wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 02:18 PM EST

PDB ID	:	8VTK
Title	:	Crystal structure of R.sphaeroides Photosynthetic Reaction Center variant Y (M210)2-chlorophenylalanine
Authors	:	Tran, K.; Mathews, I.; Boxer, S.G.
Deposited on	:	2024-01-26
Resolution	:	3.07 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:

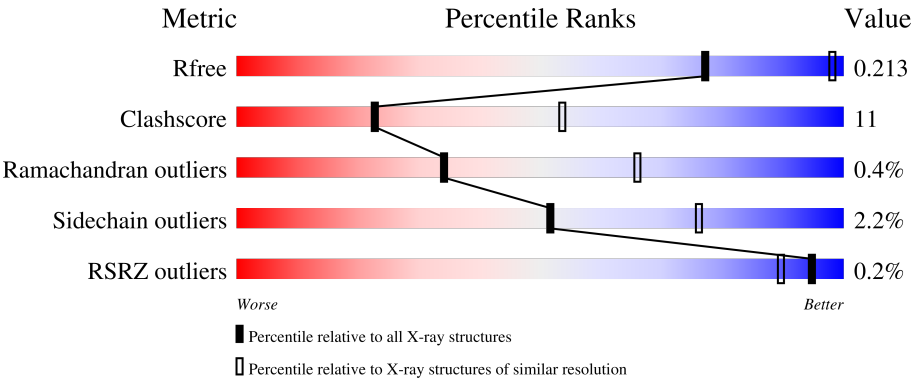
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	240	81% 18%
2	L	281	% 78% 22%
3	M	301	77% 22%

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
11	CDL	M	405	X	-	-	-
7	U10	L	305	-	-	-	X
8	CL	L	307	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 7024 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2248	1517	357	366	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	M	301	Total	C	Cl	N	O	S	0	0	0
			2396	1598	1	392	395	10			

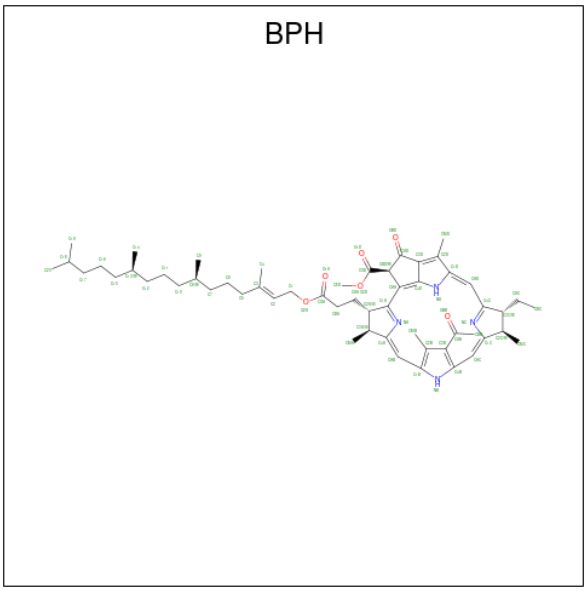
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	210	2L5	TYR	conflict	UNP P0C0Y9
M	252	VAL	TRP	conflict	UNP P0C0Y9

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

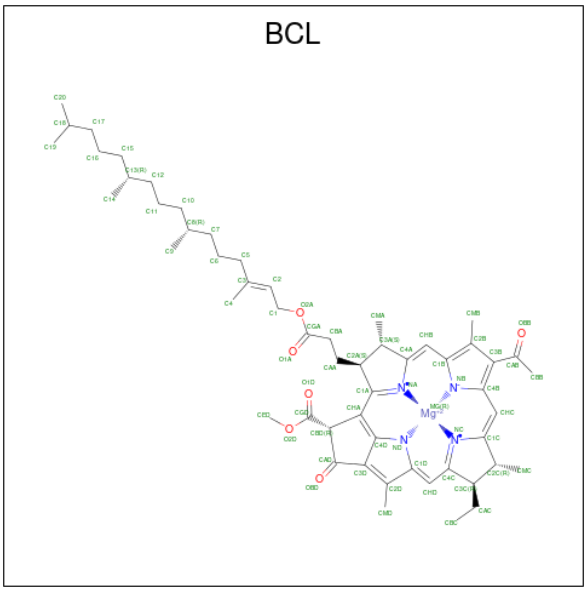
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Fe	0	0
			1	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			55	45	4	6		
5	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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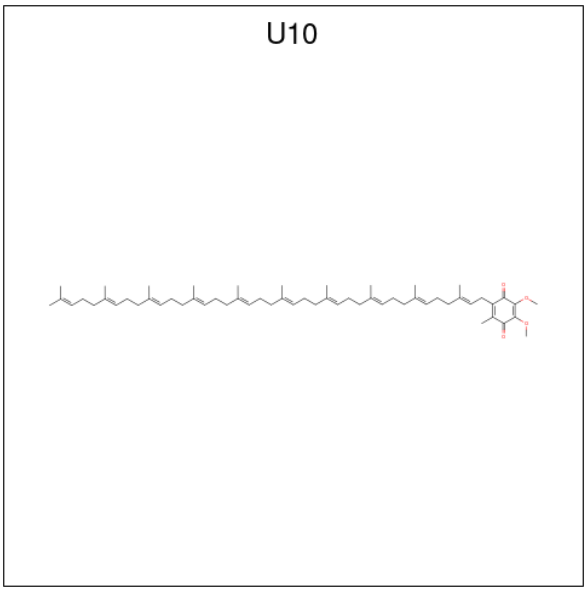
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

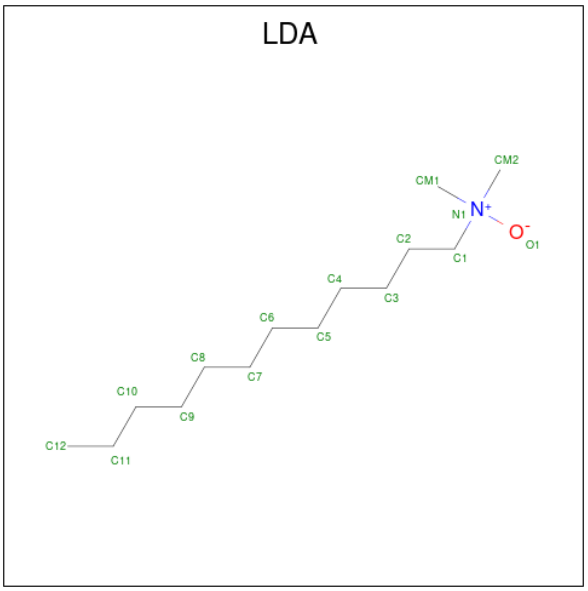


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

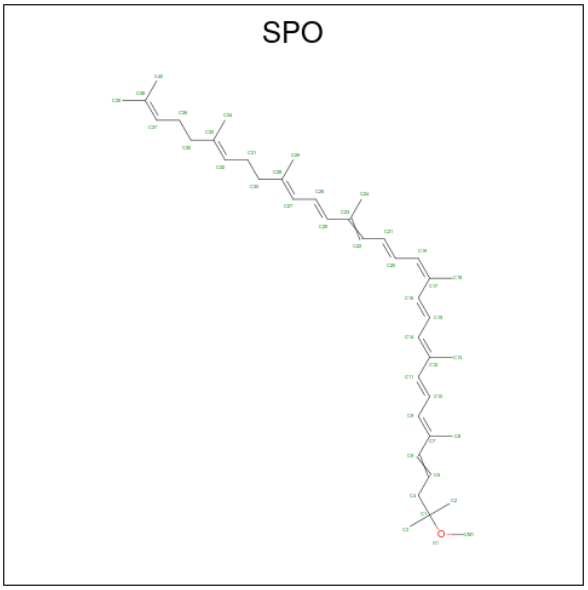
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total	Cl	0	0
			1	1		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



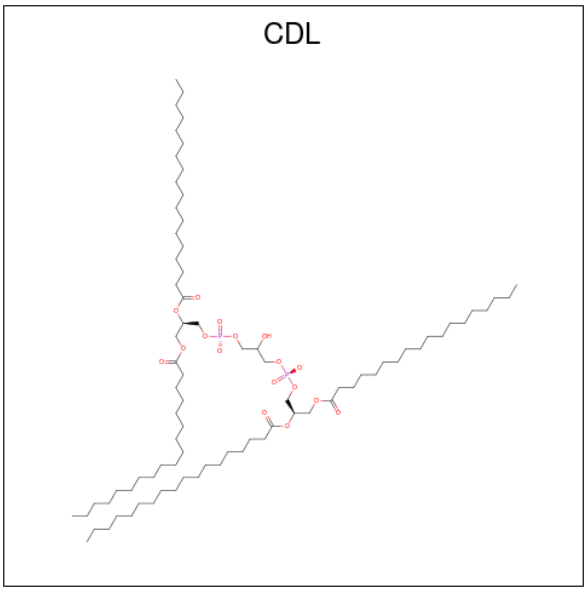
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			69	50	17	2		

- Molecule 12 is water.

