



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 12:17 am BST

PDB ID : 2HG3  
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with brominated phosphatidylcholine  
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2006-06-26  
Resolution : 2.70 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

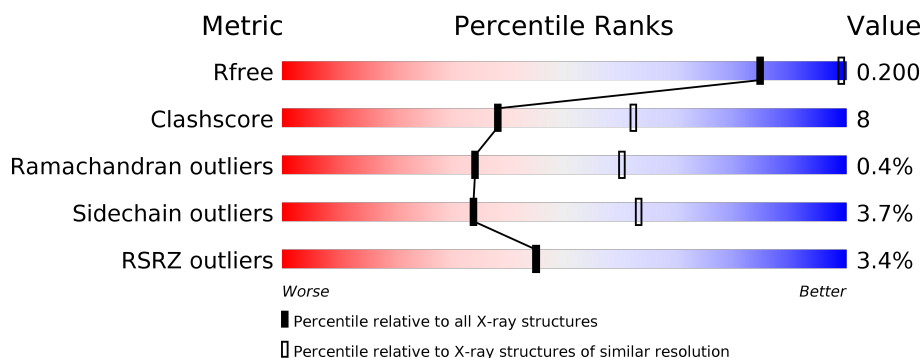
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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>3%</div> <div> <div></div> <div>91%</div> <div>9%</div> <div>.</div> </div> </div>
2	M	307	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
3	H	260	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>.</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
13	PC9	M	801	-	-	-	X
13	PC9	M	802	-	-	-	X
4	PO4	L	702	-	X	-	-
4	PO4	M	703	-	-	X	-
7	U10	L	502	-	-	-	X
9	LDA	H	901	-	-	-	X
9	LDA	H	902	-	-	-	X
9	LDA	H	903	-	-	-	X
9	LDA	H	904	-	-	-	X
9	LDA	L	905	-	-	-	X
9	LDA	L	906	-	-	-	X
9	LDA	L	908	-	-	-	X
9	LDA	L	909	-	-	-	X
9	LDA	M	920	-	-	-	X

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7921 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	4	0
			2246	1516	357	365	8			

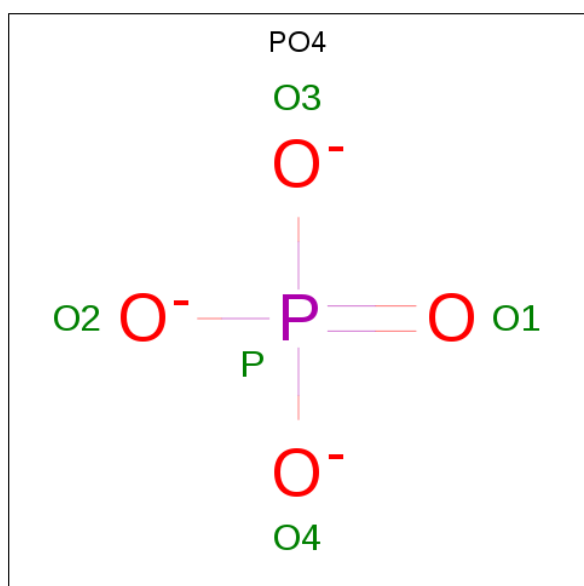
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	14	0
			2477	1654	405	407	11			

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

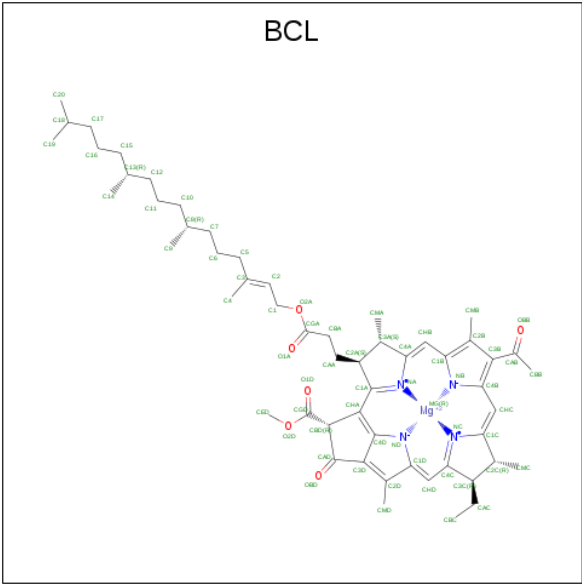
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	8	0
			1851	1181	321	338	11			

