



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 12:07 PM EDT

PDB ID : 3DTS  
Title : E(L212)A, D(L213)A, R(M233)L triple mutant structure of photosynthetic reaction center from Rhodobacter sphaeroides  
Authors : Pokkuluri, P.R.; Schiffer, M.  
Deposited on : 2008-07-15  
Resolution : 3.10 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.

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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	:	2.23.2
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)	:	2.23.2

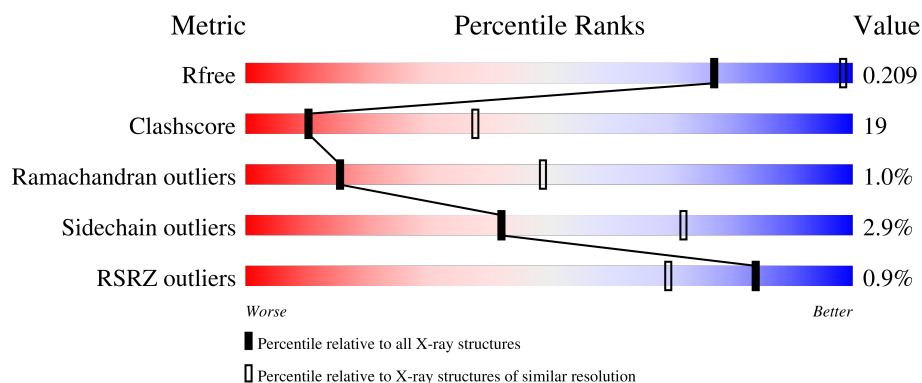
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	L	281	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 64%, yellow 35%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>64%</span> <span>35%</span> <span>.</span> </div> </div>
2	M	314	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 63%, yellow 31%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>63%</span> <span>31%</span> <span>.</span> </div> </div>
3	H	260	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 60%, yellow 30%, orange 8%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>60%</span> <span>30%</span> <span>.</span> <span>8%</span> </div> </div>

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
4	BCL	L	501	X	-	-	-
4	BCL	M	501	X	-	-	-
5	U10	L	504	-	-	-	X
6	LDA	L	709	-	-	-	X
7	BPH	M	504	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7226 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
1	L	281	Total	C	N	O	S	0	0	0
			2225	1504	355	358	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	ALA	GLU	engineered mutation	UNP P0C0Y8
L	213	ALA	ASP	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2405	1607	391	397	10			

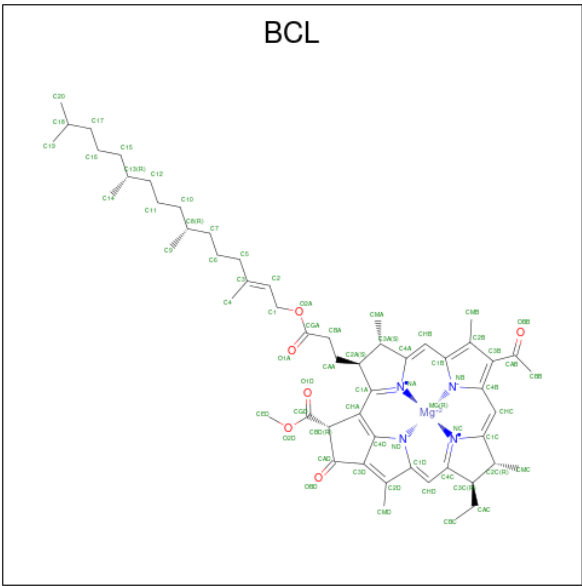
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	LEU	ARG	engineered mutation	UNP P0C0Y9
M	308	HIS	-	expression tag	UNP P0C0Y9
M	309	HIS	-	expression tag	UNP P0C0Y9
M	310	HIS	-	expression tag	UNP P0C0Y9
M	311	HIS	-	expression tag	UNP P0C0Y9
M	312	HIS	-	expression tag	UNP P0C0Y9
M	313	HIS	-	expression tag	UNP P0C0Y9
M	314	HIS	-	expression tag	UNP P0C0Y9

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

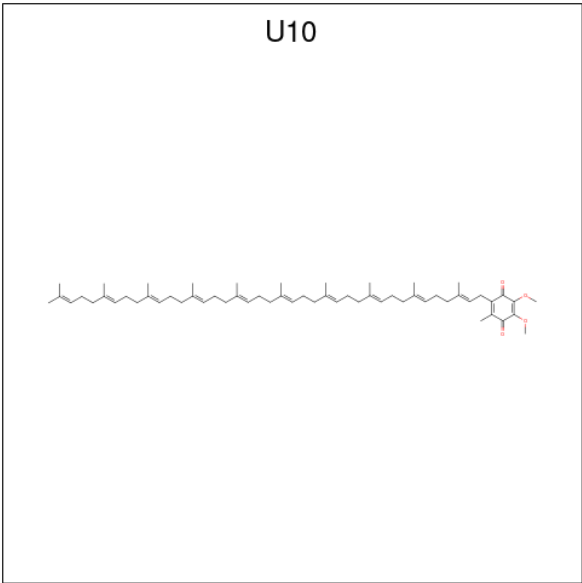
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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



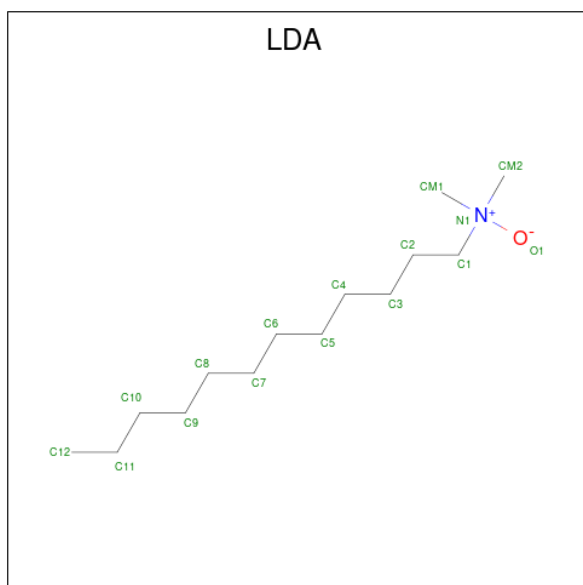
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



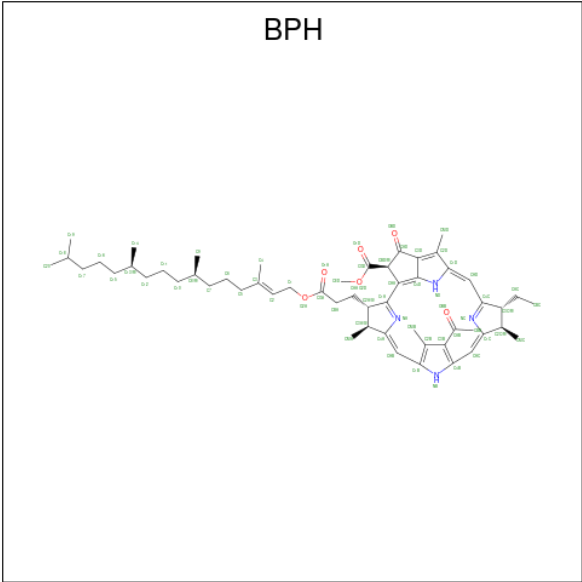
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			48	44	4		
5	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).

