	67	0	0	1	0
14	L	40	0	0	0	0
14	M	46	0	0	0	0
All	All	7365	7294	7266	28	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 28 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	1.72	0.71
4:H:302:LDA:HM21	4:H:302:LDA:H31	1.77	0.67
3:M:75:TRP:HE1	11:M:409[A]:SPN:HMA2	1.66	0.60
2:L:36:VAL:HG11	4:L:308:LDA:HM21	1.86	0.58
5:L:301:BPH:HMB1	5:L:301:BPH:HBB3	1.84	0.58

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	242/241 (100%)	240 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	L	281/281 (100%)	276 (98%)	4 (1%)	1 (0%)	30 45
3	M	303/302 (100%)	297 (98%)	6 (2%)	0	100 100
All	All	826/824 (100%)	813 (98%)	12 (2%)	1 (0%)	48 66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	31	VAL

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	199/196 (102%)	194 (98%)	5 (2%)	42 64
2	L	222/220 (101%)	217 (98%)	5 (2%)	44 66
3	M	240/236 (102%)	238 (99%)	2 (1%)	73 85
All	All	661/652 (101%)	649 (98%)	12 (2%)	51 72

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	235	LEU
2	L	271	TRP
3	M	182	HIS
2	L	274	ASN
1	H	197	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	202	HIS
3	M	259	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	LDA	M	410	-	12,15,15	0.36	0	14,17,17	0.23	0
8	UQ7	M	401	-	48,48,48	0.24	0	58,61,61	0.41	0
6	BCL	L	303	2	69,74,74	1.16	5 (7%)	83,115,115	1.28	6 (7%)
6	BCL	M	402	3	69,74,74	1.06	5 (7%)	83,115,115	1.35	6 (7%)
5	BPH	M	304	-	44,55,70	1.07	1 (2%)	43,83,101	1.74	7 (16%)
10	PO4	M	411	-	4,4,4	0.88	0	6,6,6	0.41	0
11	SPN	M	409[A]	-	40,42,42	0.14	0	50,52,52	0.54	2 (4%)
4	LDA	L	307	-	12,15,15	0.36	0	14,17,17	0.47	0
10	PO4	M	407	-	4,4,4	0.93	0	6,6,6	0.52	0
4	LDA	M	406	-	12,15,15	0.37	0	14,17,17	0.23	0
4	LDA	L	308	-	12,15,15	0.38	0	14,17,17	0.40	0
5	BPH	L	301	-	59,70,70	0.95	2 (3%)	61,101,101	1.43	7 (11%)
7	OLC	M	408[B]	-	24,24,24	0.20	0	25,25,25	0.20	0
13	CIT	M	413	-	12,12,12	1.88	6 (50%)	17,17,17	2.50	6 (35%)
6	BCL	L	302	2	69,74,74	1.07	5 (7%)	83,115,115	1.31	7 (8%)
4	LDA	H	302	-	12,15,15	0.32	0	14,17,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LDA	M	405	-	12,15,15	0.36	0	14,17,17	0.63	0
6	BCL	M	403	3	54,59,74	1.24	3 (5%)	65,97,115	1.50	9 (13%)
4	LDA	L	306	-	12,15,15	0.35	0	14,17,17	0.29	0
4	LDA	H	303	-	12,15,15	0.44	0	14,17,17	0.47	0
7	OLC	L	305	-	24,24,24	0.21	0	25,25,25	0.19	0
4	LDA	H	301	-	12,15,15	0.35	0	14,17,17	0.23	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	LDA	M	410	-	-	7/13/13/13	-
8	UQ7	M	401	-	-	4/45/69/69	0/1/1/1
6	BCL	L	303	2	-	1/41/137/137	-
6	BCL	M	402	3	-	11/41/137/137	-
5	BPH	M	304	-	-	4/19/87/105	0/5/6/6
11	SPN	M	409[A]	-	-	20/50/51/51	-
4	LDA	L	307	-	-	4/13/13/13	-
4	LDA	M	406	-	-	6/13/13/13	-
4	LDA	L	308	-	-	8/13/13/13	-
5	BPH	L	301	-	-	7/37/105/105	0/5/6/6
7	OLC	M	408[B]	-	-	7/24/24/24	-
13	CIT	M	413	-	-	7/16/16/16	-
6	BCL	L	302	2	-	3/41/137/137	-
4	LDA	H	302	-	-	6/13/13/13	-
4	LDA	M	405	-	-	5/13/13/13	-
6	BCL	M	403	3	-	0/23/119/137	-
4	LDA	L	306	-	-	4/13/13/13	-
4	LDA	H	303	-	-	8/13/13/13	-
7	OLC	L	305	-	-	15/24/24/24	-
4	LDA	H	301	-	-	5/13/13/13	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	304	BPH	C1B-C2B	5.27	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	301	BPH	C1B-C2B	4.89	1.45	1.39
6	L	303	BCL	MG-NA	4.77	2.17	2.06
6	M	403	BCL	MG-NA	4.54	2.17	2.06
6	L	302	BCL	MG-NA	4.41	2.16	2.06

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	304	BPH	C4D-CHA-CBD	-7.99	104.90	108.52
5	L	301	BPH	C4D-CHA-CBD	-7.12	105.29	108.52
13	M	413	CIT	O5-C6-C3	-6.39	113.21	122.25
13	M	413	CIT	O6-C6-C3	5.52	122.63	113.05
6	M	403	BCL	CHD-C1D-ND	-5.39	119.50	124.45

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	302	LDA	C2-C1-N1-O1
4	H	302	LDA	C2-C1-N1-CM2
4	H	302	LDA	N1-C1-C2-C3
4	H	303	LDA	C2-C1-N1-O1
4	H	303	LDA	C2-C1-N1-CM1

There are no ring outliers.

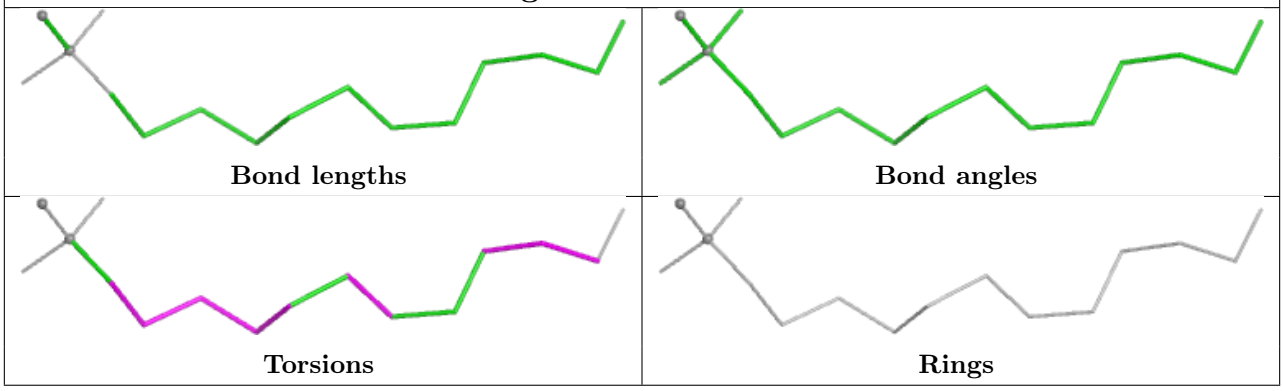
10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	303	BCL	1	0
6	M	402	BCL	1	0
5	M	304	BPH	2	0
11	M	409[A]	SPN	3	0
4	M	406	LDA	1	0
4	L	308	LDA	1	0
5	L	301	BPH	1	0
6	L	302	BCL	1	0
4	H	302	LDA	2	0
6	M	403	BCL	1	0

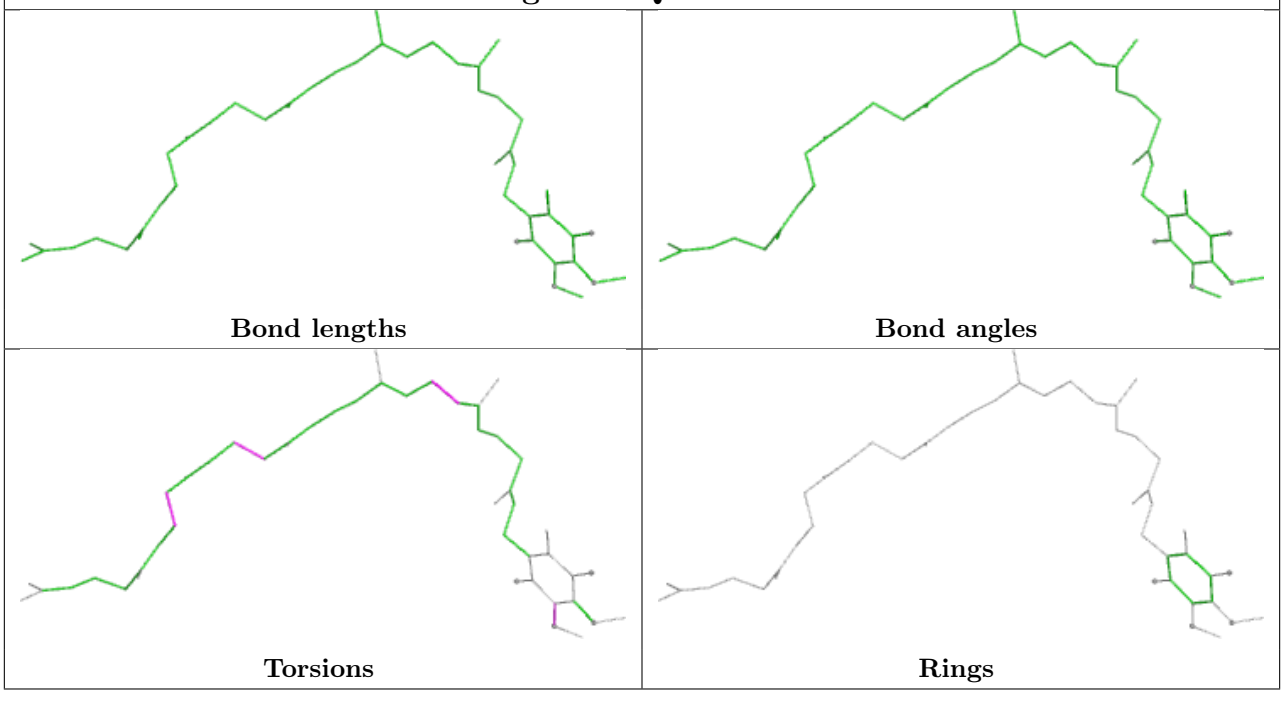
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

