



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:59 am BST

PDB ID : 1Z9J  
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides  
Authors : Thielges, M.; Uyeda, G.; Camara-Artigas, A.; Kalman, L.; Williams, J.C.; Allen, J.P.  
Deposited on : 2005-04-02  
Resolution : 4.50 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	:	2.11
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)	:	2.11

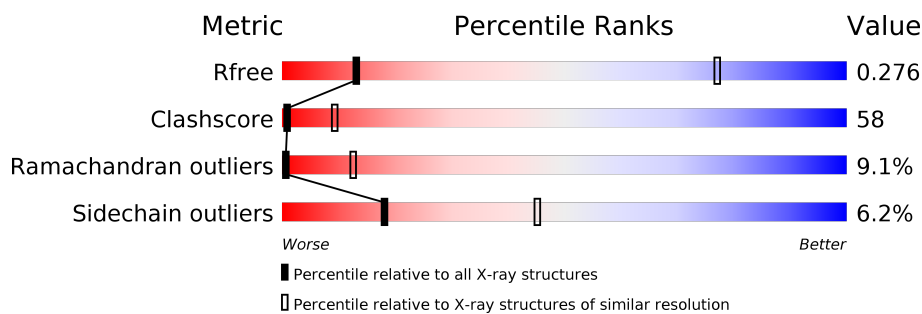
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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 on 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	281	<div> <div>25%</div> <div>62%</div> <div>12%</div> <div>.</div> </div>
2	B	307	<div> <div>26%</div> <div>62%</div> <div>10%</div> <div>..</div> </div>
3	C	260	<div> <div>36%</div> <div>49%</div> <div>7%</div> <div>8%</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6957 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	A	281	Total	C	N	O	S	0	0	0
			2234	1507	357	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	HIS	LEU	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	S	0	0	0
			2415	1609	395	402	9			

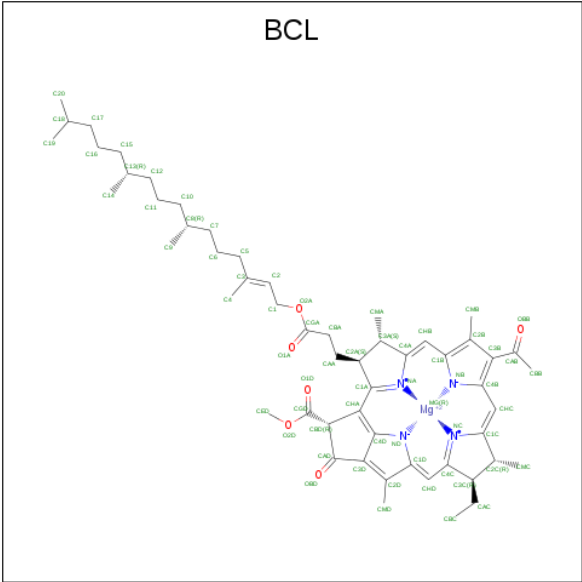
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	HIS	LEU	engineered mutation	UNP P0C0Y9
B	164	TYR	ARG	engineered mutation	UNP P0C0Y9
B	168	GLU	MET	engineered mutation	UNP P0C0Y9
B	197	HIS	PHE	engineered mutation	UNP P0C0Y9
B	288	ASP	GLY	engineered mutation	UNP P0C0Y9

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

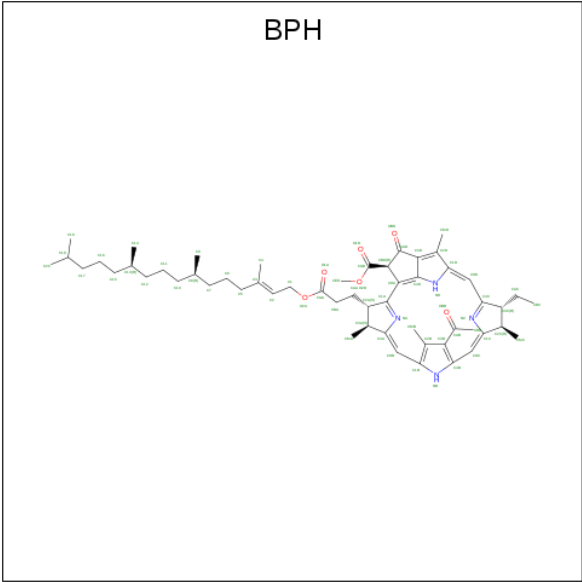
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1814	1160	311	334	9			

- 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>).



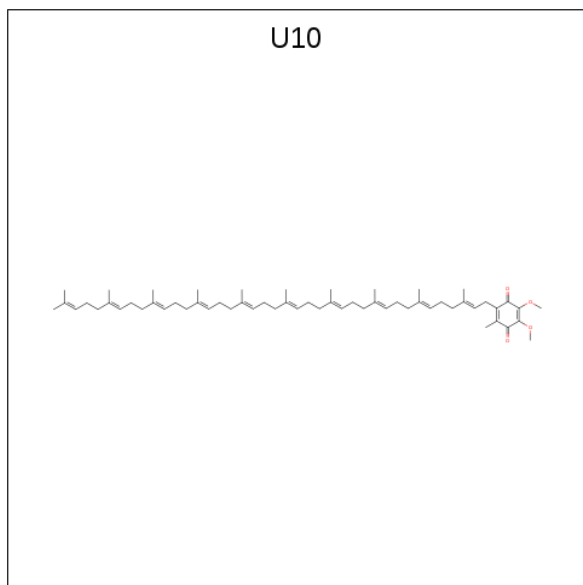
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			48	44	4		
6	B	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Fe	0	0
			1	1		

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mn	0	0
			1	1		

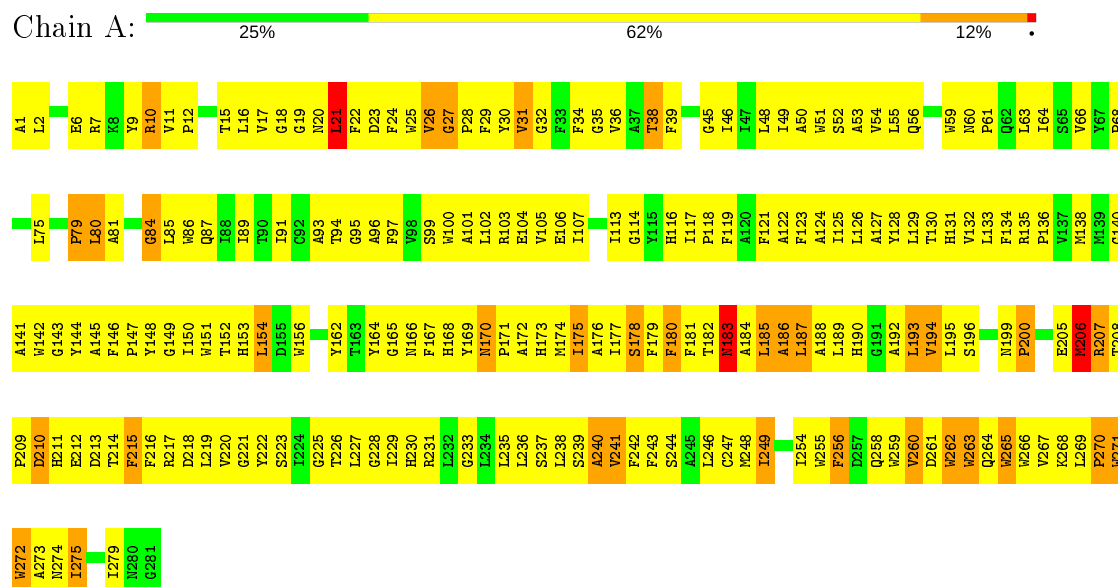
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	O	0	0
			2	2		

