



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:19 am BST

PDB ID : 1DS8  
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE CHARGE-NEUTRAL DQAQB STATE WITH THE PROTON TRANSFER INHIBITOR CD2+  
Authors : Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.  
Deposited on : 2000-01-07  
Resolution : 2.50 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

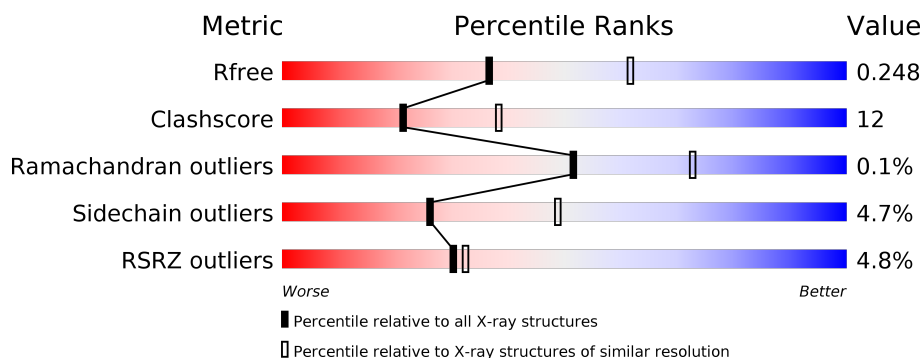
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\leq 5\%$ . 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>4%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>•</div> </div> </div>
1	R	281	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>•</div> </div> </div>
2	M	307	<div> <div>0%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>• •</div> </div> </div>
2	S	307	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>• •</div> </div> </div>
3	H	260	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
3	T	260	<div> <div>12%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 5%</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
9	LDA	S	2012	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14529 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
			2232	1507	355	362	8			
1	R	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			
2	S	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	307	ALA	ASN	CONFLICT	UNP P02953
S	307	ALA	ASN	CONFLICT	UNP P02953

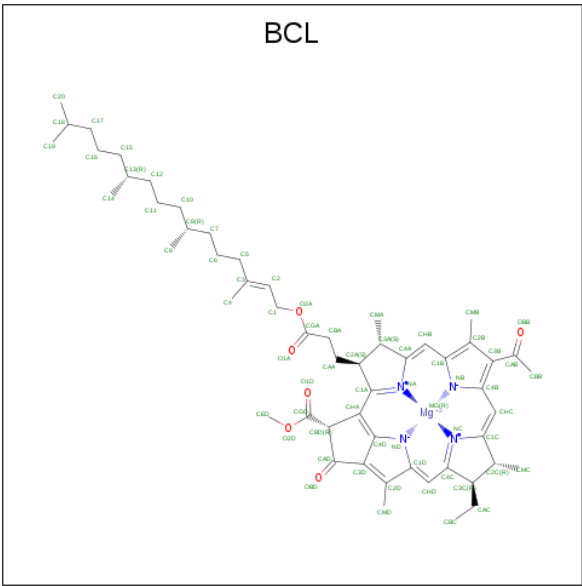
- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

There are 2 discrepancies between the modelled and reference sequences:

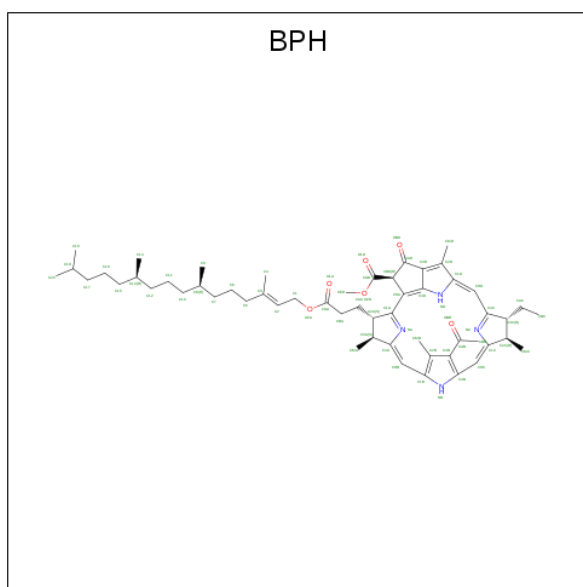
Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	CONFLICT	UNP P11846
T	8	GLN	GLY	CONFLICT	UNP P11846

- 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>).



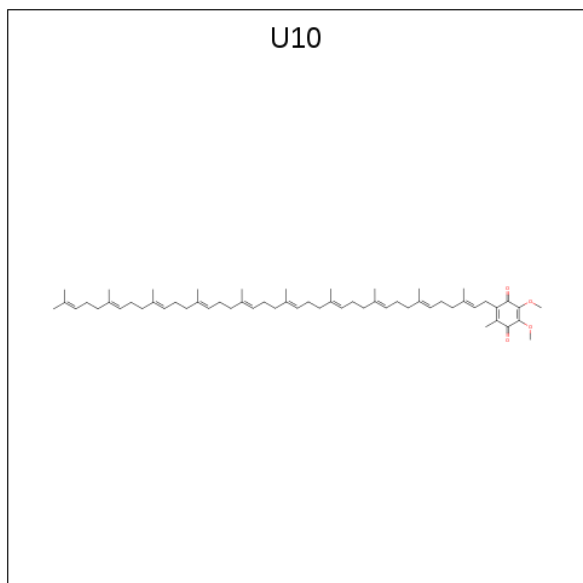
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- 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	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			51	41	4	6		
5	R	1	Total	C	N	O	0	0
			65	55	4	6		
5	S	1	Total	C	N	O	0	0
			52	42	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
			44	40	4		
6	M	1	Total	C	O	0	0
			38	34	4		
6	R	1	Total	C	O	0	0
			18	14	4		
6	S	1	Total	C	O	0	0
			32	28	4		

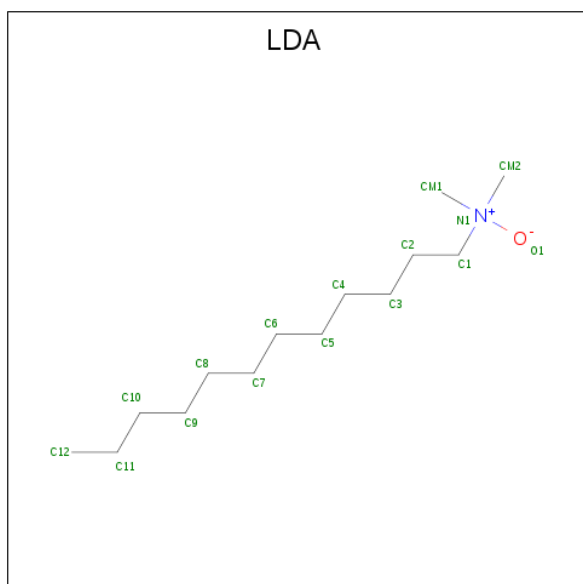
- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	S	1	Total	Fe	0	0
			1	1		
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	S	1	Total	Cl	0	0
			1	1		
8	M	1	Total	Cl	0	0
			1	1		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	S	1	Total	C	N	O	0	0
			16	14	1	1		
9	S	1	Total	C	N	O	0	0
			16	14	1	1		
9	S	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	1	Total	Cd	0	0
			1	1		
10	T	1	Total	Cd	0	0
			1	1		

- Molecule 11 is water.

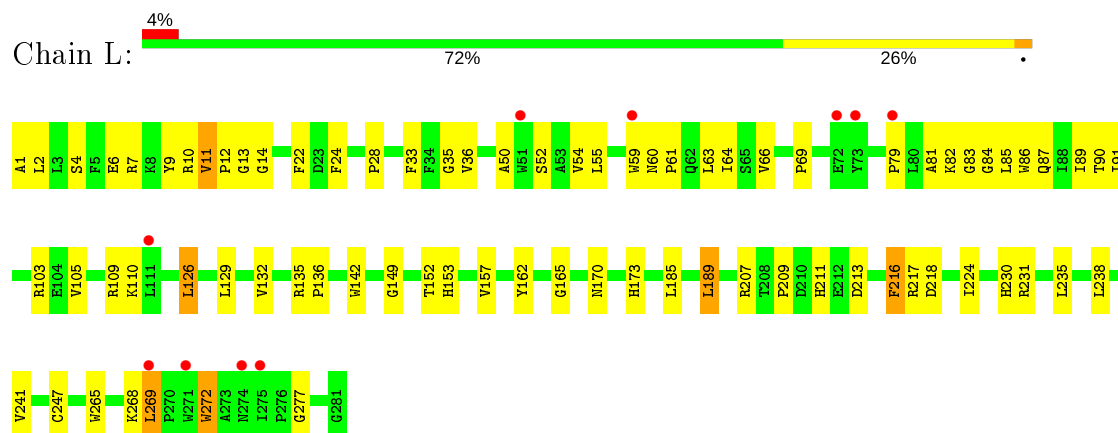
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	88	Total	O	0	0
			88	88		
11	M	133	Total	O	0	0
			133	133		
11	H	122	Total	O	0	0
			122	122		
11	R	62	Total	O	0	0
			62	62		
11	S	92	Total	O	0	0
			92	92		
11	T	85	Total	O	0	0
			85	85		



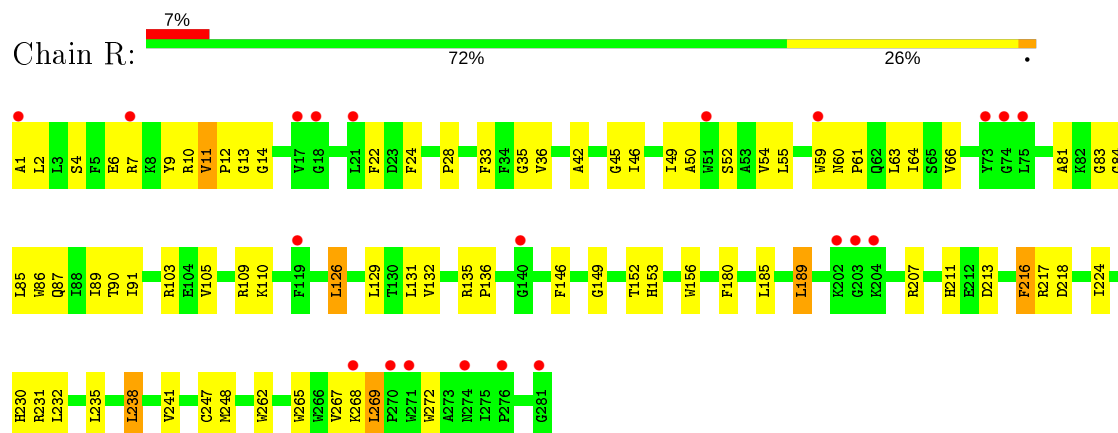
### 3 Residue-property plots [i](#)

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 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.

