



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 10:52 AM EDT

PDB ID : 1YF6  
Title : Structure of a quintuple mutant of photosynthetic reaction center from rhodobacter sphaeroides  
Authors : Paddock, M.L.; Chang, C.; Xu, Q.; Abresch, E.C.; Axelrod, H.L.  
Deposited on : 2004-12-30  
Resolution : 2.25 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

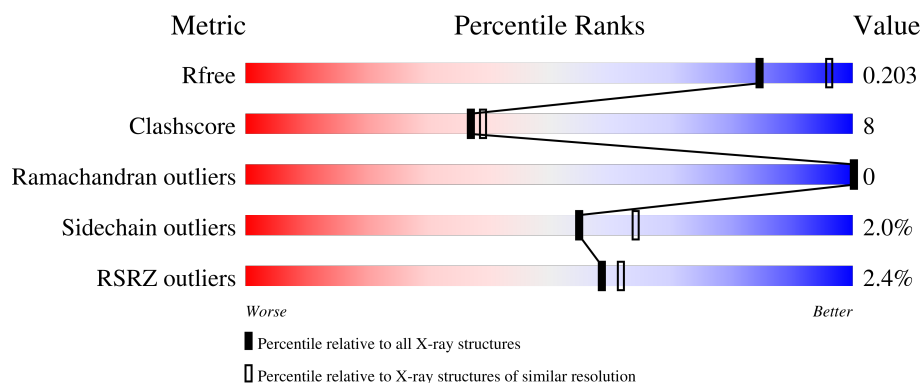
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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>0%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
2	M	307	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
3	H	260	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </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	852	X	-	-	-
4	BCL	L	854	X	-	-	-
4	BCL	M	851	X	-	-	-
4	BCL	M	853	X	-	-	-
4	BCL	M	856	X	-	-	-
9	GOL	L	869	-	X	-	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7450 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
			2233	1507	355	363	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	181	TYR	PHE	engineered mutation	UNP P02954

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2418	1615	396	397	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	203	ASP	GLY	engineered mutation	UNP P02953
M	210	PHE	TYR	engineered mutation	UNP P02953
M	214	HIS	LEU	engineered mutation	UNP P02953
M	260	TRP	ALA	engineered mutation	UNP P02953

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1814	1160	311	334	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>).



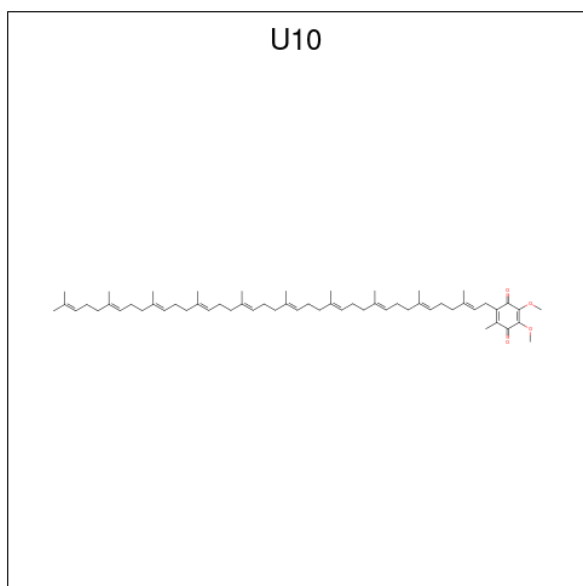
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



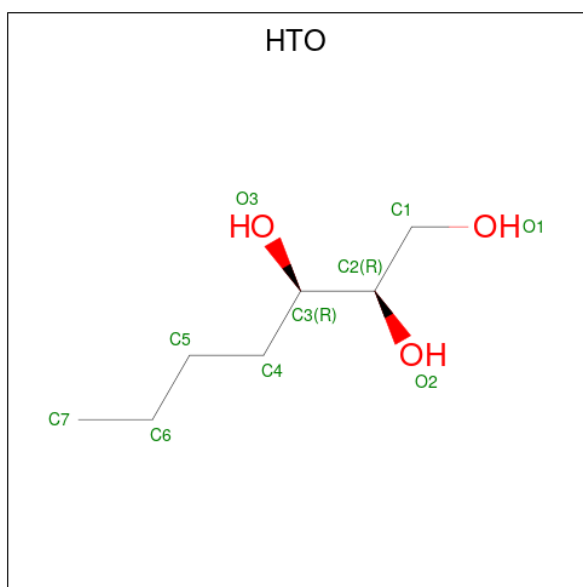
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			51	41	4	6		

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



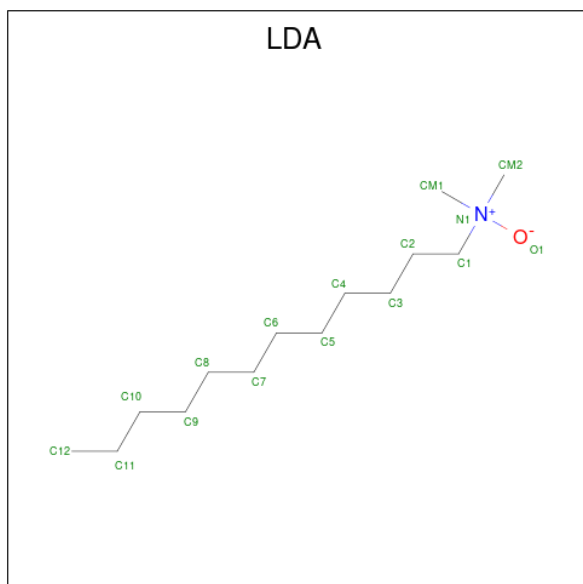
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			16	12	4		
6	L	1	Total	C	O	0	0
			15	11	4		
6	M	1	Total	C	O	0	0
			15	11	4		

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

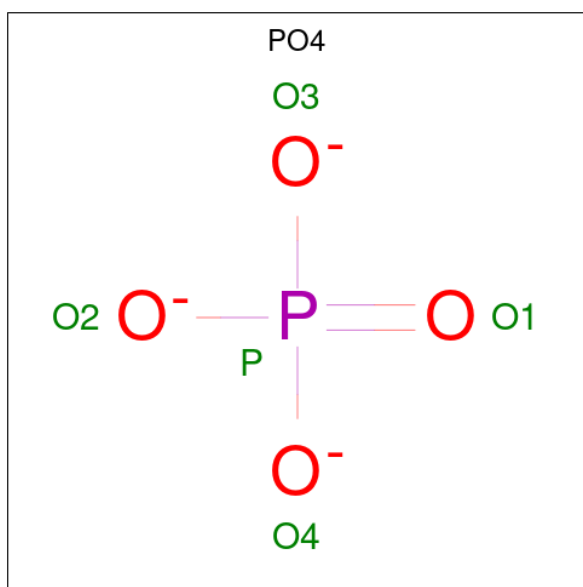
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Cl	0	0
			1	1		

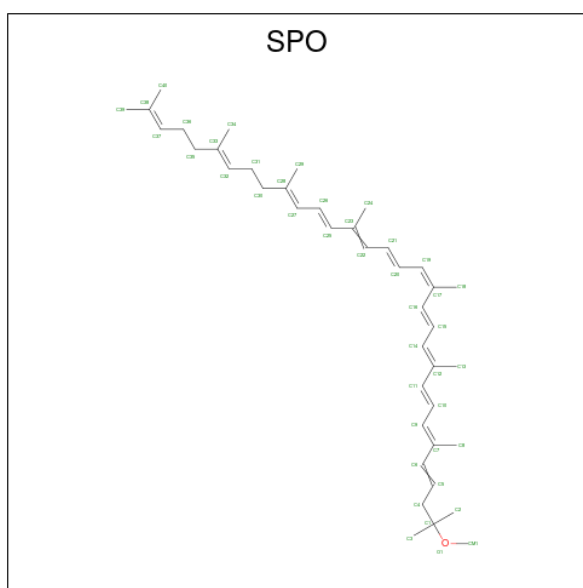
- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).





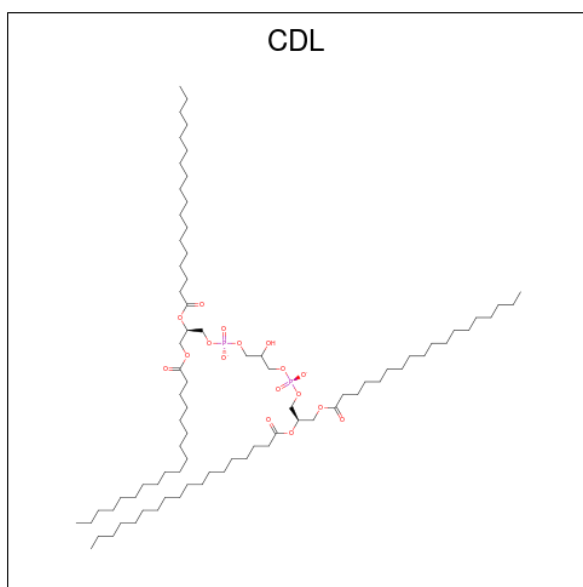
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	O	P	0	0
			5	4	1		
12	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



