



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2023 – 02:59 PM EDT

PDB ID : 4LWY  
Title : L(M196)H,H(M202)L Double Mutant Structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV  
Authors : Gabdulkhakov, A.G.  
Deposited on : 2013-07-29  
Resolution : 2.90 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.35.1  
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

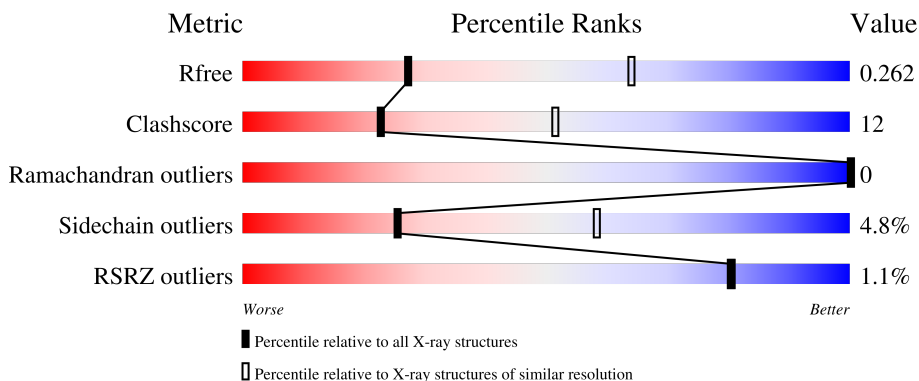
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	260	 2% 70% 23% 8%
2	L	282	 % 72% 26% .
3	M	303	 % 71% 26% .

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
12	BPH	L	303	X	-	-	-
12	BPH	M	402	X	-	-	-
12	BPH	M	404	X	-	-	-
14	CDL	M	401	-	-	-	X
4	LDA	M	411	-	-	-	X
5	UNL	L	305	-	-	-	X
5	UNL	L	307	-	-	-	X
7	DIO	H	307	-	-	-	X

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 7434 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2233	1508	355	362	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2409	1608	394	397	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9
M	196	HIS	LEU	engineered mutation	UNP P0C0Y9
M	202	LEU	HIS	engineered mutation	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



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

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

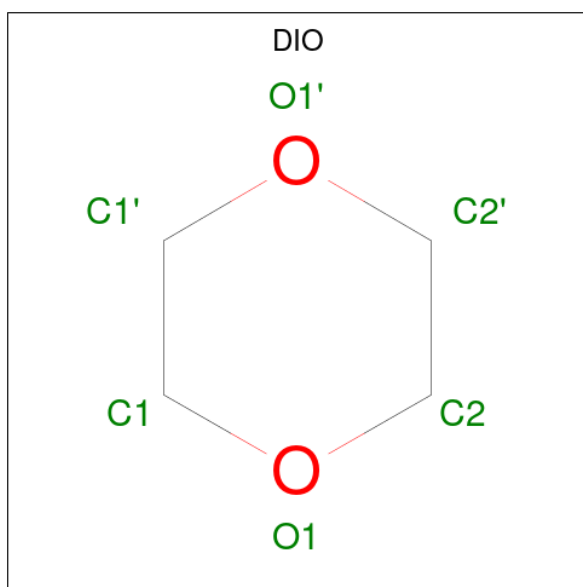
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
5	H	4	48	48	0	0
5	L	4	46	46	0	0
5	M	3	36	36	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



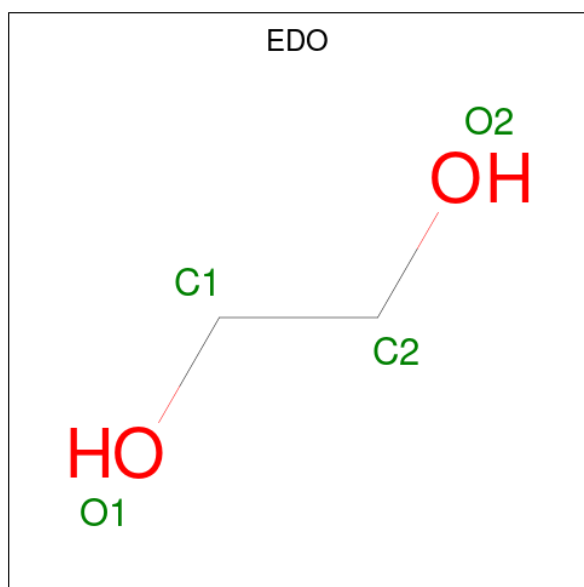
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 6 4 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 6 4 2	0	0
7	L	1	Total C O 6 4 2	0	0
7	M	1	Total C O 6 4 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C O 4 2 2	0	0
8	H	1	Total C O 4 2 2	0	0
8	H	1	Total C O 4 2 2	0	0
8	H	1	Total C O 4 2 2	0	0
8	L	1	Total C O 4 2 2	0	0
8	M	1	Total C O 4 2 2	0	0
8	M	1	Total C O 4 2 2	0	0

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).

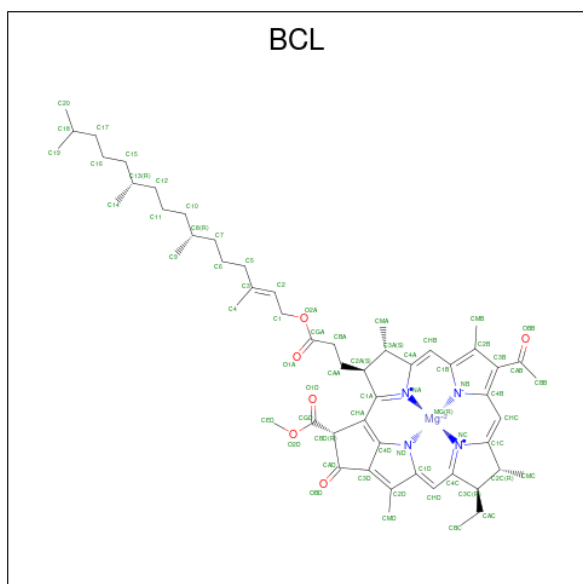


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf			
9	H	1	Total	C	N	O	0	0
			8	4	1	3		
9	L	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

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

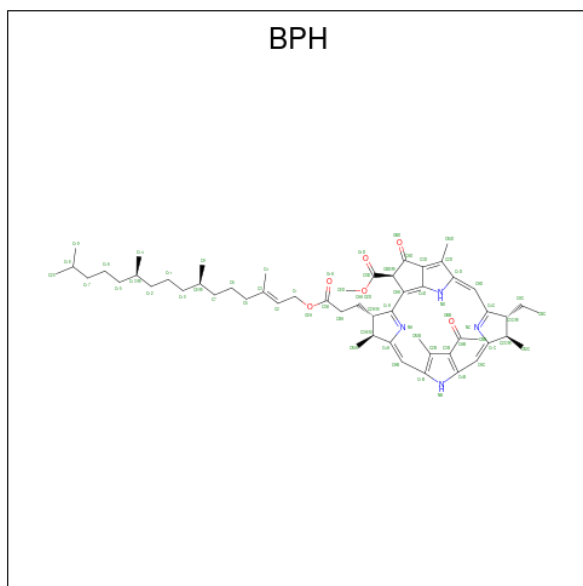
- Molecule 11 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).





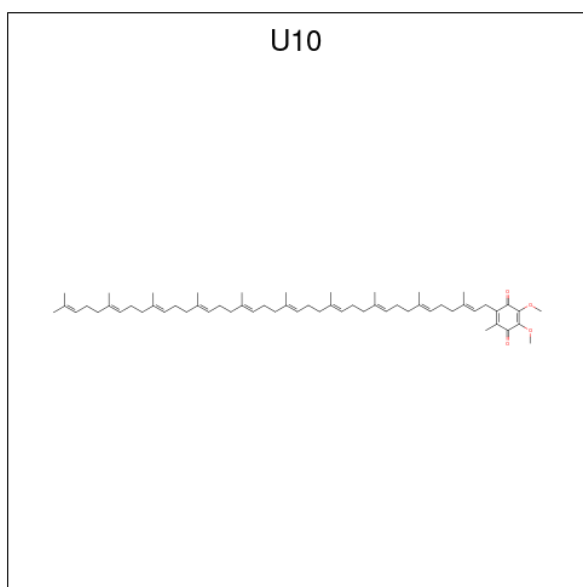
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 12 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



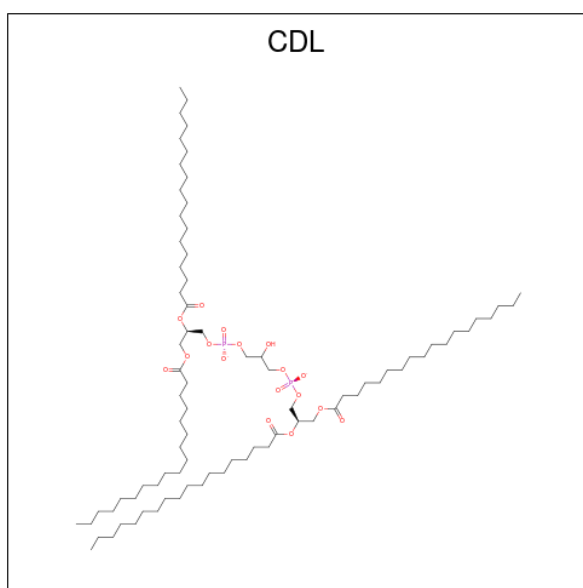
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



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

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).