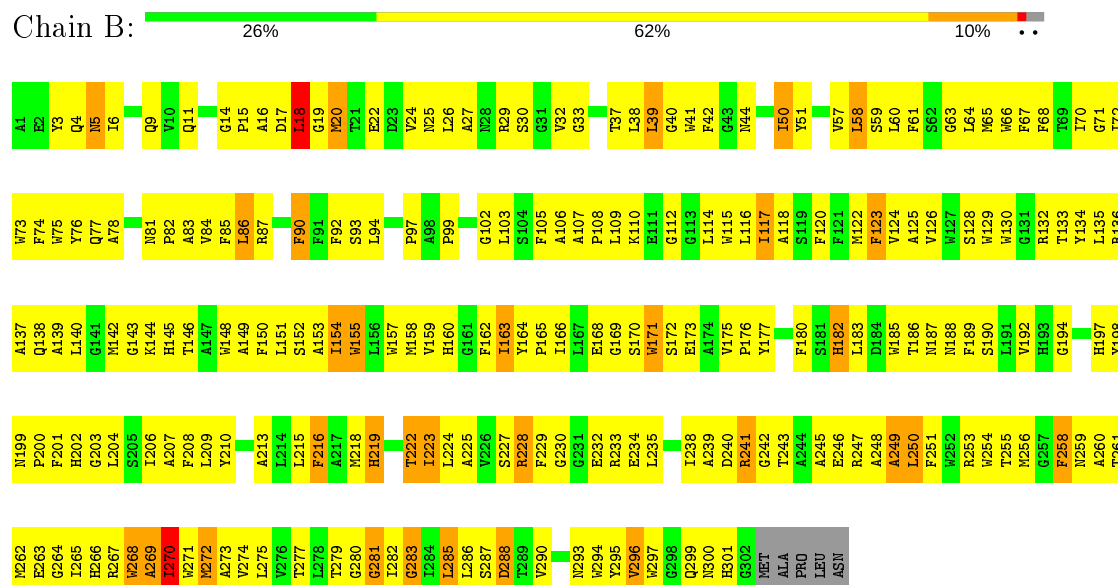
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

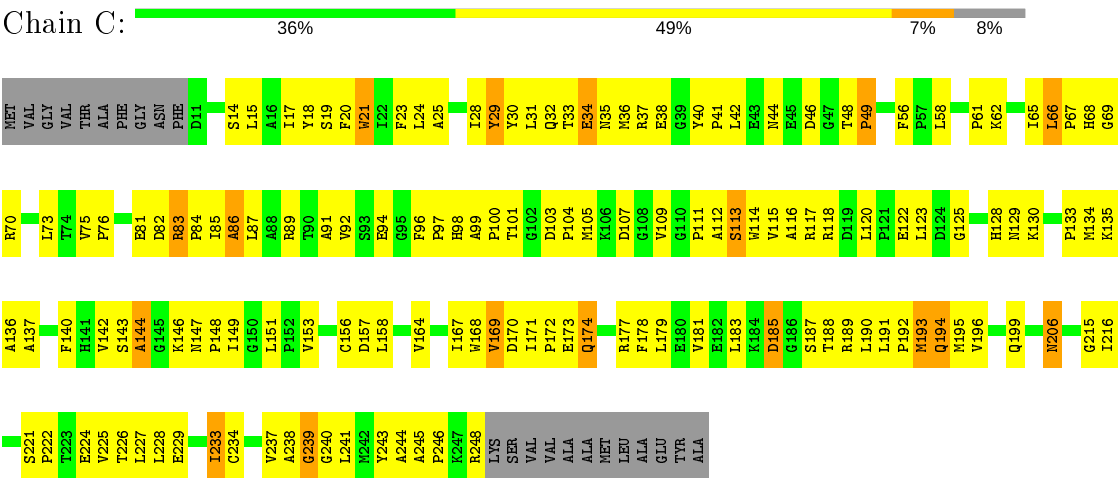
#### • Molecule 1: Reaction center protein L chain



#### • 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 42 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.84Å 203.84Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 4.50 24.90 – 4.30	Depositor EDS
% Data completeness (in resolution range)	79.9 (19.96-4.50) 80.7 (24.90-4.30)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 4.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.299 , 0.338 0.221 , 0.276	Depositor DCC
$R_{free}$ test set	712 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	145.2	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , -0.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: BCL, BPH, MN, FE, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.63	0/2323	0.80	1/3179 (0.0%)
2	B	0.63	0/2509	0.79	1/3428 (0.0%)
3	C	0.62	1/1862 (0.1%)	0.80	0/2534
All	All	0.62	1/6694 (0.0%)	0.80	2/9141 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	21	TRP	CB-CG	-5.17	1.41	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLY	N-CA-C	-5.09	100.38	113.10
2	B	285	LEU	CA-CB-CG	-5.03	103.73	115.30

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	A	2234	0	2183	329	0
2	B	2415	0	2309	368	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1814	0	1818	187	1
4	A	132	0	148	20	0
4	B	132	0	148	18	0
5	A	65	0	76	19	0
5	B	65	0	76	14	0
6	A	48	0	63	7	0
6	B	48	0	63	15	0
7	B	1	0	0	0	0
8	B	1	0	0	0	0
9	B	2	0	0	1	0
All	All	6957	0	6884	802	1

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 58.