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

- 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		

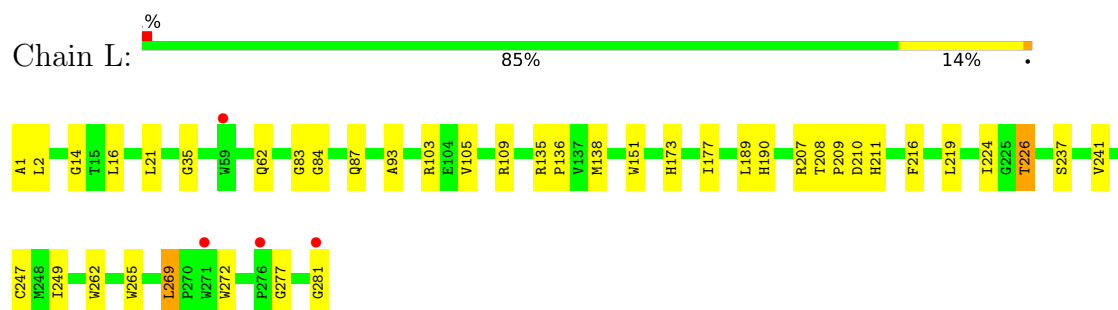
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	109	Total	O	0	0
			109	109		
15	M	108	Total	O	0	0
			108	108		
15	H	147	Total	O	0	0
			147	147		

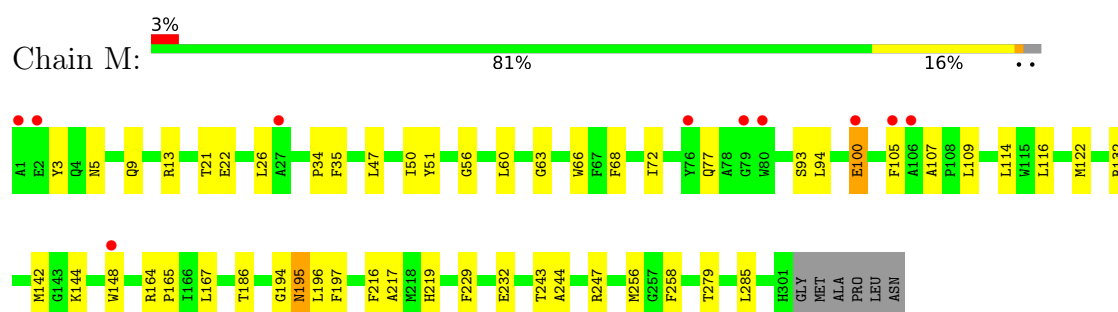
### 3 Residue-property plots

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.

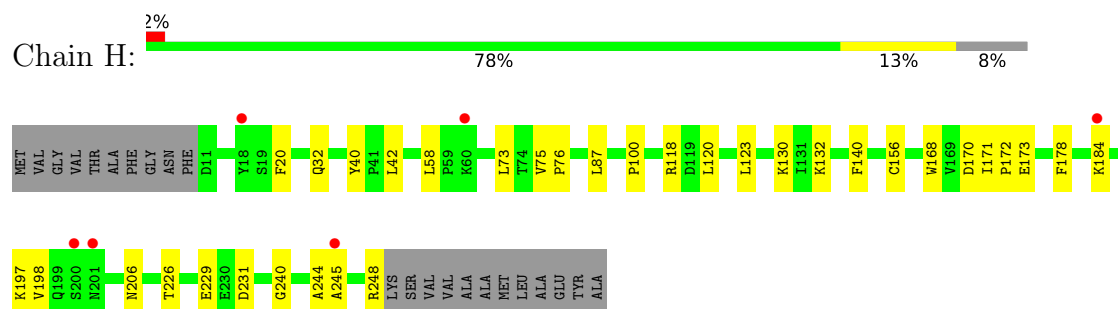
#### • Molecule 1: Reaction center protein L chain



#### • 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, $\alpha$ , $\beta$ , $\gamma$	139.44Å 139.44Å 185.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.34 – 2.25 43.20 – 2.25	Depositor EDS
% Data completeness (in resolution range)	84.8 (39.34-2.25) 84.9 (43.20-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.197 , 0.216 0.183 , 0.203	Depositor DCC
$R_{free}$ test set	4275 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.6	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	0.94	EDS
Total number of atoms	7450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, BPH, PO4, FE2, HTO, CL, CDL, U10, BCL, LDA, GOL

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	0.38	0/2321	0.55	0/3177
2	M	0.38	0/2513	0.52	0/3432
3	H	0.33	0/1862	0.59	0/2534
All	All	0.37	0/6696	0.55	0/9143

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 [i](#)

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	2233	0	2187	34	0
2	M	2418	0	2320	49	0
3	H	1814	0	1818	26	0
4	L	132	0	146	5	0
4	M	198	0	222	11	0
5	L	51	0	45	5	0
6	L	31	0	23	4	0
6	M	15	0	11	2	0
7	L	10	0	16	0	0
8	L	32	0	62	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	11	0	18	1	0
9	L	6	0	4	0	0
10	M	1	0	0	0	0
11	M	1	0	0	1	0
12	M	10	0	0	0	0
13	M	42	0	60	1	0
14	M	81	0	106	1	0
15	H	147	0	0	1	0
15	L	109	0	0	0	0
15	M	108	0	0	0	0
All	All	7450	0	7038	110	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 8.

The worst 5 of 110 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:224:ILE:H	6:L:858:U10:H4M3	1.41	0.84
4:L:854:BCL:HMB1	4:L:854:BCL:HBB2	1.63	0.78
2:M:9:GLN:NE2	3:H:198:VAL:H	1.83	0.76
2:M:77:GLN:HE22	2:M:93:SER:H	1.32	0.76
2:M:9:GLN:HE22	3:H:198:VAL:H	1.33	0.73

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%)	272 (98%)	7 (2%)	0	100	100
2	M	299/307 (97%)	289 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	236/260 (91%)	232 (98%)	4 (2%)	0	100	100
All	All	814/848 (96%)	793 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	220/220 (100%)	214 (97%)	6 (3%)	44	54
2	M	238/242 (98%)	234 (98%)	4 (2%)	60	71
3	H	193/208 (93%)	190 (98%)	3 (2%)	62	73
All	All	651/670 (97%)	638 (98%)	13 (2%)	55	64

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

Mol	Chain	Res	Type
2	M	100	GLU
2	M	195	ASN
3	H	231	ASP
3	H	73	LEU
3	H	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	206	ASN
3	H	126	HIS
2	M	77	GLN
2	M	9	GLN
2	M	195	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z  > 2$
12	PO4	M	867	-	4,4,4	1.11	0	6,6,6	1.49	1 (16%)
5	BPH	L	855	-	50,56,70	2.72	17 (34%)	59,84,101	2.46	16 (27%)
9	GOL	L	869	-	5,5,5	4.59	5 (100%)	5,5,5	5.75	3 (60%)
14	CDL	M	862	-	80,80,99	1.49	8 (10%)	86,92,111	1.59	13 (15%)
6	U10	L	858	-	16,16,63	2.13	5 (31%)	19,22,79	2.30	6 (31%)
4	BCL	M	853	2	58,74,74	2.10	8 (13%)	69,115,115	2.32	28 (40%)
6	U10	L	859	-	15,15,63	1.98	4 (26%)	19,21,79	2.31	7 (36%)
8	LDA	M	866	-	7,10,15	2.78	1 (14%)	9,12,17	1.03	0
4	BCL	M	851	2	58,74,74	2.01	11 (18%)	69,115,115	2.42	27 (39%)
4	BCL	L	854	1	58,74,74	2.21	12 (20%)	69,115,115	2.12	21 (30%)
12	PO4	M	868	-	4,4,4	0.97	0	6,6,6	0.84	0
8	LDA	L	865	-	12,15,15	2.40	1 (8%)	14,17,17	1.07	2 (14%)
4	BCL	L	852	1	58,74,74	2.20	12 (20%)	69,115,115	2.19	21 (30%)
6	U10	M	857	-	15,15,63	2.16	4 (26%)	19,21,79	2.30	7 (36%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	LDA	L	864	-	12,15,15	2.47	1 (8%)	14,17,17	1.52	1 (7%)
4	BCL	M	856	2	58,74,74	2.24	11 (18%)	69,115,115	2.01	25 (36%)
13	SPO	M	860	-	40,41,41	1.47	7 (17%)	47,50,50	3.90	13 (27%)
7	HTO	L	863	-	9,9,9	0.87	0	10,10,10	2.09	2 (20%)

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
5	BPH	L	855	-	-	8/38/89/105	0/5/6/6
9	GOL	L	869	-	-	2/4/4/4	-
14	CDL	M	862	-	-	37/91/91/110	-
6	U10	L	858	-	-	1/7/31/87	0/1/1/1
4	BCL	M	853	2	2/2/21/25	12/37/137/137	-
6	U10	L	859	-	-	1/6/30/87	0/1/1/1
8	LDA	M	866	-	-	3/8/8/13	-
4	BCL	M	851	2	2/2/21/25	11/37/137/137	-
4	BCL	L	854	1	2/2/21/25	5/37/137/137	-
8	LDA	L	865	-	-	5/13/13/13	-
4	BCL	L	852	1	2/2/21/25	13/37/137/137	-
6	U10	M	857	-	-	1/6/30/87	0/1/1/1
8	LDA	L	864	-	-	11/13/13/13	-
4	BCL	M	856	2	2/2/21/25	12/37/137/137	-
13	SPO	M	860	-	-	5/47/47/47	-
7	HTO	L	863	-	-	7/10/10/10	-

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	853	BCL	OBD-CAD	11.35	1.38	1.22
4	M	856	BCL	OBD-CAD	10.93	1.37	1.22
4	L	854	BCL	OBD-CAD	10.43	1.36	1.22
5	L	855	BPH	OBD-CAD	9.63	1.35	1.22
4	M	851	BCL	OBD-CAD	9.07	1.35	1.22

