wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 11:34 am BST

PDB ID	:	7Q7J / pdb_00007q7j
Title	:	Room temperature structure of the Rhodobacter Sphaeroides Photosynthetic Reaction Center F(M197)H mutant at 75 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	:	2.69 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 (i)) were used in the production of this report:

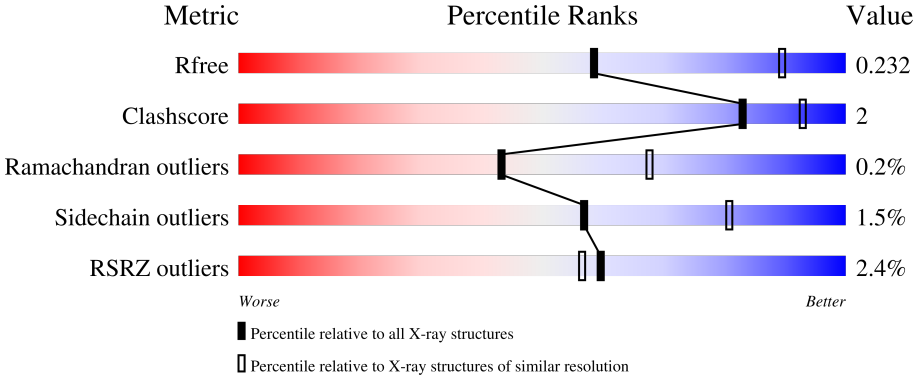
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	2%, 93%, 6%
2	L	281	3%, 96%, •
3	M	302	2%, 94%, 6%, •

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 14698 atoms, of which 7308 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
			Total	C	H	N	O	S			
1	H	240	3751	1196	1883	321	341	10	0	5	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	L	281	4447	1519	2200	357	363	8	0	2	0

There is a discrepancy between the modelled and reference sequences:

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

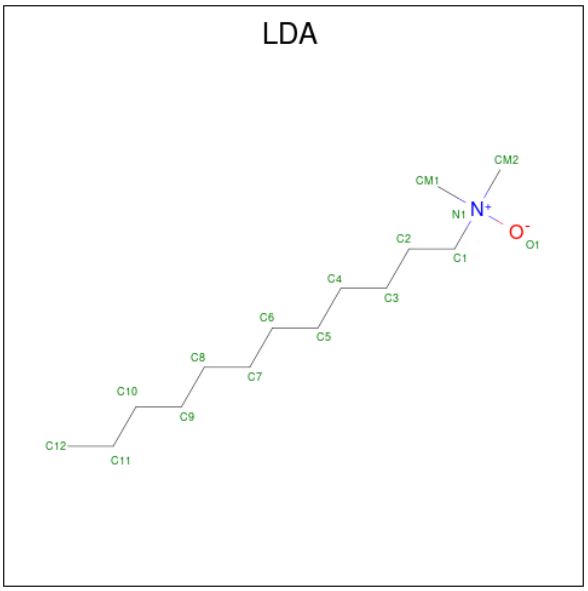
- Molecule 3 is a protein called Reaction center protein M chain.

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

There are 2 discrepancies between the modelled and reference sequences:

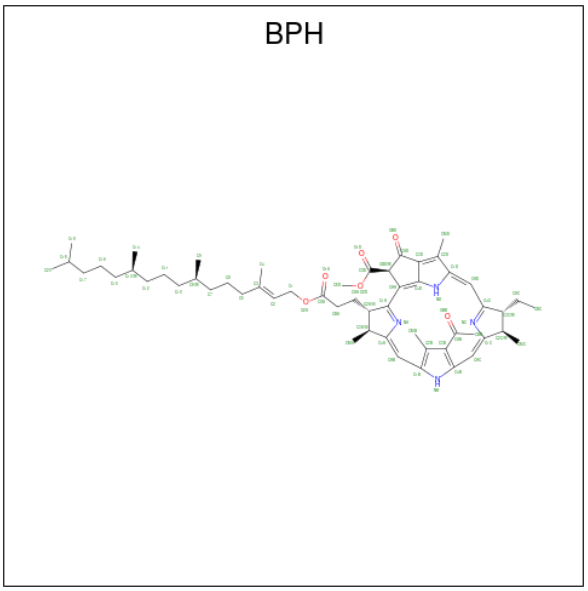
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP P0C0Y9
M	197	HIS	PHE	engineered mutation	UNP P0C0Y9

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



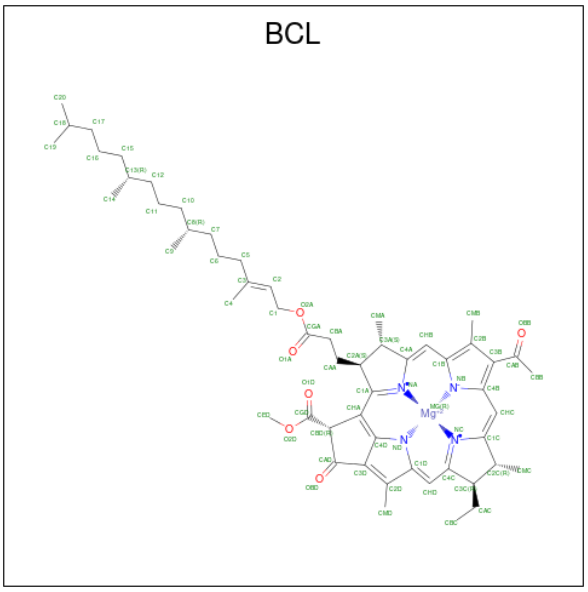
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	H	1	47	14	31	1	1	0	0
			Total	C	H	N	O		
4	H	1	47	14	31	1	1	0	0
			Total	C	H	N	O		
4	L	1	47	14	31	1	1	0	0
			Total	C	H	N	O		
4	L	1	47	14	31	1	1	0	0
			Total	C	H	N	O		
4	M	1	47	14	31	1	1	0	0
			Total	C	H	N	O		
4	M	1	47	14	31	1	1	0	0
			Total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

- 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
			Total	C	H	N	O		
5	L	1	141	55	76	4	6	0	0
			Total	C	H	N	O		
5	M	1	95	40	45	4	6	0	0

- 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
			Total	C	H	Mg	N	O		
6	L	1	140	55	74	1	4	6	0	0

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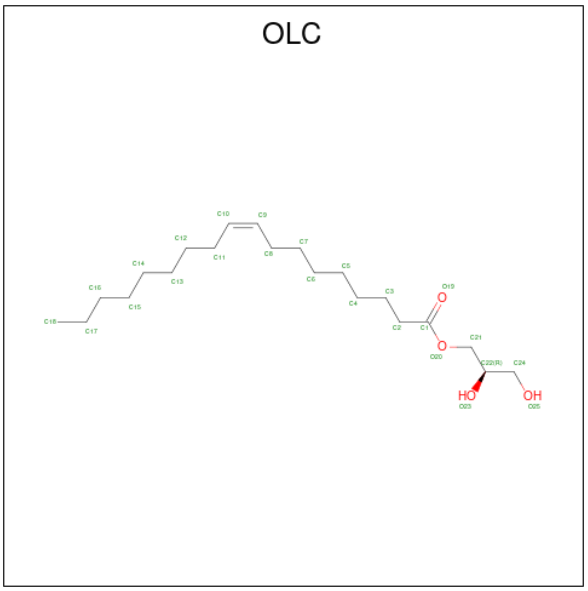
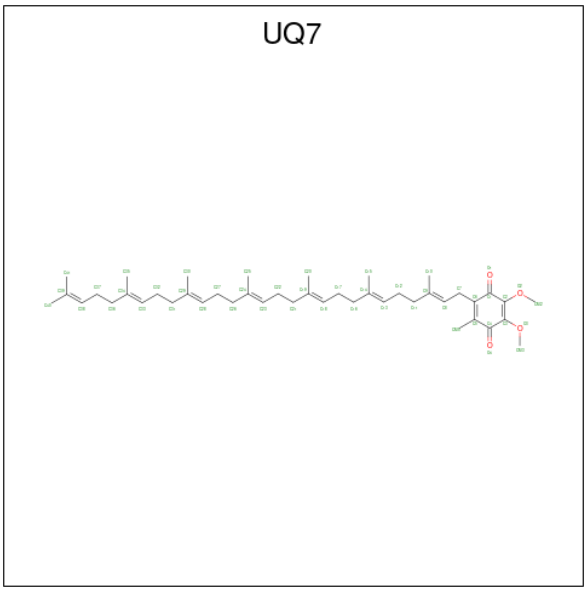
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
6	L	1	140	55	74	1	4	6	0	0
			Total	C	H	Mg	N	O		
6	M	1	140	55	74	1	4	6	0	0
			Total	C	H	Mg	N	O		
6	M	1	94	40	43	1	4	6	0	0

- 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
			Total	C	H	O		
7	L	1	65	21	40	4	0	0
			Total	C	H	O		
7	M	1	65	21	40	4	0	1

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

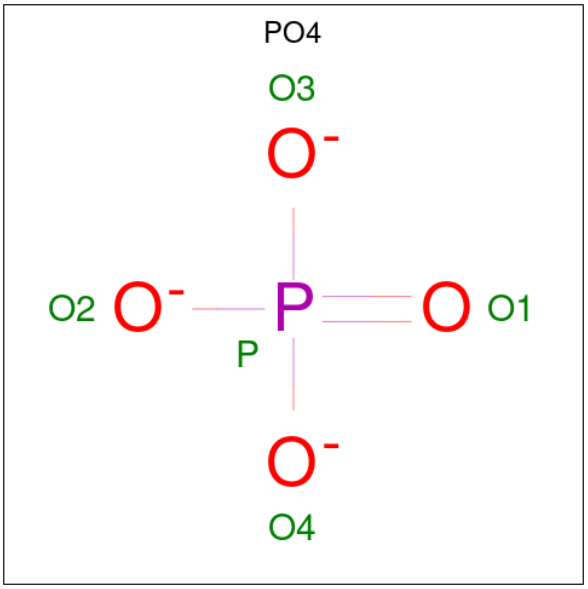


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	M	1	113	44	65	4	0	0

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

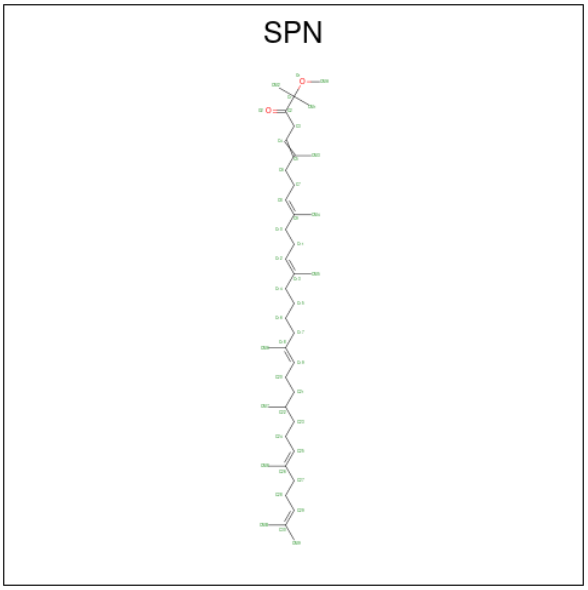
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
9	M	1	1	1	0	0

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



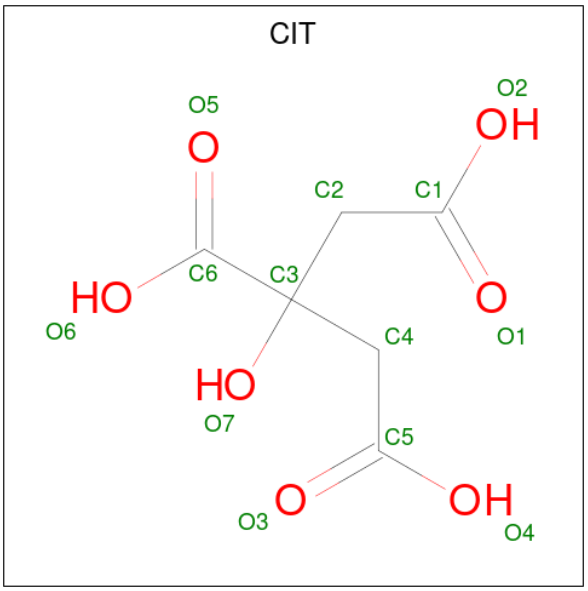
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
10	M	1	5	4	1	0	0
			Total	O	P		
10	M	1	5	4	1	0	0

- 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
			Total	C	H	O		
11	M	1	113	41	70	2	0	1

- Molecule 12 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 14 is water.

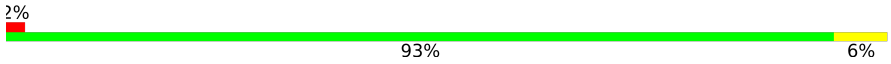
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	H	71	Total O 72 72	0	1
14	L	47	Total O 47 47	0	0
14	M	47	Total O 47 47	0	0

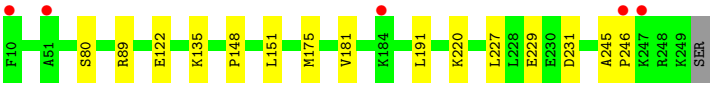
3 Residue-property plots (i)

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

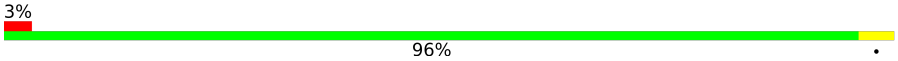
Chain H:





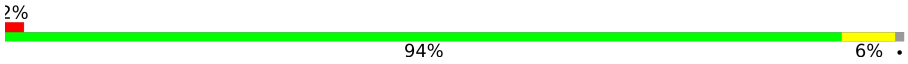
• Molecule 2: Reaction center protein L chain

Chain L:



• Molecule 3: Reaction center protein M chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.30Å 102.30Å 237.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 2.69 46.99 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.99-2.69) 88.5 (46.99-2.69)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.81 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13-2998_9999	Depositor
R, R_{free}	0.179 , 0.231 0.184 , 0.232	Depositor DCC
R_{free} test set	1436 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14698	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, LDA, SPN, FE, BCL, OLC, UQ7, CIT, CL, BPH

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	0/1928	0.31	0/2619
2	L	0.12	0/2343	0.31	0/3208
3	M	0.13	0/2542	0.31	0/3472
All	All	0.13	0/6813	0.31	0/9299

