wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 09:33 AM EDT

PDB ID	:	1NKZ
Title	:	Crystal structure of LH2 B800-850 from Rps. acidophila at 2.0 Angstrom resolution
Authors	:	Papiz, M.Z.; Prince, S.M.; Howard, T.; Cogdell, R.J.; Isaacs, N.W.
Deposited on	:	2003-01-06
Resolution	:	2.00 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:

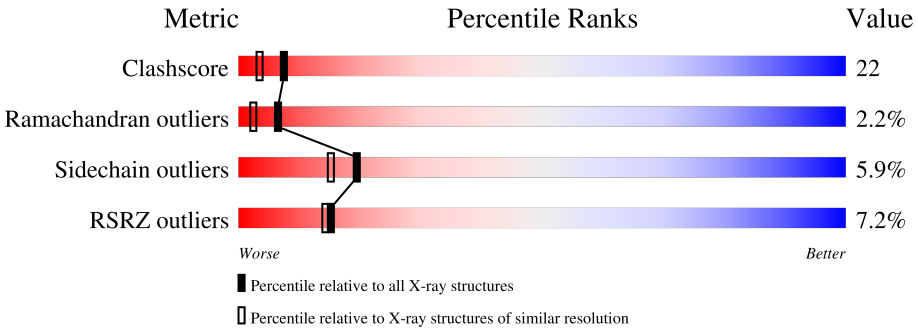
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	53	9% 72% 21% 6%
1	C	53	9% 75% 19% 6%
1	E	53	11% 74% 19% 6%
2	B	41	2% 83% 12%
2	D	41	2% 85% 10%
2	F	41	5% 88% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RG1	A	404	-	-	-	X
3	RG1	C	405	-	-	-	X
3	RG1	E	406	-	-	-	X
4	BOG	A	507	X	X	-	X
4	BOG	C	504	X	X	-	X
4	BOG	C	508	X	X	-	-
4	BOG	E	505	X	X	-	X
4	BOG	E	506	X	X	-	X
4	BOG	E	509	X	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3461 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 Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	C	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	E	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			

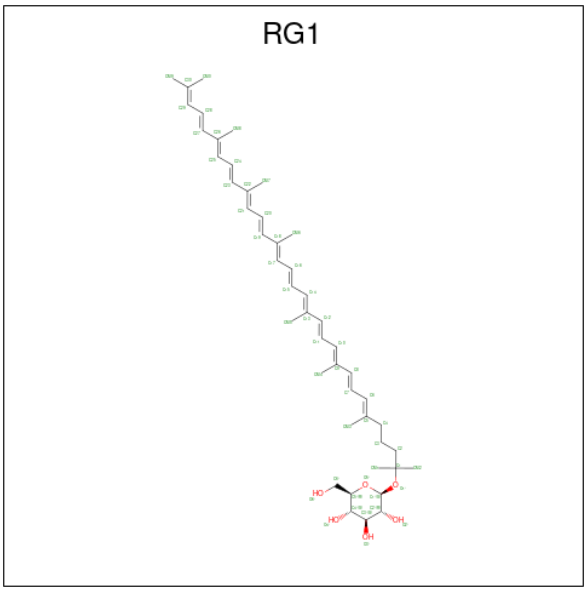
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	modified residue	UNP P26789
C	1	CXM	MET	modified residue	UNP P26789
E	1	CXM	MET	modified residue	UNP P26789

- Molecule 2 is a protein called Light-harvesting protein B-800/850, beta chain.

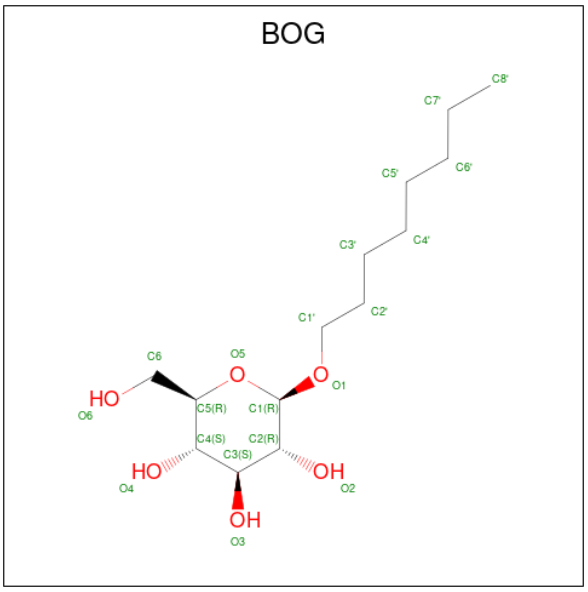
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	D	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	F	41	Total	C	N	O	0	0	0
			323	213	53	57			

- Molecule 3 is Rhodopin b-D-glucoside (three-letter code: RG1) (formula: $C_{46}H_{66}O_6$).



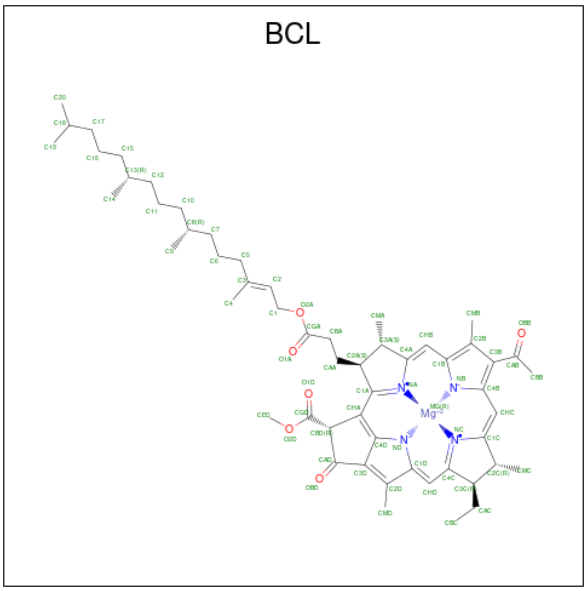
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 52 46 6	10	0
3	B	1	Total C O 52 46 6	0	0
3	C	1	Total C O 52 46 6	0	0
3	C	1	Total C O 52 46 6	10	0
3	D	1	Total C O 52 46 6	0	0
3	E	1	Total C O 52 46 6	10	0

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



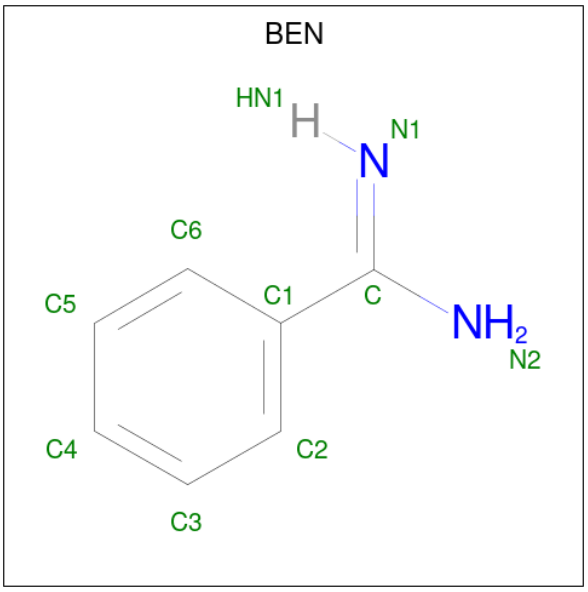
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	C	1	Total C O 20 14 6	0	0
4	C	1	Total C O 20 14 6	0	0
4	E	1	Total C O 20 14 6	0	0
4	E	1	Total C O 20 14 6	0	0
4	E	1	Total C O 20 14 6	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N 9 7 2	0	0
6	E	1	Total C N 9 7 2	0	0
6	E	1	Total C N 9 7 2	0	0

- Molecule 7 is water.

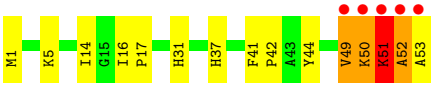
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	41	Total O 41 41	0	0
7	B	35	Total O 35 35	0	0
7	C	43	Total O 43 43	0	0
7	D	38	Total O 38 38	0	0
7	E	49	Total O 49 49	0	0
7	F	24	Total O 24 24	0	0

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.

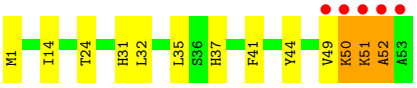
• Molecule 1: Light-harvesting protein B-800/850, alpha chain

Chain A:



• Molecule 1: Light-harvesting protein B-800/850, alpha chain

Chain C:



• Molecule 1: Light-harvesting protein B-800/850, alpha chain

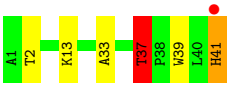
Chain E:

• Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain B:

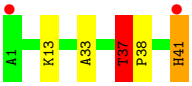
• Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain D:



• Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	117.05Å 117.05Å 298.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00 31.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (8.00-2.00) 97.8 (31.99-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.169 , 0.190 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.001 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3461	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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: BEN, RG1, CXM, BCL, BOG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.99	1/404 (0.2%)	0.68	0/556
1	C	0.51	0/404	0.68	0/556
1	E	1.18	1/404 (0.2%)	0.70	0/556
2	B	0.50	0/332	0.69	1/453 (0.2%)
2	D	0.58	0/332	0.71	1/453 (0.2%)
2	F	0.52	0/332	0.70	1/453 (0.2%)
All	All	0.78	2/2208 (0.1%)	0.69	3/3027 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	53	ALA	C-O	21.36	1.64	1.23
1	A	53	ALA	C-O	15.82	1.53	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	37	THR	N-CA-CB	-5.90	99.09	110.30
2	F	37	THR	N-CA-CB	-5.61	99.63	110.30
2	D	37	THR	N-CA-CB	-5.09	100.63	110.30

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	A	403	0	422	18	0
1	C	403	0	422	26	0
1	E	403	0	422	21	0
2	B	323	0	321	13	1
2	D	323	0	321	10	0
2	F	323	0	321	7	0
3	A	52	0	65	16	0
3	B	52	0	66	3	0
3	C	104	0	131	14	0
3	D	52	0	66	0	0
3	E	52	0	65	16	0
4	A	20	0	20	6	0
4	C	40	0	40	6	0
4	E	60	0	60	6	0
5	A	132	0	148	12	0
5	B	66	0	74	3	0
5	C	132	0	148	13	0
5	D	66	0	74	4	0
5	E	132	0	148	9	0
5	F	66	0	74	4	0
6	C	9	0	7	1	0
6	E	18	0	14	3	0
7	A	41	0	0	2	1
7	B	35	0	0	3	0
7	C	43	0	0	3	0
7	D	38	0	0	3	1
7	E	49	0	0	4	2
7	F	24	0	0	1	0
All	All	3461	0	3429	146	5

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 22.

The worst 5 of 146 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:E:53:ALA:C	1:E:53:ALA:O	1.63	1.35
1:E:9:VAL:HB	7:E:554:HOH:O	1.36	1.24
3:E:406:RG1:CM5	5:E:305:BCL:HMA3	1.84	1.08
3:A:404:RG1:CM5	5:A:301:BCL:HMA3	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:405:RG1:CM5	5:C:303:BCL:HMA3	1.91	1.01

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:537:HOH:O	7:E:553:HOH:O[4_555]	1.95	0.25
7:A:542:HOH:O	7:A:542:HOH:O[12_555]	2.07	0.13
2:B:6:GLU:OE1	2:B:13:LYS:NZ[12_555]	2.12	0.08
7:D:426:HOH:O	7:D:436:HOH:O[12_555]	2.16	0.04
7:E:520:HOH:O	7:E:553:HOH:O[4_555]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	51/53 (96%)	48 (94%)	1 (2%)	2 (4%)	3 1
1	C	51/53 (96%)	48 (94%)	1 (2%)	2 (4%)	3 1
1	E	51/53 (96%)	47 (92%)	2 (4%)	2 (4%)	3 1
2	B	39/41 (95%)	38 (97%)	1 (3%)	0	100 100
2	D	39/41 (95%)	38 (97%)	1 (3%)	0	100 100
2	F	39/41 (95%)	38 (97%)	1 (3%)	0	100 100
All	All	270/282 (96%)	257 (95%)	7 (3%)	6 (2%)	6 2

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ALA
1	C	52	ALA
1	E	52	ALA

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Mol	Chain	Res	Type
1	A	51	LYS
1	C	51	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	40/40 (100%)	37 (92%)	3 (8%)	13 9
1	C	40/40 (100%)	39 (98%)	1 (2%)	47 49
1	E	40/40 (100%)	38 (95%)	2 (5%)	24 20
2	B	33/33 (100%)	31 (94%)	2 (6%)	18 14
2	D	33/33 (100%)	30 (91%)	3 (9%)	9 5
2	F	33/33 (100%)	31 (94%)	2 (6%)	18 14
All	All	219/219 (100%)	206 (94%)	13 (6%)	19 15

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	37	THR
2	D	41	HIS
2	F	41	HIS
1	E	51	LYS
2	F	37	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	7	GLN
2	D	7	GLN
2	F	7	GLN
2	F	41	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CXM	C	1	5,1	8,10,11	0.97	1 (12%)	7,11,13	1.77	1 (14%)
1	CXM	A	1	5,1	8,10,11	0.99	1 (12%)	7,11,13	2.03	2 (28%)
1	CXM	E	1	5,1	8,10,11	0.90	1 (12%)	7,11,13	1.87	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	C	1	5,1	-	3/9/10/12	-
1	CXM	A	1	5,1	-	2/9/10/12	-
1	CXM	E	1	5,1	-	3/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	CXM	ON1-CN	2.14	1.25	1.21
1	A	1	CXM	ON1-CN	2.05	1.25	1.21
1	E	1	CXM	ON1-CN	2.04	1.25	1.21

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	CXM	ON1-CN-N	-3.98	118.32	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	CXM	ON1-CN-N	-3.73	118.72	124.85
1	E	1	CXM	ON1-CN-N	-3.66	118.85	124.85
1	A	1	CXM	C-CA-N	3.04	115.22	109.73
1	E	1	CXM	C-CA-N	2.73	114.66	109.73

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	1	CXM	C-CA-N-CN
1	A	1	CXM	CB-CA-N-CN
1	C	1	CXM	CB-CA-N-CN
1	E	1	CXM	CB-CA-N-CN
1	C	1	CXM	C-CA-CB-CG