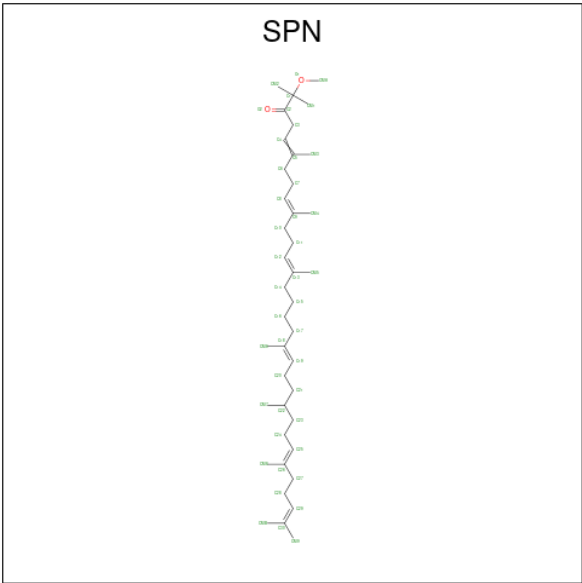


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	10	0
			65	55	4	6		

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

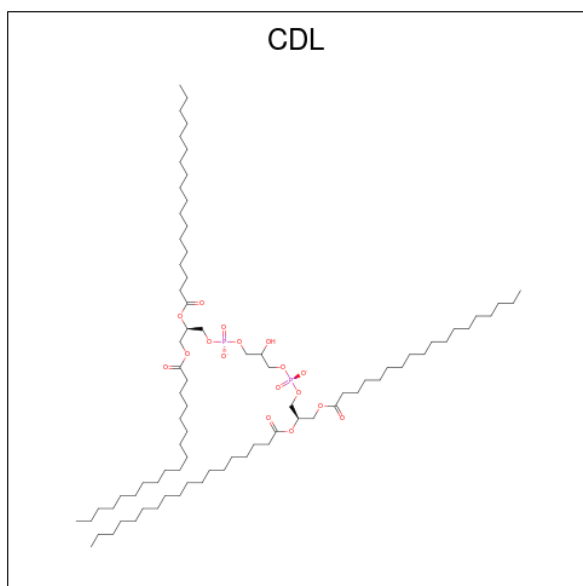
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: C<sub>41</sub>H<sub>70</sub>O<sub>2</sub>).



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

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 11 is water.

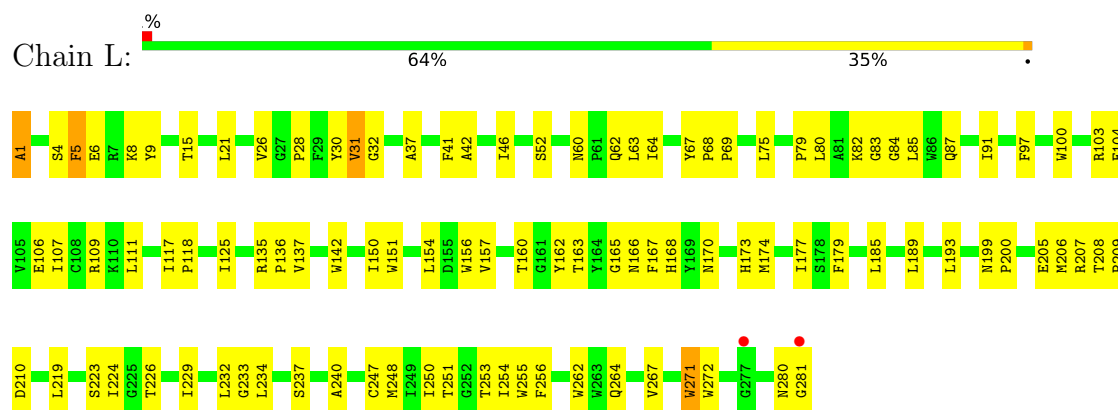
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	28	Total	O	0	0
			28	28		
11	M	27	Total	O	0	0
			27	27		
11	H	33	Total	O	0	0
			33	33		



### 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.

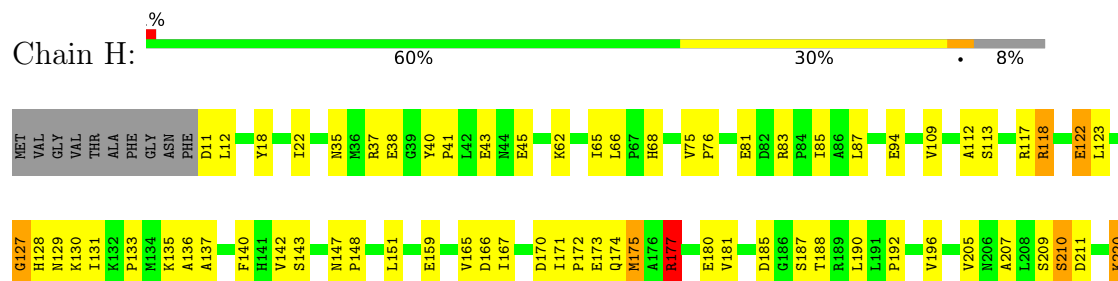
#### • Molecule 1: Reaction center protein L chain



#### • Molecule 2: Reaction center protein M chain



#### • Molecule 3: Reaction center protein H chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.30Å 141.30Å 187.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 26.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	81.0 (30.00-3.10) 80.8 (26.89-3.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 3.11Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.224 0.197 , 0.209	Depositor DCC
$R_{free}$ test set	2382 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: SPN, FE, BCL, BPH, U10, CDL, LDA

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	0.95	5/2313 (0.2%)	0.92	7/3166 (0.2%)
2	M	0.92	5/2497 (0.2%)	0.86	5/3410 (0.1%)
3	H	0.85	2/1877 (0.1%)	0.94	5/2553 (0.2%)
All	All	0.91	12/6687 (0.2%)	0.91	17/9129 (0.2%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	1	ALA	N-CA	11.39	1.69	1.46
1	L	280	ASN	C-N	-7.25	1.20	1.33
2	M	105	PHE	CE2-CZ	6.80	1.50	1.37
3	H	122	GLU	CB-CG	6.55	1.64	1.52
2	M	68	PHE	CE2-CZ	6.36	1.49	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	280	ASN	C-N-CA	10.11	143.54	122.30
1	L	280	ASN	O-C-N	-9.73	106.66	123.20
3	H	122	GLU	CB-CG-CD	-9.54	88.46	114.20
1	L	280	ASN	CA-C-N	8.30	132.79	116.20
2	M	247	ARG	NE-CZ-NH2	8.11	124.36	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	2225	0	2186	91	0
2	M	2405	0	2319	99	0
3	H	1829	0	1836	80	0
4	L	132	0	148	15	0
4	M	132	0	148	17	0
5	L	48	0	62	6	0
5	M	48	0	63	7	0
6	H	16	0	31	4	0
6	L	16	0	31	4	0
6	M	32	0	62	3	0
7	M	130	0	152	4	0
8	M	1	0	0	0	0
9	M	43	0	69	2	0
10	M	81	0	106	2	0
11	H	33	0	0	8	0
11	L	28	0	0	2	0
11	M	27	0	0	5	0
All	All	7226	0	7213	267	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 19.

The worst 5 of 267 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:1:ALA:N	1:L:1:ALA:CA	1.69	1.51
1:L:219:LEU:HA	2:M:132:ARG:HH12	1.23	1.00
1:L:154:LEU:HD11	4:L:501:BCL:HED3	1.52	0.89
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.52	0.89
5:M:505:U10:H202	6:H:703:LDA:H112	1.54	0.88

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	279/281 (99%)	249 (89%)	28 (10%)	2 (1%)	22	57
2	M	300/314 (96%)	275 (92%)	21 (7%)	4 (1%)	12	42
3	H	238/260 (92%)	220 (92%)	16 (7%)	2 (1%)	19	54
All	All	817/855 (96%)	744 (91%)	65 (8%)	8 (1%)	15	49

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	211	ASP
2	M	26	LEU
2	M	301	HIS
3	H	210	SER
1	L	4	SER

### 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	218/218 (100%)	212 (97%)	6 (3%)	43	73
2	M	236/247 (96%)	232 (98%)	4 (2%)	60	83
3	H	195/208 (94%)	186 (95%)	9 (5%)	27	59
All	All	649/673 (96%)	630 (97%)	19 (3%)	42	72