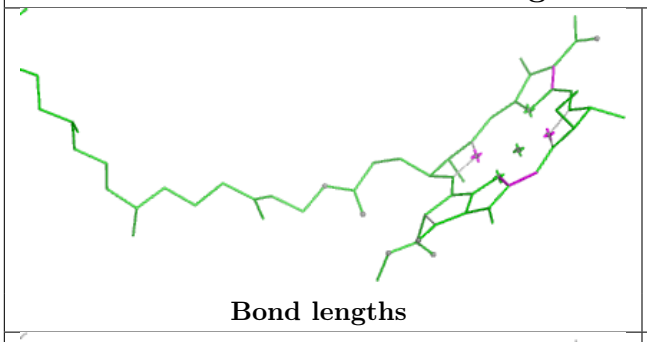
Ligand LDA M 410



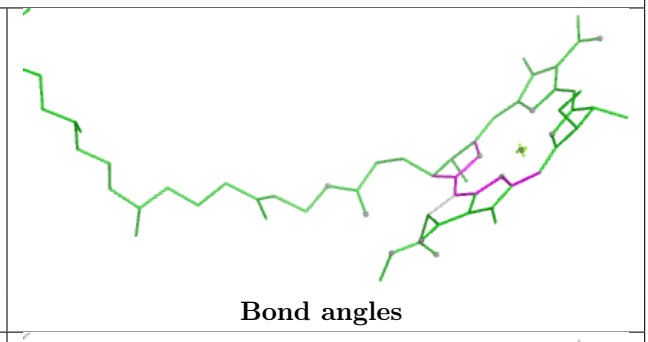
Ligand UQ7 M 401



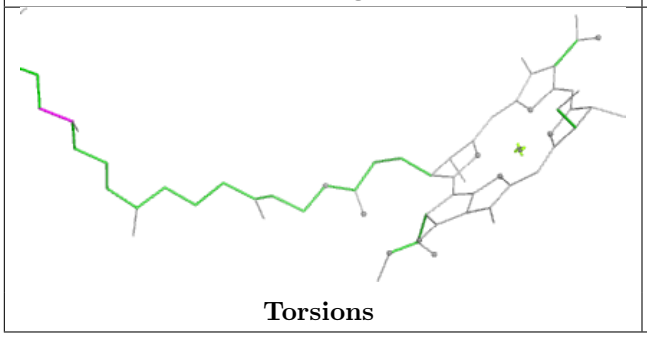
Ligand BCL L 303



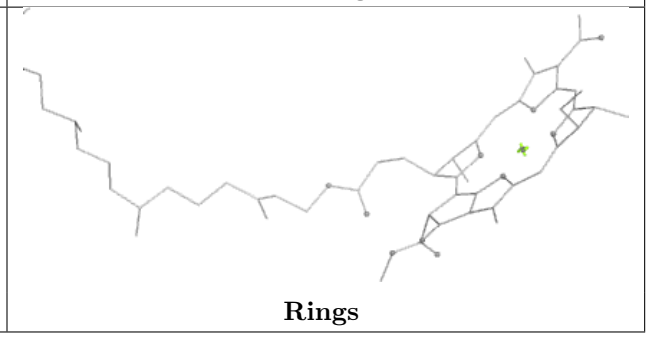
Bond lengths



Bond angles

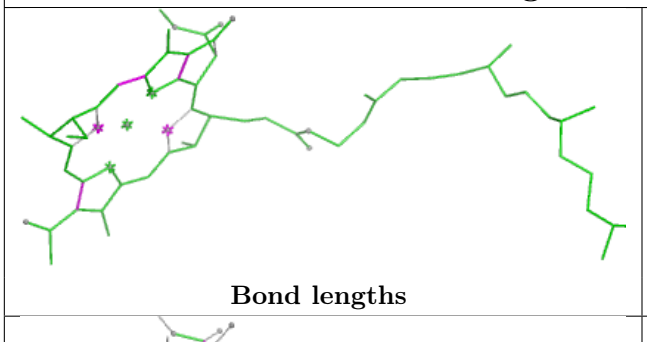


Torsions

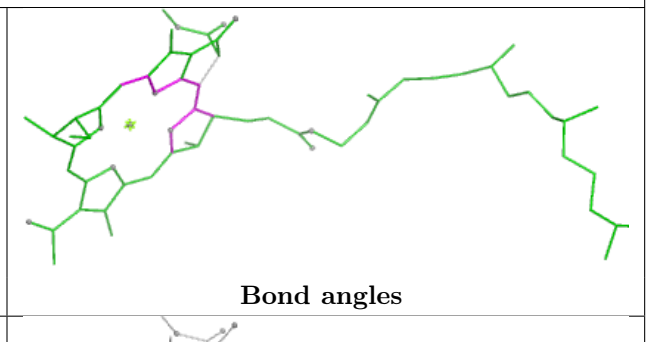


Rings

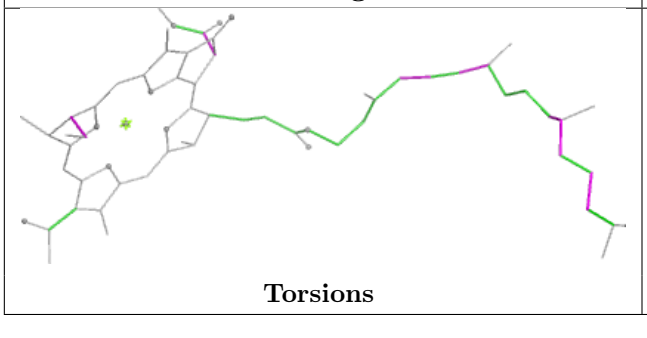
Ligand BCL M 402



Bond lengths



Bond angles

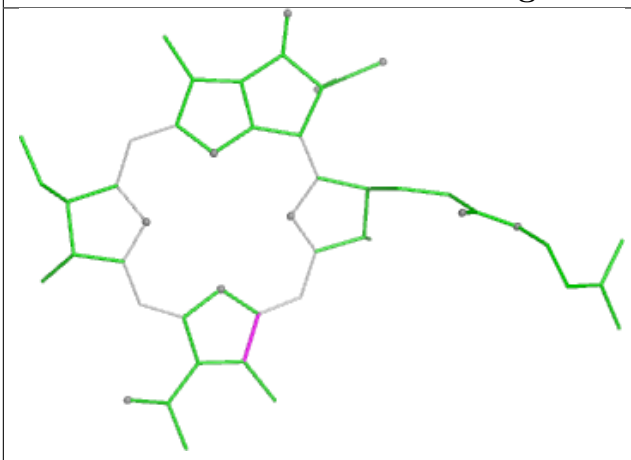


Torsions

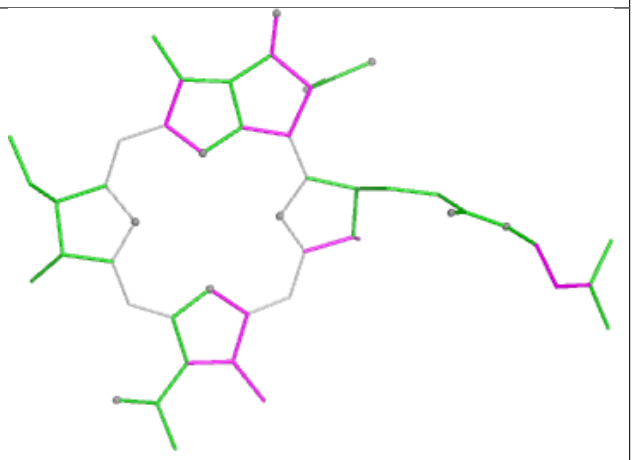


Rings

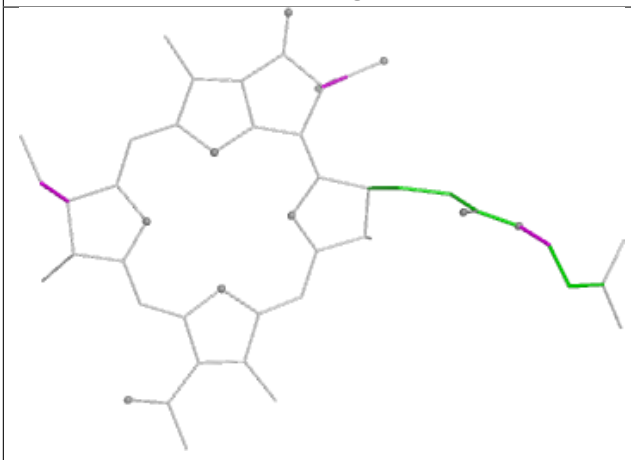
Ligand BPH M 304



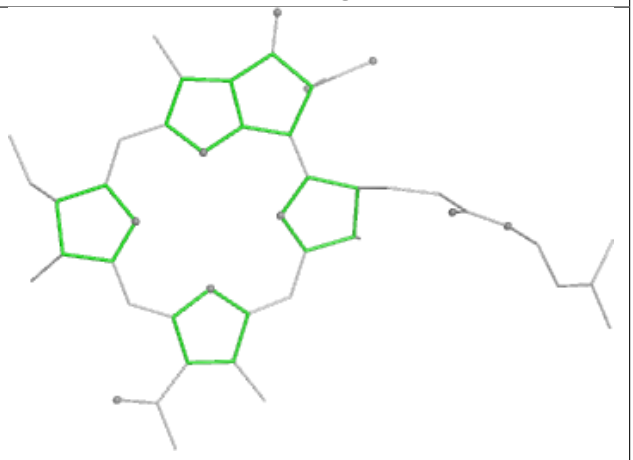
Bond lengths



Bond angles

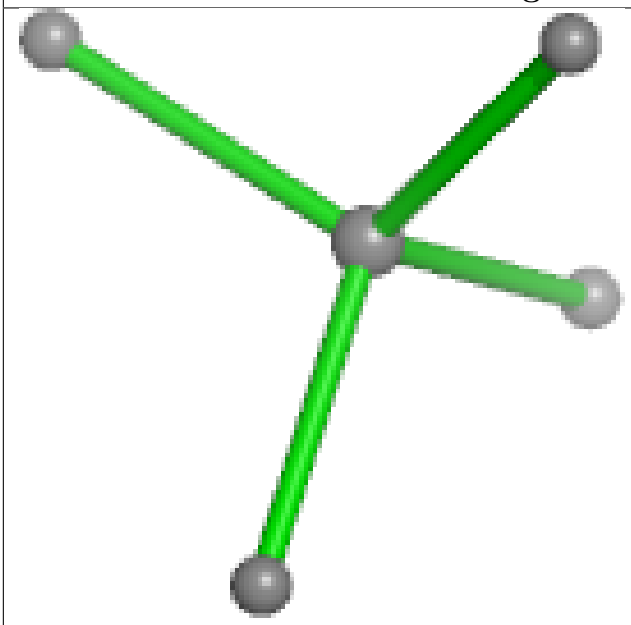


Torsions

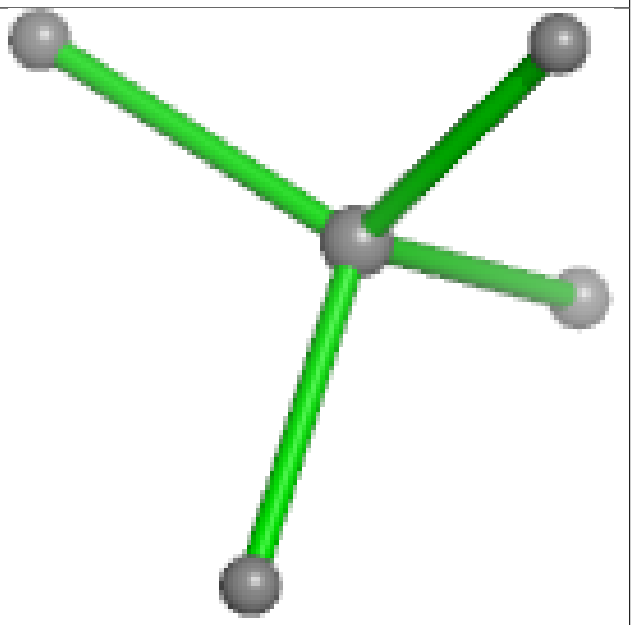


Rings

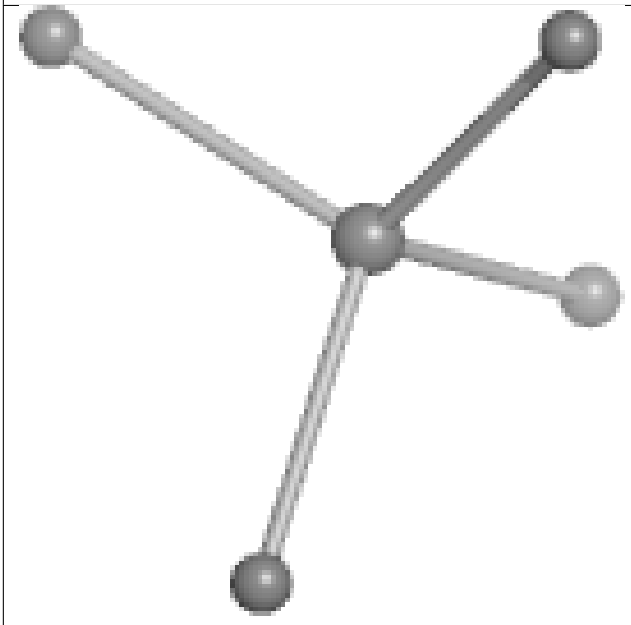
Ligand PO4 M 411



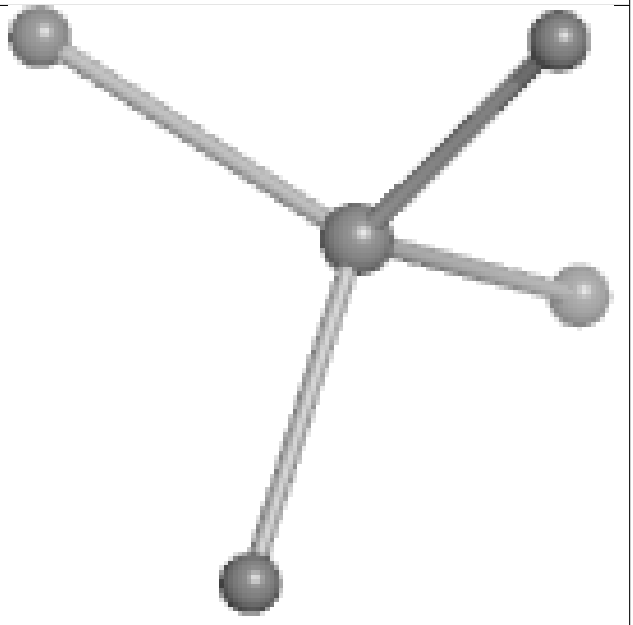
Bond lengths



Bond angles

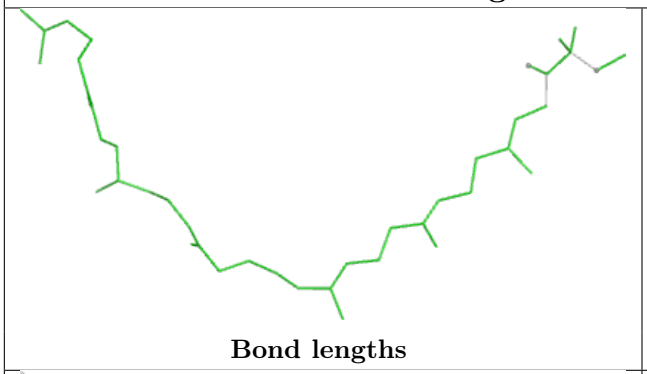


Torsions

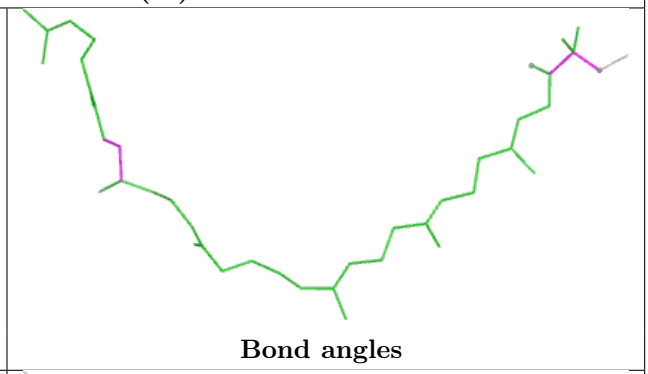


Rings

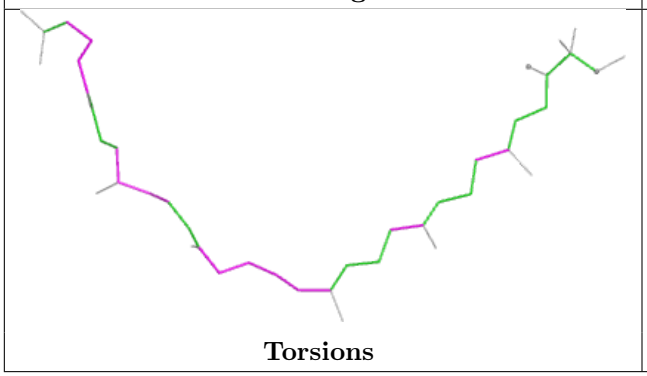
Ligand SPN M 409 (A)