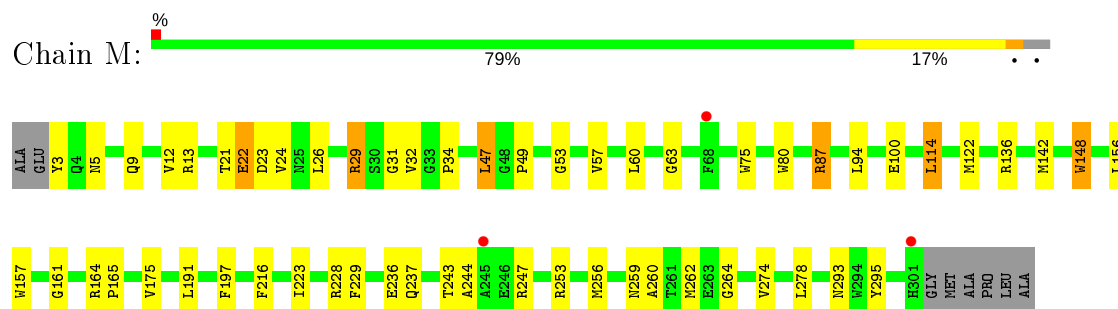
#### • Molecule 1: REACTION CENTER PROTEIN L CHAIN



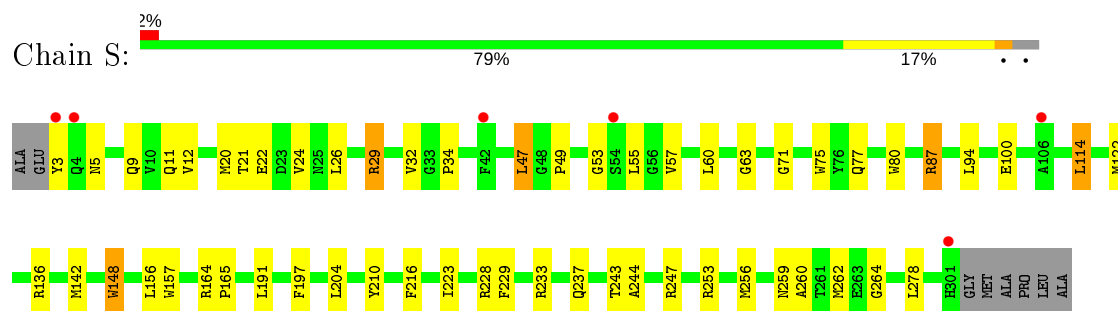
#### • Molecule 1: REACTION CENTER PROTEIN L CHAIN



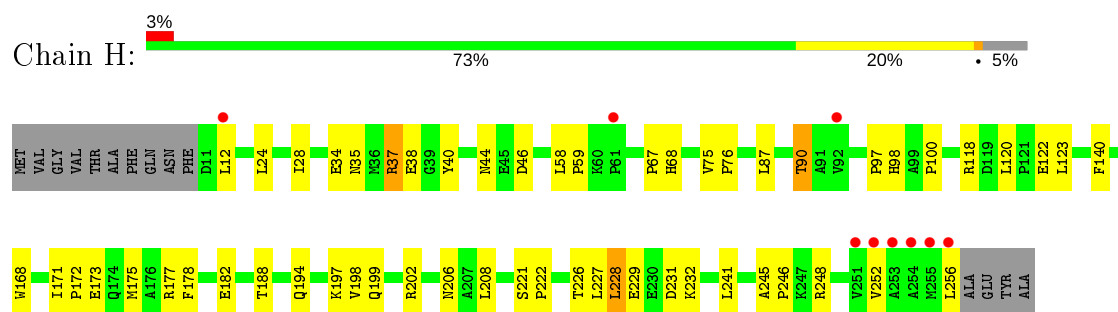
#### • Molecule 2: REACTION CENTER PROTEIN M CHAIN



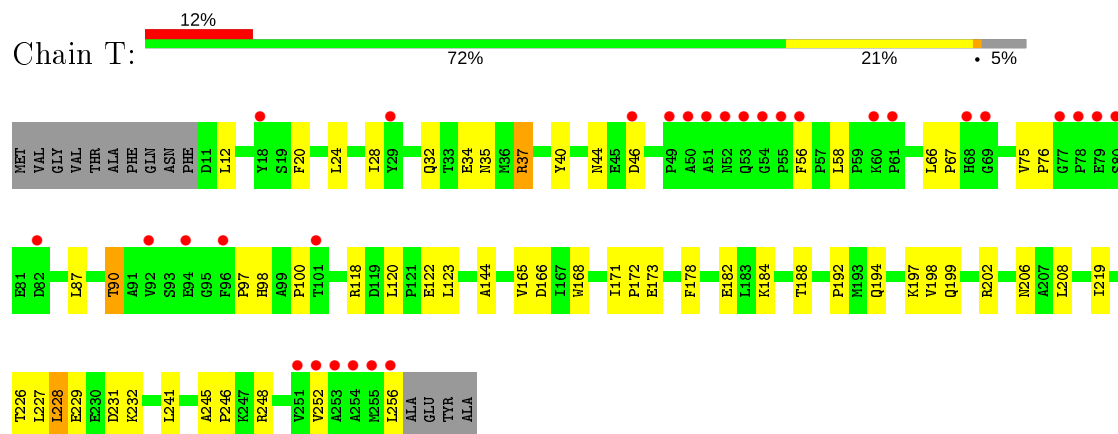
- Molecule 2: REACTION CENTER PROTEIN M CHAIN



- Molecule 3: REACTION CENTER PROTEIN H CHAIN



- Molecule 3: REACTION CENTER PROTEIN H CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.59Å 139.59Å 272.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 27.81 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.50) 99.6 (27.81-2.49)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.90 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.256 0.218 , 0.248	Depositor DCC
$R_{free}$ test set	4428 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, LDA, CL, BPH, CD, FE2, 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	L	0.39	0/2320	0.55	0/3175
1	R	0.40	0/2320	0.55	0/3175
2	M	0.41	0/2482	0.54	0/3389
2	S	0.40	0/2482	0.54	0/3389
3	H	0.35	0/1917	0.60	0/2608
3	T	0.35	0/1917	0.60	0/2608
All	All	0.39	0/13438	0.56	0/18344

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	2232	0	2187	59	0
1	R	2232	0	2187	63	0
2	M	2390	0	2304	53	0
2	S	2390	0	2304	49	0
3	H	1869	0	1884	49	0
3	T	1869	0	1884	45	0
4	L	183	0	189	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	66	0	73	8	0
4	R	183	0	189	17	0
4	S	66	0	74	6	0
5	L	65	0	76	5	0
5	M	51	0	45	5	0
5	R	65	0	76	14	0
5	S	52	0	47	4	0
6	L	44	0	57	2	0
6	M	38	0	47	2	0
6	R	18	0	15	3	0
6	S	32	0	39	2	0
7	M	1	0	0	0	0
7	S	1	0	0	0	0
8	M	1	0	0	0	0
8	S	1	0	0	0	0
9	M	48	0	93	7	0
9	S	48	0	93	5	0
10	H	1	0	0	0	0
10	T	1	0	0	0	0
11	H	122	0	0	6	0
11	L	88	0	0	7	0
11	M	133	0	0	2	0
11	R	62	0	0	2	0
11	S	92	0	0	3	0
11	T	85	0	0	3	0
All	All	14529	0	13863	333	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 333 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:M:197:PHE:HZ	4:M:1003:BCL:HBB2	1.34	0.91
2:M:197:PHE:CZ	4:M:1003:BCL:HBB2	2.11	0.86
1:L:217:ARG:HD2	11:M:1108:HOH:O	1.77	0.85
2:M:161:GLY:HA3	9:M:1014:LDA:HM12	1.62	0.82
1:R:131:LEU:HD21	4:R:2002:BCL:HED2	1.64	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	266 (95%)	12 (4%)	1 (0%)	34	54
1	R	279/281 (99%)	266 (95%)	12 (4%)	1 (0%)	34	54
2	M	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	289 (97%)	8 (3%)	0	100	100
3	H	244/260 (94%)	236 (97%)	8 (3%)	0	100	100
3	T	244/260 (94%)	234 (96%)	10 (4%)	0	100	100
All	All	1640/1696 (97%)	1579 (96%)	59 (4%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	4	SER
1	L	4	SER

### 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%)	209 (95%)	11 (5%)	24	46
1	R	220/220 (100%)	209 (95%)	11 (5%)	24	46
2	M	235/239 (98%)	222 (94%)	13 (6%)	21	41
2	S	235/239 (98%)	222 (94%)	13 (6%)	21	41
3	H	199/209 (95%)	192 (96%)	7 (4%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	T	199/209 (95%)	192 (96%)	7 (4%)	36 62
All	All	1308/1336 (98%)	1246 (95%)	62 (5%)	26 49

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	208	LEU
1	R	129	LEU
3	T	90	THR
1	R	7	ARG
1	R	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	199	GLN
3	H	206	ASN
2	S	300	ASN
3	H	194	GLN
3	T	194	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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
5	BPH	S	2005	-	51,57,70	1.25	5 (9%)	60,85,101	1.93	14 (23%)
9	LDA	M	1012	-	12,15,15	2.22	1 (8%)	14,17,17	1.42	2 (14%)
4	BCL	R	2002	1	58,74,74	1.17	4 (6%)	69,115,115	1.76	14 (20%)
5	BPH	L	1006	-	64,70,70	1.24	7 (10%)	76,101,101	1.67	14 (18%)
9	LDA	S	2013	-	12,15,15	2.35	1 (8%)	14,17,17	1.39	1 (7%)
9	LDA	M	1013	-	12,15,15	2.40	1 (8%)	14,17,17	1.37	2 (14%)
4	BCL	R	2001	2	43,59,74	1.20	6 (13%)	51,97,115	2.36	14 (27%)
6	U10	S	2008	-	32,32,63	1.70	7 (21%)	38,41,79	1.17	4 (10%)
9	LDA	M	1014	-	12,15,15	2.41	1 (8%)	14,17,17	1.41	3 (21%)
6	U10	L	1009	-	44,44,63	1.68	8 (18%)	53,56,79	1.41	9 (16%)
5	BPH	R	2006	-	64,70,70	1.11	6 (9%)	76,101,101	1.54	9 (11%)
4	BCL	M	1003	2	58,74,74	1.11	6 (10%)	69,115,115	1.76	16 (23%)
5	BPH	M	1005	-	50,56,70	1.21	7 (14%)	59,84,101	2.19	14 (23%)
4	BCL	S	2003	2	58,74,74	1.04	6 (10%)	69,115,115	2.02	14 (20%)
9	LDA	S	2014	-	12,15,15	2.55	1 (8%)	14,17,17	1.37	1 (7%)
4	BCL	L	1004	1	58,74,74	1.05	6 (10%)	69,115,115	2.21	18 (26%)
4	BCL	L	1001	2	43,59,74	1.21	6 (13%)	51,97,115	2.38	17 (33%)
4	BCL	L	1002	1	58,74,74	1.04	5 (8%)	69,115,115	1.76	14 (20%)
6	U10	M	1008	-	38,38,63	1.88	10 (26%)	46,49,79	1.30	5 (10%)
9	LDA	S	2012	-	12,15,15	2.47	1 (8%)	14,17,17	1.36	1 (7%)
4	BCL	R	2004	1	58,74,74	1.04	5 (8%)	69,115,115	2.11	12 (17%)
6	U10	R	2009	-	18,18,63	2.06	3 (16%)	22,25,79	1.46	5 (22%)

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	S	2005	-	-	10/39/90/105	0/5/6/6
9	LDA	M	1012	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	R	2002	1	-	6/37/137/137	-
5	BPH	L	1006	-	-	9/54/105/105	0/5/6/6
9	LDA	S	2013	-	-	9/13/13/13	-
9	LDA	M	1013	-	-	4/13/13/13	-
4	BCL	R	2001	2	-	2/19/119/137	-
6	U10	S	2008	-	-	2/26/50/87	0/1/1/1
9	LDA	M	1014	-	-	8/13/13/13	-
6	U10	L	1009	-	-	13/41/65/87	0/1/1/1
5	BPH	R	2006	-	-	6/54/105/105	0/5/6/6
4	BCL	M	1003	2	-	4/37/137/137	-
5	BPH	M	1005	-	-	6/38/89/105	0/5/6/6
4	BCL	S	2003	2	-	3/37/137/137	-
9	LDA	S	2014	-	-	7/13/13/13	-
4	BCL	L	1004	1	-	3/37/137/137	-
4	BCL	L	1001	2	-	3/19/119/137	-
4	BCL	L	1002	1	-	2/37/137/137	-
6	U10	M	1008	-	-	3/33/57/87	0/1/1/1
9	LDA	S	2012	-	-	5/13/13/13	-
4	BCL	R	2004	1	-	7/37/137/137	-
6	U10	R	2009	-	-	2/9/33/87	0/1/1/1

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	2014	LDA	O1-N1	-8.50	1.22	1.42
9	S	2012	LDA	O1-N1	-8.18	1.23	1.42
9	M	1014	LDA	O1-N1	-8.16	1.23	1.42
9	M	1013	LDA	O1-N1	-7.96	1.23	1.42
9	S	2013	LDA	O1-N1	-7.88	1.23	1.42

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1004	BCL	C4D-C3D-CAD	-10.10	102.84	108.47
4	S	2003	BCL	C4D-C3D-CAD	-9.79	103.01	108.47
4	R	2004	BCL	C4D-C3D-CAD	-9.36	103.25	108.47
4	R	2001	BCL	C4D-C3D-CAD	-8.62	103.66	108.47
4	L	1001	BCL	C4D-C3D-CAD	-8.29	103.84	108.47

There are no chirality outliers.