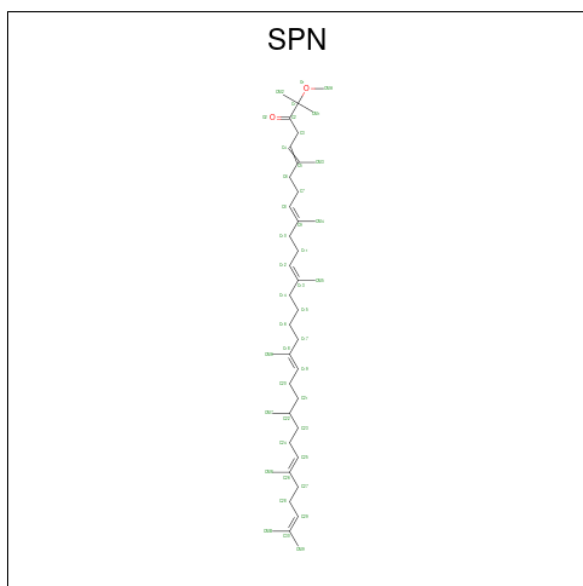


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 15 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 16 is SPEROIDENONE (three-letter code: SPN) (formula:  $C_{41}H_{70}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total C O 43 41 2	0	0

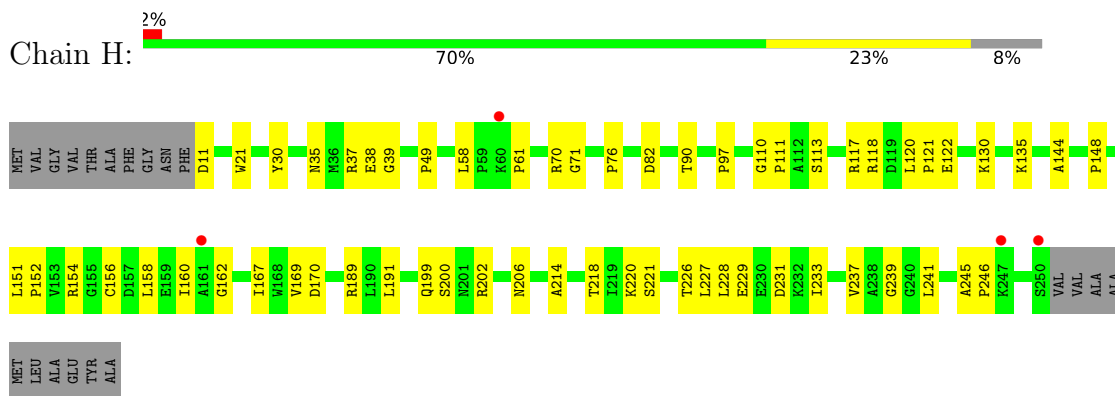
- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	11	Total O 11 11	0	0
17	L	10	Total O 10 10	0	0
17	M	18	Total O 18 18	0	0

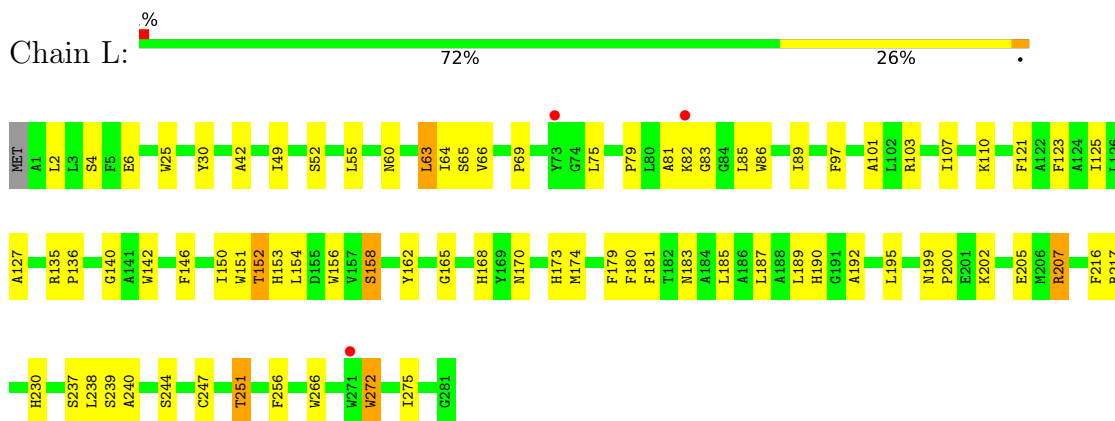
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

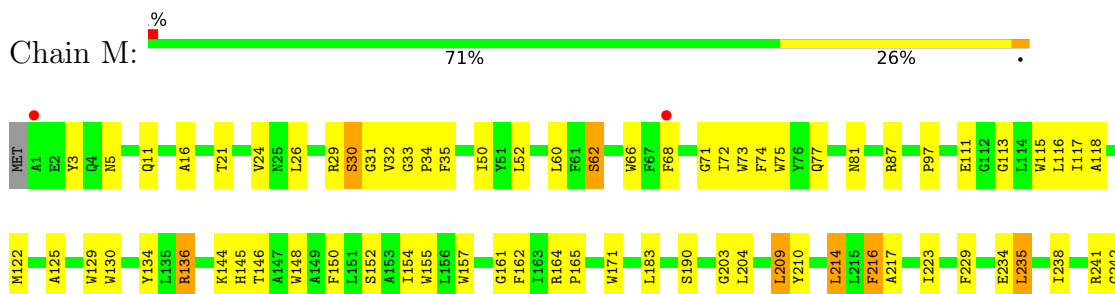
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.04Å 140.04Å 184.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.19 – 2.90 43.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.19-2.90) 99.8 (43.19-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, $R_{free}$	0.214 , 0.262 0.214 , 0.262	Depositor DCC
$R_{free}$ test set	2335 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.066 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: UNL, BCL, EDO, LDA, FE, SPN, CDL, PO4, BPH, K, TRS, U10, DIO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	H	0.43	0/1877	0.63	0/2553
2	L	0.46	0/2321	0.60	0/3177
3	M	0.44	0/2501	0.59	0/3415
All	All	0.44	0/6699	0.60	0/9145

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1836	39	0
2	L	2233	0	2189	63	0
3	M	2409	0	2323	71	0
4	H	16	0	31	2	0
4	M	80	0	155	9	0
5	H	48	0	0	0	0
5	L	46	0	0	0	0
5	M	36	0	0	0	0
6	H	5	0	0	0	0
6	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	6	0	8	0	0
7	L	12	0	16	3	0
7	M	6	0	8	1	0
8	H	16	0	24	3	0
8	L	4	0	6	1	0
8	M	8	0	12	1	0
9	H	8	0	12	1	0
9	L	8	0	12	0	0
10	H	1	0	0	0	0
11	L	132	0	148	11	0
11	M	66	0	74	4	0
12	L	65	0	76	10	0
12	M	130	0	152	11	0
13	L	48	0	63	1	0
13	M	48	0	63	5	0
14	M	81	0	106	6	0
15	M	1	0	0	0	0
16	M	43	0	70	5	0
17	H	11	0	0	0	0
17	L	10	0	0	0	0
17	M	18	0	0	1	0
All	All	7434	0	7384	170	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 12.

The worst 5 of 170 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)
3:M:34:PRO:HA	4:M:412:LDA:H71	1.55	0.89
2:L:200:PRO:HD2	7:L:309:DIO:H22	1.64	0.80
1:H:202:ARG:HH12	9:H:312:TRS:H21	1.53	0.73
2:L:42:ALA:HA	12:L:303:BPH:H9C3	1.71	0.73
2:L:65:SER:HB2	2:L:152:THR:HG21	1.70	0.72

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
2	L	279/282 (99%)	261 (94%)	18 (6%)	0	100	100
3	M	300/303 (99%)	280 (93%)	20 (7%)	0	100	100
All	All	817/845 (97%)	774 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	188 (96%)	7 (4%)	35	69
2	L	220/221 (100%)	208 (94%)	12 (6%)	21	53
3	M	236/237 (100%)	224 (95%)	12 (5%)	24	56
All	All	651/666 (98%)	620 (95%)	31 (5%)	25	58

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	216	PHE
3	M	216	PHE
2	L	256	PHE
3	M	258	PHE
3	M	136	ARG