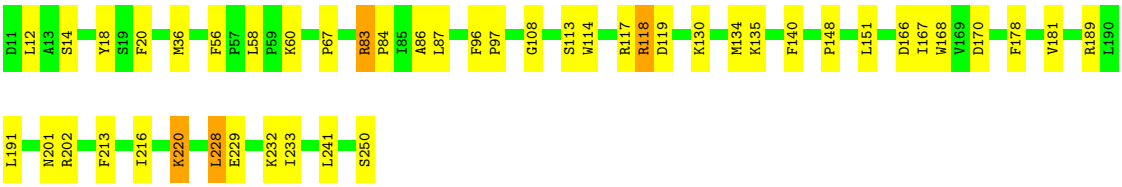
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	5	Total	O	0	0
			5	5		
12	L	4	Total	O	0	0
			4	4		
12	M	10	Total	O	0	0
			10	10		

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.

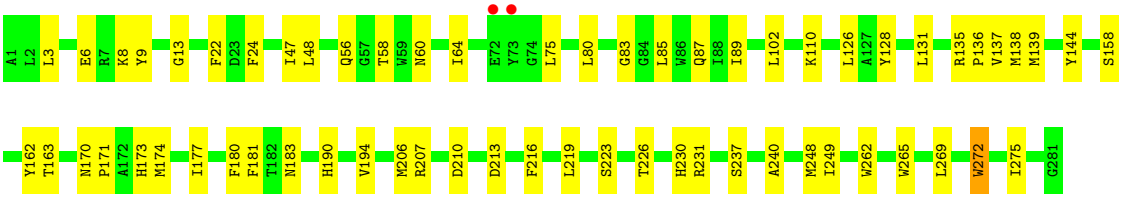
• Molecule 1: Reaction center protein H chain

Chain H:



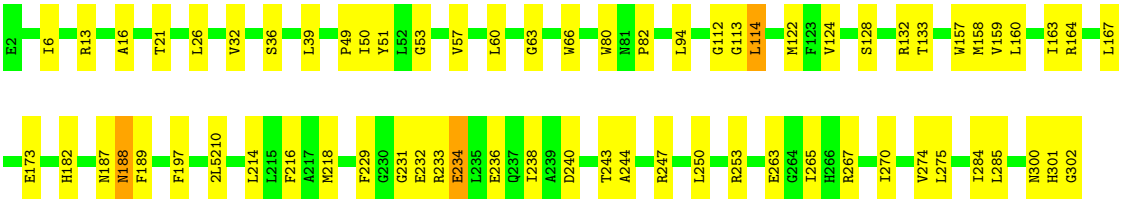
• Molecule 2: Reaction center protein L chain

Chain L:



• Molecule 3: Reaction center protein M chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.95Å 140.95Å 186.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.76 – 3.07 39.76 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.76-3.07) 91.1 (39.76-3.07)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.177 , 0.213 0.181 , 0.213	Depositor DCC
R_{free} test set	2036 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: SPO, 2L5, CDL, FE, BCL, CL, LDA, U10, 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	0.60	0/1877	0.73	0/2553
2	L	0.60	0/2336	0.68	0/3197
3	M	0.59	0/2472	0.70	1/3372 (0.0%)
All	All	0.60	0/6685	0.70	1/9122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	234	GLU	OE1-CD-OE2	-7.75	114.00	123.30

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	1829	0	1836	49	0
2	L	2248	0	2200	45	0
3	M	2396	0	2307	55	0
4	L	1	0	0	0	0
5	L	120	0	129	12	0
6	L	132	0	148	10	0
6	M	117	0	115	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	18	0	15	3	0
8	L	1	0	0	2	0
9	M	32	0	62	3	0
10	M	42	0	60	1	0
11	M	69	0	82	3	0
12	H	5	0	0	0	0
12	L	4	0	0	1	0
12	M	10	0	0	1	0
All	All	7024	0	6954	160	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 11.

The worst 5 of 160 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:119:ASP:OD2	1:H:220:LYS:NZ	1.68	1.26
2:L:230:HIS:NE2	3:M:234:GLU:OE2	1.72	1.22
1:H:83:ARG:NH2	1:H:108:GLY:O	1.75	1.19
1:H:229:GLU:O	1:H:233:ILE:HD12	1.59	1.02
1:H:117:ARG:O	1:H:228:LEU:HD12	1.62	0.99

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	238/240 (99%)	228 (96%)	10 (4%)	0	100 100
2	L	281/281 (100%)	271 (96%)	10 (4%)	0	100 100
3	M	298/301 (99%)	280 (94%)	15 (5%)	3 (1%)	15 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	817/822 (99%)	779 (95%)	35 (4%)	3 (0%)	34 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	113	GLY
3	M	301	HIS
3	M	232	GLU

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	195/195 (100%)	189 (97%)	6 (3%)	40 69
2	L	222/220 (101%)	217 (98%)	5 (2%)	50 75
3	M	235/235 (100%)	231 (98%)	4 (2%)	60 82
All	All	652/650 (100%)	637 (98%)	15 (2%)	52 75

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

Mol	Chain	Res	Type
2	L	126[B]	LEU
3	M	188	ASN
2	L	207	ARG
3	M	216	PHE
3	M	114	LEU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	2L5	M	210	3	11,12,13	0.92	1 (9%)	11,15,17	0.53	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
3	2L5	M	210	3	-	2/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	210	2L5	O-C	2.99	1.31	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	2L5	CA-C13-C14-C15
3	M	210	2L5	CA-C13-C14-C16

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
6	BCL	M	406	-	49,59,74	1.93	11 (22%)	60,97,115	1.84	15 (25%)
6	BCL	L	306	-	64,74,74	1.44	7 (10%)	78,115,115	1.59	13 (16%)
9	LDA	M	402	-	12,15,15	2.05	1 (8%)	14,17,17	0.53	0
11	CDL	M	405	-	68,68,99	1.26	11 (16%)	74,80,111	1.01	6 (8%)
5	BPH	L	304	-	51,70,70	0.98	1 (1%)	52,101,101	1.36	8 (15%)
6	BCL	M	401	-	64,74,74	1.42	7 (10%)	78,115,115	1.52	11 (14%)
7	U10	L	305	-	18,18,63	2.45	7 (38%)	22,25,79	1.66	4 (18%)
9	LDA	M	403	-	12,15,15	1.92	1 (8%)	14,17,17	0.71	0
10	SPO	M	404	-	40,41,41	0.56	1 (2%)	47,50,50	0.71	1 (2%)
5	BPH	L	302	-	41,60,70	0.95	2 (4%)	40,89,101	1.72	9 (22%)
6	BCL	L	303	-	64,74,74	1.65	11 (17%)	78,115,115	1.62	15 (19%)

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
6	BCL	M	406	-	-	1/19/119/137	-
6	BCL	L	306	-	-	4/37/137/137	-
11	CDL	M	405	-	1/1/9/9	33/79/79/110	-
9	LDA	M	402	-	-	6/13/13/13	-
5	BPH	L	304	-	-	5/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	M	401	-	-	1/37/137/137	-
7	U10	L	305	-	-	2/9/33/87	0/1/1/1
9	LDA	M	403	-	-	6/13/13/13	-
10	SPO	M	404	-	-	6/47/47/47	-
5	BPH	L	302	-	-	5/25/93/105	0/5/6/6
6	BCL	L	303	-	-	3/37/137/137	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	402	LDA	O1-N1	-6.98	1.25	1.42
6	M	406	BCL	C1B-NB	6.62	1.41	1.35
9	M	403	LDA	O1-N1	-6.58	1.26	1.42
6	L	303	BCL	C1B-NB	5.62	1.40	1.35
6	M	401	BCL	C1B-NB	5.46	1.40	1.35

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	302	BPH	C1-C2-C3	-5.72	116.15	126.04
6	M	406	BCL	CHD-C1D-ND	-5.66	119.26	124.45
6	M	401	BCL	CHD-C1D-ND	-5.19	119.68	124.45
6	L	303	BCL	CHD-C1D-ND	-5.04	119.82	124.45
6	L	306	BCL	CHD-C1D-ND	-4.97	119.89	124.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	405	CDL	CA4

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	403	LDA	C2-C1-N1-O1
9	M	403	LDA	C2-C1-N1-CM1
11	M	405	CDL	CA3-OA5-PA1-OA4
11	M	405	CDL	CB2-OB2-PB2-OB4
11	M	405	CDL	CB3-OB5-PB2-OB3

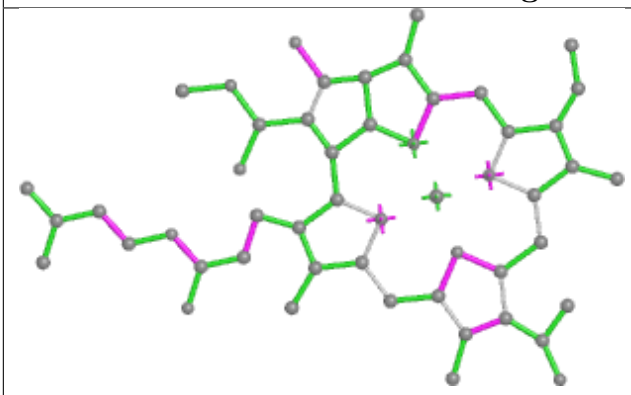
There are no ring outliers.