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	159	GLU
3	H	225	VAL
3	H	231	ASP
3	H	220	LYS
2	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	300	ASN
3	H	68	HIS
3	H	206	ASN
2	M	28	ASN
2	M	44	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 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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
4	BCL	M	501	2	58,74,74	1.58	10 (17%)	69,115,115	2.55	27 (39%)
6	LDA	M	701	-	12,15,15	2.57	1 (8%)	14,17,17	0.40	0
4	BCL	L	501	-	58,74,74	1.39	9 (15%)	69,115,115	2.24	14 (20%)
10	CDL	M	800	-	80,80,99	0.48	0	86,92,111	0.93	5 (5%)
5	U10	M	505	-	48,48,63	2.46	21 (43%)	58,61,79	1.30	7 (12%)
6	LDA	M	704	-	12,15,15	2.06	1 (8%)	14,17,17	0.52	0
4	BCL	L	502	1	58,74,74	1.61	10 (17%)	69,115,115	2.62	14 (20%)
6	LDA	H	703	-	12,15,15	2.41	1 (8%)	14,17,17	0.65	0
6	LDA	L	709	-	12,15,15	2.40	1 (8%)	14,17,17	0.49	0
7	BPH	M	504	-	64,70,70	1.34	8 (12%)	76,101,101	2.29	29 (38%)
4	BCL	M	502	2	58,74,74	1.31	7 (12%)	69,115,115	1.93	13 (18%)
9	SPN	M	600	-	40,42,42	3.76	18 (45%)	50,52,52	2.58	16 (32%)
5	U10	L	504	-	48,48,63	1.94	13 (27%)	58,61,79	2.89	18 (31%)
7	BPH	M	503	-	64,70,70	1.30	9 (14%)	76,101,101	1.92	19 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	M	501	2	2/2/21/25	15/37/137/137	-
6	LDA	M	701	-	-	8/13/13/13	-
4	BCL	L	501	-	1/1/21/25	10/37/137/137	-
7	BPH	M	503	-	-	5/54/105/105	0/5/6/6
10	CDL	M	800	-	-	30/91/91/110	-
5	U10	M	505	-	-	10/45/69/87	0/1/1/1
6	LDA	M	704	-	-	5/13/13/13	-
4	BCL	L	502	1	-	6/37/137/137	-
6	LDA	H	703	-	-	5/13/13/13	-
6	LDA	L	709	-	-	4/13/13/13	-
4	BCL	M	502	2	-	8/37/137/137	-
9	SPN	M	600	-	-	19/50/51/51	-
5	U10	L	504	-	-	11/45/69/87	0/1/1/1
7	BPH	M	504	-	1/1/18/22	16/54/105/105	0/5/6/6



The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C4-C5	8.92	1.54	1.33
9	M	600	SPN	C19-C18	8.82	1.54	1.33
6	M	701	LDA	O1-N1	-8.77	1.21	1.42
9	M	600	SPN	C8-C9	8.46	1.53	1.33
6	H	703	LDA	O1-N1	-8.33	1.22	1.42

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	504	U10	C32-C33-C34	14.67	162.97	127.66
4	L	502	BCL	C4B-C3B-CAB	-11.04	105.81	127.13
4	L	502	BCL	OBB-CAB-C3B	9.29	136.48	119.99
4	L	501	BCL	C4A-NA-C1A	8.47	110.52	106.71
4	L	502	BCL	C4A-NA-C1A	8.39	110.48	106.71

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	501	BCL	C13
4	M	501	BCL	C13
4	M	501	BCL	C8
7	M	504	BPH	C8

5 of 152 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	501	BCL	C2C-C3C-CAC-CBC
4	L	501	BCL	C4C-C3C-CAC-CBC
4	M	501	BCL	C1-C2-C3-C4
5	L	504	U10	C12-C13-C14-C15
5	L	504	U10	C12-C13-C14-C16

There are no ring outliers.

14 monomers are involved in 57 short contacts:

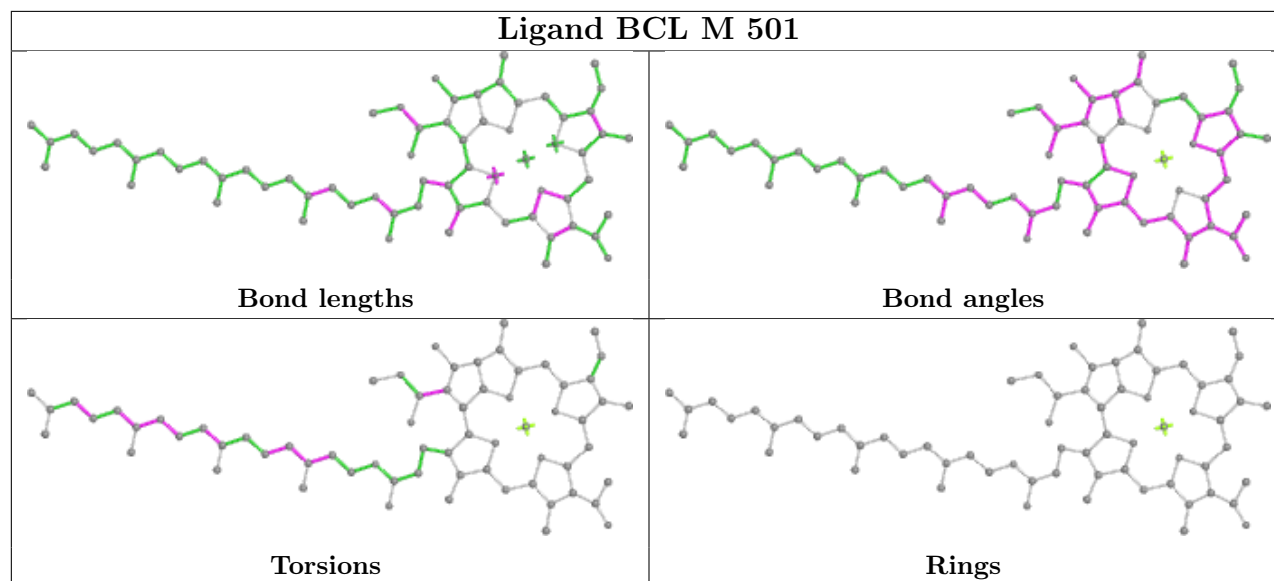
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	501	BCL	6	0
6	M	701	LDA	2	0
4	L	501	BCL	7	0
10	M	800	CDL	2	0
5	M	505	U10	7	0