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	860	SPO	C18-C17-C19	-15.96	100.57	122.92
13	M	860	SPO	C16-C17-C19	14.57	141.30	118.94
13	M	860	SPO	C20-C21-C22	-10.89	101.16	123.47
9	L	869	GOL	O3-C3-C2	10.51	160.59	110.20
5	L	855	BPH	OBD-CAD-CBD	-8.20	114.18	125.89

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	852	BCL	C13
4	L	852	BCL	C8
4	L	854	BCL	C13
4	L	854	BCL	C8
4	M	851	BCL	C13

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	852	BCL	C11-C12-C13-C14
4	M	851	BCL	C12-C13-C15-C16
5	L	855	BPH	C4B-C3B-CAB-CBB
5	L	855	BPH	C2B-C3B-CAB-CBB
5	L	855	BPH	C2-C3-C5-C6

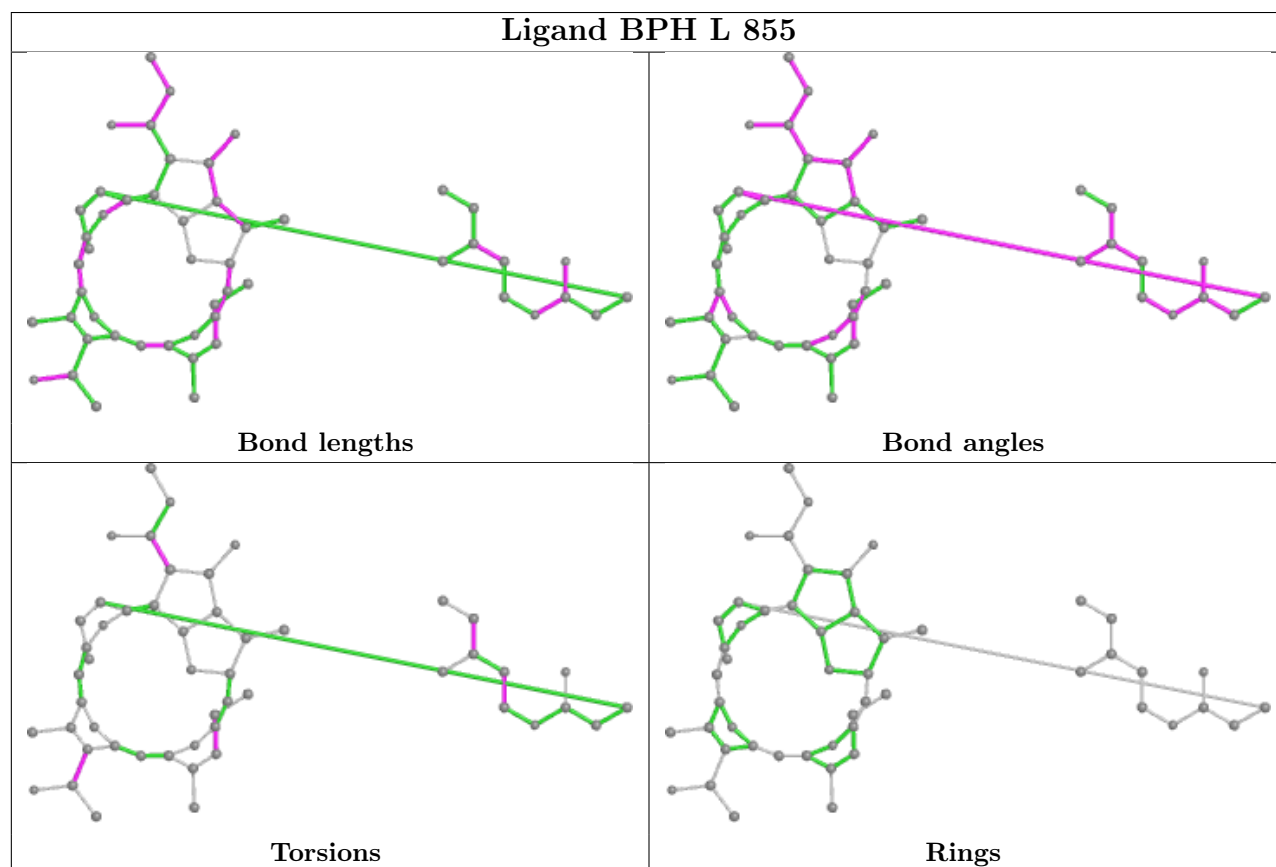
There are no ring outliers.

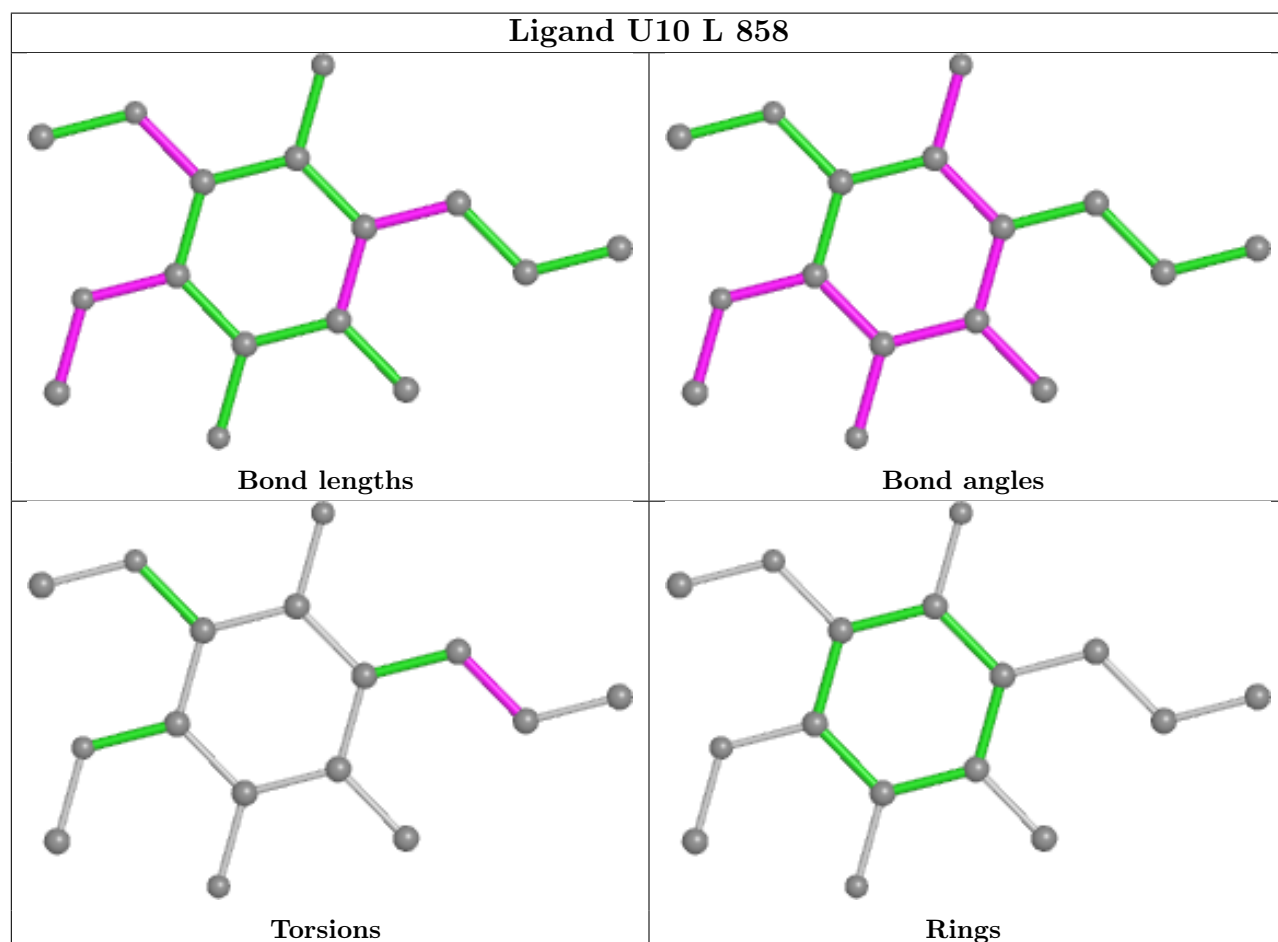
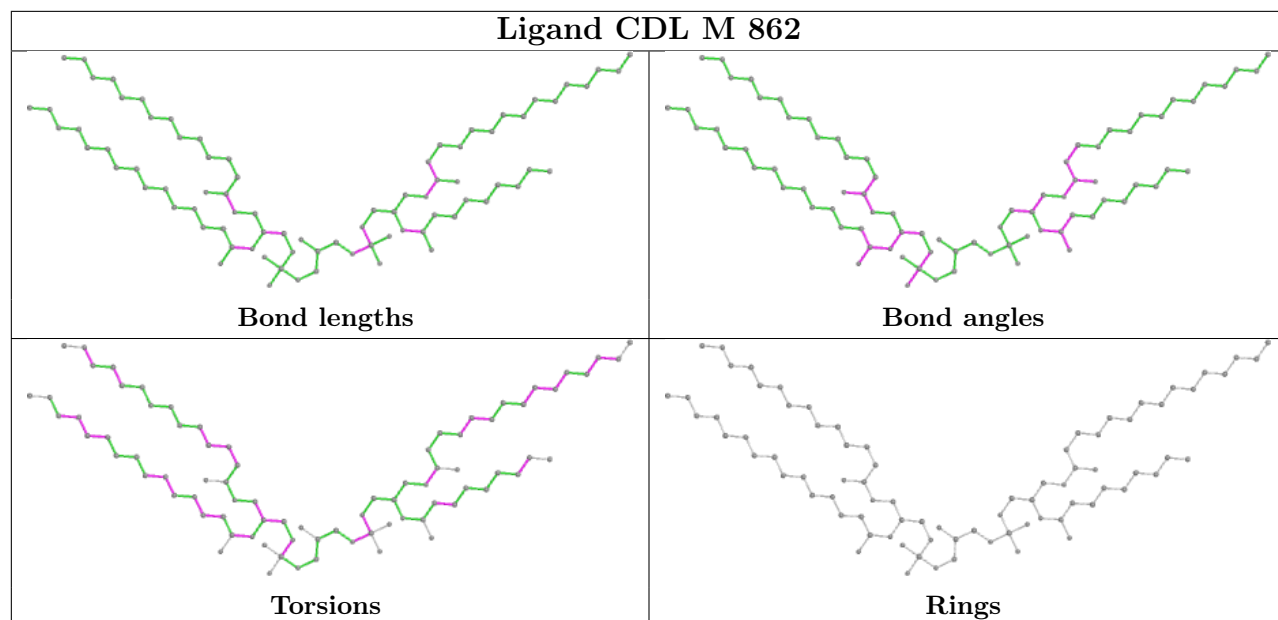
11 monomers are involved in 30 short contacts:

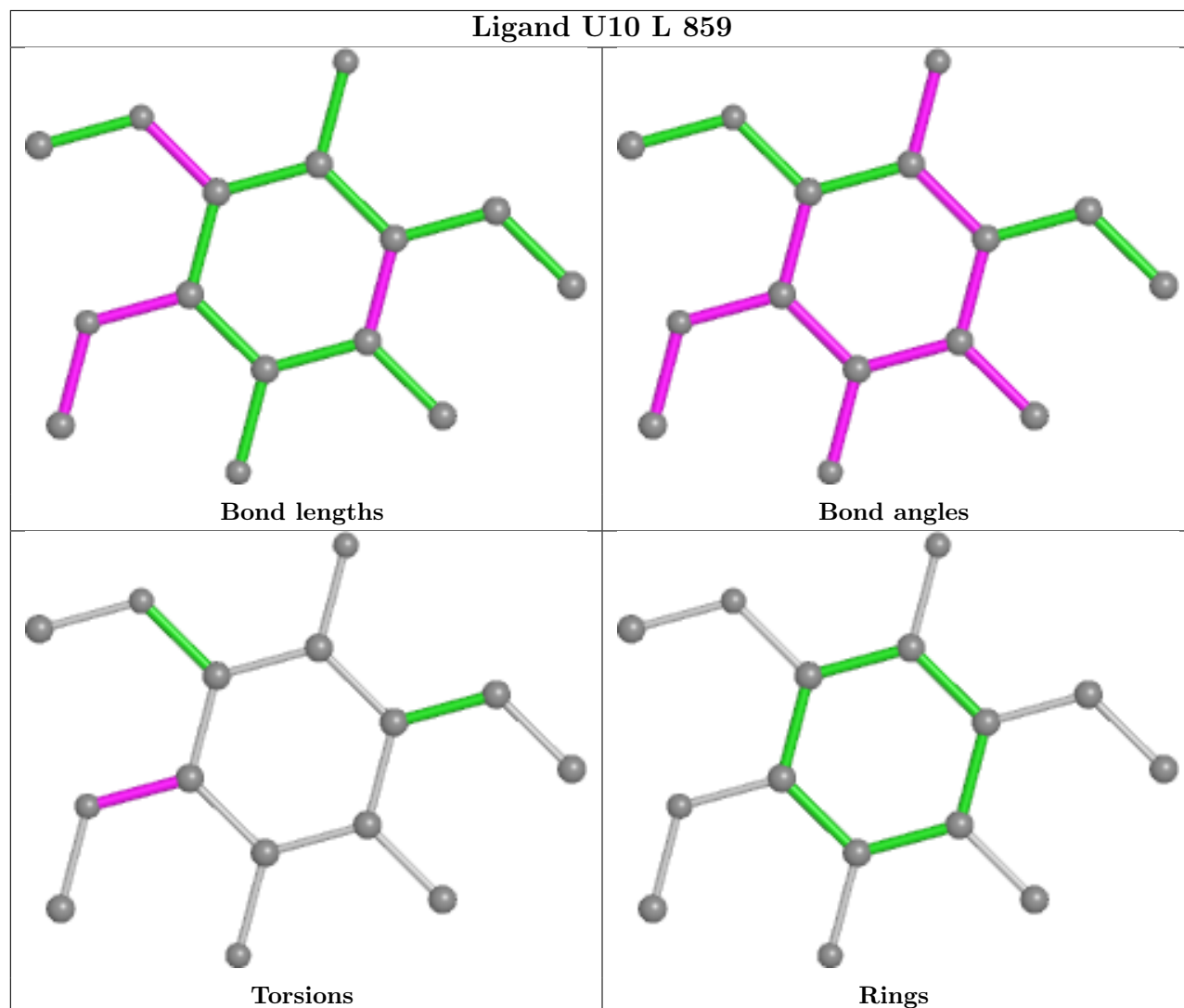
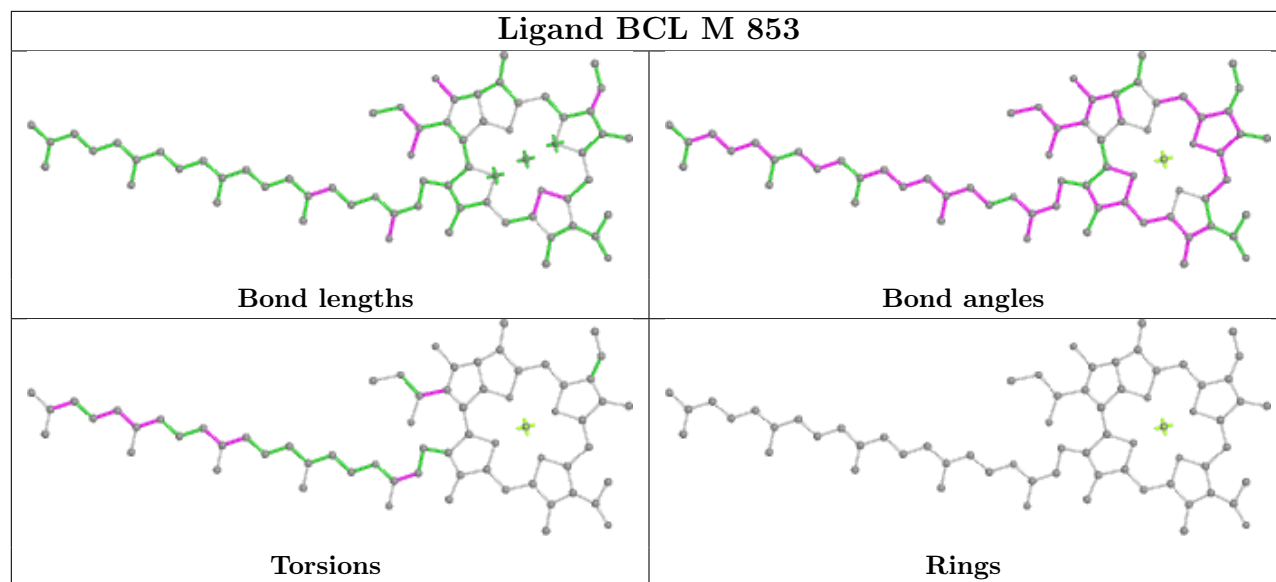
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	855	BPH	5	0
14	M	862	CDL	1	0
6	L	858	U10	4	0
4	M	853	BCL	4	0
8	M	866	LDA	1	0
4	M	851	BCL	2	0
4	L	854	BCL	3	0
4	L	852	BCL	3	0
6	M	857	U10	2	0
4	M	856	BCL	5	0
13	M	860	SPO	1	0