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)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	BEN	C	510	-	9,9,9	1.33	1 (11%)	7,11,11	0.79	0
5	BCL	D	304	2	58,74,74	2.09	14 (24%)	69,115,115	2.41	23 (33%)
5	BCL	A	307	1	58,74,74	2.18	14 (24%)	69,115,115	2.21	19 (27%)
4	BOG	C	504	-	20,20,20	5.53	14 (70%)	25,25,25	4.07	17 (68%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BCL	E	309	1	58,74,74	2.29	15 (25%)	69,115,115	2.33	21 (30%)
5	BCL	C	303	1	58,74,74	2.09	15 (25%)	69,115,115	2.22	19 (27%)
5	BCL	E	305	1	58,74,74	2.05	14 (24%)	69,115,115	2.32	23 (33%)
3	RG1	B	401	-	52,52,52	1.49	5 (9%)	64,67,67	1.70	11 (17%)
5	BCL	F	306	2	58,74,74	2.10	15 (25%)	69,115,115	2.55	21 (30%)
3	RG1	C	405	-	52,52,52	1.81	6 (11%)	64,67,67	2.66	14 (21%)
4	BOG	A	507	-	20,20,20	5.55	14 (70%)	25,25,25	5.00	17 (68%)
4	BOG	E	505	-	20,20,20	5.53	14 (70%)	25,25,25	3.91	16 (64%)
5	BCL	B	302	2	58,74,74	2.11	14 (24%)	69,115,115	2.58	21 (30%)
3	RG1	A	404	-	52,52,52	1.80	6 (11%)	64,67,67	2.66	18 (28%)
5	BCL	C	308	1	58,74,74	2.20	14 (24%)	69,115,115	2.19	20 (28%)
4	BOG	E	506	-	20,20,20	5.54	14 (70%)	25,25,25	4.03	17 (68%)
4	BOG	E	509	-	20,20,20	5.52	15 (75%)	25,25,25	4.26	17 (68%)
5	BCL	A	301	1	58,74,74	2.12	15 (25%)	69,115,115	2.38	21 (30%)
3	RG1	D	402	-	52,52,52	1.32	4 (7%)	64,67,67	1.39	7 (10%)
3	RG1	E	406	-	52,52,52	1.77	7 (13%)	64,67,67	2.58	16 (25%)
3	RG1	C	403	-	52,52,52	1.28	3 (5%)	64,67,67	1.37	6 (9%)
4	BOG	C	508	-	20,20,20	5.52	14 (70%)	25,25,25	3.91	17 (68%)
6	BEN	E	511	-	9,9,9	1.34	1 (11%)	7,11,11	0.71	0
6	BEN	E	512	-	9,9,9	1.39	1 (11%)	7,11,11	0.81	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
6	BEN	C	510	-	-	4/4/4/4	0/1/1/1
5	BCL	D	304	2	-	8/37/137/137	-
5	BCL	A	307	1	-	8/37/137/137	-
4	BOG	C	504	-	4/4/5/5	7/11/31/31	0/1/1/1
5	BCL	E	309	1	-	8/37/137/137	-
5	BCL	C	303	1	-	6/37/137/137	-
5	BCL	E	305	1	-	6/37/137/137	-
3	RG1	B	401	-	-	4/51/71/71	0/1/1/1
5	BCL	F	306	2	-	7/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RG1	C	405	-	-	24/51/71/71	0/1/1/1
4	BOG	A	507	-	4/4/5/5	6/11/31/31	0/1/1/1
4	BOG	E	505	-	4/4/5/5	9/11/31/31	0/1/1/1
5	BCL	B	302	2	-	7/37/137/137	-
3	RG1	A	404	-	-	24/51/71/71	0/1/1/1
5	BCL	C	308	1	-	8/37/137/137	-
4	BOG	E	506	-	4/4/5/5	6/11/31/31	0/1/1/1
4	BOG	E	509	-	4/4/5/5	7/11/31/31	0/1/1/1
5	BCL	A	301	1	-	6/37/137/137	-
3	RG1	D	402	-	-	4/51/71/71	0/1/1/1
3	RG1	C	403	-	-	4/51/71/71	0/1/1/1
3	RG1	E	406	-	-	25/51/71/71	0/1/1/1
4	BOG	C	508	-	4/4/5/5	9/11/31/31	0/1/1/1
6	BEN	E	511	-	-	1/4/4/4	0/1/1/1
6	BEN	E	512	-	-	2/4/4/4	0/1/1/1

The worst 5 of 249 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	506	BOG	O1-C1	-9.98	1.23	1.40
4	A	507	BOG	O1-C1	-9.93	1.23	1.40
4	C	504	BOG	O1-C1	-9.90	1.23	1.40
4	C	508	BOG	O1-C1	-9.89	1.23	1.40
4	E	505	BOG	O1-C1	-9.82	1.23	1.40

The worst 5 of 361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	507	BOG	O1-C1'-C2'	16.10	166.00	109.56
3	C	405	RG1	C25-C24-C23	14.35	167.99	123.22
3	A	404	RG1	C25-C24-C23	14.23	167.61	123.22
3	E	406	RG1	C25-C24-C23	13.04	163.92	123.22
5	F	306	BCL	C4A-NA-C1A	-13.02	100.85	106.71

5 of 24 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	507	BOG	C5
4	A	507	BOG	C3

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Mol	Chain	Res	Type	Atom
4	A	507	BOG	C4
4	A	507	BOG	C2
4	C	504	BOG	C5

5 of 200 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	RG1	C2'-C1'-O1'-C1
3	A	404	RG1	O5'-C1'-O1'-C1
3	A	404	RG1	CM2-C1-O1'-C1'
3	A	404	RG1	C2-C1-O1'-C1'
3	A	404	RG1	C3-C4-C5-CM3

There are no ring outliers.

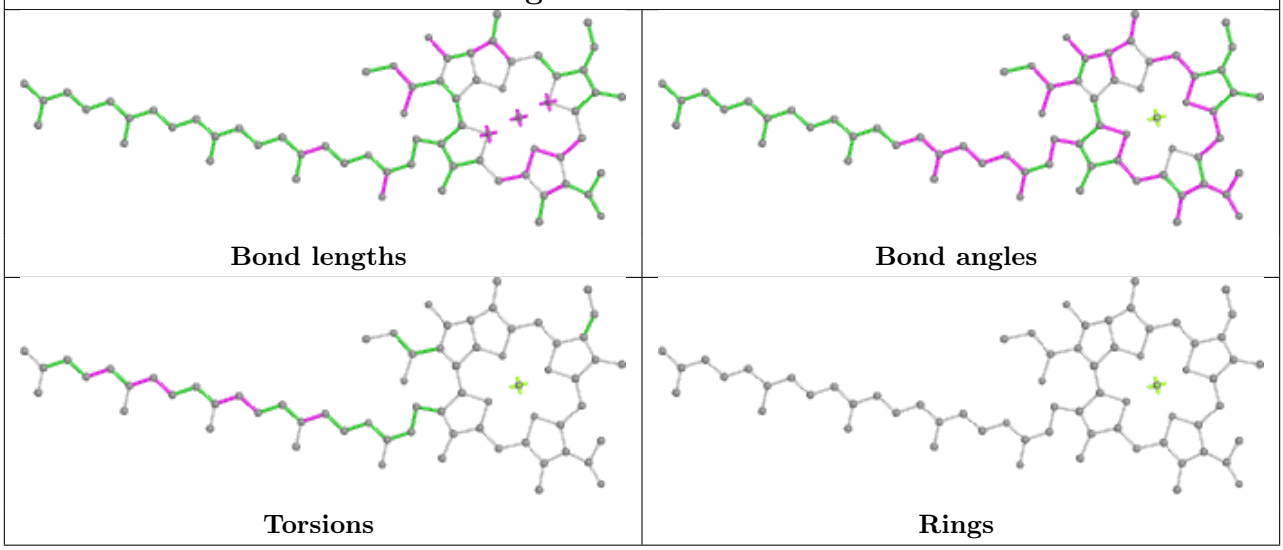
22 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	510	BEN	1	0
5	D	304	BCL	4	0
5	A	307	BCL	3	0
4	C	504	BOG	4	0
5	E	309	BCL	3	0
5	C	303	BCL	8	0
5	E	305	BCL	6	0
3	B	401	RG1	3	0
5	F	306	BCL	4	0
3	C	405	RG1	14	0
4	A	507	BOG	6	0
4	E	505	BOG	2	0
5	B	302	BCL	3	0
3	A	404	RG1	16	0
5	C	308	BCL	5	0
4	E	506	BOG	3	0
4	E	509	BOG	1	0
5	A	301	BCL	9	0
3	E	406	RG1	16	0
4	C	508	BOG	2	0
6	E	511	BEN	1	0
6	E	512	BEN	2	0

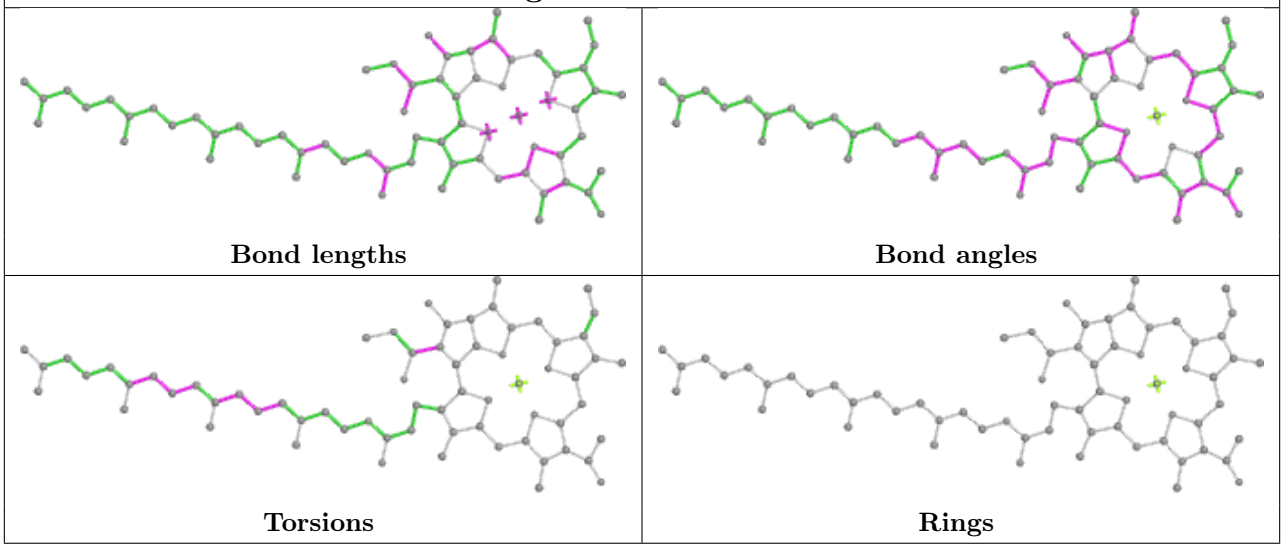
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

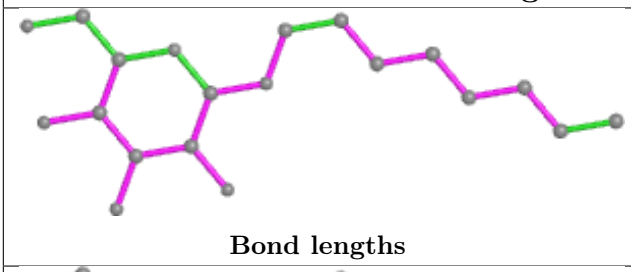
Ligand BCL D 304



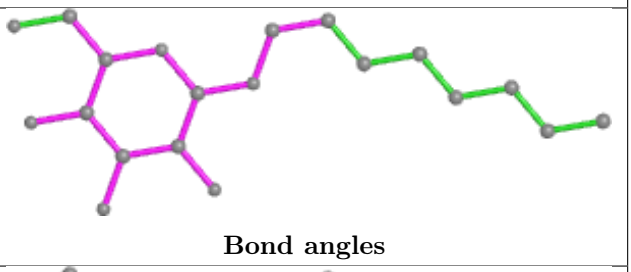
Ligand BCL A 307



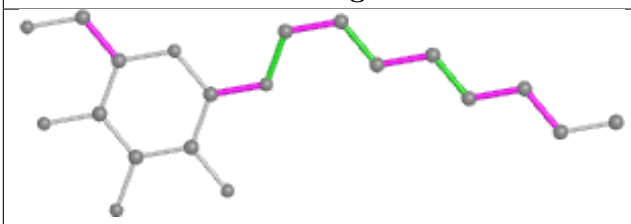
Ligand BOG C 504



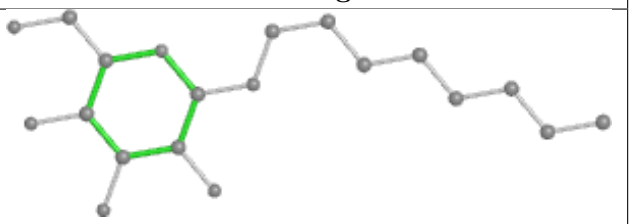
Bond lengths



Bond angles

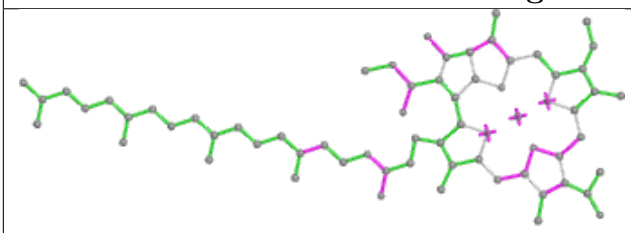


Torsions



Rings

Ligand BCL E 309



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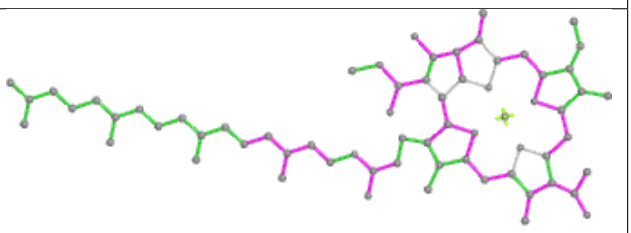
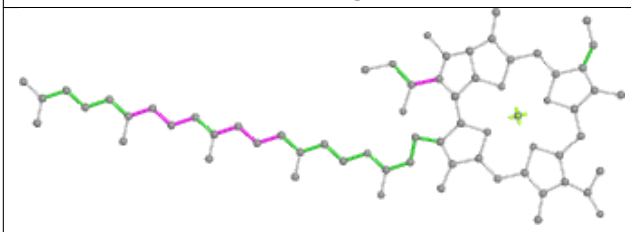


Bond angles



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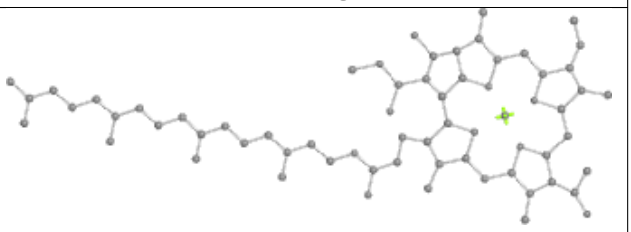
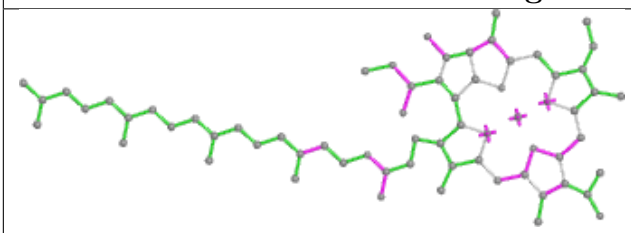
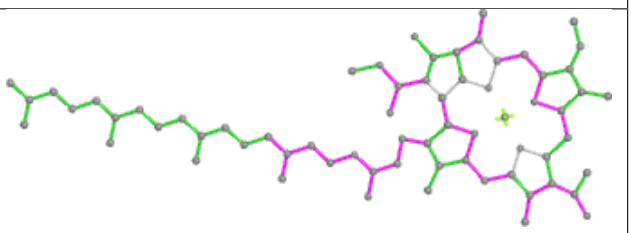