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1868	1883	1875	5	0
2	L	2247	2200	2194	5	0
3	M	2435	2340	2326	14	0
4	H	32	62	62	3	0
4	L	32	62	62	0	0
4	M	80	155	155	2	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	117	115	4	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	2	0
9	M	1	0	0	0	0
10	M	10	0	0	0	0
11	M	43	70	70	6	0
12	M	13	5	5	1	0
13	M	1	0	0	0	0
14	H	72	0	0	0	0
14	L	47	0	0	0	0
14	M	47	0	0	0	0
All	All	7390	7308	7277	35	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 35 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	1.70	0.72
4:H:301:LDA:H123	8:M:401:UQ7:H202	1.72	0.70
3:M:51:TYR:HH	12:M:414:CIT:HO7	1.47	0.62
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.82	0.62
5:M:304:BPH:HBC3	5:M:304:BPH:HHD	1.83	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	243/241 (101%)	236 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	281/281 (100%)	274 (98%)	5 (2%)	2 (1%)	18	41
3	M	303/302 (100%)	295 (97%)	8 (3%)	0	100	100
All	All	827/824 (100%)	805 (97%)	20 (2%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	270	PRO
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	200/196 (102%)	195 (98%)	5 (2%)	42	71
2	L	222/220 (101%)	217 (98%)	5 (2%)	44	73
3	M	240/236 (102%)	240 (100%)	0	100	100
All	All	662/652 (102%)	652 (98%)	10 (2%)	57	81

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	247	CYS
2	L	271	TRP
2	L	274	ASN
1	H	175	MET
1	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	68	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
10	PO4	M	407	-	4,4,4	0.90	0	6,6,6	0.47	0
4	LDA	M	405	-	12,15,15	0.44	0	14,17,17	0.19	0
4	LDA	M	410	-	12,15,15	0.38	0	14,17,17	0.15	0
4	LDA	M	406	-	12,15,15	0.39	0	14,17,17	0.47	0
4	LDA	M	412	-	12,15,15	0.32	0	14,17,17	0.43	0
7	OLC	M	408[B]	-	24,24,24	0.17	0	25,25,25	0.14	0
4	LDA	H	301	-	12,15,15	0.31	0	14,17,17	0.43	0
10	PO4	M	413	-	4,4,4	0.90	0	6,6,6	0.42	0
4	LDA	H	302	-	12,15,15	0.48	0	14,17,17	0.42	0
4	LDA	L	307	-	12,15,15	0.36	0	14,17,17	0.37	0
5	BPH	M	304	-	44,55,70	1.13	4 (9%)	43,83,101	1.69	7 (16%)
6	BCL	L	302	2	69,74,74	1.08	4 (5%)	83,115,115	1.28	7 (8%)
6	BCL	M	402	3	69,74,74	1.06	5 (7%)	83,115,115	1.37	6 (7%)
8	UQ7	M	401	-	48,48,48	0.24	0	58,61,61	0.39	0
5	BPH	L	301	-	59,70,70	0.97	2 (3%)	61,101,101	1.42	6 (9%)
6	BCL	M	403	3	54,59,74	1.21	3 (5%)	65,97,115	1.49	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	BCL	L	303	2	69,74,74	1.15	5 (7%)	83,115,115	1.27	6 (7%)
4	LDA	L	306	-	12,15,15	0.44	0	14,17,17	0.28	0
12	CIT	M	414	-	12,12,12	1.11	2 (16%)	17,17,17	1.12	2 (11%)
7	OLC	L	305	-	24,24,24	0.23	0	25,25,25	0.18	0
11	SPN	M	409[A]	-	40,42,42	0.19	0	50,52,52	0.59	1 (2%)
4	LDA	M	411	-	12,15,15	0.33	0	14,17,17	0.89	2 (14%)

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	405	-	-	6/13/13/13	-
4	LDA	M	410	-	-	4/13/13/13	-
4	LDA	M	406	-	-	8/13/13/13	-
4	LDA	M	412	-	-	8/13/13/13	-
7	OLC	M	408[B]	-	-	9/24/24/24	-
4	LDA	H	301	-	-	4/13/13/13	-
4	LDA	H	302	-	-	6/13/13/13	-
4	LDA	L	307	-	-	5/13/13/13	-
5	BPH	M	304	-	-	2/19/87/105	0/5/6/6
6	BCL	L	302	2	-	1/41/137/137	-
6	BCL	M	402	3	-	11/41/137/137	-
8	UQ7	M	401	-	-	7/45/69/69	0/1/1/1
5	BPH	L	301	-	-	8/37/105/105	0/5/6/6
6	BCL	M	403	3	-	0/23/119/137	-
6	BCL	L	303	2	-	2/41/137/137	-
4	LDA	L	306	-	-	10/13/13/13	-
12	CIT	M	414	-	-	6/16/16/16	-
7	OLC	L	305	-	-	15/24/24/24	-
11	SPN	M	409[A]	-	-	21/50/51/51	-
4	LDA	M	411	-	-	9/13/13/13	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	304	BPH	C1B-C2B	5.20	1.45	1.39
5	L	301	BPH	C1B-C2B	5.08	1.45	1.39
6	L	303	BCL	MG-NA	4.73	2.17	2.06
6	L	302	BCL	MG-NA	4.49	2.16	2.06
6	M	403	BCL	MG-NA	4.39	2.16	2.06

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	301	BPH	C4D-CHA-CBD	-7.49	105.13	108.52
5	M	304	BPH	C4D-CHA-CBD	-7.18	105.27	108.52
6	M	403	BCL	CHD-C1D-ND	-5.03	119.83	124.45
6	M	403	BCL	C4D-CHA-C1A	4.99	127.32	121.25
6	M	402	BCL	CHD-C1D-ND	-4.97	119.88	124.45

There are no chirality outliers.

5 of 142 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	LDA	N1-C1-C2-C3
4	H	302	LDA	C2-C1-N1-O1
4	H	302	LDA	C2-C1-N1-CM2
4	L	306	LDA	N1-C1-C2-C3
4	M	405	LDA	C2-C1-N1-O1

There are no ring outliers.

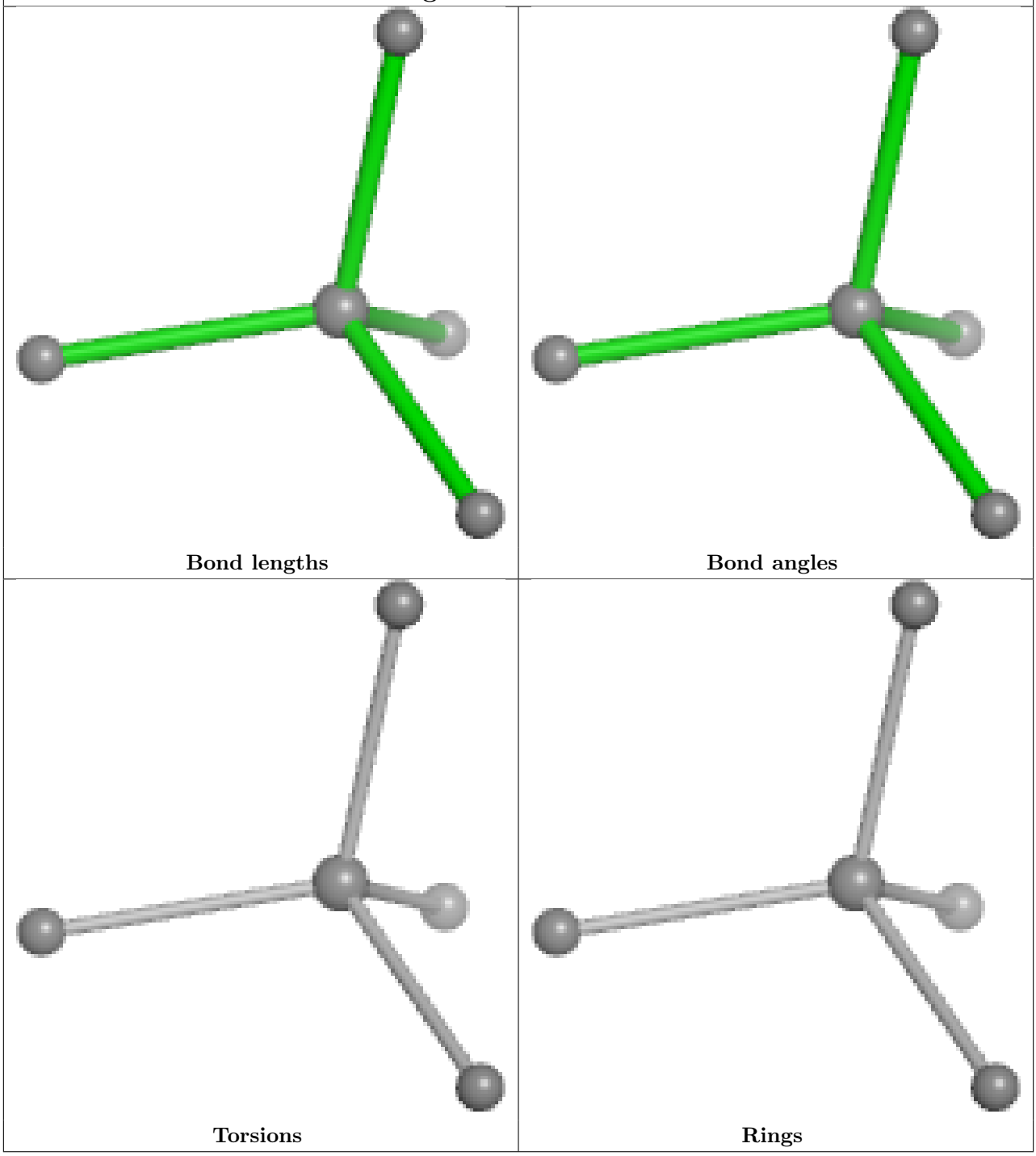
11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	405	LDA	1	0
4	M	410	LDA	1	0
4	H	301	LDA	3	0
5	M	304	BPH	2	0
6	L	302	BCL	2	0
6	M	402	BCL	1	0
8	M	401	UQ7	2	0
5	L	301	BPH	1	0
6	M	403	BCL	3	0
12	M	414	CIT	1	0
11	M	409[A]	SPN	6	0

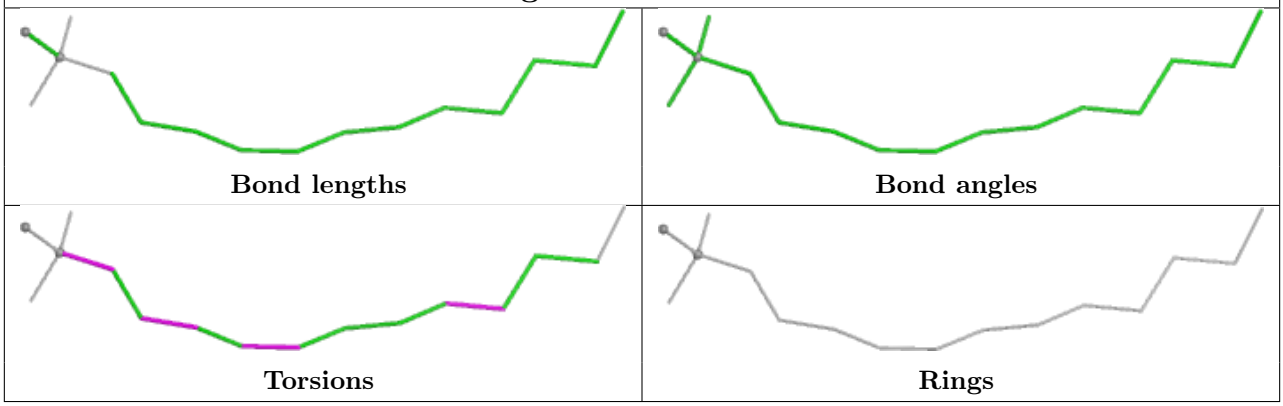
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