11 monomers are involved in 37 short contacts:

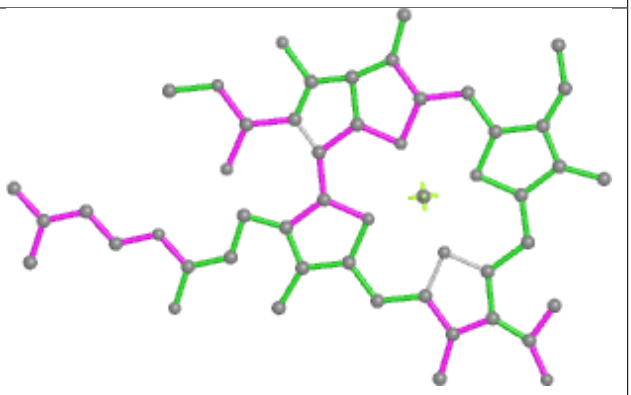
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	406	BCL	3	0
6	L	306	BCL	7	0
9	M	402	LDA	2	0
11	M	405	CDL	3	0
5	L	304	BPH	3	0
6	M	401	BCL	9	0
7	L	305	U10	3	0
9	M	403	LDA	1	0
10	M	404	SPO	1	0
5	L	302	BPH	9	0
6	L	303	BCL	4	0

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.

