wwPDB X-ray Structure Validation Summary Report (i)

Feb 8, 2024 – 08:37 AM EST

PDB ID	:	2HIT
Title	:	Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylethanolamine
Authors	:	Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on	:	2006-06-29
Resolution	:	2.75 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:

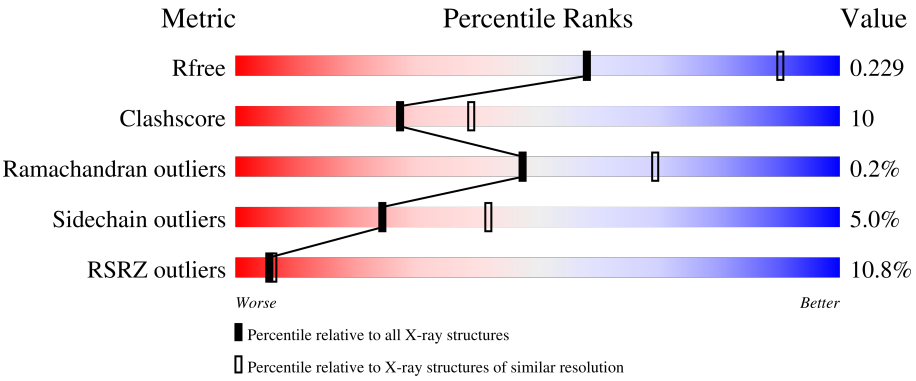
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	L	281	9% 86% 12% ·
2	M	307	14% 79% 18% ··
3	H	260	8% 77% 14% · 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
10	PO4	M	706	-	-	-	X
11	CDL	M	800	-	-	-	X
12	PEW	M	802	-	-	-	X
13	LDA	H	901	-	-	X	X
13	LDA	H	903	-	-	-	X
13	LDA	H	904	-	-	-	X
13	LDA	M	902	-	-	-	X
13	LDA	M	907	-	-	-	X
13	LDA	M	920	-	-	X	X
15	PEV	H	801[A]	-	-	-	X
15	PEV	H	801[B]	-	-	-	X
6	U10	L	502	-	-	-	X
9	CL	H	703	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 7851 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 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	281	2256	1523	360	365	8	0	4	0

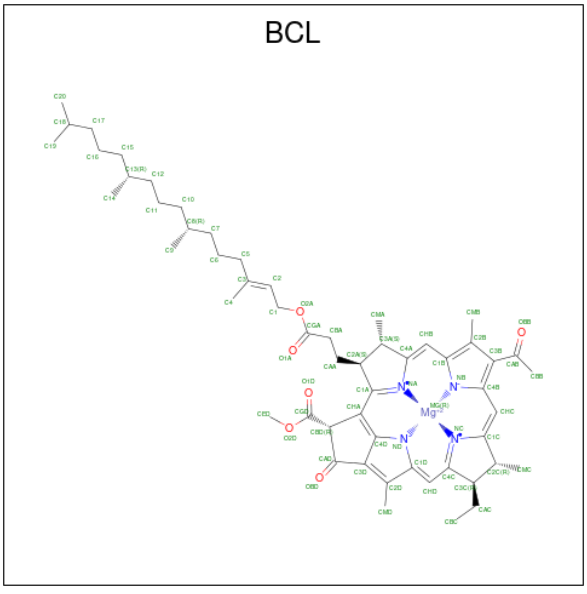
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2477	1650	405	411	11	0	12	0

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

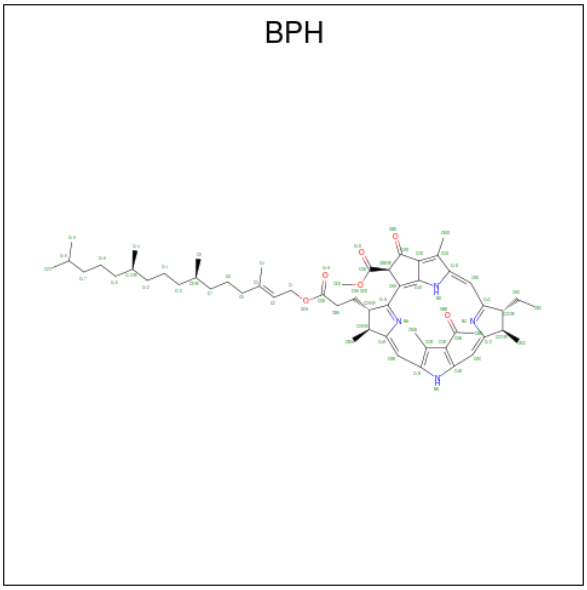
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	243	1876	1199	323	343	11	0	6	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



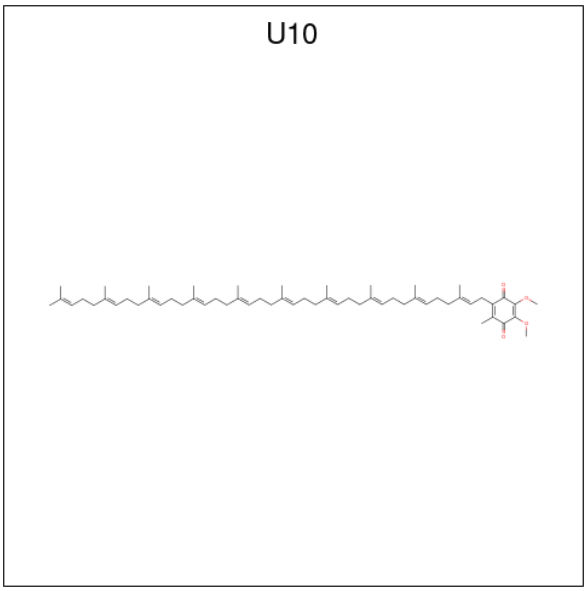
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



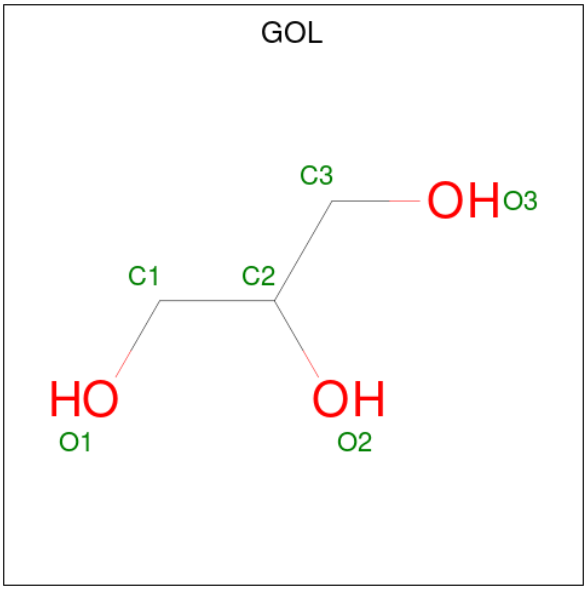
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 48 44 4	0	0
6	M	1	Total C O 48 44 4	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 6 3 3	0	0
7	H	1	Total C O 6 3 3	0	0

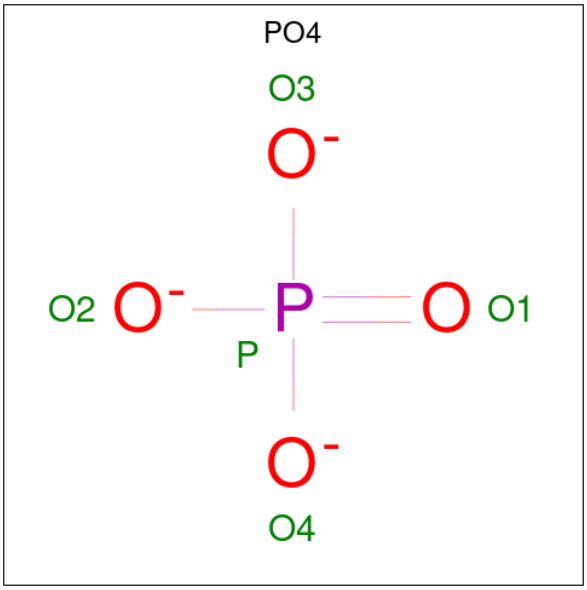
- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

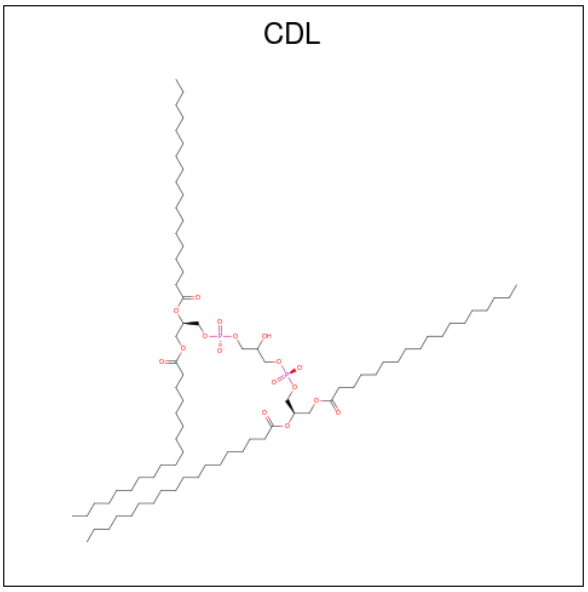
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	2	Total Cl 2 2	0	0
9	H	1	Total Cl 1 1	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



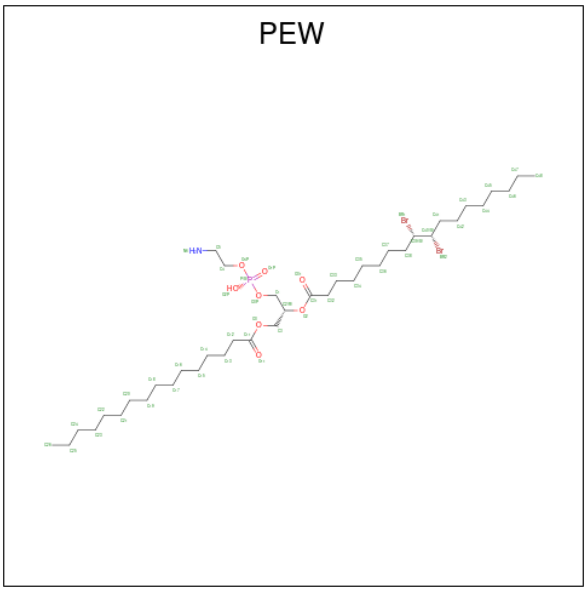
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total O P 5 4 1	0	0
10	M	1	Total O P 5 4 1	0	0
10	H	1	Total O P 5 4 1	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
11	M	1	81	62	17	2	0	0

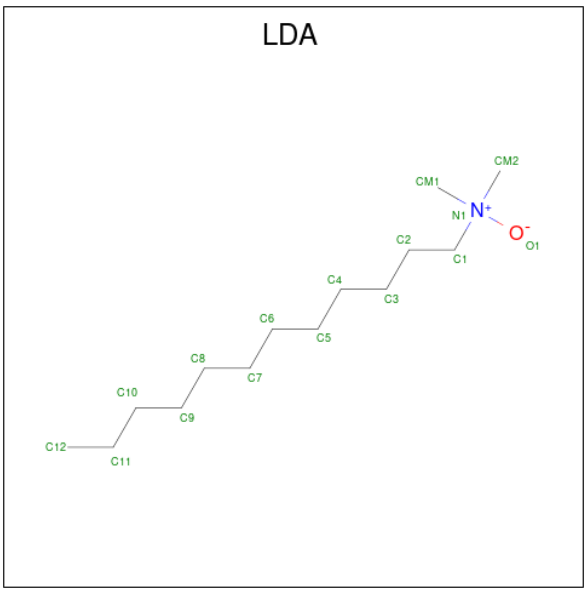
- Molecule 12 is (1R)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (9S,10S)-9,10-DIBROMOOCTADECANOATE (three-letter code: PEW) (formula: $C_{39}H_{76}Br_2NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	P		
12	M	1	51	2	39	1	8	1	0	0

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

$C_{14}H_{31}NO$).