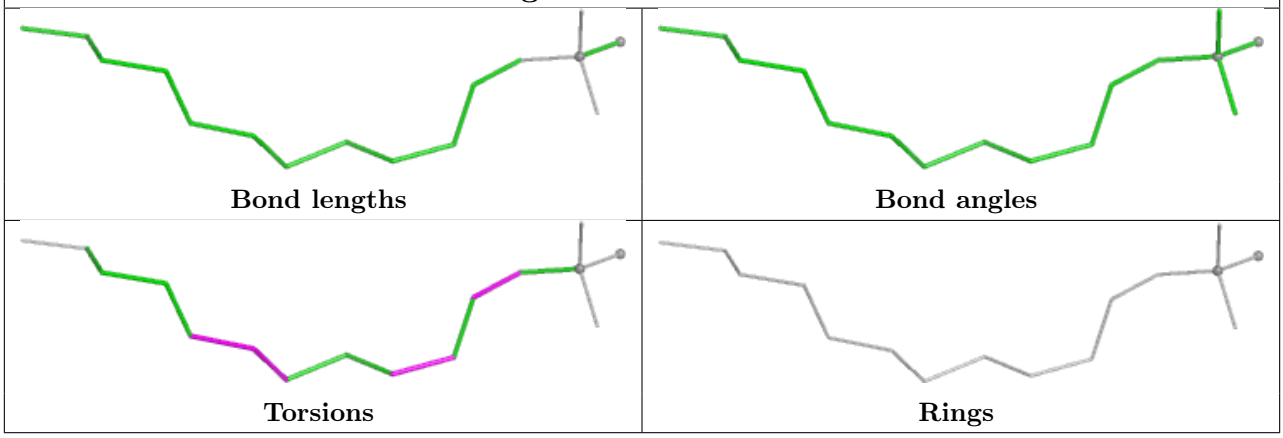
Ligand PO4 M 407



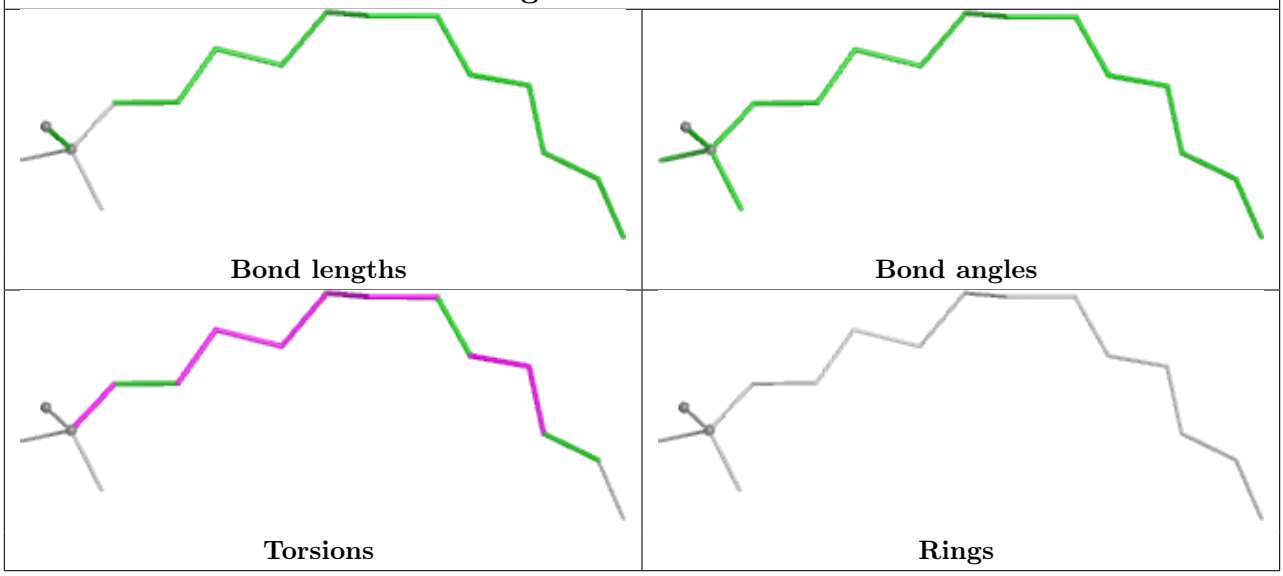
Ligand LDA M 405



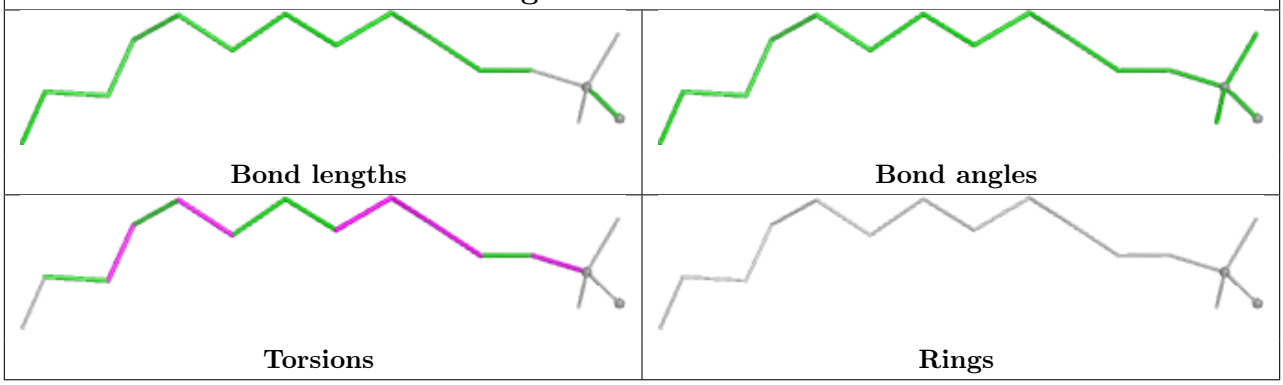
Ligand LDA M 410



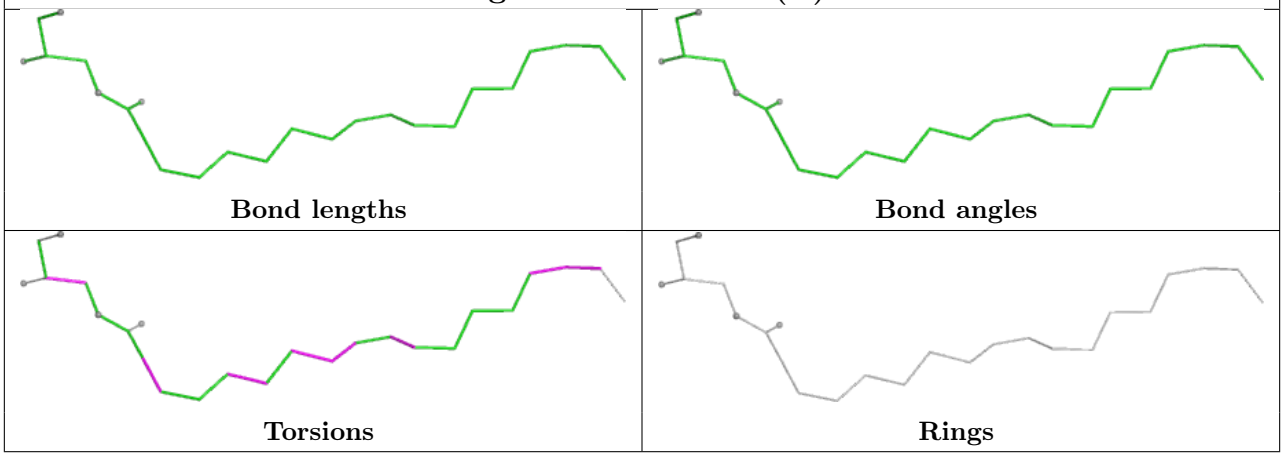
Ligand LDA M 406



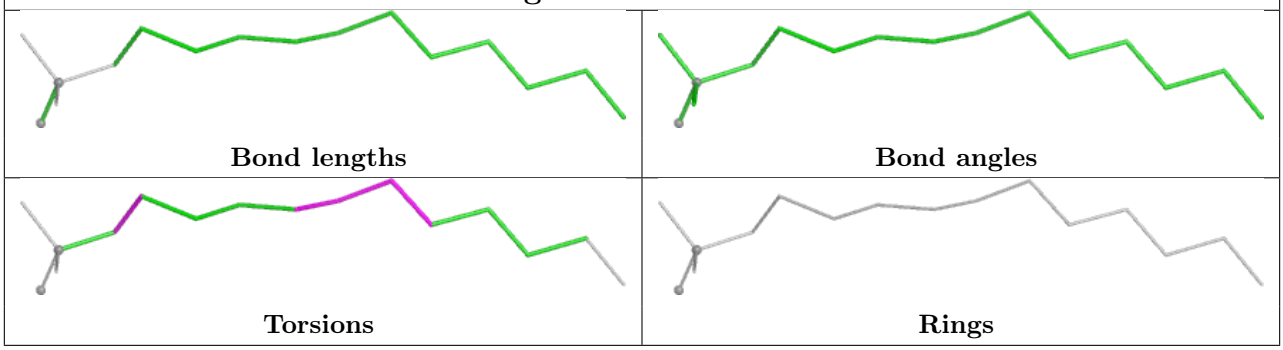
Ligand LDA M 412



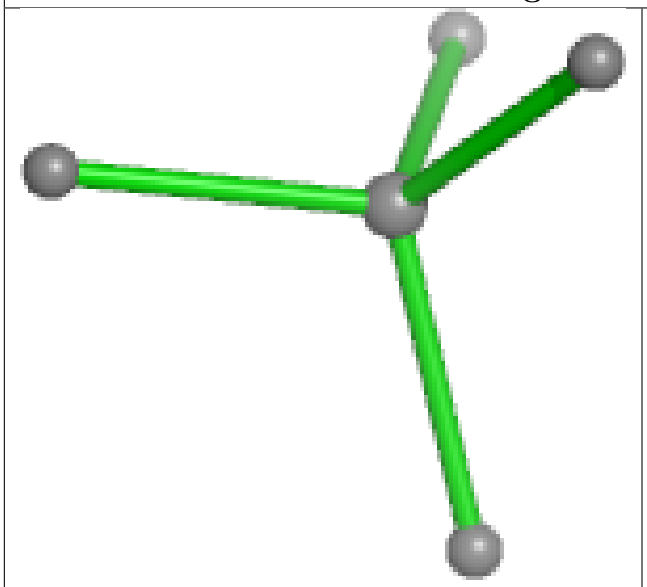
Ligand OLC M 408 (B)



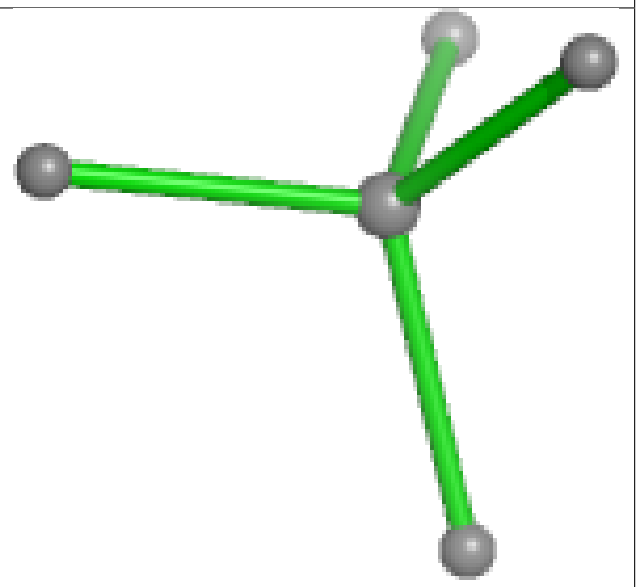
Ligand LDA H 301



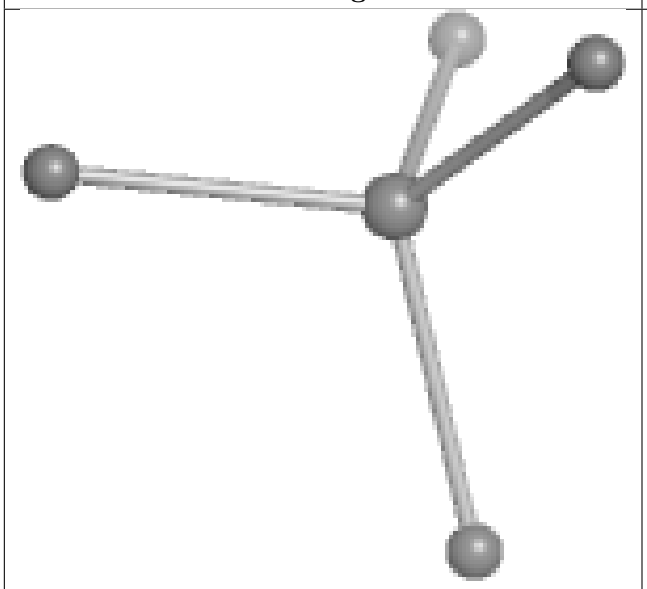
Ligand PO4 M 413



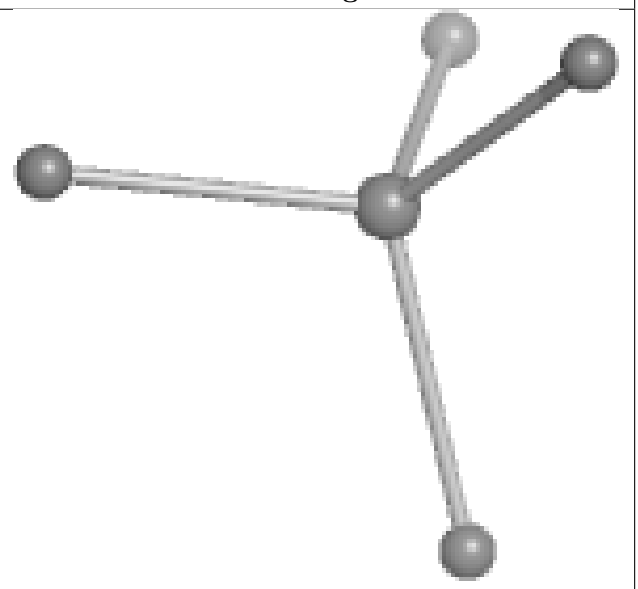
Bond lengths



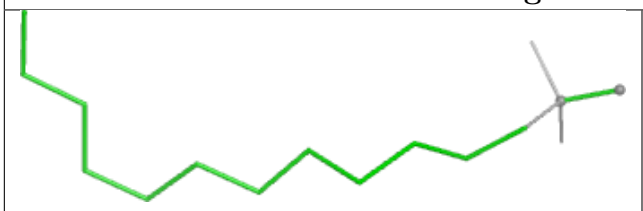
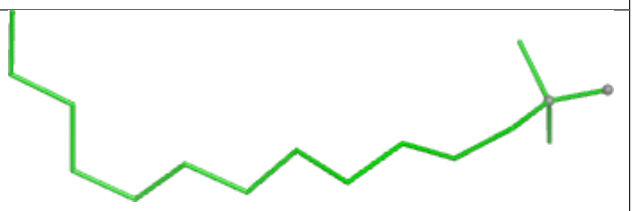
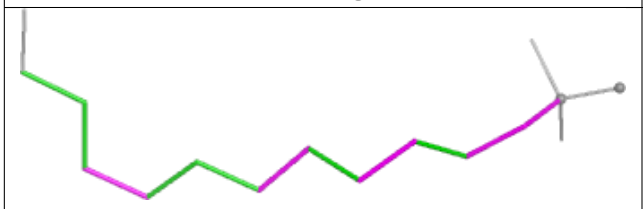
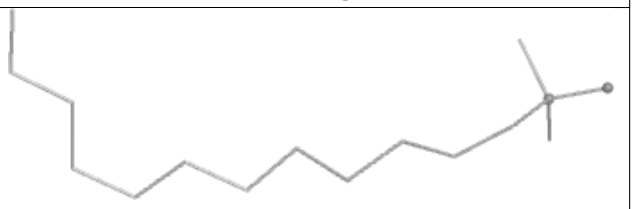
Bond angles

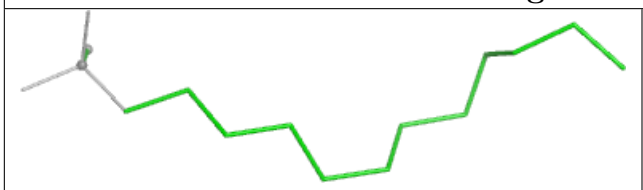
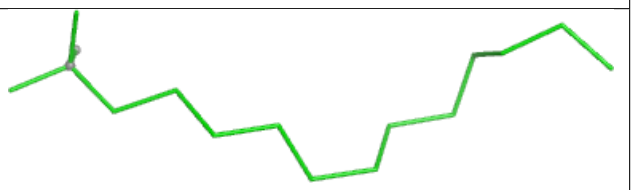
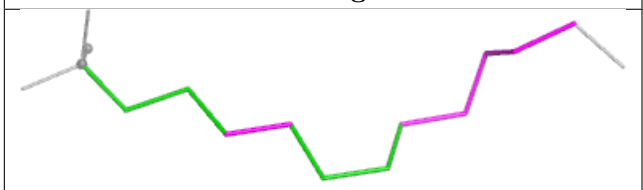
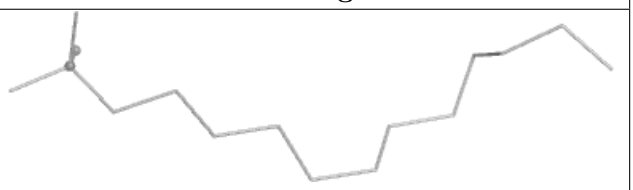