Rings

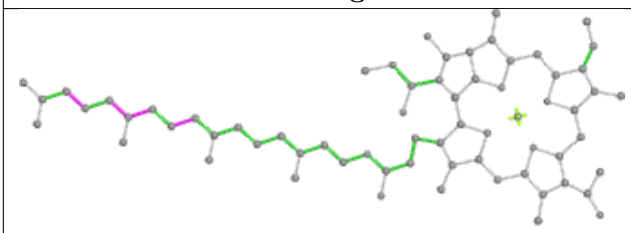
Ligand BCL C 303



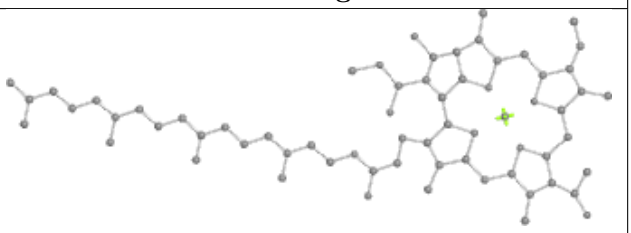
Bond lengths



Bond angles

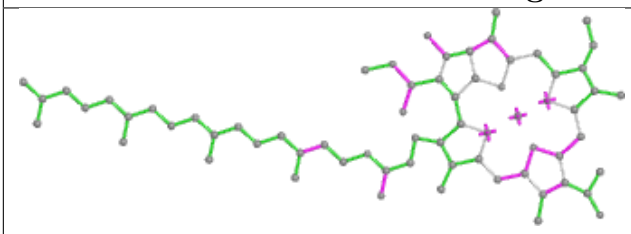


Torsions



Rings

Ligand BCL E 305



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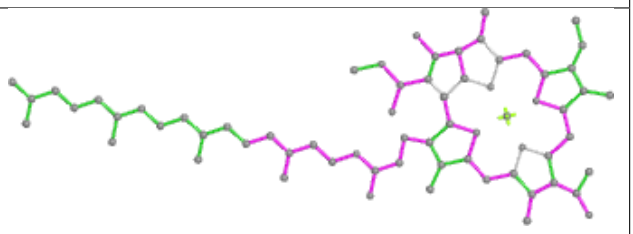
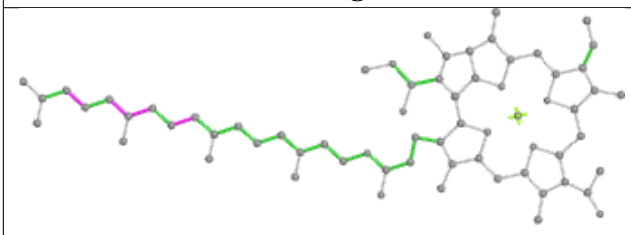
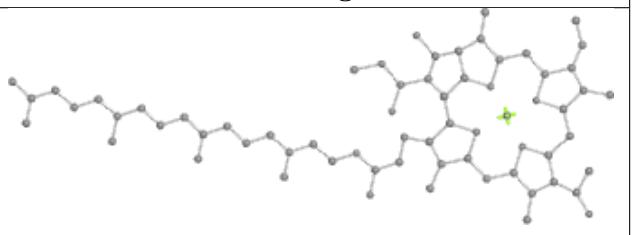


Bond angles

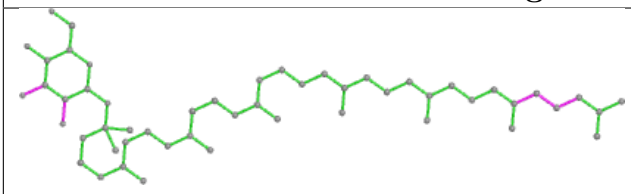


Torsions

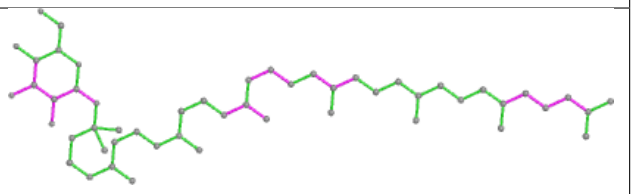


Rings

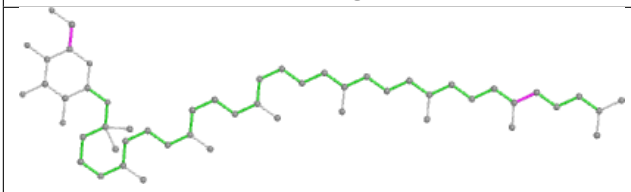
Ligand RG1 B 401



Bond lengths



Bond angles



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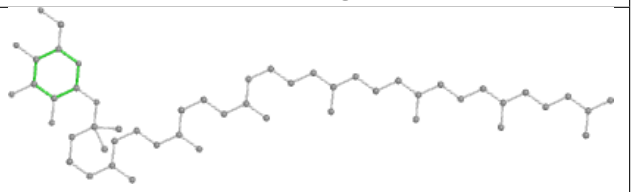
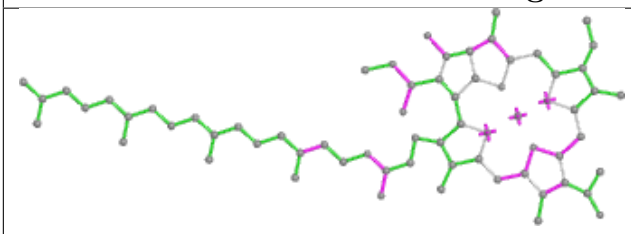
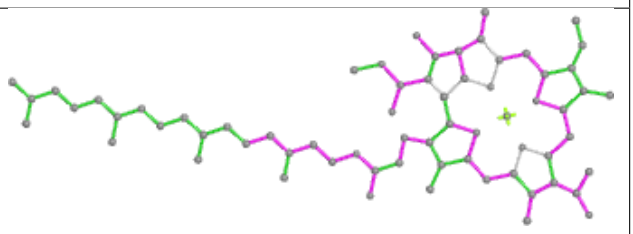


Rings

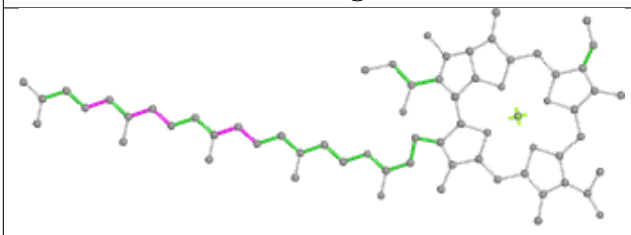
Ligand BCL F 306



Bond lengths



Bond angles



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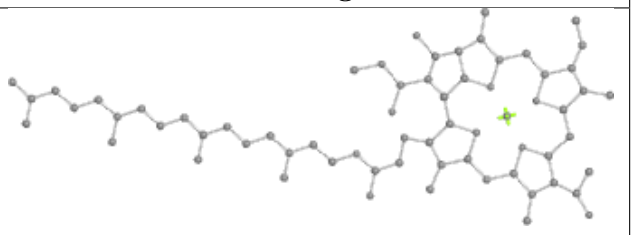
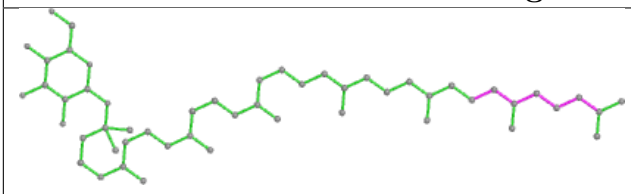
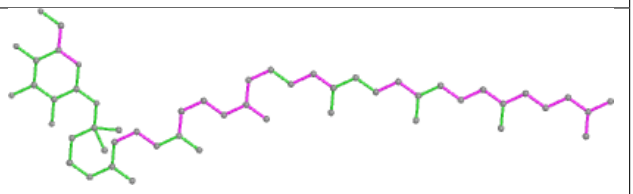
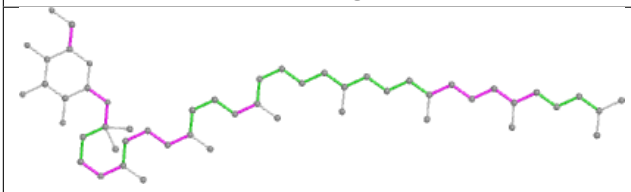


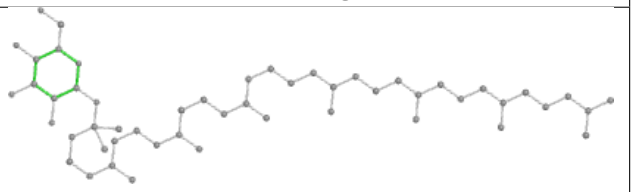
Rings

Ligand RG1 C 405

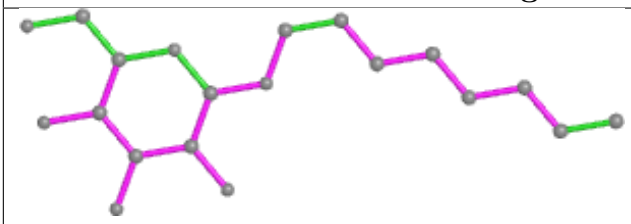

Bond lengths

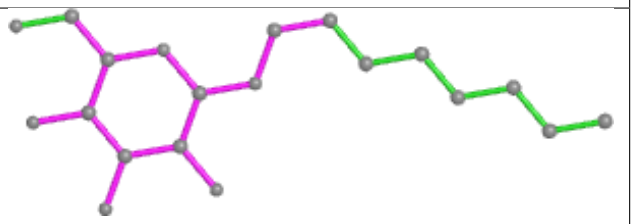

Bond angles

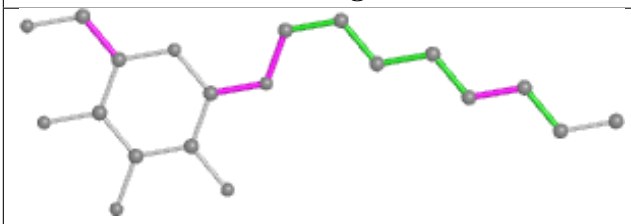

Torsions

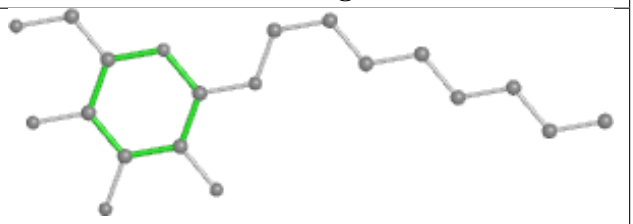

Rings

Ligand BOG A 507

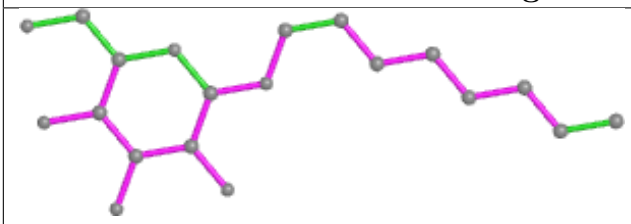

Bond lengths

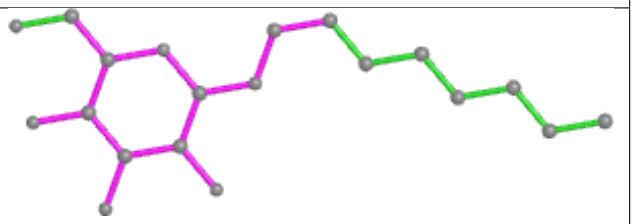

Bond angles

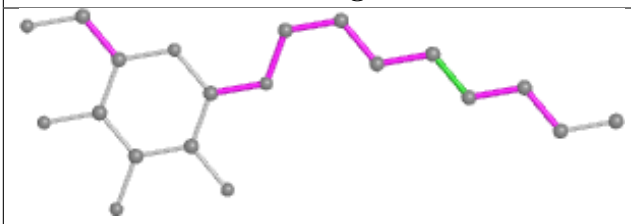

Torsions

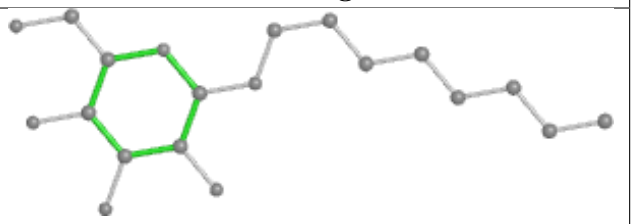

Rings

Ligand BOG E 505

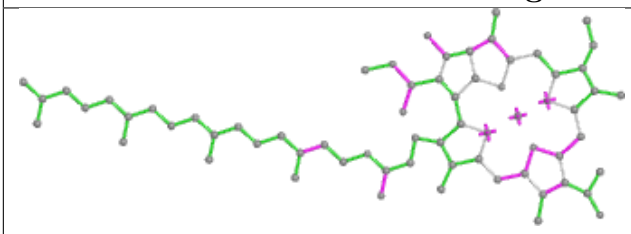

Bond lengths


Bond angles

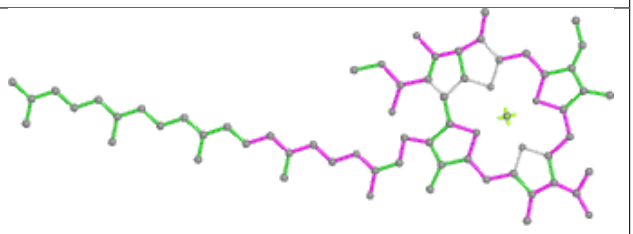

Torsions


Rings

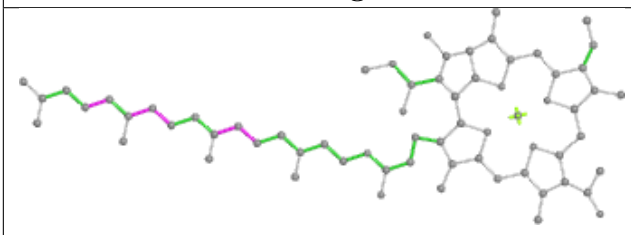
Ligand BCL B 302



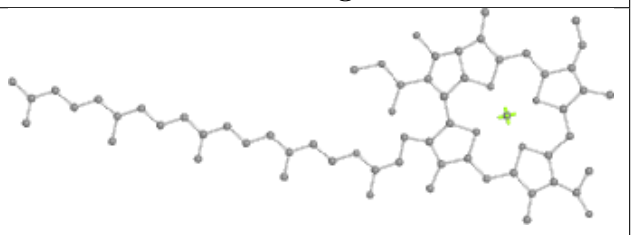
Bond lengths



Bond angles

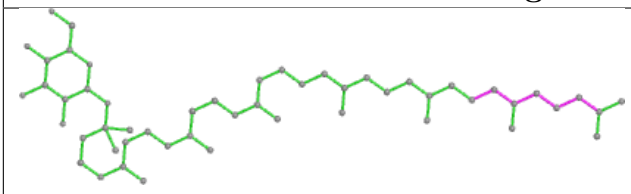


Torsions

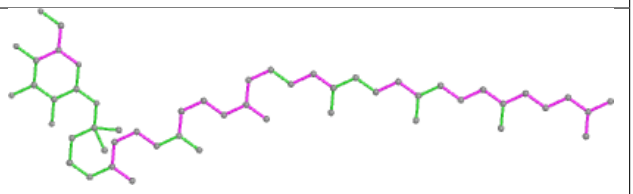


Rings

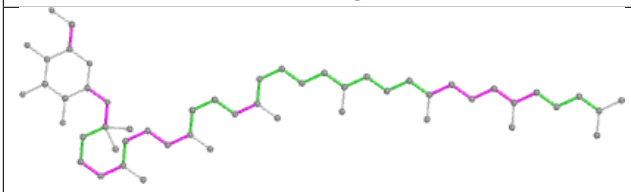
Ligand RG1 A 404



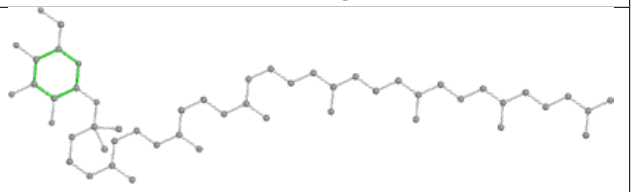
Bond lengths



Bond angles

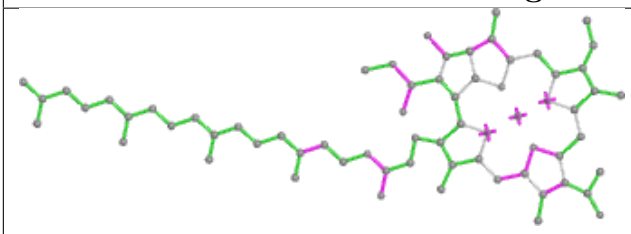


Torsions

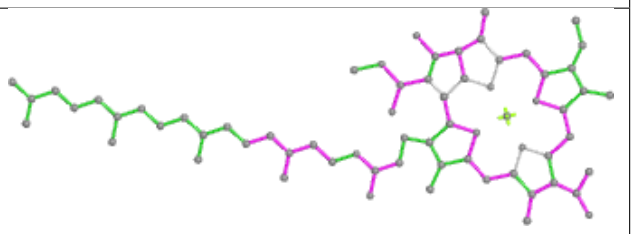


Rings

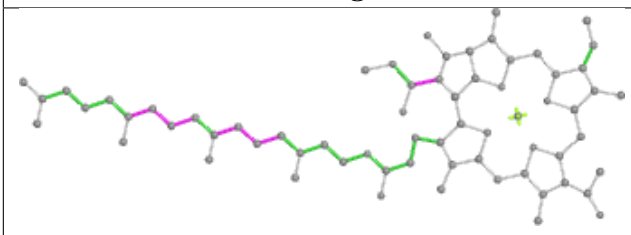
Ligand BCL C 308



Bond lengths



Bond angles



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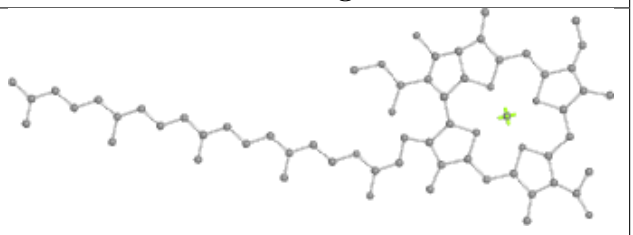
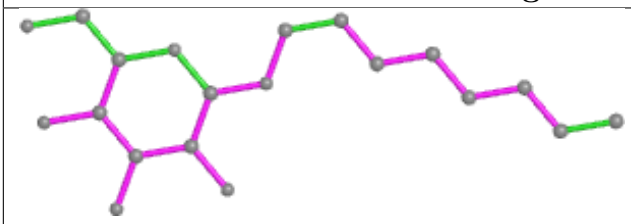
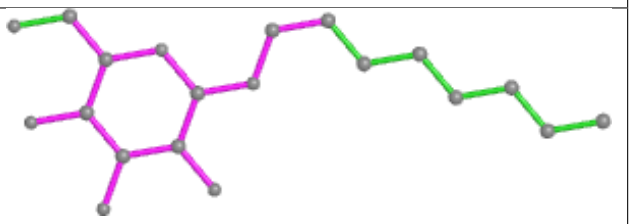