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

Mol	Chain	Res	Type
3	M	77	GLN

### 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 45 ligands modelled in this entry, 11 are unknown and 2 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PO4	M	416	-	4,4,4	0.84	0	6,6,6	0.43	0
8	EDO	M	420	-	3,3,3	0.52	0	2,2,2	0.20	0
8	EDO	H	309	-	3,3,3	0.44	0	2,2,2	0.55	0
12	BPH	M	404	-	51,70,70	0.81	3 (5%)	52,101,101	1.39	7 (13%)
8	EDO	H	308	-	3,3,3	0.47	0	2,2,2	0.28	0
4	LDA	M	410	-	12,15,15	2.08	1 (8%)	14,17,17	0.60	0
11	BCL	L	302	-	58,74,74	1.29	5 (8%)	69,115,115	1.69	14 (20%)
7	DIO	H	307	-	6,6,6	0.86	0	6,6,6	0.76	0
11	BCL	L	301	-	58,74,74	1.31	3 (5%)	69,115,115	1.71	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EDO	H	311	-	3,3,3	0.54	0	2,2,2	0.17	0
13	U10	M	406	-	48,48,63	2.64	14 (29%)	58,61,79	1.84	14 (24%)
16	SPN	M	407	-	40,42,42	1.22	6 (15%)	50,52,52	1.66	13 (26%)
8	EDO	M	419	-	3,3,3	0.51	0	2,2,2	0.28	0
8	EDO	L	311	-	3,3,3	0.55	0	2,2,2	0.09	0
14	CDL	M	401	-	80,80,99	0.90	4 (5%)	86,92,111	1.30	7 (8%)
6	PO4	M	417	-	4,4,4	0.87	0	6,6,6	0.35	0
12	BPH	M	402	-	51,70,70	0.80	3 (5%)	52,101,101	1.31	7 (13%)
11	BCL	M	403	-	58,74,74	1.42	6 (10%)	69,115,115	1.84	15 (21%)
4	LDA	M	412	-	12,15,15	2.04	1 (8%)	14,17,17	0.35	0
7	DIO	L	310	-	6,6,6	0.70	0	6,6,6	1.07	0
9	TRS	H	312	-	7,7,7	0.30	0	9,9,9	0.34	0
9	TRS	L	312	-	7,7,7	0.32	0	9,9,9	0.30	0
4	LDA	H	301	-	12,15,15	2.03	1 (8%)	14,17,17	0.55	0
4	LDA	M	408	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
4	LDA	M	411	-	12,15,15	2.07	1 (8%)	14,17,17	0.38	0
13	U10	L	304	-	48,48,63	2.60	13 (27%)	58,61,79	1.84	15 (25%)
7	DIO	M	418	-	6,6,6	0.85	0	6,6,6	0.85	0
4	LDA	M	409	-	12,15,15	2.04	1 (8%)	14,17,17	0.43	0
8	EDO	H	310	-	3,3,3	0.46	0	2,2,2	0.48	0
12	BPH	L	303	-	51,70,70	0.81	2 (3%)	52,101,101	1.30	8 (15%)
7	DIO	L	309	-	6,6,6	0.81	0	6,6,6	0.80	0
6	PO4	H	306	-	4,4,4	0.93	0	6,6,6	0.31	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	M	420	-	-	1/1/1/1	-
12	BPH	M	404	-	2/2/18/22	5/37/105/105	0/5/6/6
8	EDO	H	309	-	-	0/1/1/1	-
8	EDO	H	308	-	-	0/1/1/1	-
4	LDA	M	410	-	-	1/13/13/13	-
11	BCL	L	302	-	-	7/37/137/137	-
7	DIO	H	307	-	-	-	0/1/1/1
11	BCL	L	301	-	-	10/37/137/137	-
8	EDO	H	311	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	U10	M	406	-	-	12/45/69/87	0/1/1/1
16	SPN	M	407	-	-	17/50/51/51	-
8	EDO	M	419	-	-	1/1/1/1	-
8	EDO	L	311	-	-	0/1/1/1	-
14	CDL	M	401	-	-	44/91/91/110	-
12	BPH	M	402	-	2/2/18/22	7/37/105/105	0/5/6/6
11	BCL	M	403	-	-	7/37/137/137	-
4	LDA	M	412	-	-	6/13/13/13	-
7	DIO	L	310	-	-	-	0/1/1/1
9	TRS	H	312	-	-	6/9/9/9	-
9	TRS	L	312	-	-	7/9/9/9	-
4	LDA	H	301	-	-	8/13/13/13	-
4	LDA	M	408	-	-	2/13/13/13	-
4	LDA	M	411	-	-	7/13/13/13	-
13	U10	L	304	-	-	11/45/69/87	0/1/1/1
4	LDA	M	409	-	-	5/13/13/13	-
7	DIO	M	418	-	-	-	0/1/1/1
8	EDO	H	310	-	-	0/1/1/1	-
12	BPH	L	303	-	2/2/18/22	11/37/105/105	0/5/6/6
7	DIO	L	309	-	-	-	0/1/1/1

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	408	LDA	O1-N1	-7.13	1.25	1.42
4	M	410	LDA	O1-N1	-7.11	1.25	1.42
4	M	411	LDA	O1-N1	-7.07	1.25	1.42
4	H	301	LDA	O1-N1	-6.97	1.25	1.42
4	M	412	LDA	O1-N1	-6.96	1.25	1.42

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	403	BCL	C1C-NC-C4C	6.48	109.62	106.71
11	L	301	BCL	C1C-NC-C4C	5.95	109.38	106.71
13	L	304	U10	C7-C8-C9	-5.69	117.32	126.79
11	L	302	BCL	CMB-C2B-C1B	-4.99	120.80	128.46
11	L	301	BCL	O2D-CGD-CBD	4.89	119.96	111.27

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	L	303	BPH	C13
12	L	303	BPH	C8
12	M	402	BPH	C13
12	M	402	BPH	C8
12	M	404	BPH	C13

5 of 175 torsion outliers are listed below:

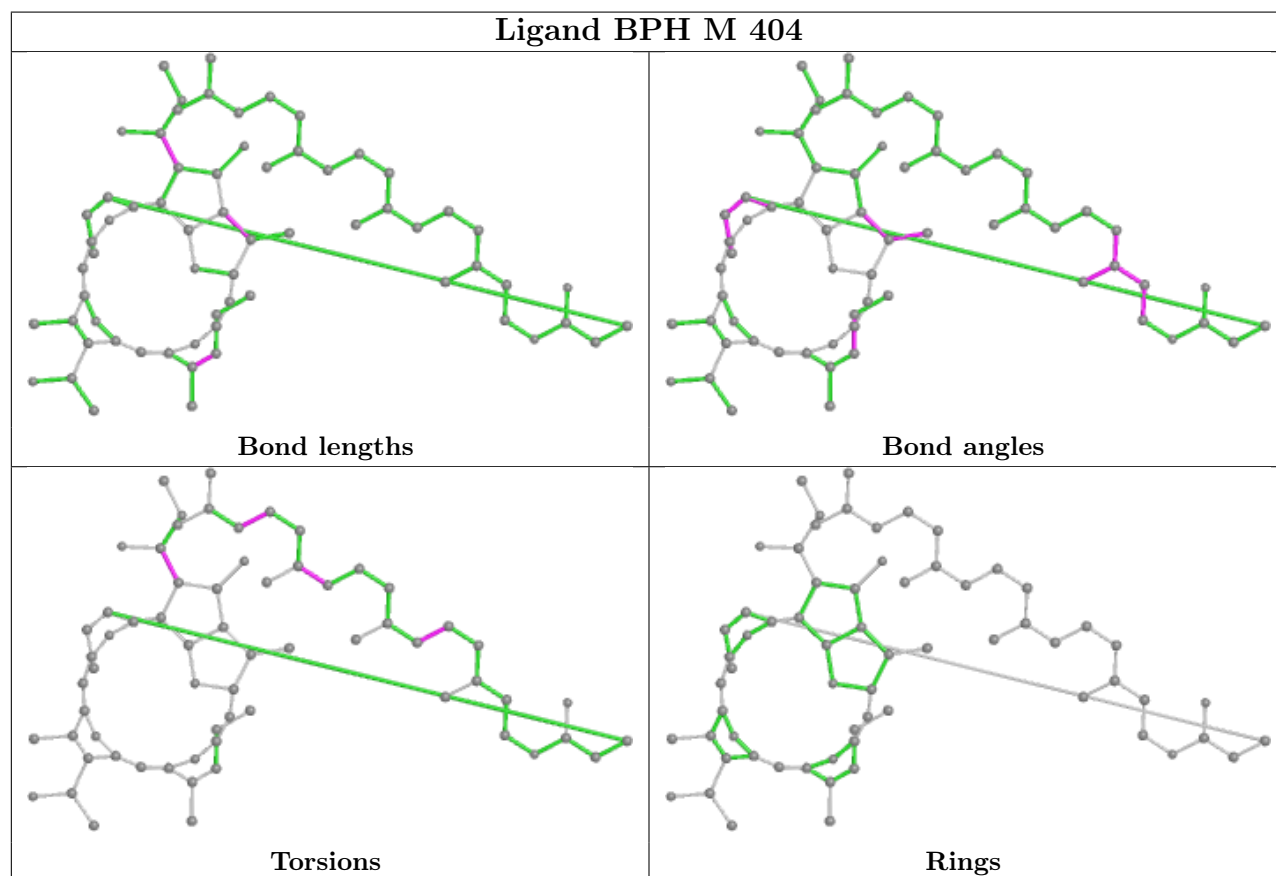
Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C2-C1-N1-O1
4	H	301	LDA	C2-C1-N1-CM1
4	H	301	LDA	C2-C1-N1-CM2
4	M	409	LDA	N1-C1-C2-C3
9	H	312	TRS	C2-C-C1-O1