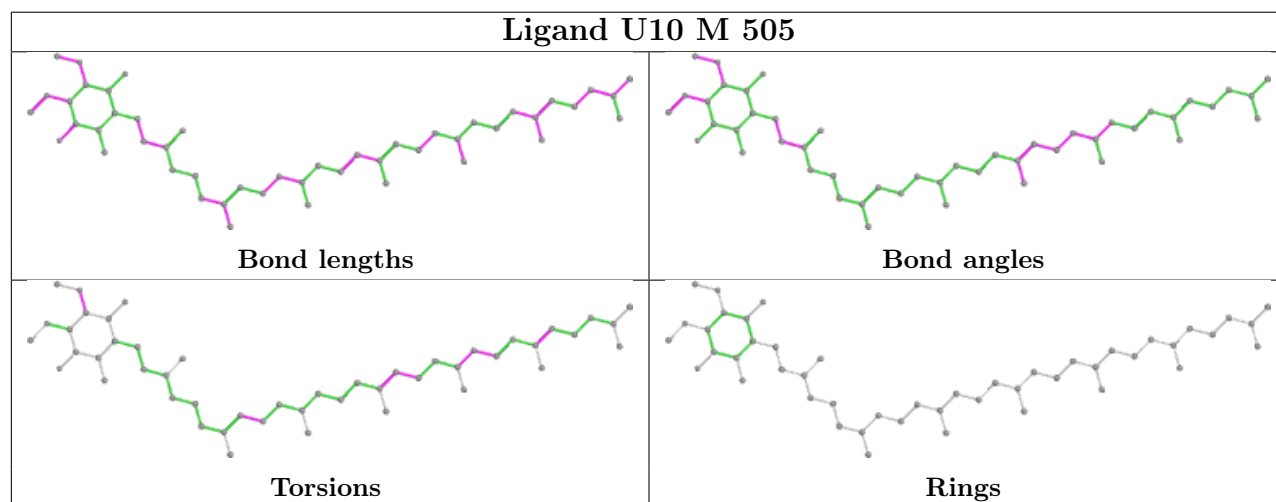
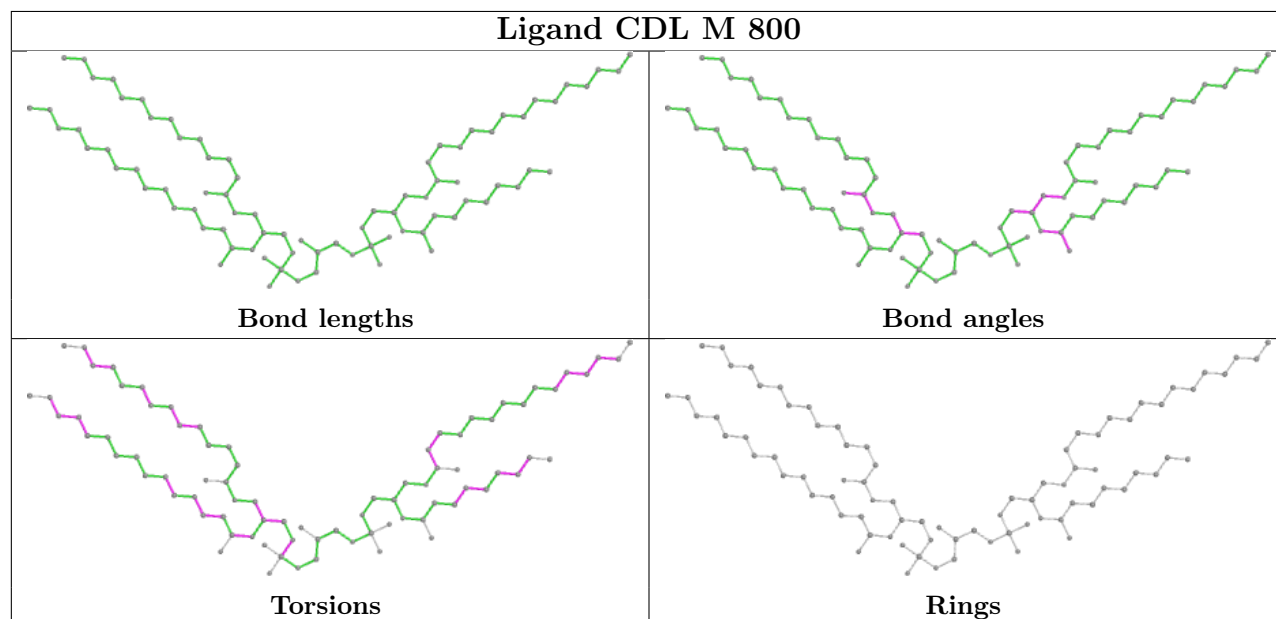
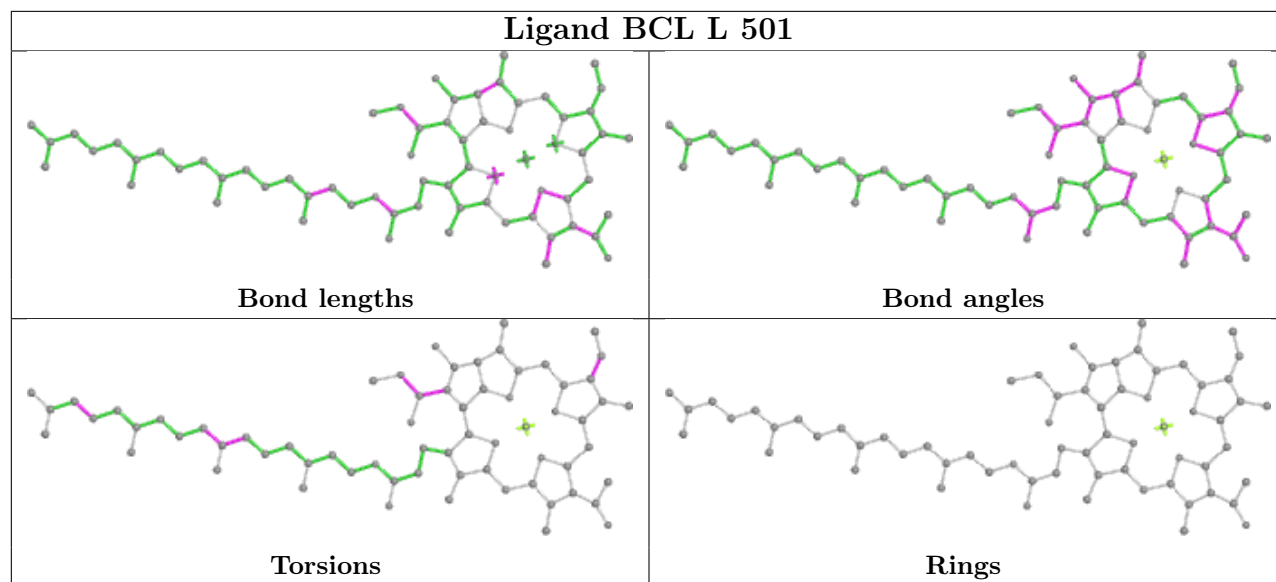
*Continued on next page...*

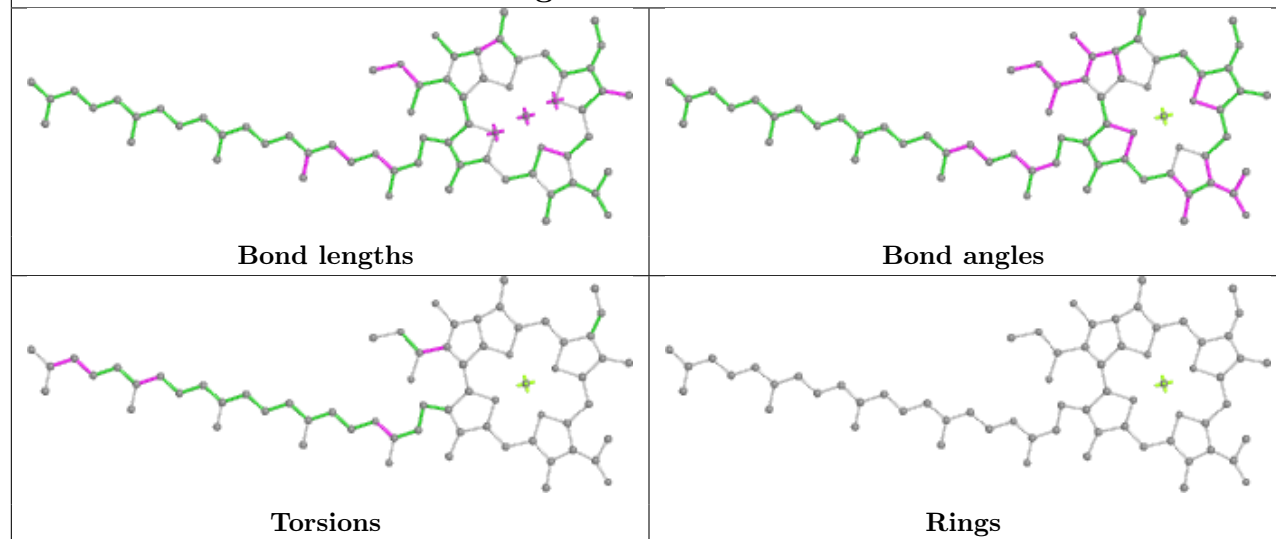
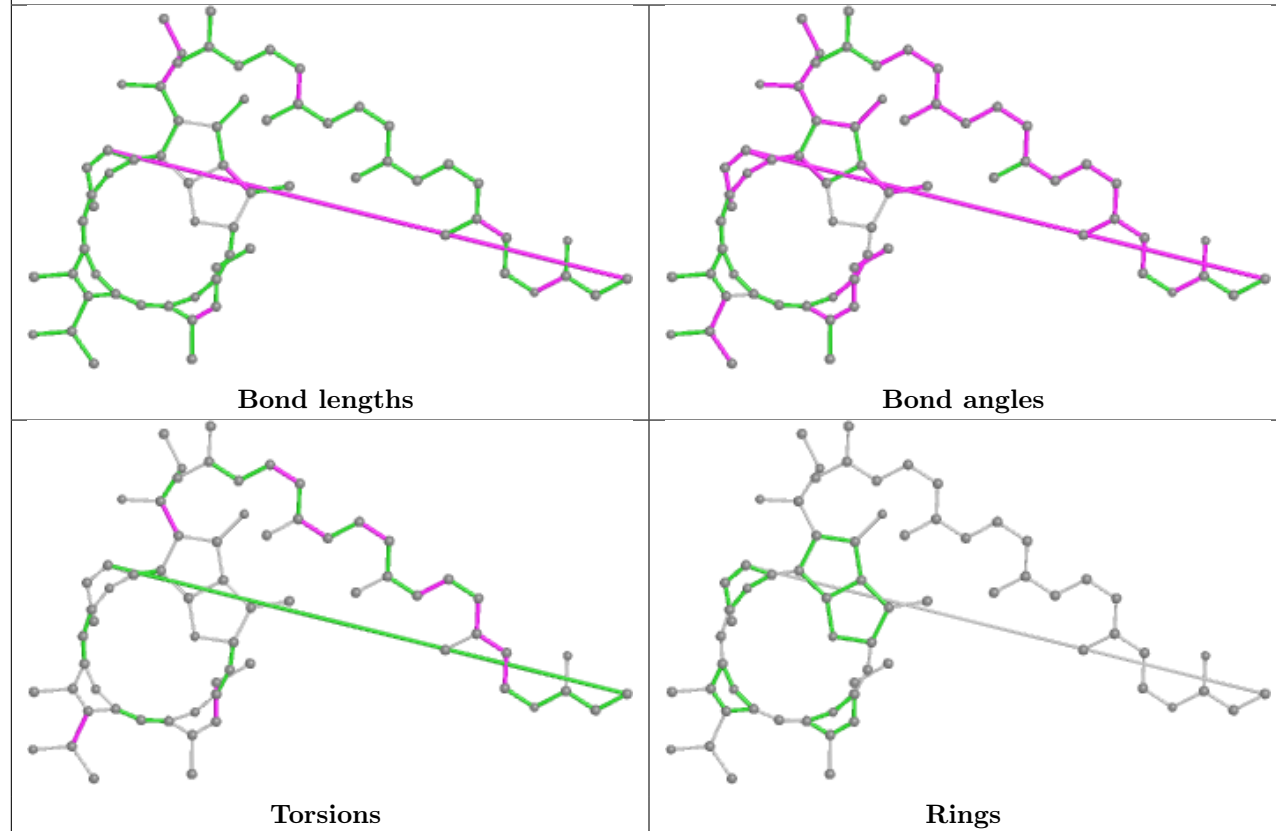
*Continued from previous page...*