Torsions

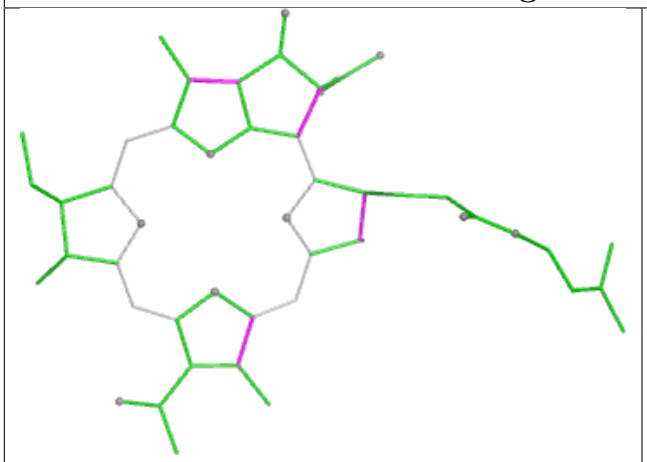


Rings

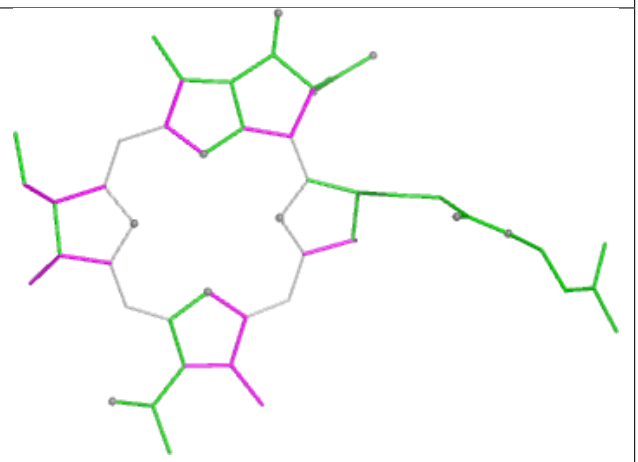
Ligand LDA H 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LDA L 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