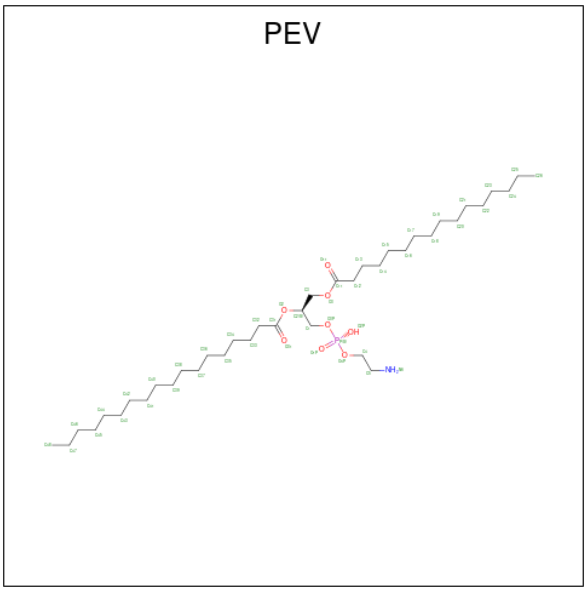


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C N O 16 14 1 1	0	0
13	M	1	Total C N O 16 14 1 1	0	0
13	M	1	Total C N O 16 14 1 1	0	0
13	H	1	Total C N O 16 14 1 1	0	0
13	H	1	Total C N O 16 14 1 1	0	0
13	H	1	Total C N O 16 14 1 1	0	0

- Molecule 14 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	H	1	Total K 1 1	0	0

- Molecule 15 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: $C_{39}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	C	N	O	P	0	1
			98	78	2	16	2		

- Molecule 16 is water.

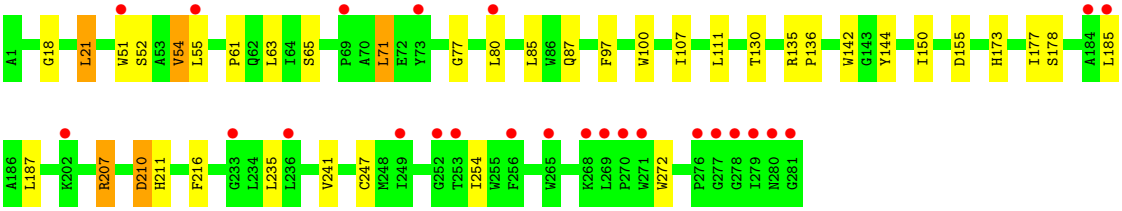
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	91	Total	O	0	0
			91	91		
16	M	118	Total	O	0	0
			118	118		
16	H	185	Total	O	0	0
			185	185		

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.

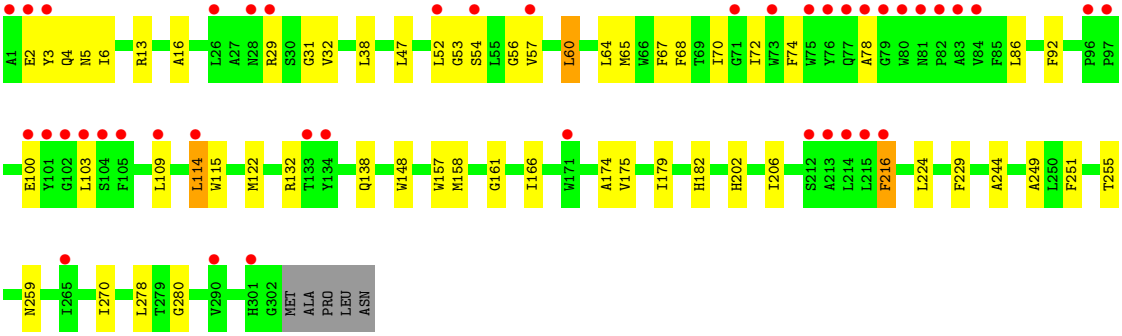
• Molecule 1: Reaction center protein L chain

Chain L:



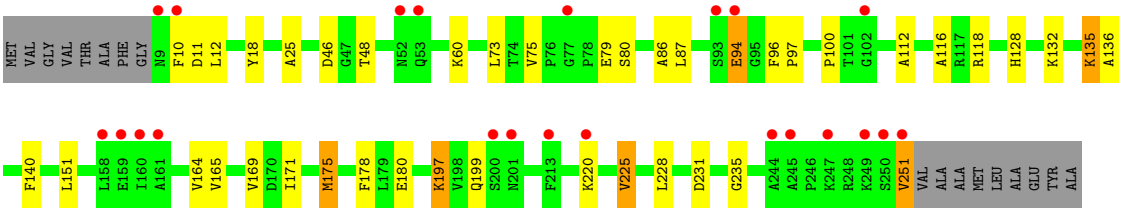
• Molecule 2: Reaction center protein M chain

Chain M:



• Molecule 3: Reaction center protein H chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.29Å 139.29Å 183.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.01 – 2.75 46.01 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.01-2.75) 100.0 (46.01-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.222 0.186 , 0.229	Depositor DCC
R_{free} test set	2689 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	68.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 106.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7851	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, PO4, CDL, GOL, U10, K, CL, BCL, PEW, LDA, BPH, PEV

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	L	0.87	0/2357	0.80	2/3228 (0.1%)
2	M	0.89	0/2617	0.84	2/3569 (0.1%)
3	H	0.92	1/1952 (0.1%)	0.87	3/2653 (0.1%)
All	All	0.89	1/6926 (0.0%)	0.84	7/9450 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	5.10	1.59	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	210	ASP	CB-CG-OD1	9.16	126.55	118.30
2	M	29	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	M	29	ARG	NE-CZ-NH2	-5.93	117.34	120.30
3	H	118[A]	ARG	NE-CZ-NH1	-5.49	117.55	120.30
3	H	118[B]	ARG	NE-CZ-NH1	-5.49	117.55	120.30

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	L	2256	0	2215	32	0
2	M	2477	0	2381	47	0
3	H	1876	0	1893	28	0
4	L	132	0	148	10	0
4	M	132	0	148	14	0
5	L	65	0	76	3	0
5	M	65	0	76	9	0
6	L	48	0	63	7	0
6	M	48	0	63	0	0
7	H	6	0	8	1	0
7	L	6	0	8	0	0
8	M	1	0	0	0	0
9	H	1	0	0	0	0
9	M	2	0	0	0	0
10	H	5	0	0	1	0
10	M	10	0	0	2	0
11	M	81	0	106	2	0
12	M	51	0	73	11	0
13	H	48	0	93	17	0
13	M	48	0	93	13	0
14	H	1	0	0	0	0
15	H	98	0	154	13	0
16	H	185	0	0	6	0
16	L	91	0	0	1	0
16	M	118	0	0	0	0
All	All	7851	0	7598	152	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 10.

The worst 5 of 152 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:L:135[B]:ARG:HB3	1:L:136:PRO:HD3	1.18	1.16
11:M:800:CDL:H231	13:H:904:LDA:HM12	1.28	1.15
15:H:801[B]:PEV:H442	13:H:901:LDA:H121	1.10	1.05
1:L:135[B]:ARG:HB3	1:L:136:PRO:CD	1.87	1.02
1:L:135[B]:ARG:HG3	1:L:135[B]:ARG:HH21	1.28	0.95

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	L	283/281 (101%)	268 (95%)	14 (5%)	1 (0%)	34 53
2	M	313/307 (102%)	299 (96%)	14 (4%)	0	100 100
3	H	247/260 (95%)	237 (96%)	9 (4%)	1 (0%)	34 53
All	All	843/848 (99%)	804 (95%)	37 (4%)	2 (0%)	47 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	86	ALA
1	L	54	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	224/220 (102%)	214 (96%)	10 (4%)	27 46
2	M	249/240 (104%)	236 (95%)	13 (5%)	23 39
3	H	204/208 (98%)	191 (94%)	13 (6%)	17 31
All	All	677/668 (101%)	641 (95%)	36 (5%)	24 38

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	135	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	251	VAL
3	H	175	MET
3	H	220	LYS
2	M	60[A]	LEU

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

Mol	Chain	Res	Type
2	M	4	GLN
2	M	28	ASN
2	M	202	HIS
3	H	9	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CDL	M	800	-	80,80,99	1.30	5 (6%)	86,92,111	1.25	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	L	707	-	5,5,5	0.46	0	5,5,5	0.57	0
4	BCL	L	312	1	64,74,74	1.31	5 (7%)	78,115,115	1.35	11 (14%)
13	LDA	H	903	-	12,15,15	1.97	1 (8%)	14,17,17	0.56	0
4	BCL	L	314	1	64,74,74	1.05	4 (6%)	78,115,115	1.85	21 (26%)
5	BPH	L	402	-	51,70,70	1.14	5 (9%)	52,101,101	1.75	12 (23%)
13	LDA	H	901	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
10	PO4	M	706	-	4,4,4	0.91	0	6,6,6	0.90	0
10	PO4	M	704	-	4,4,4	0.64	0	6,6,6	1.71	2 (33%)
6	U10	M	501	-	48,48,63	1.17	3 (6%)	58,61,79	1.55	11 (18%)
5	BPH	M	401	-	51,70,70	0.83	1 (1%)	52,101,101	2.07	17 (32%)
6	U10	L	502	-	48,48,63	1.22	3 (6%)	58,61,79	1.75	13 (22%)
10	PO4	H	705	-	4,4,4	1.05	0	6,6,6	0.66	0
7	GOL	H	708	-	5,5,5	0.31	0	5,5,5	0.68	0
13	LDA	M	902	-	12,15,15	1.86	1 (8%)	14,17,17	0.59	0
13	LDA	H	904	-	12,15,15	2.00	1 (8%)	14,17,17	0.57	0
4	BCL	M	311	2	64,74,74	1.25	5 (7%)	78,115,115	1.53	15 (19%)
15	PEV	H	801[B]	-	48,48,48	0.95	2 (4%)	51,53,53	1.05	4 (7%)
4	BCL	M	313	2	64,74,74	1.40	5 (7%)	78,115,115	1.82	17 (21%)
13	LDA	M	907	-	12,15,15	2.00	1 (8%)	14,17,17	0.70	0
12	PEW	M	802	-	50,50,50	0.96	3 (6%)	53,57,57	1.32	5 (9%)
15	PEV	H	801[A]	-	48,48,48	0.91	1 (2%)	51,53,53	1.04	4 (7%)
13	LDA	M	920	-	12,15,15	1.93	1 (8%)	14,17,17	1.11	1 (7%)