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



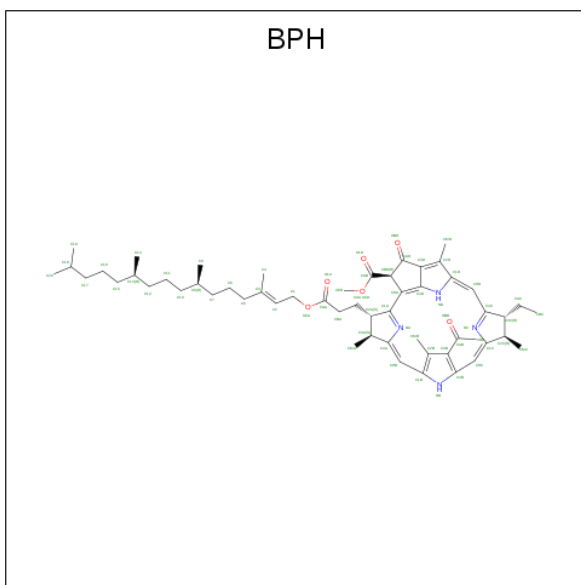
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O P 5 4 1	0	0
4	L	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



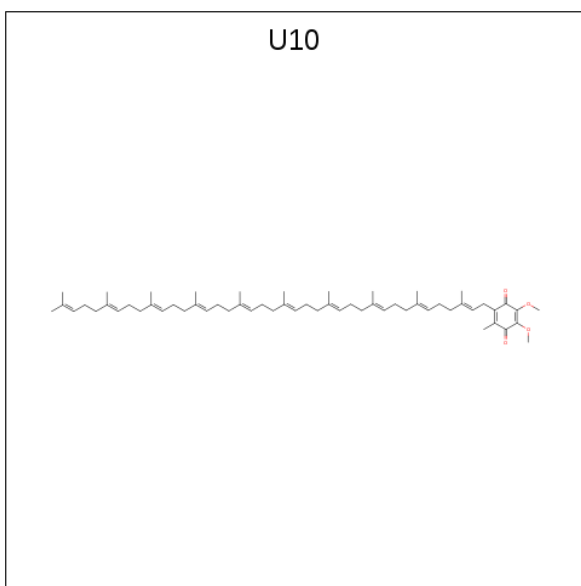
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



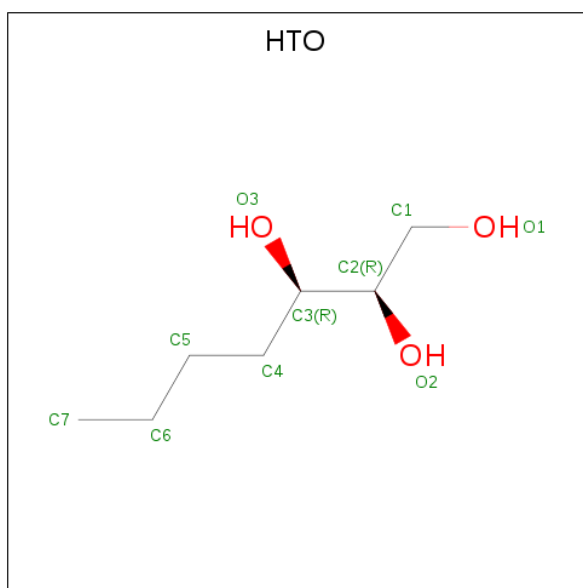
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



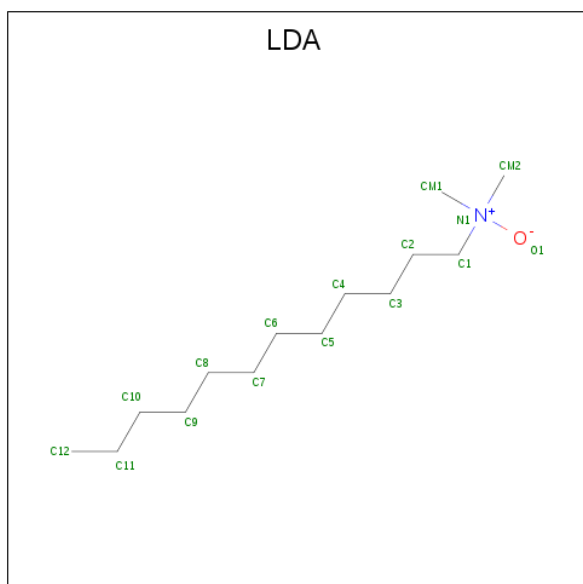
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



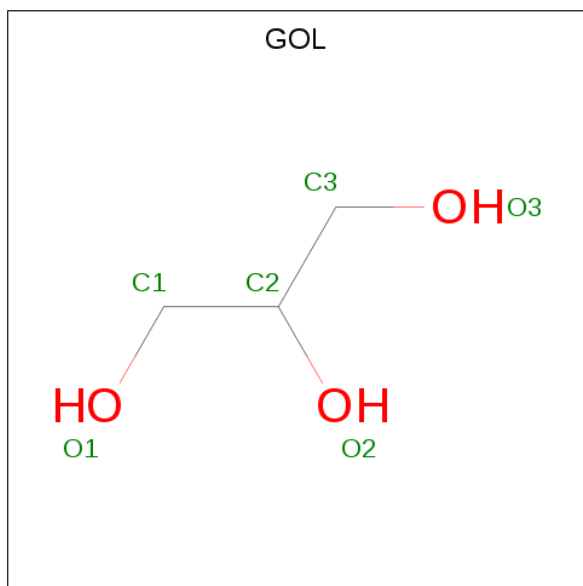
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			16	14	1	1		