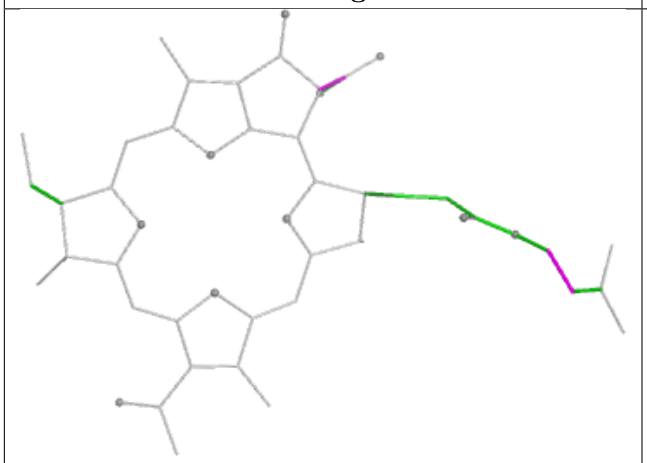
Ligand BPH M 304



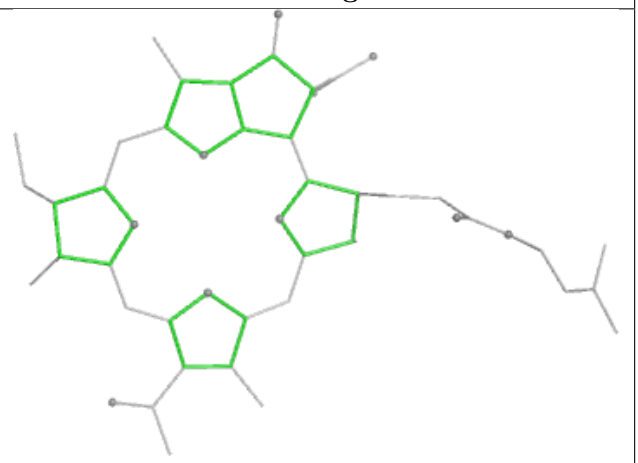
Bond lengths



Bond angles

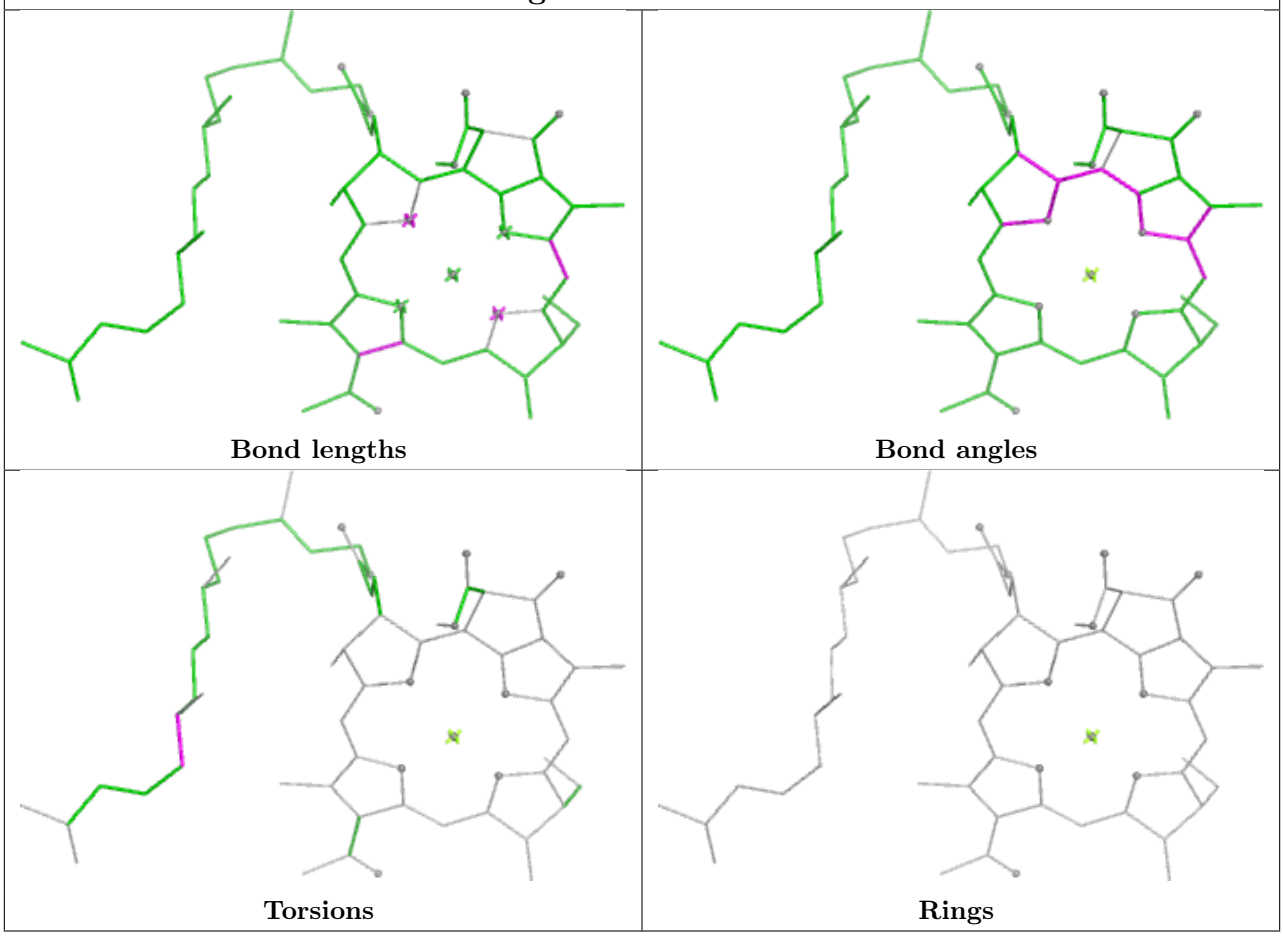


Torsions

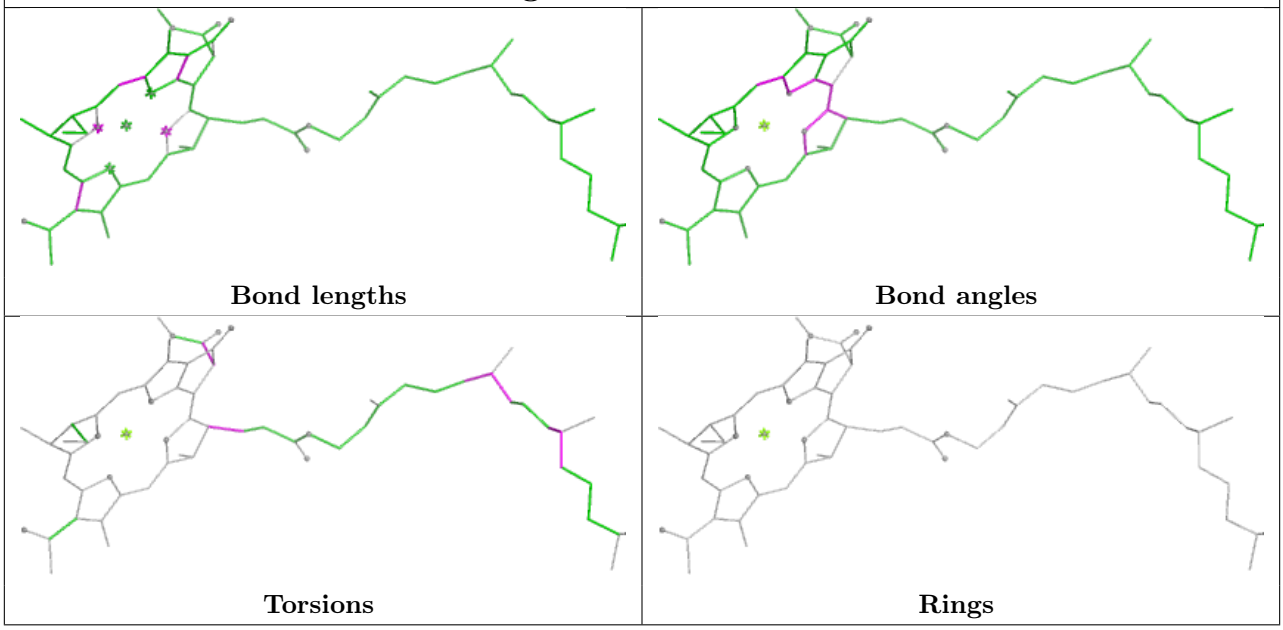


Rings

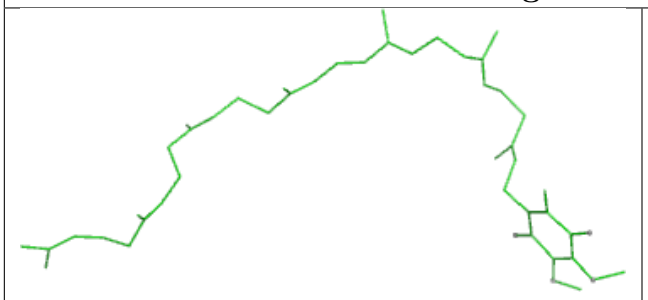
Ligand BCL L 302



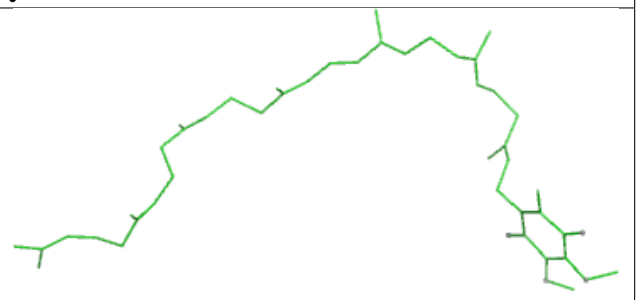
Ligand BCL M 402



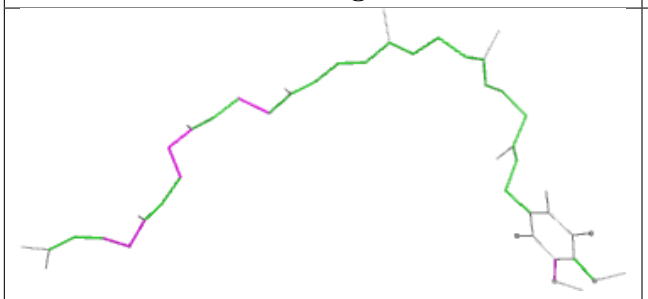
Ligand UQ7 M 401



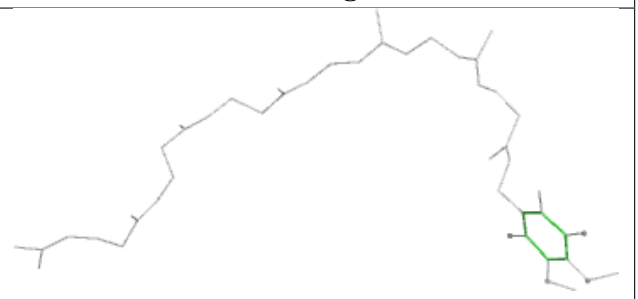
Bond lengths



Bond angles

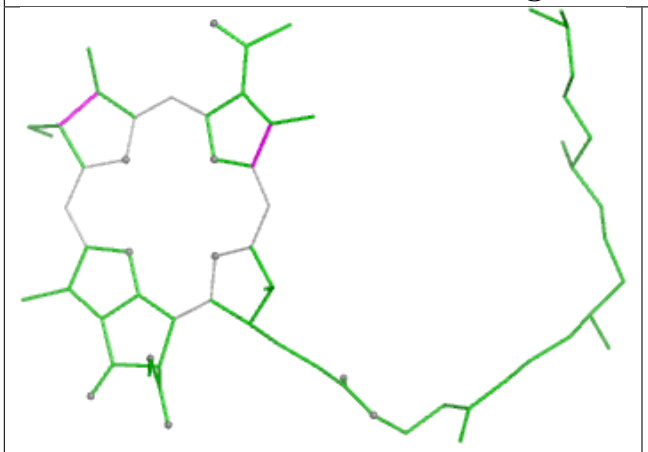


Torsions

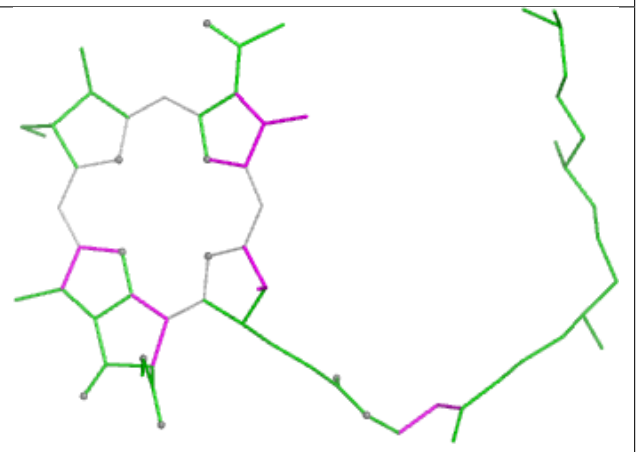


Rings

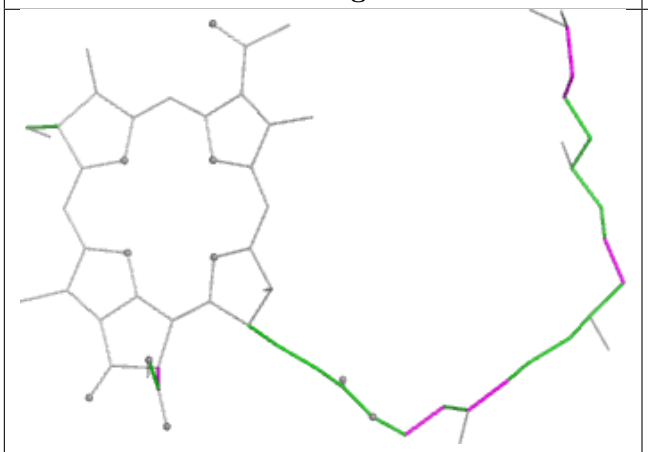
Ligand BPH L 301



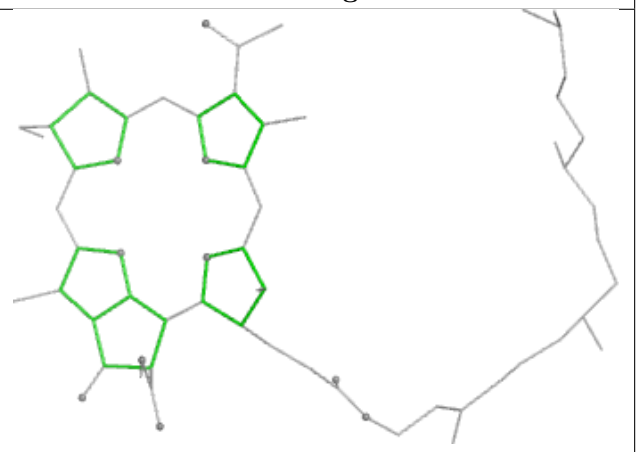
Bond lengths



Bond angles

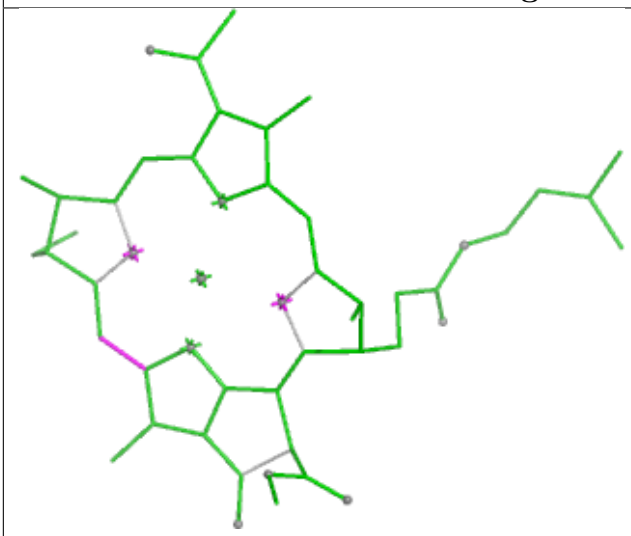


Torsions

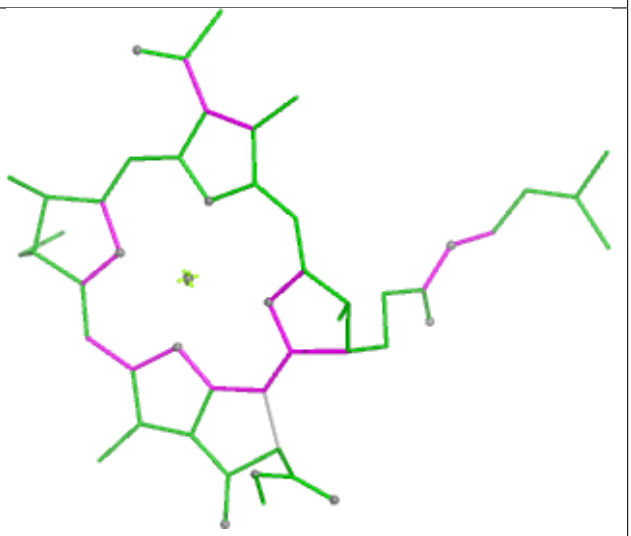


Rings

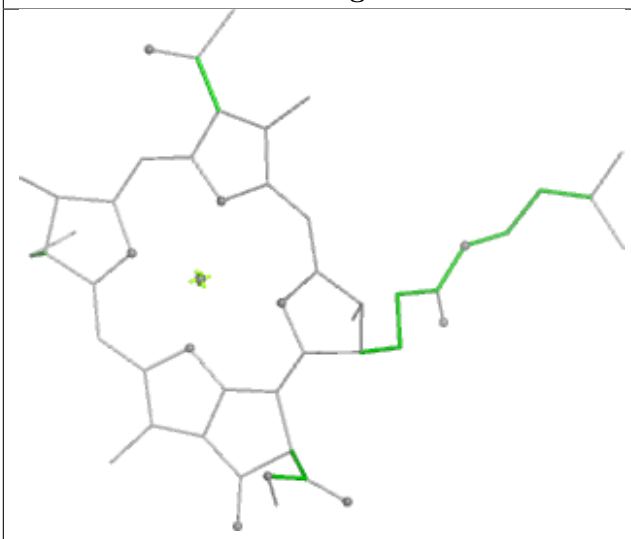
Ligand BCL M 403



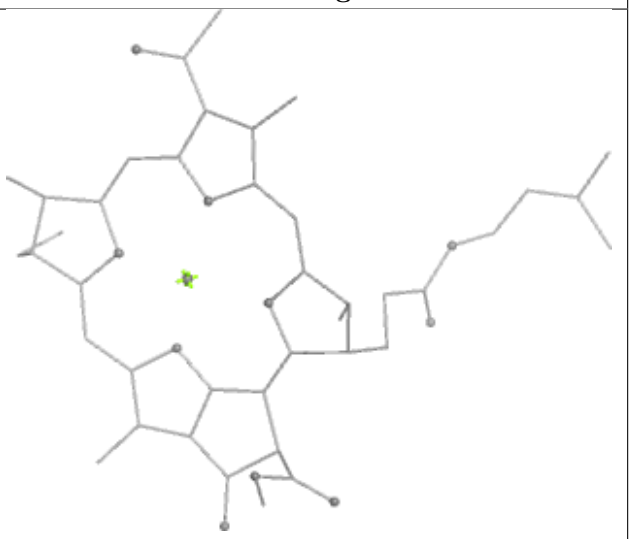
Bond lengths



Bond angles

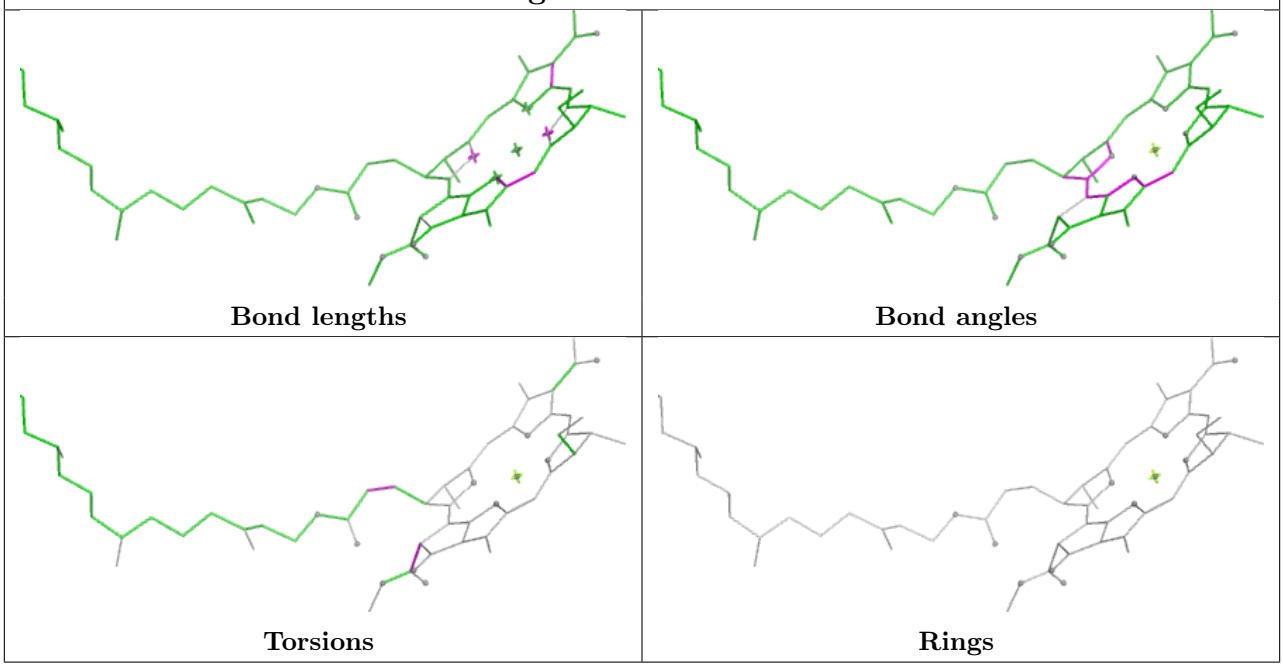


Torsions

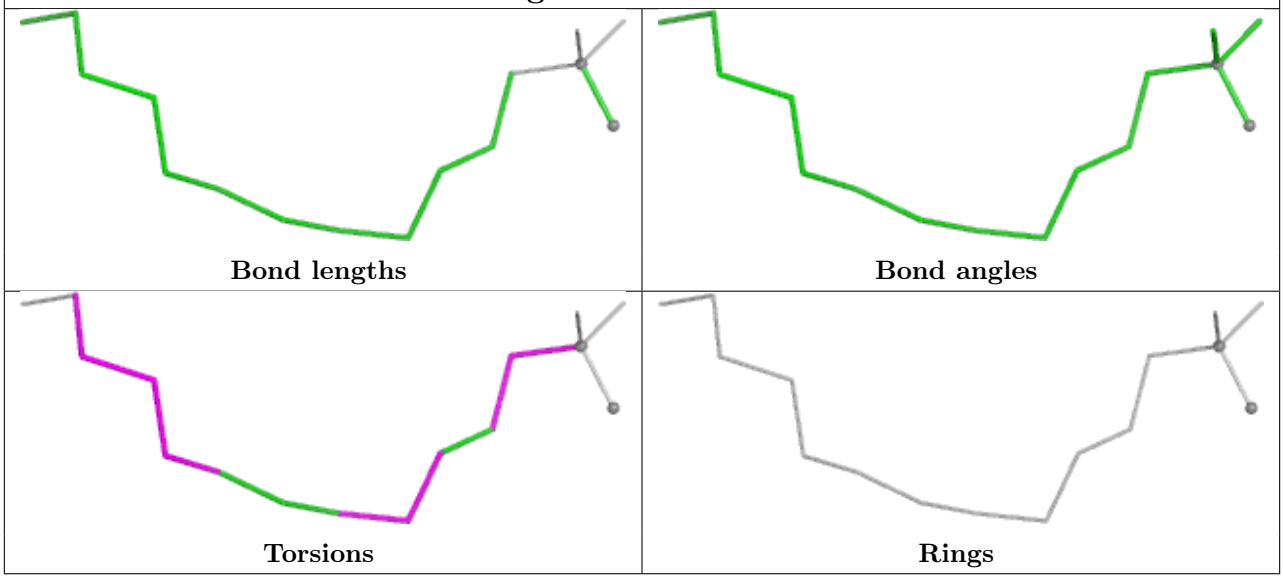


Rings

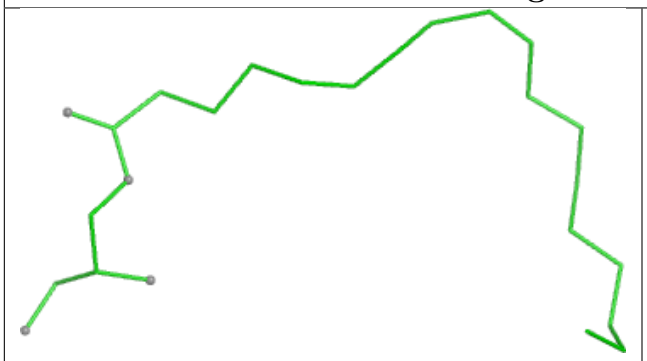
Ligand BCL L 303



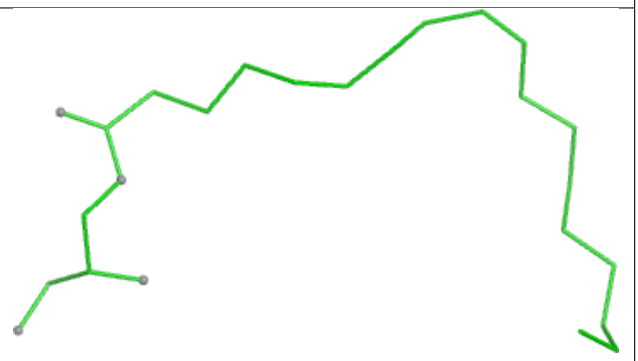
Ligand LDA L 306



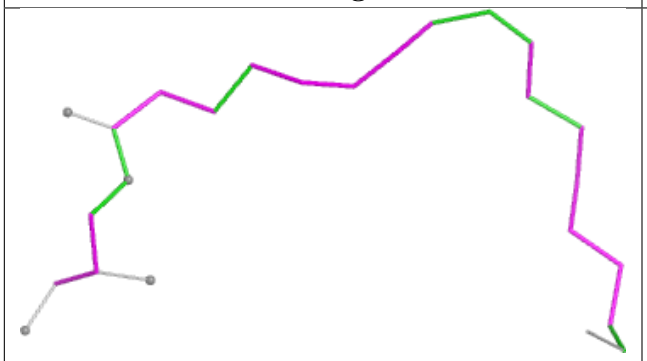
Ligand OLC L 305



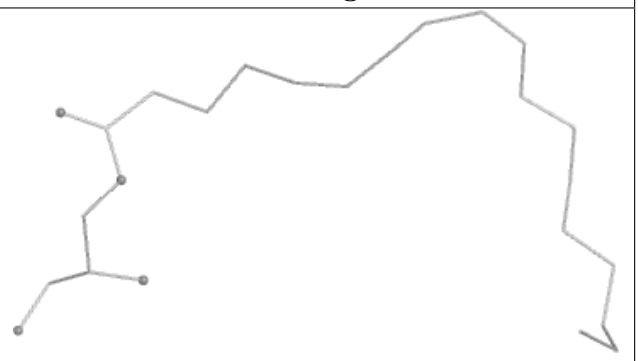
Bond lengths



Bond angles

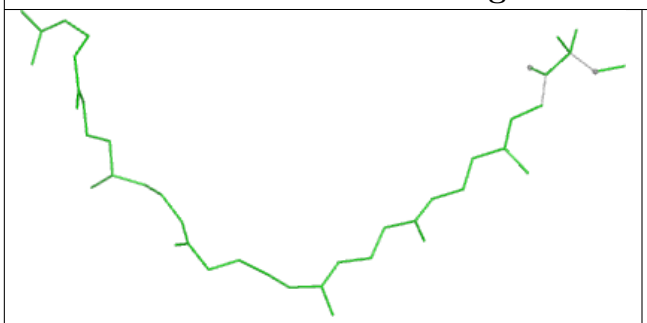


Torsions

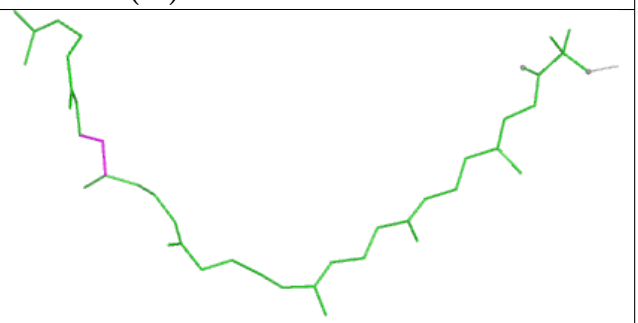


Rings

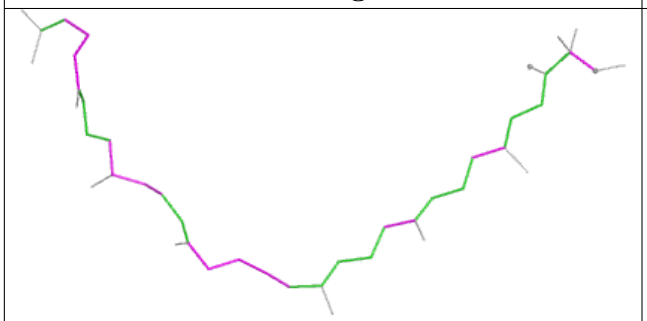
Ligand SPN M 409 (A)



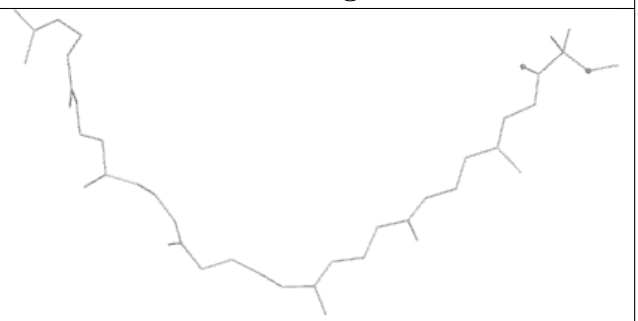
Bond lengths



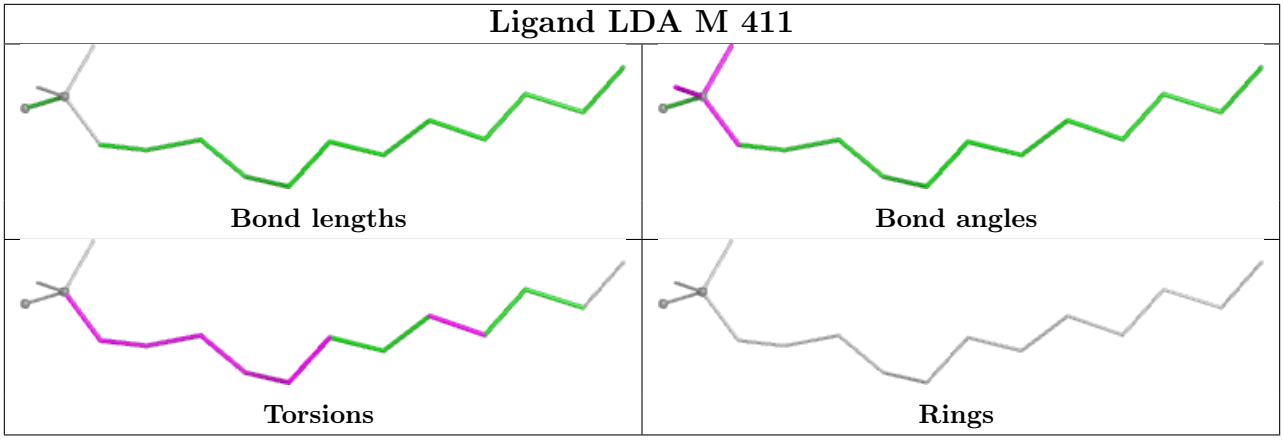
Bond angles



Torsions



Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	0.02	5 (2%)	63	61	22, 44, 77, 138	4 (1%)
2	L	281/281 (100%)	-0.16	8 (2%)	55	51	24, 41, 88, 125	1 (0%)
3	M	300/302 (99%)	-0.13	7 (2%)	61	58	20, 42, 73, 117	3 (1%)
All	All	821/824 (99%)	-0.10	20 (2%)	59	56	20, 43, 79, 138	8 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	148[A]	TRP	6.0
1	H	184[A]	LYS	5.1
1	H	10	PHE	4.5
2	L	51[A]	TRP	4.5
2	L	265	TRP	4.3

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

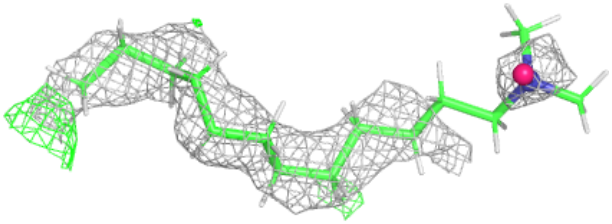
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

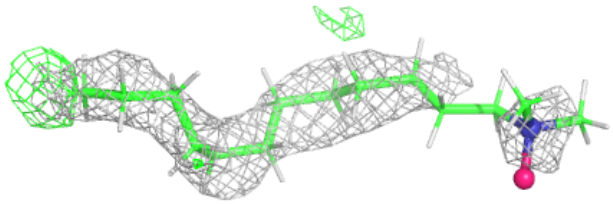
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LDA	L	307	16/16	0.75	0.21	44,55,63,64	47
4	LDA	H	302	16/16	0.77	0.28	80,98,110,110	0