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
11	CDL	M	800	-	-	37/91/91/110	-
7	GOL	L	707	-	-	4/4/4/4	-
4	BCL	L	312	1	-	5/37/137/137	-
13	LDA	H	903	-	-	2/13/13/13	-
4	BCL	L	314	1	-	6/37/137/137	-
5	BPH	L	402	-	-	5/37/105/105	0/5/6/6
13	LDA	H	901	-	-	6/13/13/13	-
6	U10	M	501	-	-	6/45/69/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	M	401	-	-	16/37/105/105	0/5/6/6
6	U10	L	502	-	-	13/45/69/87	0/1/1/1
7	GOL	H	708	-	-	1/4/4/4	-
13	LDA	M	902	-	-	3/13/13/13	-
13	LDA	H	904	-	-	6/13/13/13	-
4	BCL	M	311	2	-	11/37/137/137	-
15	PEV	H	801[B]	-	-	28/52/52/52	-
4	BCL	M	313	2	-	8/37/137/137	-
13	LDA	M	907	-	-	7/13/13/13	-
12	PEW	M	802	-	-	29/57/57/57	-
15	PEV	H	801[A]	-	-	20/52/52/52	-
13	LDA	M	920	-	-	7/13/13/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	901	LDA	O1-N1	-6.94	1.25	1.42
13	M	907	LDA	O1-N1	-6.83	1.26	1.42
13	H	904	LDA	O1-N1	-6.80	1.26	1.42
13	H	903	LDA	O1-N1	-6.75	1.26	1.42
13	M	920	LDA	O1-N1	-6.63	1.26	1.42

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	401	BPH	OBD-CAD-CBD	-7.03	115.51	125.82
5	L	402	BPH	O2D-CGD-CBD	6.52	119.25	111.00
5	M	401	BPH	O2D-CGD-CBD	6.49	119.22	111.00
6	L	502	U10	C25-C24-C26	6.33	125.93	115.27
12	M	802	PEW	O2-C31-C32	5.37	123.08	111.50

There are no chirality outliers.

5 of 220 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	311	BCL	C11-C12-C13-C14
5	M	401	BPH	C4C-C3C-CAC-CBC
5	M	401	BPH	C2C-C3C-CAC-CBC
7	L	707	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	M	800	CDL	CA2-C1-CB2-OB2

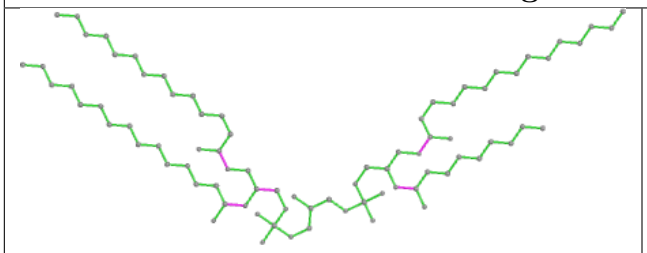
There are no ring outliers.

20 monomers are involved in 78 short contacts:

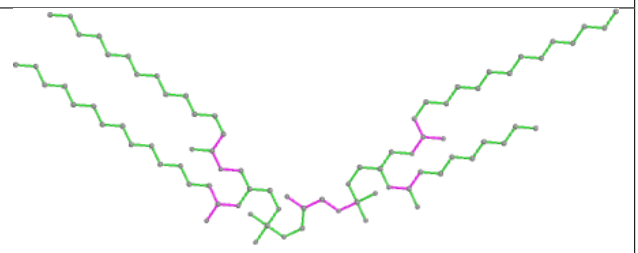
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	800	CDL	2	0
4	L	312	BCL	6	0
13	H	903	LDA	5	0
4	L	314	BCL	4	0
5	L	402	BPH	3	0
13	H	901	LDA	10	0
10	M	706	PO4	1	0
10	M	704	PO4	1	0
5	M	401	BPH	9	0
6	L	502	U10	7	0
10	H	705	PO4	1	0
7	H	708	GOL	1	0
13	M	902	LDA	2	0
13	H	904	LDA	3	0
4	M	311	BCL	5	0
15	H	801[B]	PEV	4	0
4	M	313	BCL	9	0
12	M	802	PEW	11	0
15	H	801[A]	PEV	9	0
13	M	920	LDA	11	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.

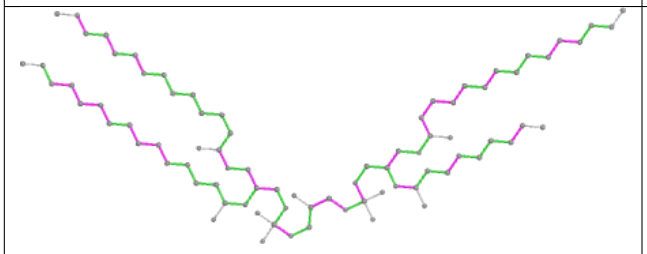
Ligand CDL M 800



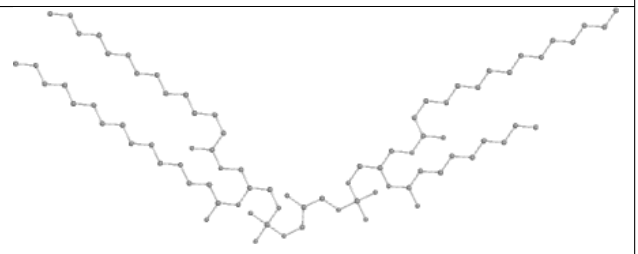
Bond lengths



Bond angles

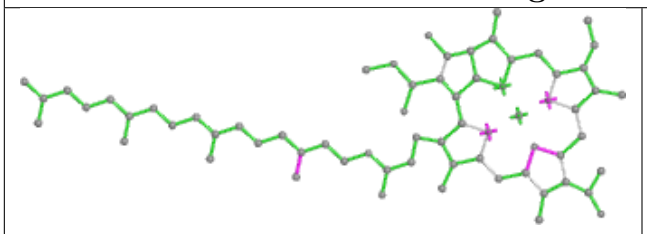


Torsions



Rings

Ligand BCL L 312



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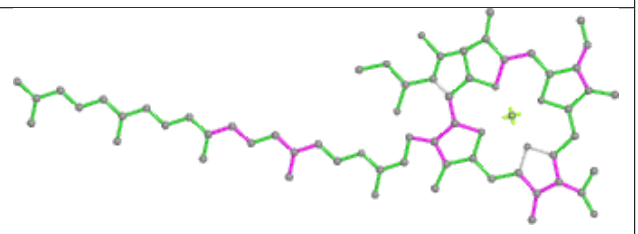
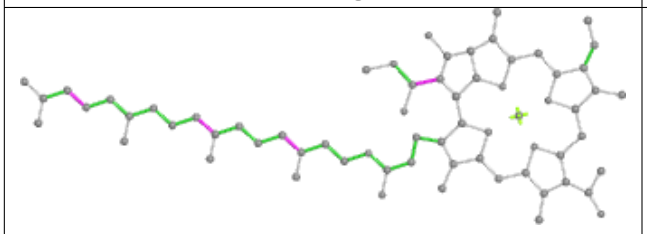


Bond angles



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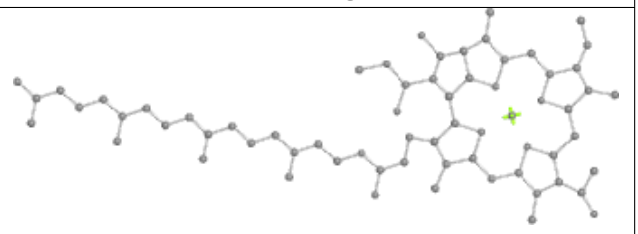
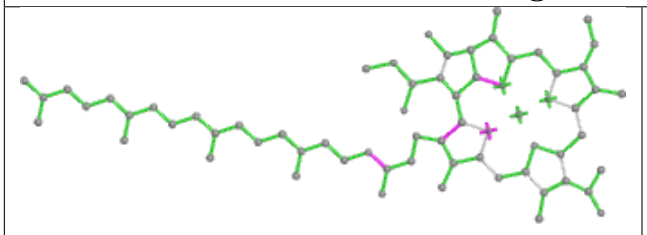


Rings

Ligand BCL L 314



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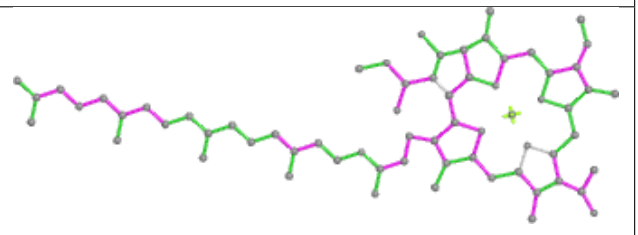
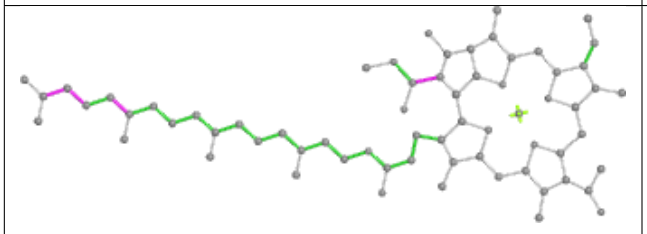