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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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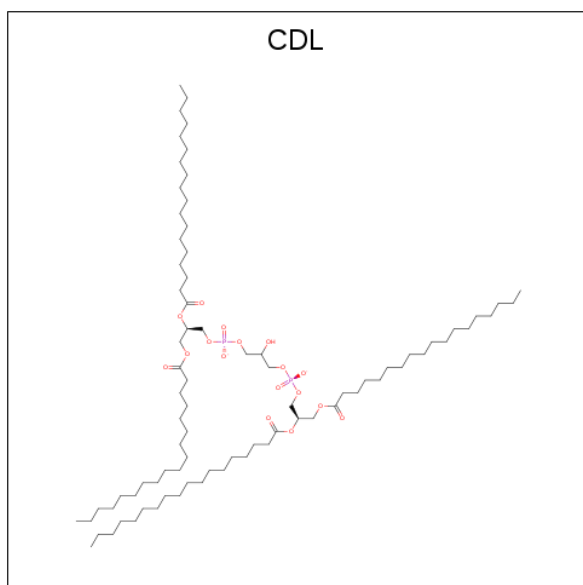
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

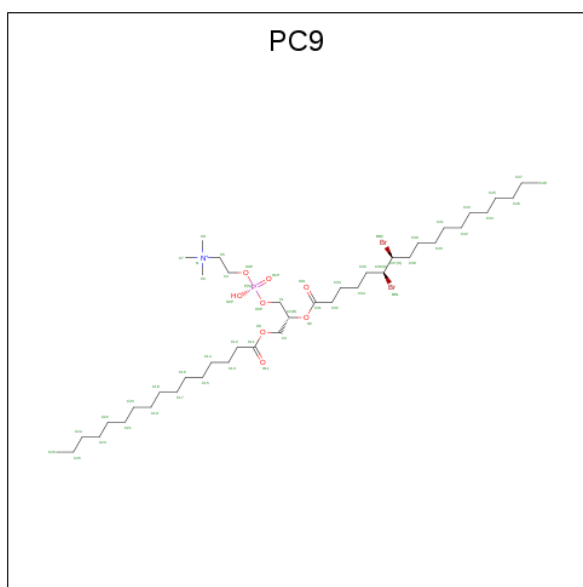
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

- Molecule 13 is (7R,14S)-14,15-DIBROMO-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC9) (formula: C<sub>42</sub>H<sub>83</sub>Br<sub>2</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	M	1	Total	Br	C	N	O	P	0	0
			54	2	42	1	8	1		
13	M	1	Total	Br	C	N	O	P	0	0
			54	2	42	1	8	1		

- Molecule 14 is POTASSIUM ION (three-letter code: K) (formula: K).

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

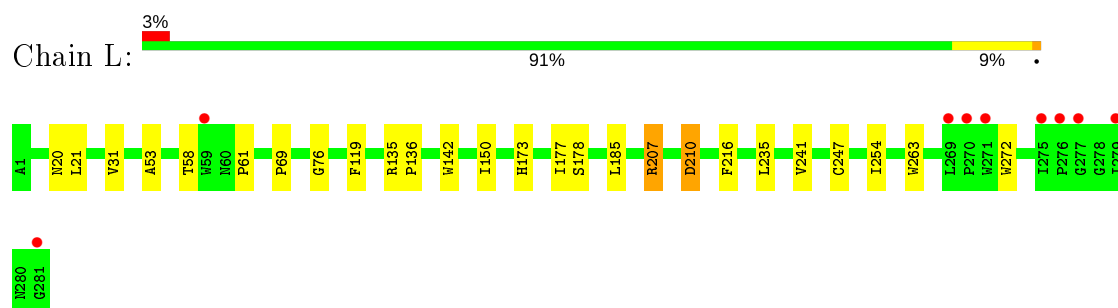
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	104	Total	O	0	0
			104	104		
15	M	141	Total	O	0	0
			141	141		
15	H	207	Total	O	0	0
			207	207		

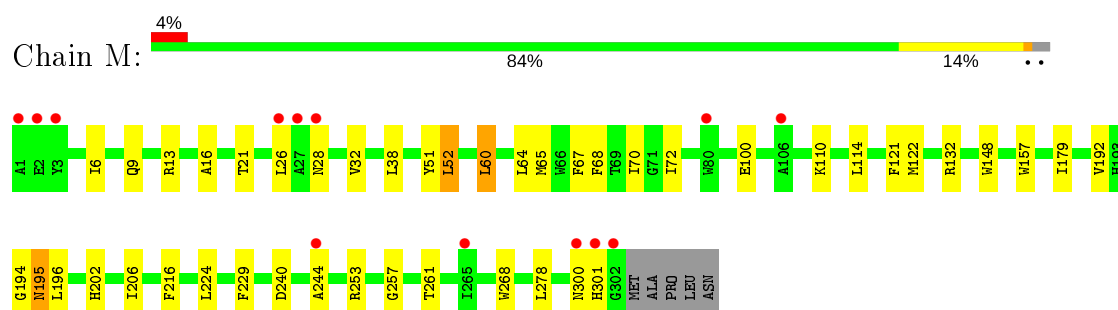
### 3 Residue-property plots [i](#)

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.