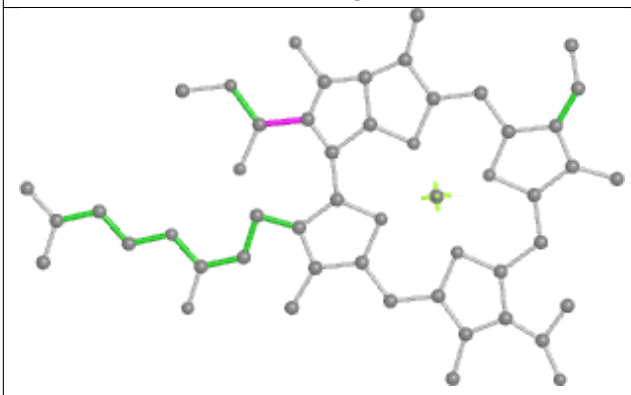
Ligand BCL M 406



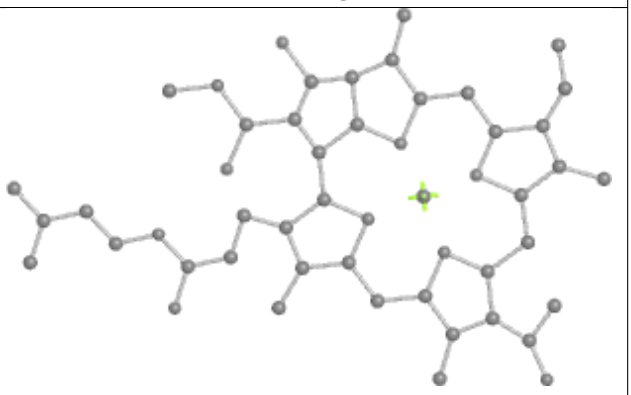
Bond lengths



Bond angles

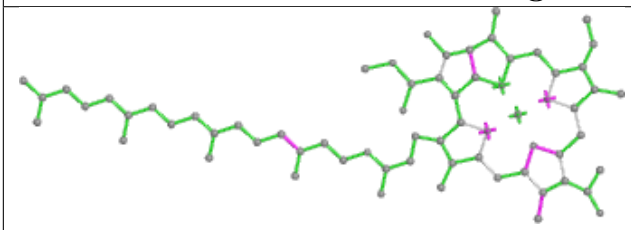


Torsions

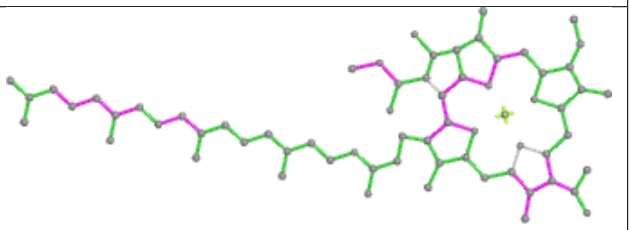


Rings

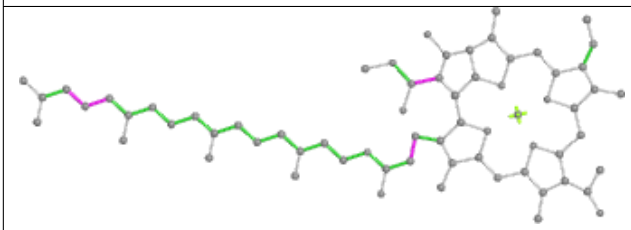
Ligand BCL L 306



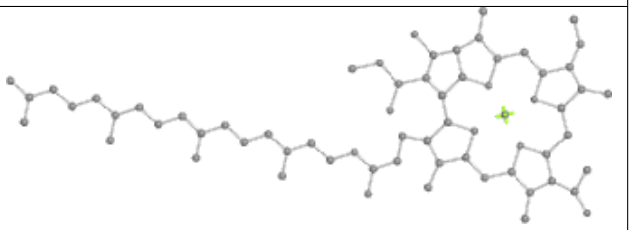
Bond lengths



Bond angles

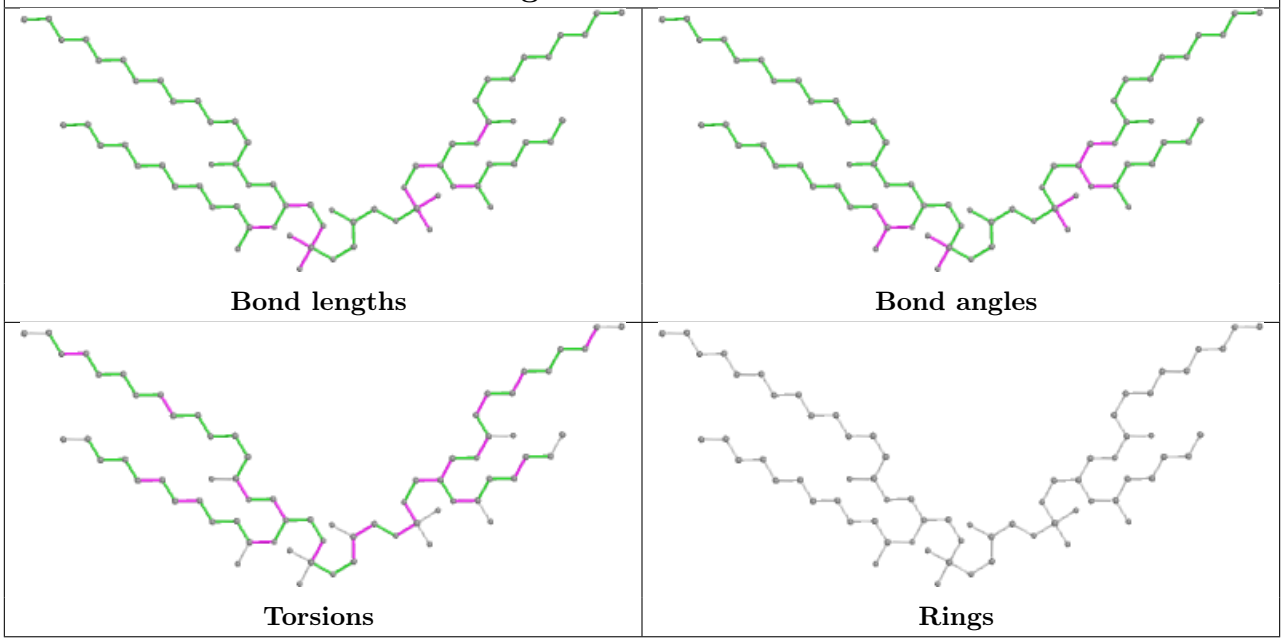


Torsions

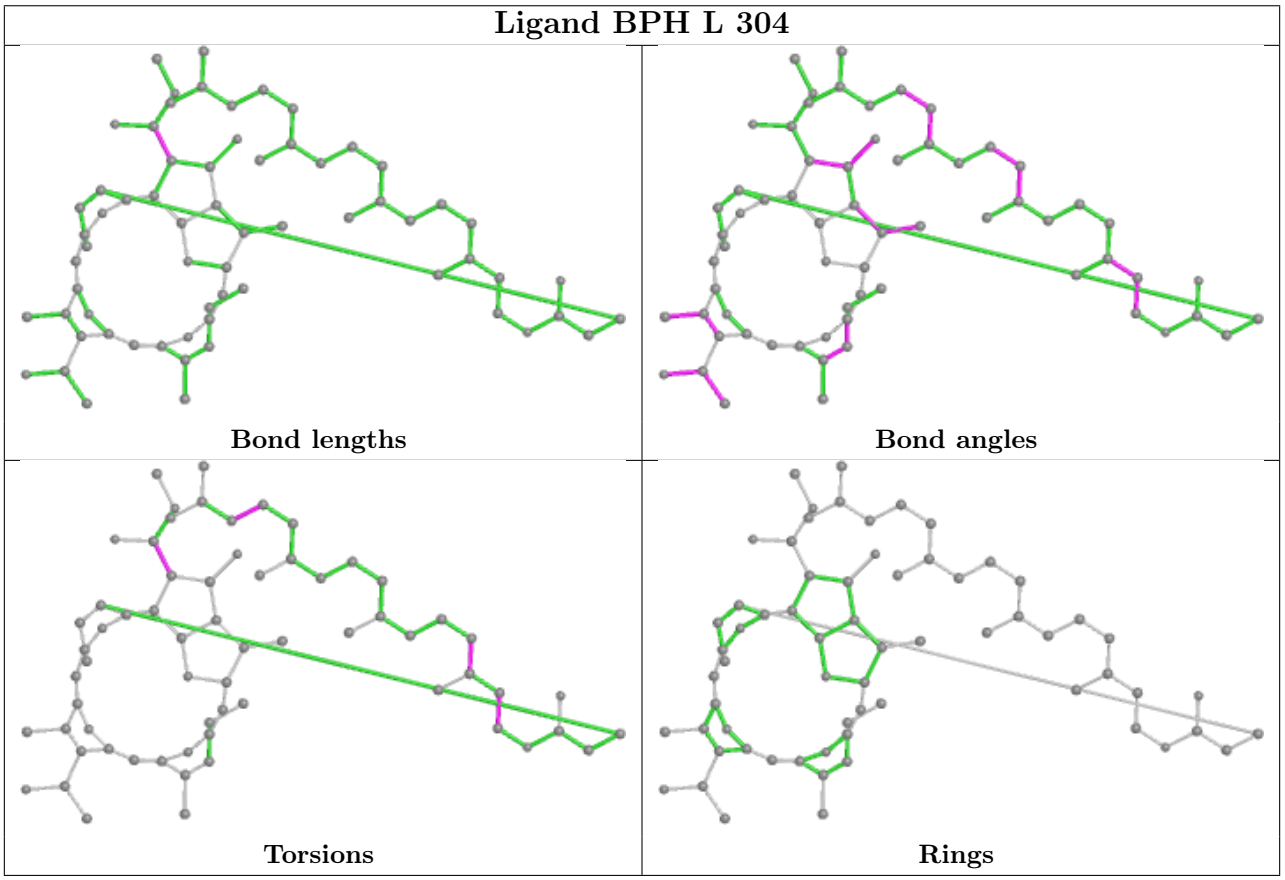


Rings

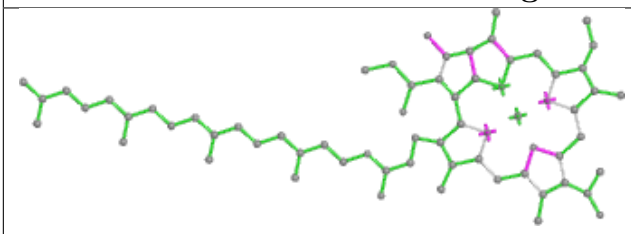
Ligand CDL M 405



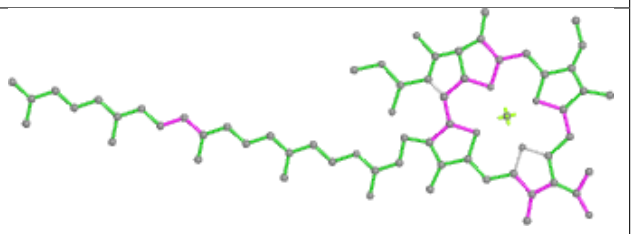
Ligand BPH L 304



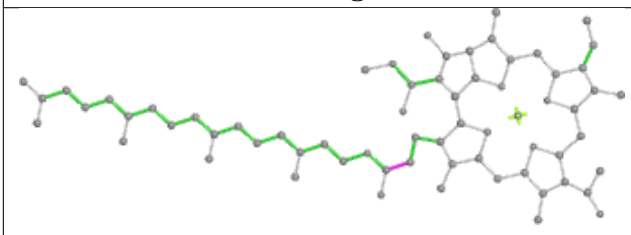
Ligand BCL M 401



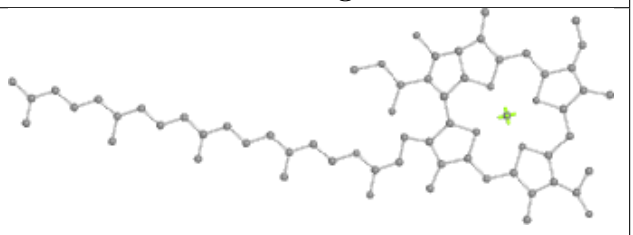
Bond lengths



Bond angles

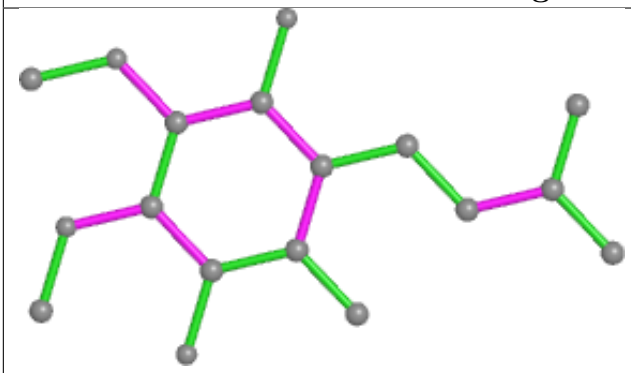


Torsions

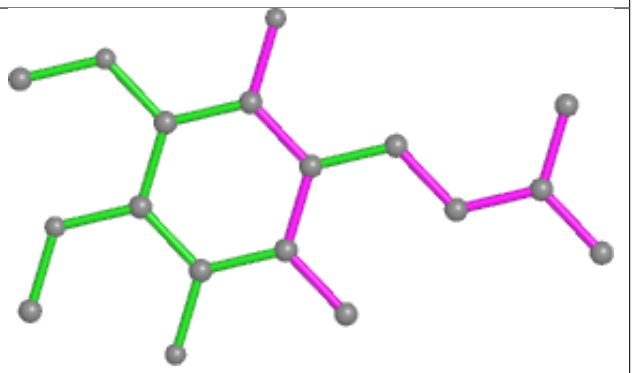


Rings

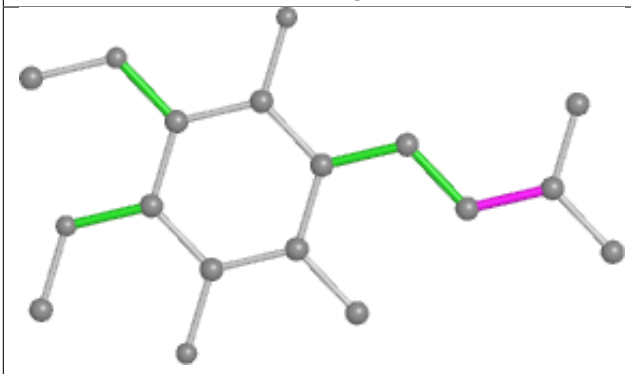
Ligand U10 L 305



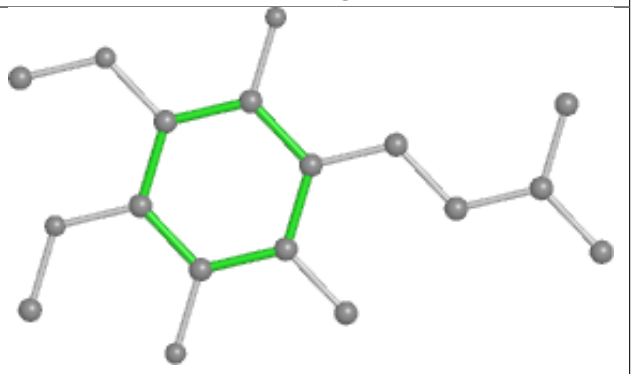
Bond lengths



Bond angles

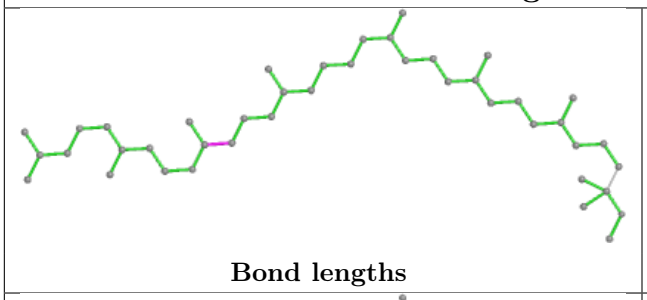