Bond angles



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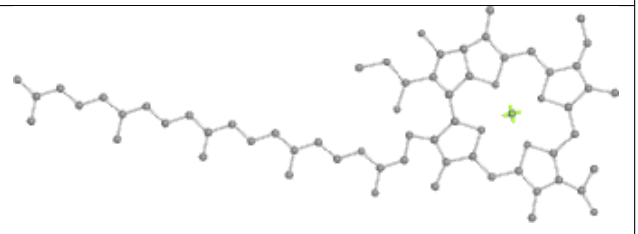
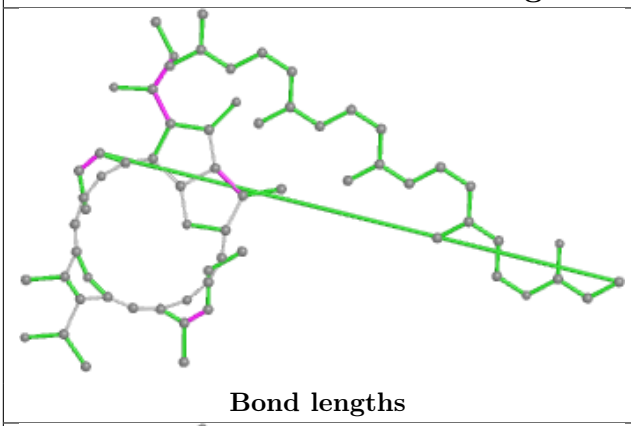
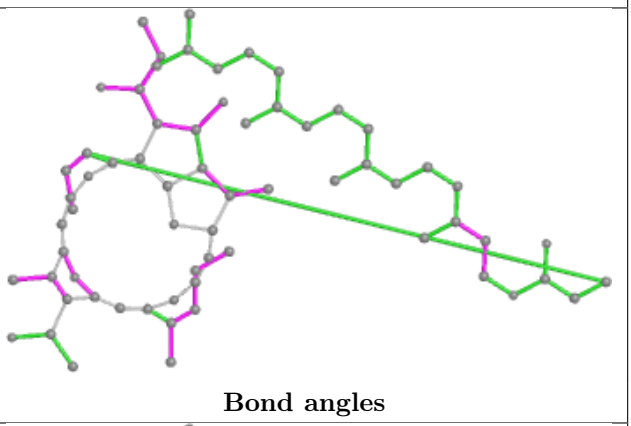


Rings

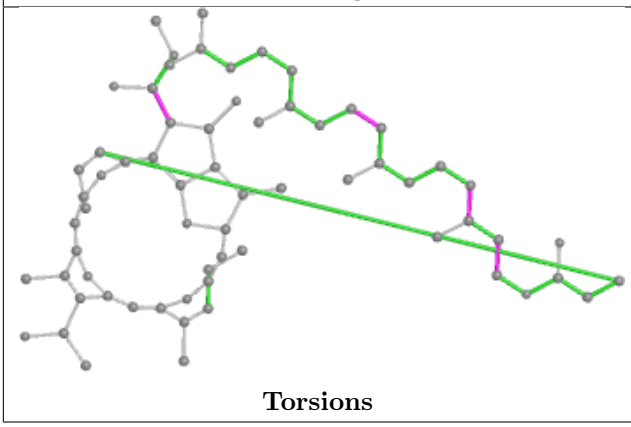
Ligand BPH L 402



Bond lengths



Bond angles



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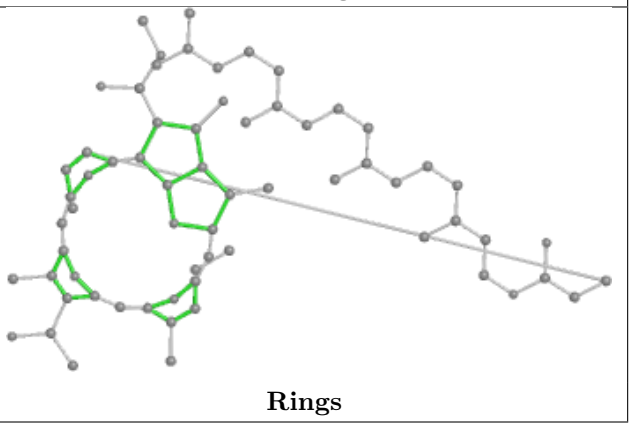
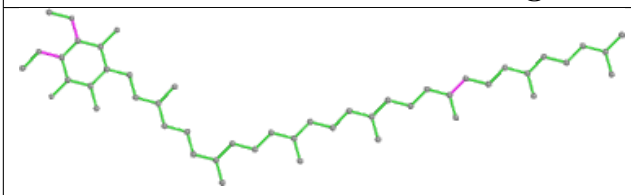
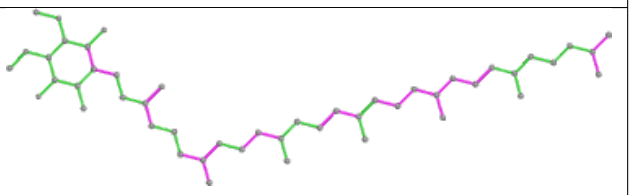


Rings

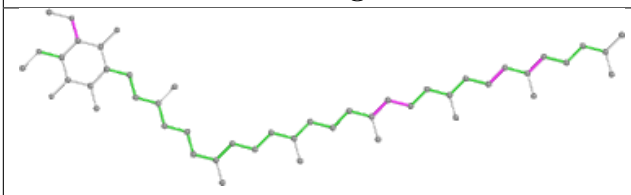
Ligand U10 M 501



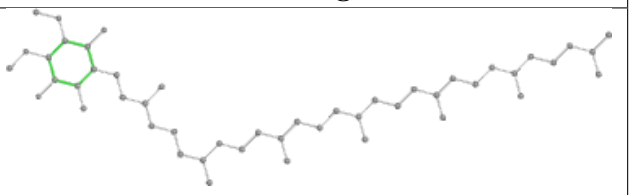
Bond lengths



Bond angles

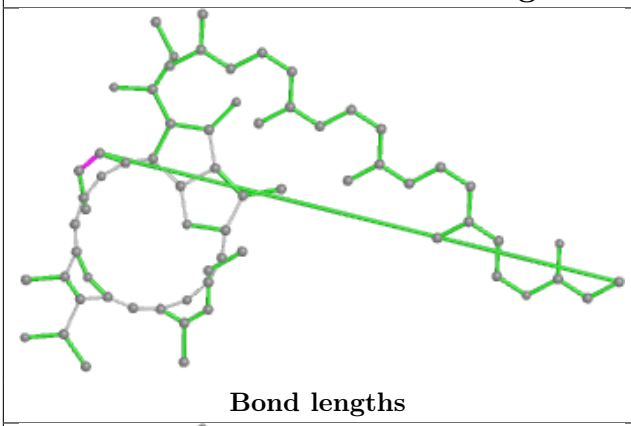


Torsions



Rings

Ligand BPH M 401



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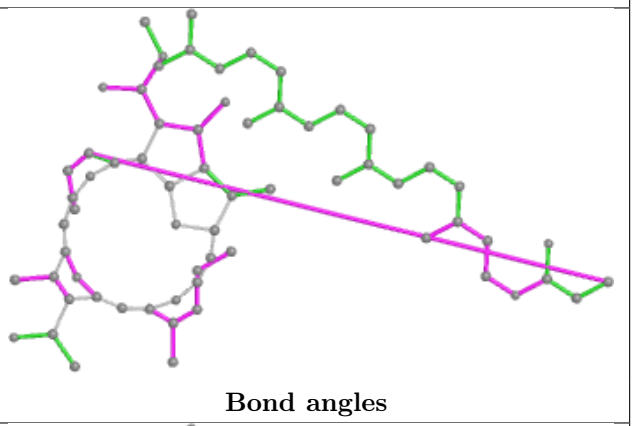
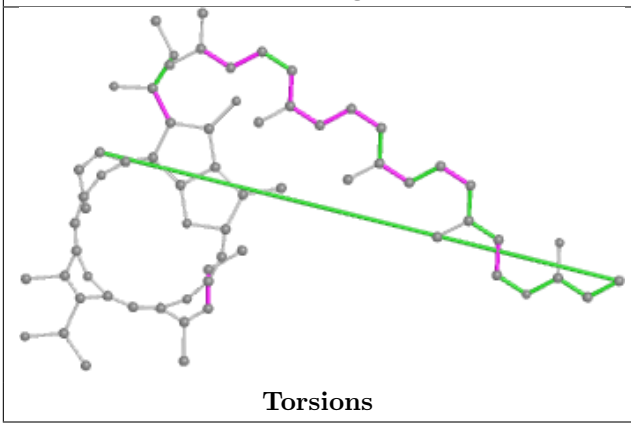


Bond angles



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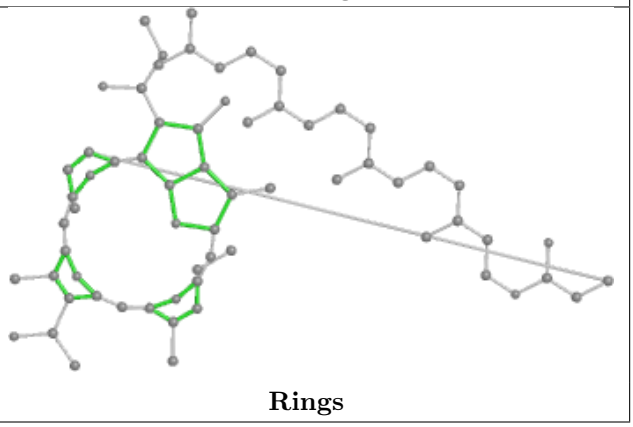
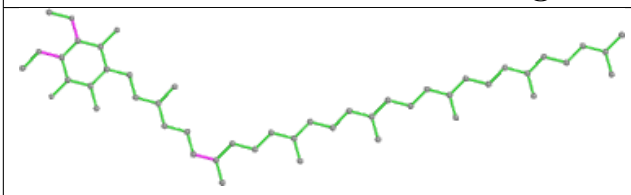


Rings

Ligand U10 L 502



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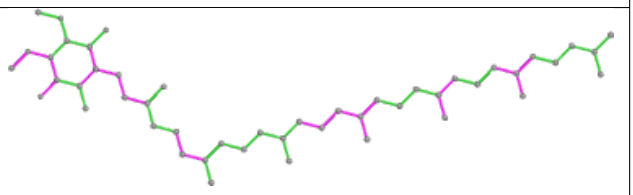
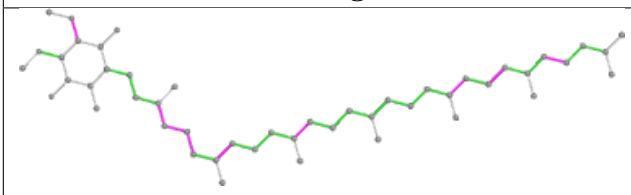


Bond angles



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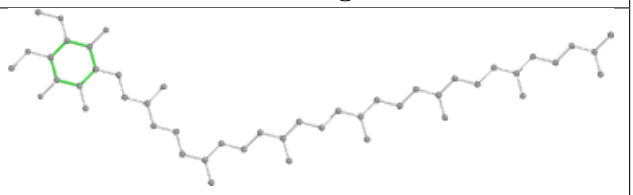
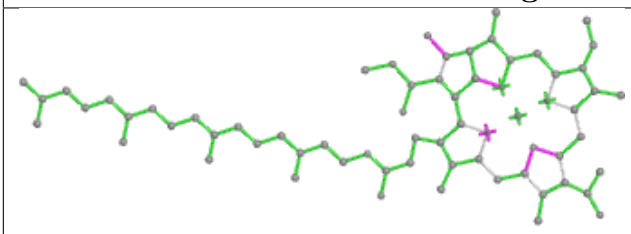