4	LDA	M	410	16/16	0.79	0.22	74,90,103,104	0
4	LDA	M	412	16/16	0.80	0.26	58,74,91,92	47
12	CIT	M	414	13/13	0.80	0.18	85,86,104,104	0
4	LDA	M	405	16/16	0.81	0.25	54,77,92,93	0
4	LDA	M	411	16/16	0.81	0.23	80,97,108,108	0
11	SPN	M	409[A]	43/43	0.83	0.22	21,52,67,67	113
4	LDA	L	306	16/16	0.83	0.24	75,90,106,107	0
10	PO4	M	413	5/5	0.85	0.15	77,78,78,78	5
7	OLC	M	408[B]	25/25	0.87	0.17	44,56,67,67	65
7	OLC	L	305	25/25	0.88	0.21	57,83,102,102	0
4	LDA	M	406	16/16	0.89	0.16	51,63,65,65	0
10	PO4	M	407	5/5	0.90	0.14	64,66,69,70	0
4	LDA	H	301	16/16	0.92	0.12	55,67,75,77	0
6	BCL	M	403	51/66	0.94	0.09	28,34,67,77	0
8	UQ7	M	401	48/48	0.94	0.12	31,57,83,89	0
6	BCL	M	402	66/66	0.94	0.10	30,42,80,83	0
5	BPH	M	304	50/65	0.95	0.08	27,37,52,54	0
6	BCL	L	302	66/66	0.95	0.09	30,39,69,72	0
6	BCL	L	303	66/66	0.95	0.08	27,38,61,66	0
5	BPH	L	301	65/65	0.95	0.09	24,34,49,53	0
13	CL	M	415	1/1	0.95	0.16	38,38,38,38	0
9	FE	M	404	1/1	0.99	0.03	20,20,20,20	0

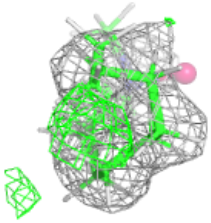
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

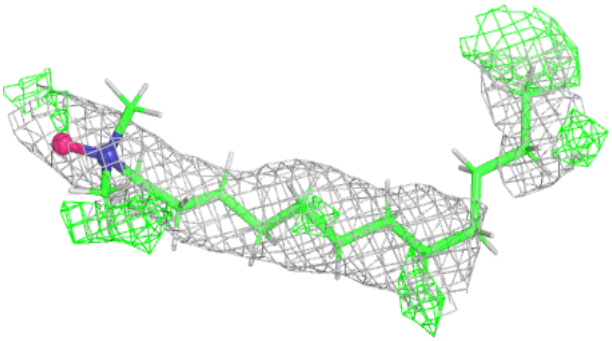


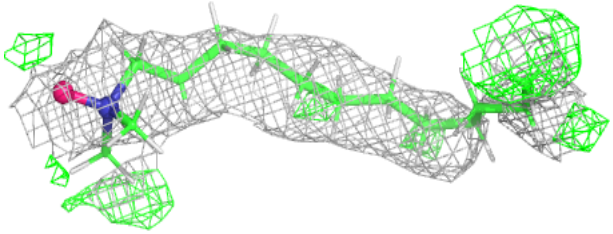


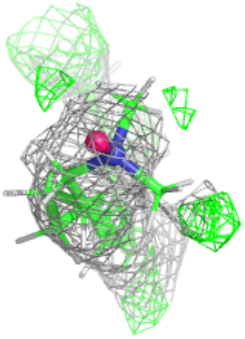


Electron density around LDA H 302:

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

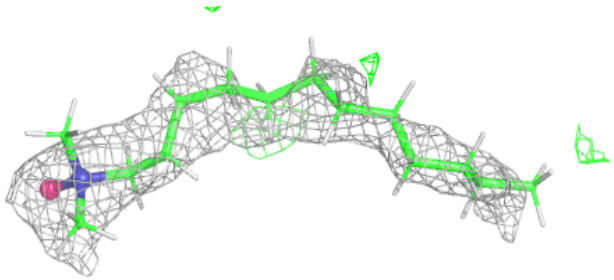


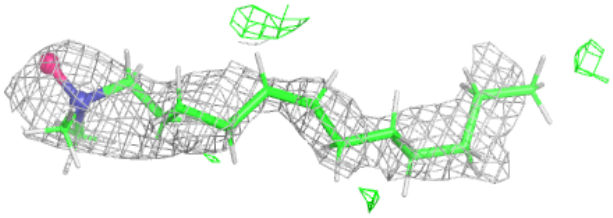


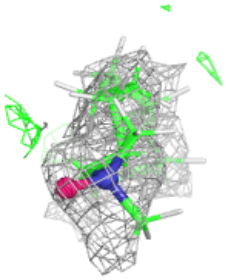


Electron density around LDA M 410:

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

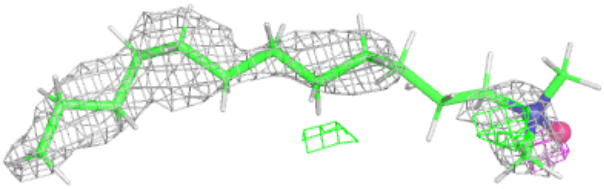


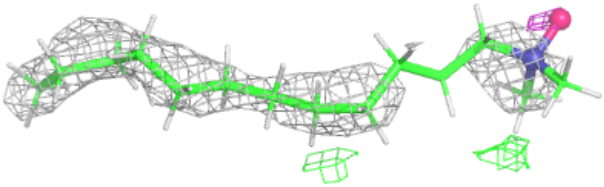


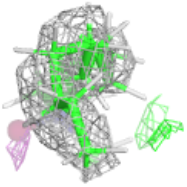


Electron density around LDA M 412:

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

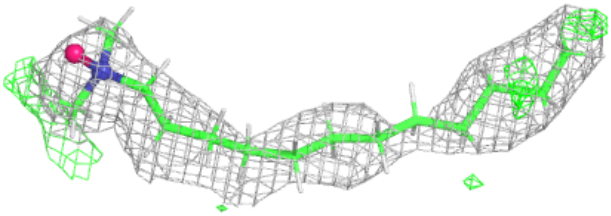


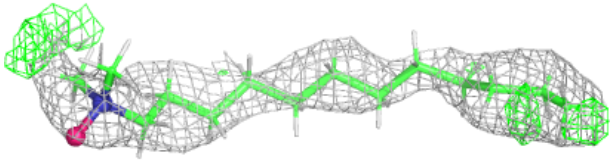


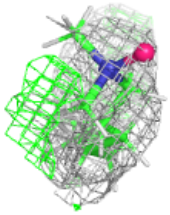


Electron density around LDA M 405:

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

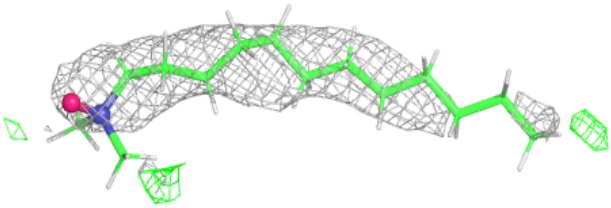


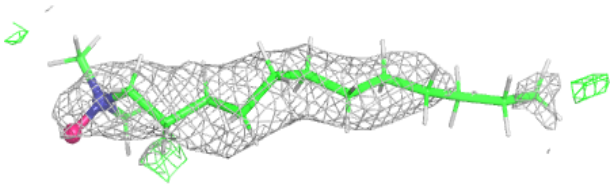


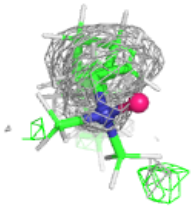


Electron density around LDA M 411:

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

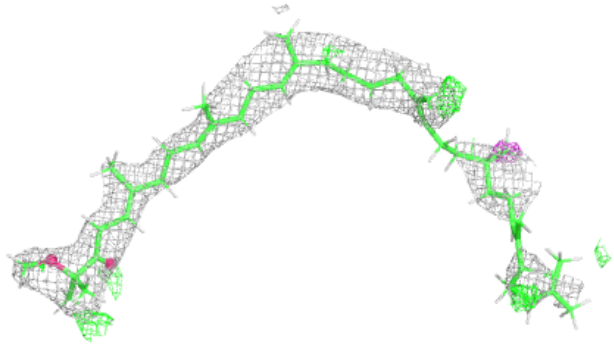


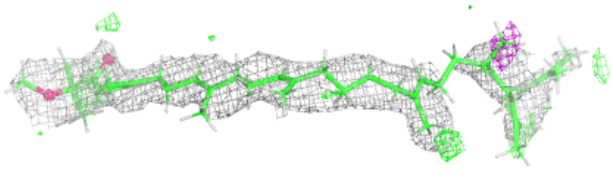


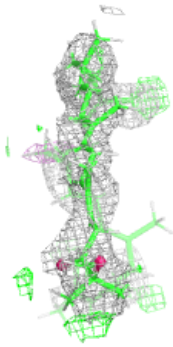


Electron density around SPN M 409 (A):