5 of 121 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	S	2005	BPH	C4C-C3C-CAC-CBC
5	S	2005	BPH	C4B-C3B-CAB-OB
5	S	2005	BPH	C2-C3-C5-C6
5	S	2005	BPH	C4-C3-C5-C6
5	S	2005	BPH	C3-C5-C6-C7

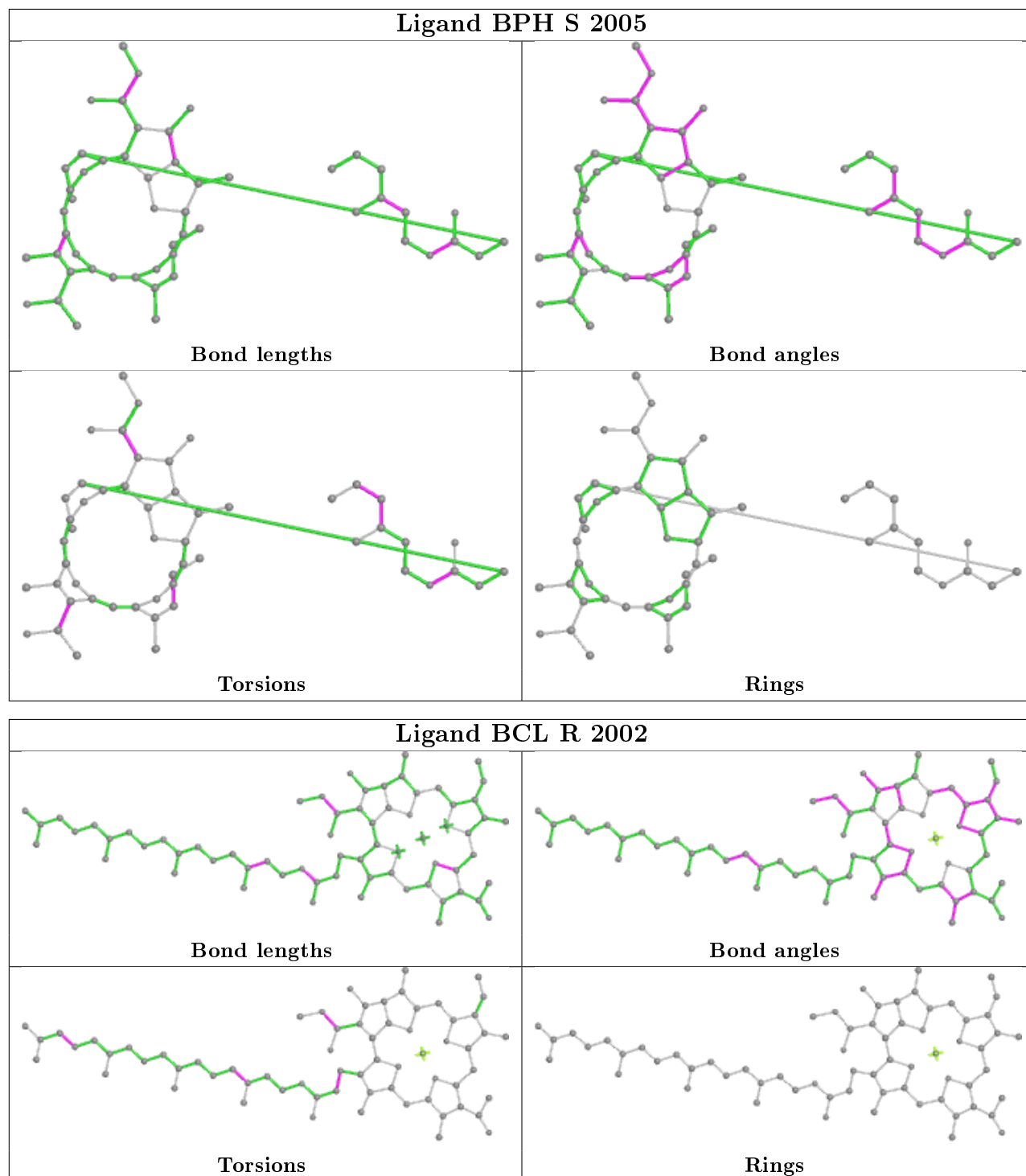
There are no ring outliers.

22 monomers are involved in 84 short contacts:

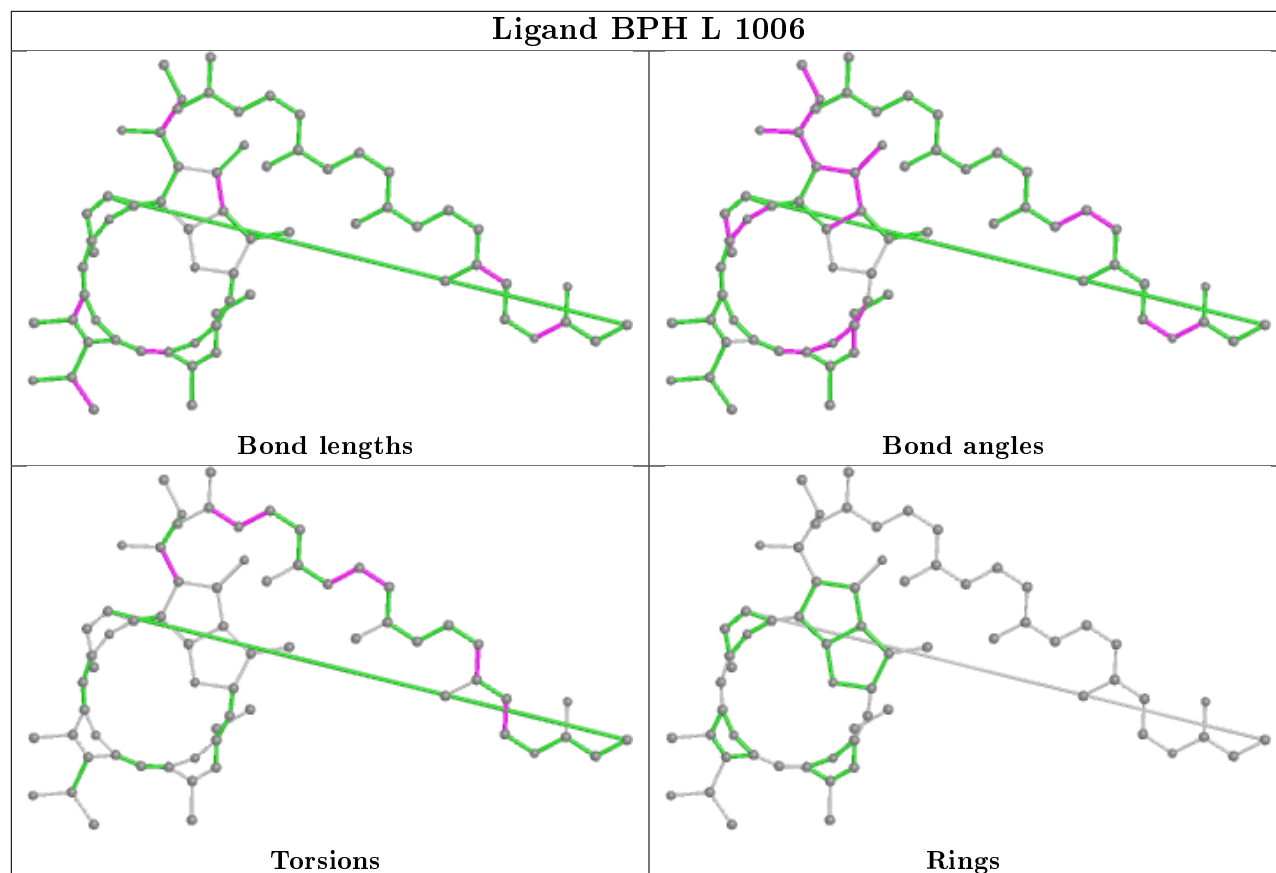
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	2005	BPH	4	0
9	M	1012	LDA	1	0
4	R	2002	BCL	9	0
5	L	1006	BPH	5	0
9	S	2013	LDA	1	0
9	M	1013	LDA	1	0
4	R	2001	BCL	3	0
6	S	2008	U10	2	0
9	M	1014	LDA	5	0
6	L	1009	U10	2	0
5	R	2006	BPH	14	0
4	M	1003	BCL	8	0
5	M	1005	BPH	5	0
4	S	2003	BCL	6	0
9	S	2014	LDA	2	0
4	L	1004	BCL	7	0
4	L	1001	BCL	4	0
4	L	1002	BCL	9	0
6	M	1008	U10	2	0
9	S	2012	LDA	2	0
4	R	2004	BCL	6	0
6	R	2009	U10	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

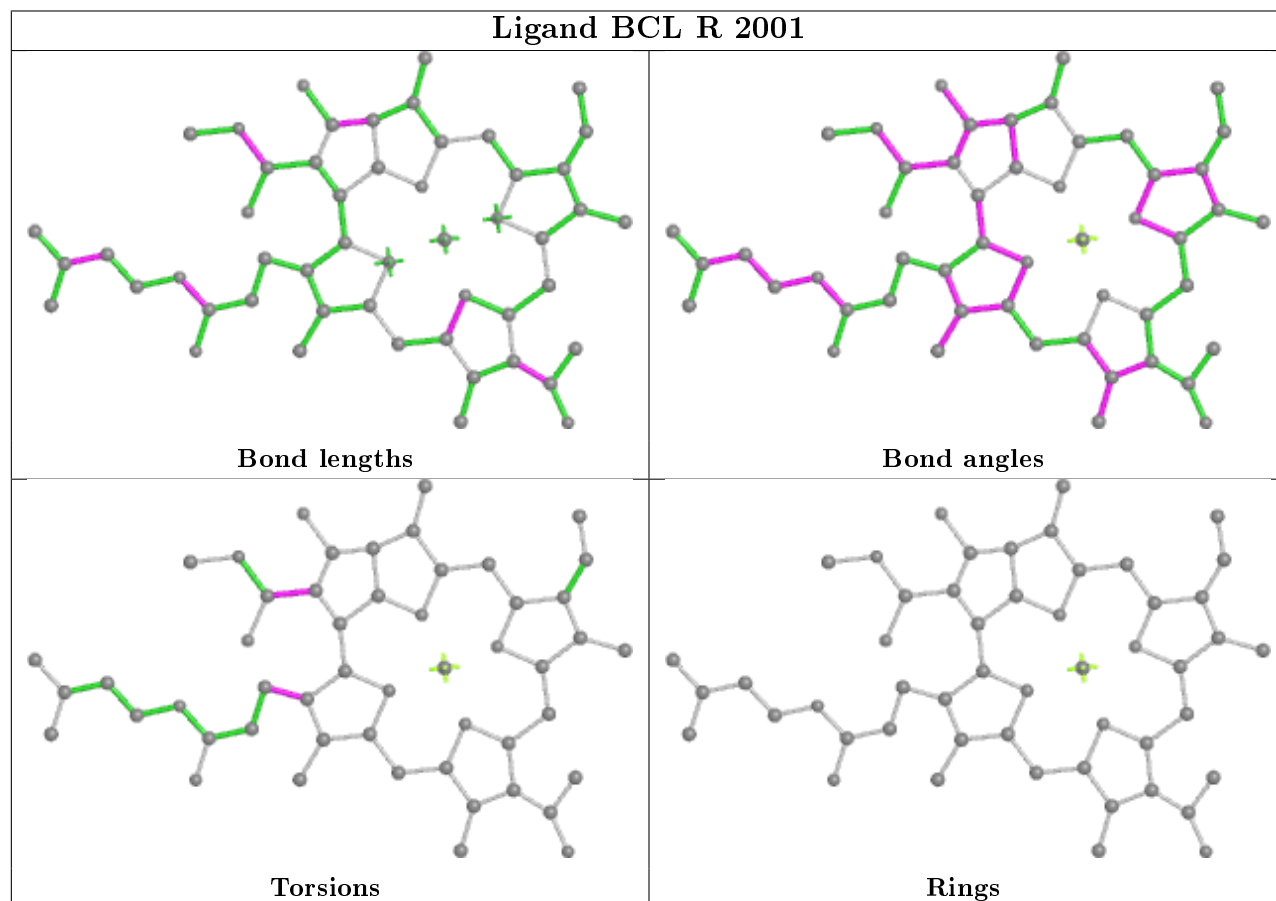
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