Rings

Ligand BCL M 311



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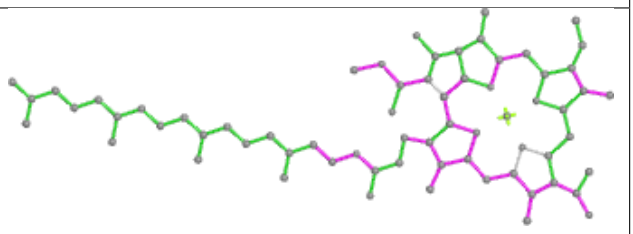

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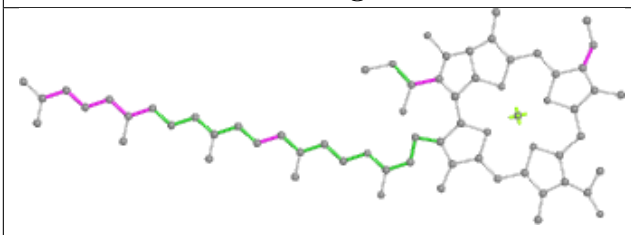

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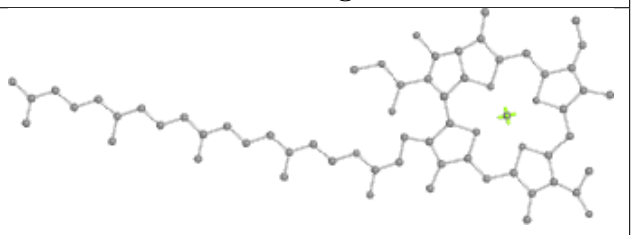
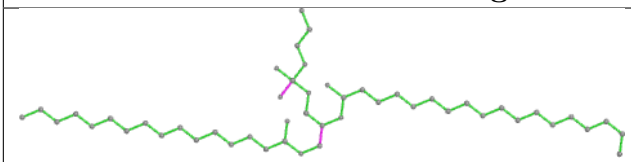
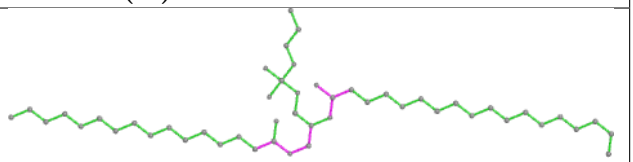


Rings

Ligand PEV H 801 (B)



Bond lengths



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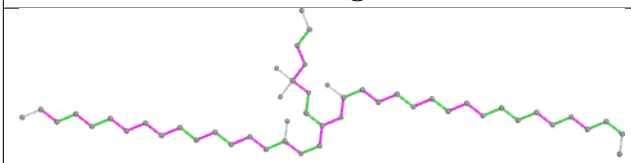
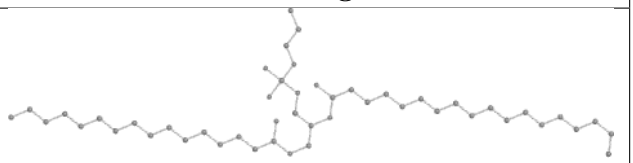
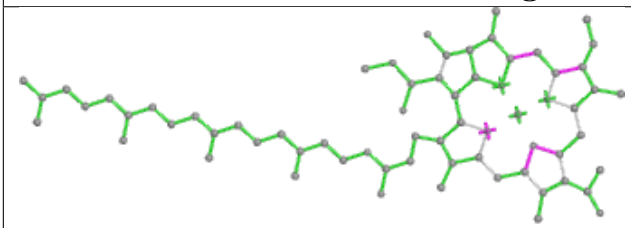


Torsions

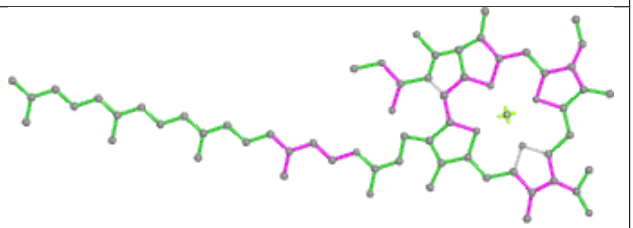


Rings

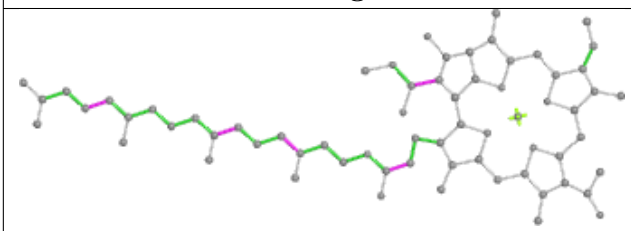
Ligand BCL M 313



Bond lengths



Bond angles



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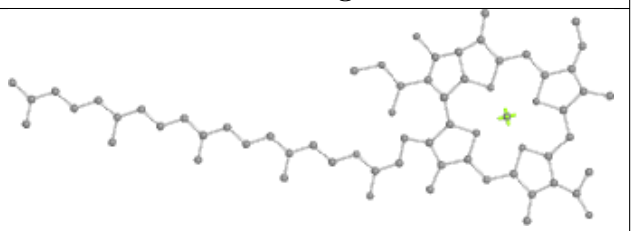
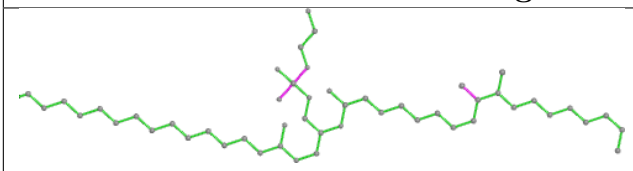
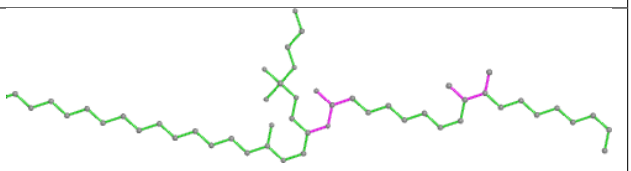
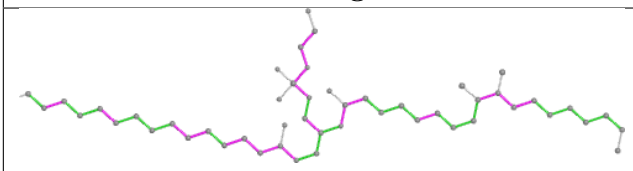


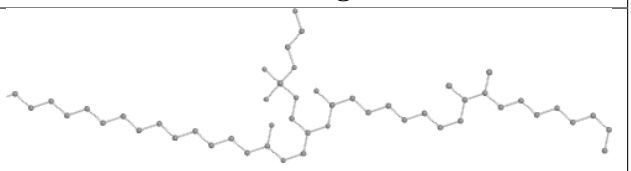
Rings

Ligand PEW M 802

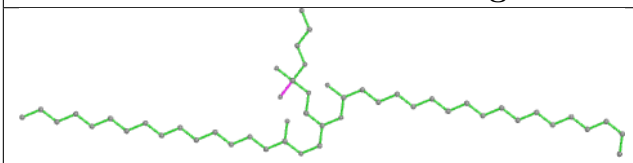

Bond lengths

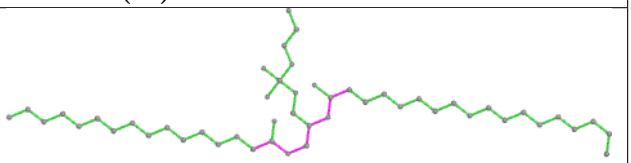

Bond angles

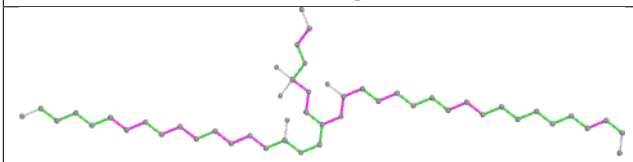

Torsions

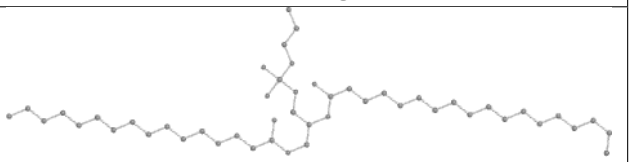

Rings

Ligand PEV H 801 (A)


Bond lengths


Bond angles


Torsions


Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	L	281/281 (100%)	0.35	25 (8%) 9 11	63, 73, 81, 90	0
2	M	302/307 (98%)	0.64	42 (13%) 2 3	63, 72, 82, 106	0
3	H	243/260 (93%)	0.37	22 (9%) 9 10	61, 72, 86, 111	0
All	All	826/848 (97%)	0.46	89 (10%) 5 6	61, 73, 83, 111	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	8.5
3	H	9	ASN	8.4
2	M	80	TRP	6.1
2	M	102	GLY	6.0
2	M	2[A]	GLU	5.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

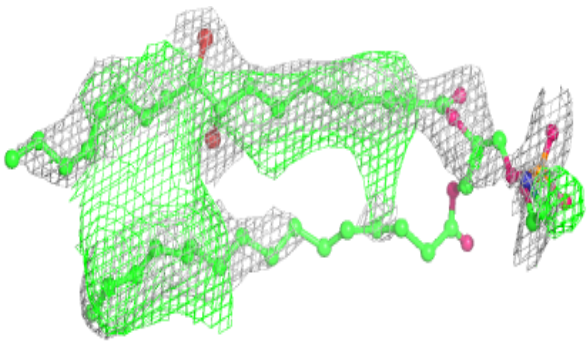
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