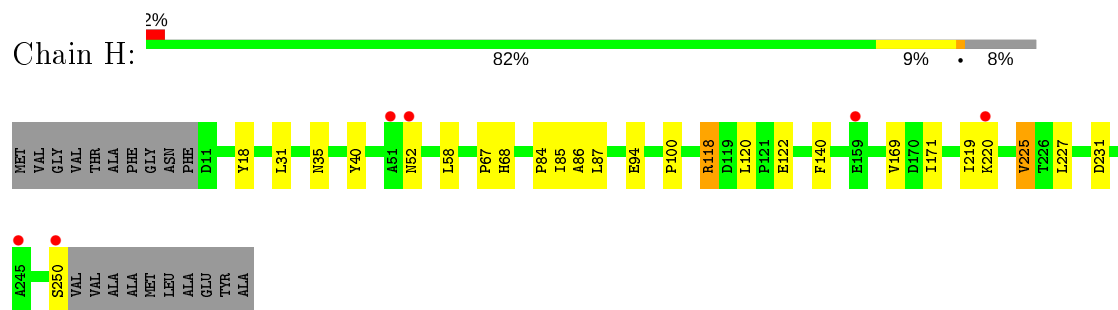
- Molecule 1: Reaction center protein L chain



- Molecule 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, $\alpha$ , $\beta$ , $\gamma$	139.84Å 139.84Å 184.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.35 – 2.70 34.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.35-2.70) 99.7 (34.35-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.164 , 0.199 0.169 , 0.200	Depositor DCC
$R_{free}$ test set	2852 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 78.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, PC9, CDL, BPH, K, HTO, FE, U10, PO4

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	0.85	0/2351	0.77	3/3217 (0.1%)
2	M	0.88	0/2628	0.79	1/3584 (0.0%)
3	H	0.96	2/1945 (0.1%)	0.83	0/2642
All	All	0.89	2/6924 (0.0%)	0.79	4/9443 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	6.36	1.61	1.51
3	H	94	GLU	CD-OE2	6.10	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASP	CB-CG-OD1	6.91	124.52	118.30
1	L	207	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	L	207	ARG	NE-CZ-NH1	-5.51	117.54	120.30
2	M	240	ASP	CB-CG-OD1	5.16	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2246	0	2207	14	0
2	M	2477	0	2389	39	0
3	H	1851	0	1866	16	0
4	L	10	0	0	0	0
4	M	10	0	0	2	0
5	L	132	0	148	5	0
5	M	132	0	148	14	0
6	L	65	0	76	3	0
6	M	65	0	76	4	0
7	L	48	0	63	8	0
7	M	48	0	63	1	0
8	L	10	0	16	0	0
9	H	64	0	124	7	0
9	L	64	0	124	10	0
9	M	32	0	62	7	0
10	H	12	0	16	0	0
10	L	12	0	16	0	0
11	M	1	0	0	0	0
12	M	81	0	106	3	0
13	M	108	0	160	23	0
14	H	1	0	0	0	0
15	H	207	0	0	0	0
15	L	104	0	0	0	0
15	M	141	0	0	5	0
All	All	7921	0	7660	116	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 116 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)
13:M:801:PC9:H261	9:H:903:LDA:H121	1.33	1.05
2:M:257:GLY:O	13:M:801:PC9:H32	1.64	0.98
5:M:311:BCL:H41	13:M:802:PC9:H441	1.45	0.97
3:H:118[B]:ARG:HD3	3:H:120:LEU:HD12	1.65	0.79
3:H:84:PRO:O	3:H:85:ILE:HD13	1.85	0.76

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	283/281 (101%)	272 (96%)	10 (4%)	1 (0%)	34	60
2	M	314/307 (102%)	298 (95%)	15 (5%)	1 (0%)	41	66
3	H	246/260 (95%)	240 (98%)	5 (2%)	1 (0%)	34	60
All	All	843/848 (99%)	810 (96%)	30 (4%)	3 (0%)	34	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN
3	H	86	ALA
1	L	31	VAL

### 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	224/220 (102%)	215 (96%)	9 (4%)	31	60
2	M	250/240 (104%)	239 (96%)	11 (4%)	28	56
3	H	203/208 (98%)	197 (97%)	6 (3%)	41	70
All	All	677/668 (101%)	651 (96%)	26 (4%)	34	62