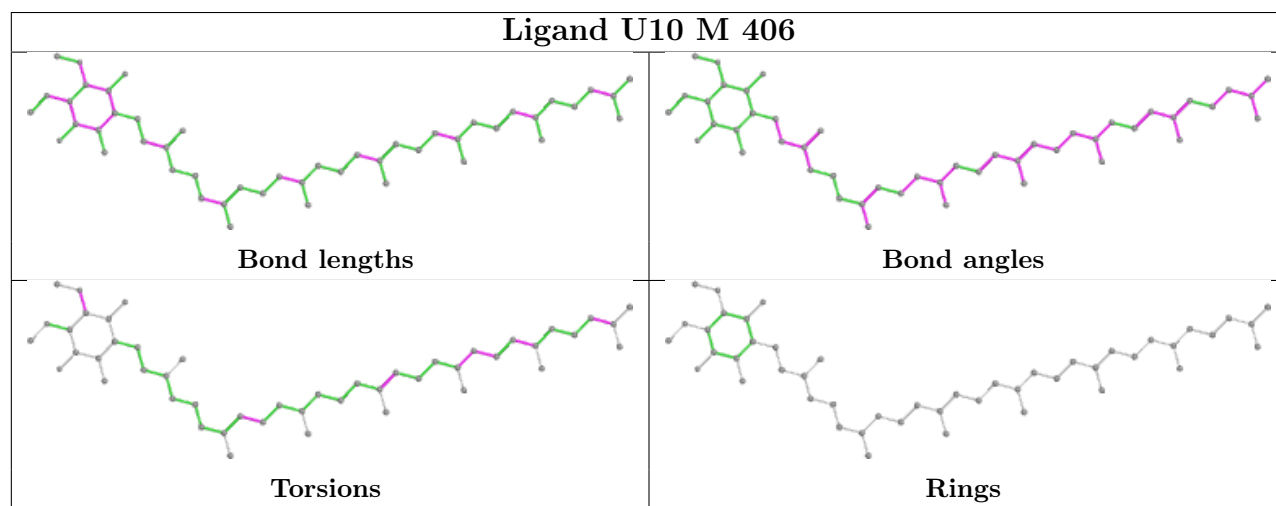
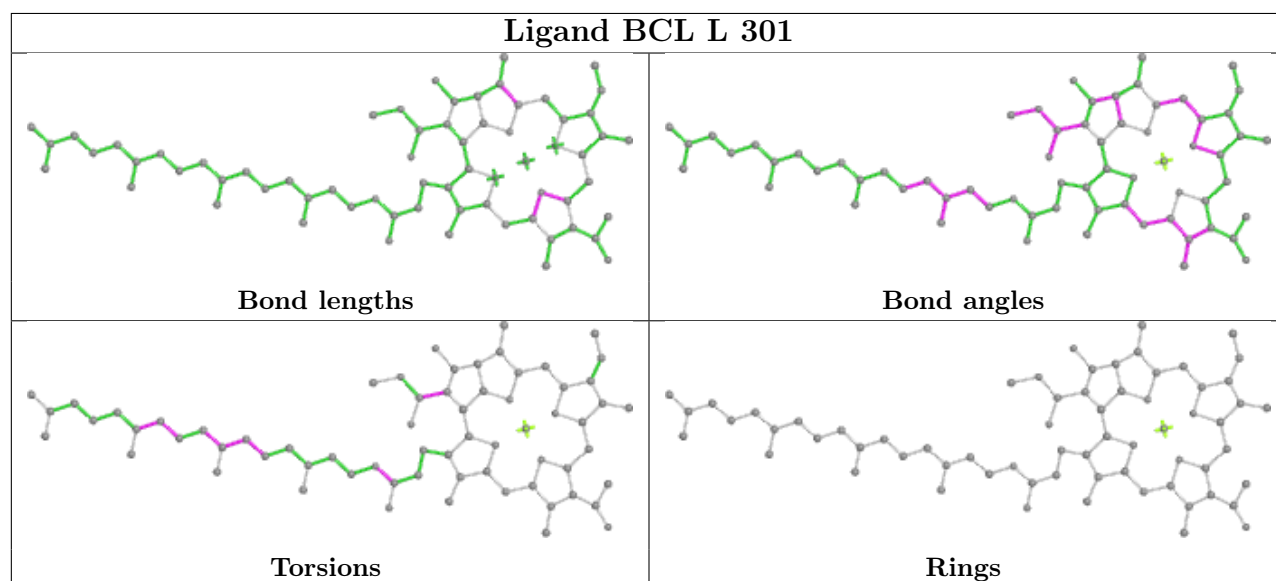
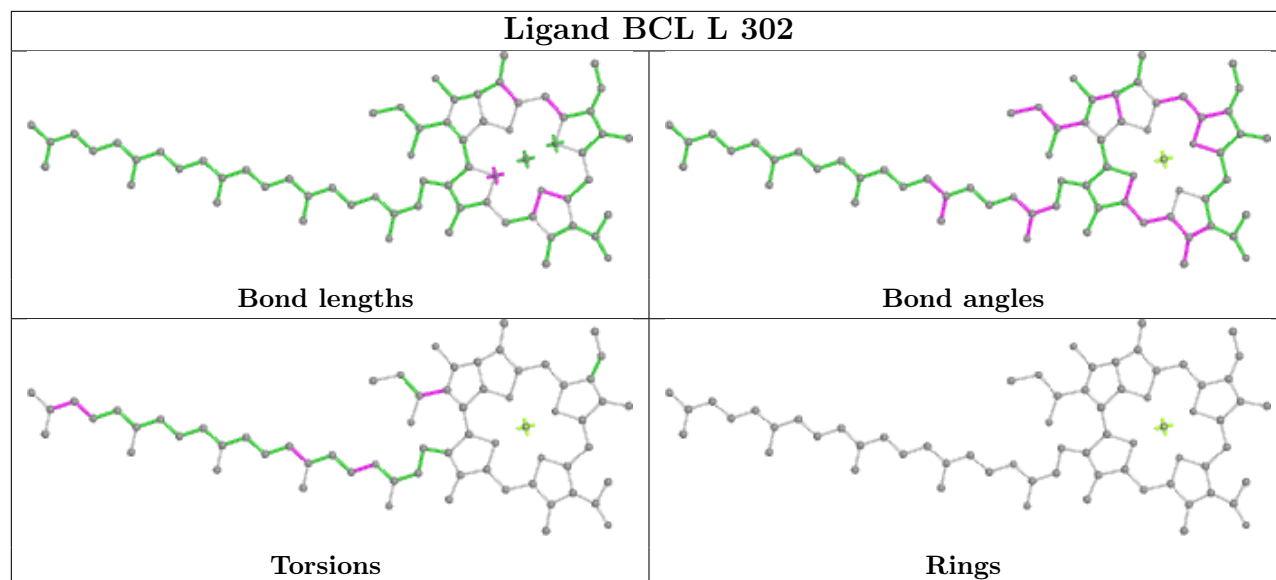
There are no ring outliers.

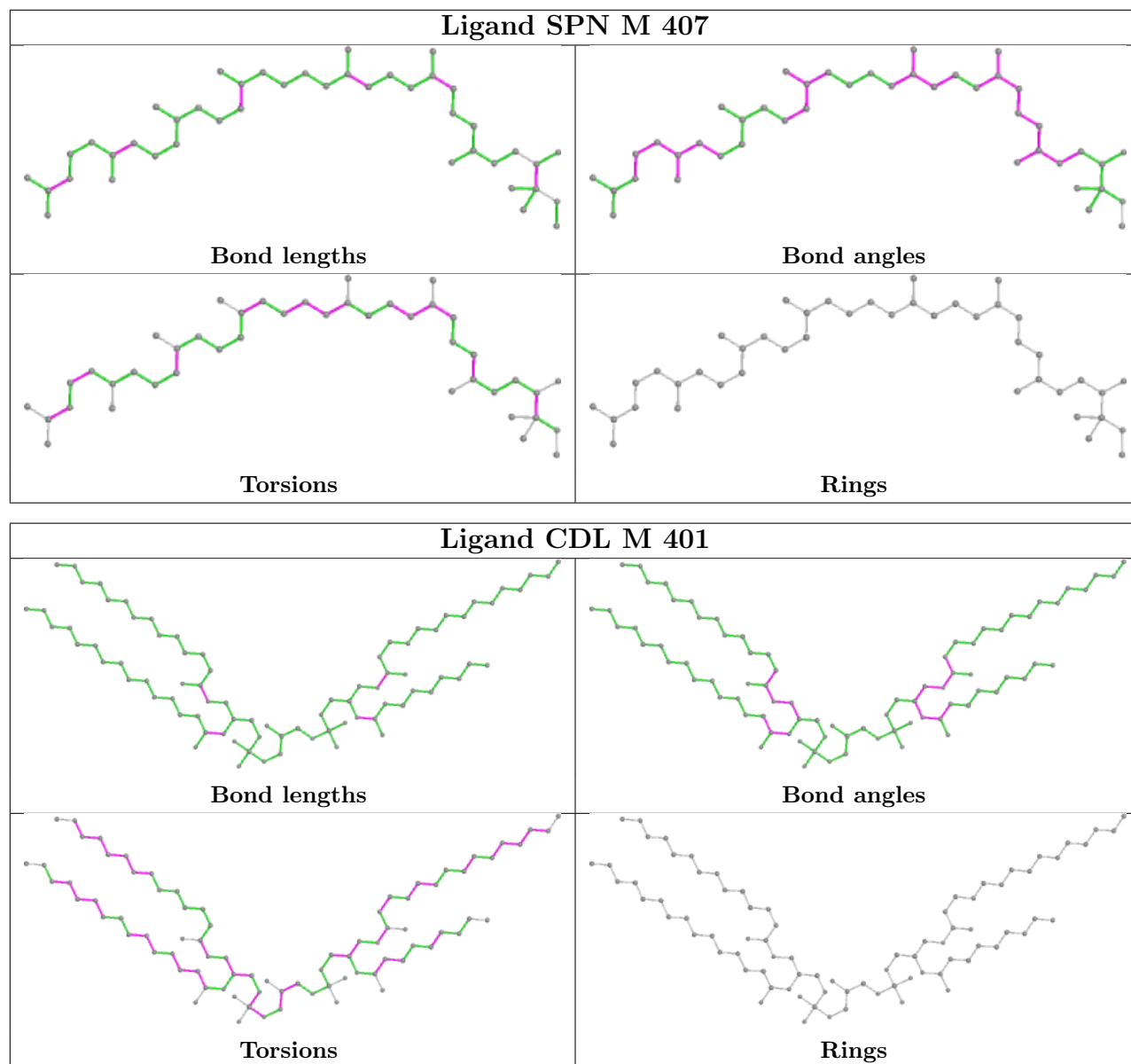
21 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	404	BPH	7	0
4	M	410	LDA	1	0
11	L	302	BCL	6	0
11	L	301	BCL	5	0
8	H	311	EDO	1	0
13	M	406	U10	5	0
16	M	407	SPN	5	0
8	M	419	EDO	1	0
8	L	311	EDO	1	0
14	M	401	CDL	6	0
12	M	402	BPH	5	0
11	M	403	BCL	4	0
4	M	412	LDA	4	0
9	H	312	TRS	1	0
4	H	301	LDA	2	0
4	M	408	LDA	4	0
13	L	304	U10	1	0
7	M	418	DIO	1	0
8	H	310	EDO	2	0
12	L	303	BPH	10	0
7	L	309	DIO	3	0