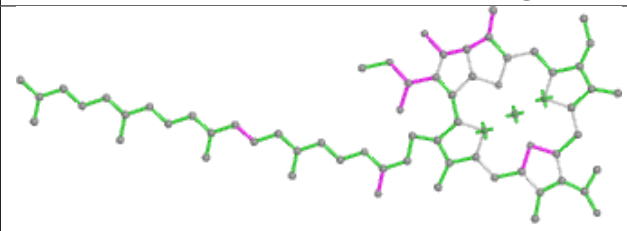
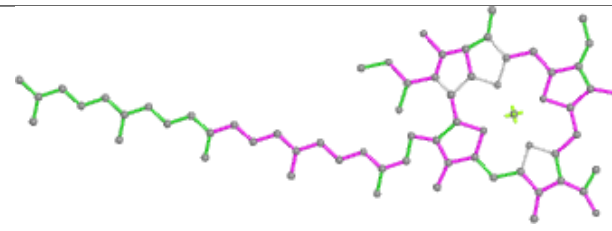
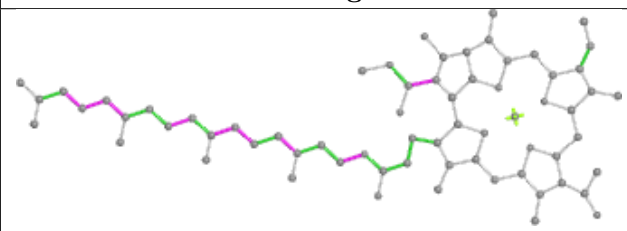
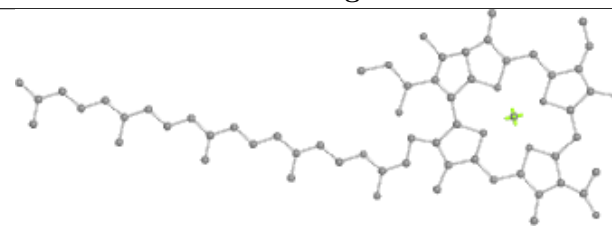
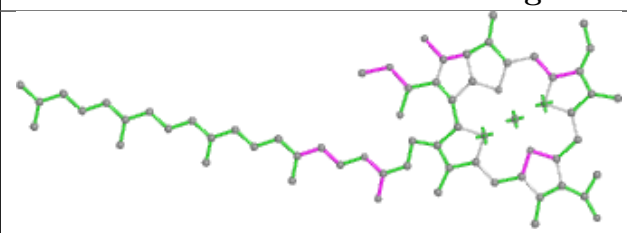
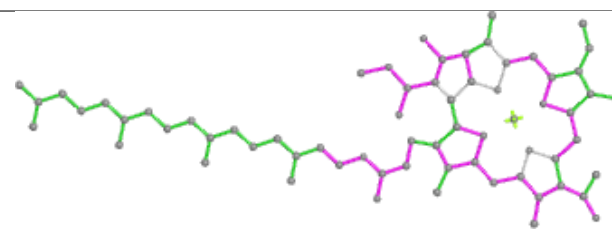
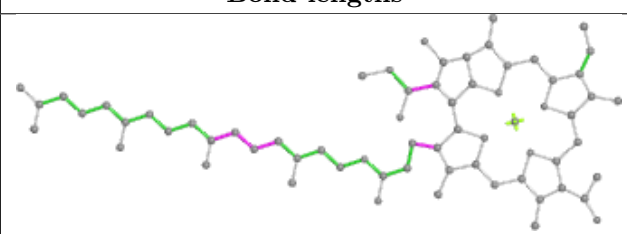
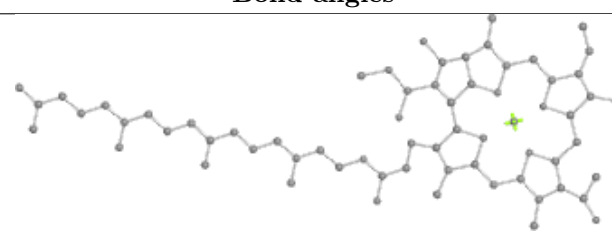
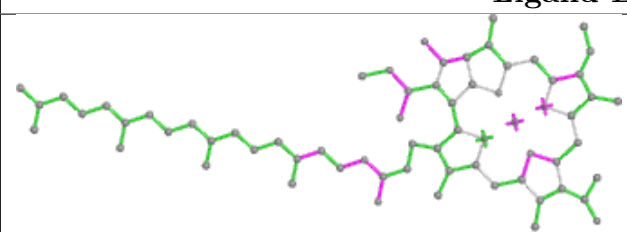
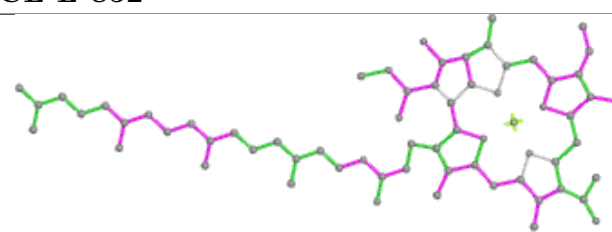
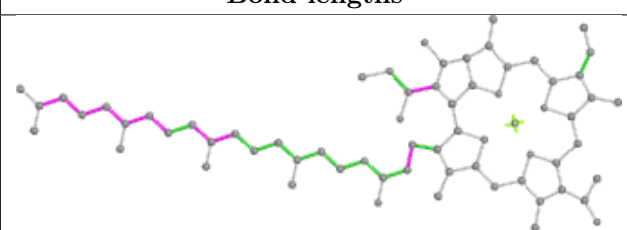
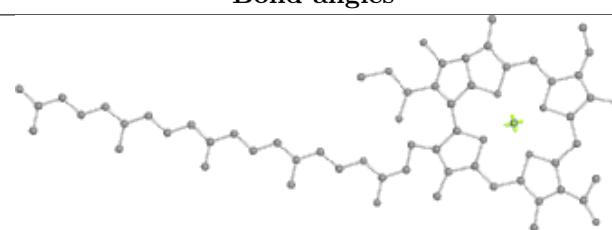
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