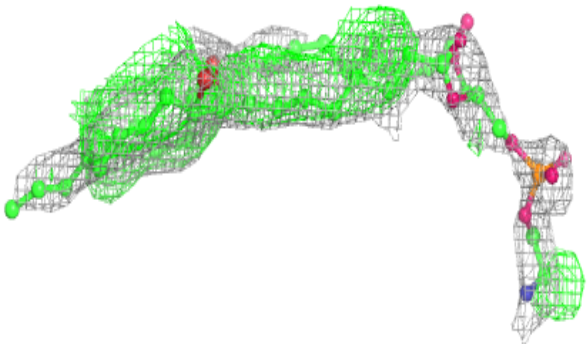
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	LDA	H	903	16/16	0.11	1.17	76,79,84,84	16
13	LDA	H	904	16/16	0.27	0.87	75,78,87,87	16
12	PEW	M	802	51/51	0.31	0.72	62,74,82,84	51
13	LDA	M	902	16/16	0.46	0.79	73,77,87,88	16
10	PO4	M	706	5/5	0.61	0.47	73,73,75,75	5
11	CDL	M	800	81/100	0.68	0.57	51,71,89,91	81
15	PEV	H	801[A]	49/49	0.68	0.96	50,72,79,80	49
15	PEV	H	801[B]	49/49	0.68	0.96	48,75,85,85	49
6	U10	L	502	48/63	0.69	0.58	60,69,77,78	48
13	LDA	M	920	16/16	0.70	0.53	52,61,74,75	16
13	LDA	H	901	16/16	0.73	0.51	74,77,85,86	16
10	PO4	H	705	5/5	0.75	0.39	80,80,80,81	5
9	CL	H	703	1/1	0.78	0.89	72,72,72,72	1
13	LDA	M	907	16/16	0.79	0.42	74,80,85,87	16
6	U10	M	501	48/63	0.84	0.33	64,76,99,100	0
7	GOL	L	707	6/6	0.85	0.53	69,78,79,79	6
10	PO4	M	704	5/5	0.90	0.31	69,69,75,76	5
9	CL	M	702	1/1	0.91	0.40	66,66,66,66	1
5	BPH	M	401	65/65	0.91	0.21	63,75,122,124	0
7	GOL	H	708	6/6	0.91	0.51	75,75,76,76	6
4	BCL	L	312	66/66	0.94	0.19	58,70,77,84	0
4	BCL	L	314	66/66	0.94	0.22	56,68,80,86	0
4	BCL	M	311	66/66	0.94	0.22	64,73,127,128	0
5	BPH	L	402	65/65	0.94	0.22	59,71,75,75	0
4	BCL	M	313	66/66	0.96	0.19	61,69,90,101	0
9	CL	M	701	1/1	0.97	0.23	71,71,71,71	1
14	K	H	700	1/1	0.99	0.10	66,66,66,66	0
8	FE	M	500	1/1	1.00	0.19	72,72,72,72	0

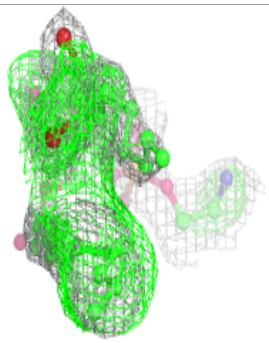
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEW M 802:

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

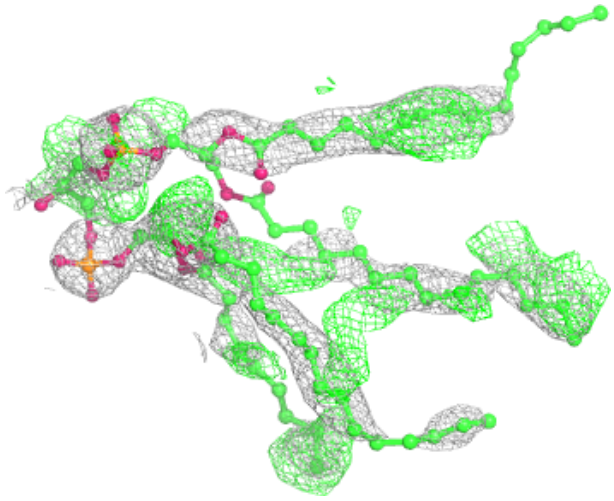


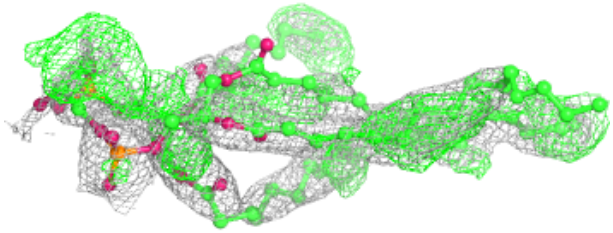


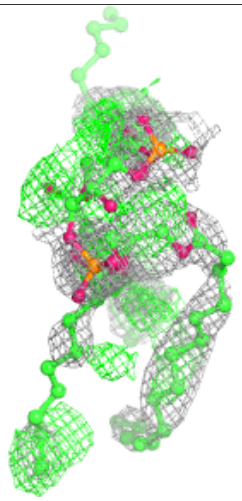


Electron density around CDL M 800:

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

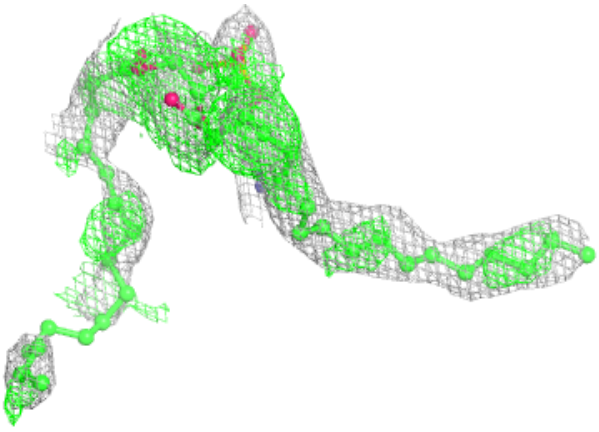


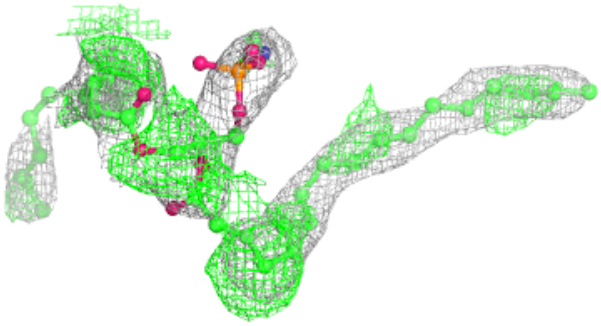


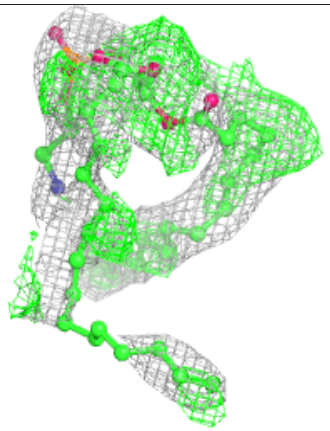


Electron density around PEV H 801 (A):