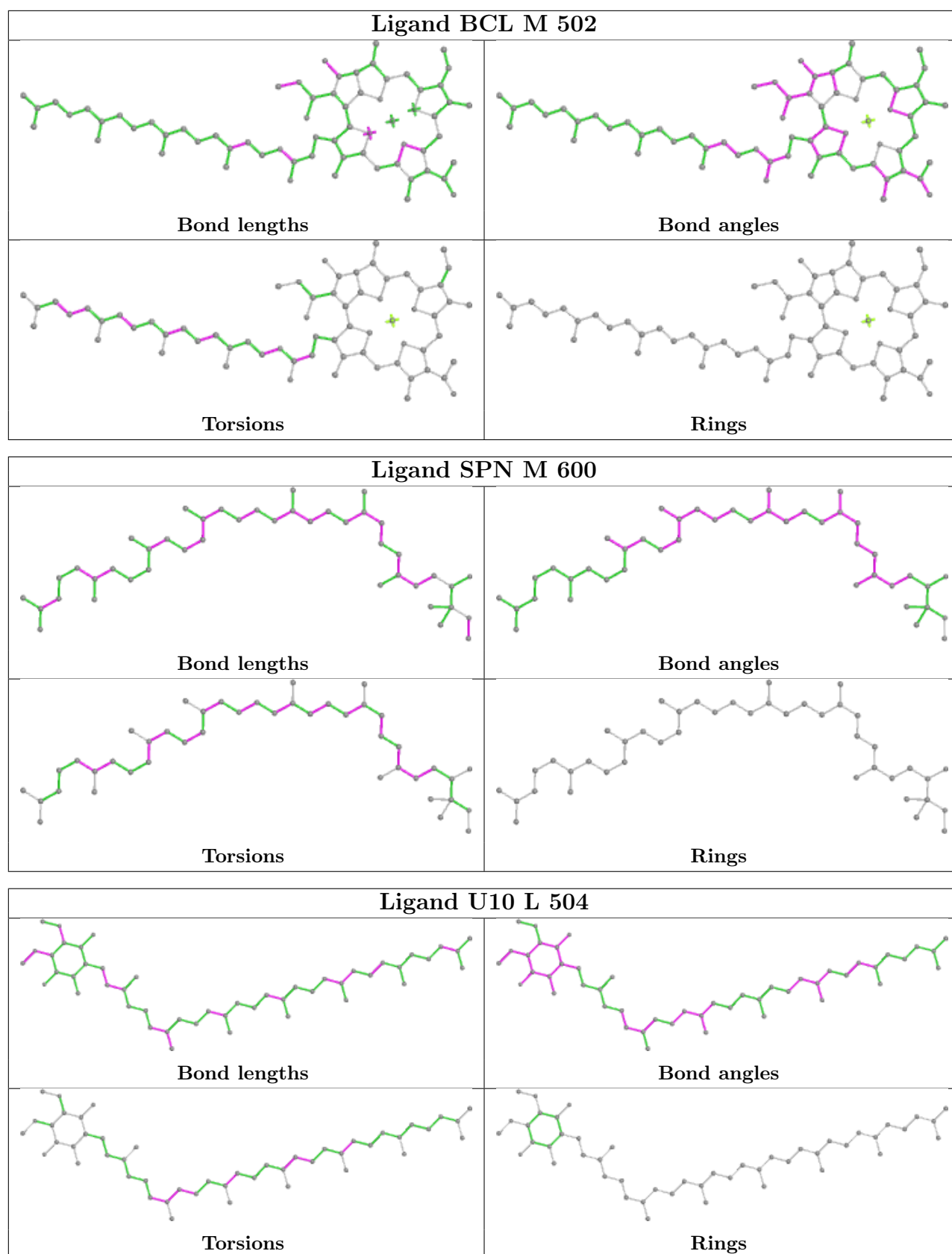
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	704	LDA	1	0
4	L	502	BCL	10	0
6	H	703	LDA	4	0
6	L	709	LDA	4	0
7	M	504	BPH	2	0
4	M	502	BCL	13	0
9	M	600	SPN	2	0
5	L	504	U10	6	0
7	M	503	BPH	2	0

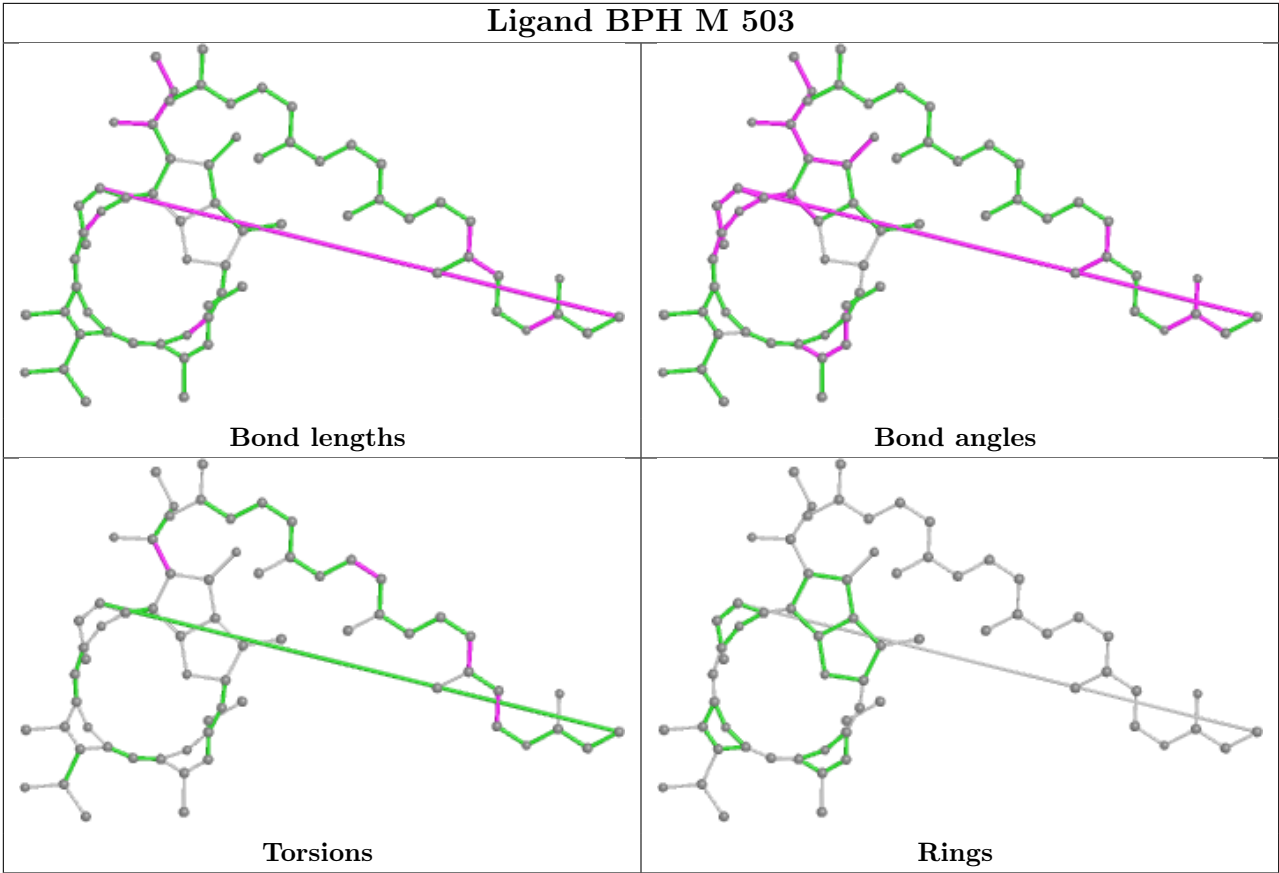
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