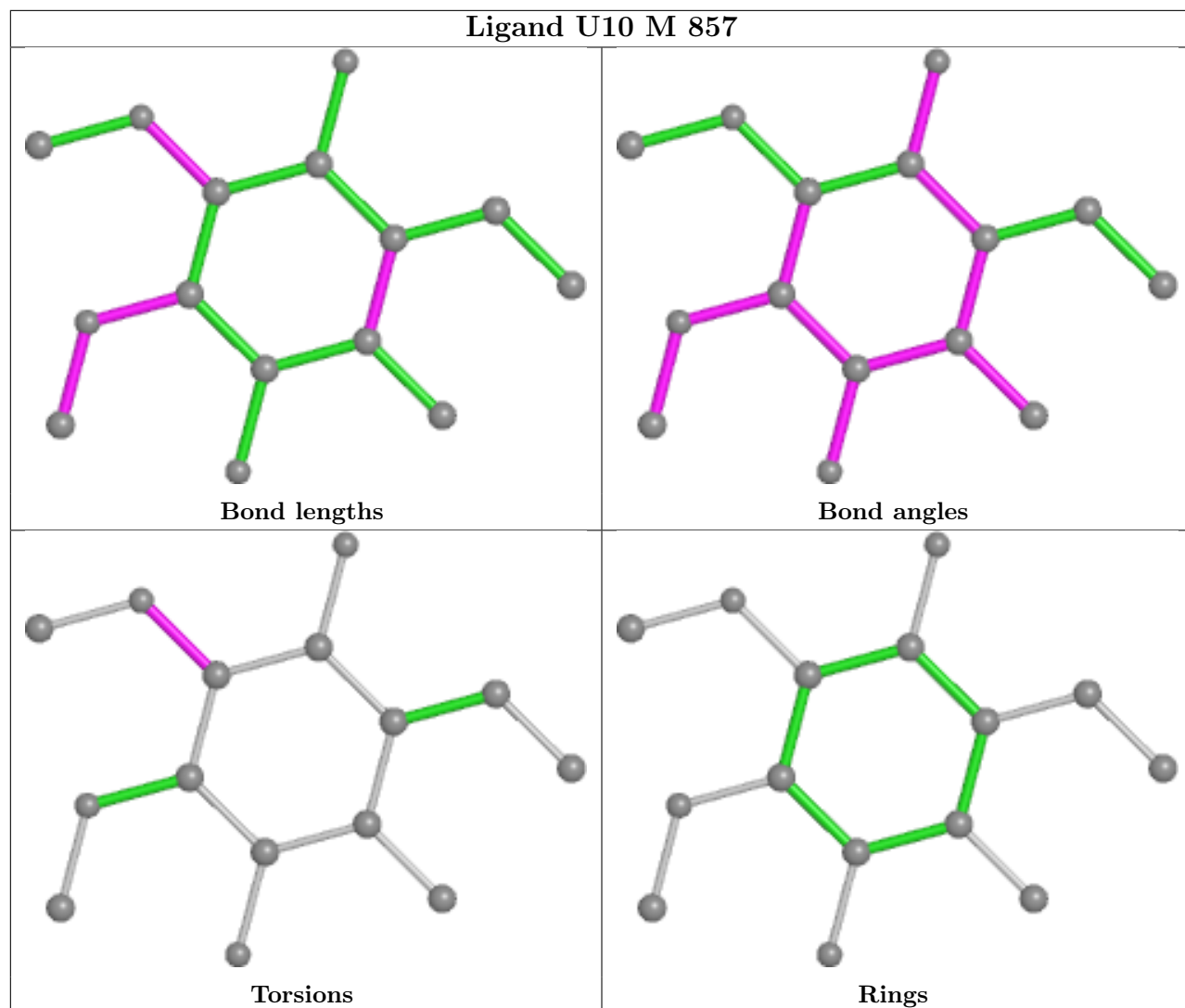




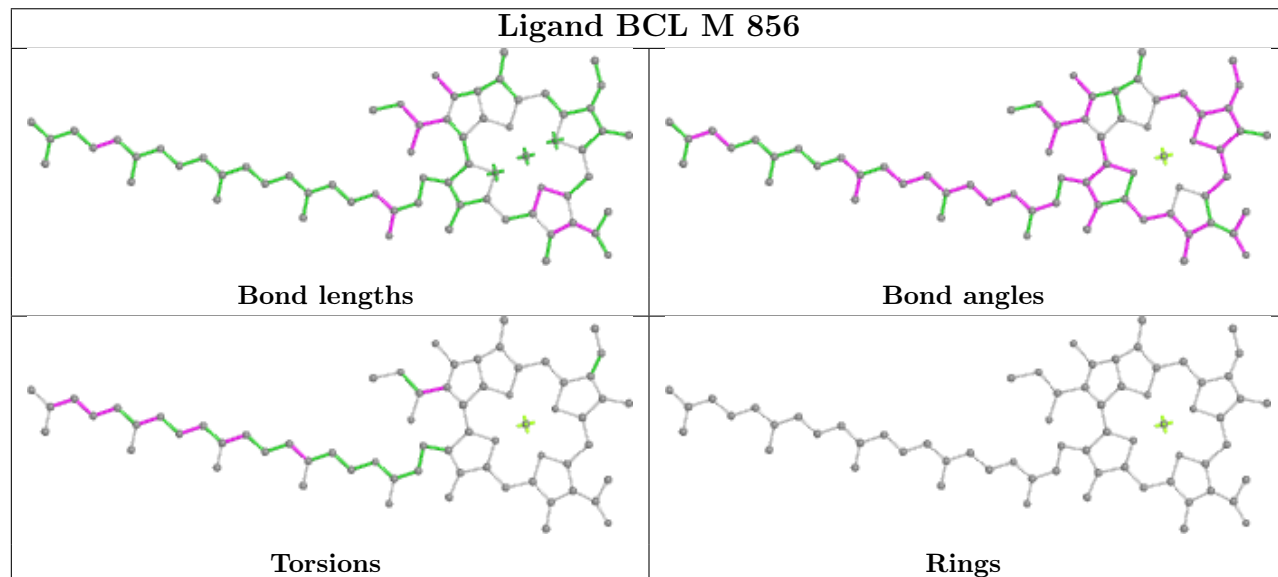


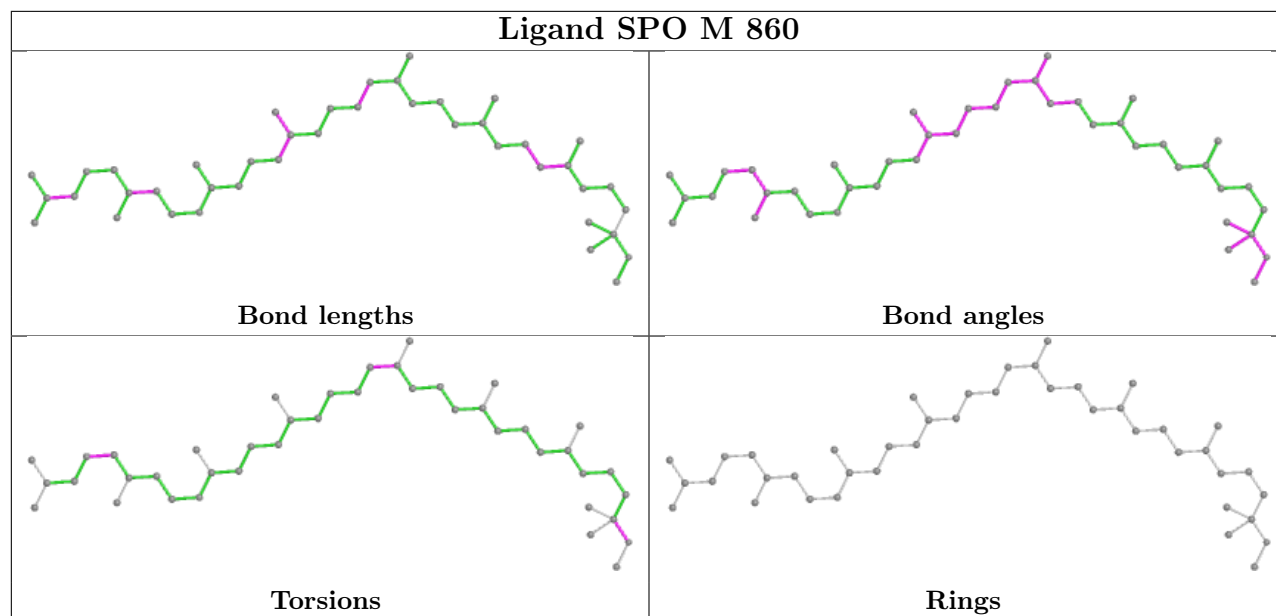
Ligand BCL M 851	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL L 854	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL L 852	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

## Ligand U10 M 857



## Ligand BCL M 856





## 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	L	281/281 (100%)	-0.44	4 (1%) 75 77	18, 26, 48, 57	0
2	M	301/307 (98%)	-0.19	10 (3%) 46 48	17, 30, 49, 72	0
3	H	238/260 (91%)	-0.40	6 (2%) 57 60	20, 29, 43, 71	0
All	All	820/848 (96%)	-0.34	20 (2%) 59 62	17, 28, 48, 72	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	5.6
3	H	18	TYR	3.3
3	H	60	LYS	3.3
2	M	2	GLU	3.0
1	L	281	GLY	2.7

### 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](#)

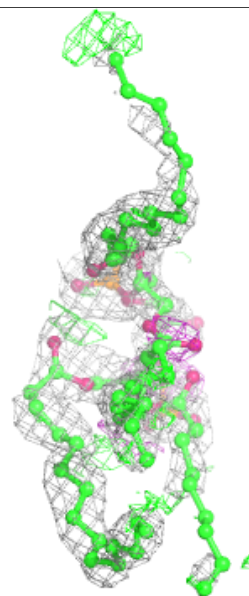
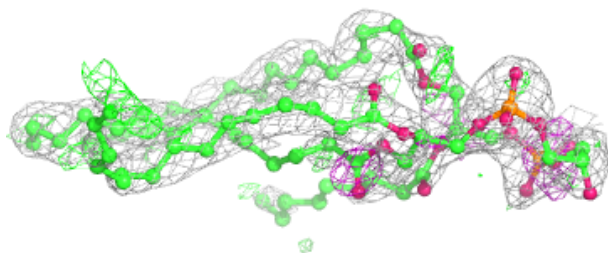
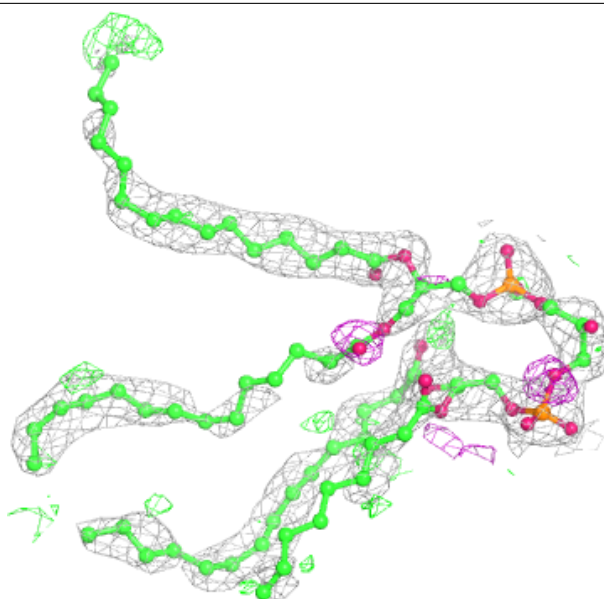
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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
8	LDA	L	864	16/16	0.66	0.34	54,66,74,74	0
8	LDA	L	865	16/16	0.67	0.39	70,73,78,79	0
8	LDA	M	866	11/16	0.73	0.34	77,79,83,83	0
14	CDL	M	862	81/100	0.75	0.29	61,72,89,93	0
6	U10	M	857	15/63	0.80	0.23	59,63,65,66	0
9	GOL	L	869	6/6	0.83	0.29	50,54,56,58	0
7	HTO	L	863	10/10	0.84	0.23	59,61,62,63	0
6	U10	L	858	16/63	0.84	0.19	34,38,43,45	0
13	SPO	M	860	42/42	0.91	0.14	27,35,58,61	0
6	U10	L	859	15/63	0.93	0.15	40,44,48,49	0
12	PO4	M	867	5/5	0.95	0.22	67,68,68,69	0
5	BPH	L	855	51/65	0.96	0.11	22,27,42,46	0
4	BCL	L	854	66/66	0.96	0.11	19,23,50,51	0
4	BCL	M	851	66/66	0.96	0.13	17,23,66,68	0
4	BCL	M	853	66/66	0.96	0.14	19,24,44,53	0
12	PO4	M	868	5/5	0.97	0.11	57,58,59,59	0
4	BCL	L	852	66/66	0.97	0.11	15,22,43,52	0
4	BCL	M	856	66/66	0.97	0.12	12,20,32,34	0
10	FE2	M	850	1/1	1.00	0.12	19,19,19,19	0
11	CL	M	861	1/1	1.00	0.17	24,24,24,24	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.