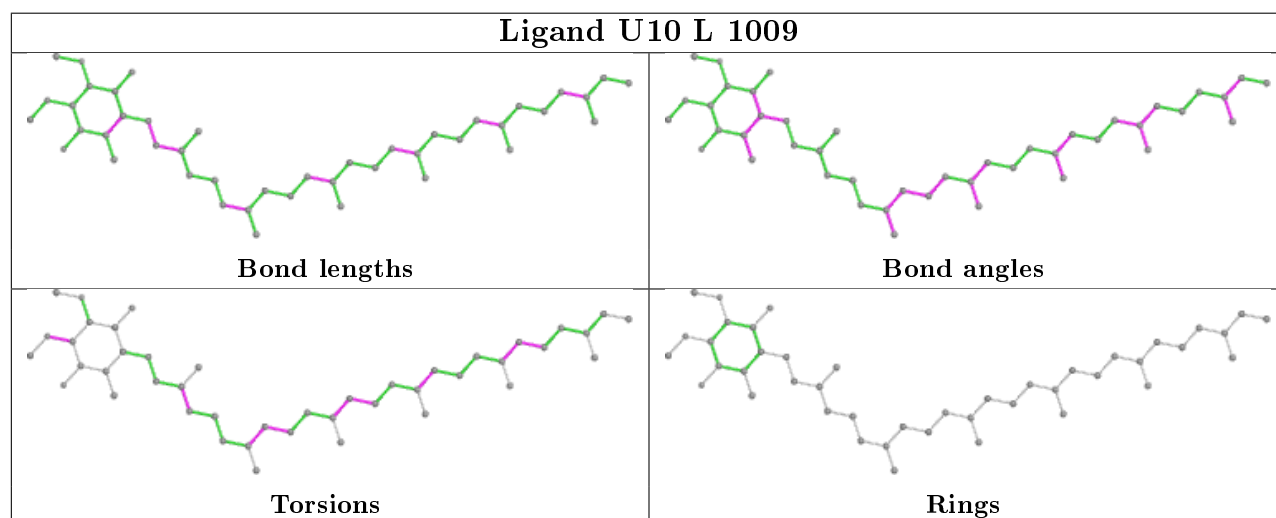
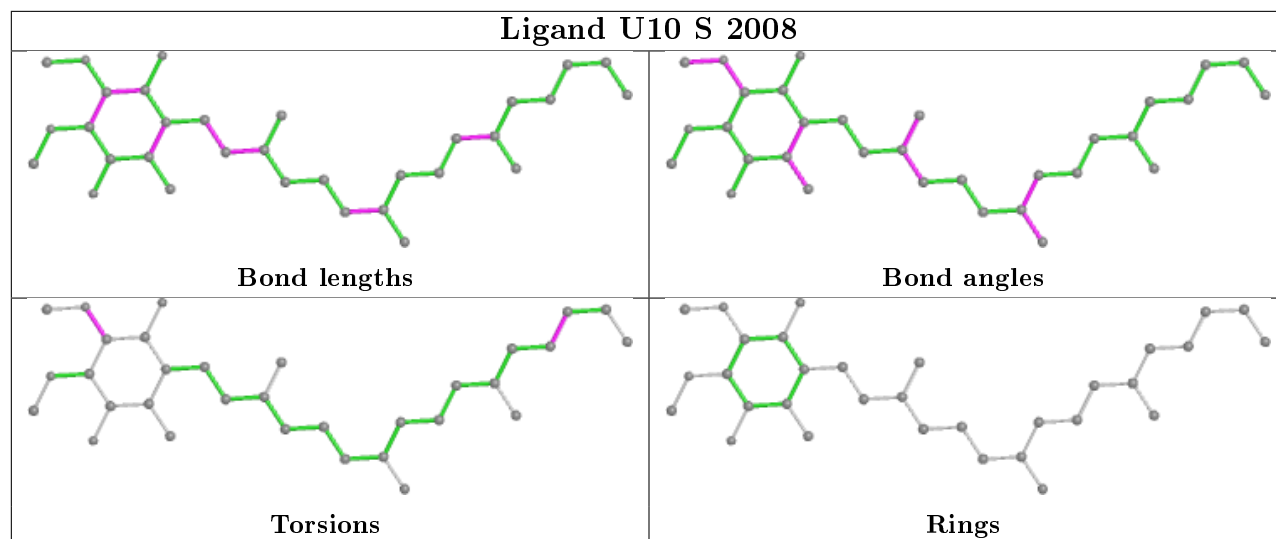


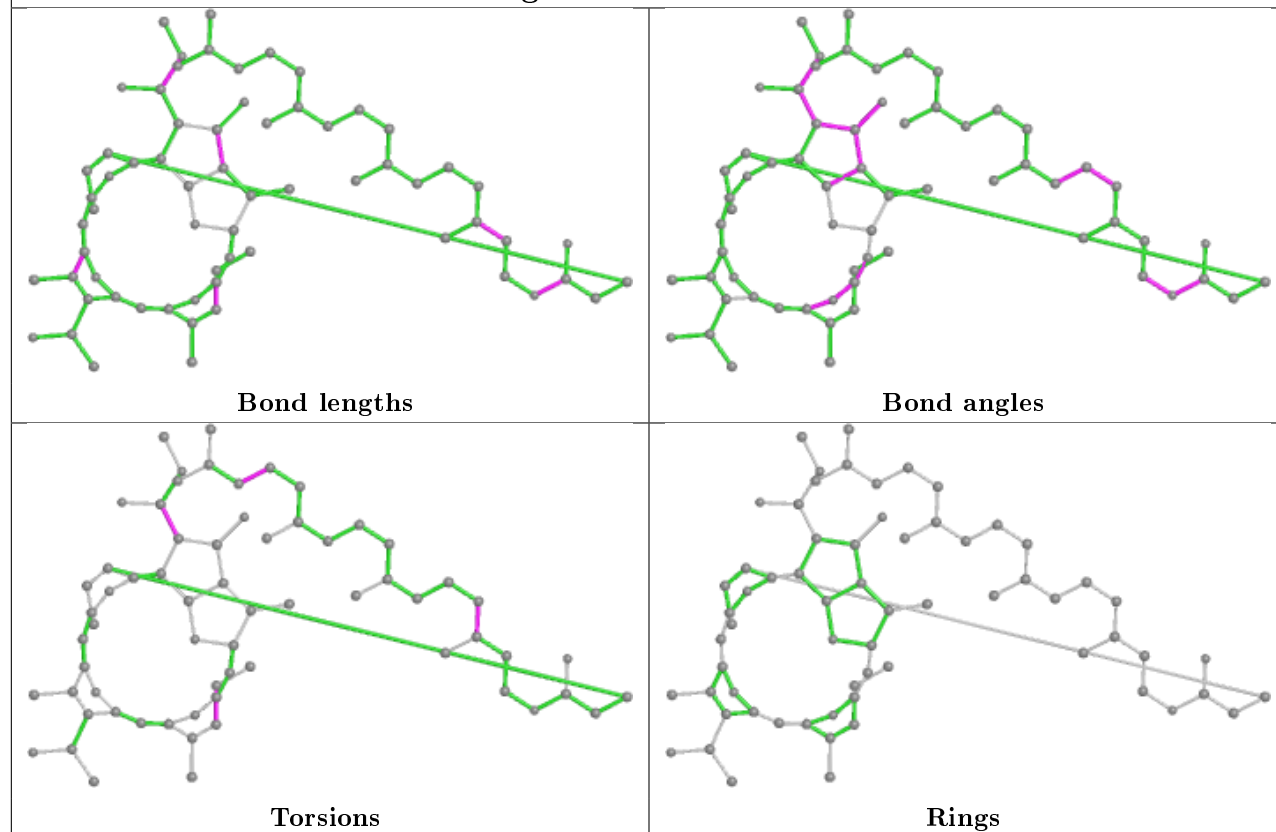
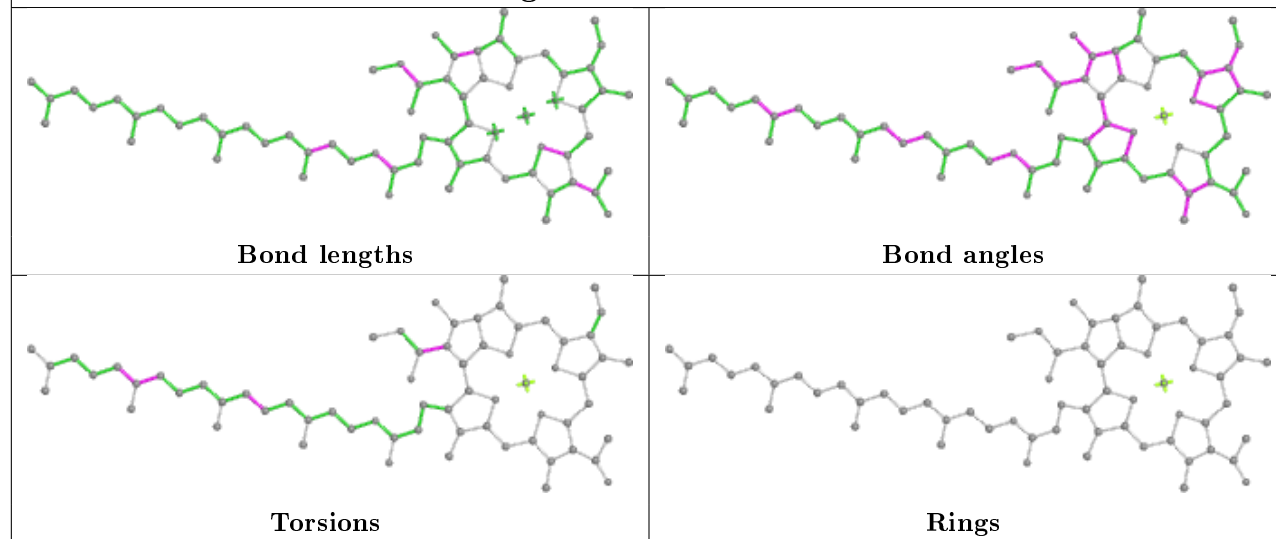
## Ligand BPH L 1006