**Ligand BCL L 502****Ligand BPH M 504**





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	280:ASN	C	281:GLY	N	1.20

## 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	L	281/281 (100%)	-0.67	2 (0%) 87 75	24, 43, 83, 99	0
2	M	302/314 (96%)	-0.62	3 (0%) 82 67	25, 51, 87, 109	0
3	H	240/260 (92%)	-0.53	2 (0%) 86 72	25, 48, 74, 109	0
All	All	823/855 (96%)	-0.61	7 (0%) 84 69	24, 47, 84, 109	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	4.8
2	M	1	ALA	3.3
3	H	249	LYS	2.7
2	M	2	GLU	2.3
1	L	277	GLY	2.3

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

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

### 6.3 Carbohydrates [i](#)

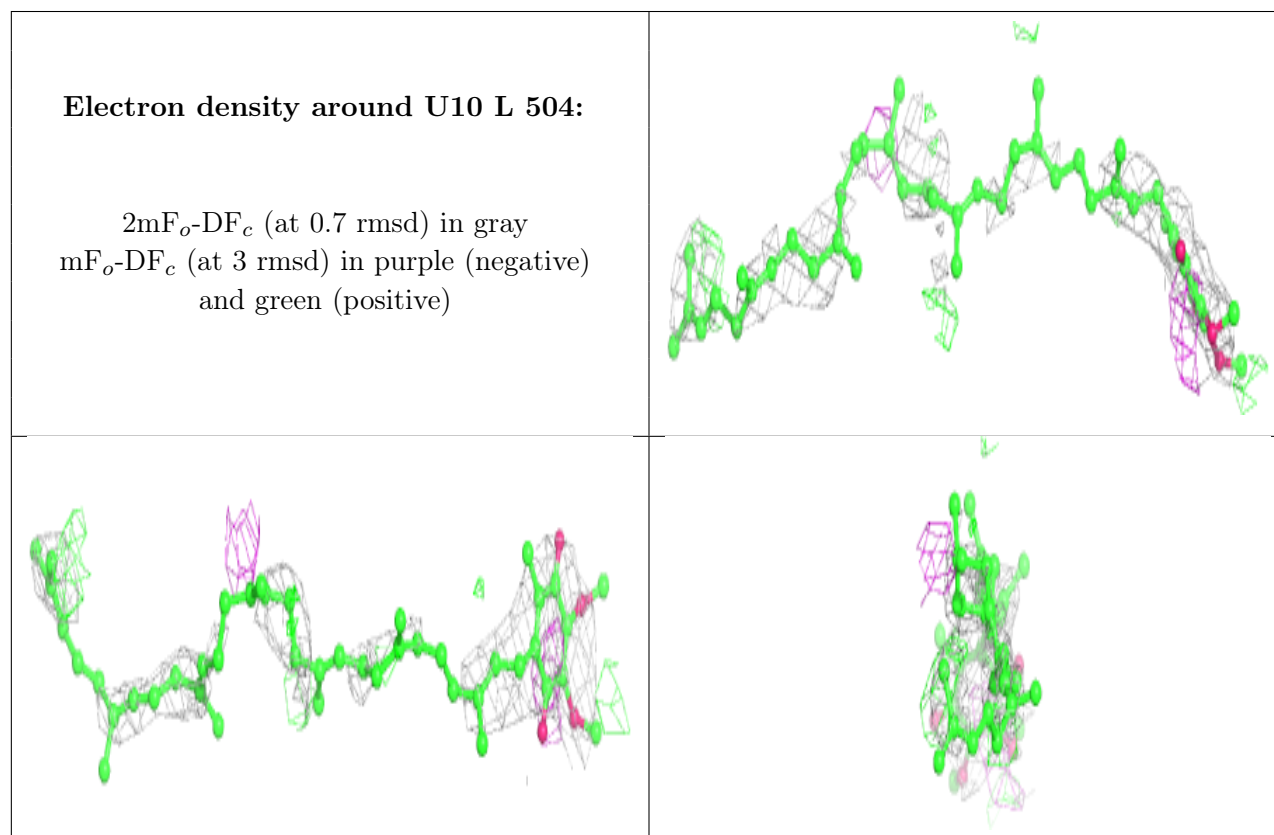
There are no monosaccharides in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
5	U10	L	504	48/63	0.78	0.50	76,89,95,96	0
6	LDA	L	709	16/16	0.79	0.59	104,109,119,120	0
6	LDA	M	704	16/16	0.79	0.33	90,97,121,122	0
10	CDL	M	800	81/100	0.84	0.37	25,68,82,85	81
9	SPN	M	600	43/43	0.86	0.28	44,64,91,94	0
6	LDA	M	701	16/16	0.90	0.24	57,75,79,82	0
6	LDA	H	703	16/16	0.92	0.26	64,74,87,89	0
4	BCL	M	501	66/66	0.93	0.21	31,41,88,91	0
5	U10	M	505	48/63	0.94	0.20	30,45,77,79	0
7	BPH	M	504	65/65	0.95	0.17	22,53,71,79	10
4	BCL	L	501	66/66	0.96	0.16	19,33,55,59	0
4	BCL	L	502	66/66	0.97	0.15	22,33,42,49	0
8	FE	M	500	1/1	0.97	0.10	36,36,36,36	0
4	BCL	M	502	66/66	0.97	0.16	27,37,69,75	0
7	BPH	M	503	65/65	0.97	0.15	25,37,47,50	0

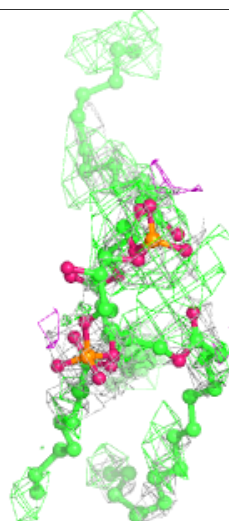
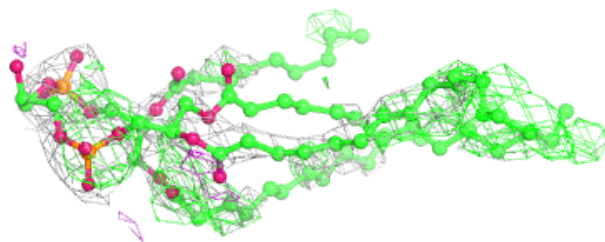
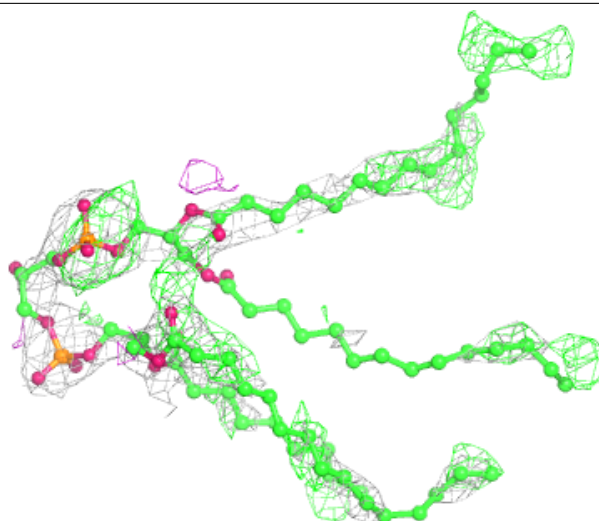
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





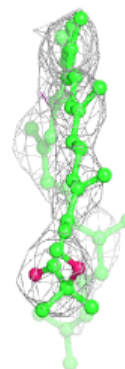
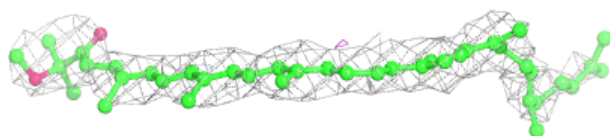
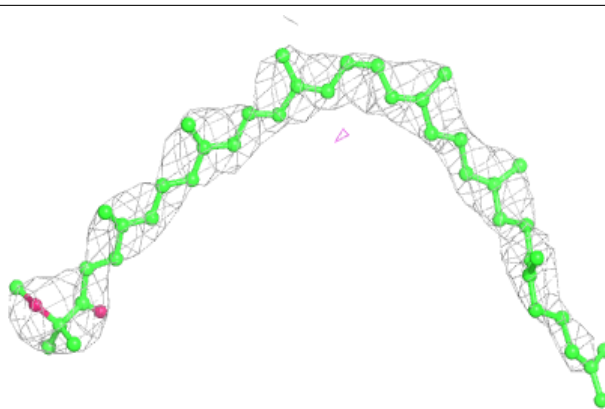
**Electron density around CDL M 800:**