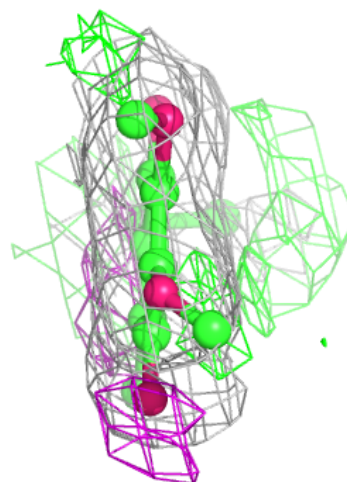
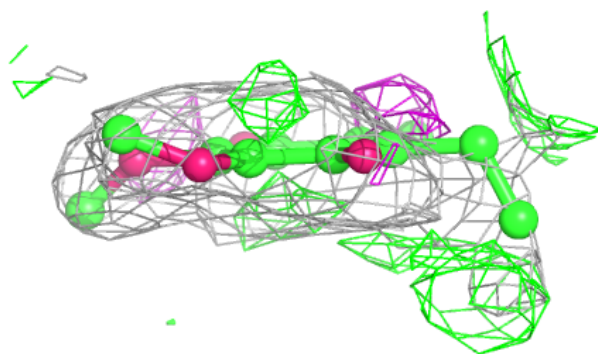
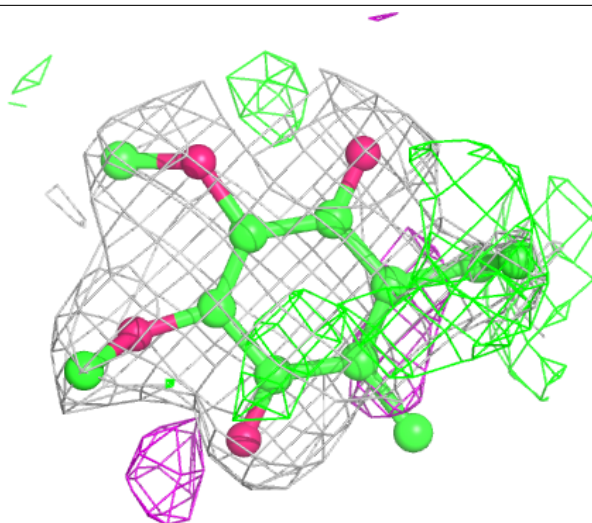
**Electron density around CDL M 862:**

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



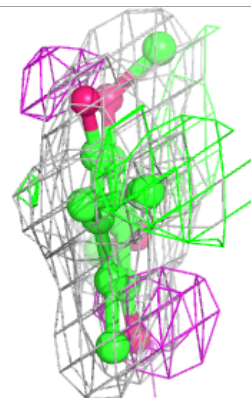
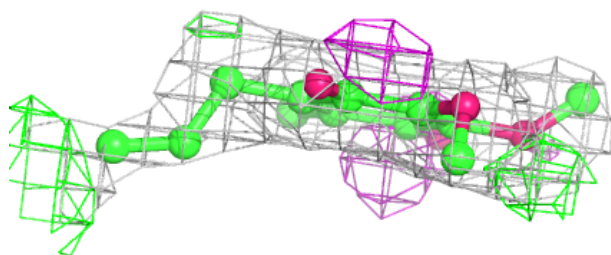
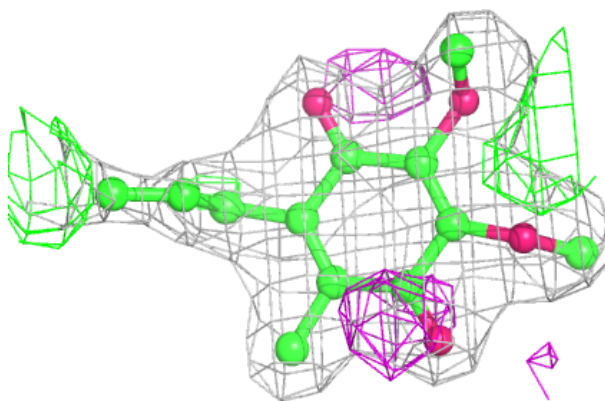
**Electron density around U10 M 857:**

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

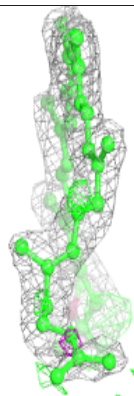
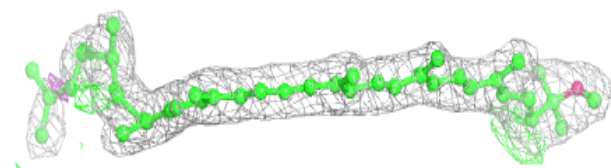
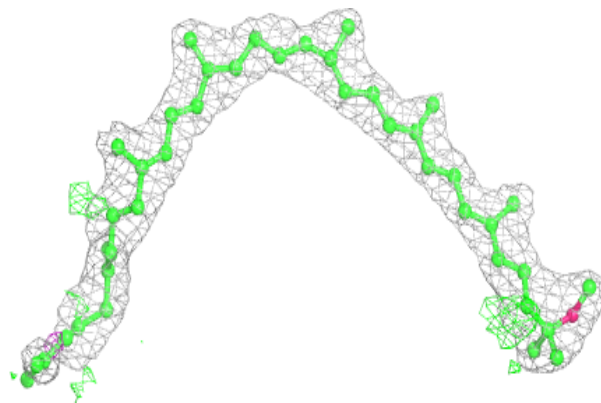


**Electron density around U10 L 858:**

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

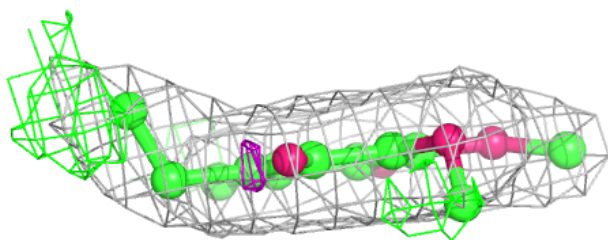
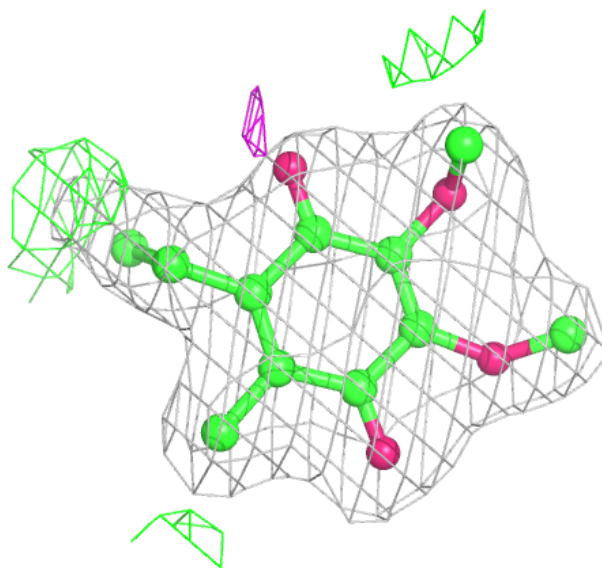
**Electron density around SPO M 860:**

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



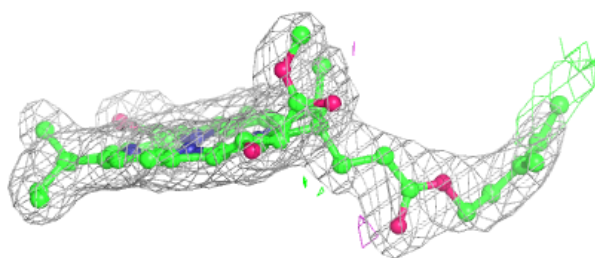
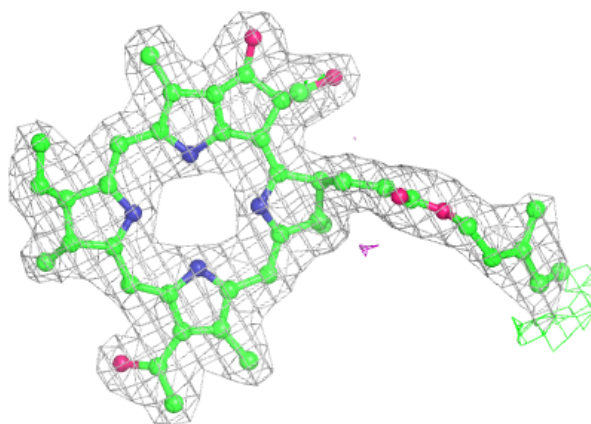
**Electron density around U10 L 859:**

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



**Electron density around BPH L 855:**

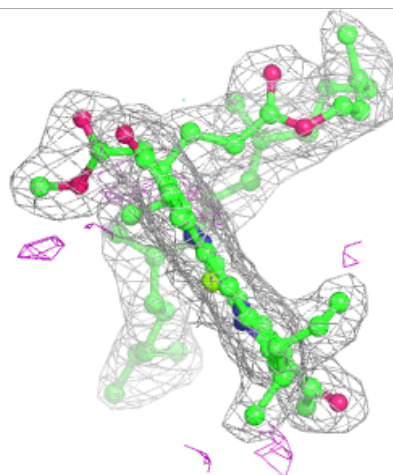
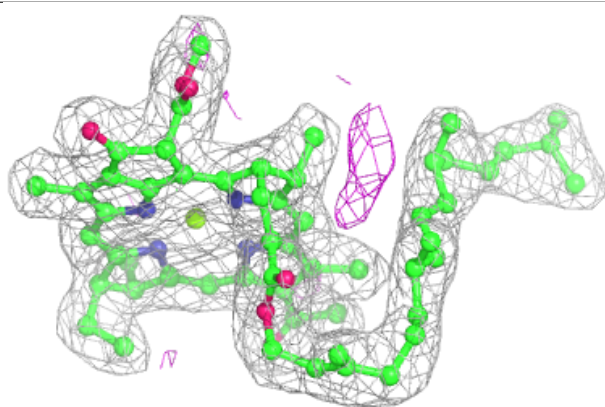
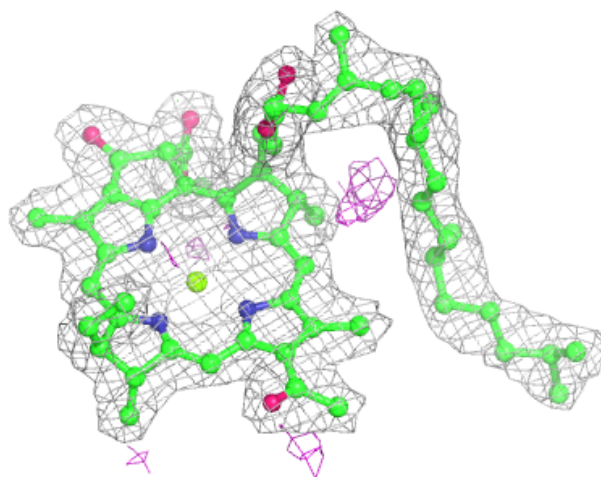
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BCL L 854:**