Torsions

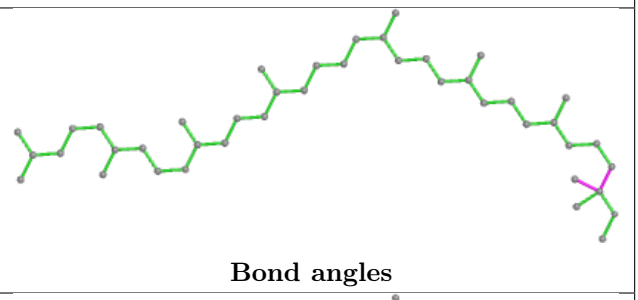


Rings

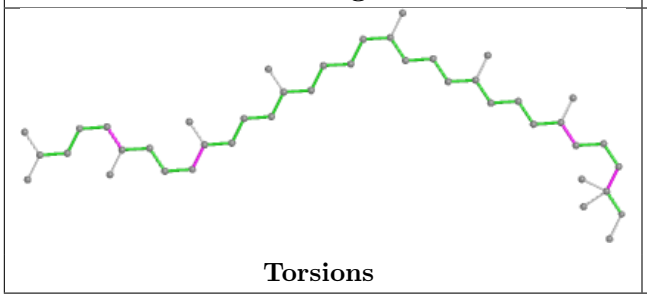
Ligand SPO M 404



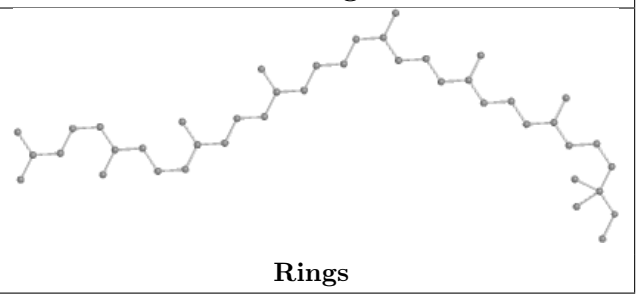
Bond lengths



Bond angles

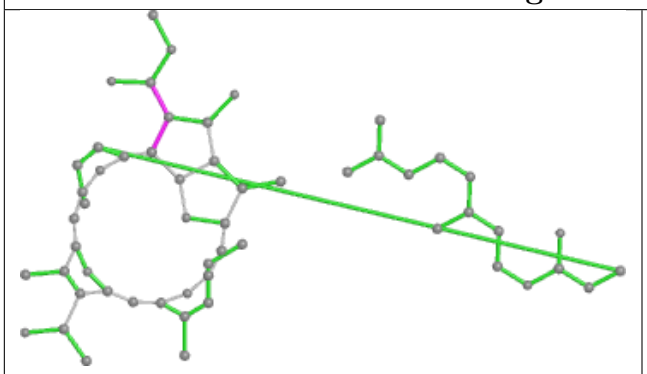


Torsions

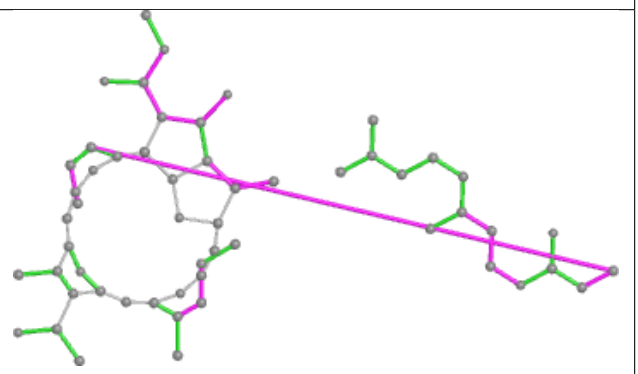


Rings

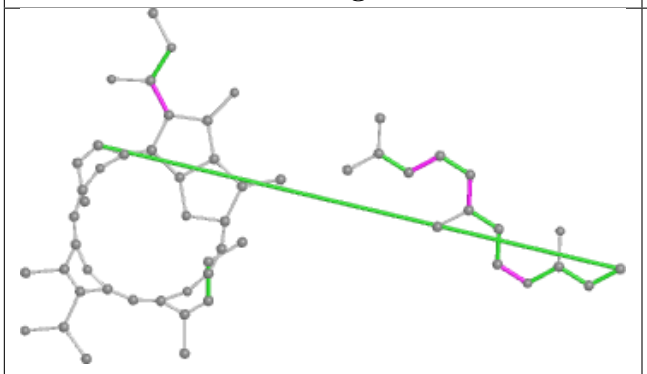
Ligand BPH L 302



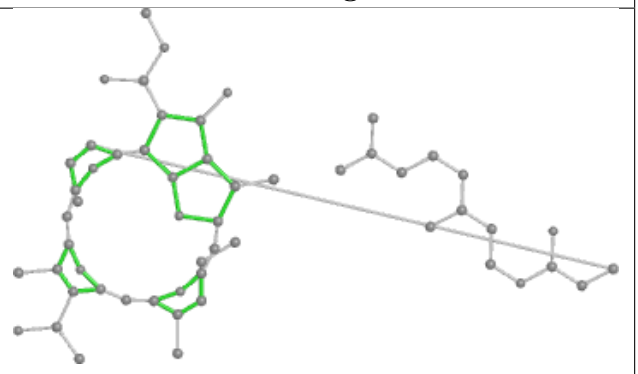
Bond lengths



Bond angles

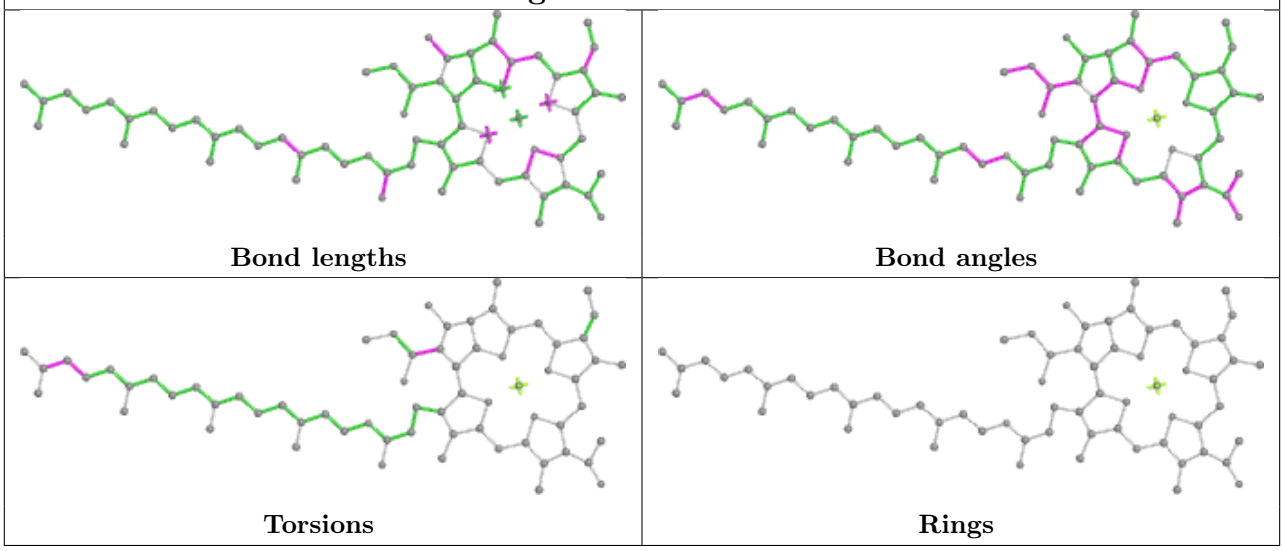


Torsions



Rings

Ligand BCL L 303



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	240/240 (100%)	-0.54	0 100 100	50, 62, 89, 132	0
2	L	281/281 (100%)	-0.71	2 (0%) 87 74	42, 57, 93, 117	0
3	M	300/301 (99%)	-0.75	0 100 100	43, 62, 91, 120	0
All	All	821/822 (99%)	-0.67	2 (0%) 95 89	42, 60, 91, 132	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	72	GLU	2.4
2	L	73	TYR	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2L5	M	210	12/13	0.98	0.13	44,49,52,53	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