The worst 5 of 802 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)
2:B:64:LEU:HD21	5:B:854:BPH:H112	1.32	1.10
2:B:267:ARG:O	2:B:270:ILE:HG22	1.65	0.96
1:A:171:PRO:HA	1:A:174:MET:HG3	1.48	0.95
2:B:242:GLY:HA2	3:C:117:ARG:HD2	1.49	0.94
1:A:114:GLY:H	2:B:225:ALA:HB1	1.32	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:HIS:NE2	3:C:128:HIS:NE2[5_656]	2.18	0.02

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/281 (99%)	199 (71%)	51 (18%)	29 (10%)	0	9
2	B	300/307 (98%)	202 (67%)	69 (23%)	29 (10%)	0	11
3	C	236/260 (91%)	175 (74%)	45 (19%)	16 (7%)	1	17
All	All	815/848 (96%)	576 (71%)	165 (20%)	74 (9%)	1	12

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	80	LEU
1	A	186	ALA
1	A	200	PRO
1	A	215	PHE

### 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	A	220/220 (100%)	201 (91%)	19 (9%)	10	35
2	B	237/241 (98%)	223 (94%)	14 (6%)	19	47
3	C	193/208 (93%)	186 (96%)	7 (4%)	35	60
All	All	650/669 (97%)	610 (94%)	40 (6%)	18	45

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	TRP
2	B	86	LEU
3	C	185	ASP
2	B	42	PHE
2	B	90	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	202	HIS
2	B	259	ASN
3	C	68	HIS
2	B	188	ASN
3	C	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	B	853	1	58,74,74	1.47	10 (17%)	69,115,115	2.10	22 (31%)
6	U10	B	856	-	48,48,63	2.43	13 (27%)	58,61,79	2.06	19 (32%)
5	BPH	B	854	-	64,70,70	1.51	11 (17%)	76,101,101	1.89	19 (25%)
4	BCL	B	852	2	58,74,74	1.53	12 (20%)	69,115,115	2.00	16 (23%)
4	BCL	A	850	-	58,74,74	1.66	13 (22%)	69,115,115	1.98	17 (24%)
5	BPH	A	855	-	64,70,70	1.30	8 (12%)	76,101,101	1.80	17 (22%)
6	U10	A	857	-	48,48,63	2.70	16 (33%)	58,61,79	2.07	18 (31%)
4	BCL	A	851	1	58,74,74	1.54	12 (20%)	69,115,115	1.82	11 (15%)

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	B	853	1	-	12/37/137/137	-
6	U10	B	856	-	-	12/45/69/87	0/1/1/1
5	BPH	B	854	-	-	11/54/105/105	0/5/6/6
4	BCL	B	852	2	-	11/37/137/137	-
4	BCL	A	850	-	-	8/37/137/137	-
5	BPH	A	855	-	-	12/54/105/105	0/5/6/6
6	U10	A	857	-	-	12/45/69/87	0/1/1/1
4	BCL	A	851	1	-	6/37/137/137	-

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	856	U10	C6-C1	10.41	1.54	1.35
6	A	857	U10	C6-C1	10.08	1.53	1.35
4	A	851	BCL	C3D-C2D	5.50	1.49	1.39
4	B	852	BCL	C3D-C2D	5.44	1.49	1.39
4	A	850	BCL	C3B-C2B	5.02	1.48	1.39

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	853	BCL	CMB-C2B-C1B	-6.89	117.88	128.46
4	A	850	BCL	CMB-C2B-C1B	-6.70	118.16	128.46
4	B	853	BCL	CAA-C2A-C1A	-6.68	90.10	111.97
4	A	851	BCL	CMB-C2B-C1B	-6.64	118.25	128.46
4	B	852	BCL	CMB-C2B-C1B	-6.41	118.61	128.46

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

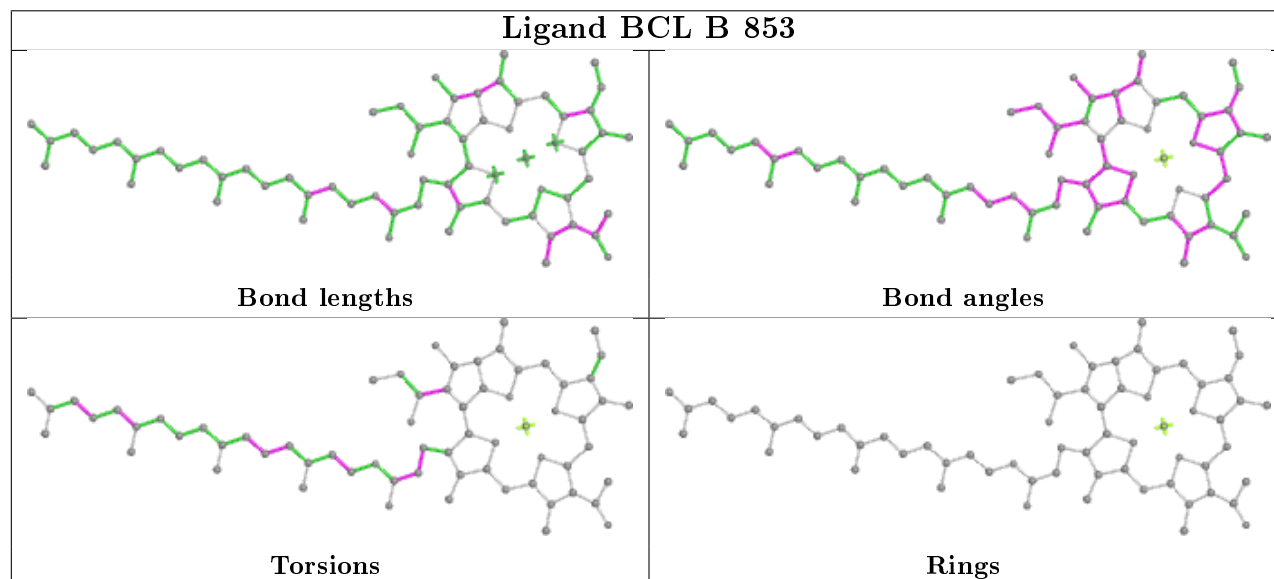
Mol	Chain	Res	Type	Atoms
6	B	856	U10	C20-C19-C21-C22
6	B	856	U10	C19-C21-C22-C23
5	B	854	BPH	C4C-C3C-CAC-CBC
5	B	854	BPH	C2C-C3C-CAC-CBC
5	B	854	BPH	C4B-C3B-CAB-CBB