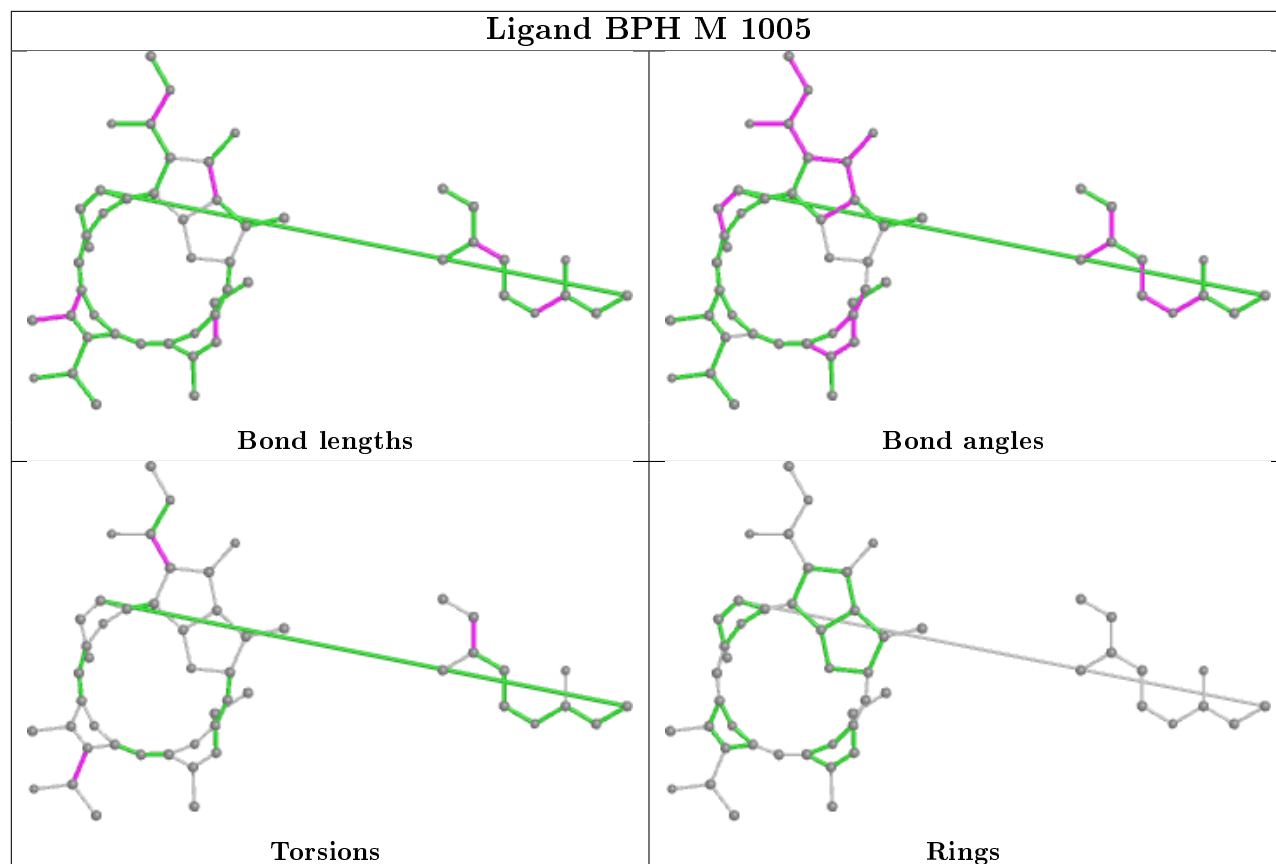
## Ligand BCL R 2001



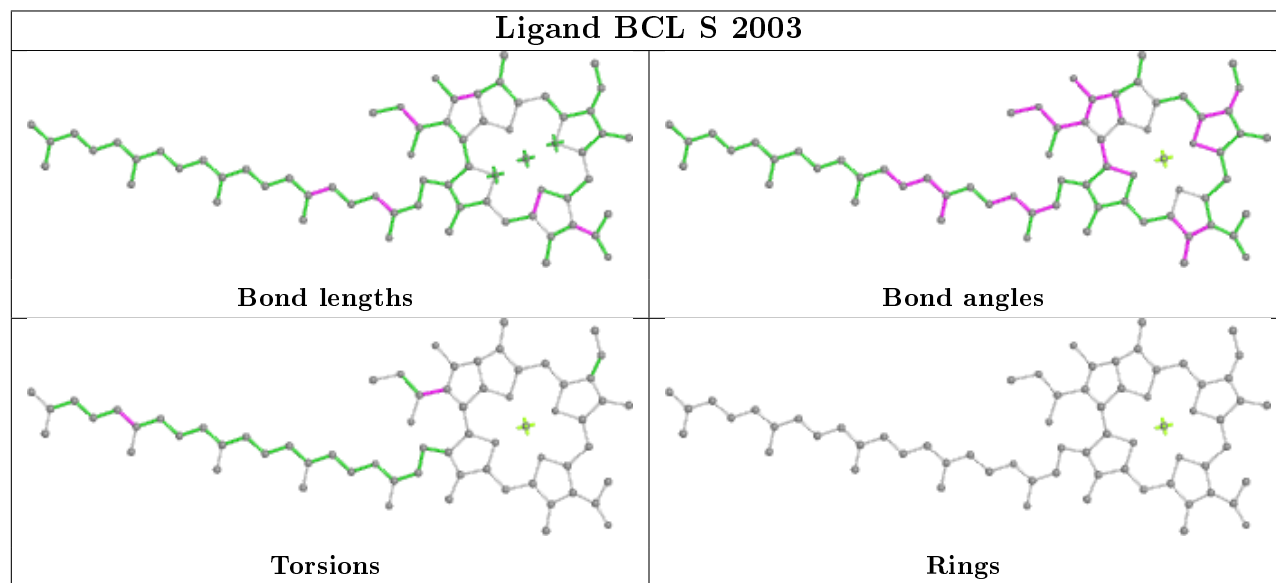


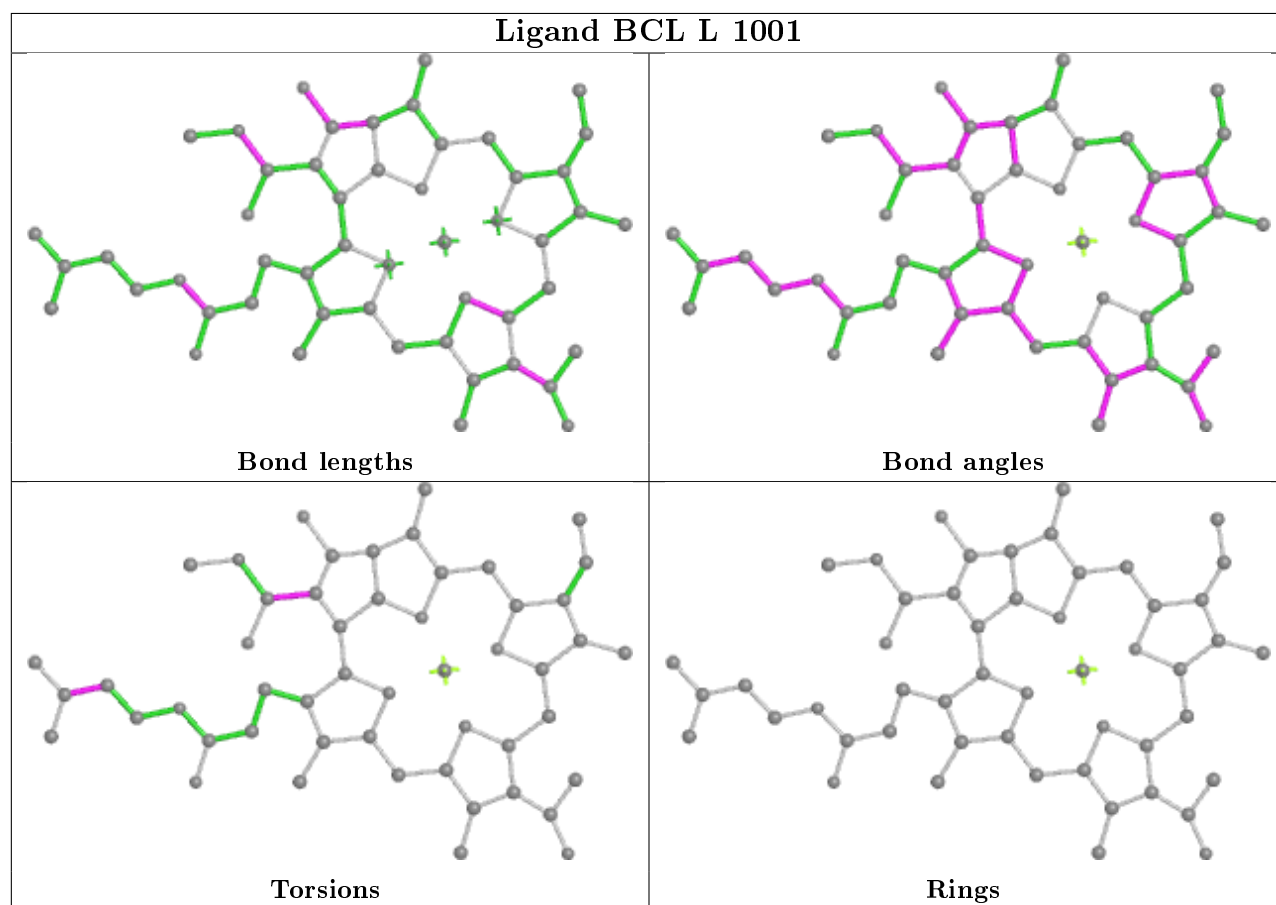
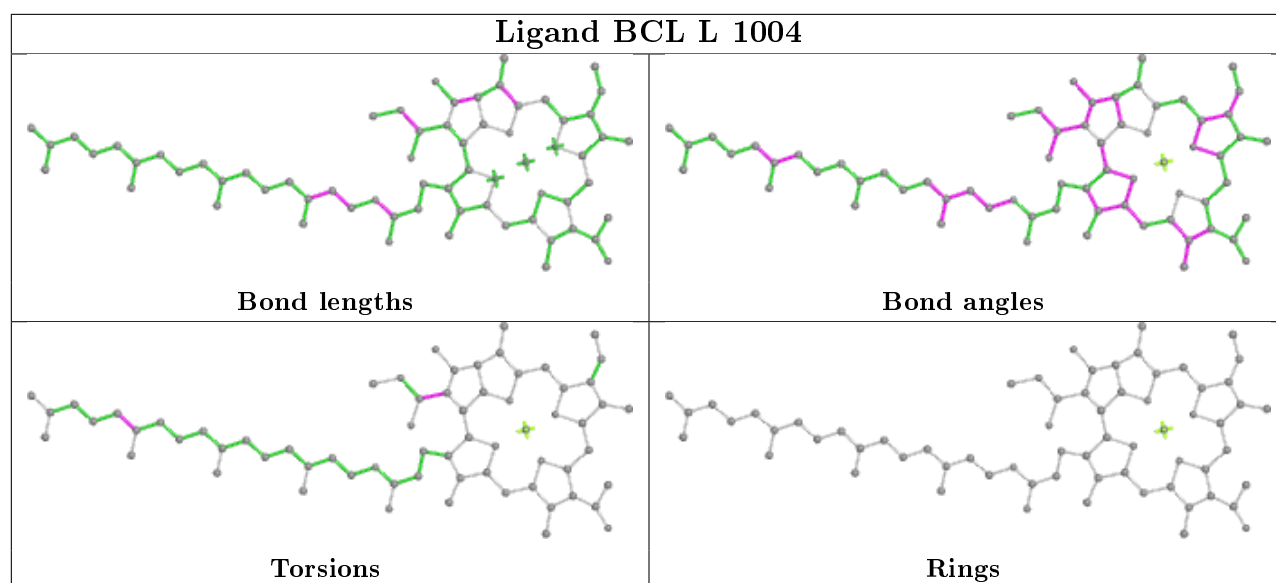
**Ligand BPH R 2006****Ligand BCL M 1003**

## Ligand BPH M 1005

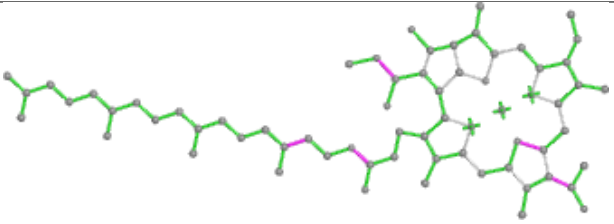
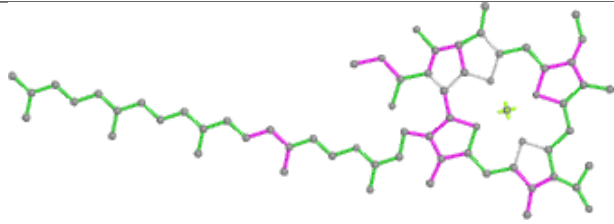
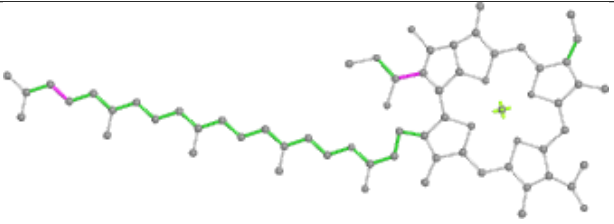
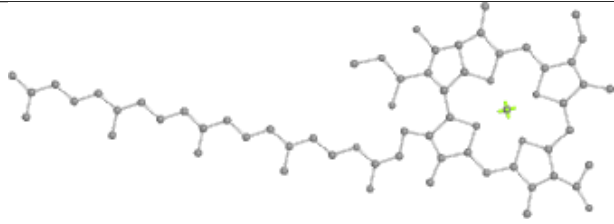
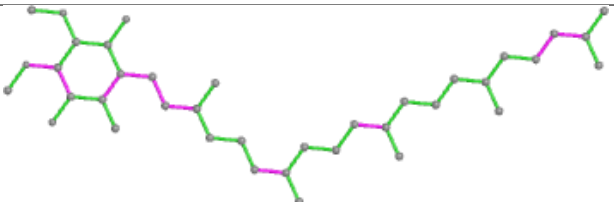
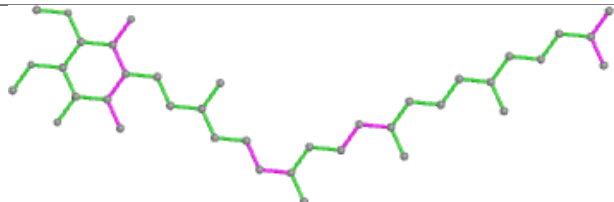
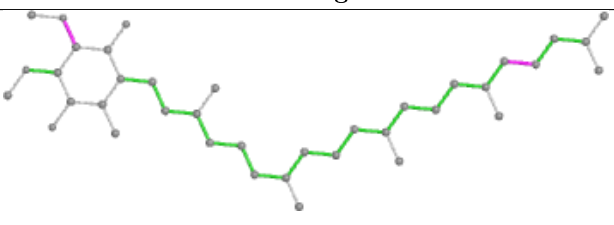
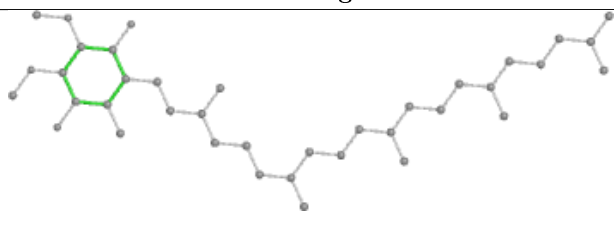
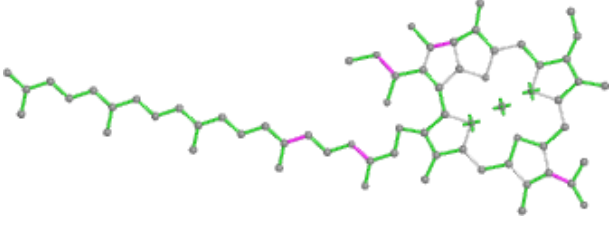
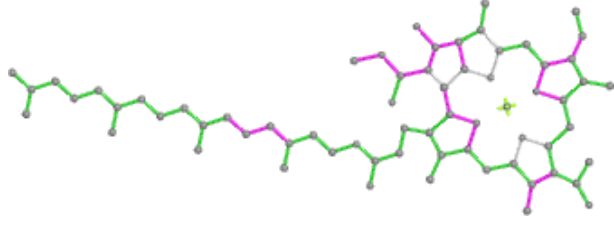
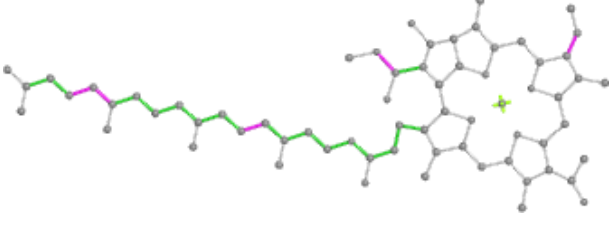
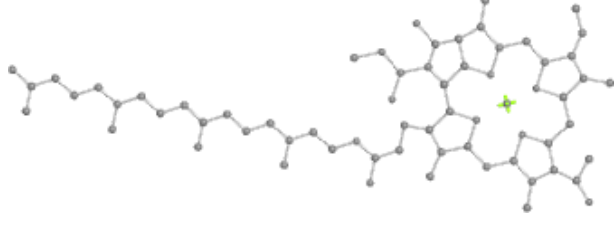