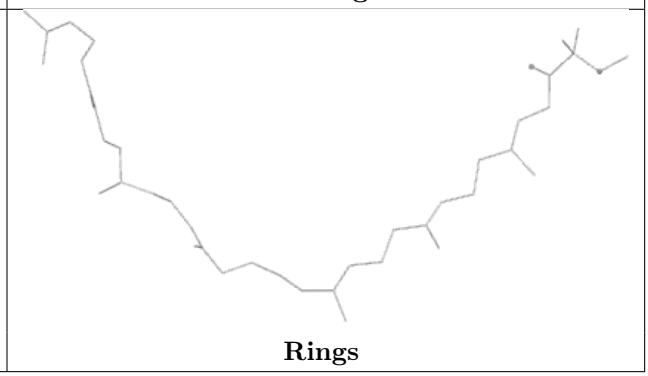
Bond lengths



Bond angles

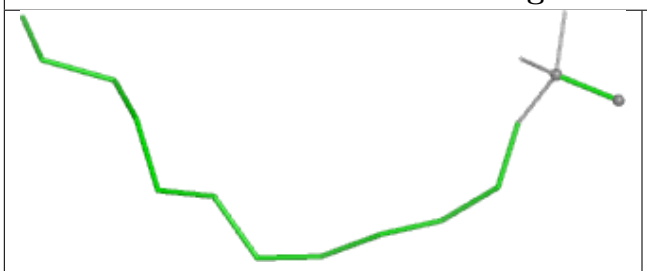


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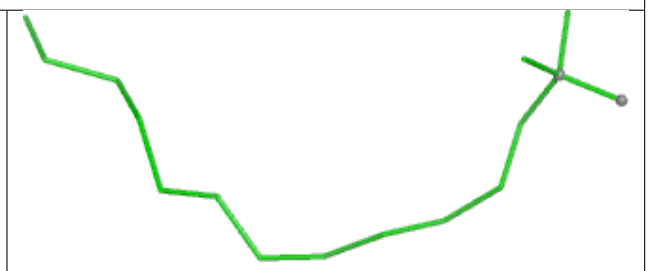


Rings

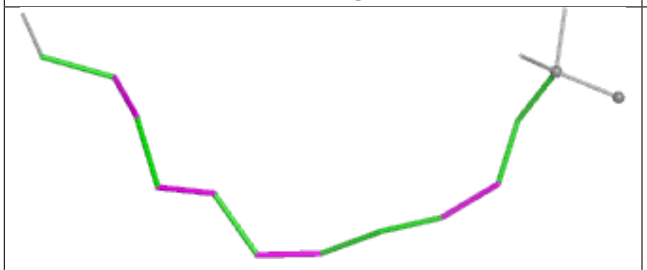
Ligand LDA L 307



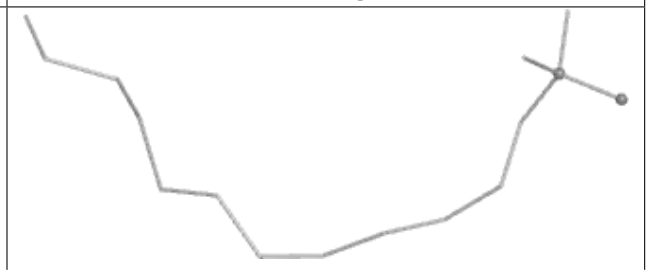
Bond lengths



Bond angles

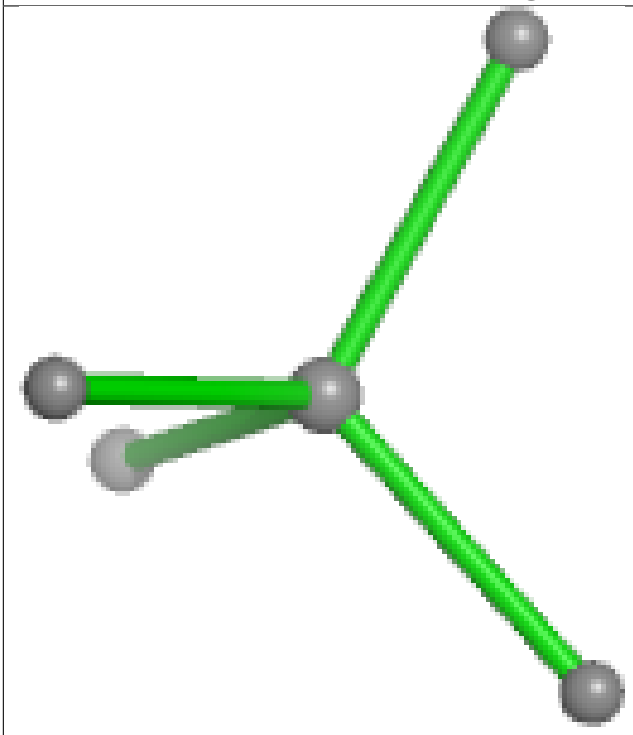


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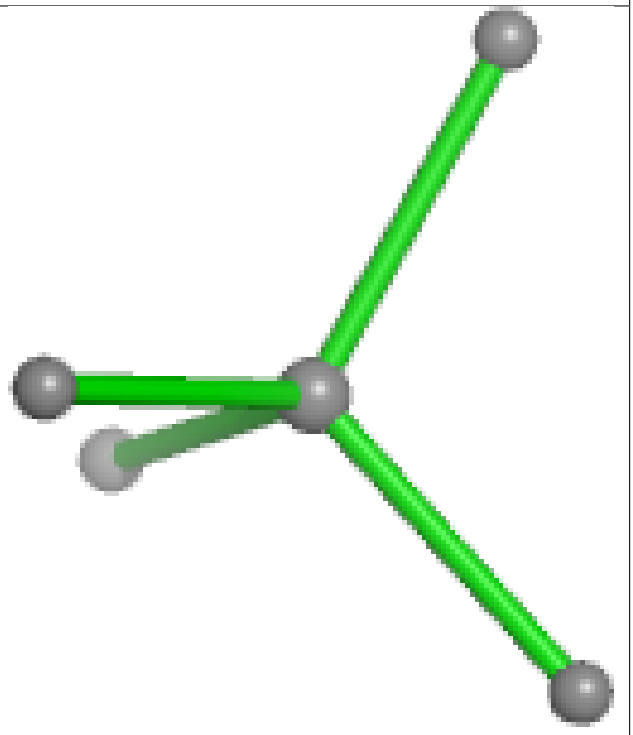


Rings

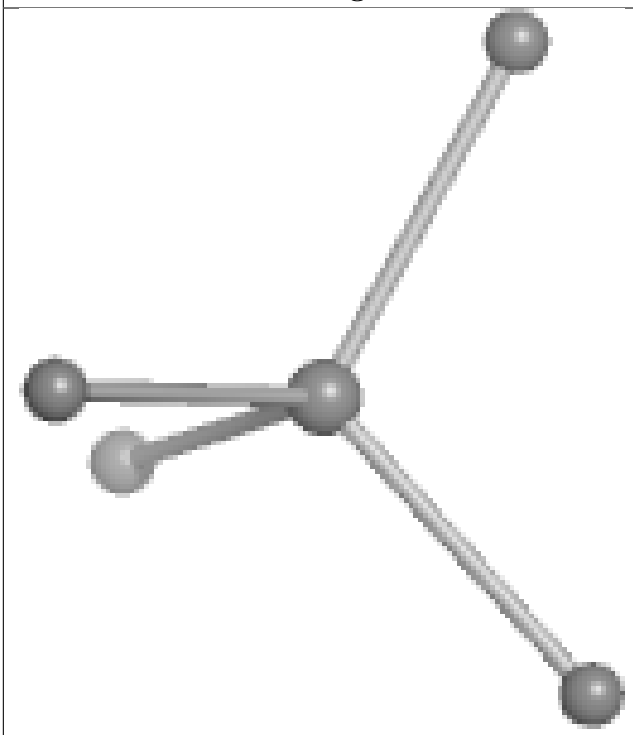
Ligand PO4 M 407



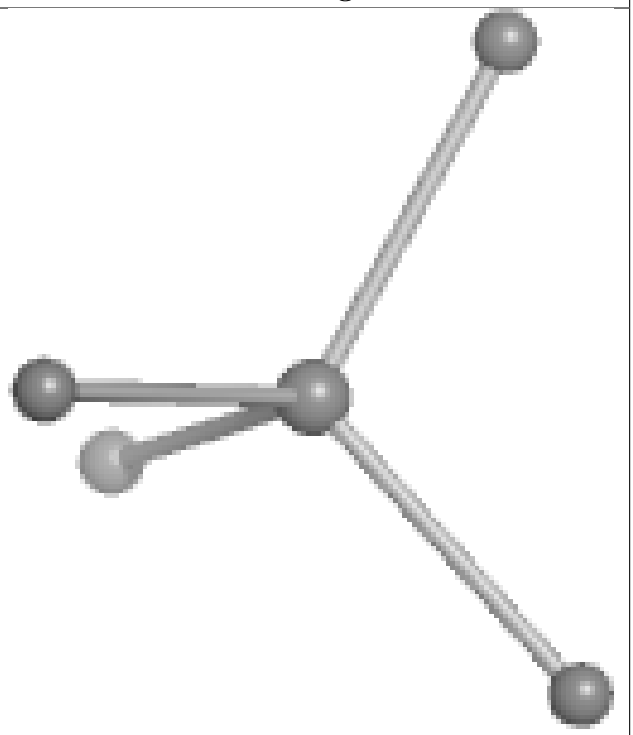
Bond lengths



Bond angles

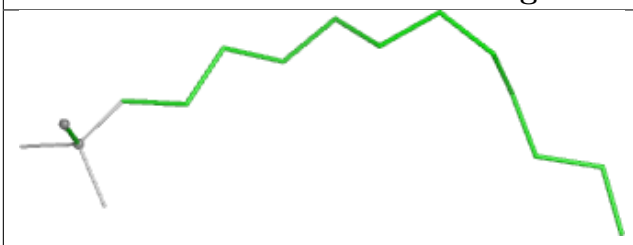


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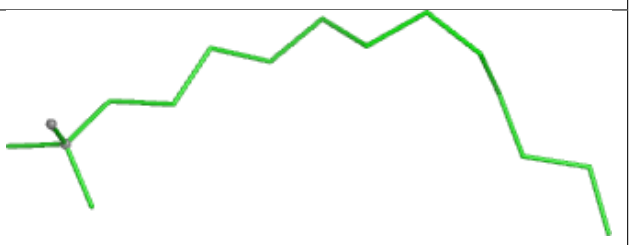