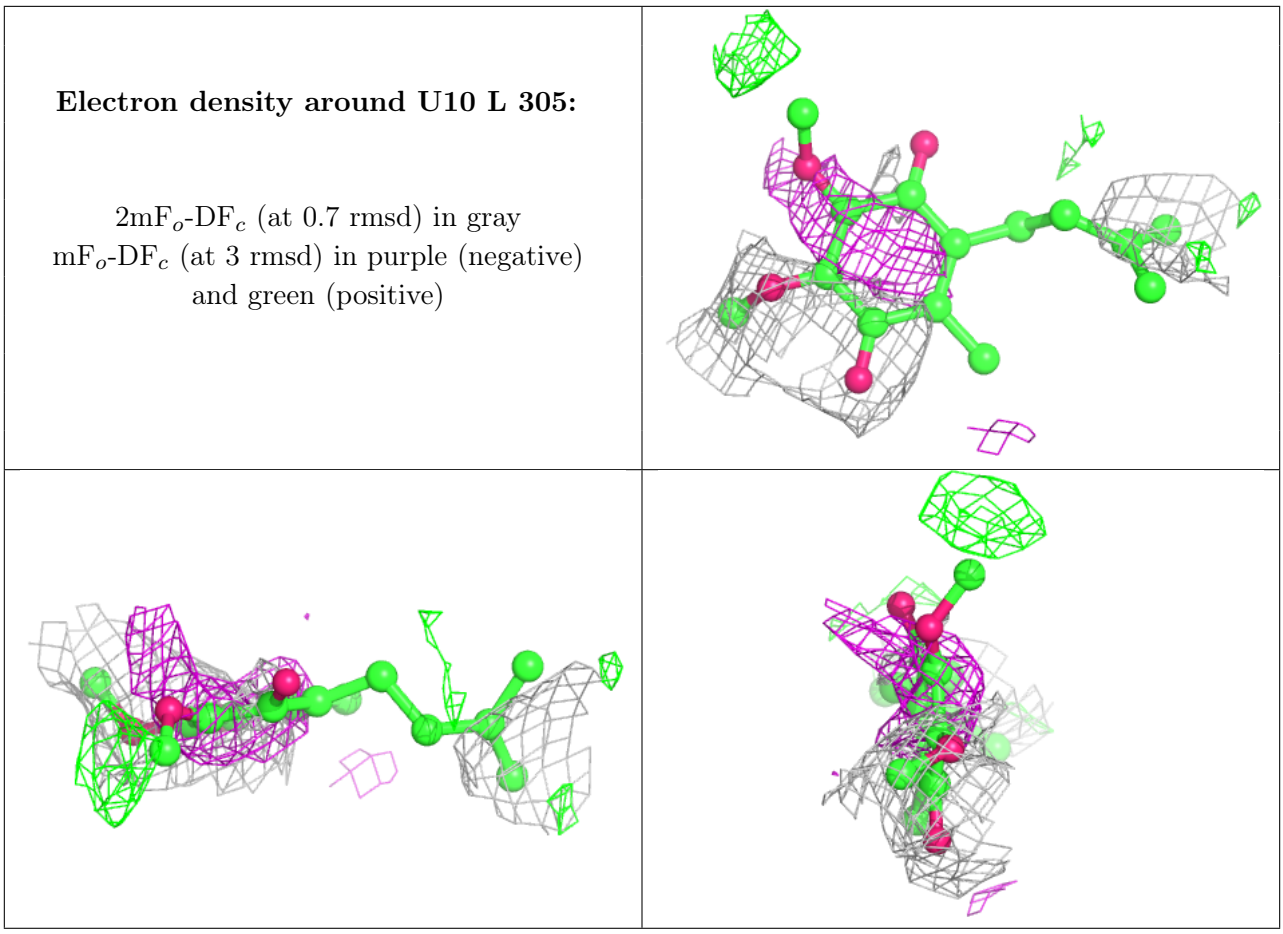
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	U10	L	305	18/63	0.60	0.49	117,136,151,152	0
9	LDA	M	402	16/16	0.85	0.45	82,86,103,105	0
9	LDA	M	403	16/16	0.85	0.27	66,86,111,111	0
8	CL	L	307	1/1	0.86	0.22	109,109,109,109	0
4	FE	L	301	1/1	0.90	0.16	130,130,130,130	0
11	CDL	M	405	69/100	0.90	0.35	64,93,116,123	0
10	SPO	M	404	42/42	0.96	0.29	49,66,82,92	0
5	BPH	L	302	55/65	0.97	0.16	36,54,71,85	0
6	BCL	M	401	66/66	0.97	0.18	36,49,66,83	0
5	BPH	L	304	65/65	0.98	0.14	36,50,59,64	0
6	BCL	M	406	51/66	0.98	0.15	41,50,66,71	0
6	BCL	L	303	66/66	0.98	0.14	42,49,66,68	0
6	BCL	L	306	66/66	0.98	0.16	42,50,59,66	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.

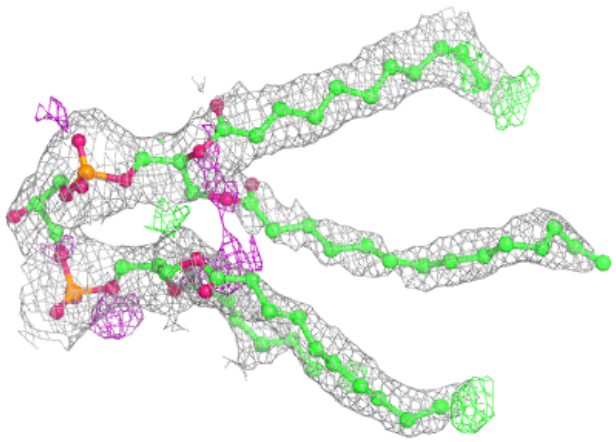
Electron density around U10 L 305:

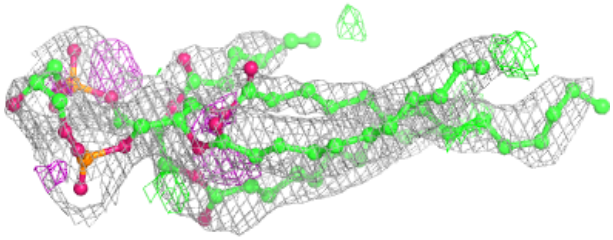
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

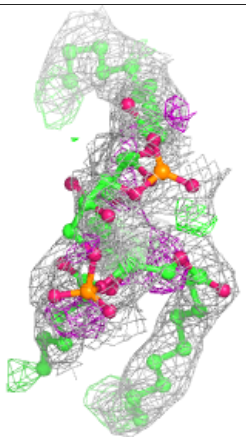


Electron density around CDL M 405:

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

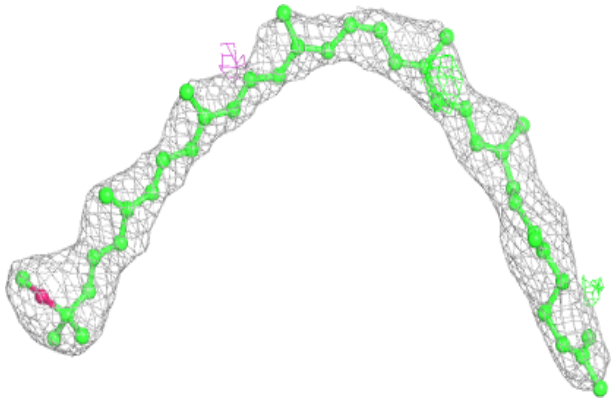


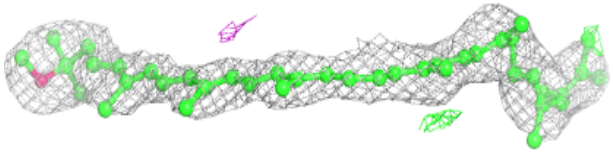


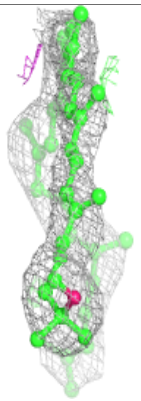


Electron density around SPO M 404:

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

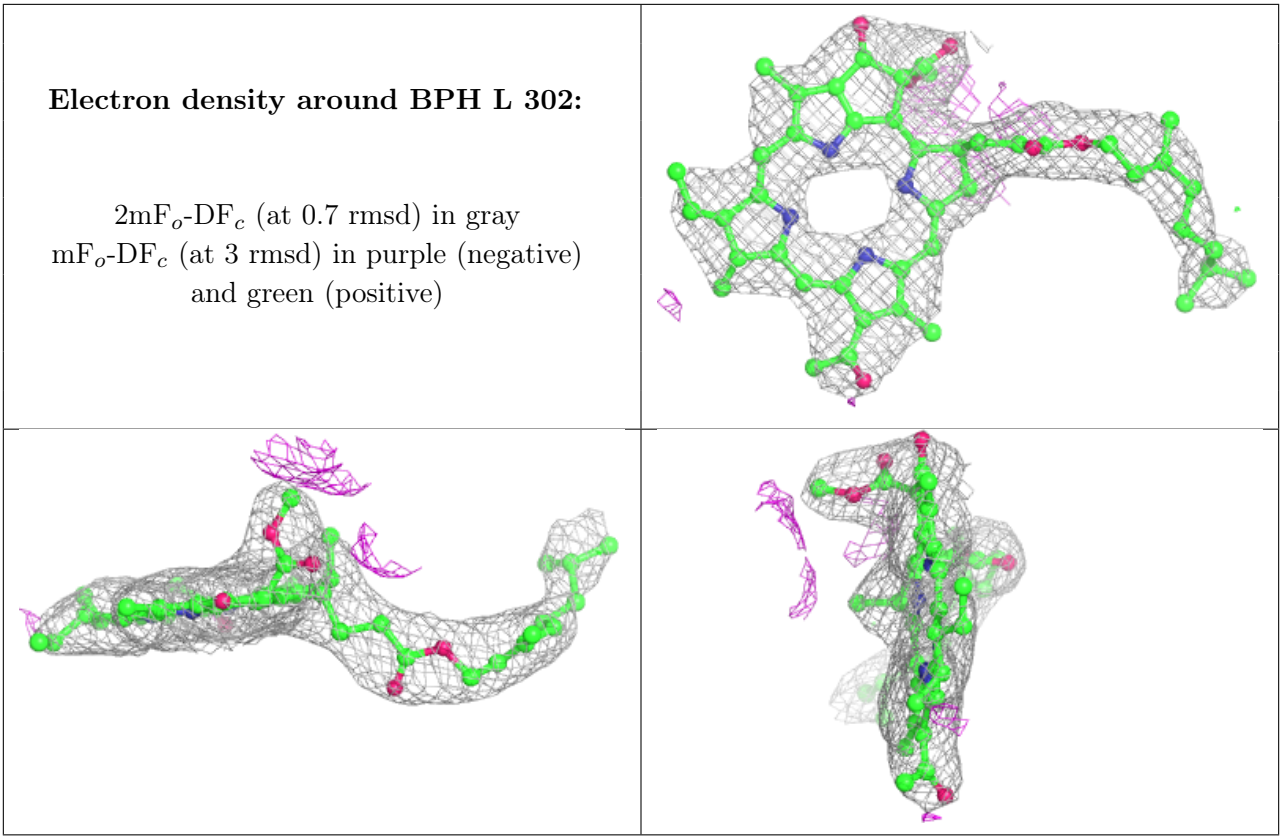






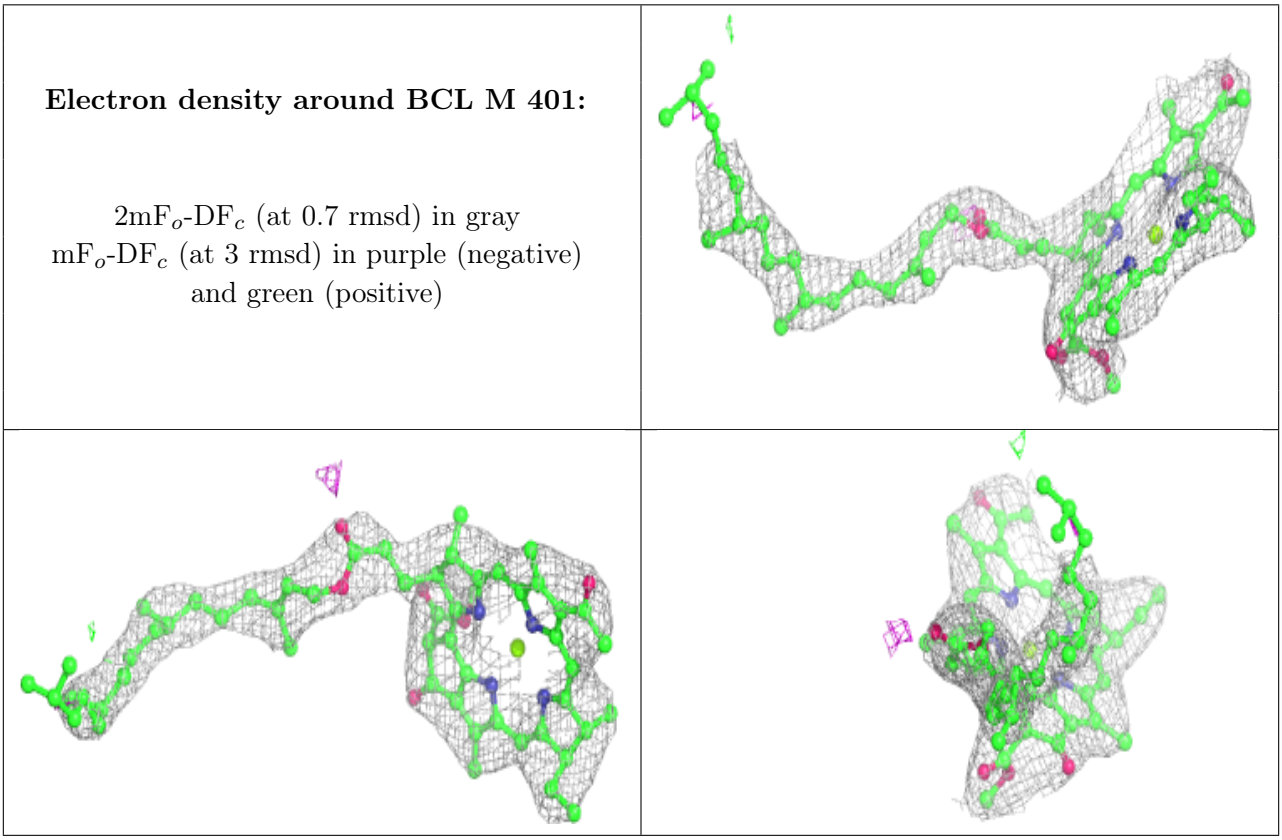
Electron density around BPH L 302:

$2mF_o$-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 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 L 304:

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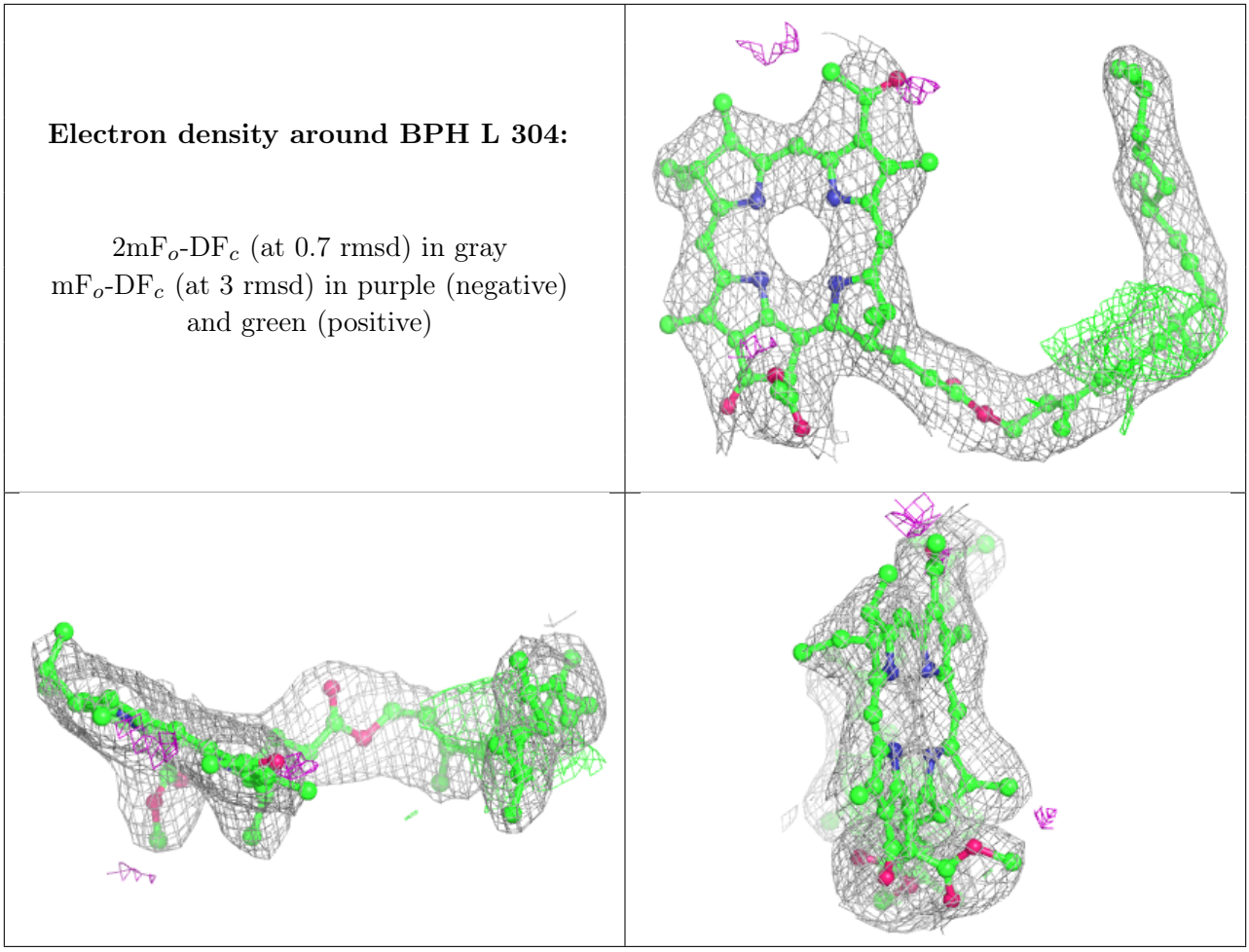
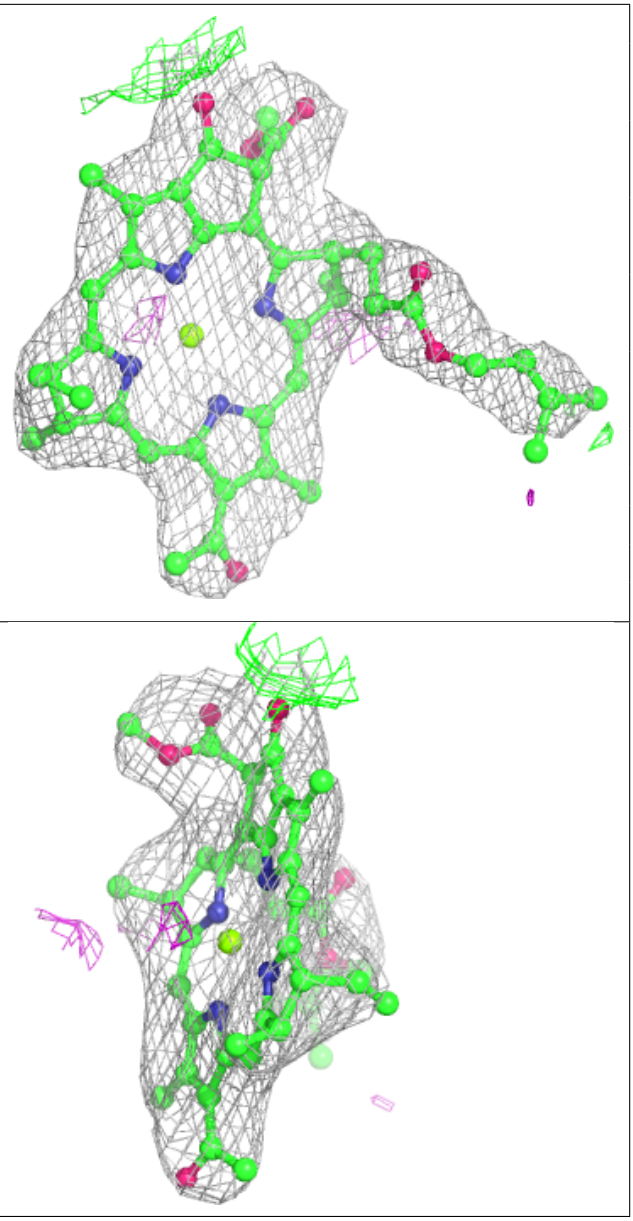
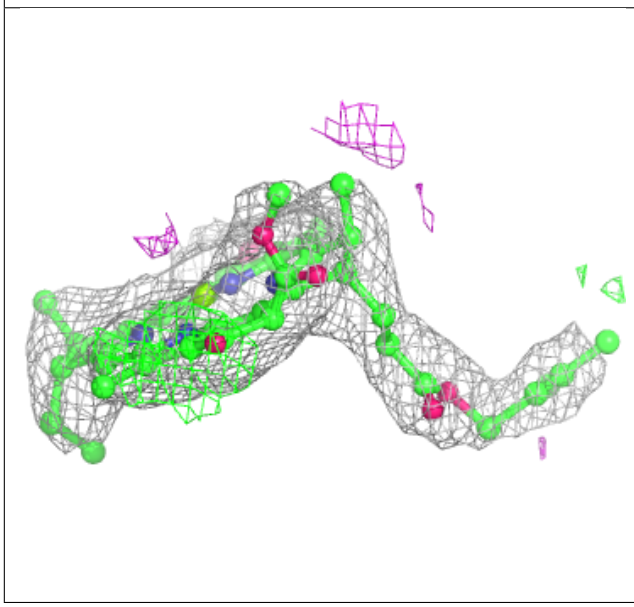
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCL M 406:

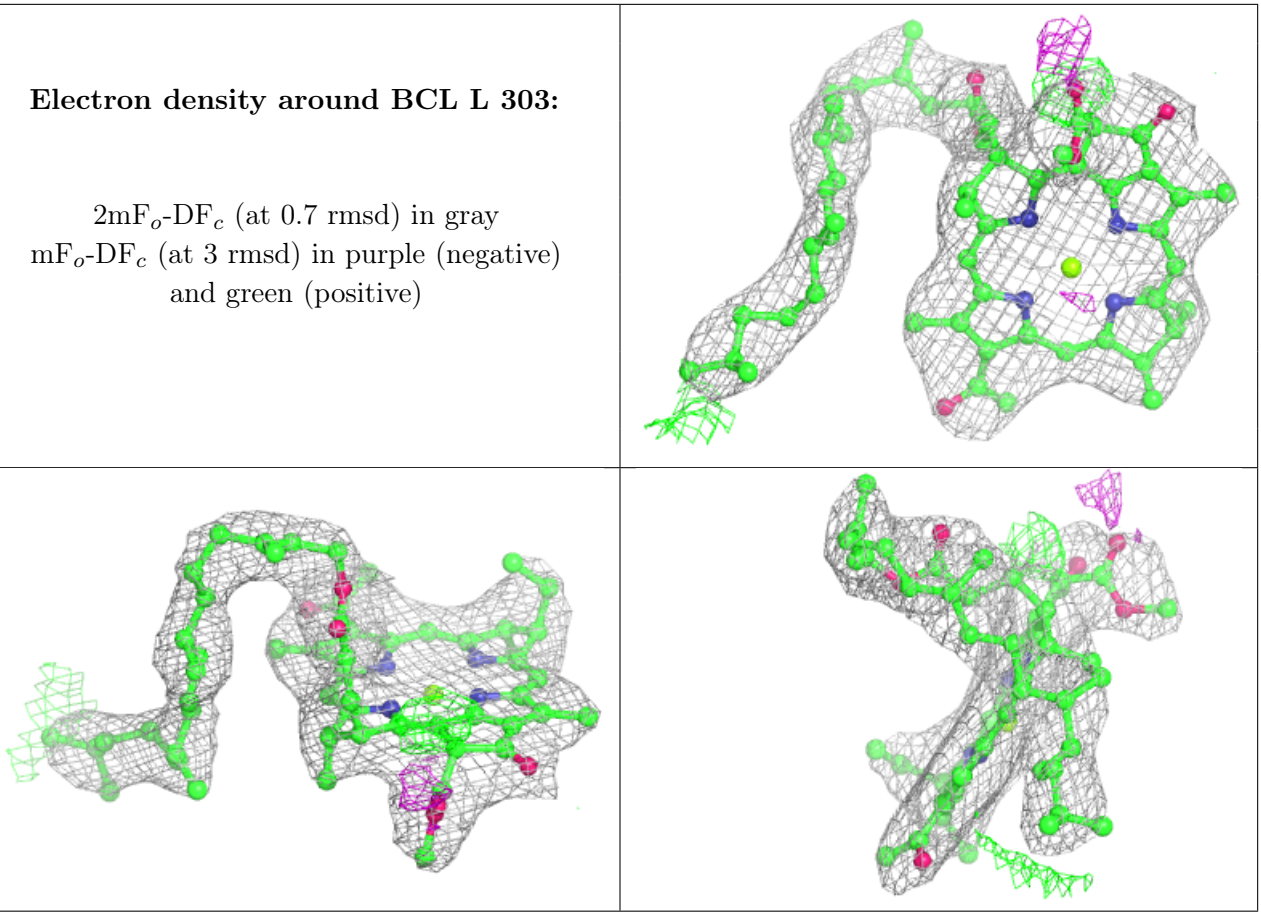
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





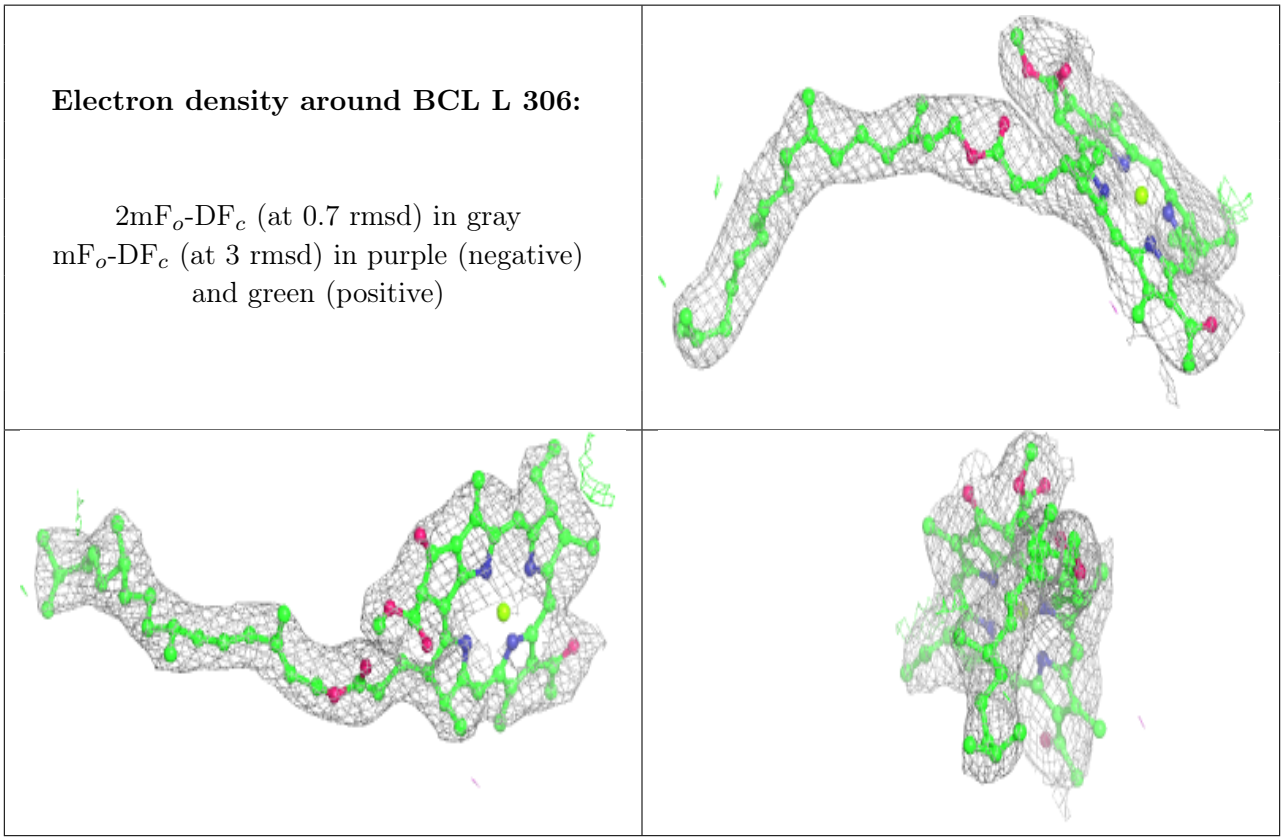
Electron density around BCL L 303:

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



Electron density around BCL 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)



6.5 Other polymers (i)

There are no such residues in this entry.