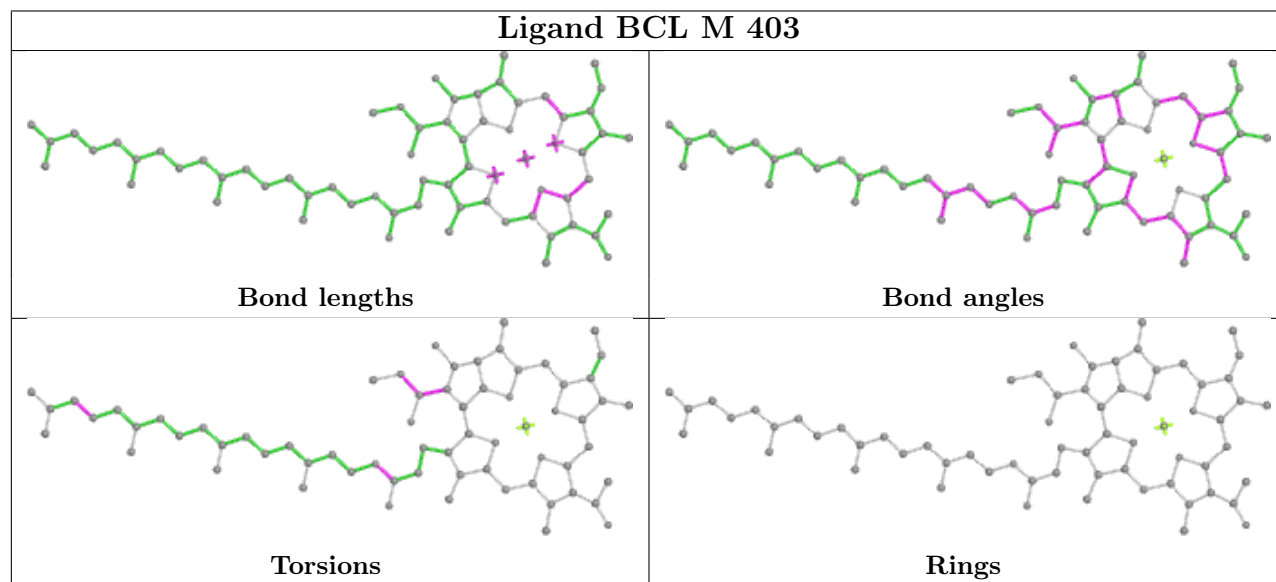
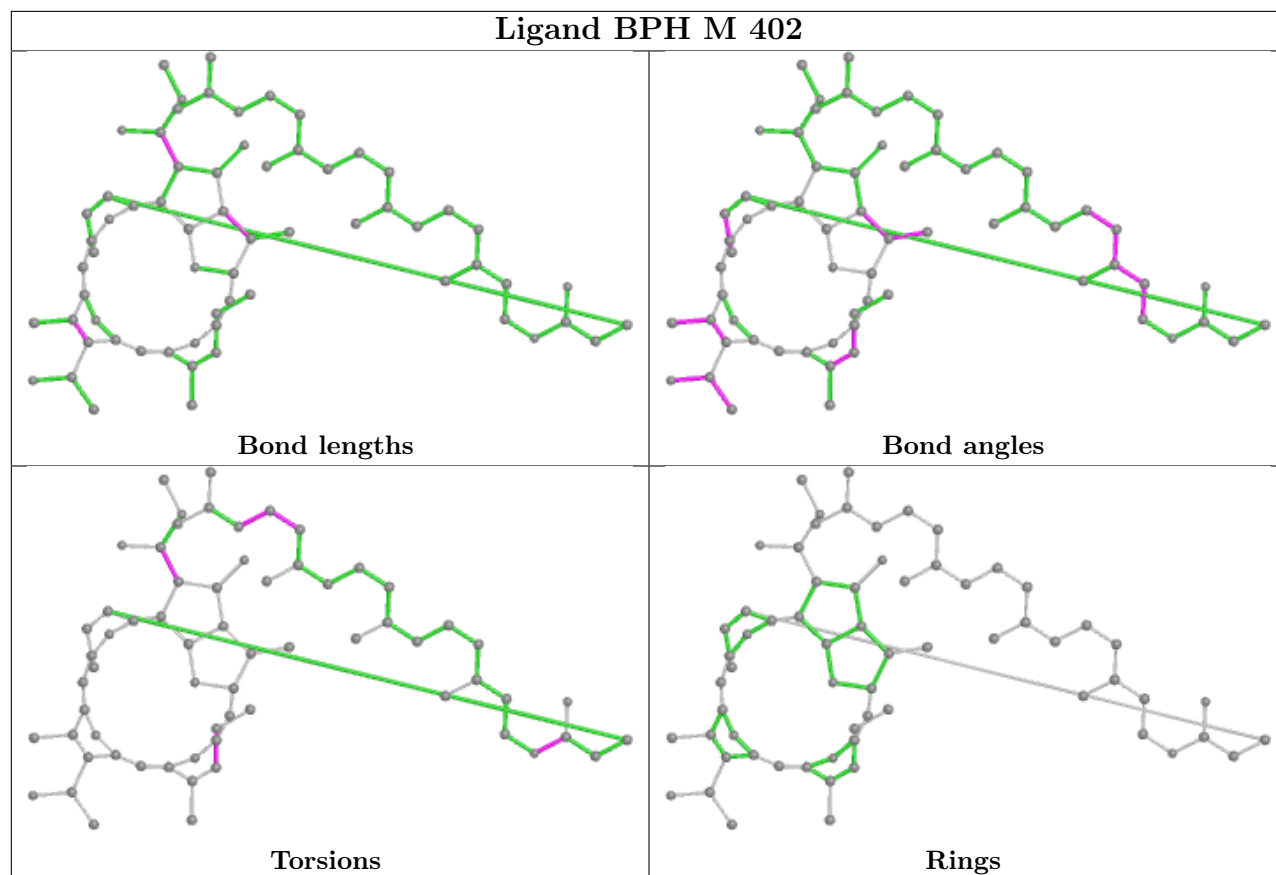
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