Rings

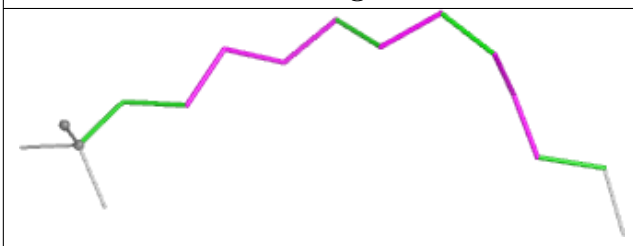
Ligand LDA M 406



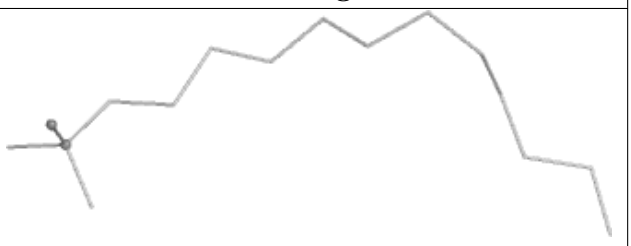
Bond lengths



Bond angles

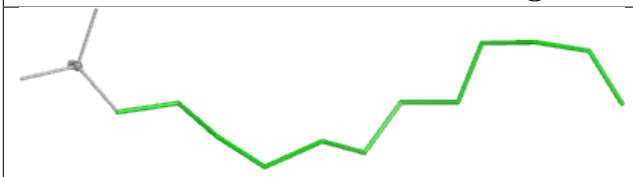


Torsions

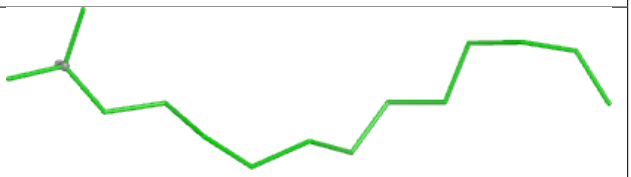


Rings

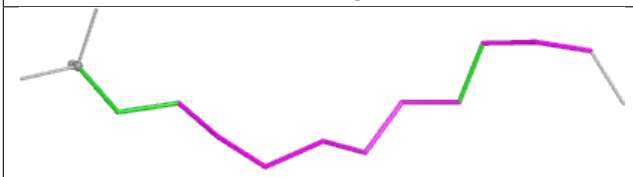
Ligand LDA L 308



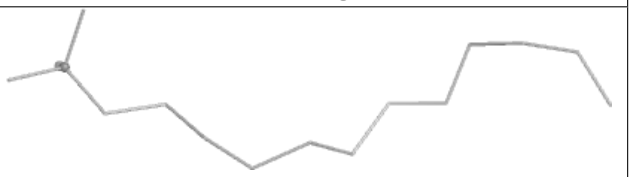
Bond lengths



Bond angles

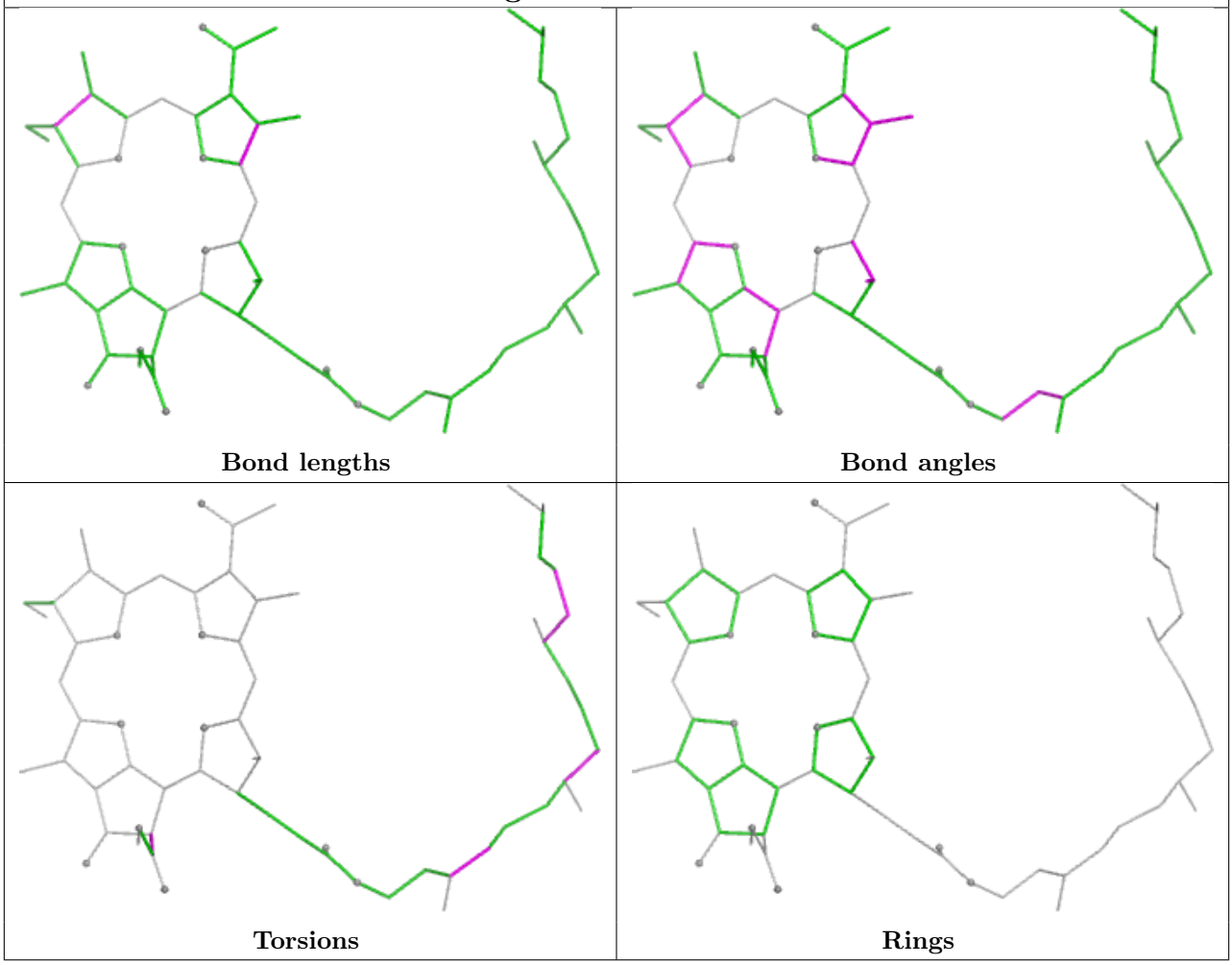


Torsions

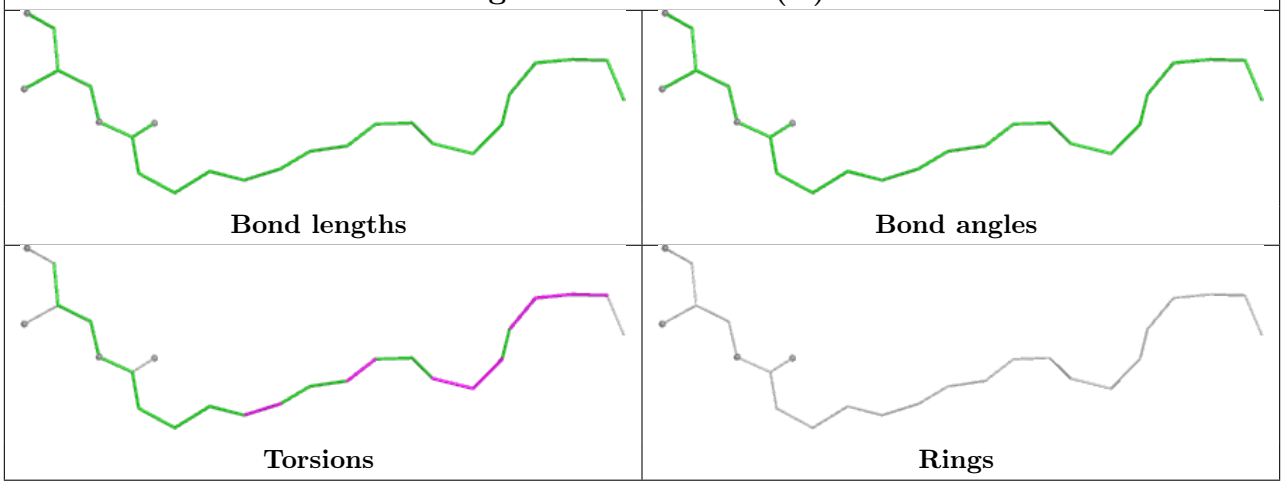


Rings

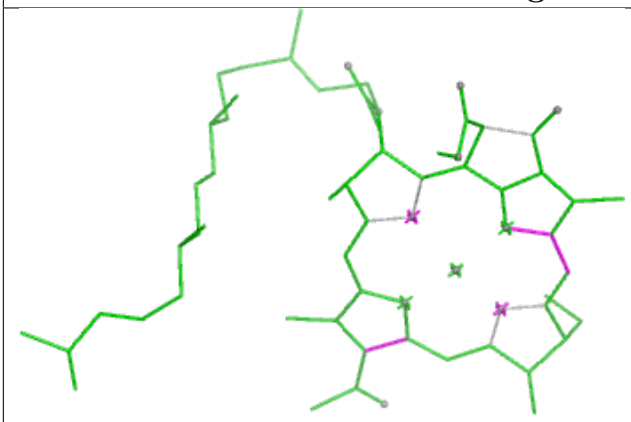
Ligand BPH L 301



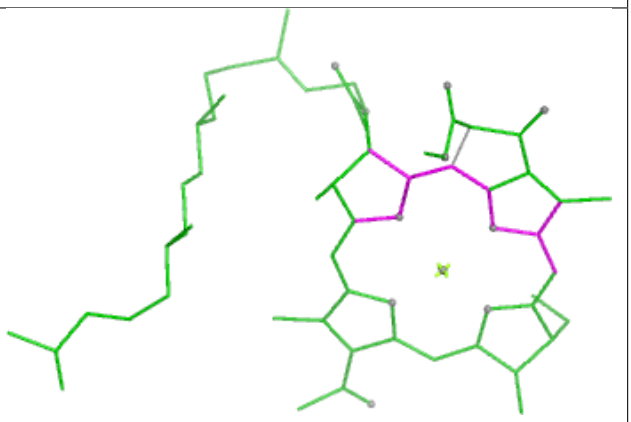
Ligand OLC M 408 (B)