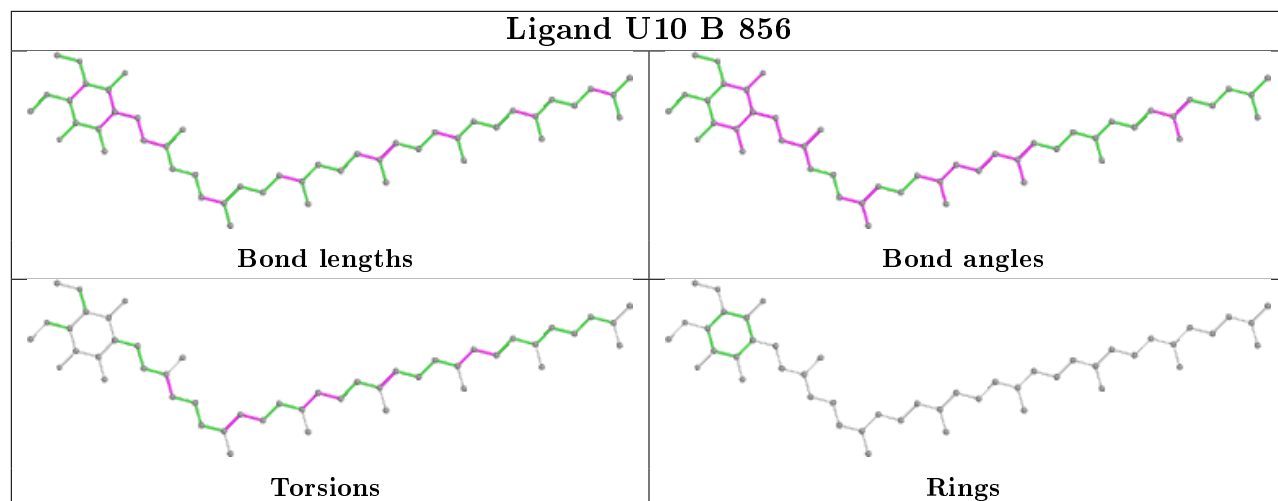
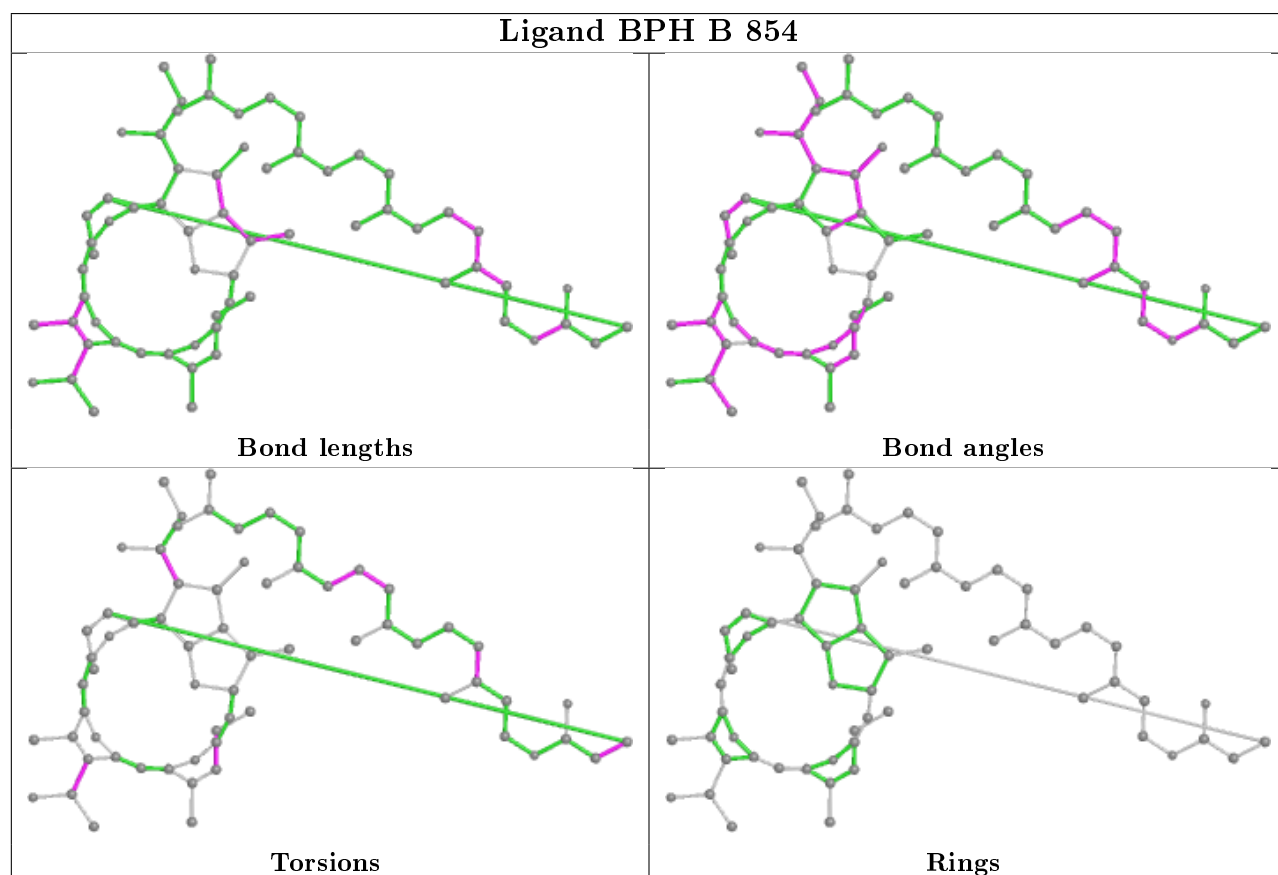
There are no ring outliers.

8 monomers are involved in 87 short contacts:

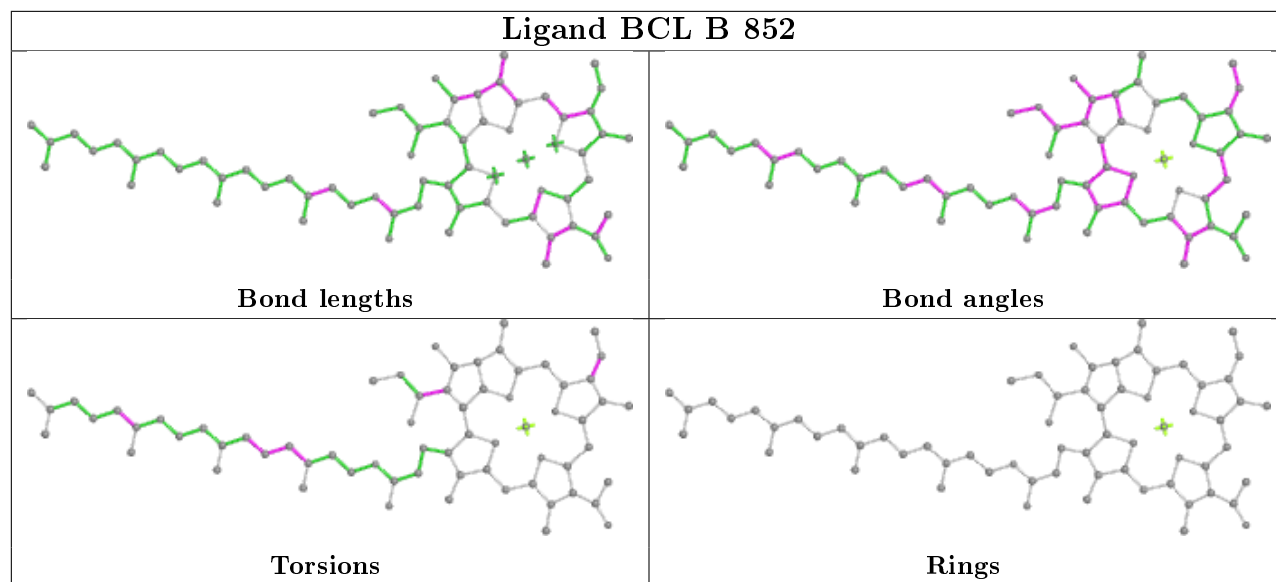
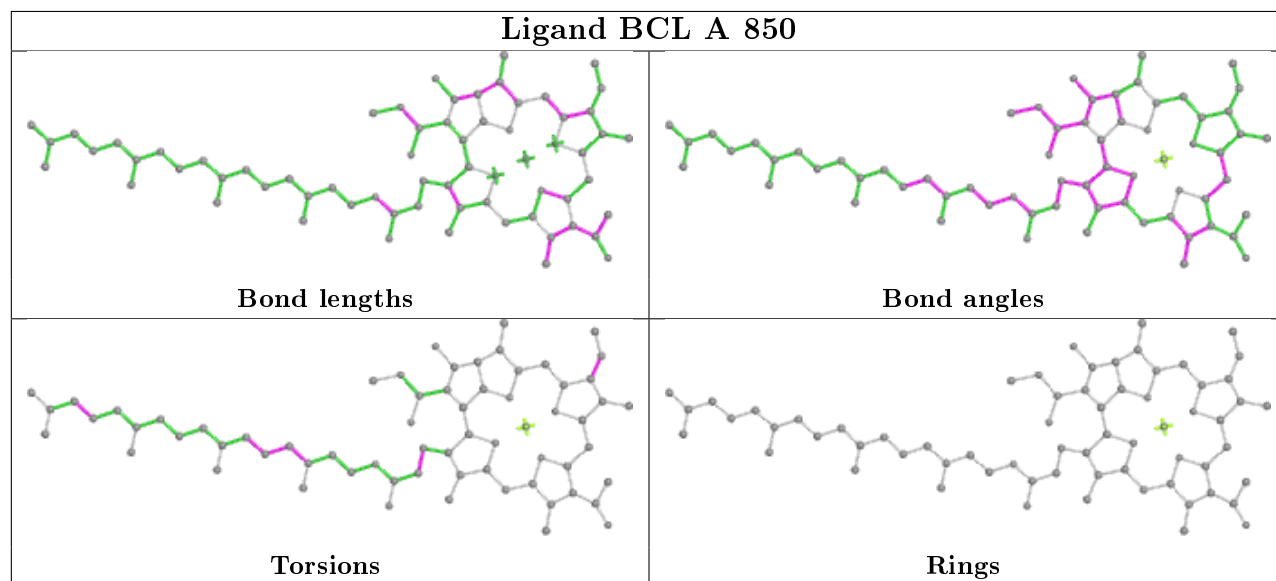
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	853	BCL	11	0
6	B	856	U10	15	0
5	B	854	BPH	14	0
4	B	852	BCL	9	0
4	A	850	BCL	11	0
5	A	855	BPH	19	0
6	A	857	U10	7	0
4	A	851	BCL	11	0

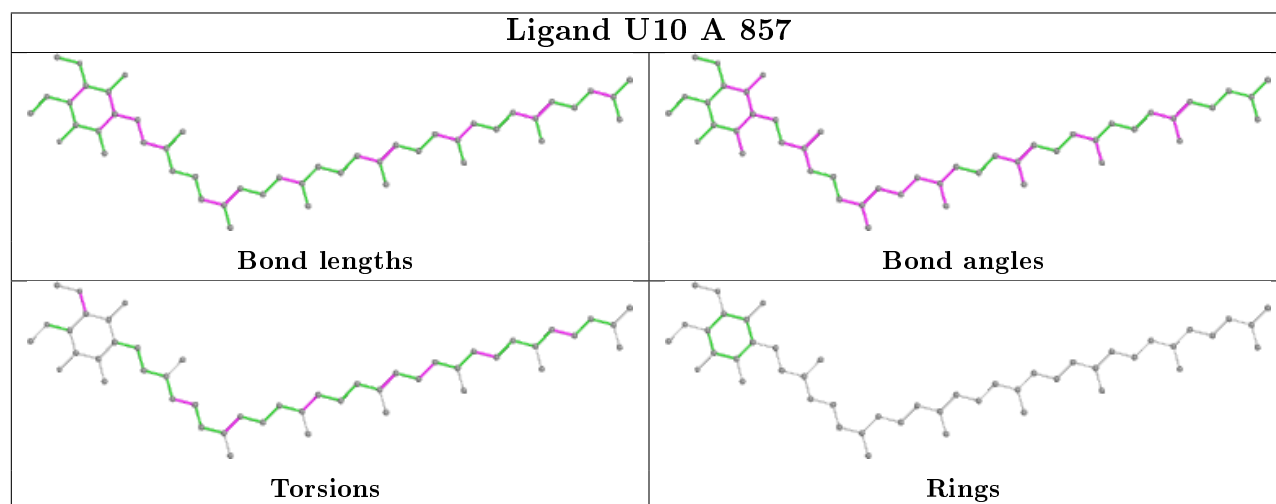
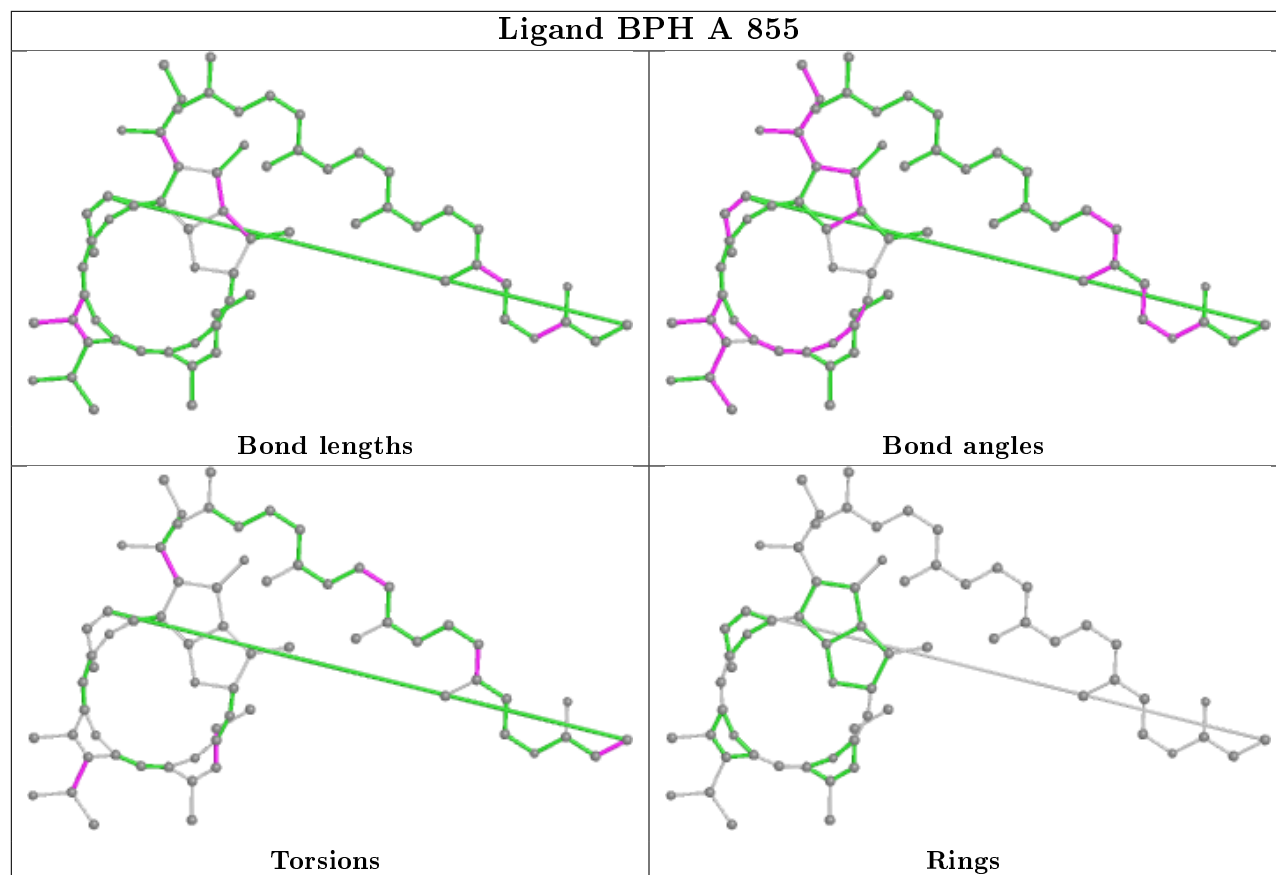
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