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



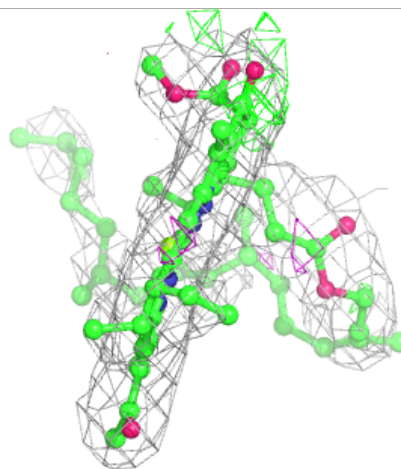
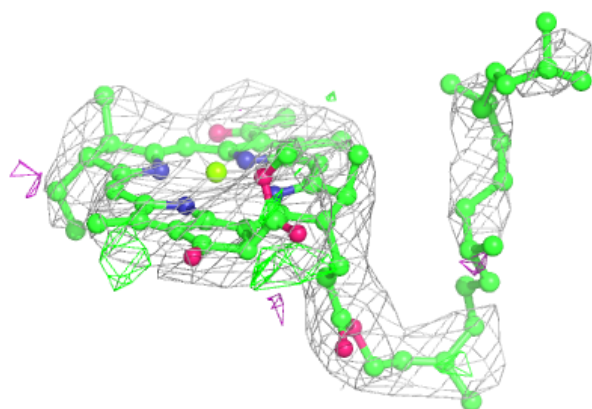
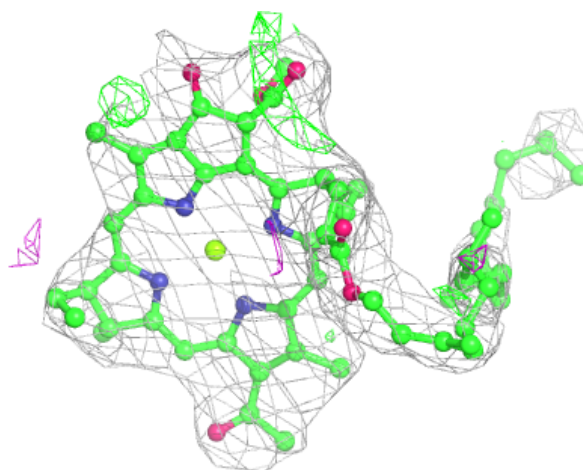
**Electron density around SPN M 600:**

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



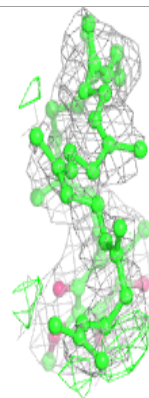
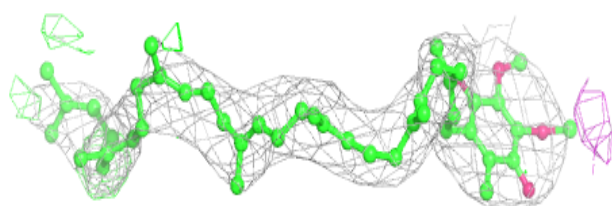
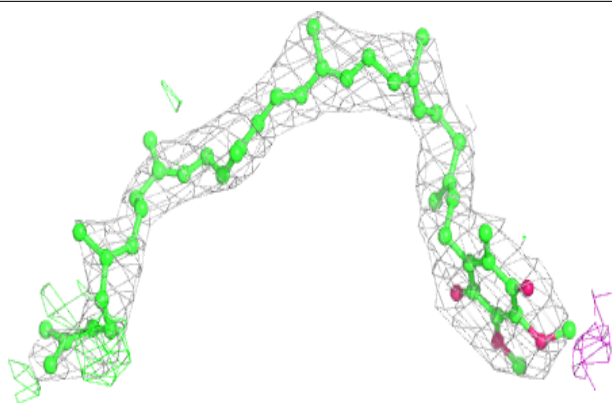
**Electron density around BCL M 501:**

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

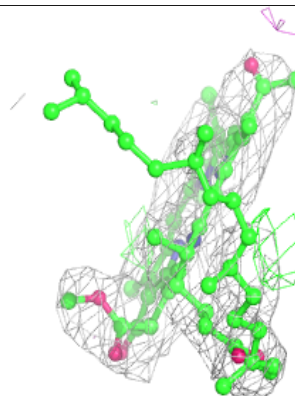
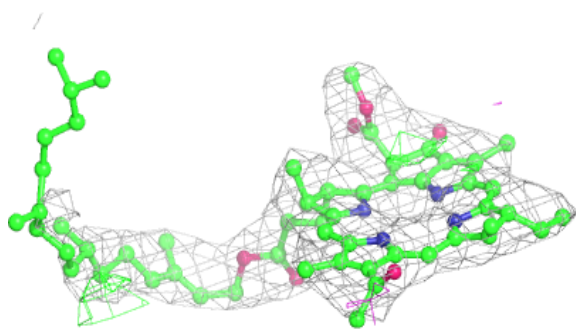
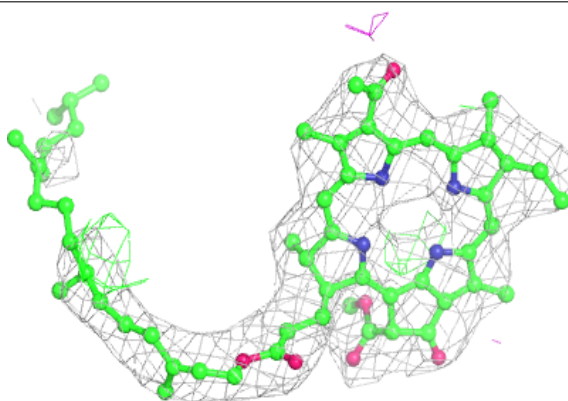


**Electron density around U10 M 505:**

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

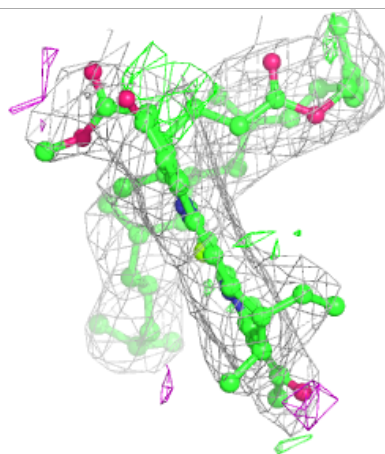
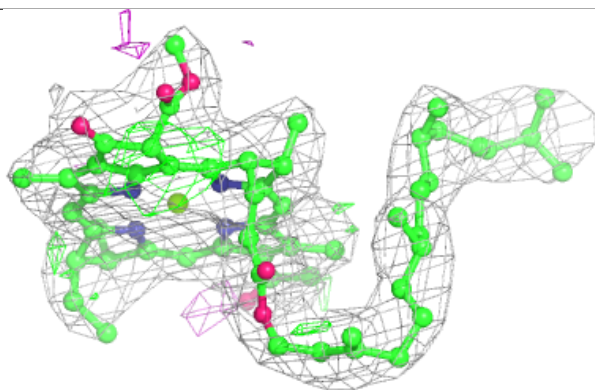
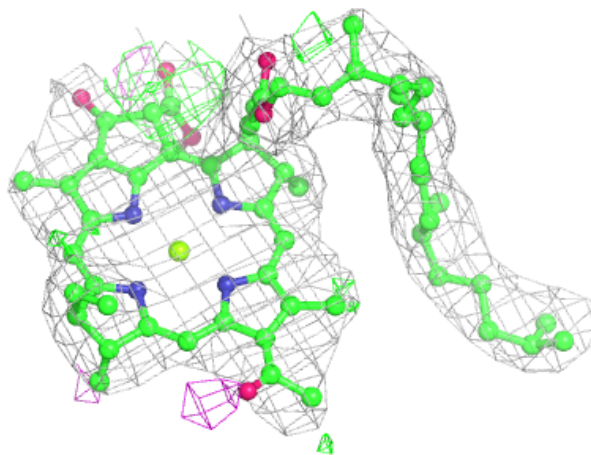
**Electron density around BPH M 504:**