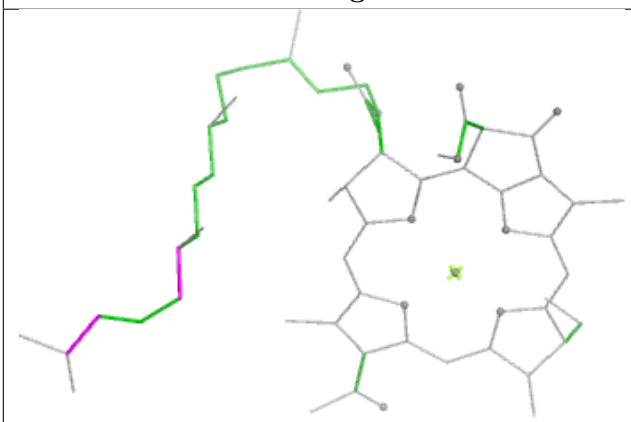
Ligand BCL L 302



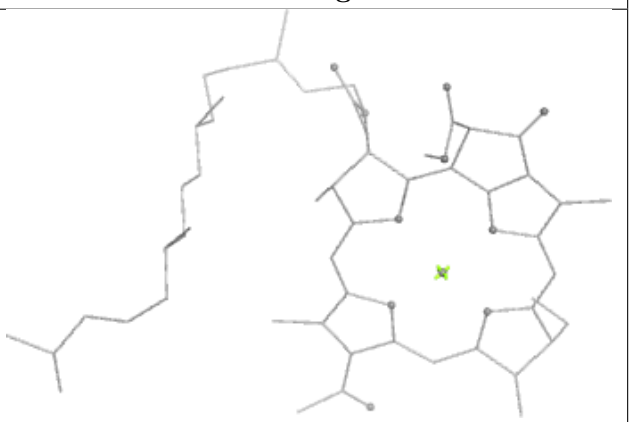
Bond lengths



Bond angles

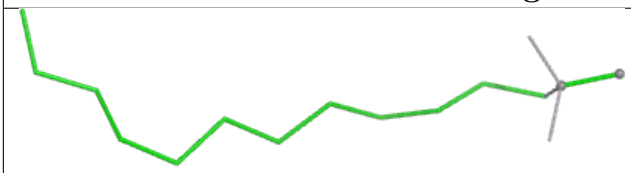


Torsions

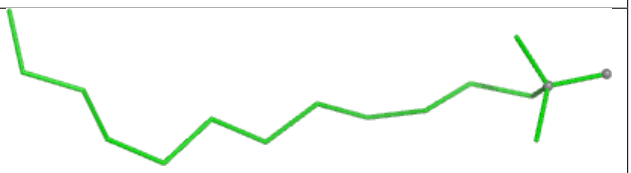


Rings

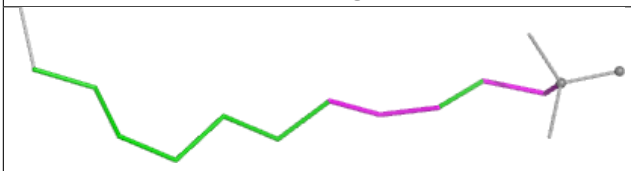
Ligand LDA H 302



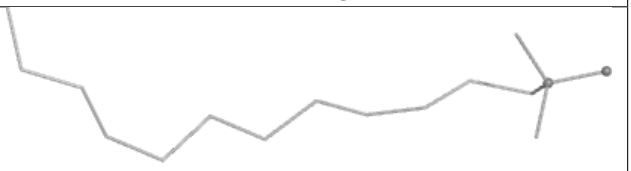
Bond lengths



Bond angles

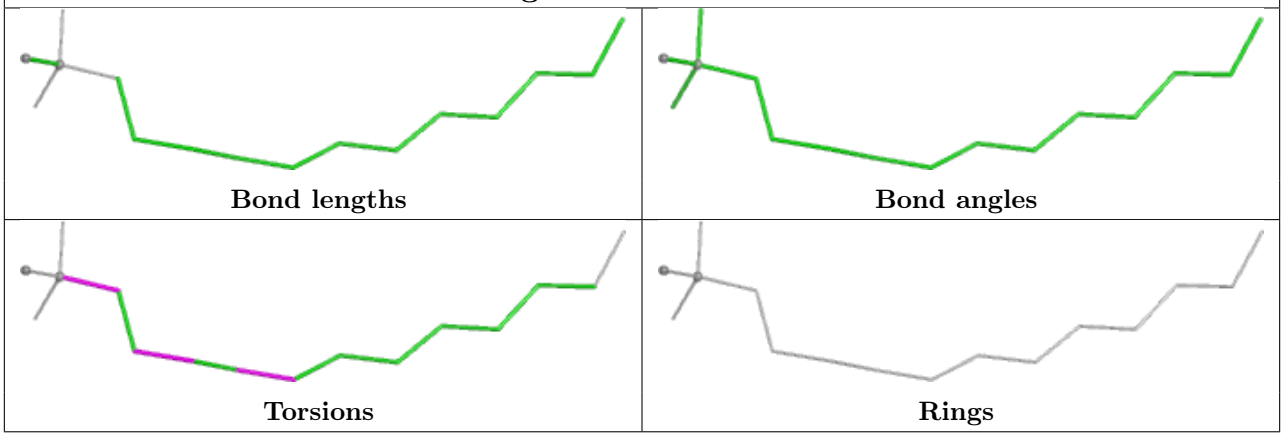


Torsions

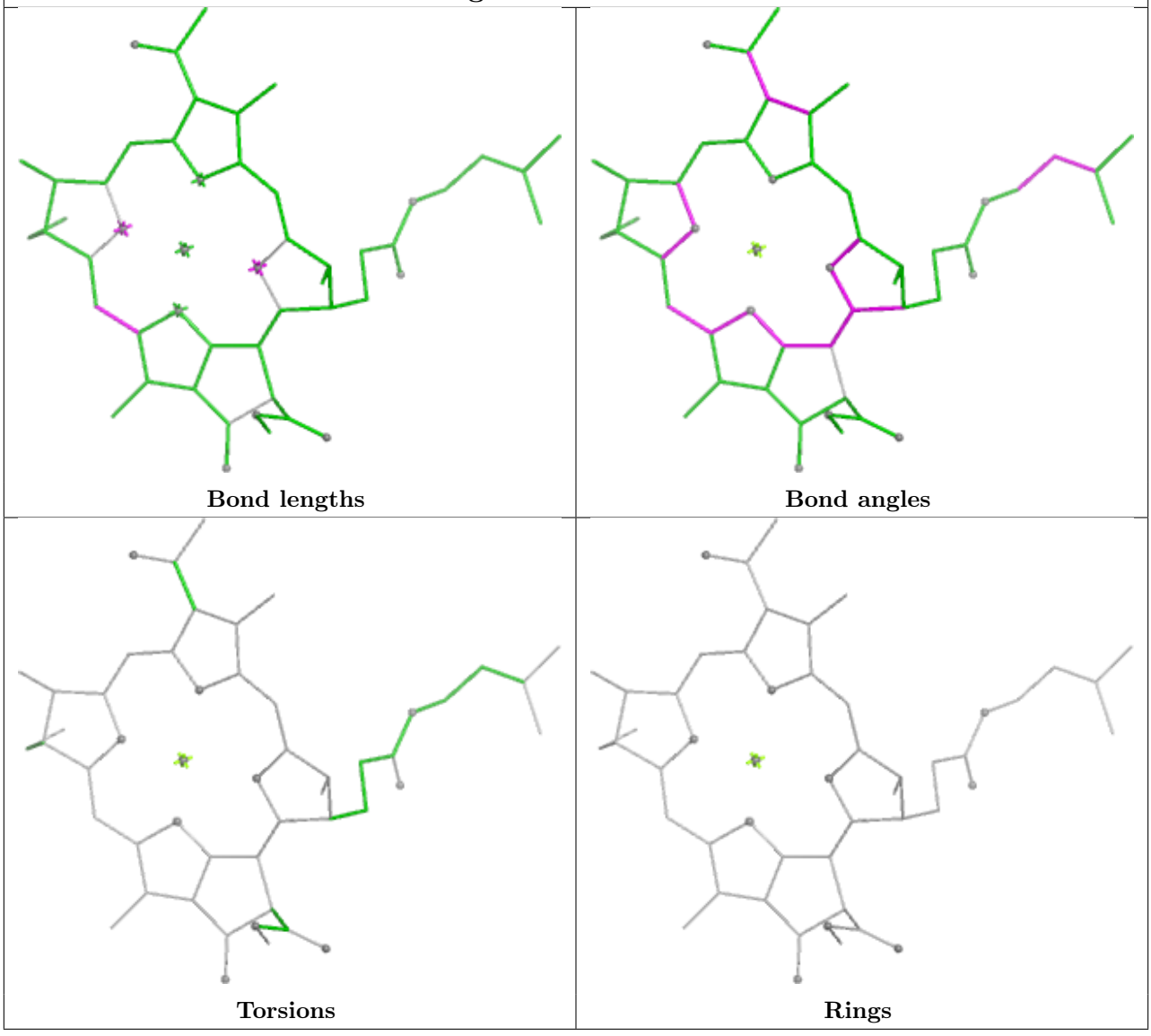


Rings

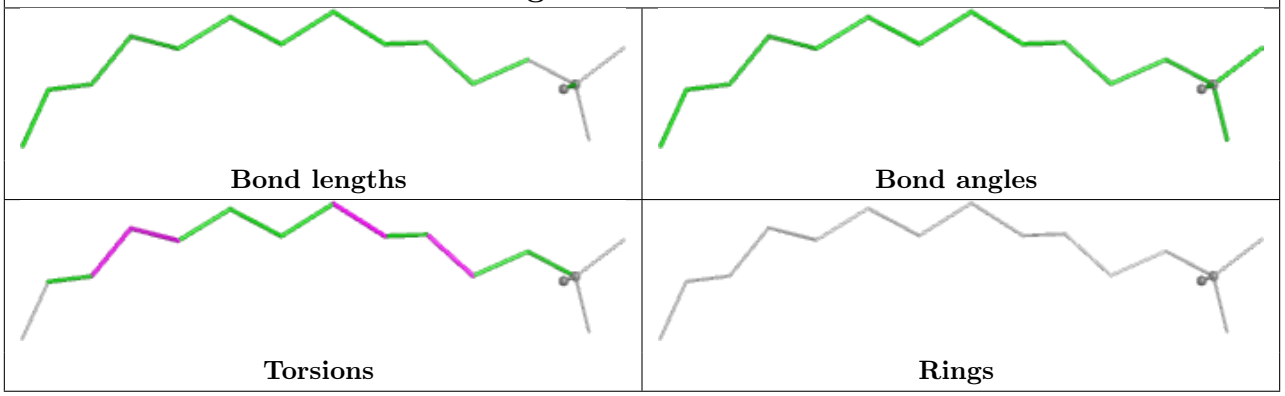
Ligand LDA M 405



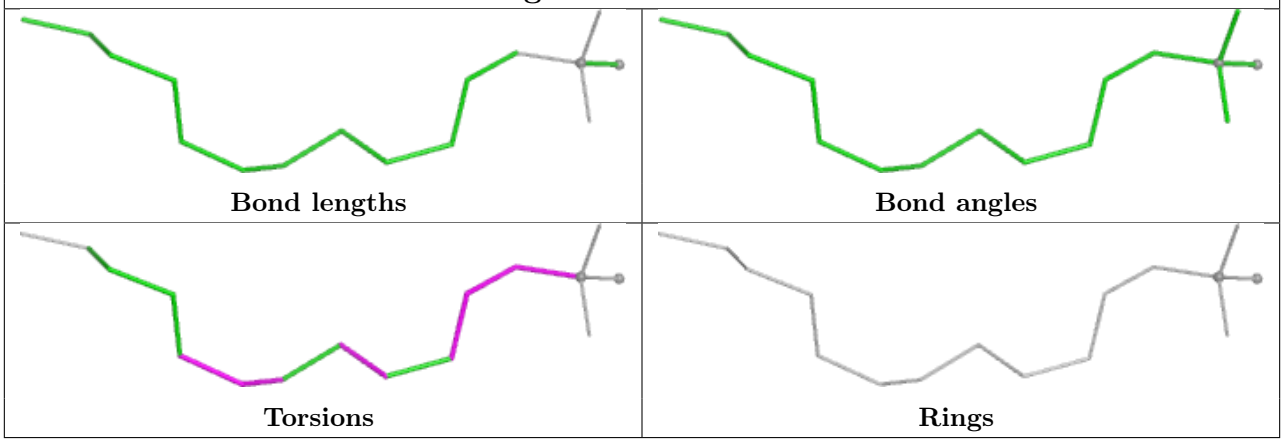
Ligand BCL M 403



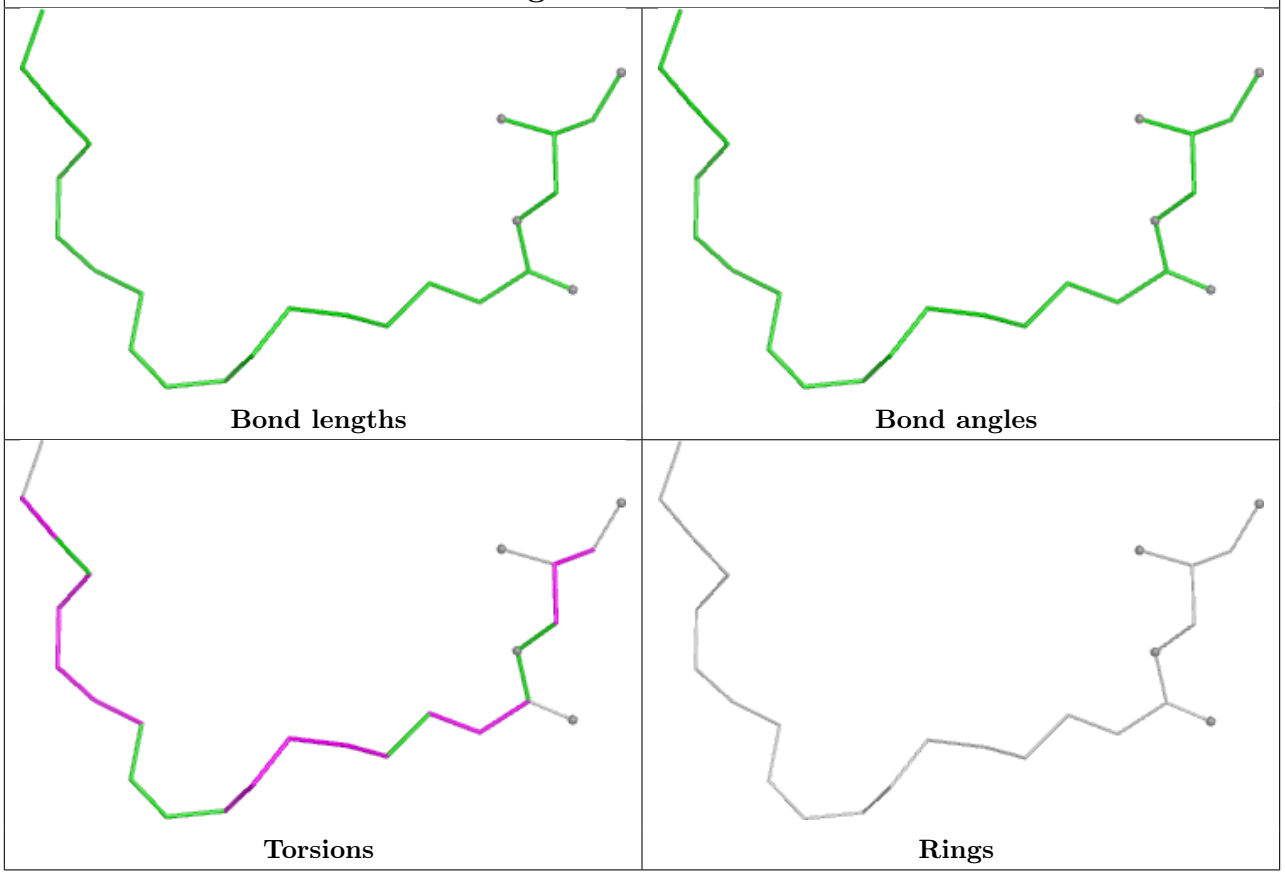
Ligand LDA L 306



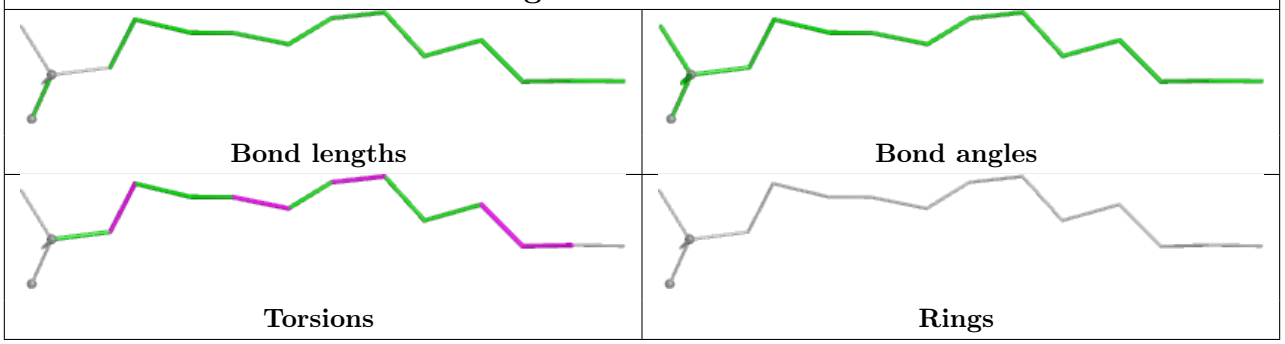
Ligand LDA H 303



Ligand OLC L 305



Ligand LDA H 301



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%)	-0.10	3 (1%)	75	71	23, 50, 83, 143	3 (1%)
2	L	281/281 (100%)	-0.14	8 (2%)	55	48	27, 48, 96, 139	1 (0%)
3	M	300/302 (99%)	-0.22	5 (1%)	69	64	25, 49, 80, 122	3 (1%)
All	All	821/824 (99%)	-0.16	16 (1%)	66	61	23, 50, 87, 143	7 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	51[A]	TRP	5.3
3	M	68[A]	PHE	5.0
2	L	59	TRP	4.7
3	M	148[A]	TRP	4.6
3	M	2	GLU	3.9

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 oligosaccharides in this entry.