Rings

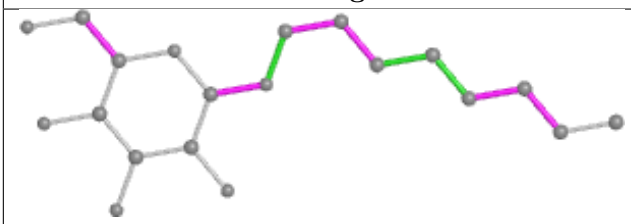
Ligand BOG E 506



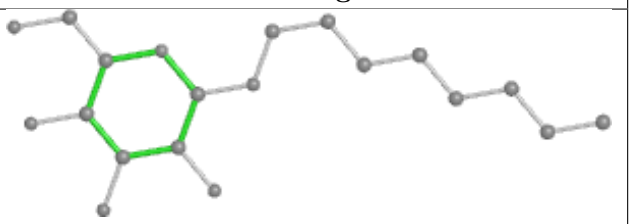
Bond lengths



Bond angles

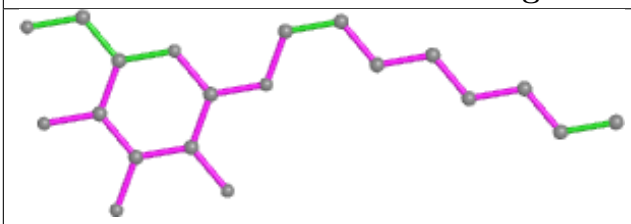


Torsions

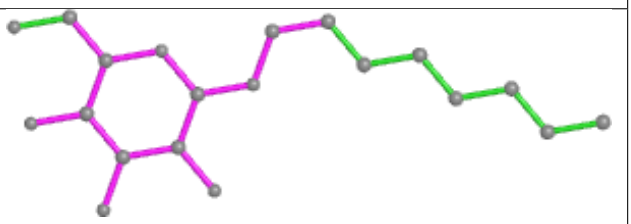


Rings

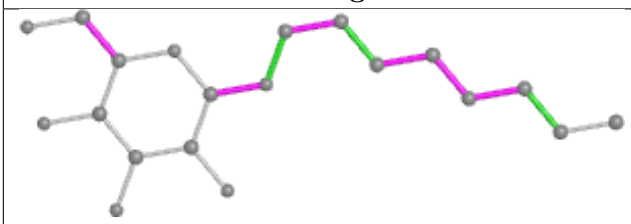
Ligand BOG E 509



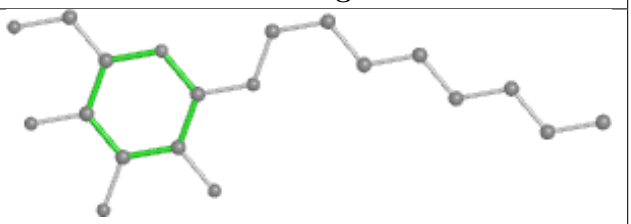
Bond lengths



Bond angles

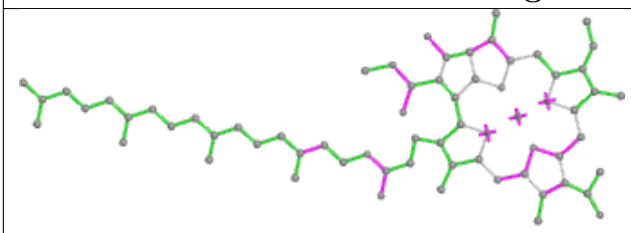


Torsions

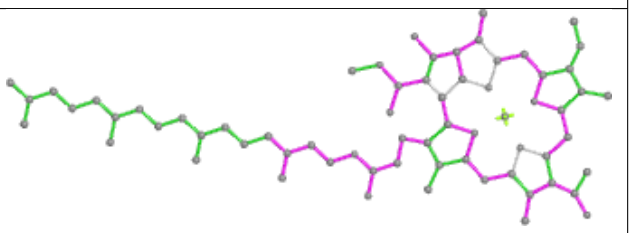


Rings

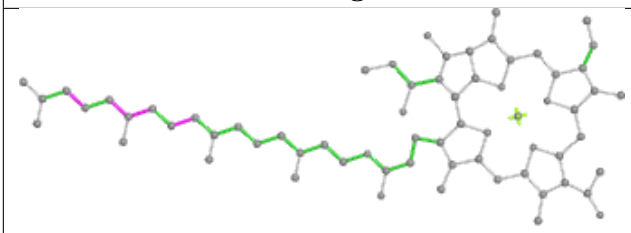
Ligand BCL A 301



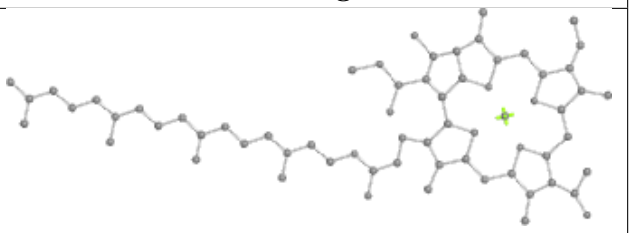
Bond lengths



Bond angles

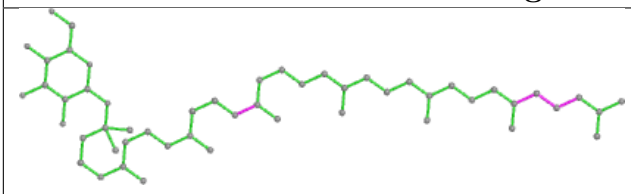


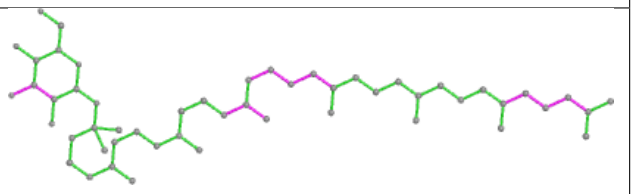
Torsions

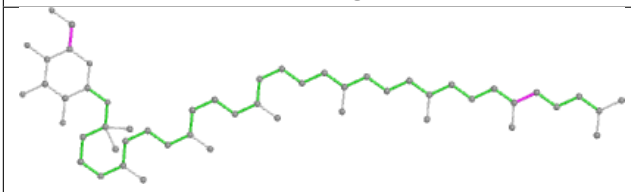


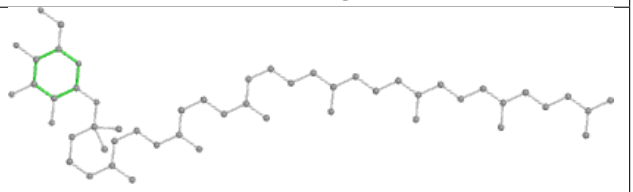
Rings

Ligand RG1 D 402

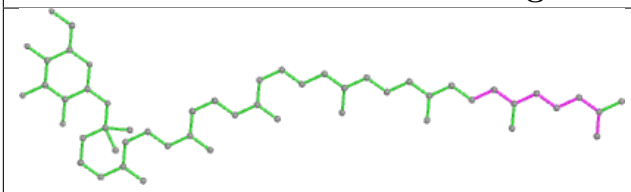

Bond lengths

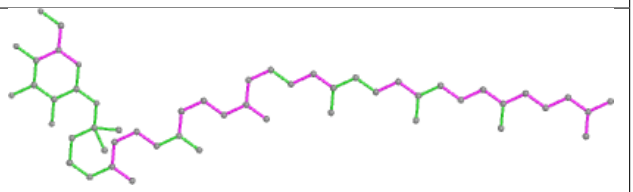

Bond angles

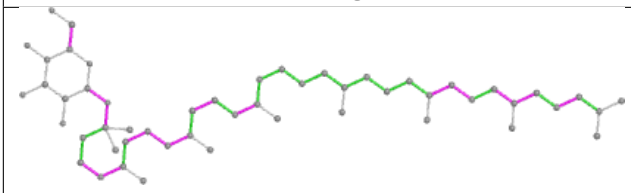

Torsions

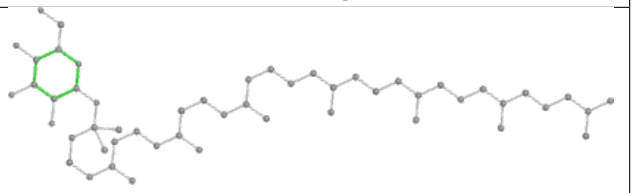

Rings

Ligand RG1 E 406

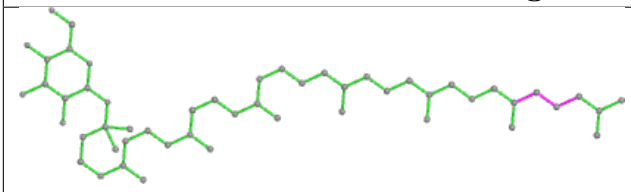

Bond lengths

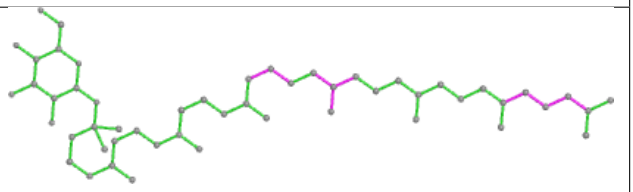

Bond angles

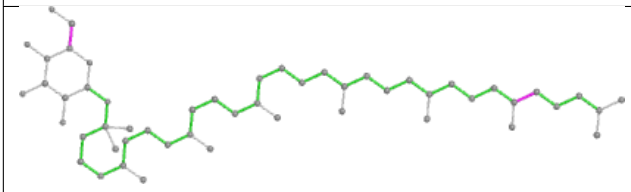

Torsions

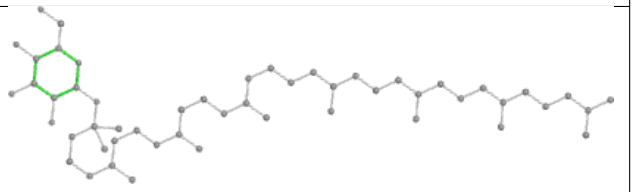

Rings

Ligand RG1 C 403

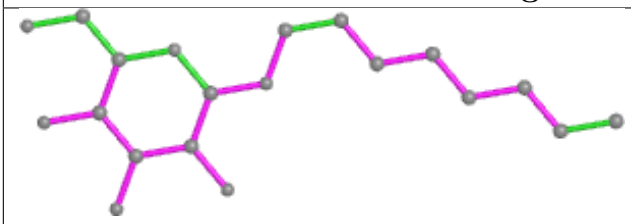

Bond lengths


Bond angles

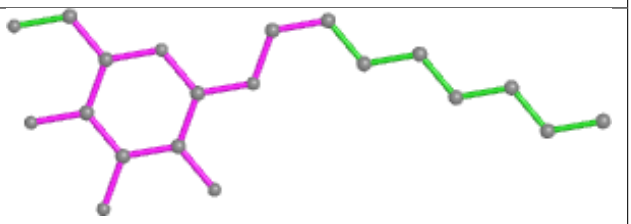

Torsions


Rings

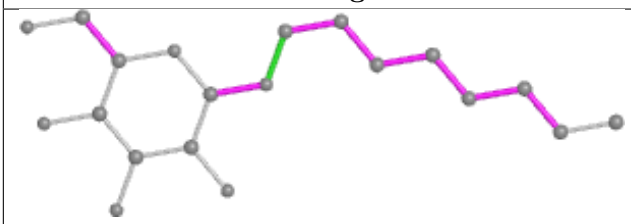
Ligand BOG C 508



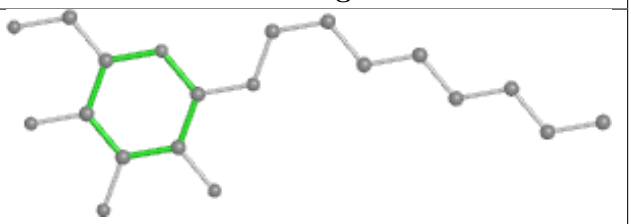
Bond lengths



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	52/53 (98%)	0.43	5 (9%)	8	7	14, 18, 50, 51	0
1	C	52/53 (98%)	0.35	5 (9%)	8	7	14, 18, 50, 51	0
1	E	52/53 (98%)	0.69	6 (11%)	4	4	14, 18, 50, 51	0
2	B	41/41 (100%)	-0.25	1 (2%)	59	57	16, 18, 22, 35	0
2	D	41/41 (100%)	-0.27	1 (2%)	59	57	16, 18, 23, 35	0
2	F	41/41 (100%)	-0.25	2 (4%)	29	28	16, 18, 23, 35	0
All	All	279/282 (98%)	0.16	20 (7%)	15	14	14, 18, 44, 51	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	52	ALA	13.8
1	E	51	LYS	13.6
1	A	51	LYS	10.7
1	E	49	VAL	10.0
1	A	49	VAL	9.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CXM	C	1	11/12	0.94	0.12	14,17,20,20	0
1	CXM	A	1	11/12	0.97	0.07	15,17,20,20	0
1	CXM	E	1	11/12	0.97	0.13	13,16,20,20	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