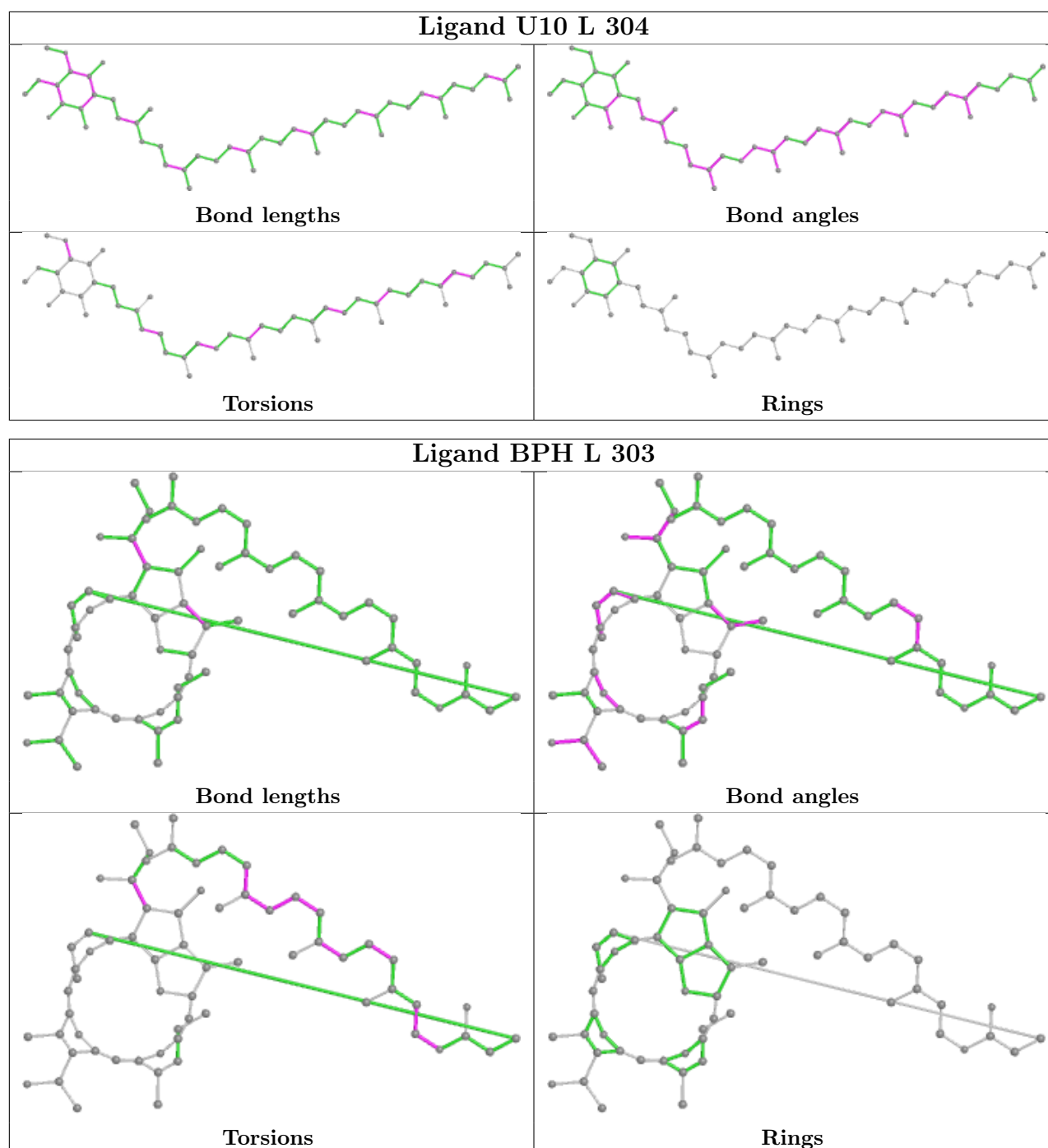












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	240/260 (92%)	-0.41	4 (1%) 70 69	19, 45, 74, 127	0
2	L	281/282 (99%)	-0.32	3 (1%) 80 80	13, 42, 83, 130	0
3	M	302/303 (99%)	-0.30	2 (0%) 87 87	18, 45, 84, 118	0
All	All	823/845 (97%)	-0.34	9 (1%) 80 80	13, 44, 82, 130	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	4.5
1	H	247	LYS	3.1
3	M	1	ALA	2.7
2	L	82	LYS	2.2
3	M	68	PHE	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no 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<sup>th</sup> 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.

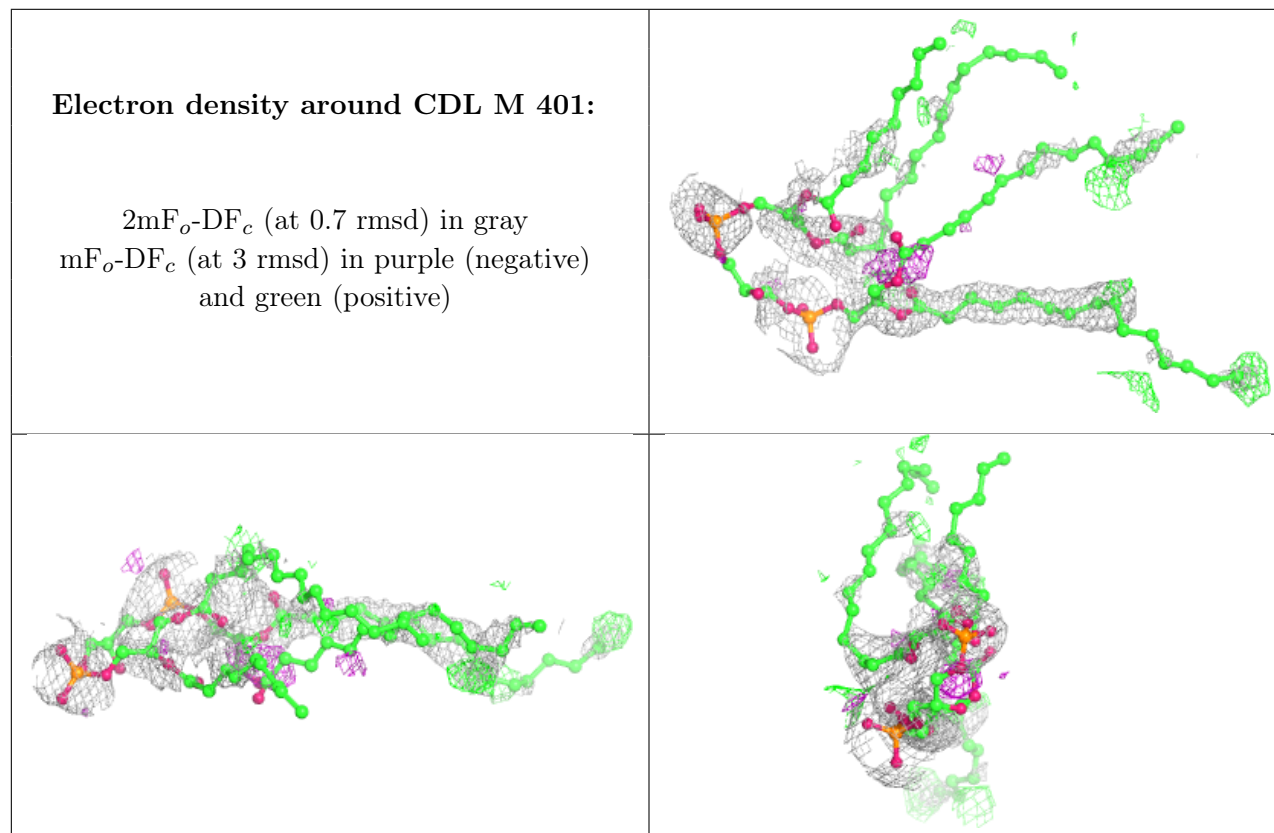
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	LDA	M	411	16/16	0.63	0.93	63,106,135,139	0
8	EDO	H	311	4/4	0.71	0.37	58,60,62,63	0
5	UNL	L	308	12/-	0.73	0.36	39,70,76,79	0
7	DIO	H	307	6/6	0.75	0.60	100,102,102,102	0
5	UNL	L	307	10/-	0.76	0.91	53,79,104,107	0
5	UNL	L	305	12/-	0.76	0.83	67,78,91,94	0
5	UNL	M	414	12/-	0.79	0.32	45,66,80,85	0
4	LDA	M	412	16/16	0.80	0.34	63,87,99,105	0
14	CDL	M	401	81/100	0.80	0.48	58,97,140,158	0
5	UNL	H	304	12/-	0.81	0.51	39,53,80,83	0
5	UNL	M	415	12/-	0.82	0.69	70,82,90,92	0
9	TRS	H	312	8/8	0.83	0.26	76,84,92,102	0
8	EDO	M	419	4/4	0.84	0.29	60,73,77,78	0
5	UNL	H	303	12/-	0.85	0.55	43,54,70,73	0
5	UNL	M	413	12/-	0.85	0.25	32,47,55,58	0
5	UNL	L	306	12/-	0.85	0.38	35,54,67,68	0
4	LDA	M	410	16/16	0.85	0.29	48,66,88,98	0
9	TRS	L	312	8/8	0.85	0.39	73,77,88,89	0
6	PO4	M	416	5/5	0.85	0.13	95,108,121,134	0
4	LDA	M	409	16/16	0.86	0.46	34,45,80,83	0
5	UNL	H	305	12/-	0.86	0.38	54,66,81,82	0
6	PO4	M	417	5/5	0.86	0.22	94,102,115,118	0
7	DIO	L	310	6/6	0.87	0.23	64,68,73,82	0
5	UNL	H	302	12/-	0.87	0.41	53,59,78,82	0
10	K	H	313	1/1	0.88	0.15	64,64,64,64	0
13	U10	L	304	48/63	0.88	0.24	53,70,84,90	0
8	EDO	H	310	4/4	0.88	0.34	61,65,68,70	0
6	PO4	H	306	5/5	0.89	0.16	94,105,115,120	0
8	EDO	H	308	4/4	0.89	0.18	79,79,82,86	0
8	EDO	L	311	4/4	0.90	0.20	68,73,73,81	0
13	U10	M	406	48/63	0.91	0.24	28,39,57,64	0
7	DIO	M	418	6/6	0.91	0.36	99,104,105,112	0
12	BPH	M	404	65/65	0.92	0.26	39,54,101,113	0
16	SPN	M	407	43/43	0.92	0.40	30,52,74,78	0
7	DIO	L	309	6/6	0.93	0.32	34,36,40,46	6
4	LDA	H	301	16/16	0.94	0.18	48,58,63,69	0
12	BPH	L	303	65/65	0.95	0.18	25,31,44,51	0
8	EDO	H	309	4/4	0.95	0.17	55,56,59,61	0
4	LDA	M	408	16/16	0.95	0.18	45,55,64,66	0
8	EDO	M	420	4/4	0.96	0.19	37,40,46,47	0
11	BCL	M	403	66/66	0.97	0.16	19,24,37,41	0
11	BCL	L	301	66/66	0.97	0.17	21,34,65,72	0
12	BPH	M	402	65/65	0.97	0.16	27,33,55,67	0