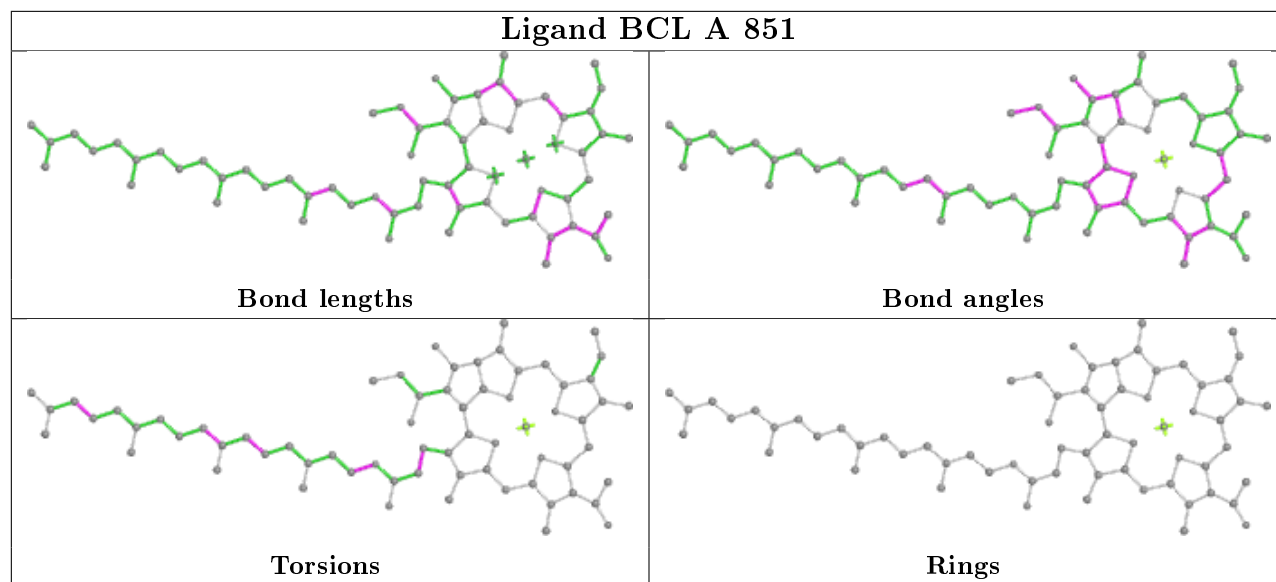


**Ligand U10 B 856****Ligand BPH B 854**



**Ligand BCL B 852****Ligand BCL A 850**





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

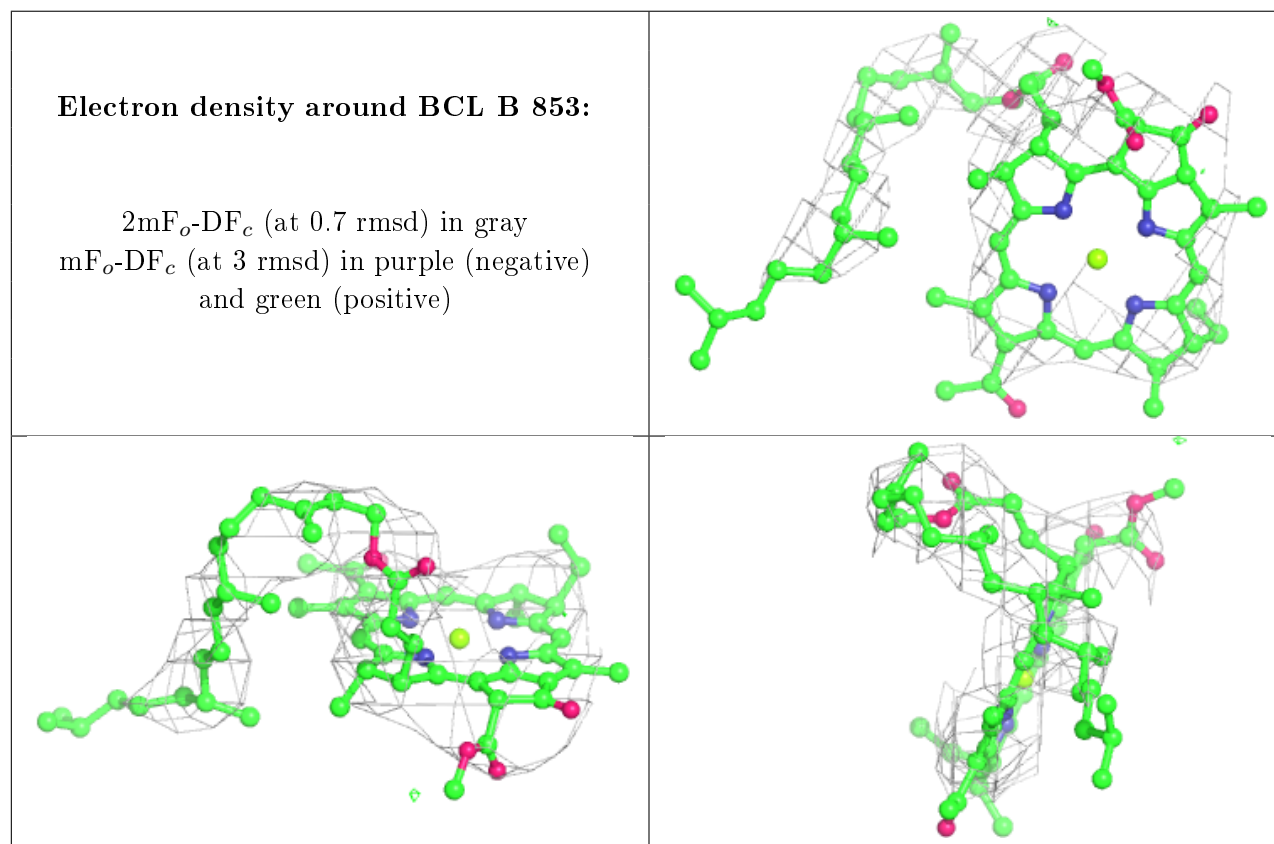
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