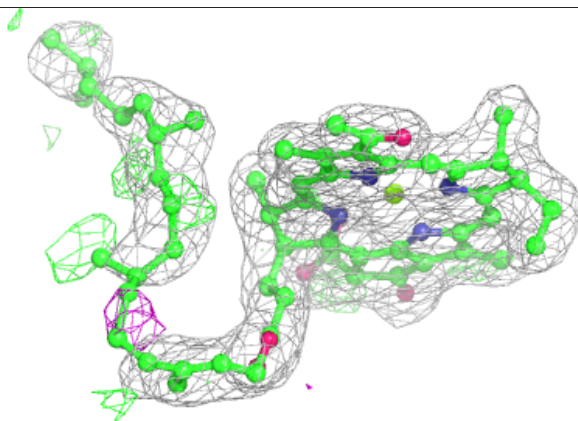
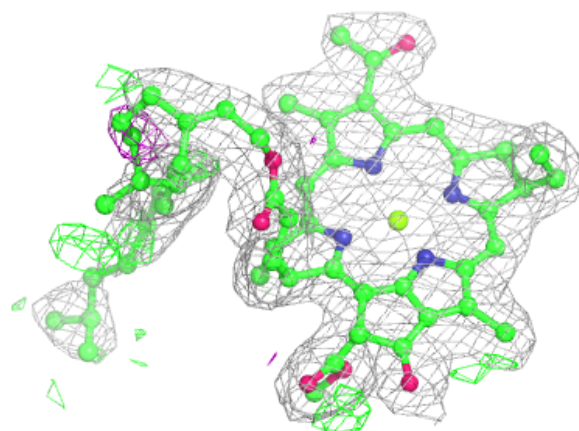
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



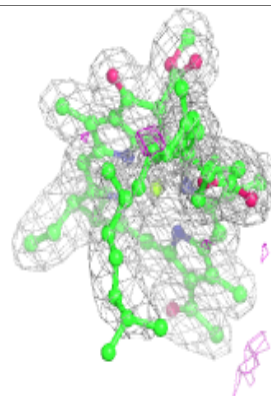
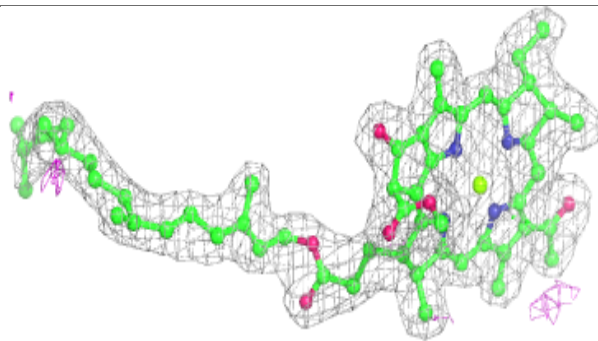
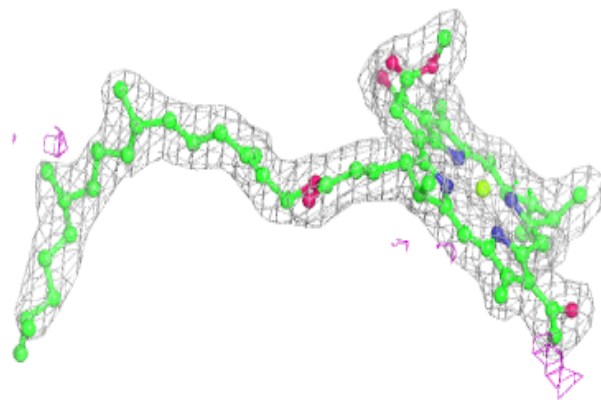


**Electron density around BCL M 851:**

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

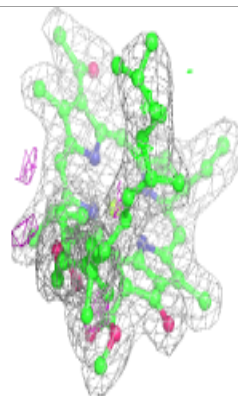
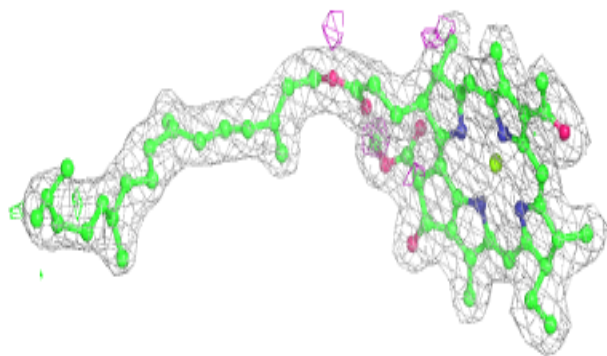
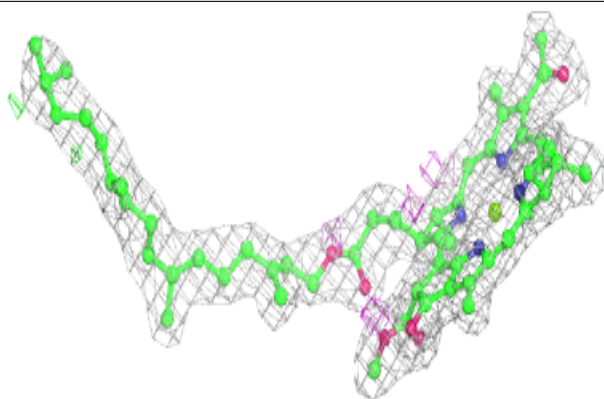
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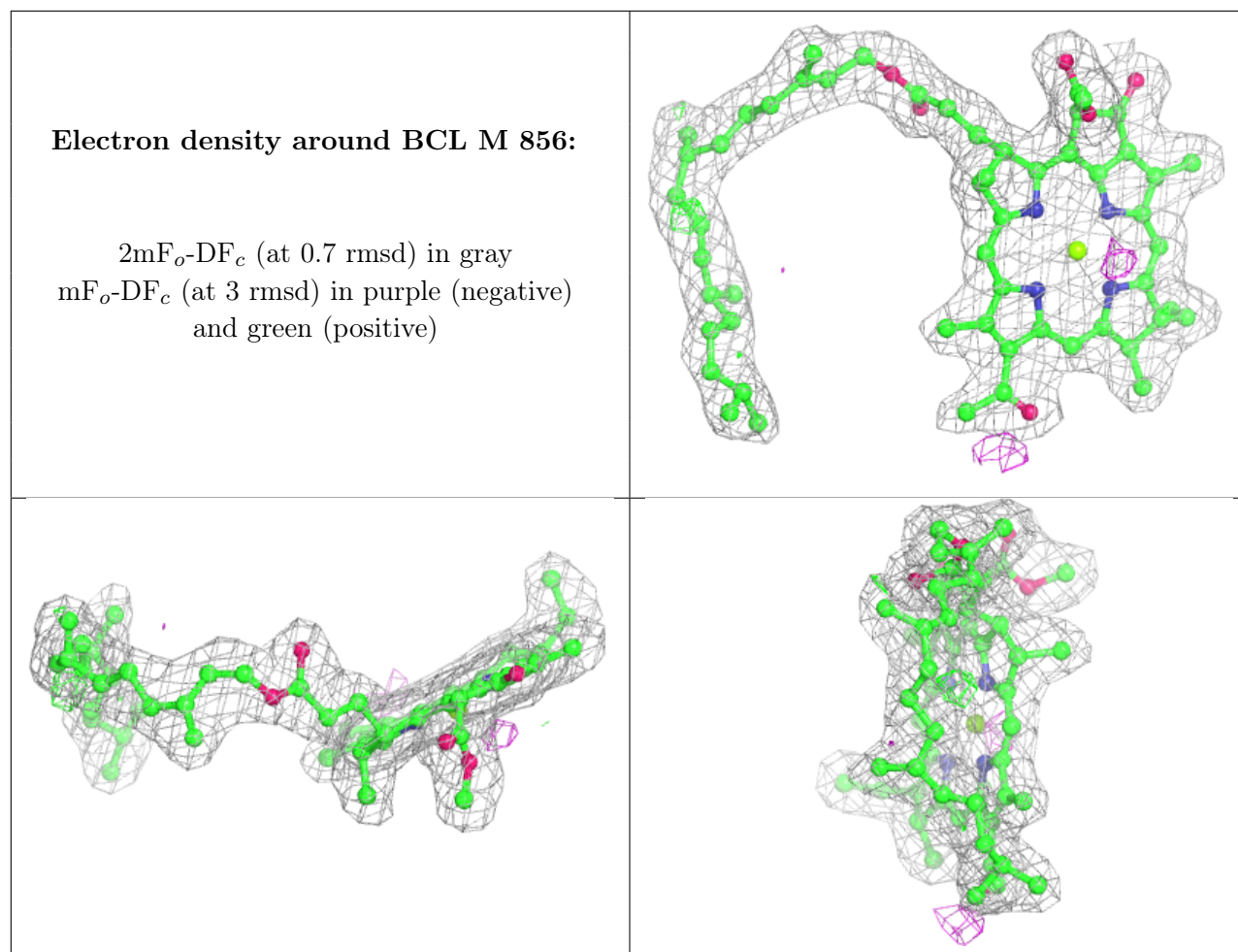
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCL L 852:**

$2mF_o-DF_c$  (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.