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	60[A]	LEU
2	M	114	LEU
3	H	231	ASP
2	M	60[B]	LEU
2	M	100	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	274	ASN
2	M	28	ASN
3	H	68	HIS

### 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 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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	BCL	L	314	1	58,74,74	0.87	1 (1%)	69,115,115	1.67	16 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BCL	M	311	2	58,74,74	1.36	3 (5%)	69,115,115	1.83	21 (30%)
9	LDA	H	902	-	12,15,15	1.98	1 (8%)	14,17,17	0.55	0
4	PO4	M	703	-	4,4,4	0.82	0	6,6,6	0.45	0
9	LDA	L	909	-	12,15,15	2.03	1 (8%)	14,17,17	0.60	0
5	BCL	M	313	2	58,74,74	1.48	4 (6%)	69,115,115	1.71	15 (21%)
12	CDL	M	800	-	80,80,99	1.30	4 (5%)	86,92,111	1.40	10 (11%)
7	U10	M	501	-	48,48,63	1.08	2 (4%)	58,61,79	1.78	14 (24%)
9	LDA	H	904	-	12,15,15	2.04	1 (8%)	14,17,17	0.49	0
10	GOL	H	709	-	5,5,5	0.54	0	5,5,5	0.22	0
13	PC9	M	802	-	53,53,53	1.03	4 (7%)	59,63,63	1.44	6 (10%)
9	LDA	L	906	-	12,15,15	1.70	1 (8%)	14,17,17	0.49	0
5	BCL	L	312	1	58,74,74	1.30	5 (8%)	69,115,115	1.22	6 (8%)
9	LDA	H	901	-	12,15,15	1.99	1 (8%)	14,17,17	0.56	0
4	PO4	M	704	-	4,4,4	1.91	1 (25%)	6,6,6	1.16	0
6	BPH	M	401	-	64,70,70	1.04	4 (6%)	76,101,101	1.83	18 (23%)
4	PO4	L	701	-	4,4,4	0.94	0	6,6,6	0.68	0
10	GOL	L	708	-	5,5,5	0.54	0	5,5,5	0.32	0
9	LDA	L	905	-	12,15,15	1.98	1 (8%)	14,17,17	0.41	0
10	GOL	H	706	-	5,5,5	0.29	0	5,5,5	0.94	0
9	LDA	H	903	-	12,15,15	2.02	1 (8%)	14,17,17	0.53	0
6	BPH	L	402	-	64,70,70	0.81	1 (1%)	76,101,101	1.38	10 (13%)
10	GOL	L	707	-	5,5,5	0.70	0	5,5,5	1.00	0
7	U10	L	502	-	48,48,63	1.33	7 (14%)	58,61,79	1.83	16 (27%)
9	LDA	M	907	-	12,15,15	1.92	1 (8%)	14,17,17	0.76	1 (7%)
13	PC9	M	801	-	53,53,53	1.12	6 (11%)	59,63,63	1.52	9 (15%)
9	LDA	M	920	-	12,15,15	1.76	1 (8%)	14,17,17	0.89	1 (7%)
9	LDA	L	908	-	12,15,15	1.92	1 (8%)	14,17,17	0.56	0
8	HTO	L	705	-	9,9,9	0.63	0	10,10,10	0.71	0
4	PO4	L	702	-	4,4,4	4.04	3 (75%)	6,6,6	1.25	1 (16%)

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	BCL	M	311	2	-	9/37/137/137	-

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LDA	H	902	-	-	6/13/13/13	-
9	LDA	L	909	-	-	9/13/13/13	-
5	BCL	M	313	2	-	5/37/137/137	-
12	CDL	M	800	-	-	40/91/91/110	-
7	U10	M	501	-	-	6/45/69/87	0/1/1/1
9	LDA	H	904	-	-	4/13/13/13	-
10	GOL	H	709	-	-	4/4/4/4	-
13	PC9	M	802	-	-	34/60/60/60	-
9	LDA	L	906	-	-	10/13/13/13	-
5	BCL	L	312	1	-	6/37/137/137	-
9	LDA	H	901	-	-	4/13/13/13	-
5	BCL	L	314	1	-	5/37/137/137	-
6	BPH	M	401	-	-	18/54/105/105	0/5/6/6
10	GOL	L	708	-	-	4/4/4/4	-
9	LDA	L	905	-	-	7/13/13/13	-
10	GOL	H	706	-	-	2/4/4/4	-
9	LDA	H	903	-	-	8/13/13/13	-
6	BPH	L	402	-	-	10/54/105/105	0/5/6/6
10	GOL	L	707	-	-	4/4/4/4	-
7	U10	L	502	-	-	9/45/69/87	0/1/1/1
9	LDA	M	907	-	-	7/13/13/13	-
13	PC9	M	801	-	-	29/60/60/60	-
9	LDA	M	920	-	-	5/13/13/13	-
9	LDA	L	908	-	-	6/13/13/13	-
8	HTO	L	705	-	-	0/10/10/10	-