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



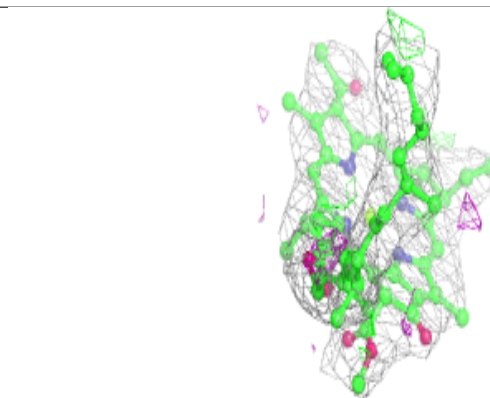
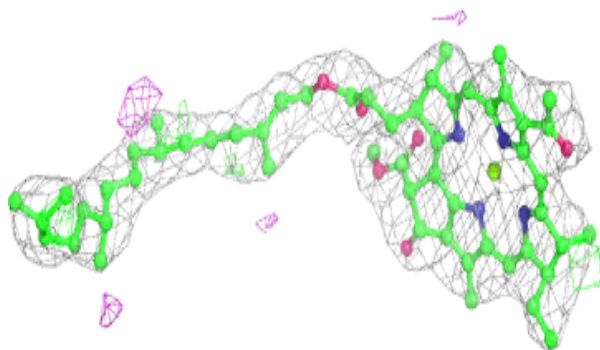
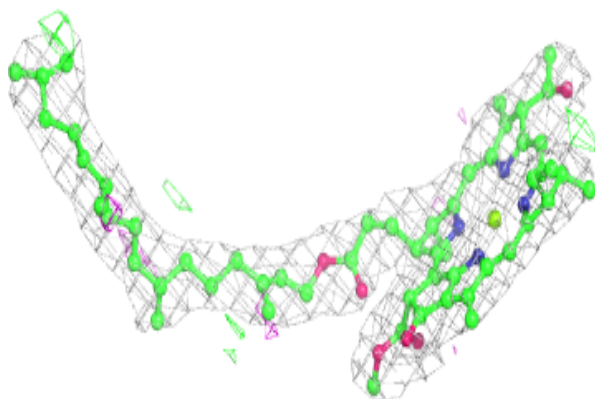
**Electron density around BCL L 501:**

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

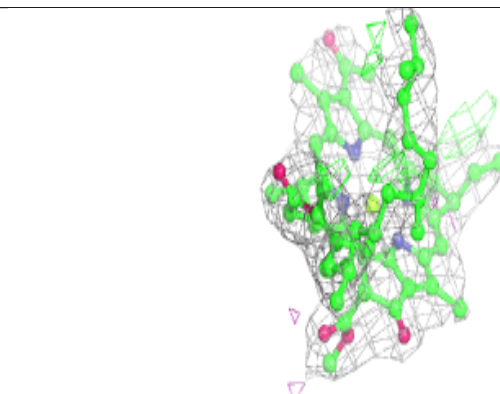
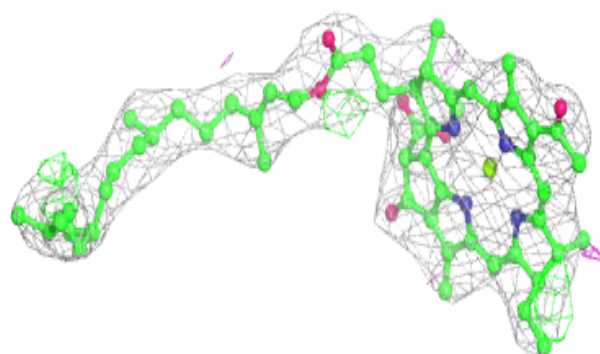
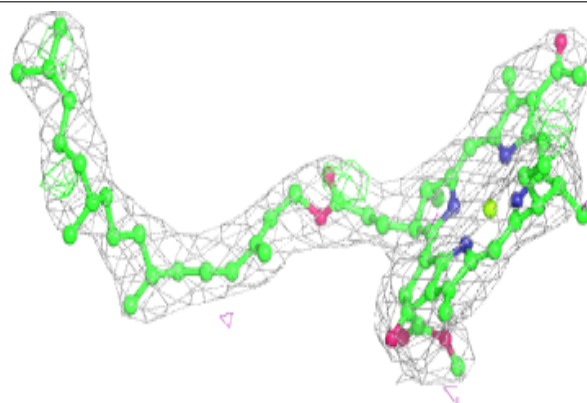


**Electron density around BCL L 502:**

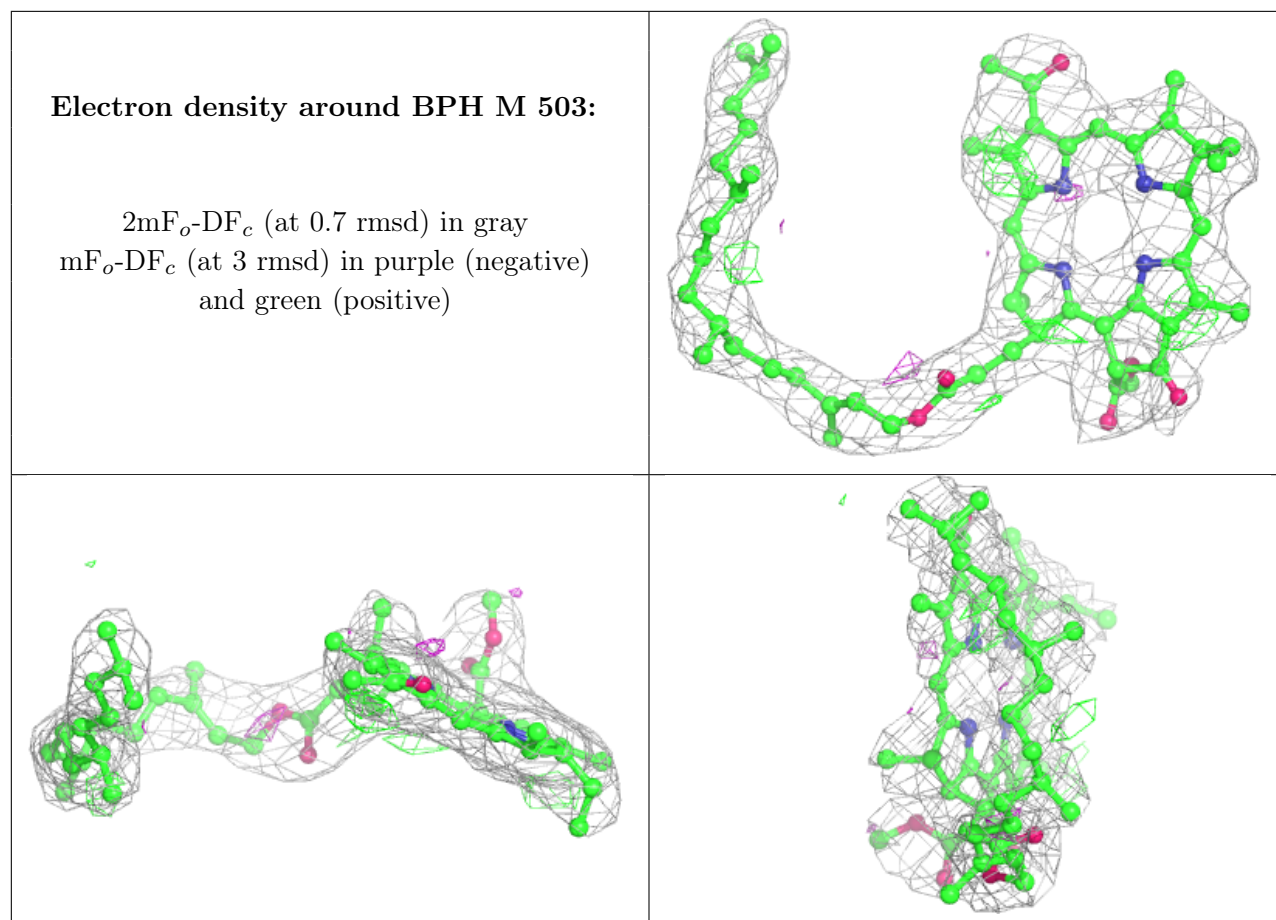
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCL M 502:**

$2mF_o-DF_c$  (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.