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

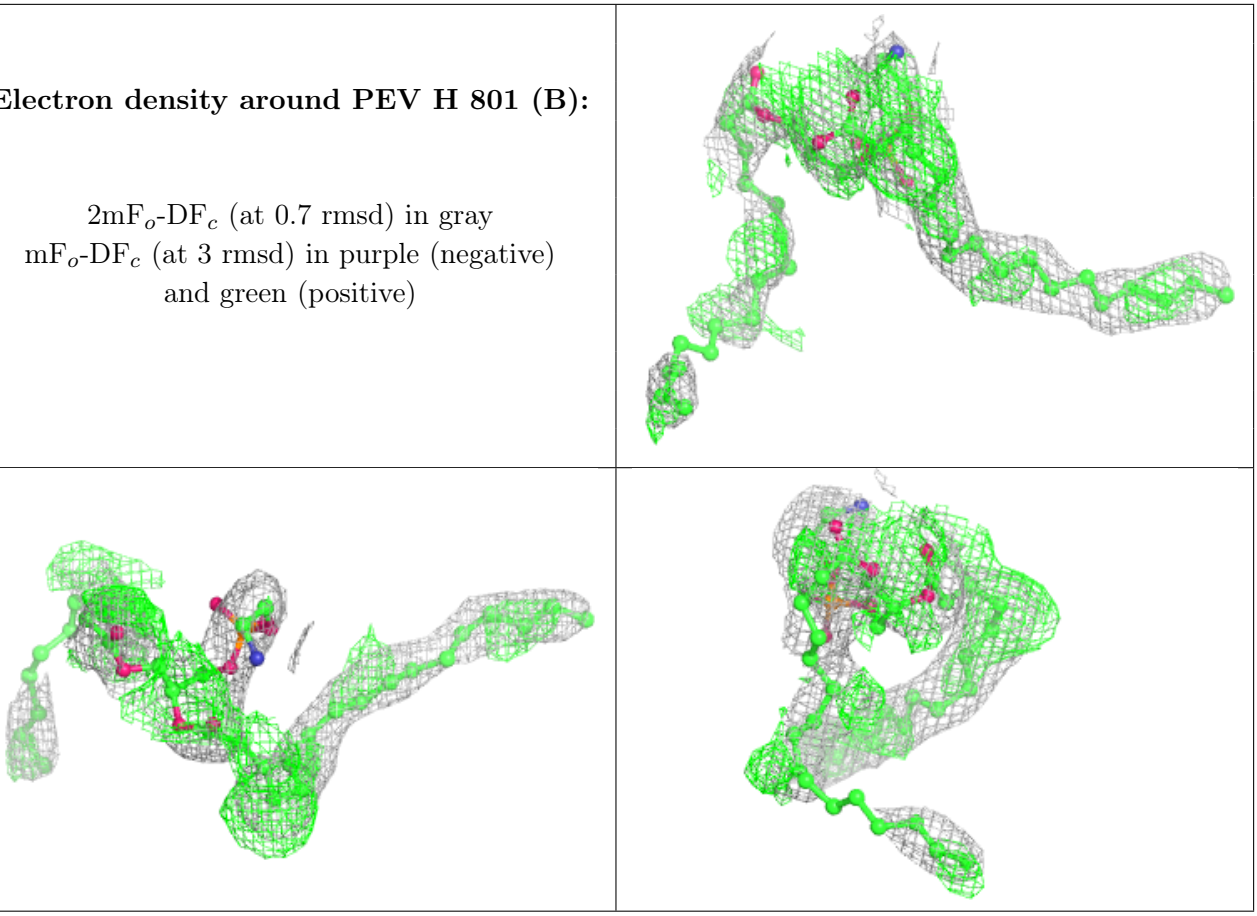






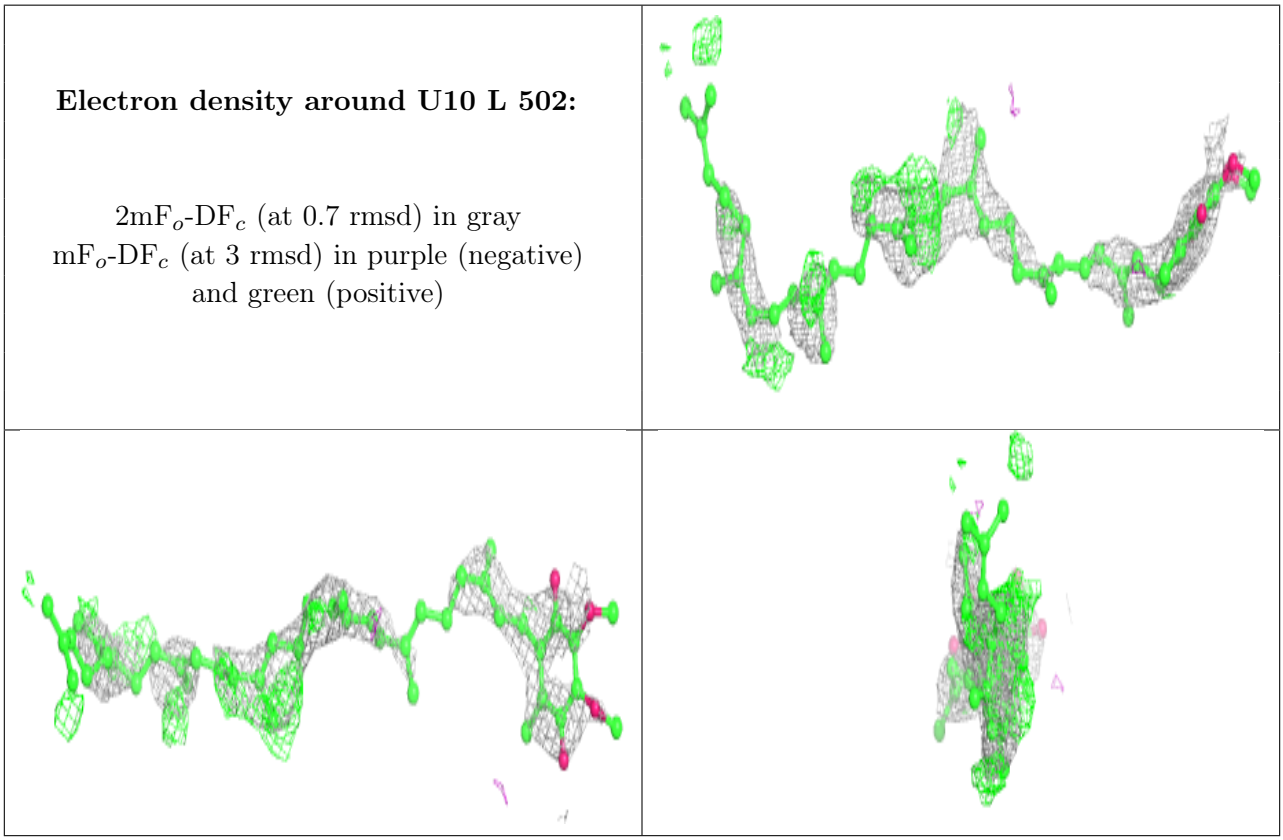
Electron density around PEV H 801 (B):

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



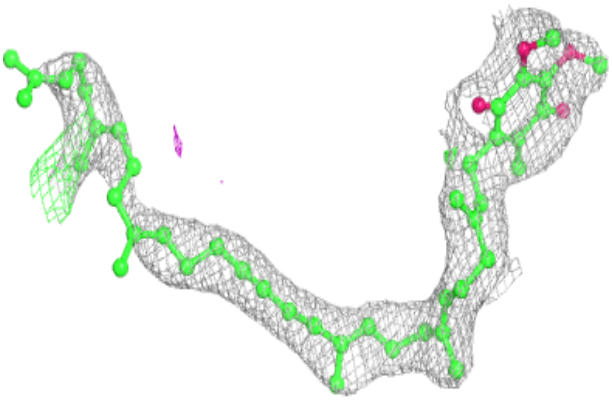
Electron density around U10 L 502:

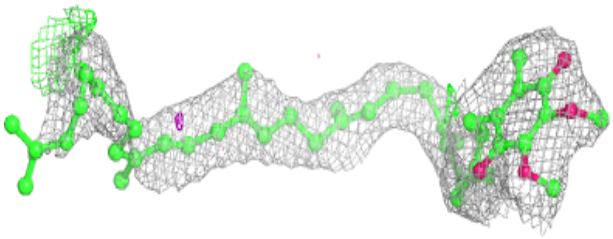
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

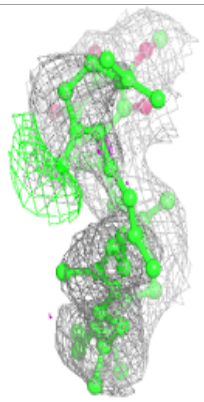


Electron density around U10 M 501:

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

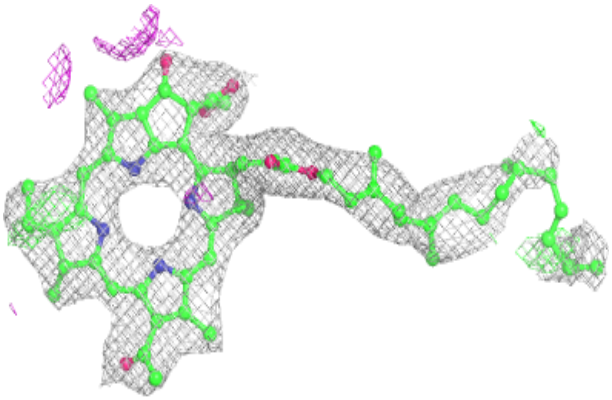


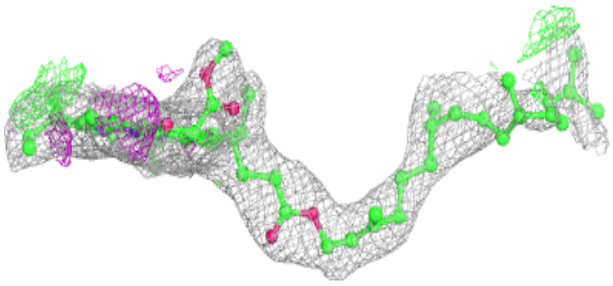




Electron density around BPH M 401:

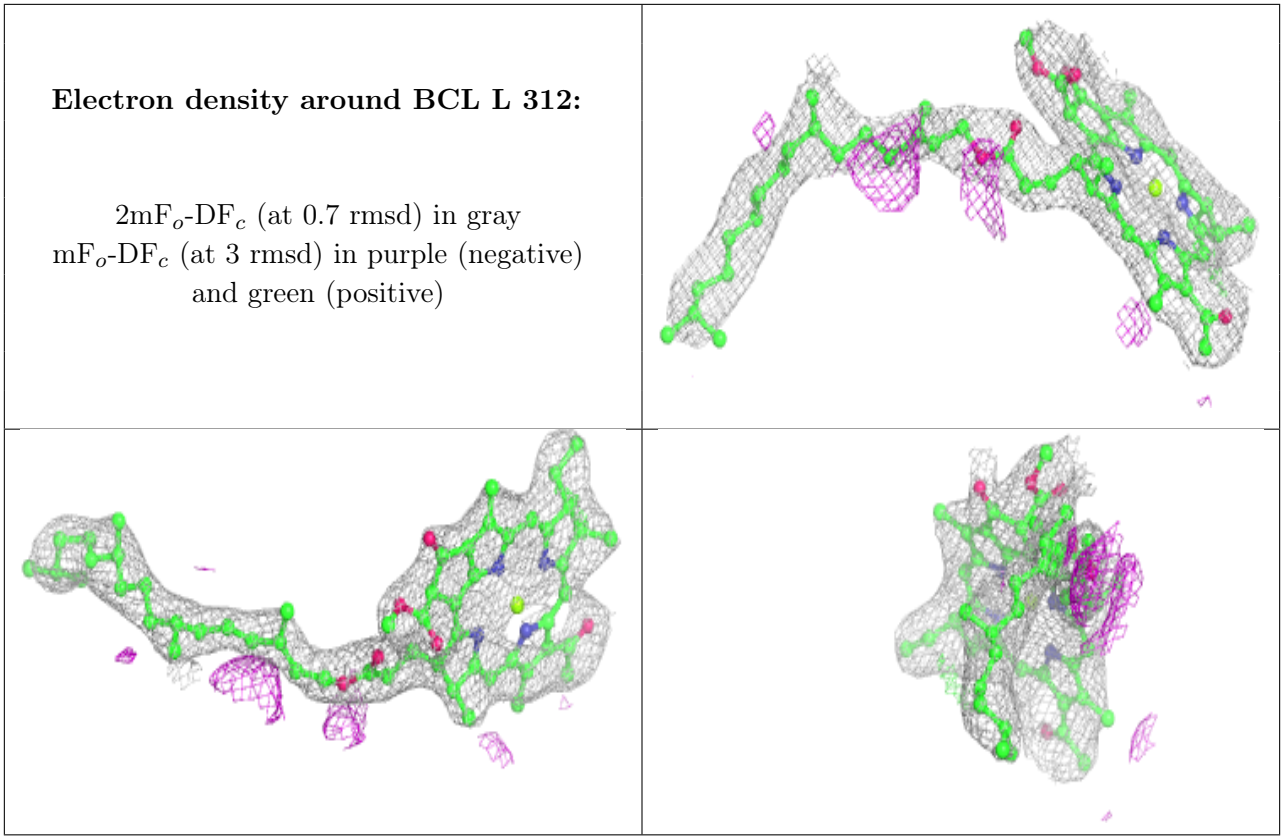
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





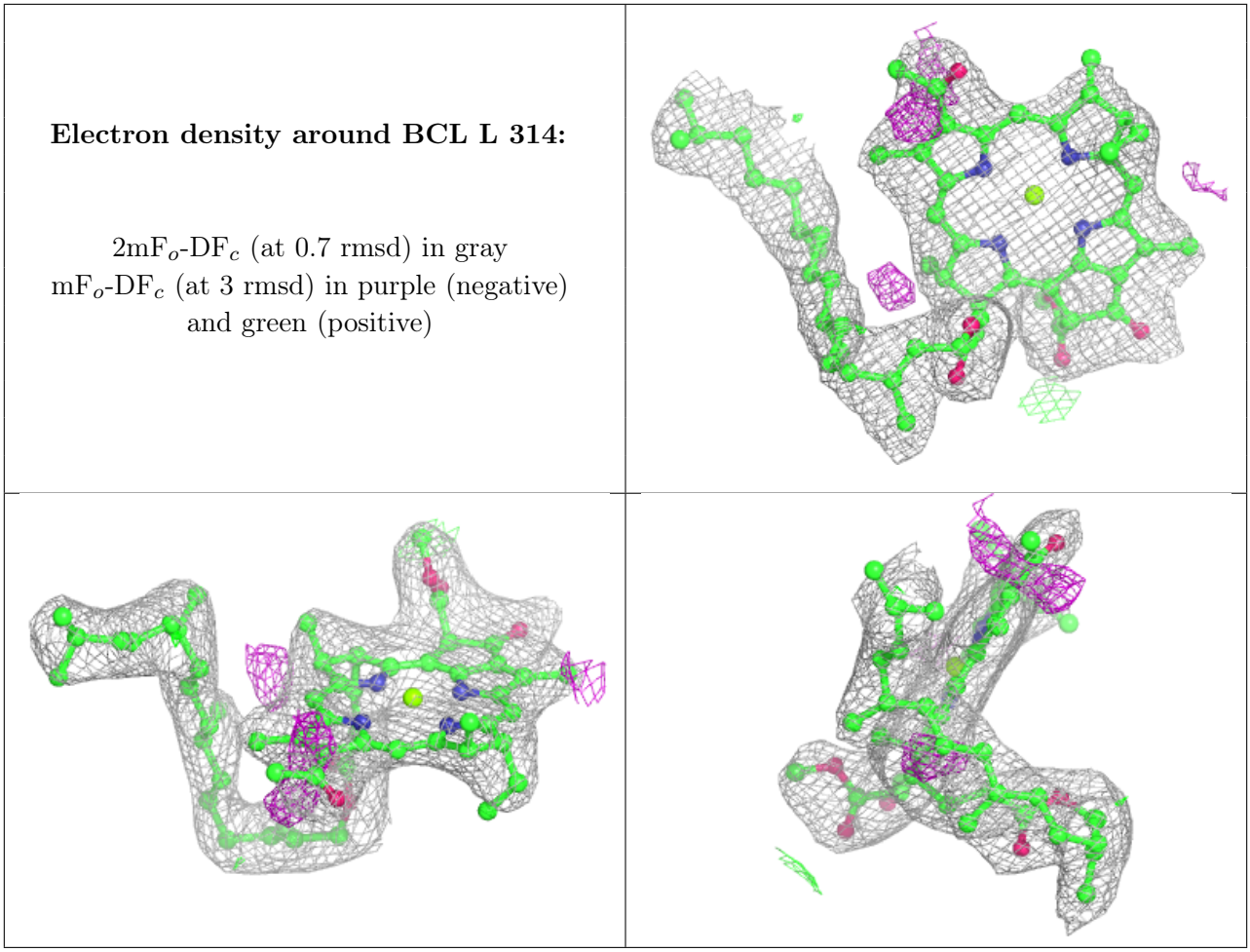
Electron density around BCL L 312:

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



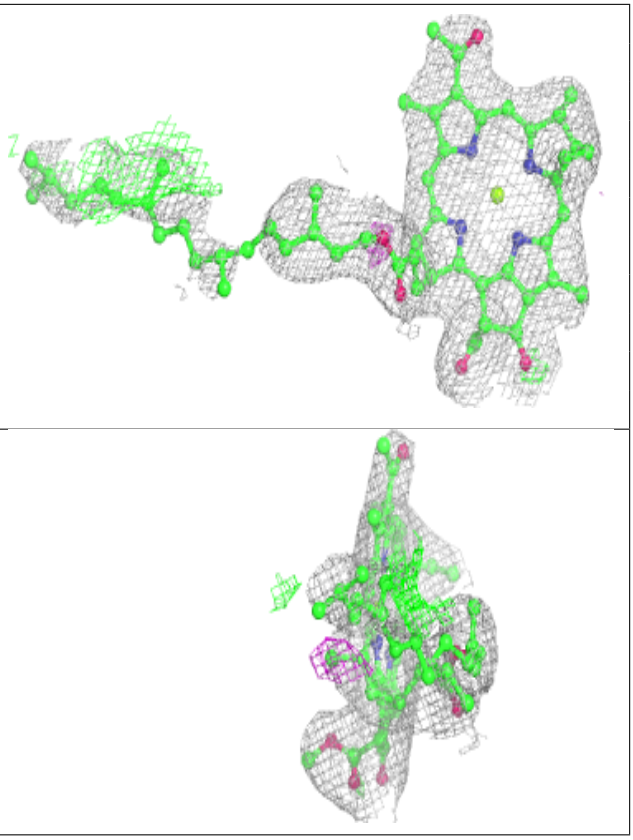
Electron density around BCL L 314:

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



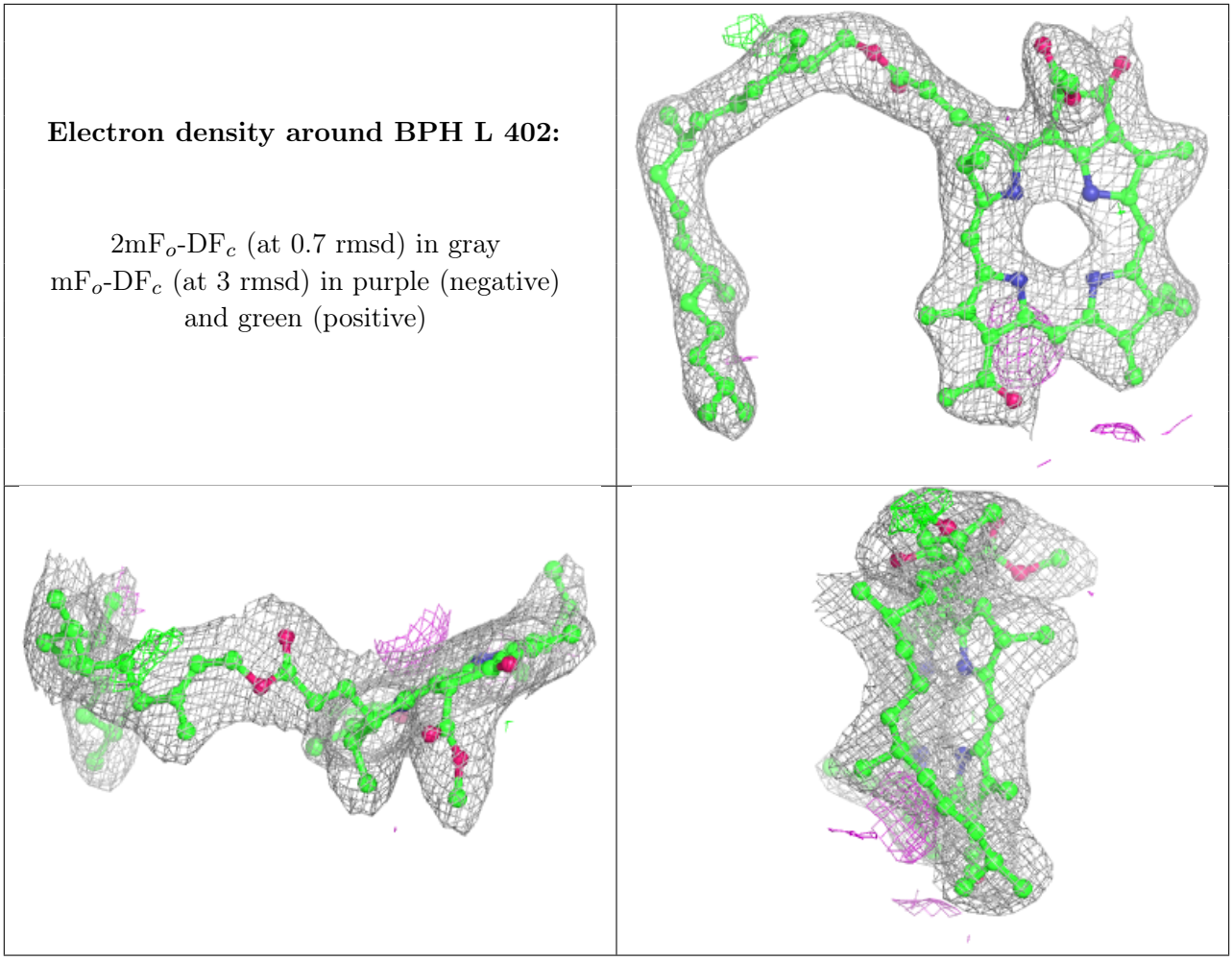
Electron density around BCL M 311:

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



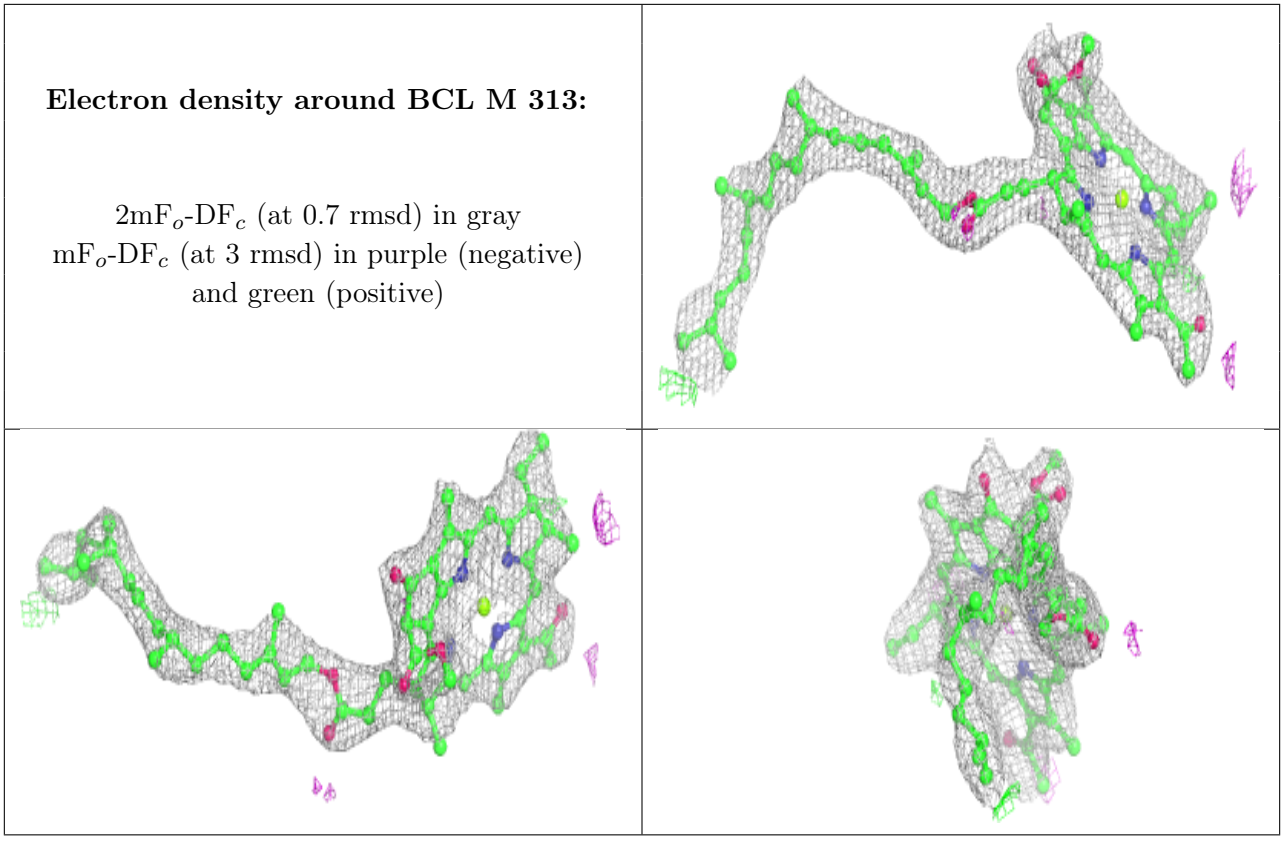
Electron density around BPH L 402:

$2mF_o$-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 M 313:

$2mF_o$-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.