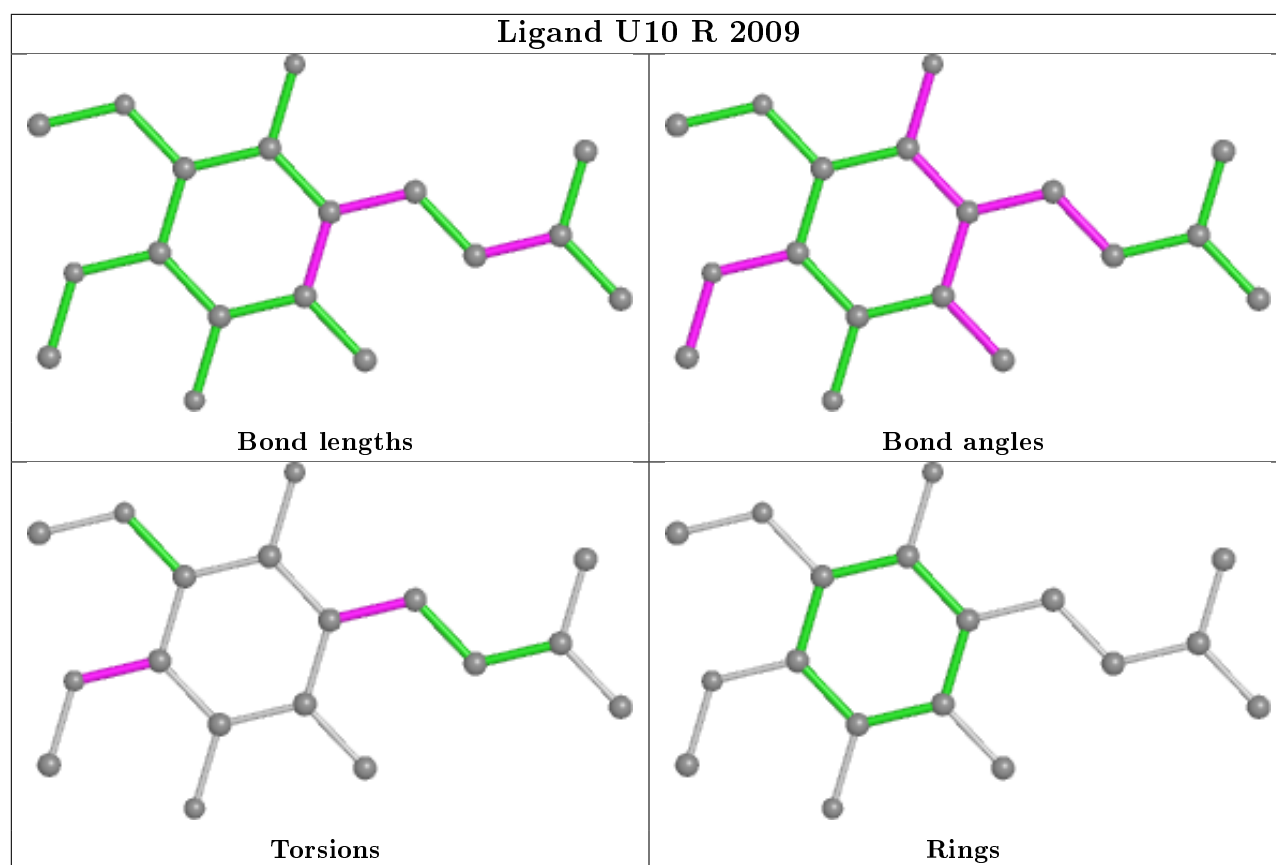
## Ligand BCL S 2003







Ligand BCL L 1002	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand U10 M 1008	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL R 2004	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



## 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%)	0.29	10 (3%) 42 46	26, 43, 67, 75	0
1	R	281/281 (100%)	0.15	21 (7%) 14 14	26, 44, 67, 75	0
2	M	299/307 (97%)	0.08	3 (1%) 82 84	28, 36, 48, 67	0
2	S	299/307 (97%)	-0.12	6 (2%) 65 68	29, 37, 49, 67	0
3	H	246/260 (94%)	0.09	9 (3%) 41 45	33, 43, 66, 82	0
3	T	246/260 (94%)	0.39	30 (12%) 4 3	34, 44, 66, 82	0
All	All	1652/1696 (97%)	0.14	79 (4%) 30 32	26, 40, 65, 82	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	301	HIS	6.5
2	M	301	HIS	6.1
3	H	255	MET	5.4
3	H	252	VAL	5.1
3	T	69	GLY	5.1

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

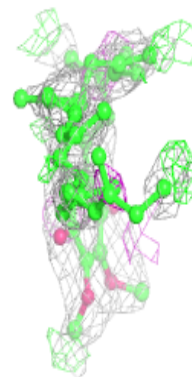
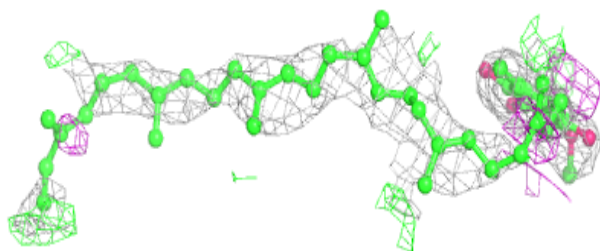
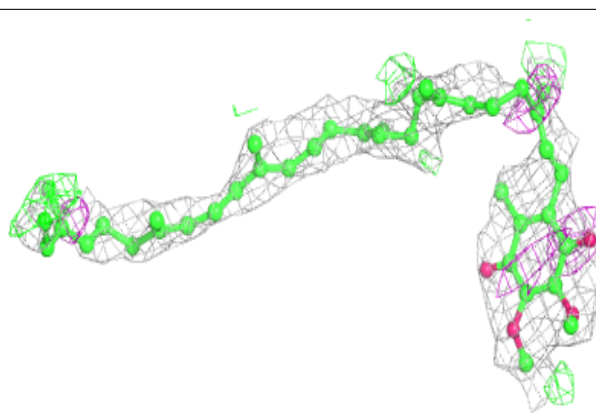
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	LDA	S	2012	16/16	0.61	0.42	50,54,58,58	0
9	LDA	S	2013	16/16	0.67	0.28	58,59,63,63	0
6	U10	L	1009	44/63	0.68	0.36	67,78,87,87	0
9	LDA	S	2014	16/16	0.69	0.27	54,57,60,60	0
9	LDA	M	1014	16/16	0.70	0.39	51,52,55,55	0
9	LDA	M	1012	16/16	0.76	0.25	54,56,59,59	0
9	LDA	M	1013	16/16	0.77	0.24	47,51,55,55	0
6	U10	R	2009	18/63	0.79	0.27	61,62,63,63	0
6	U10	M	1008	38/63	0.92	0.18	27,30,45,45	0
5	BPH	R	2006	65/65	0.92	0.17	42,45,51,51	0
5	BPH	L	1006	65/65	0.92	0.16	26,30,39,39	0
4	BCL	R	2002	66/66	0.93	0.19	36,38,43,44	0
4	BCL	L	1002	66/66	0.94	0.18	27,32,33,36	0
4	BCL	R	2001	51/66	0.94	0.13	30,32,41,43	0
4	BCL	S	2003	66/66	0.94	0.17	33,34,48,49	0
4	BCL	R	2004	66/66	0.94	0.15	30,33,53,54	0
6	U10	S	2008	32/63	0.94	0.17	41,43,46,47	0
4	BCL	L	1004	66/66	0.95	0.15	25,27,43,44	0
4	BCL	M	1003	66/66	0.95	0.19	27,29,39,43	0
5	BPH	S	2005	52/65	0.96	0.12	30,32,41,41	0
5	BPH	M	1005	51/65	0.96	0.14	23,25,33,34	0
4	BCL	L	1001	51/66	0.96	0.15	26,28,33,34	0
8	CL	S	2011	1/1	0.96	0.20	59,59,59,59	0
8	CL	M	1011	1/1	0.97	0.18	48,48,48,48	0
10	CD	H	1010	1/1	0.99	0.05	41,41,41,41	0
7	FE2	M	1007	1/1	0.99	0.12	28,28,28,28	0
7	FE2	S	2007	1/1	0.99	0.05	32,32,32,32	0
10	CD	T	2010	1/1	0.99	0.04	53,53,53,53	0

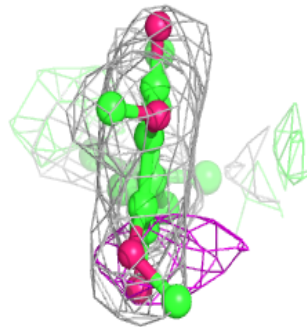
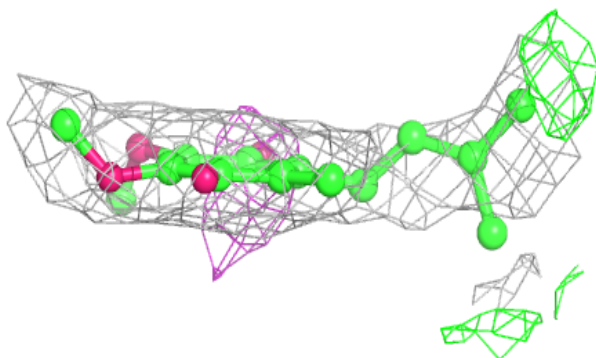
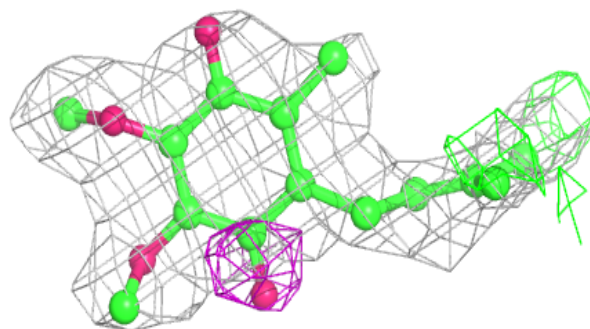
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around U10 L 1009:**

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

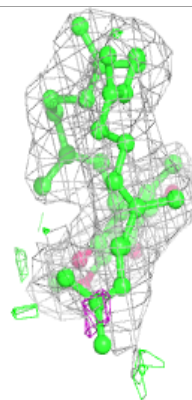
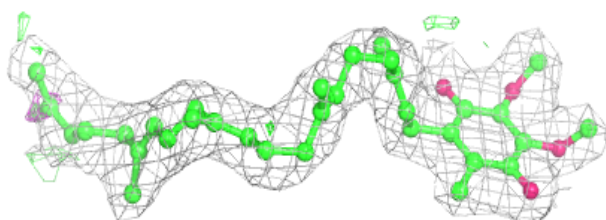
**Electron density around U10 R 2009:**

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and green (positive)