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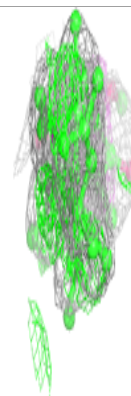
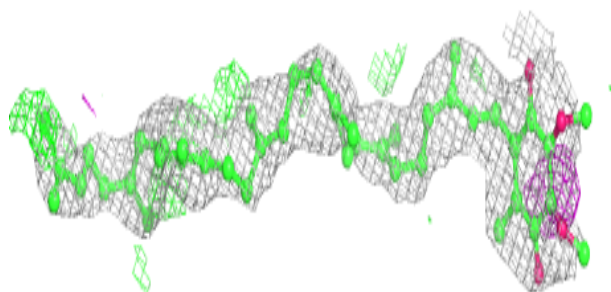
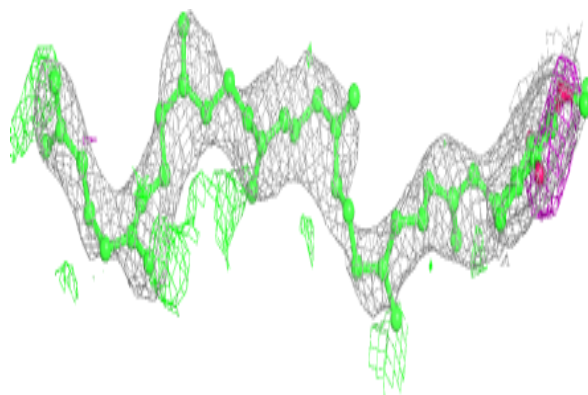
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	BCL	L	302	66/66	0.97	0.16	24,32,42,46	0
15	FE	M	405	1/1	1.00	0.15	25,25,25,25	0

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

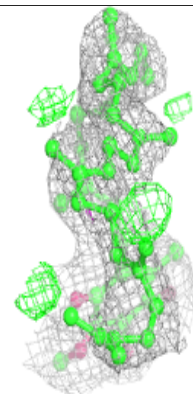
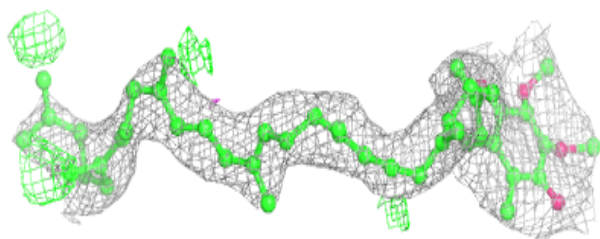
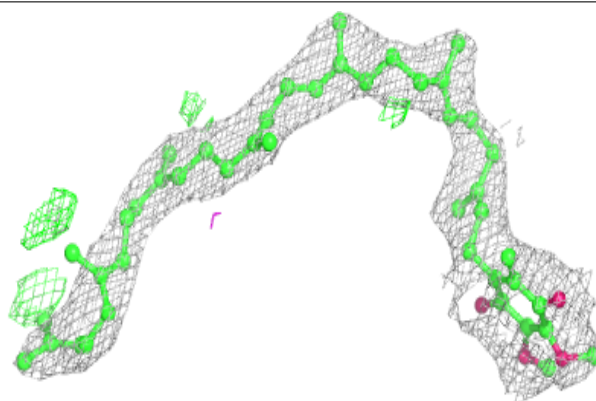


**Electron density around U10 L 304:**

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

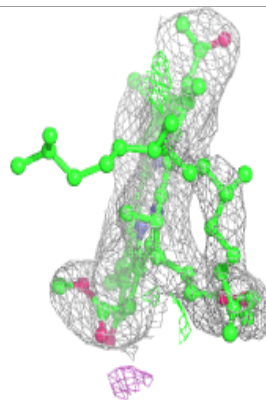
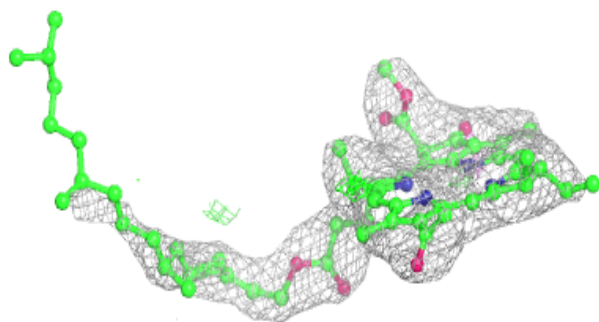
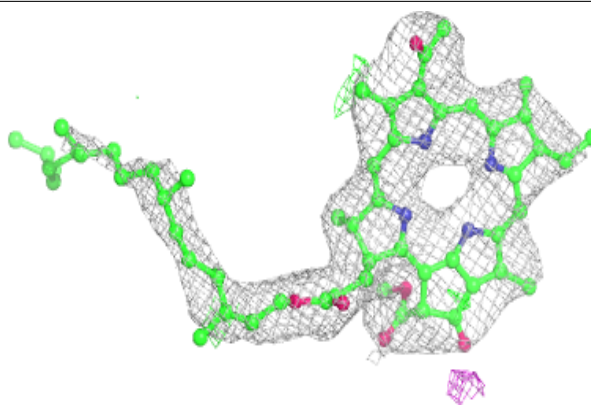
**Electron density around U10 M 406:**

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

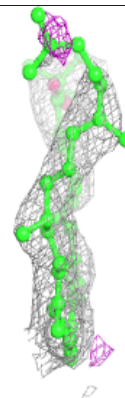
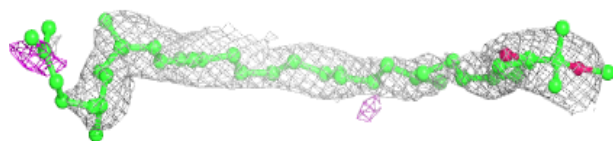
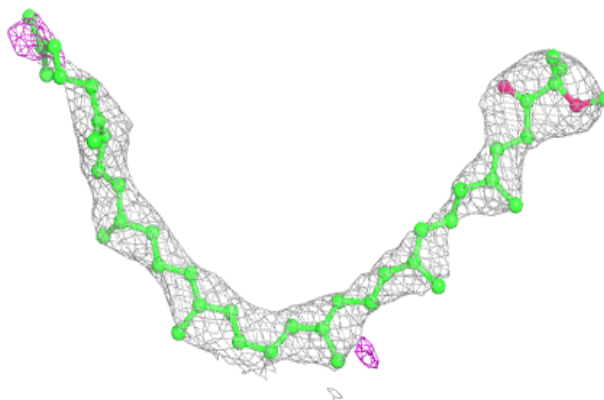


**Electron density around BPH M 404:**

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

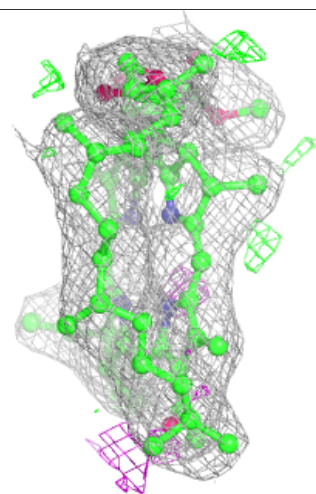
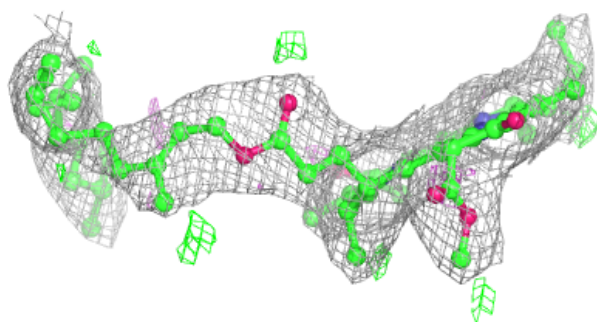
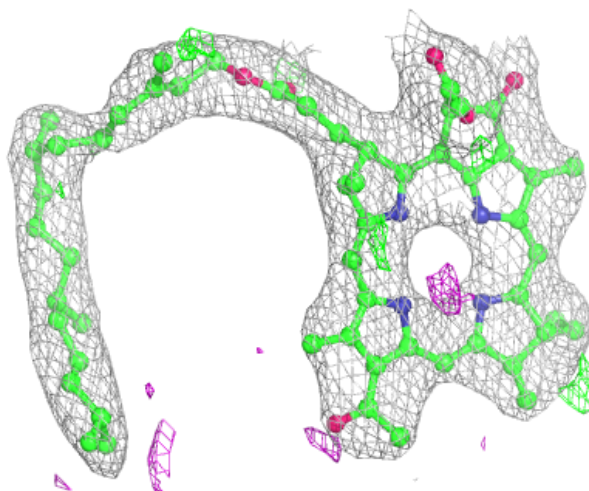
**Electron density around SPN M 407:**