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

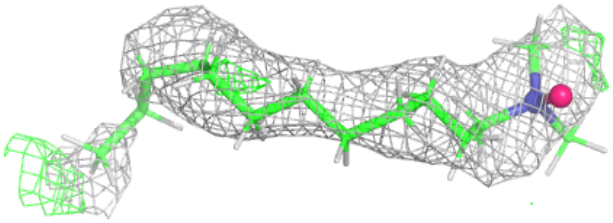


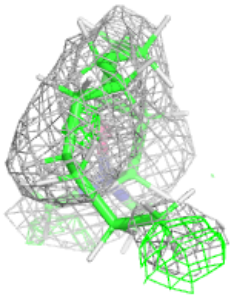




Electron density around LDA L 306:

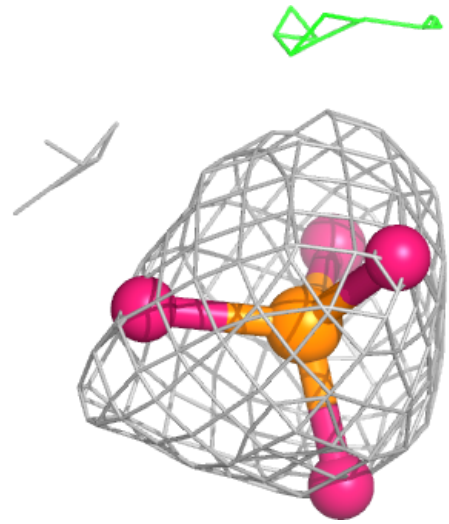
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

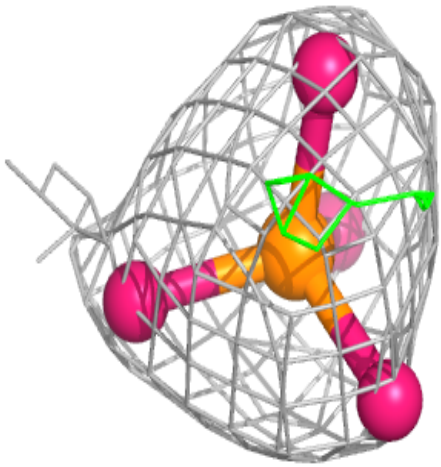


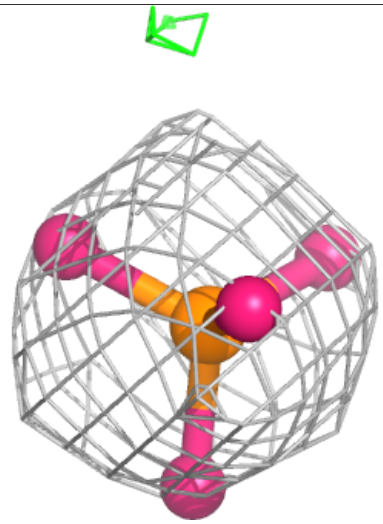


Electron density around PO4 M 413:

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

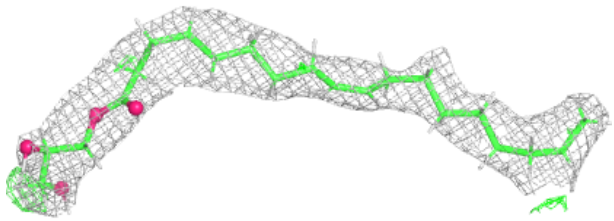


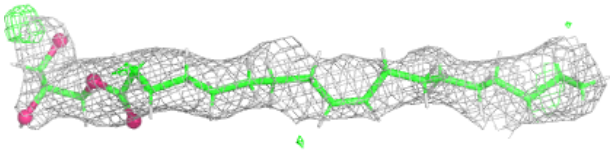


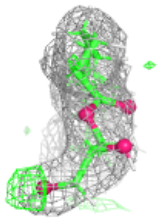


Electron density around OLC M 408 (B):

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

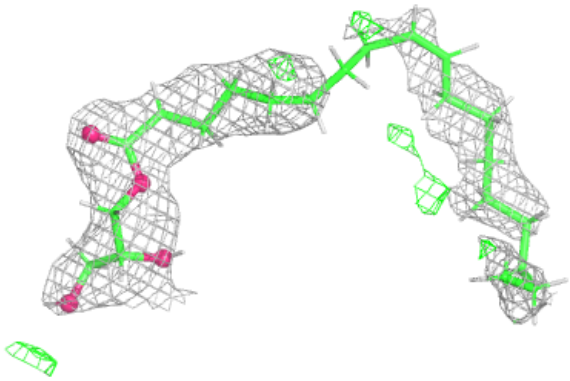


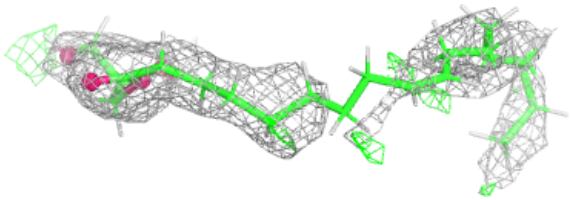


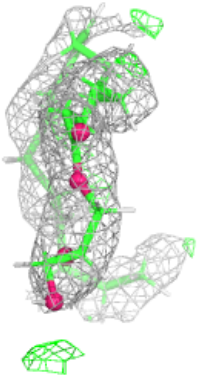


Electron density around OLC L 305:

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

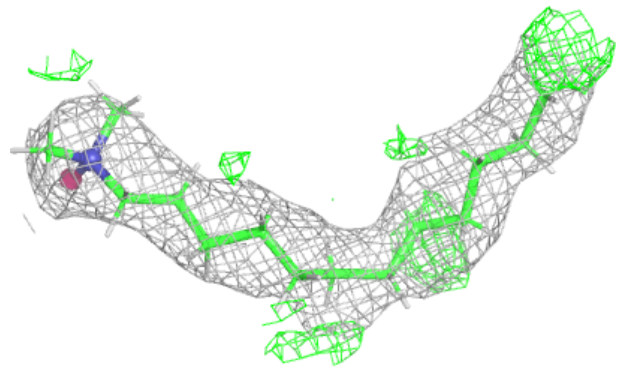


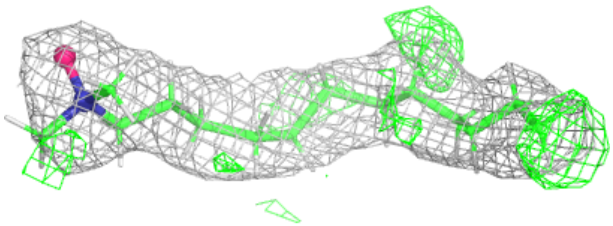


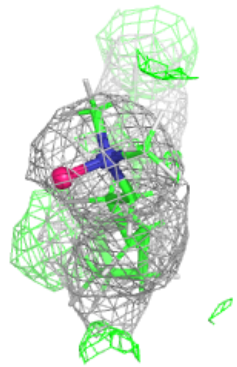


Electron density around LDA M 406:

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

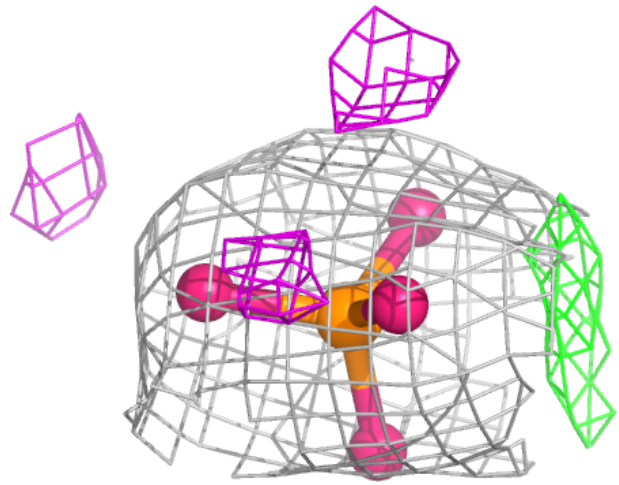


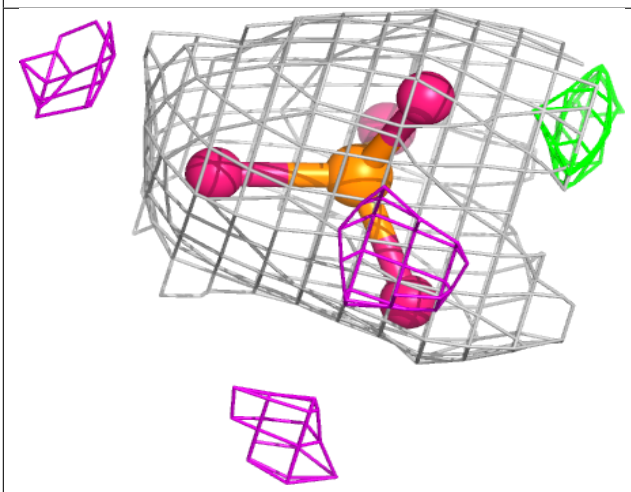


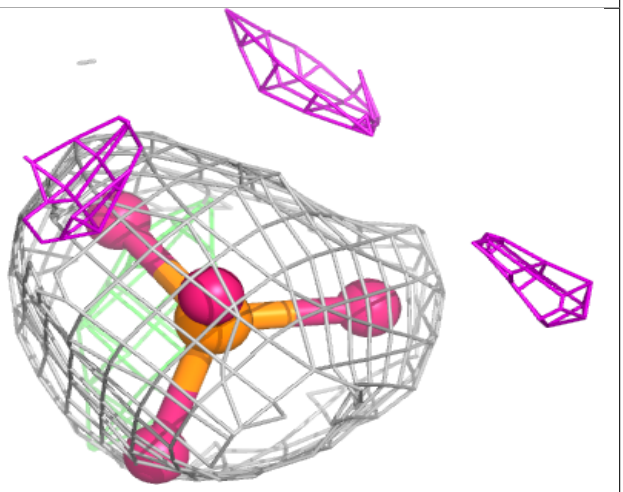


Electron density around PO4 M 407:

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

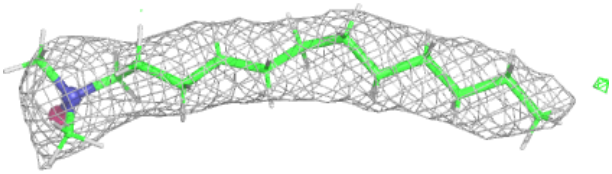


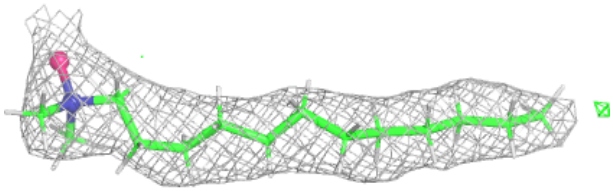


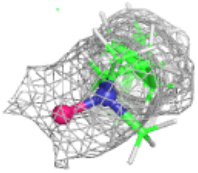


Electron density around LDA H 301:

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

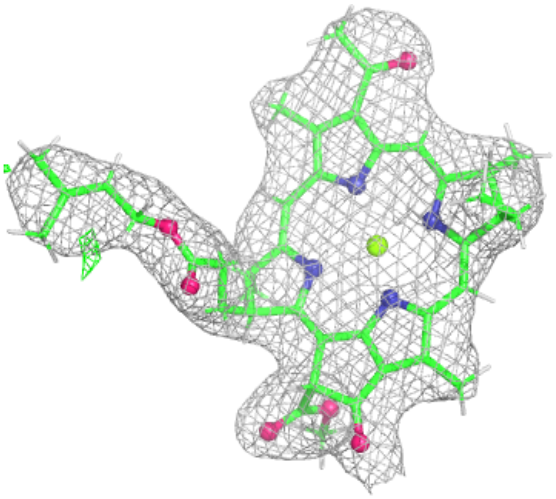


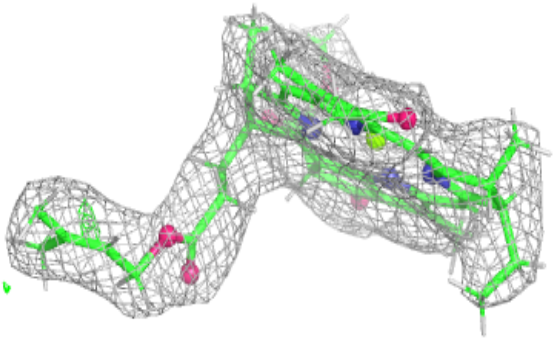


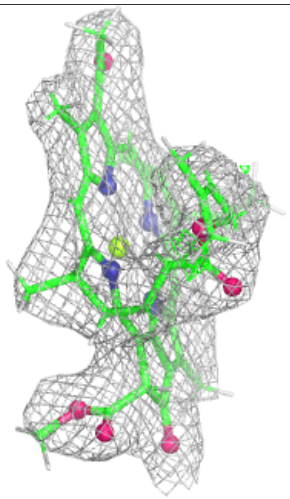


Electron density around BCL M 403:

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

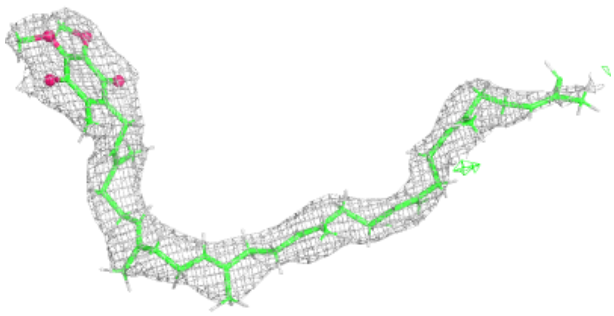


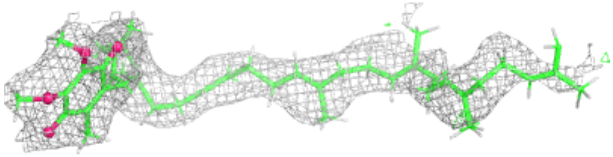




Electron density around UQ7 M 401:

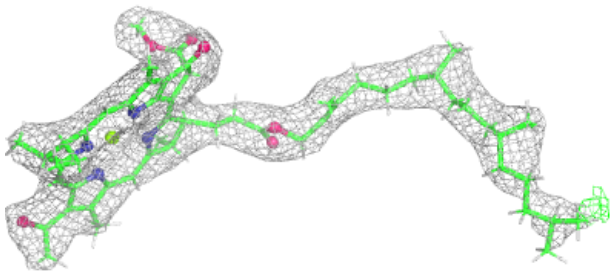
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

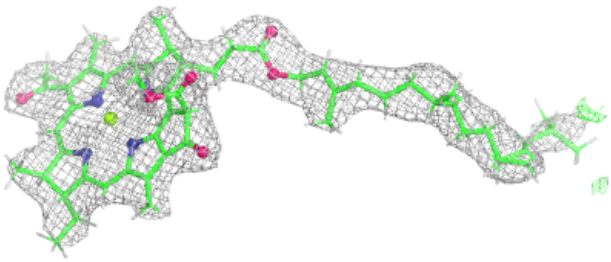


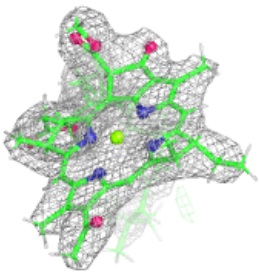


Electron density around BCL M 402:

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

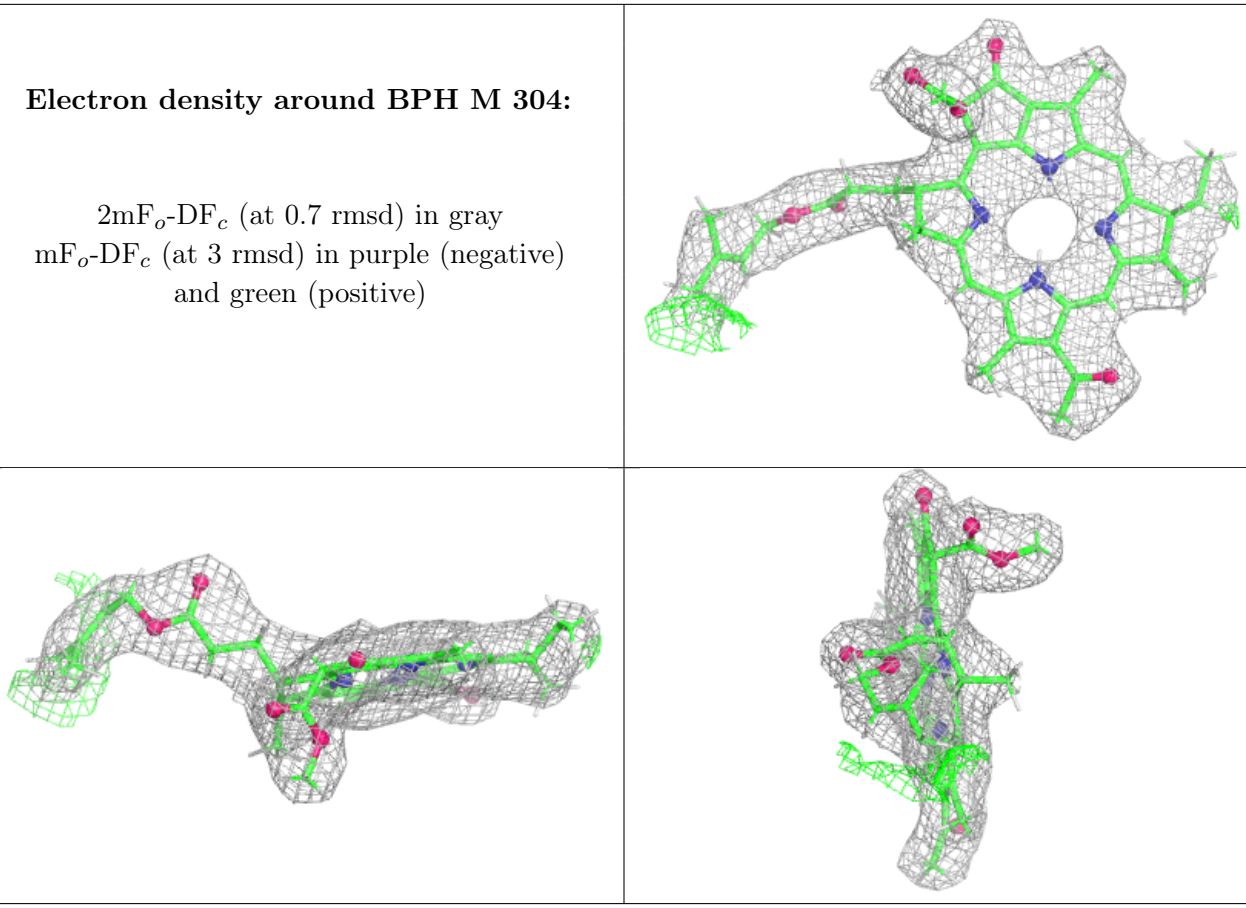






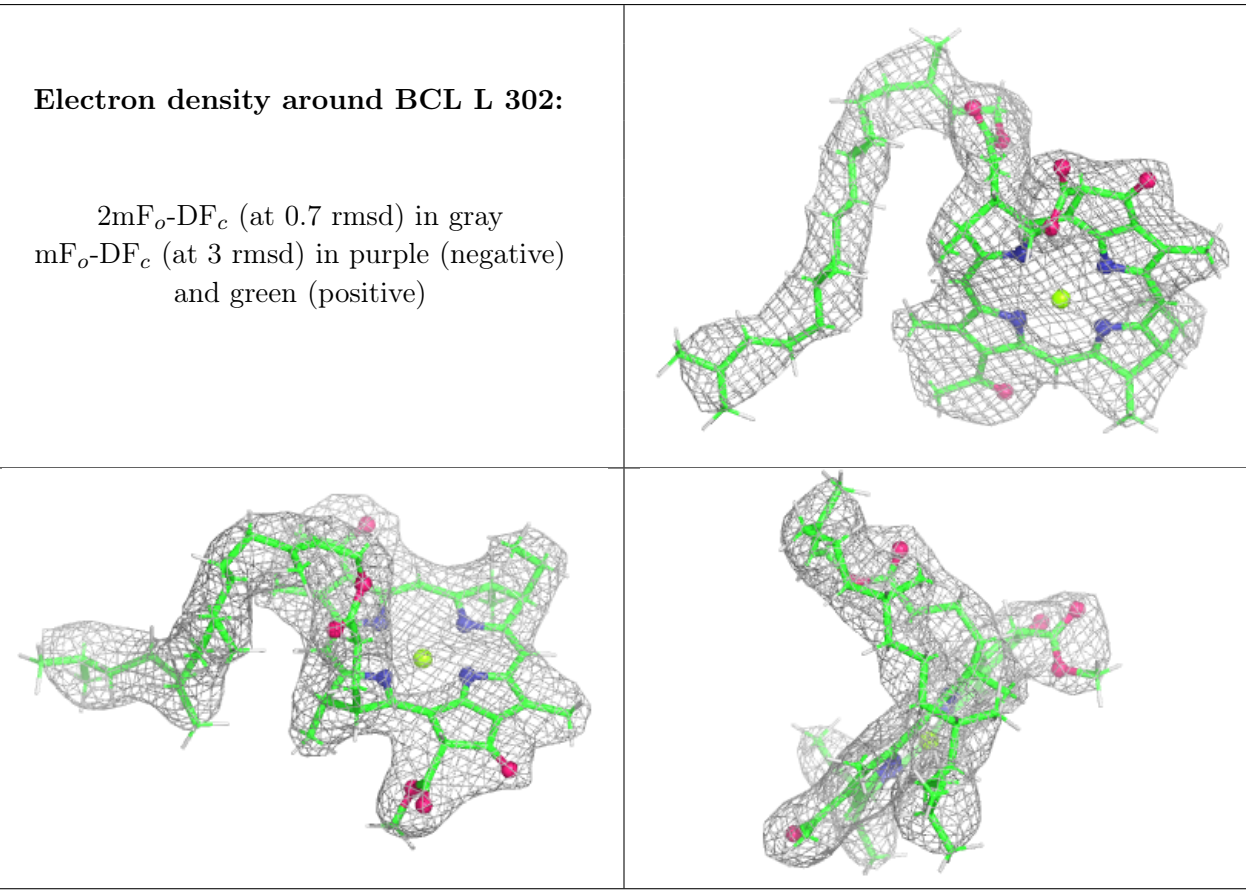
Electron density around BPH M 304:

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



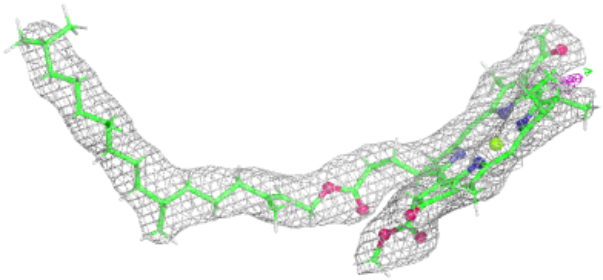
Electron density around BCL L 302:

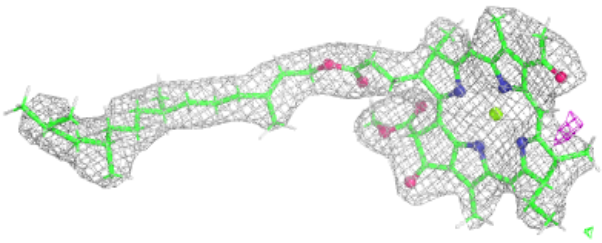
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

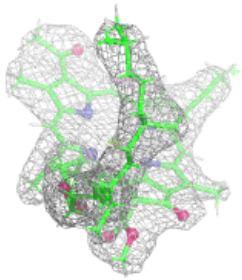


Electron density around BCL L 303:

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

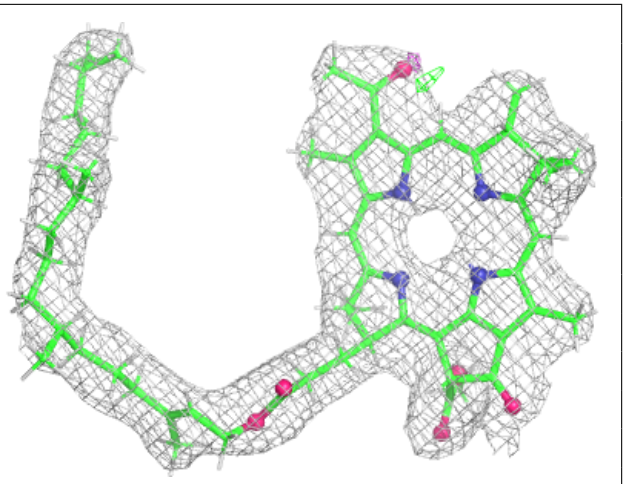


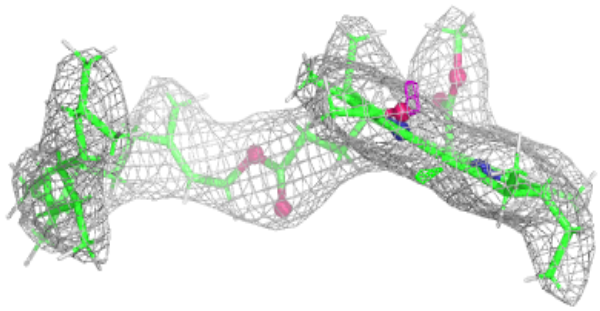


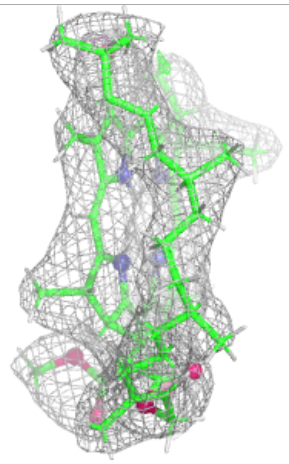


Electron density around BPH L 301:

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

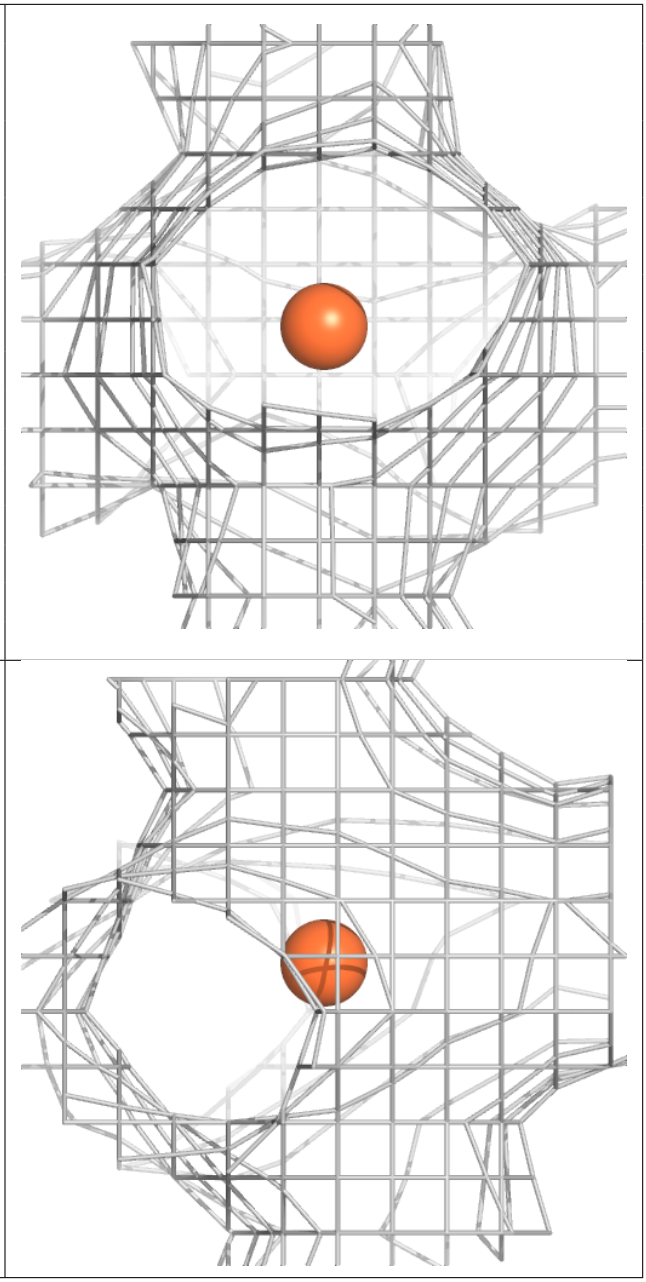






Electron density around FE M 404:

$2mF_o$-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 (i)

There are no such residues in this entry.