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	313	BCL	MG-NA	8.01	2.25	2.06
4	L	702	PO4	P-O1	7.05	1.67	1.50
9	H	904	LDA	O1-N1	-6.97	1.25	1.42
9	H	903	LDA	O1-N1	-6.92	1.26	1.42
9	H	901	LDA	O1-N1	-6.78	1.26	1.42

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	313	BCL	C4D-C3D-CAD	-6.27	104.97	108.47
7	L	502	U10	C25-C24-C26	6.06	125.46	115.27
13	M	802	PC9	O2-C31-C32	5.97	124.38	111.50
12	M	800	CDL	OB6-CB5-C51	5.93	124.28	111.50
6	M	401	BPH	C4D-C3D-CAD	-5.53	104.37	107.87

There are no chirality outliers.

5 of 251 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	H	902	LDA	C2-C1-N1-CM2
9	L	909	LDA	N1-C1-C2-C3
12	M	800	CDL	CA2-OA2-PA1-OA3
12	M	800	CDL	CA2-OA2-PA1-OA4
12	M	800	CDL	OB6-CB4-CB6-OB8

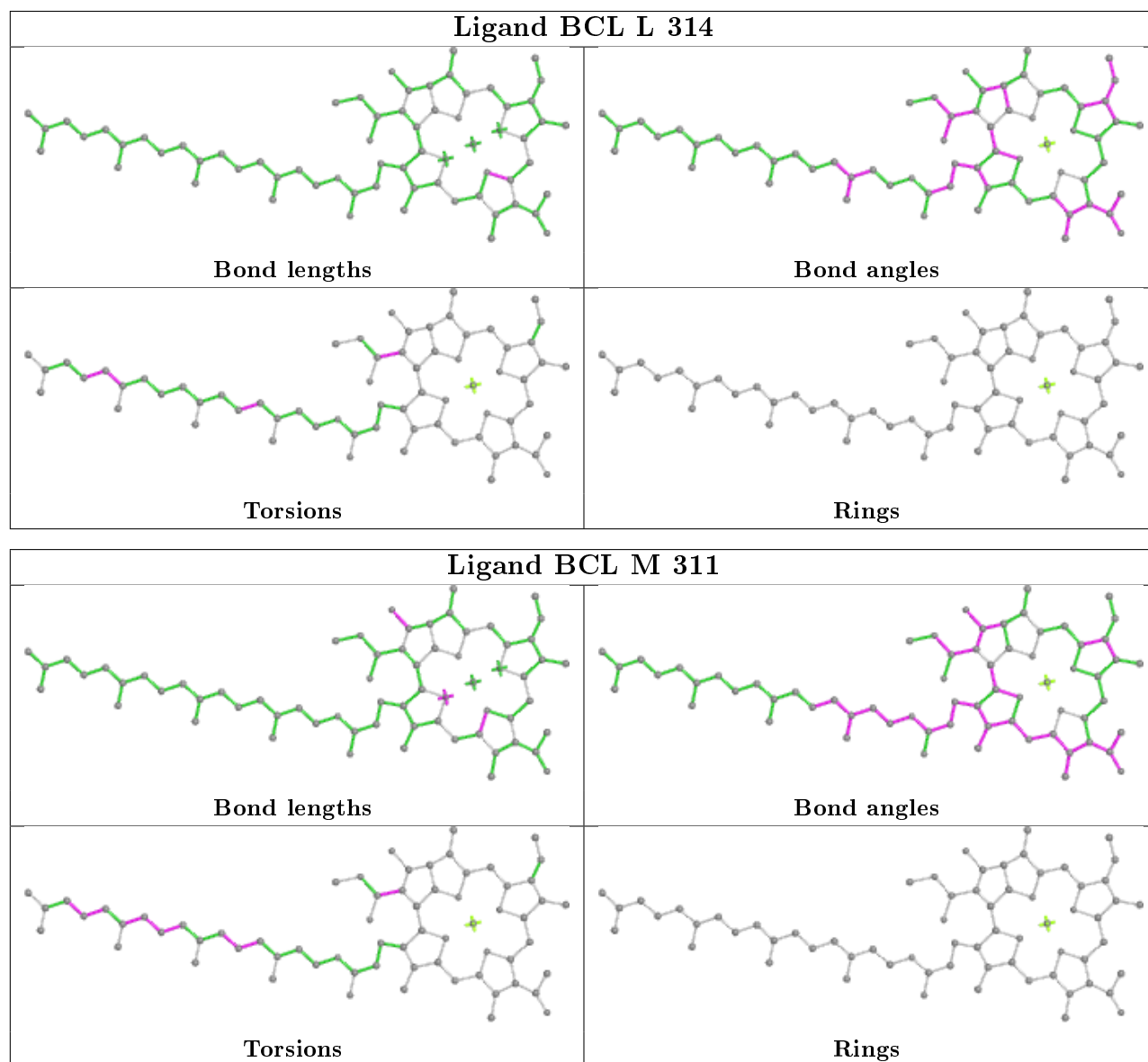
There are no ring outliers.