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



**Electron density around BPH L 303:**

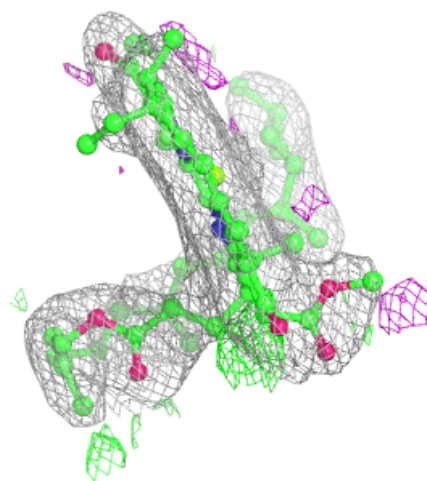
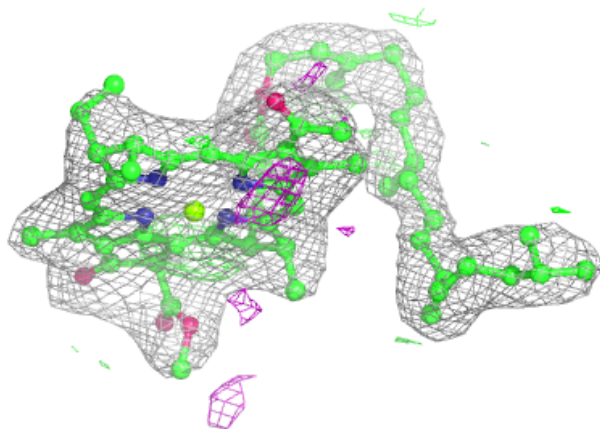
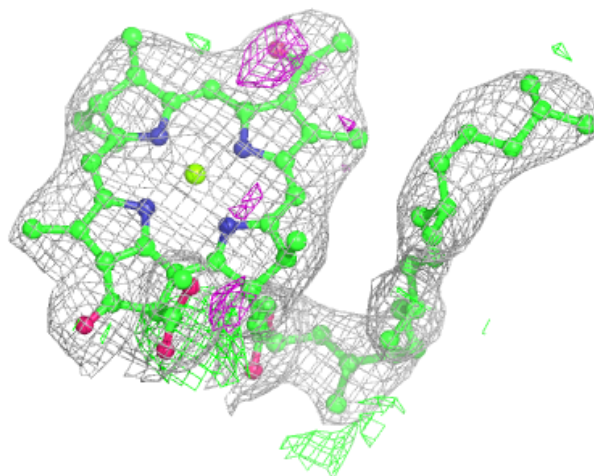
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





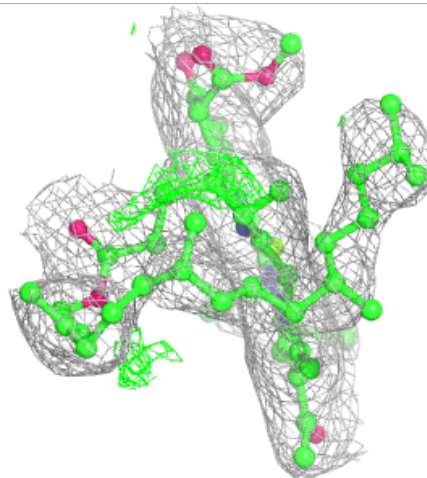
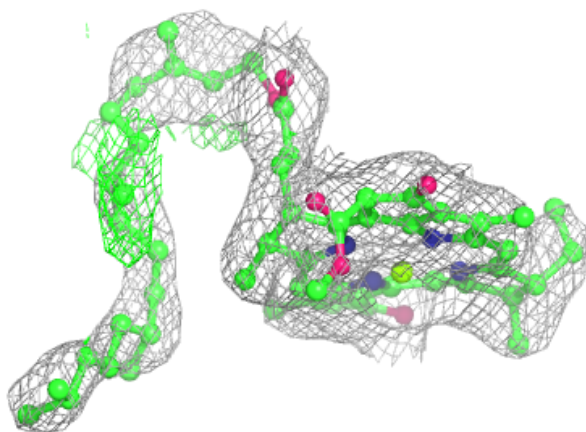
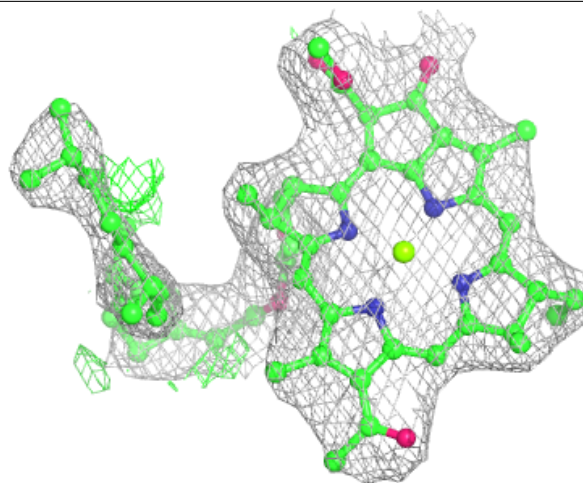
**Electron density around BCL M 403:**

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



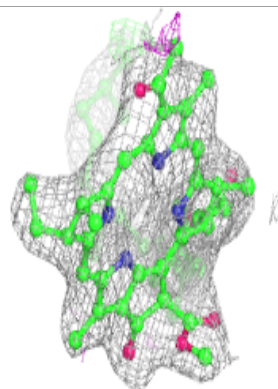
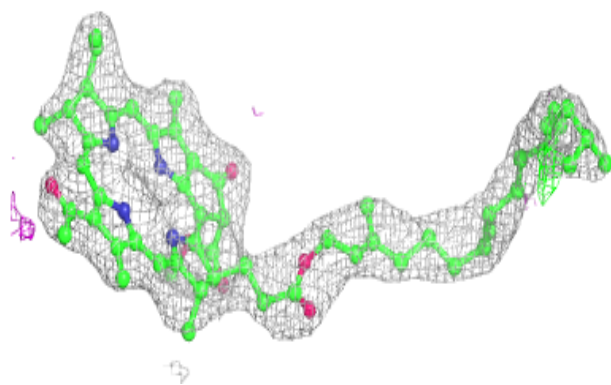
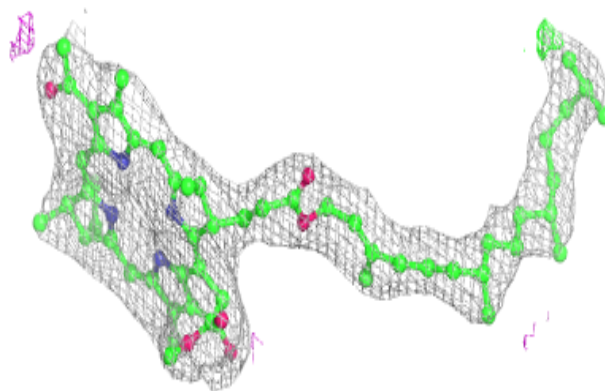
**Electron density around BCL L 301:**

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

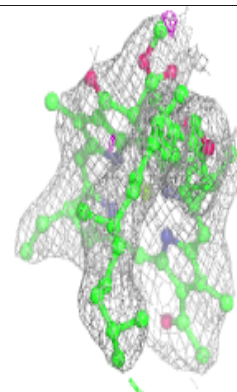
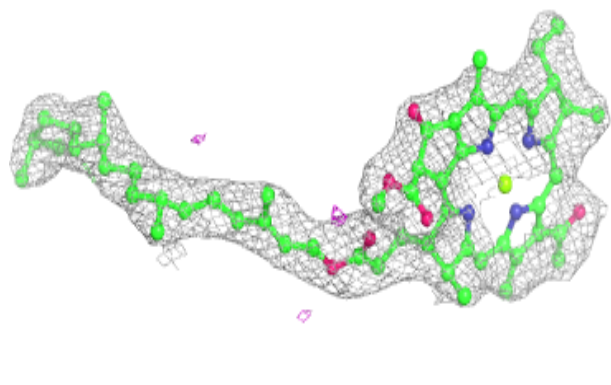
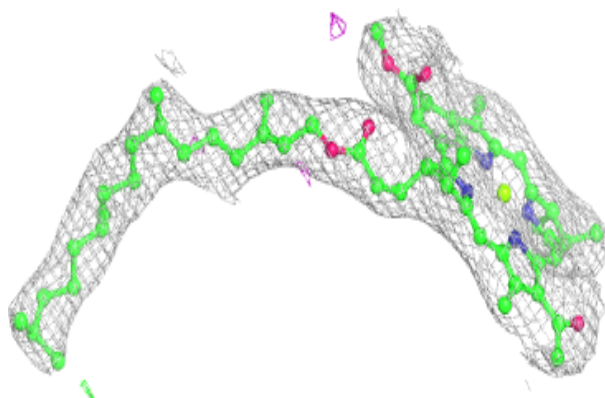


**Electron density around BPH M 402:**

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

**Electron density around BCL L 302:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.