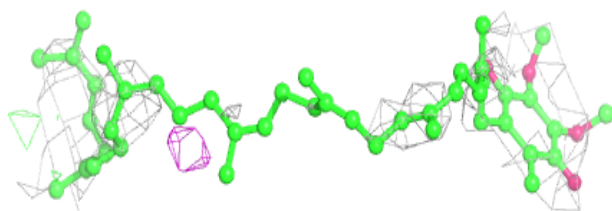
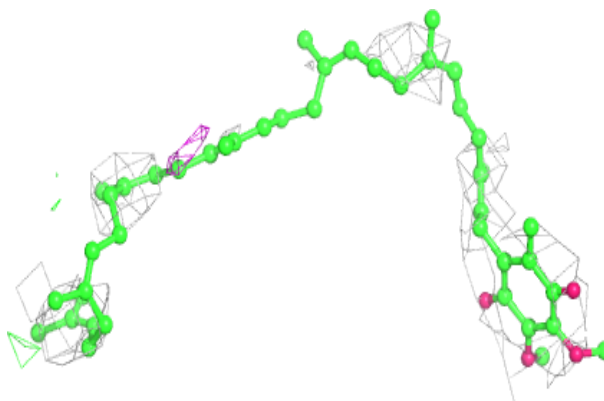
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

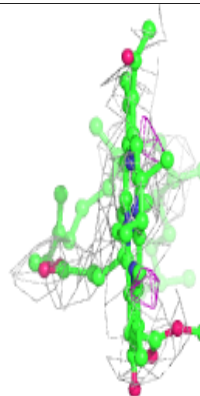
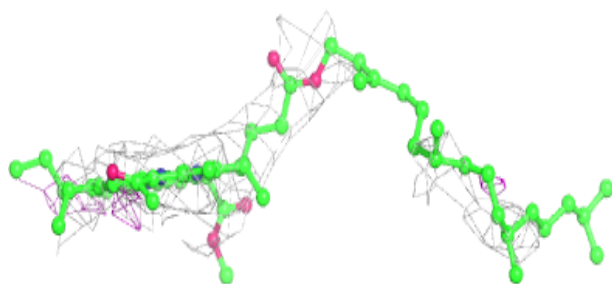
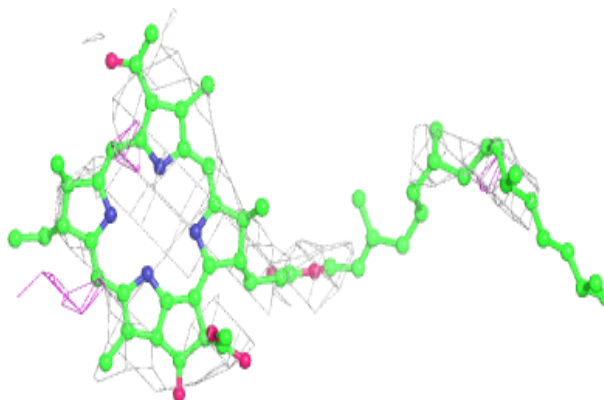


**Electron density around U10 B 856:**

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

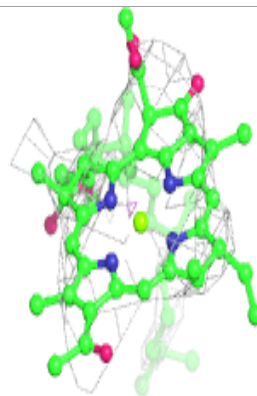
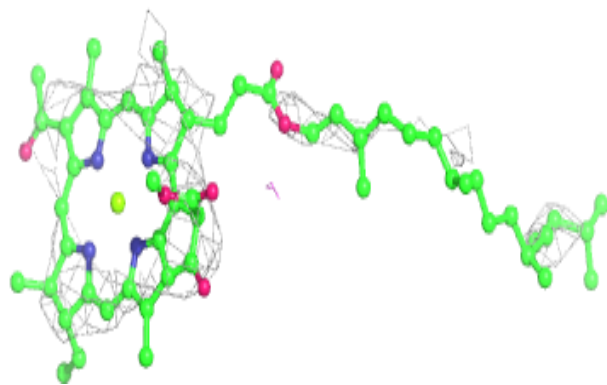
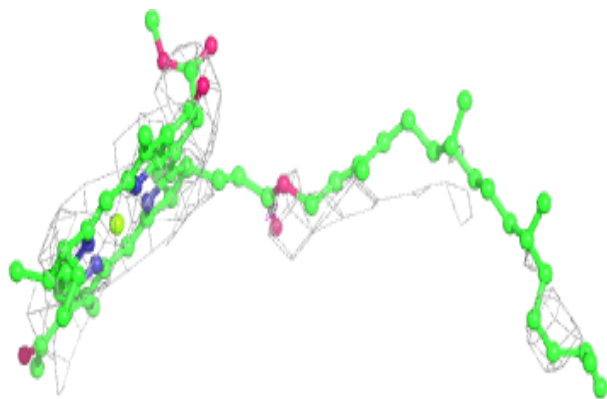
**Electron density around BPH B 854:**