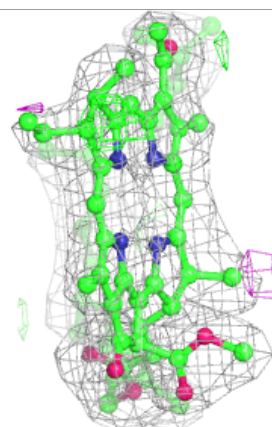
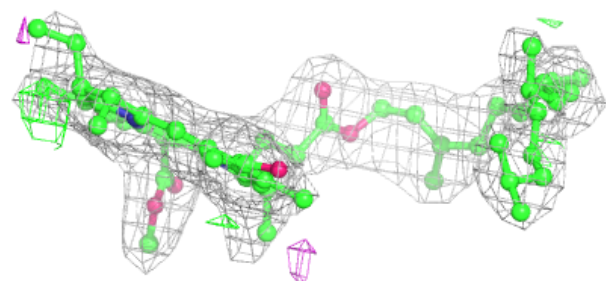
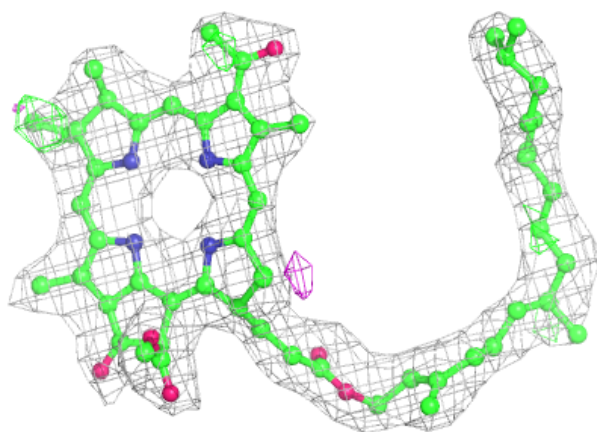


**Electron density around U10 M 1008:**

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and green (positive)

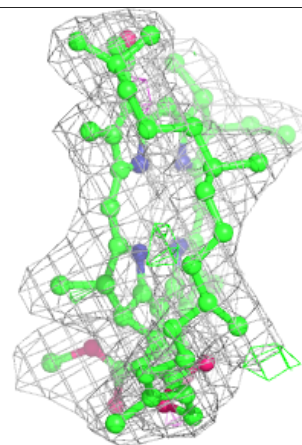
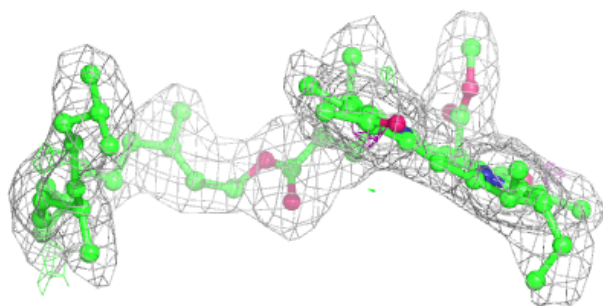
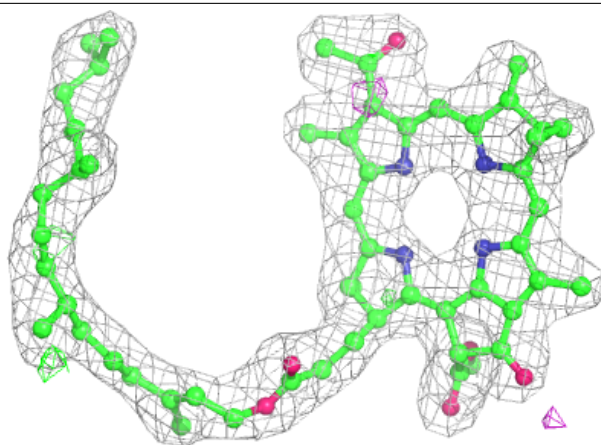
**Electron density around BPH R 2006:**

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and green (positive)

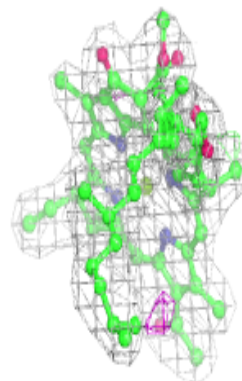
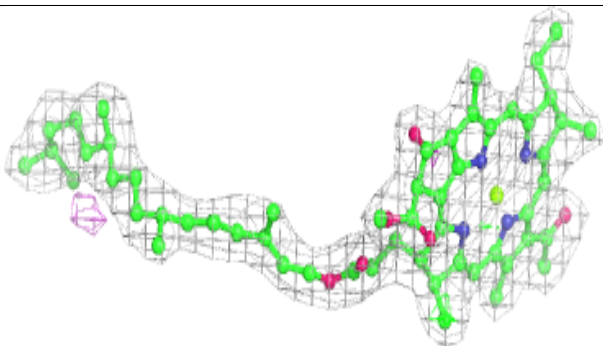
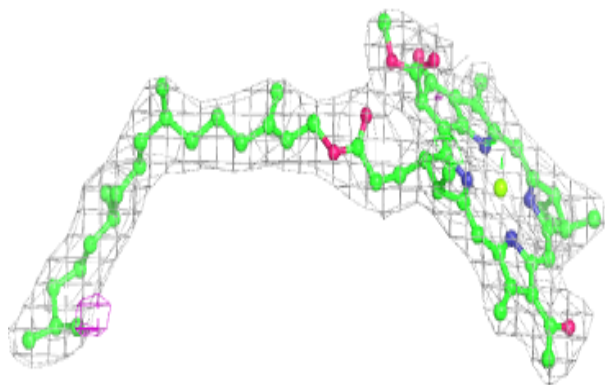


**Electron density around BPH L 1006:**

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

**Electron density around BCL R 2002:**

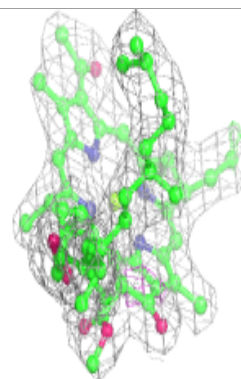
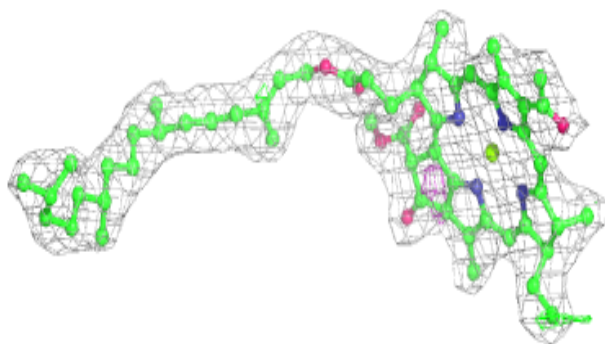
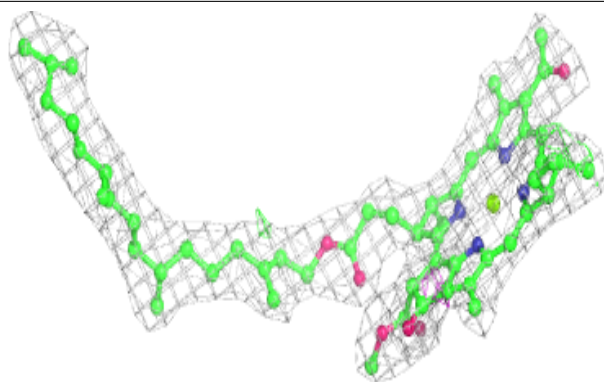
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BCL L 1002:**

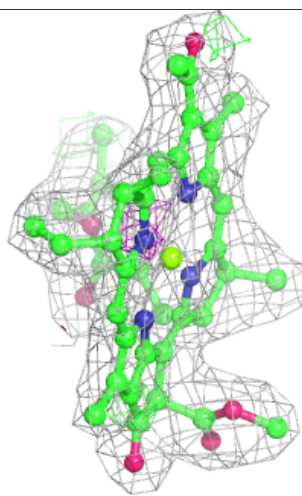
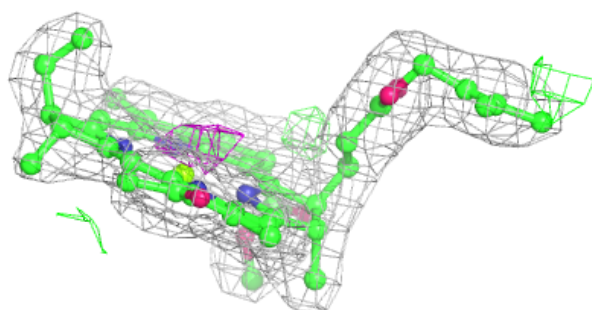
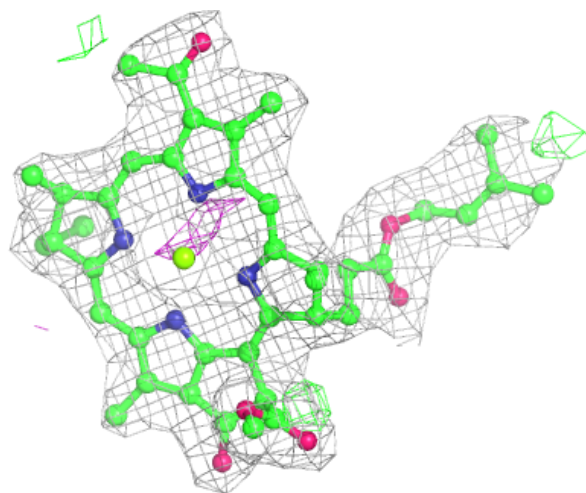
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





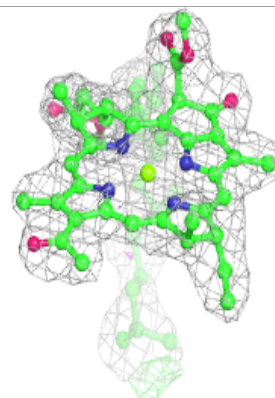
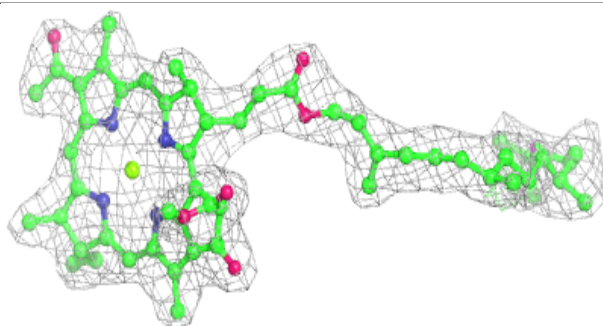
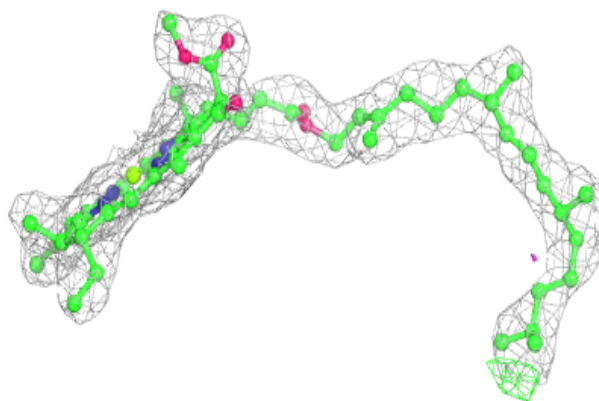
**Electron density around BCL R 2001:**

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

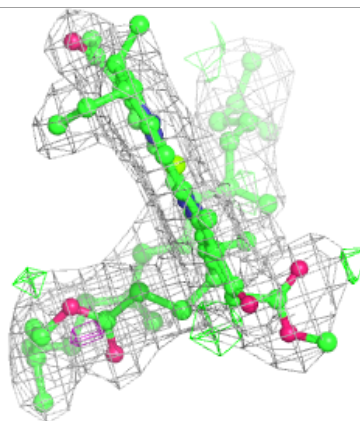
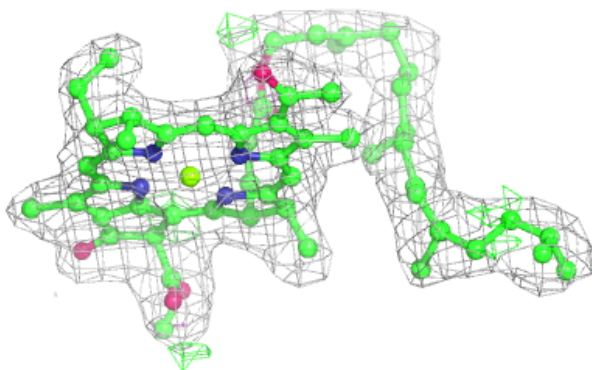
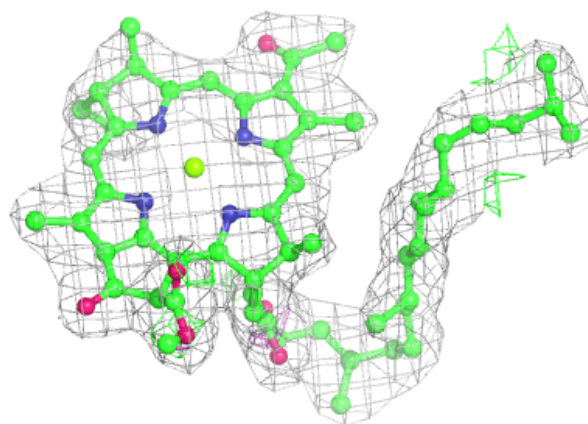