6.4 Ligands

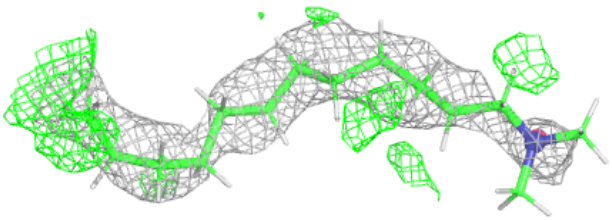
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

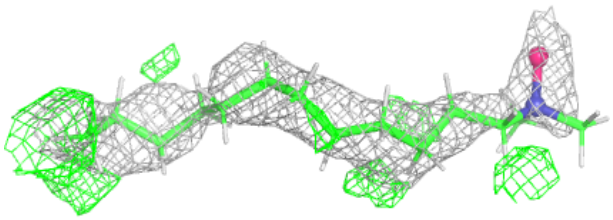
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LDA	L	308	16/16	0.74	0.25	38,48,58,58	47
4	LDA	L	306	16/16	0.75	0.26	58,84,124,124	0
13	CIT	M	413	13/13	0.77	0.19	45,48,57,57	18
4	LDA	M	410	16/16	0.80	0.24	82,102,129,129	0
4	LDA	H	302	16/16	0.80	0.24	39,50,61,63	47
4	LDA	M	405	16/16	0.82	0.27	70,87,95,95	0
10	PO4	M	411	5/5	0.84	0.16	82,82,82,82	5
11	SPN	M	409[A]	43/43	0.84	0.26	33,70,98,98	113
4	LDA	M	406	16/16	0.84	0.17	52,65,68,68	0
4	LDA	L	307	16/16	0.85	0.28	90,110,136,136	0
7	OLC	L	305	25/25	0.87	0.23	63,95,115,115	0
4	LDA	H	303	16/16	0.87	0.17	57,73,89,89	47
7	OLC	M	408[B]	25/25	0.89	0.20	58,79,98,98	65
4	LDA	H	301	16/16	0.91	0.14	55,68,78,80	0
10	PO4	M	407	5/5	0.92	0.13	65,65,69,69	0
6	BCL	M	402	66/66	0.94	0.09	40,49,70,73	0
8	UQ7	M	401	48/48	0.94	0.15	33,65,115,120	0
5	BPH	M	304	50/65	0.95	0.07	34,42,52,53	0
6	BCL	M	403	51/66	0.95	0.07	29,38,56,57	0
6	BCL	L	303	66/66	0.95	0.09	35,46,88,102	0
5	BPH	L	301	65/65	0.96	0.07	27,40,53,56	0
12	CL	M	412	1/1	0.96	0.10	70,70,70,70	0
6	BCL	L	302	66/66	0.96	0.09	34,44,80,83	0
9	FE	M	404	1/1	1.00	0.03	24,24,24,24	0

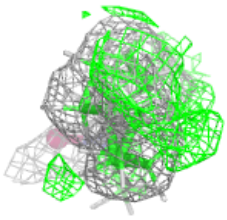
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LDA L 308:

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

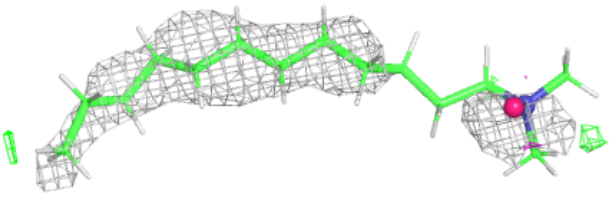


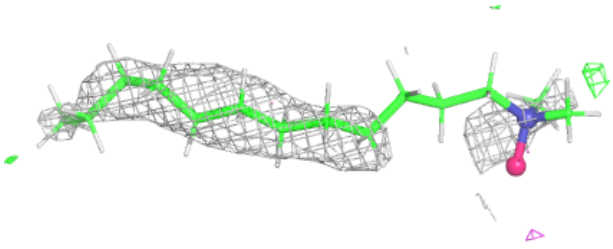


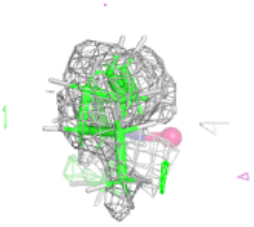


Electron density around LDA L 306:

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

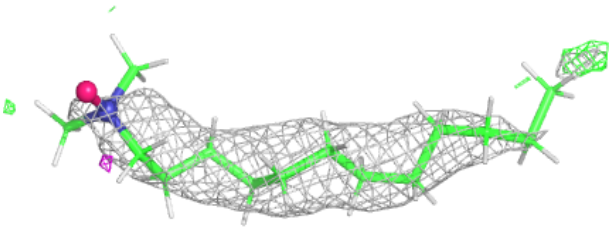


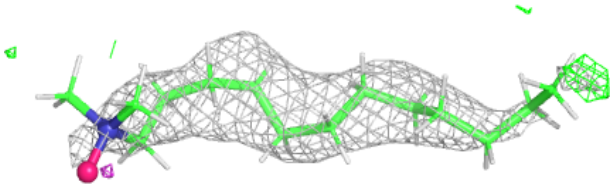


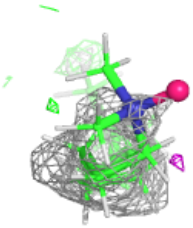


Electron density around LDA M 410:

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

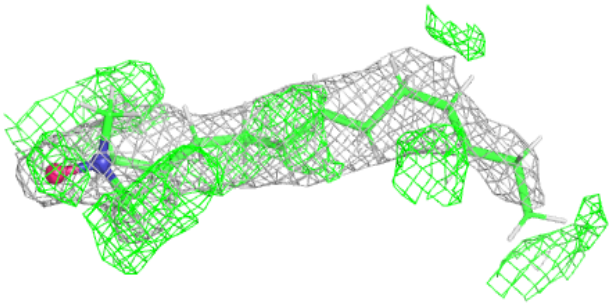


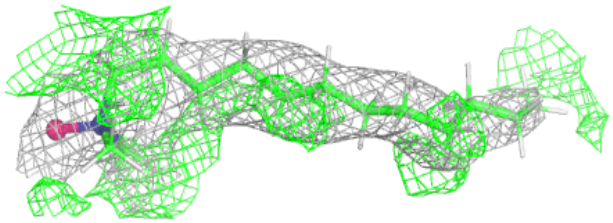


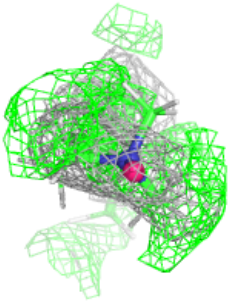


Electron density around LDA H 302:

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

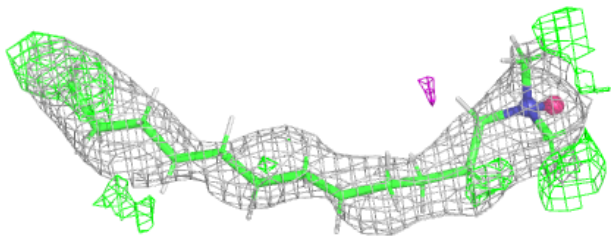


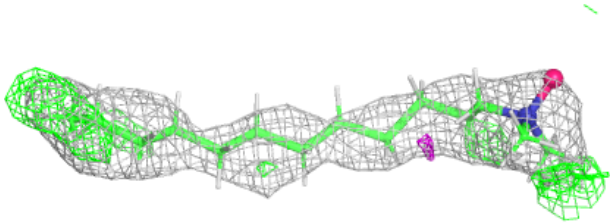


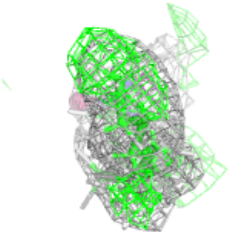


Electron density around LDA M 405:

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

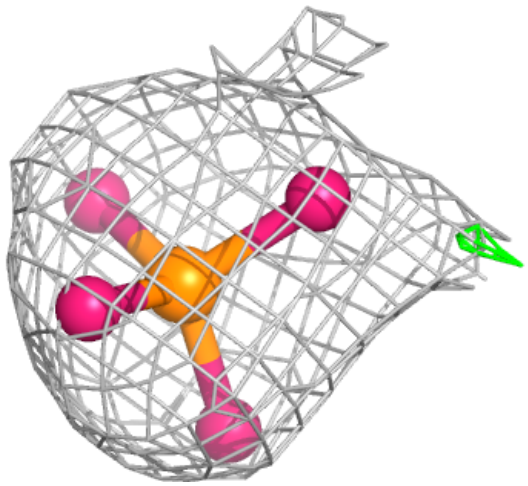


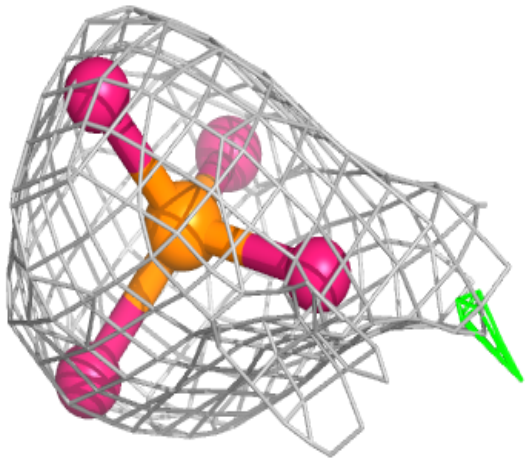


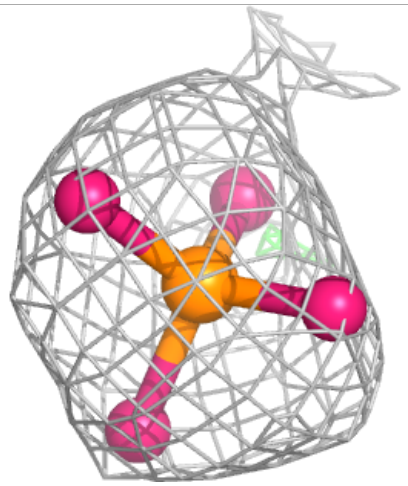


Electron density around PO4 M 411:

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

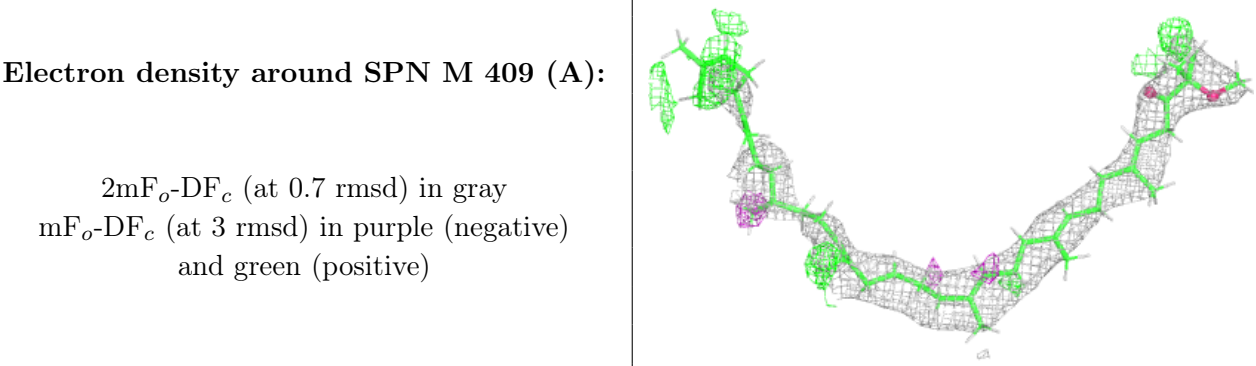


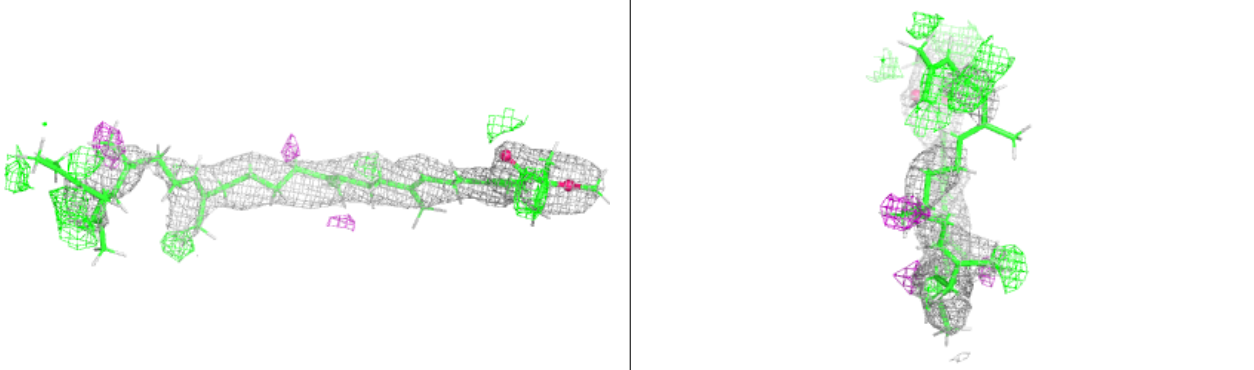




Electron density around SPN M 409 (A):

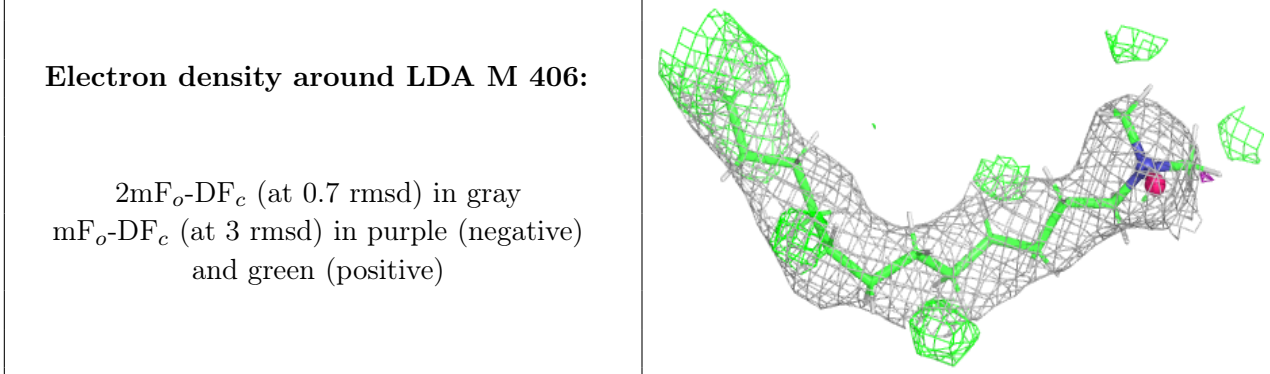
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

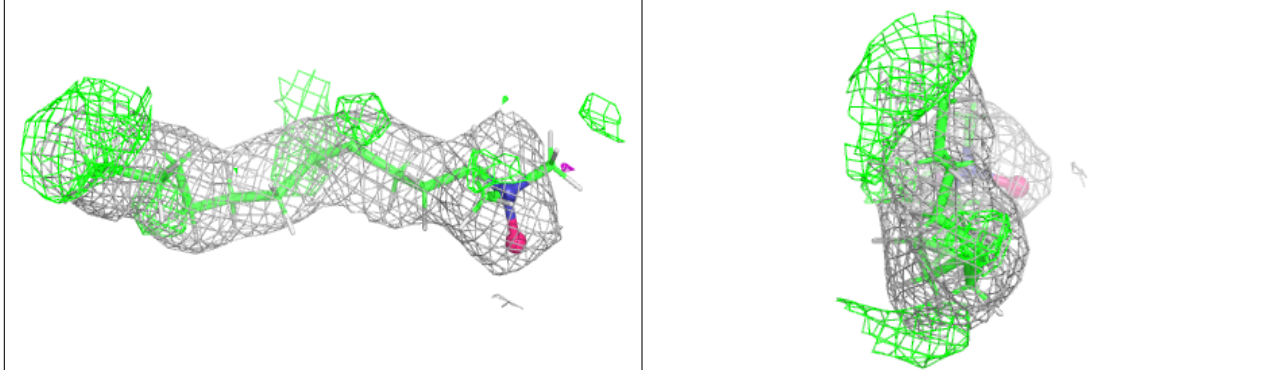




Electron density around LDA M 406:

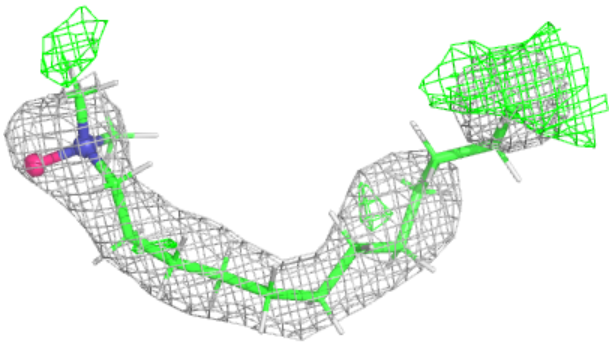
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

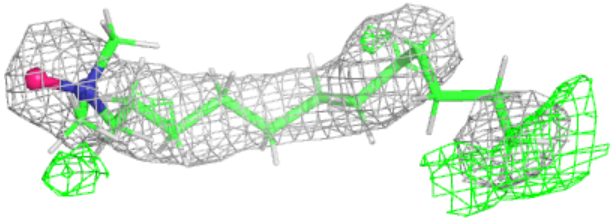


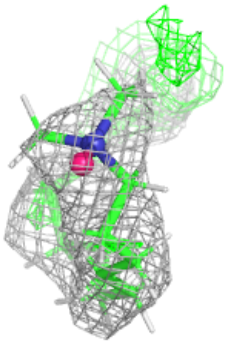


Electron density around LDA L 307:

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

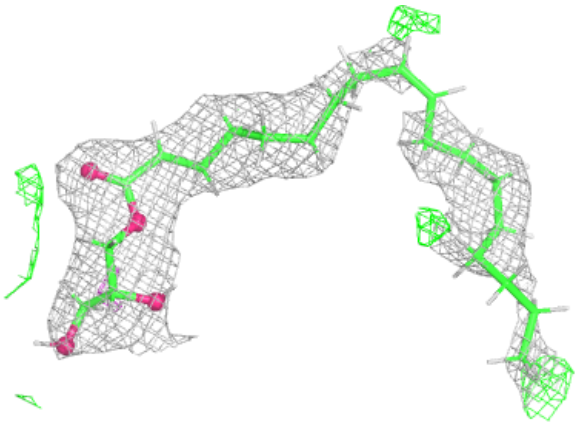


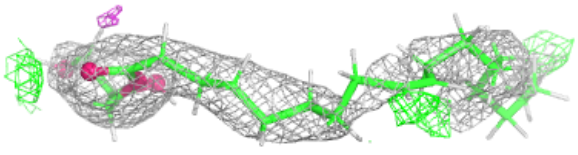




Electron density around OLC L 305:

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

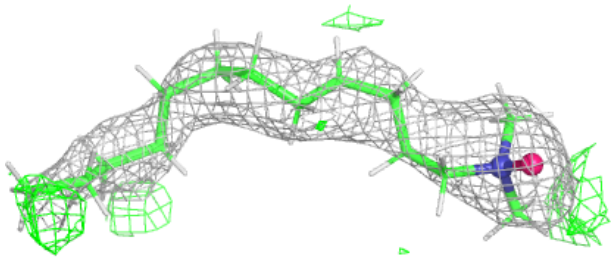


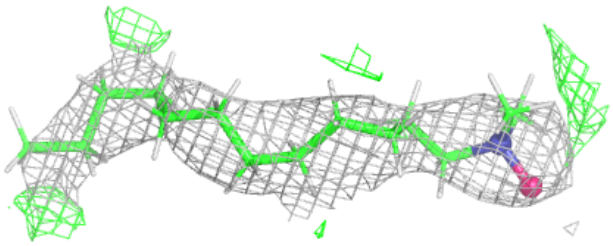


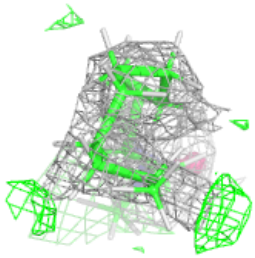


Electron density around LDA H 303:

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

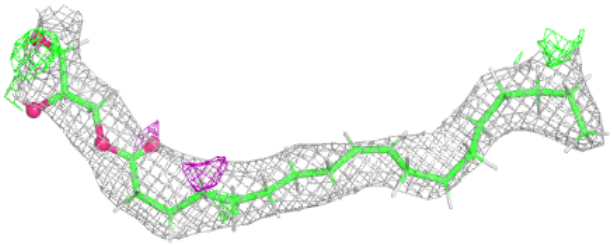


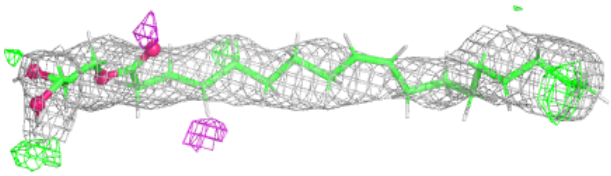


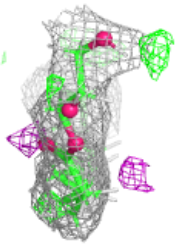


Electron density around OLC M 408 (B):

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

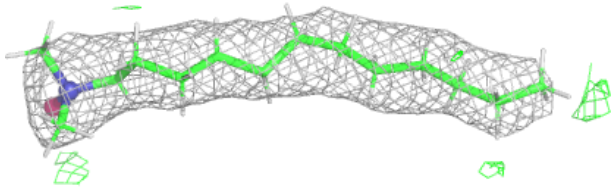


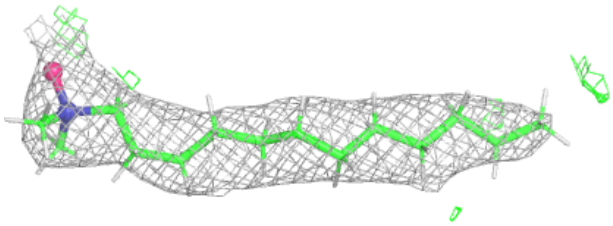


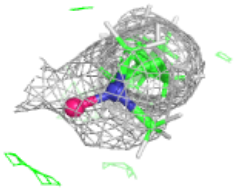


Electron density around LDA H 301:

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

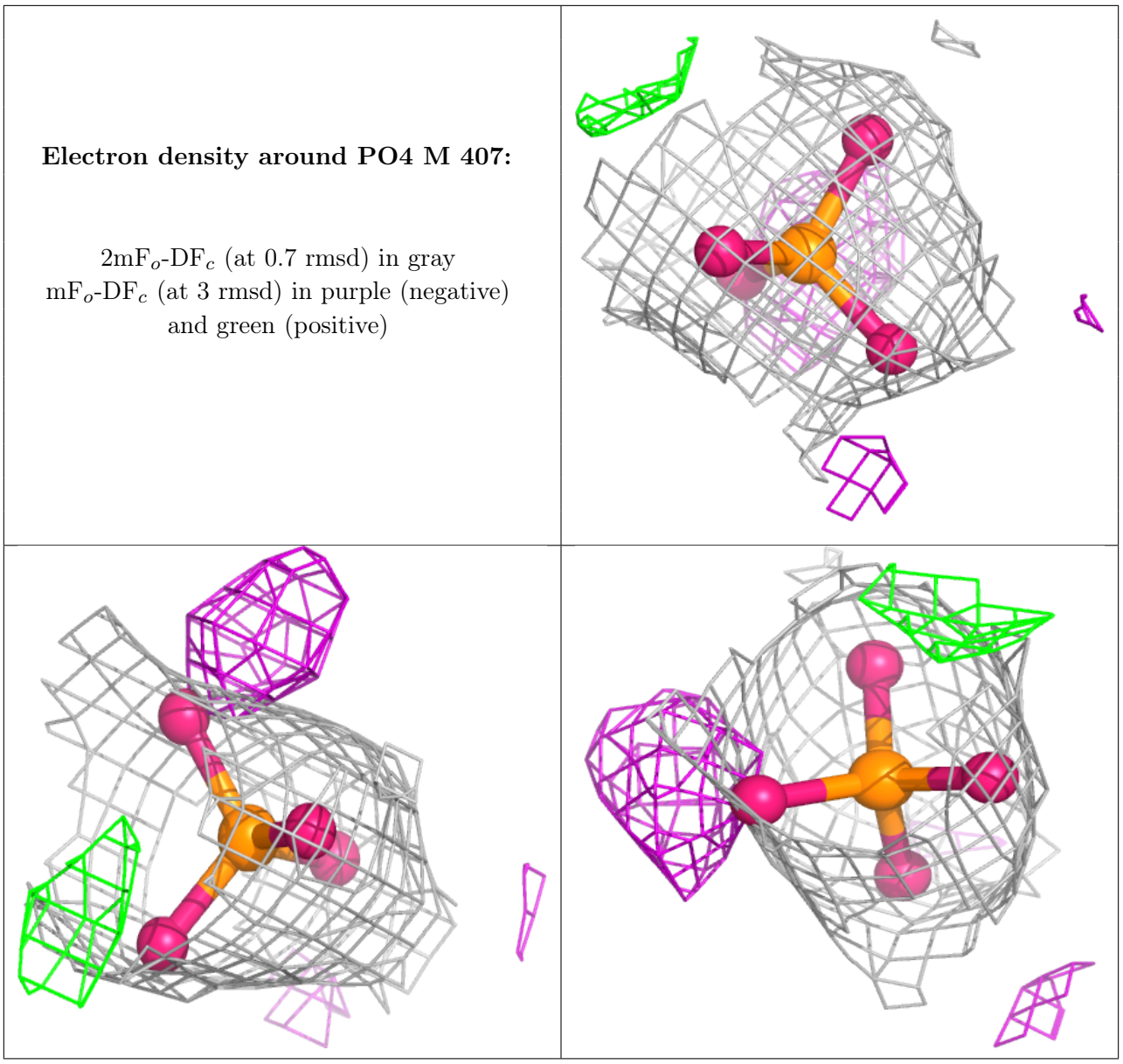






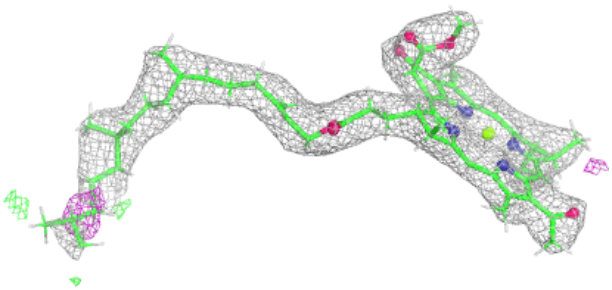
Electron density around PO4 M 407:

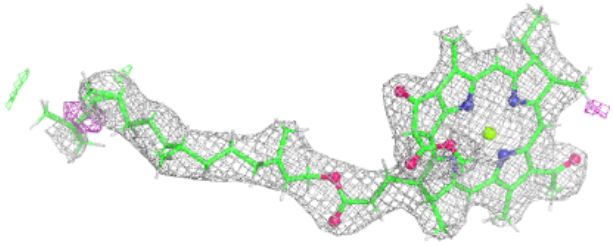
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

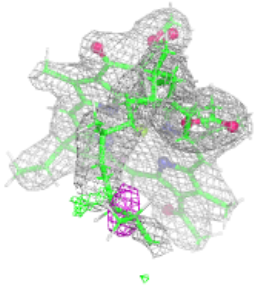


Electron density around BCL M 402:

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

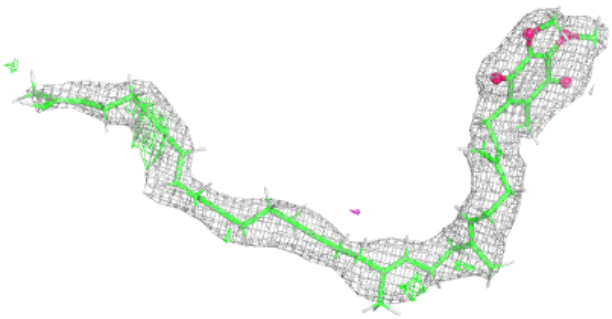


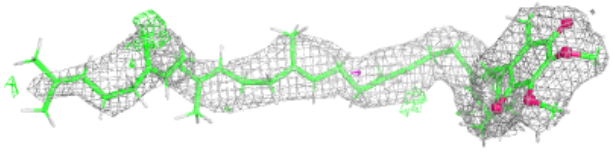


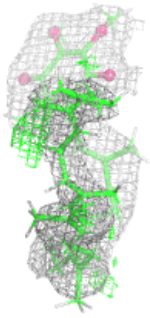


Electron density around UQ7 M 401:

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

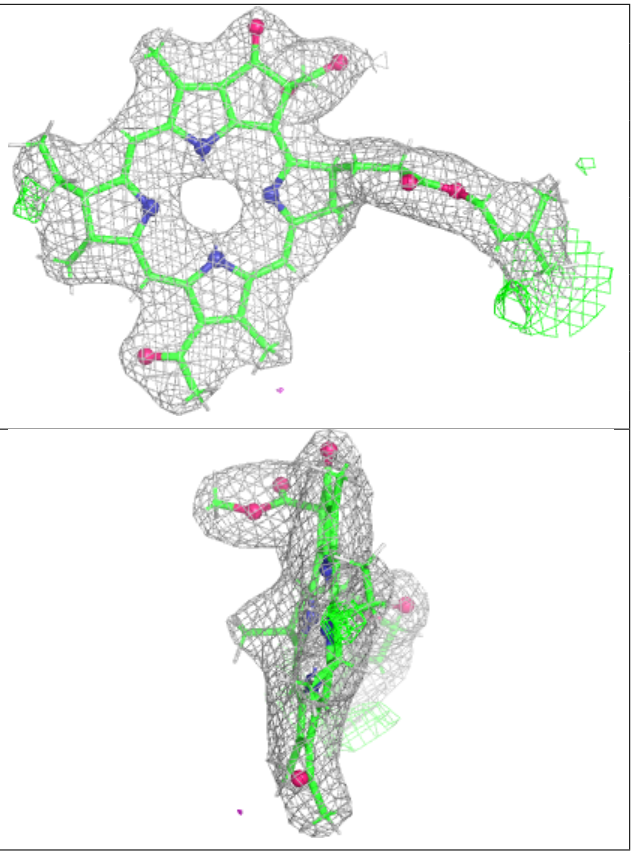






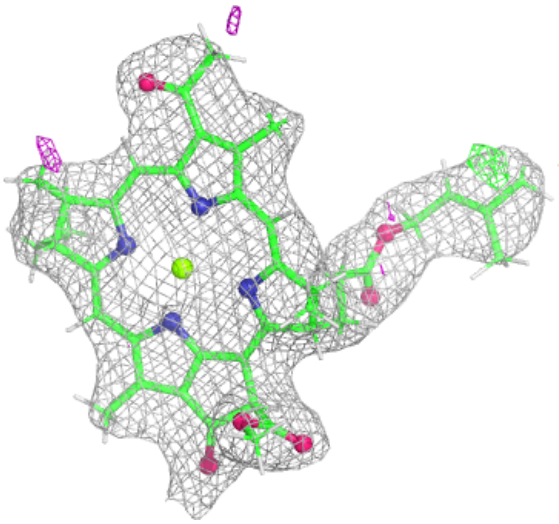
Electron density around BPH M 304:

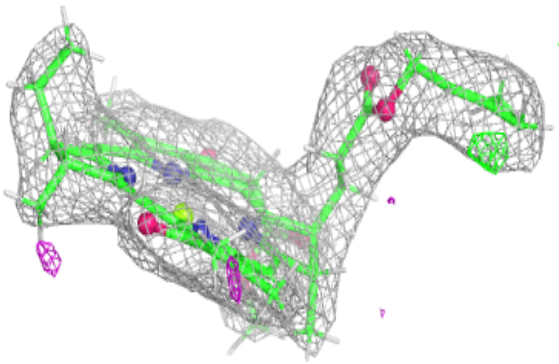
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

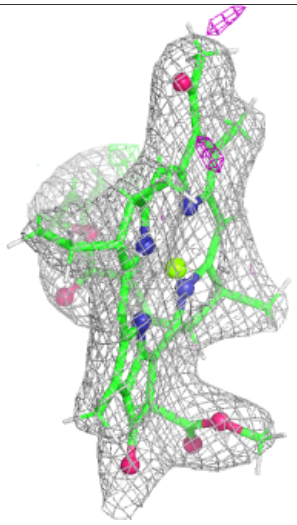


Electron density around BCL M 403:

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

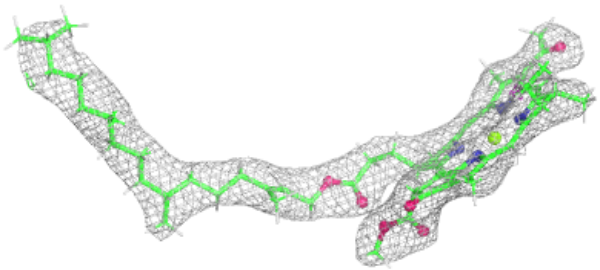




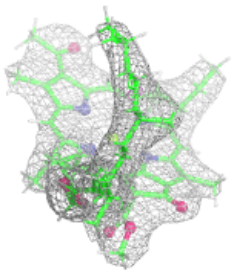


Electron density around BCL L 303:

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

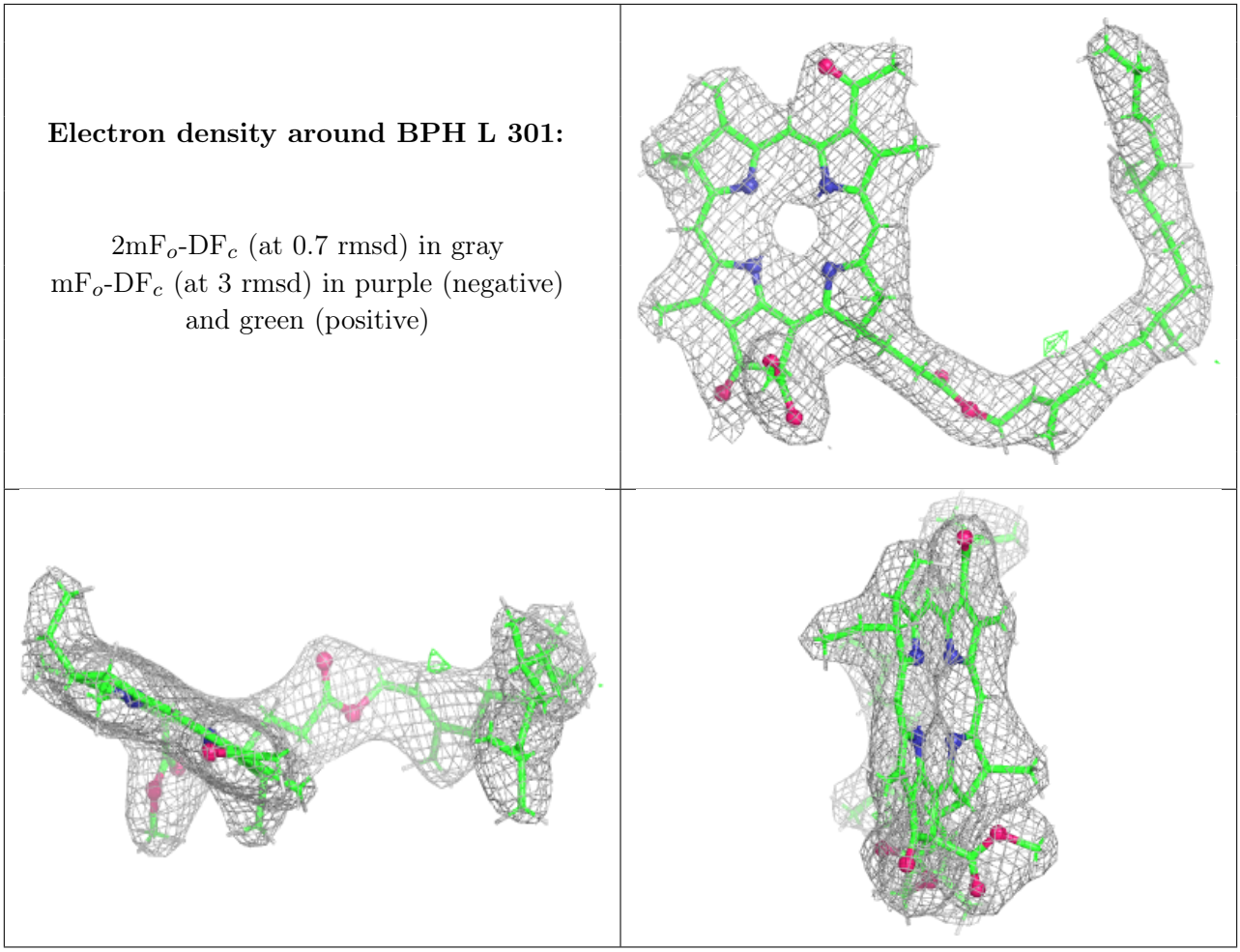






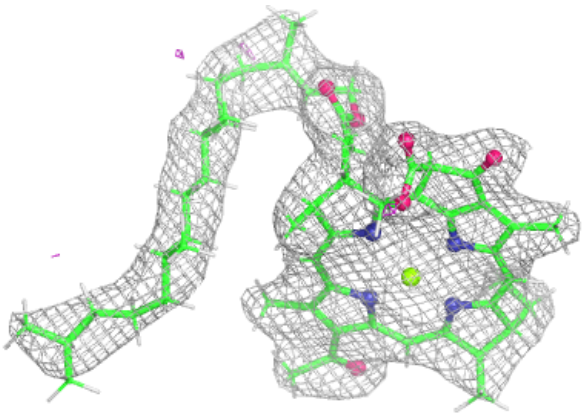
Electron density around BPH L 301:

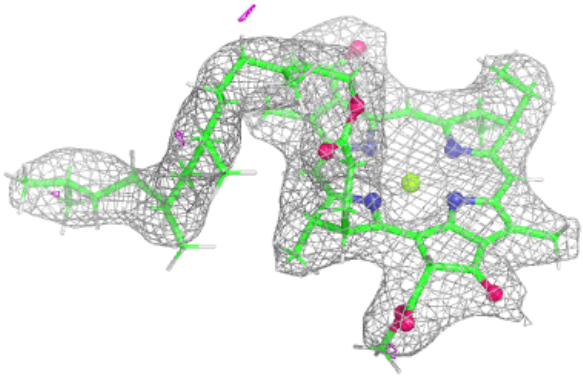
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

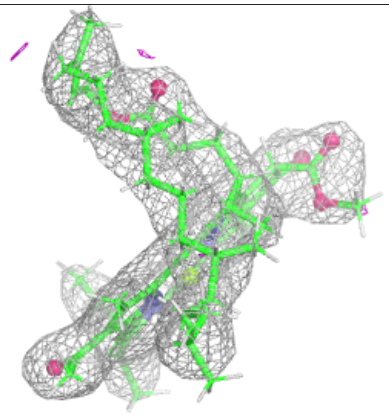


Electron density around BCL L 302:

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

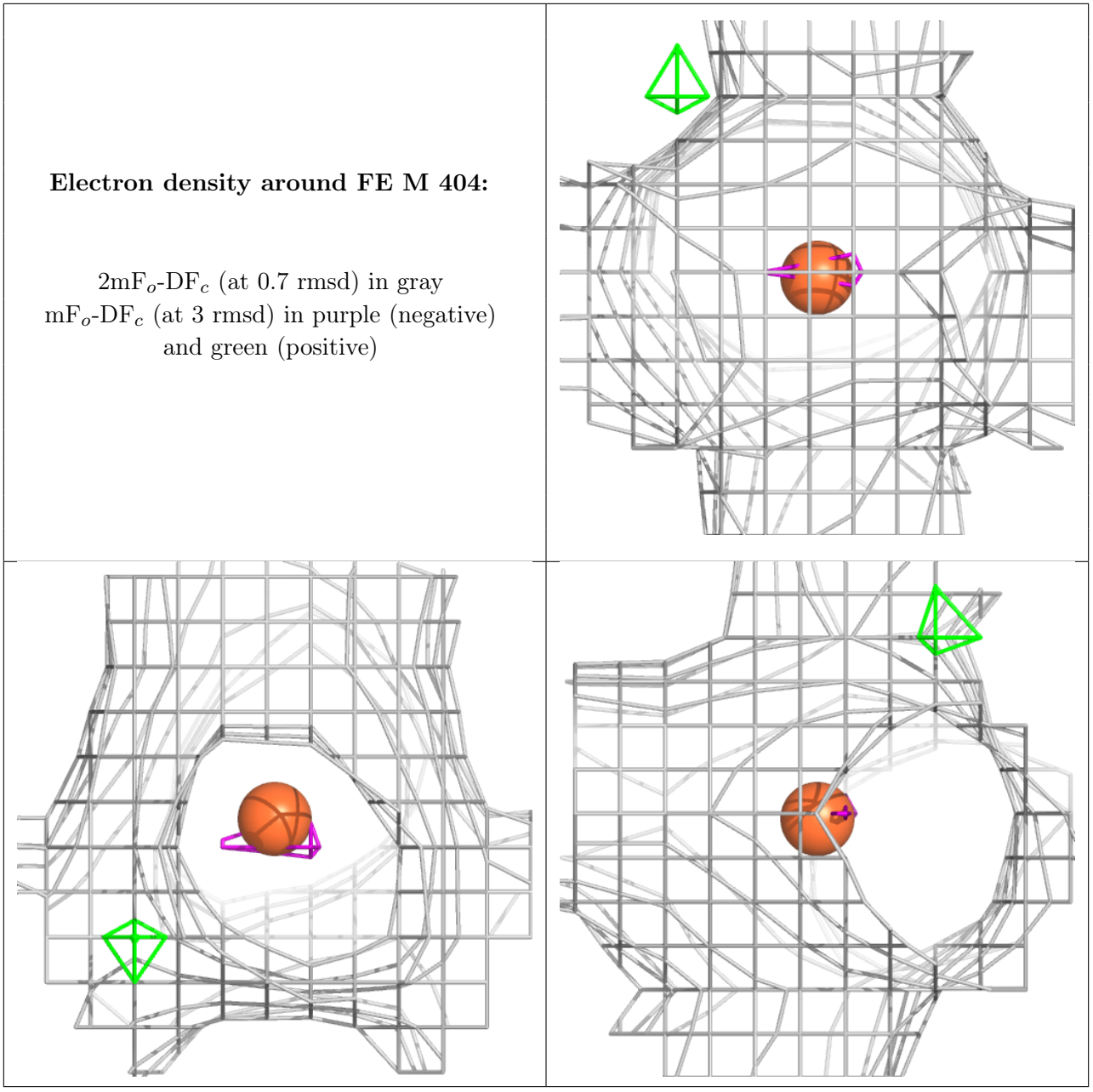






Electron density around FE M 404:

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



6.5 Other polymers

There are no such residues in this entry.