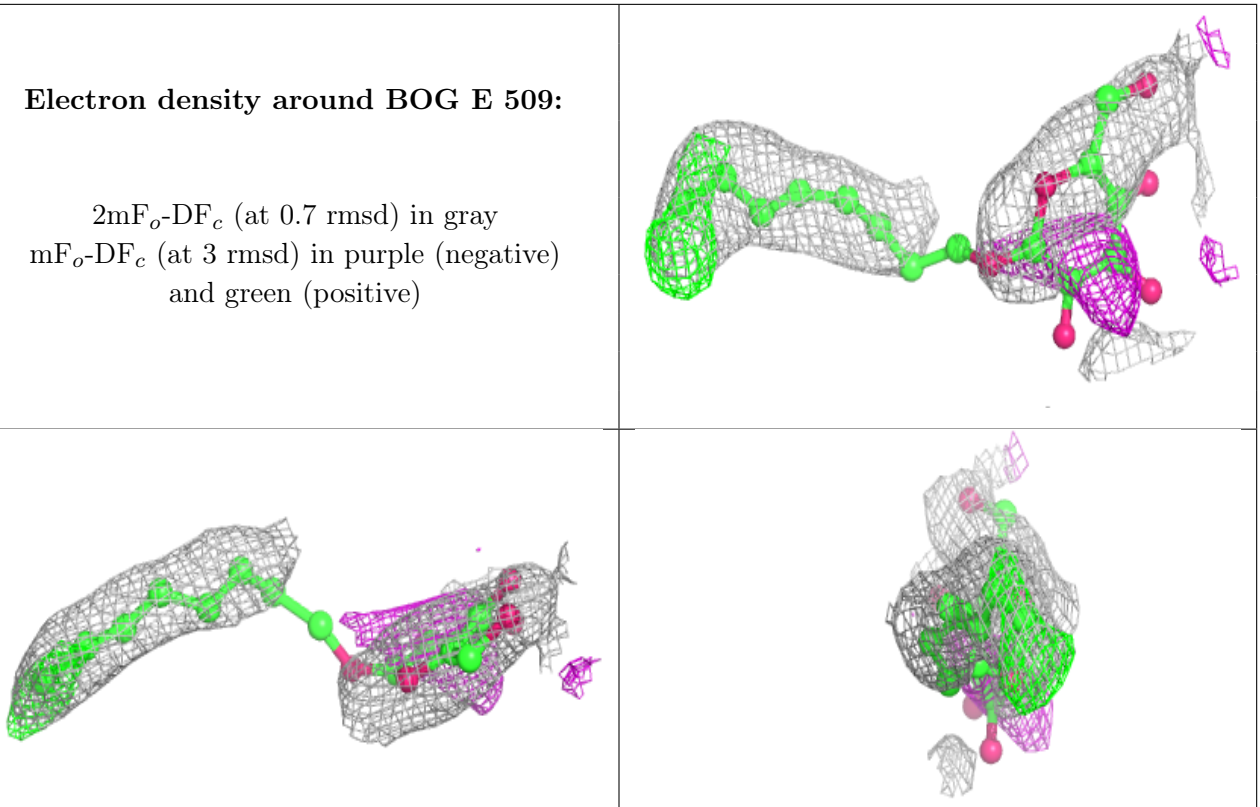
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BOG	E	509	20/20	0.28	0.40	81,100,105,106	0
4	BOG	A	507	20/20	0.31	0.57	88,104,108,108	0
4	BOG	C	508	20/20	0.35	0.37	79,96,102,104	0
4	BOG	E	505	20/20	0.43	0.46	99,111,116,116	0
3	RG1	C	405	52/52	0.43	0.63	39,57,63,63	52
4	BOG	C	504	20/20	0.49	0.46	86,101,103,104	0
4	BOG	E	506	20/20	0.50	0.45	89,102,105,105	0
3	RG1	E	406	52/52	0.53	0.56	40,57,63,64	52
3	RG1	A	404	52/52	0.54	0.56	40,57,63,63	52
6	BEN	E	511	9/9	0.62	0.28	77,80,83,83	0
6	BEN	E	512	9/9	0.65	0.37	76,79,80,80	0
6	BEN	C	510	9/9	0.68	0.35	73,76,78,79	0
3	RG1	C	403	52/52	0.80	0.19	13,16,29,31	0
3	RG1	B	401	52/52	0.81	0.20	13,16,29,31	0
3	RG1	D	402	52/52	0.87	0.17	13,16,28,31	0
5	BCL	E	309	66/66	0.90	0.13	11,16,37,43	0
5	BCL	A	307	66/66	0.91	0.12	11,17,38,43	0
5	BCL	C	308	66/66	0.91	0.12	11,16,38,43	0
5	BCL	D	304	66/66	0.95	0.12	13,16,29,36	0
5	BCL	B	302	66/66	0.95	0.10	12,16,29,36	0
5	BCL	F	306	66/66	0.95	0.10	13,16,29,36	0
5	BCL	E	305	66/66	0.96	0.10	13,17,21,24	0
5	BCL	A	301	66/66	0.96	0.12	13,16,22,24	0
5	BCL	C	303	66/66	0.96	0.12	13,16,22,23	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.

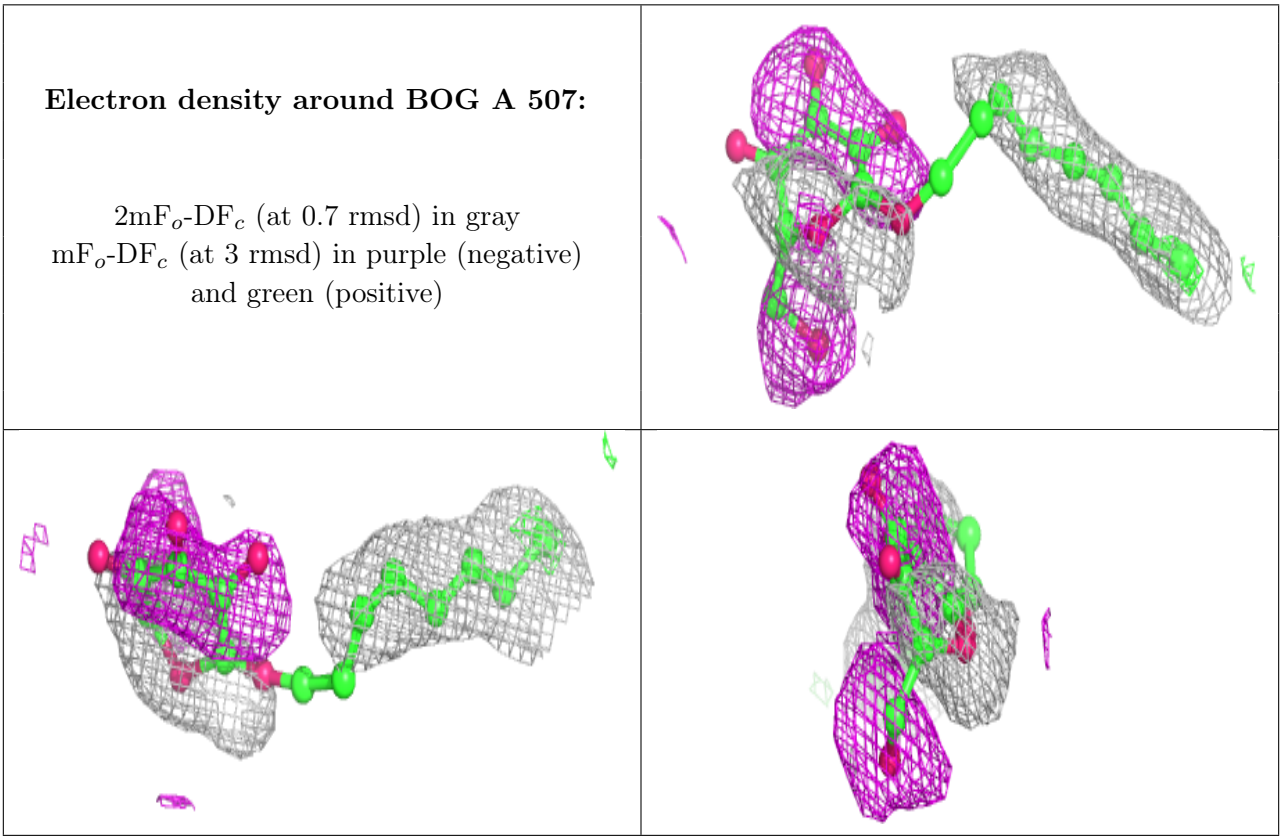
Electron density around BOG E 509:

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



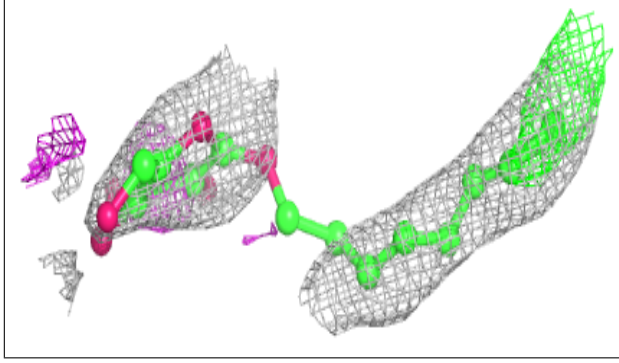
Electron density around BOG A 507:

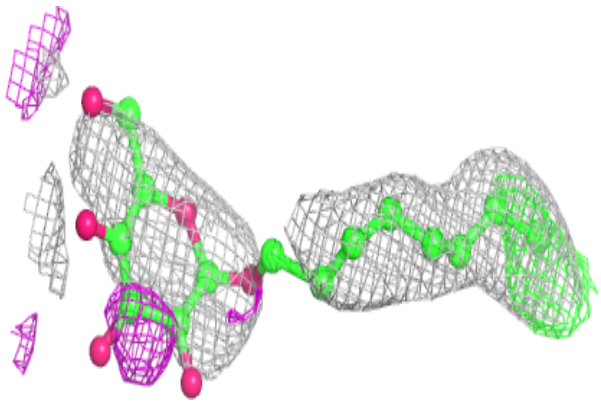
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

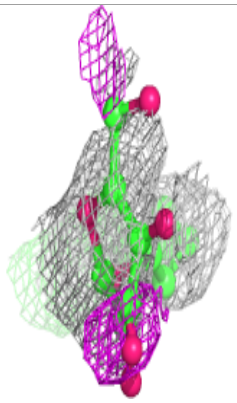


Electron density around BOG C 508:

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

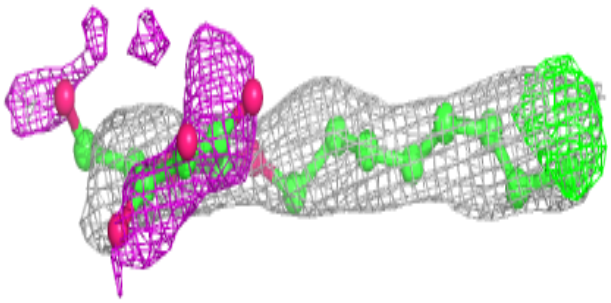


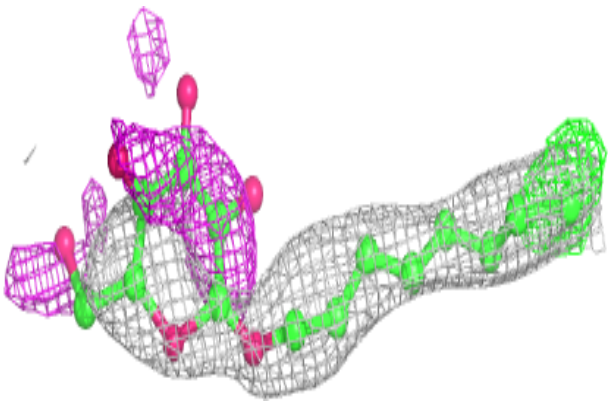


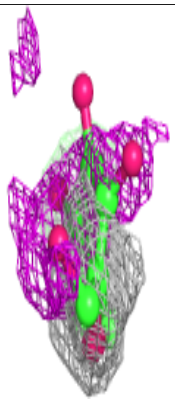


Electron density around BOG E 505:

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

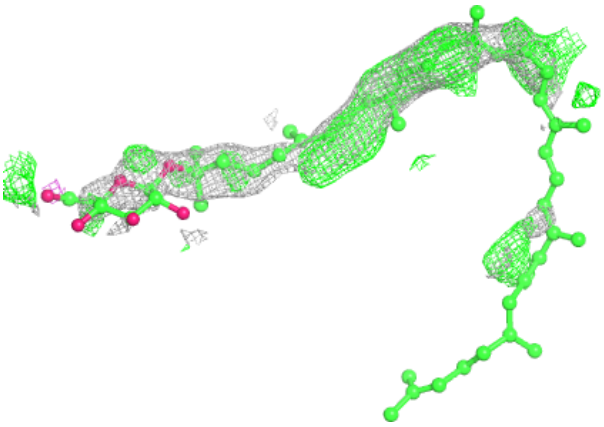


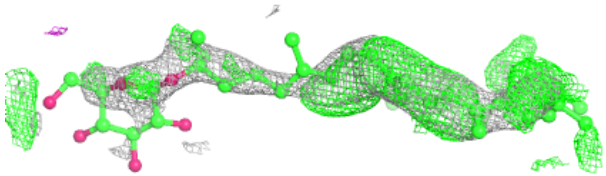


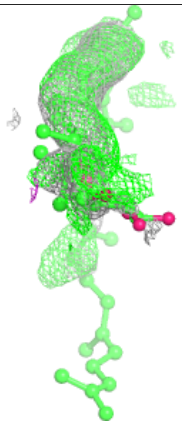


Electron density around RG1 C 405:

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

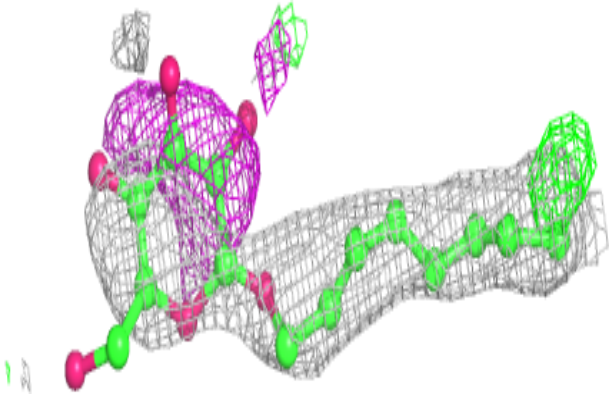


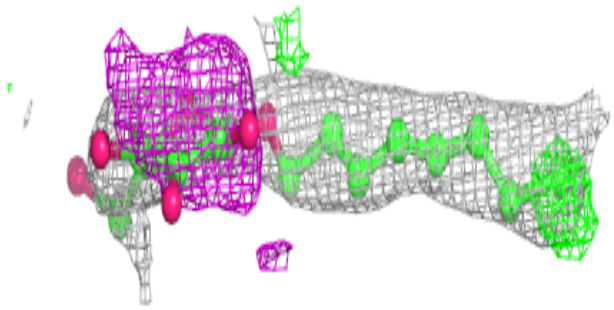


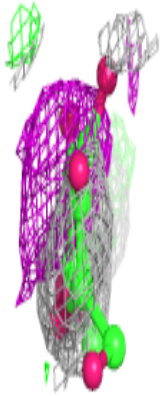


Electron density around BOG C 504:

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

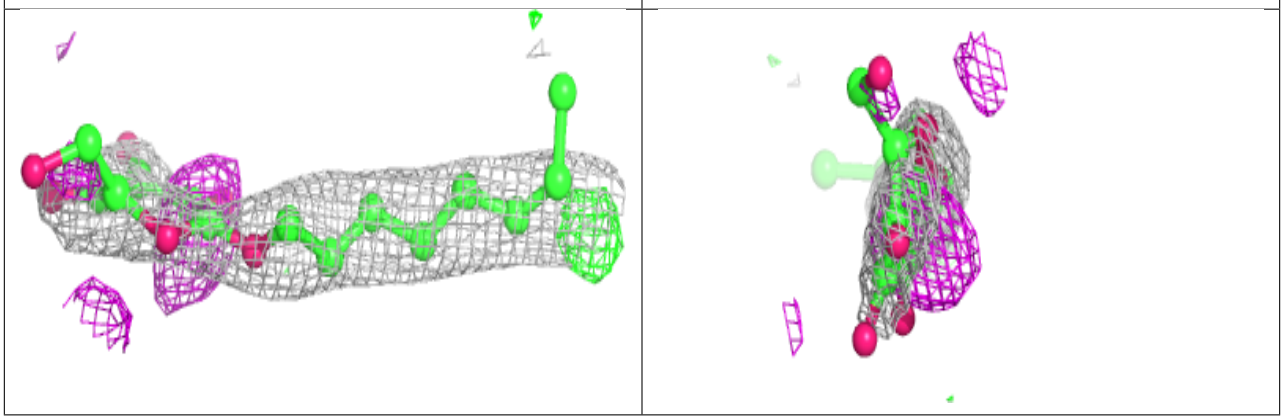






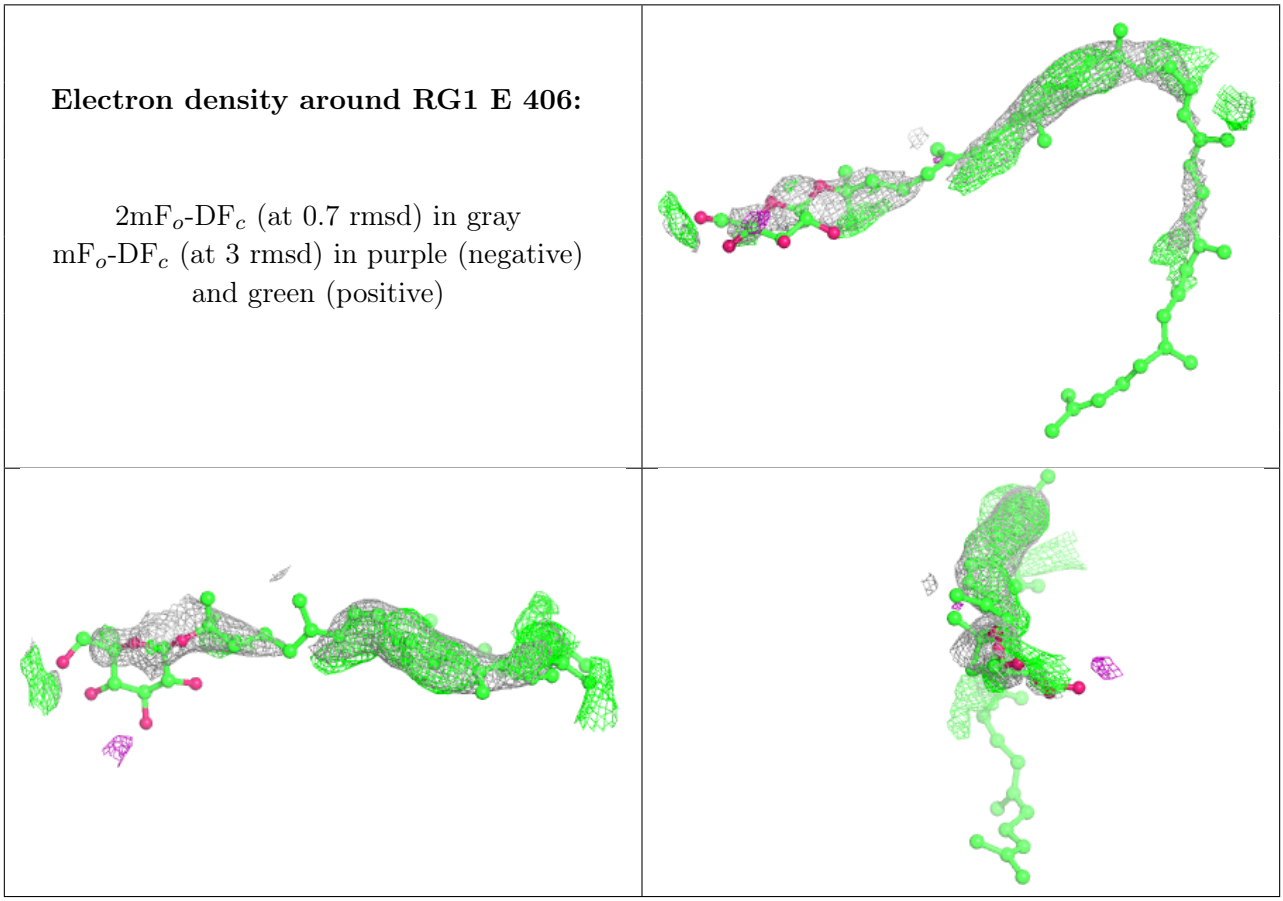
Electron density around BOG E 506:

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



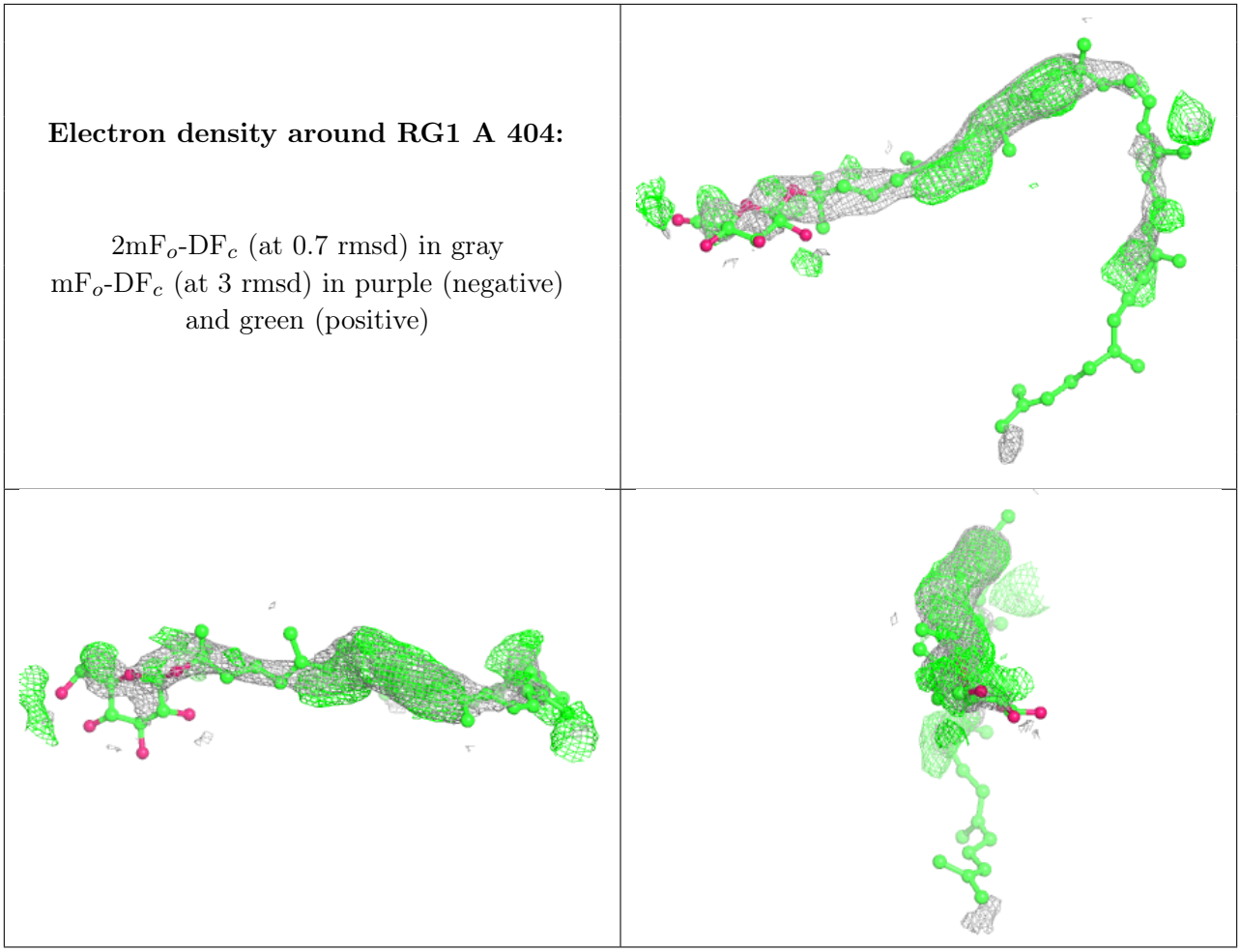
Electron density around RG1 E 406:

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



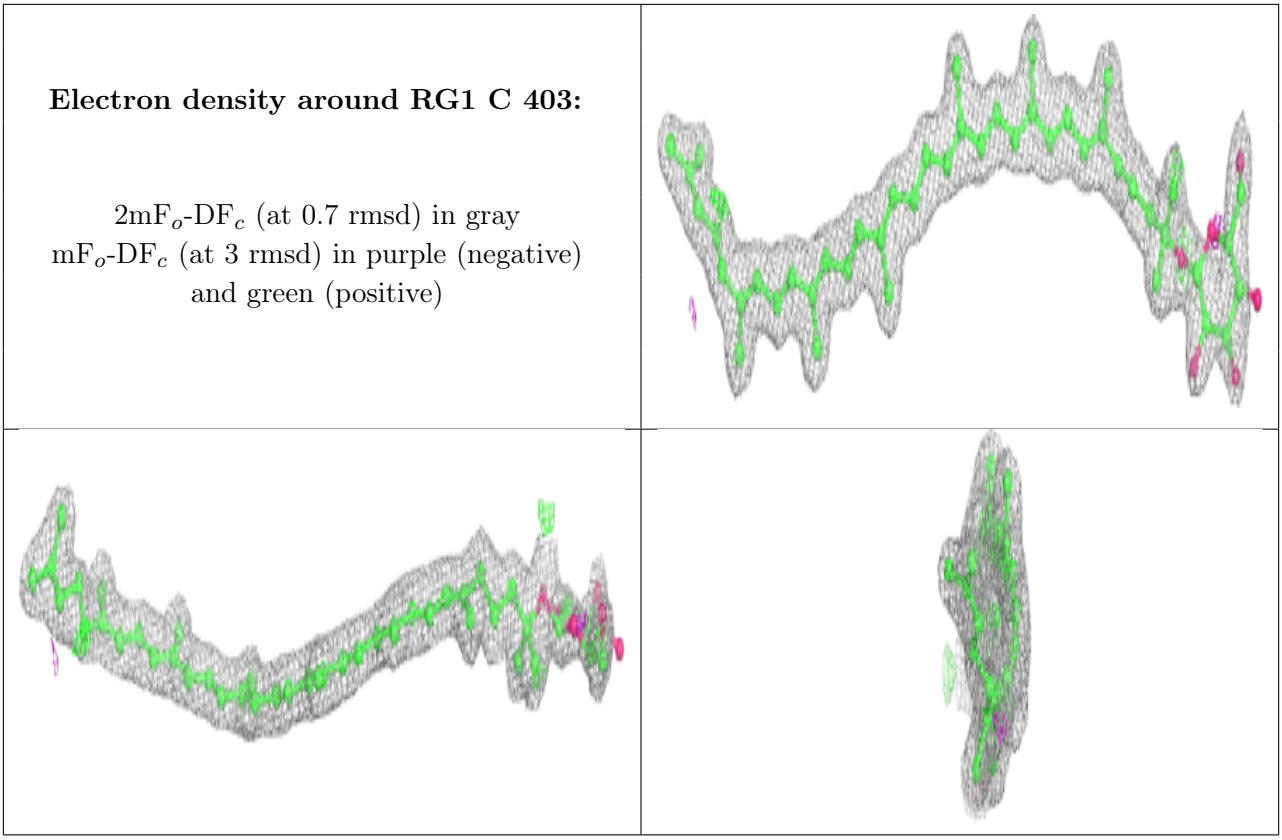
Electron density around RG1 A 404:

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



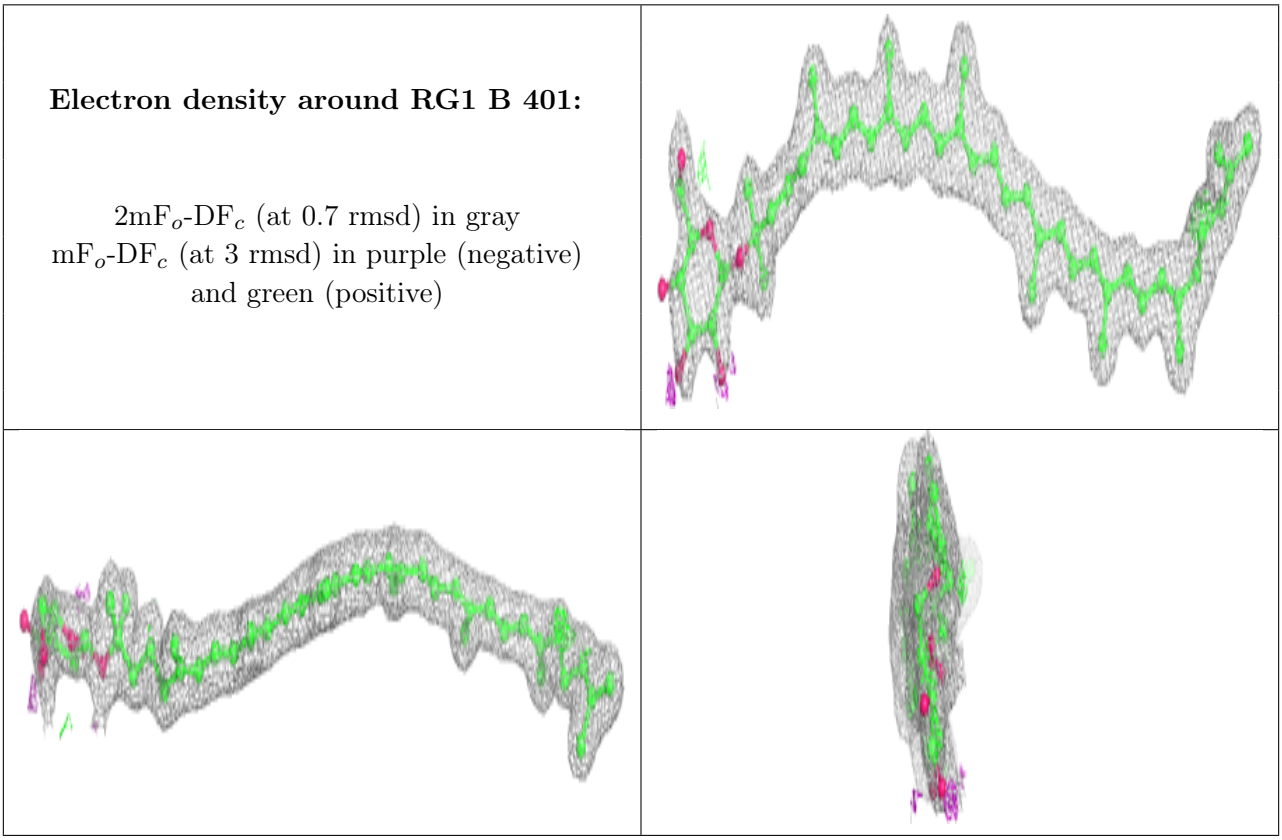
Electron density around RG1 C 403:

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



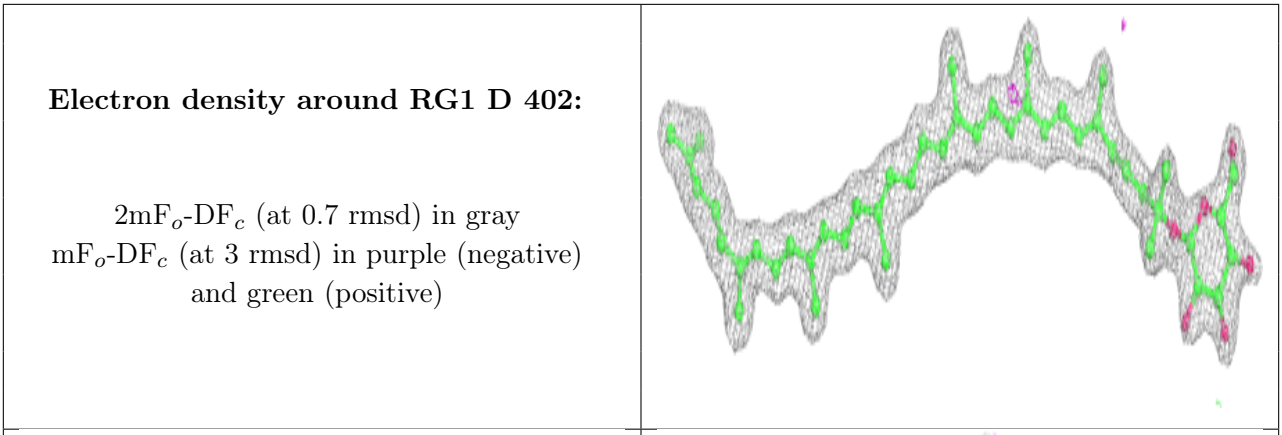
Electron density around RG1 B 401:

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



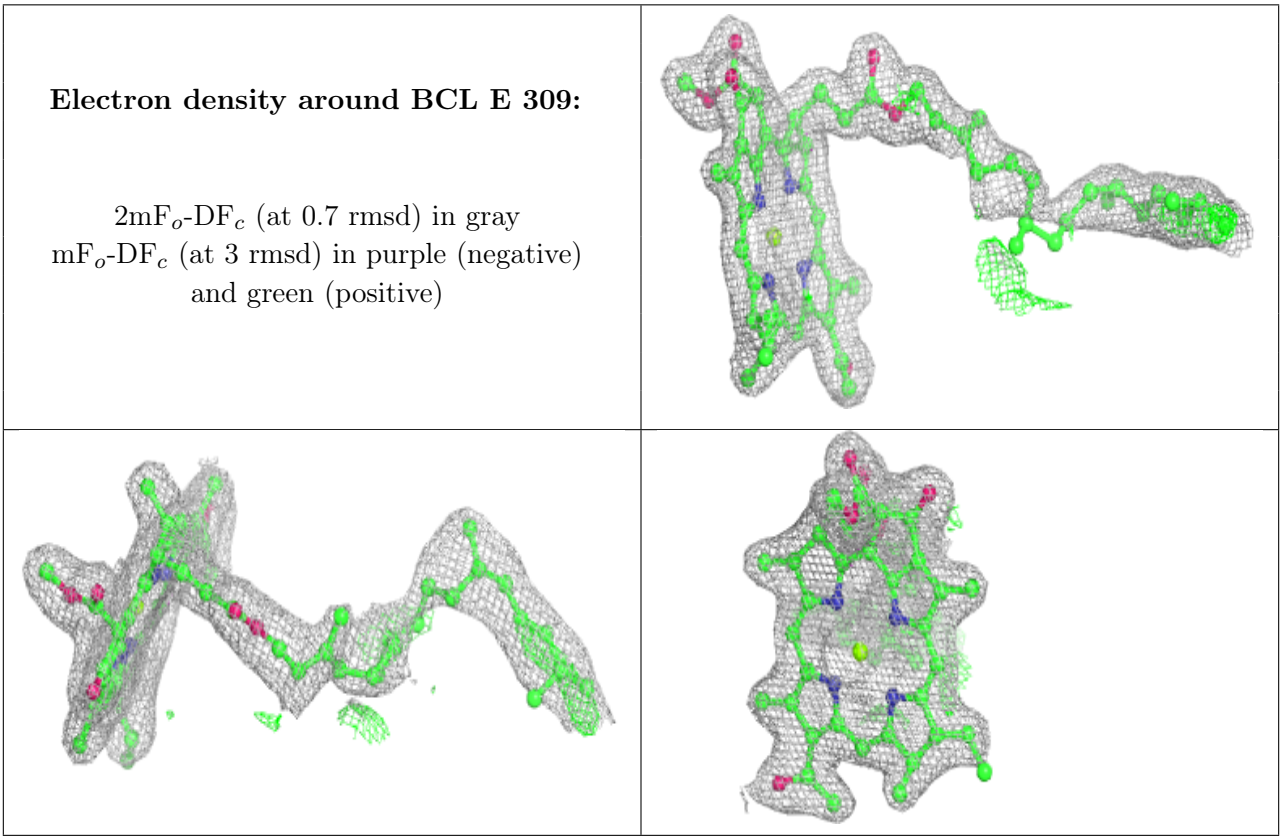
Electron density around RG1 D 402:

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



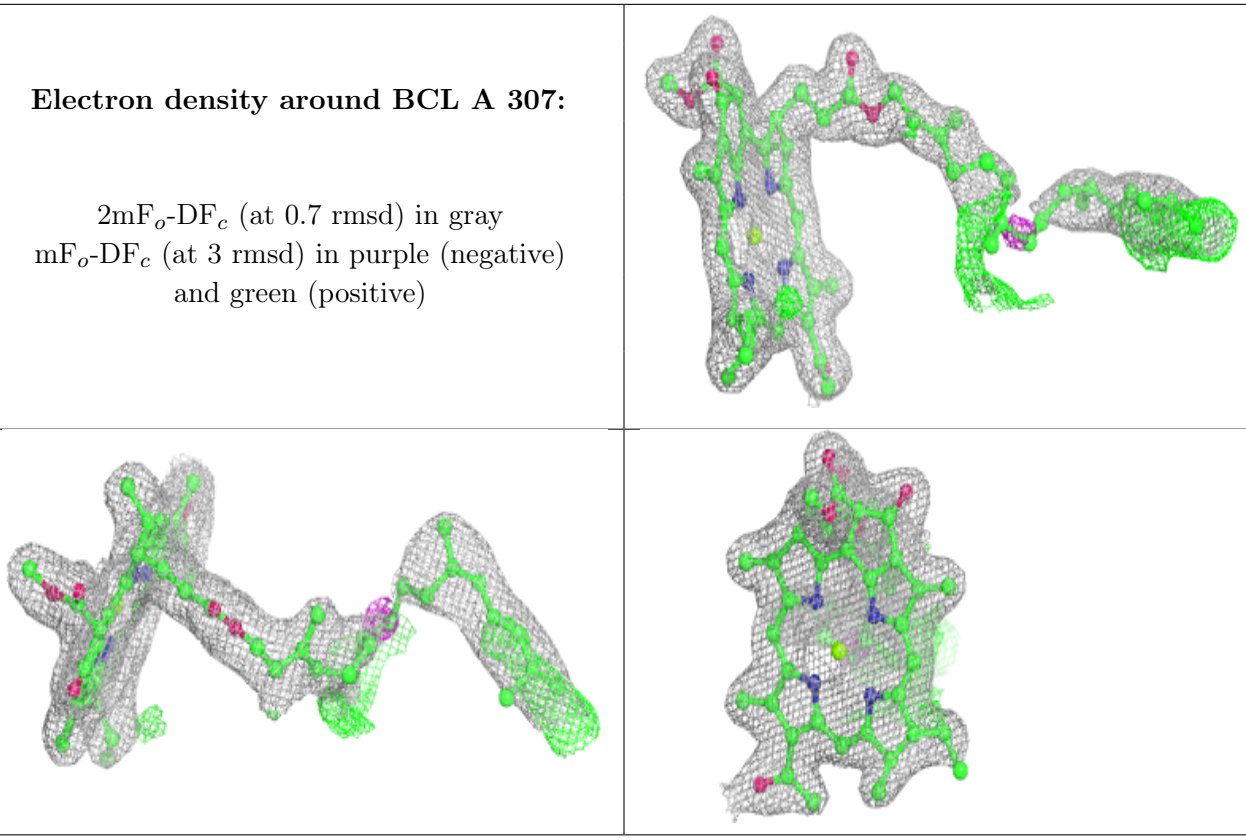
Electron density around BCL E 309:

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



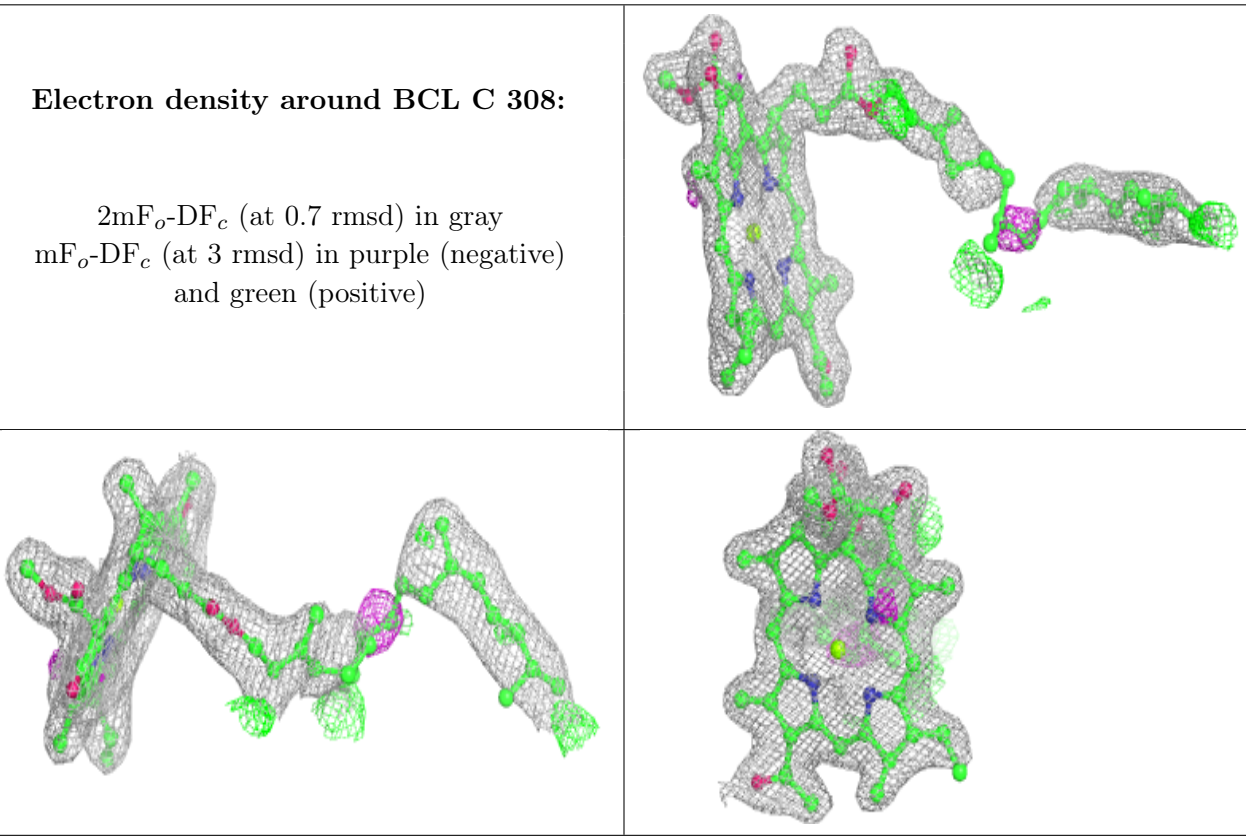
Electron density around BCL A 307:

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



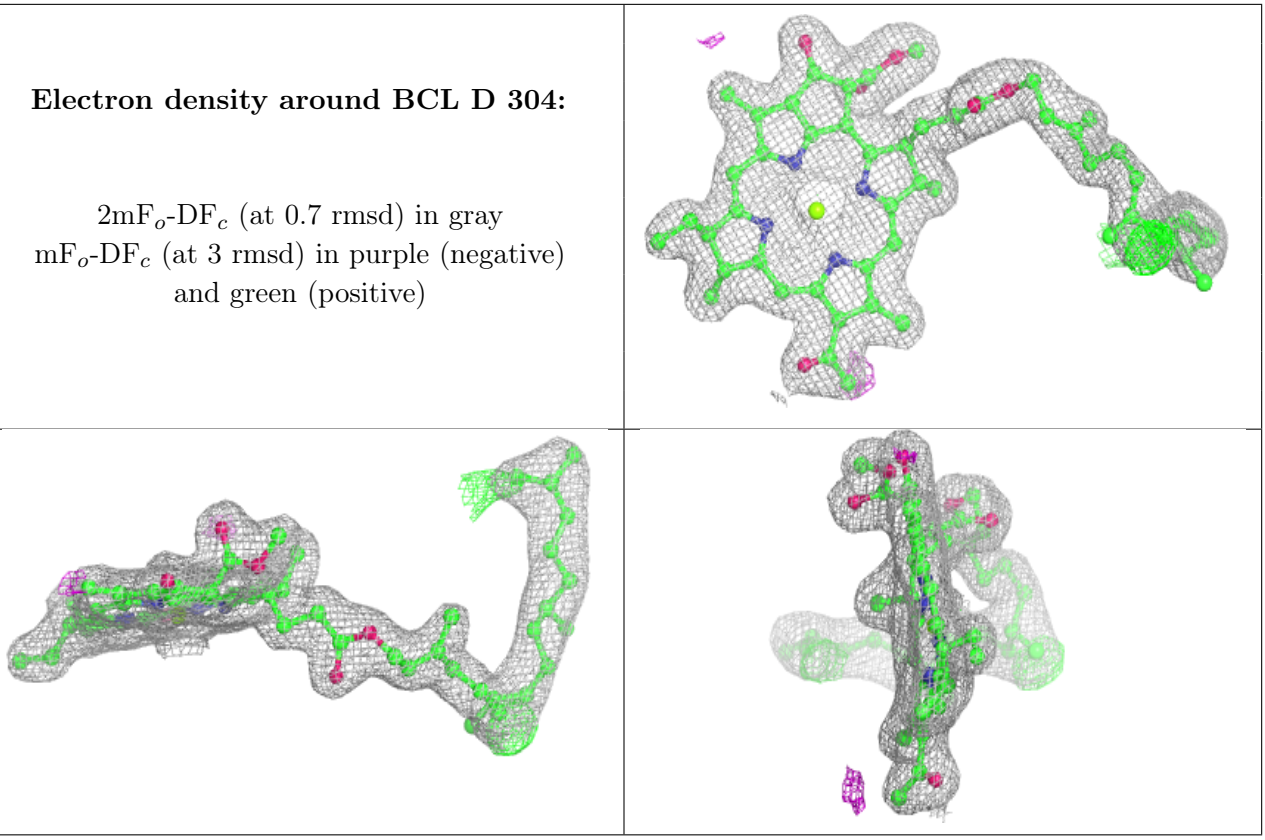
Electron density around BCL C 308:

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



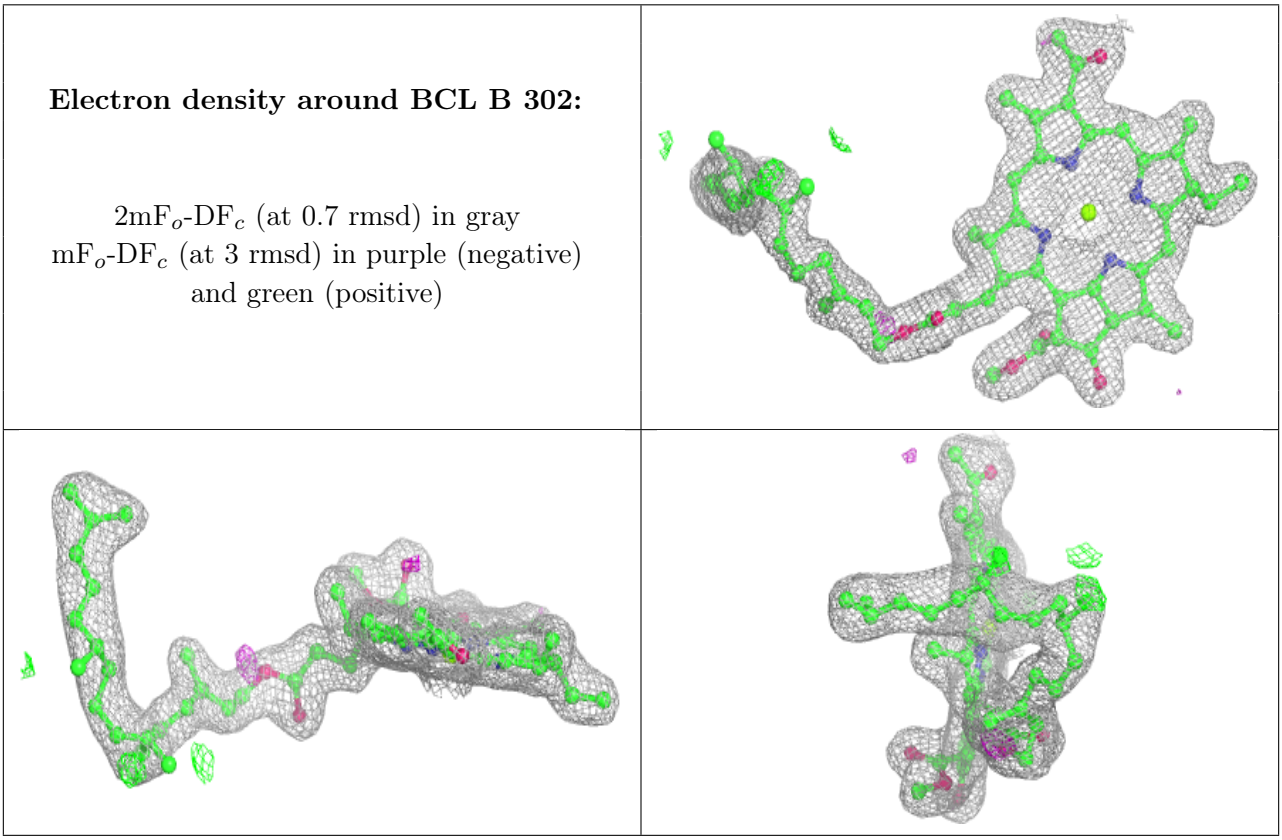
Electron density around BCL D 304:

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



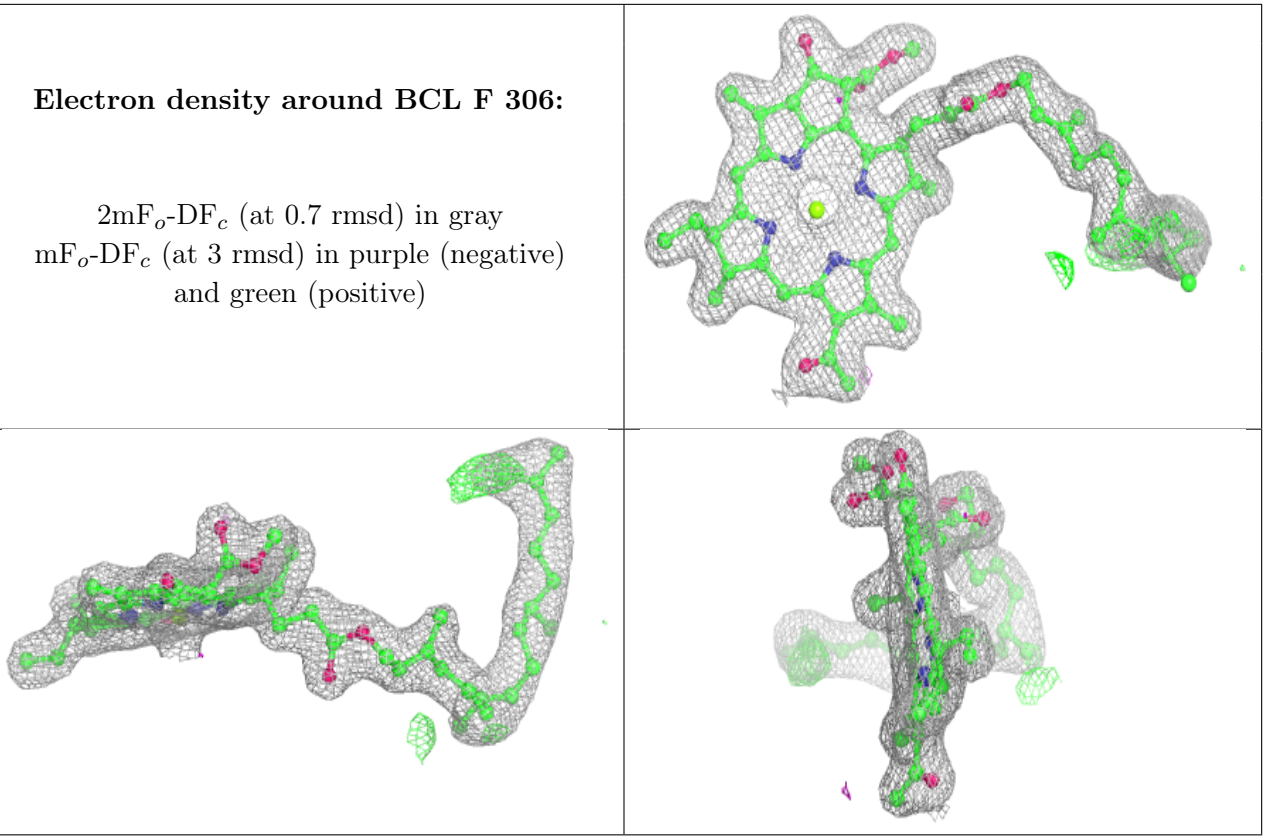
Electron density around BCL B 302:

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



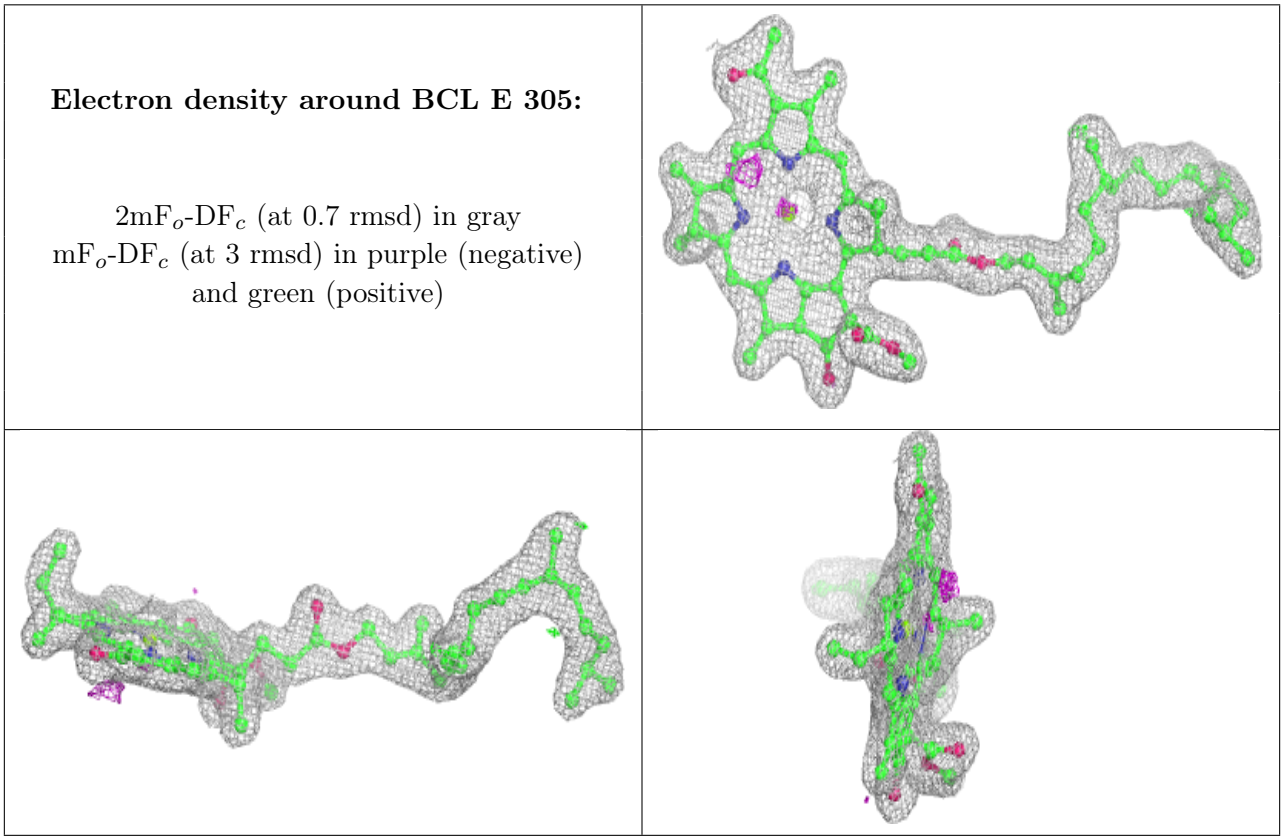
Electron density around BCL F 306:

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



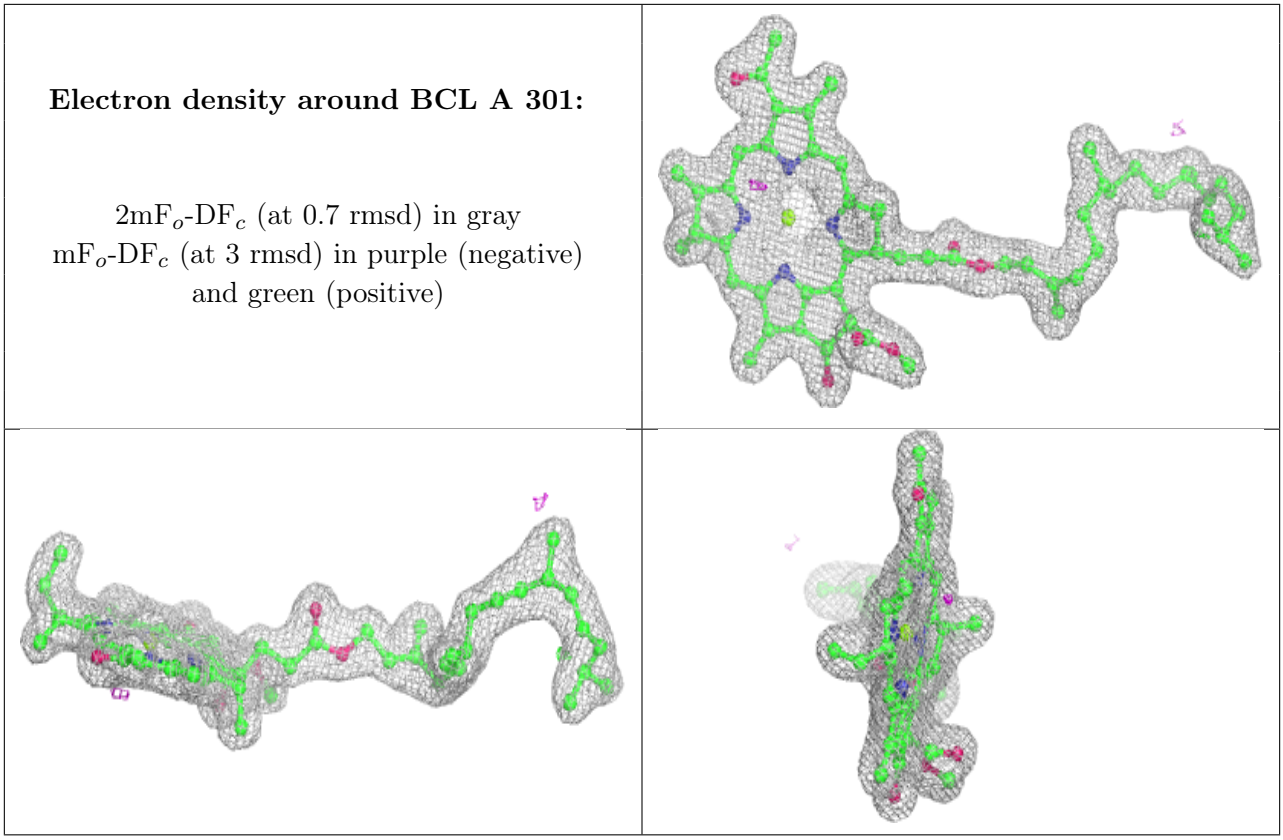
Electron density around BCL E 305:

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



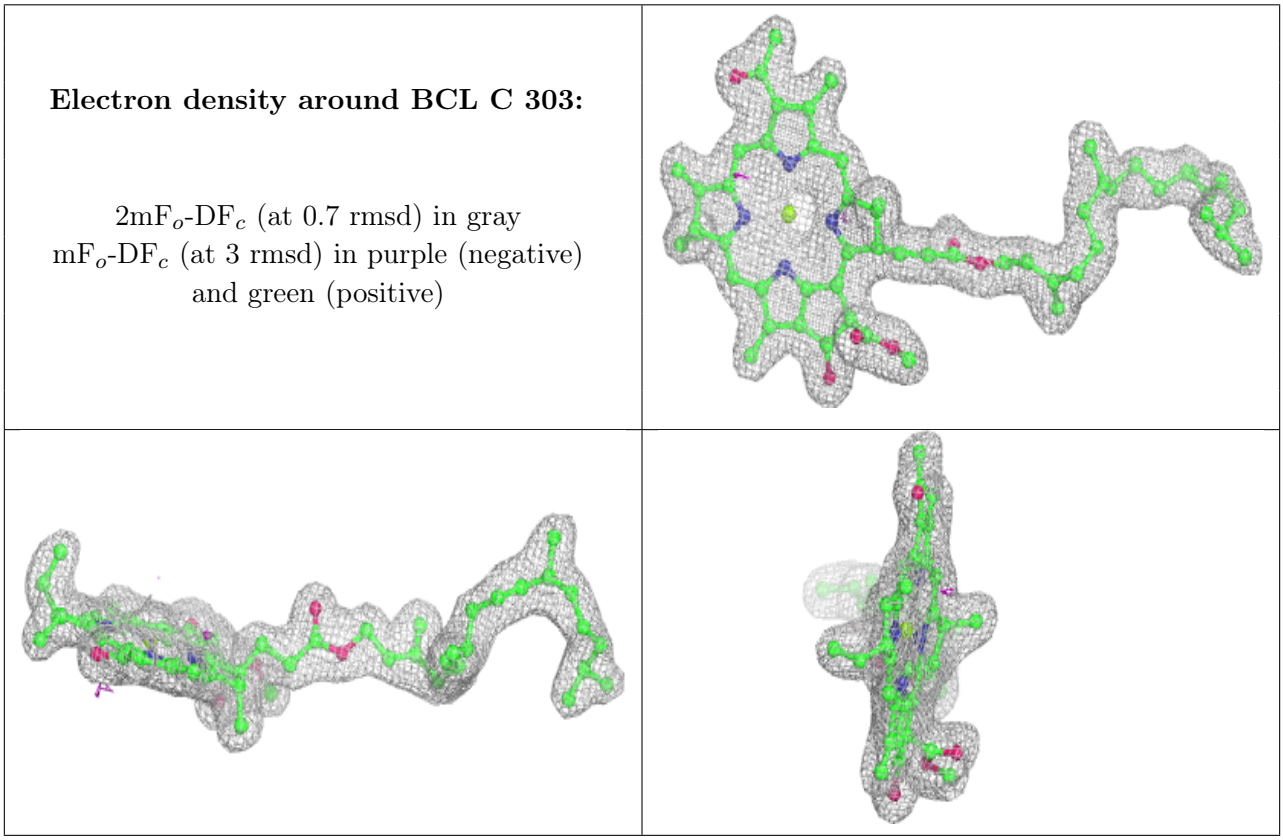
Electron density around BCL A 301:

$2mF_o$-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 C 303:

$2mF_o$-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.