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



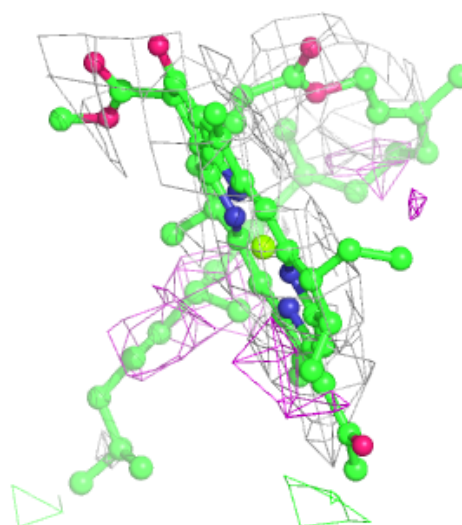
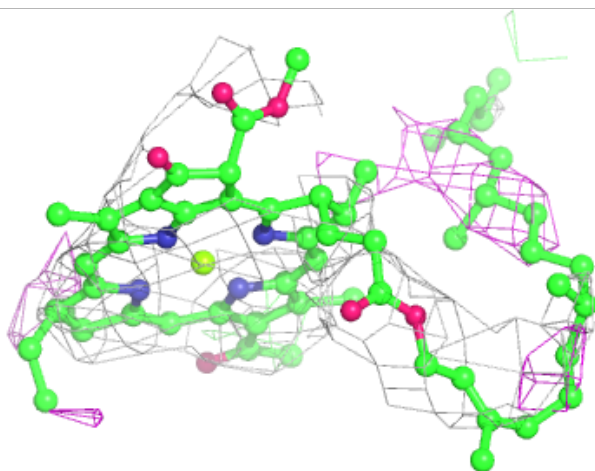
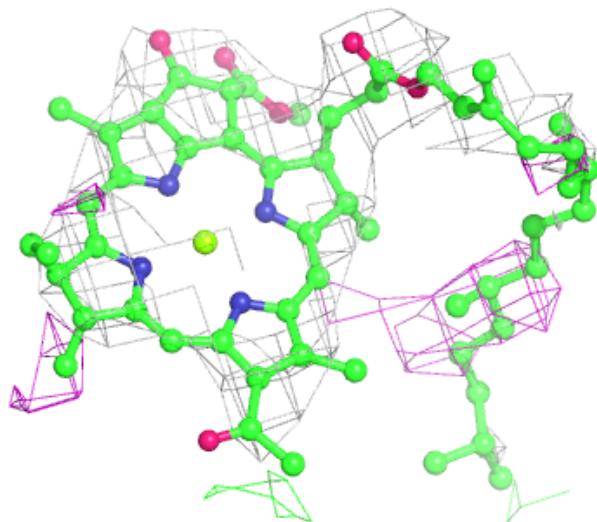
**Electron density around BCL B 852:**

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



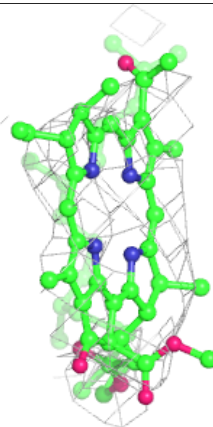
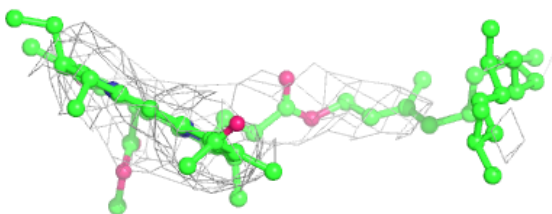
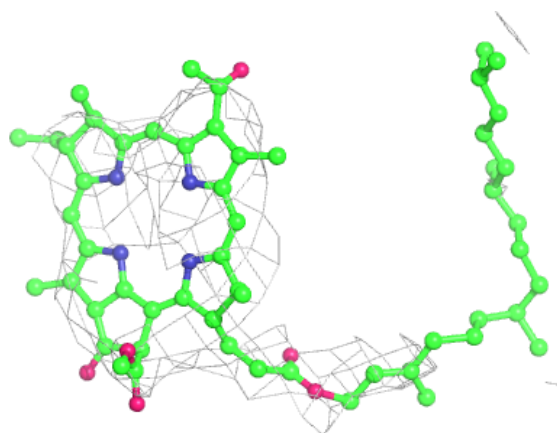
**Electron density around BCL A 850:**

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



**Electron density around BPH A 855:**

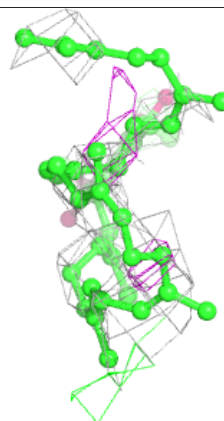
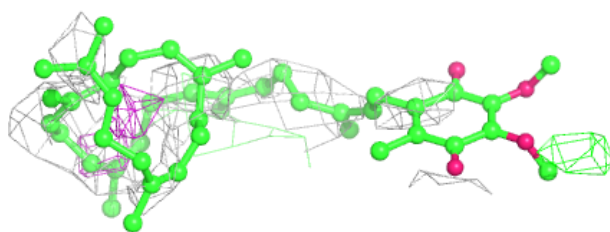
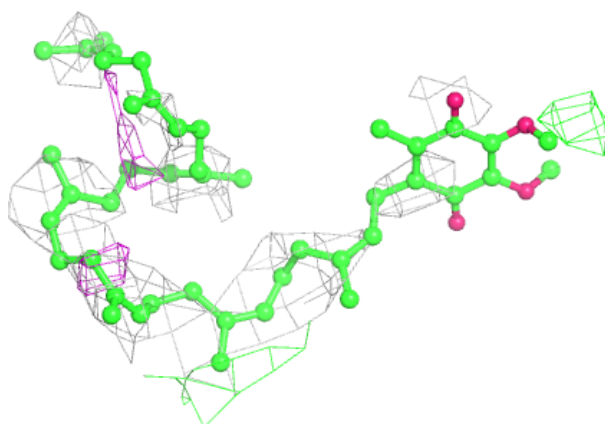
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



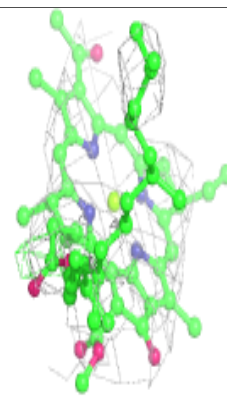
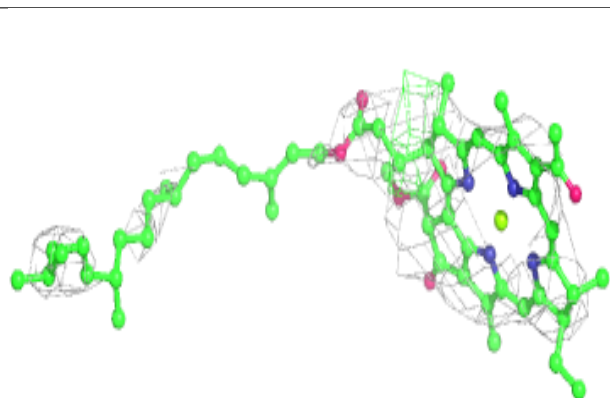
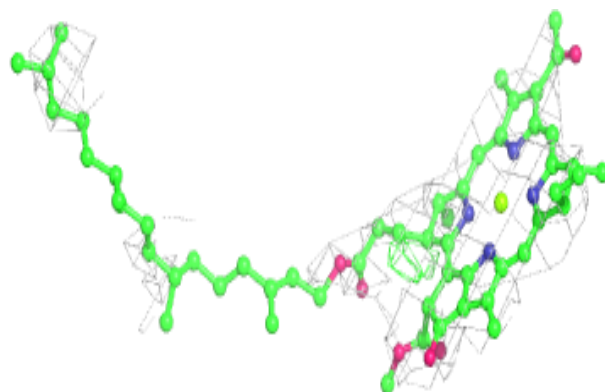


**Electron density around U10 A 857:**

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

**Electron density around BCL A 851:**

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



## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.