**Electron density around BCL S 2003:**

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

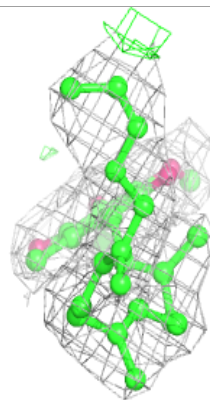
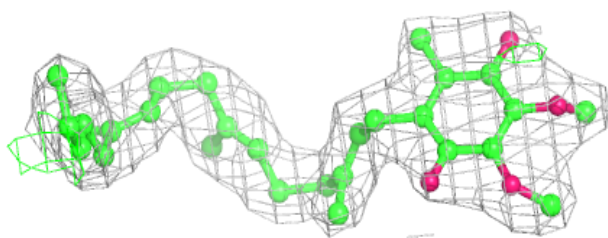
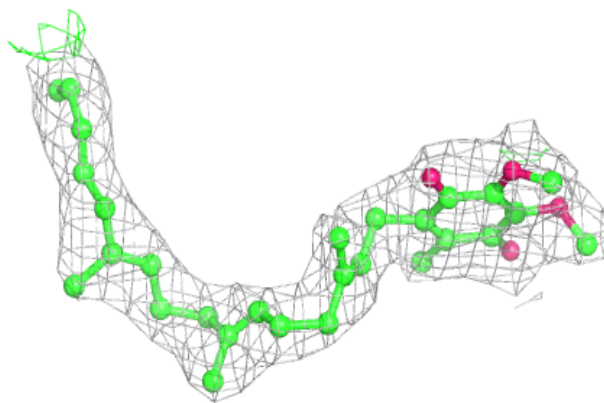
**Electron density around BCL R 2004:**

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



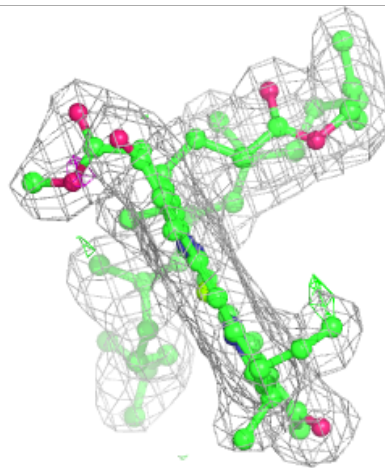
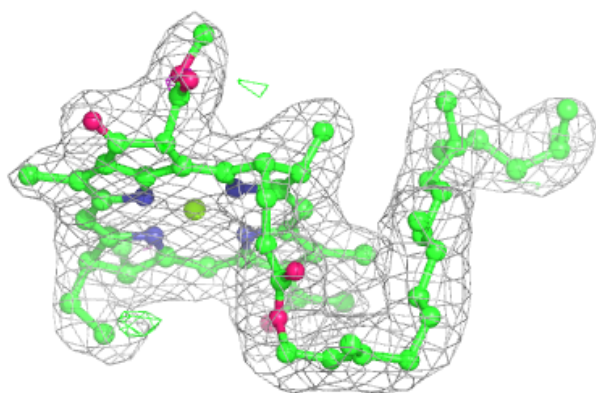
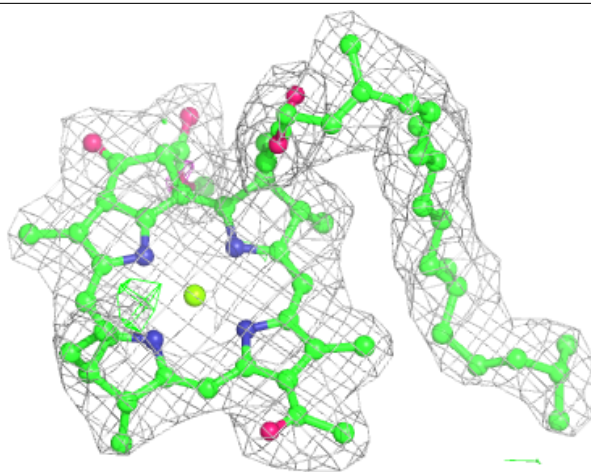
**Electron density around U10 S 2008:**

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



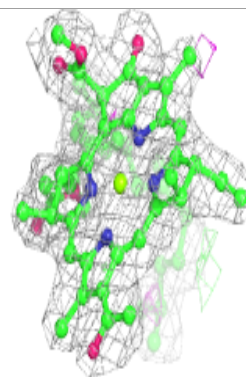
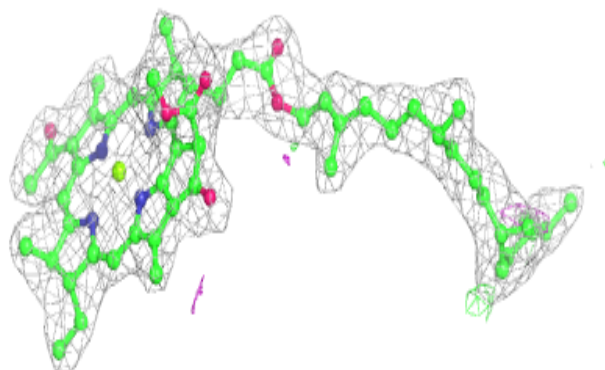
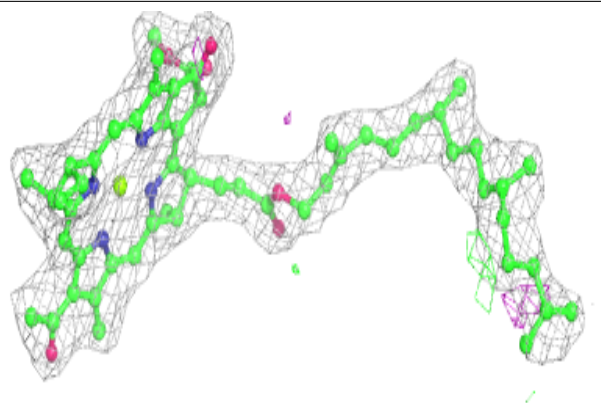
**Electron density around BCL L 1004:**

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



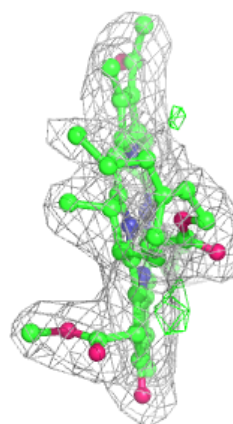
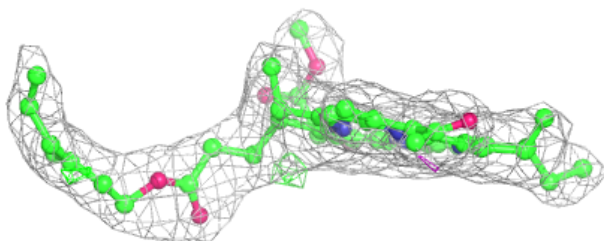
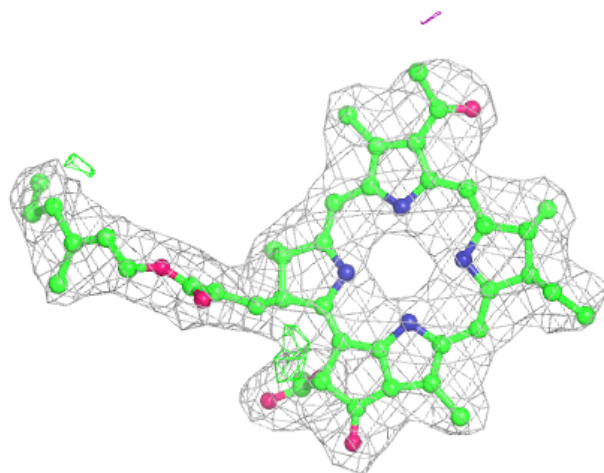
**Electron density around BCL M 1003:**

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



**Electron density around BPH S 2005:**

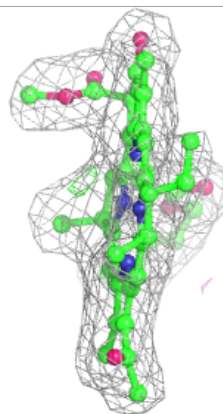
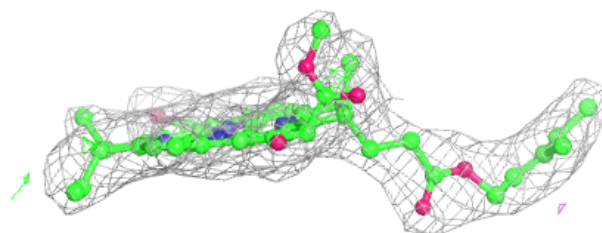
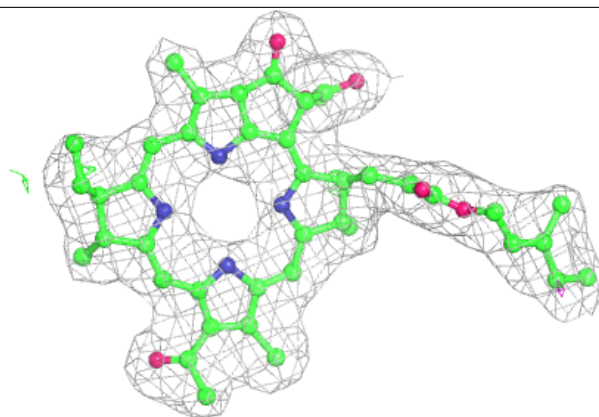
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





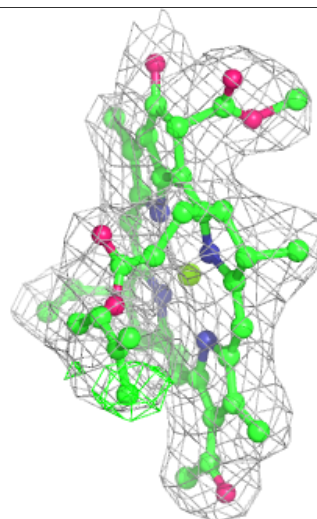
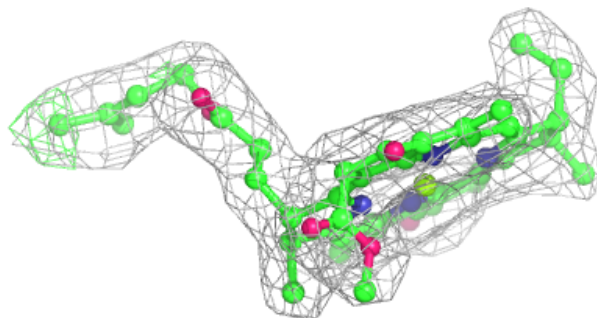
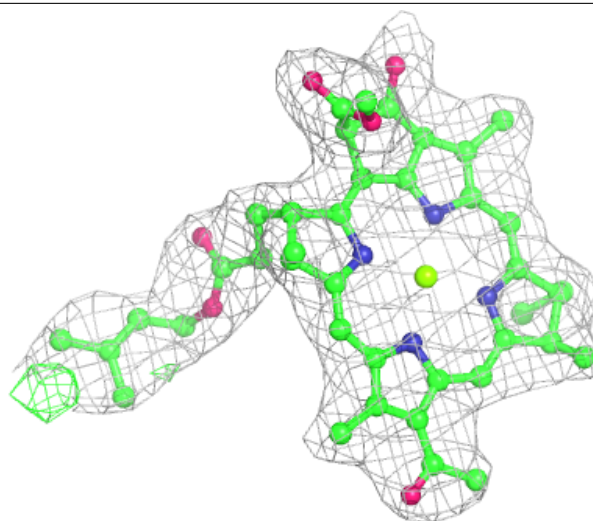
**Electron density around BPH M 1005:**

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



**Electron density around BCL L 1001:**

$2mF_o-DF_c$  (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.