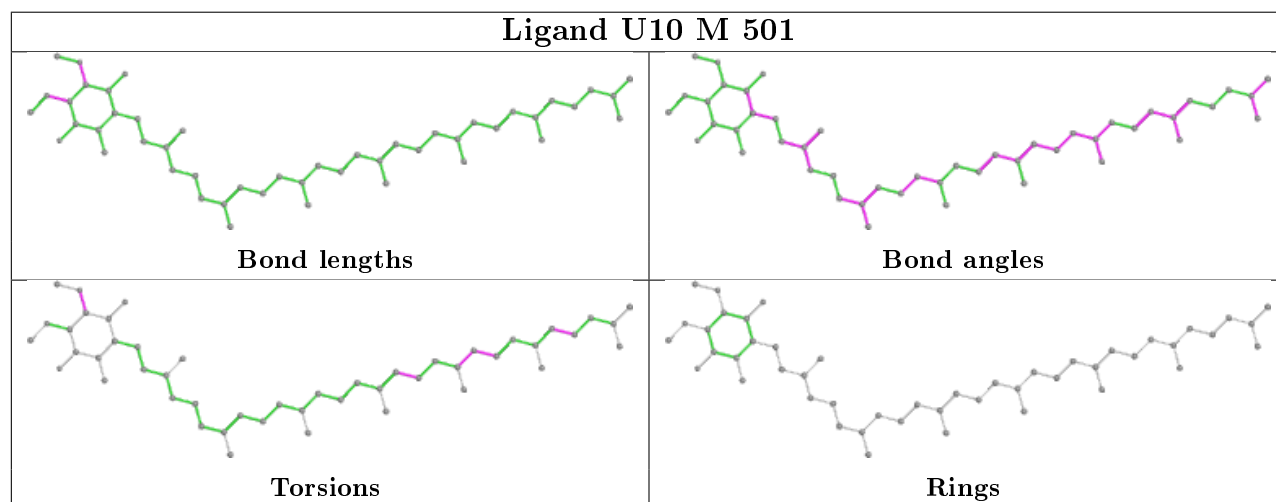
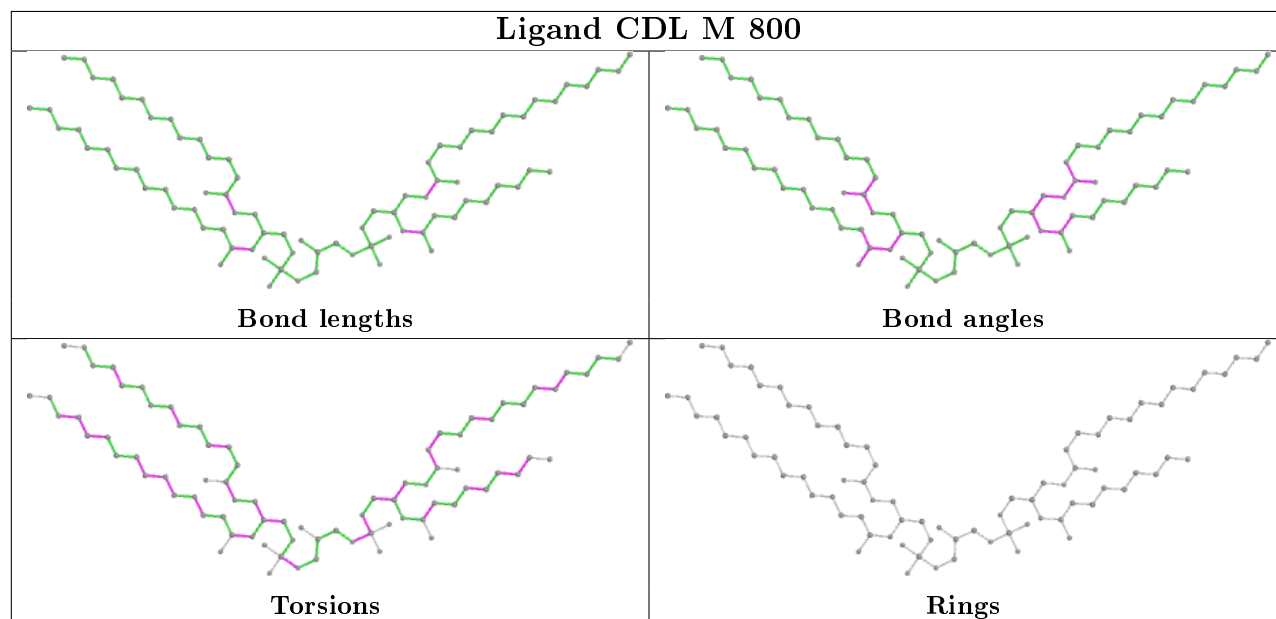
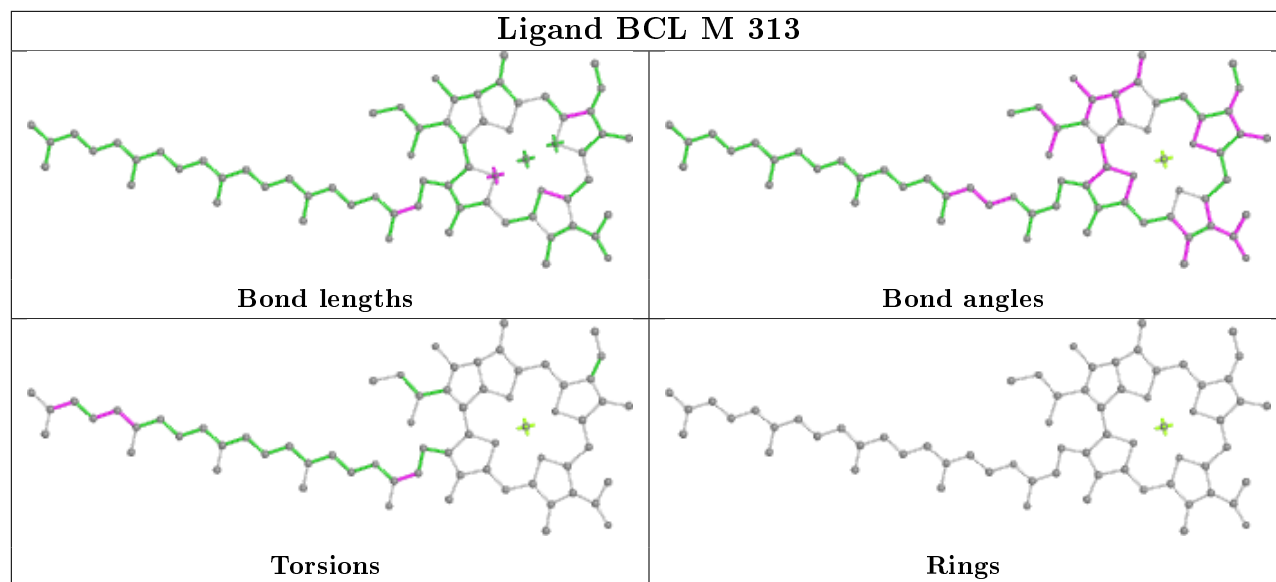
19 monomers are involved in 75 short contacts:

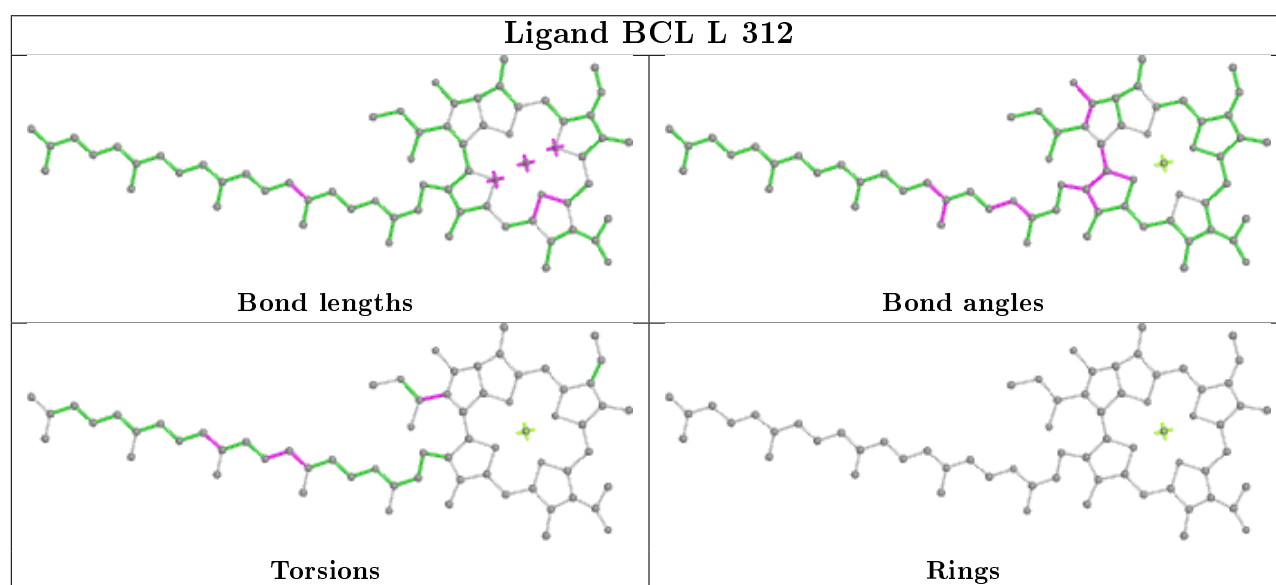
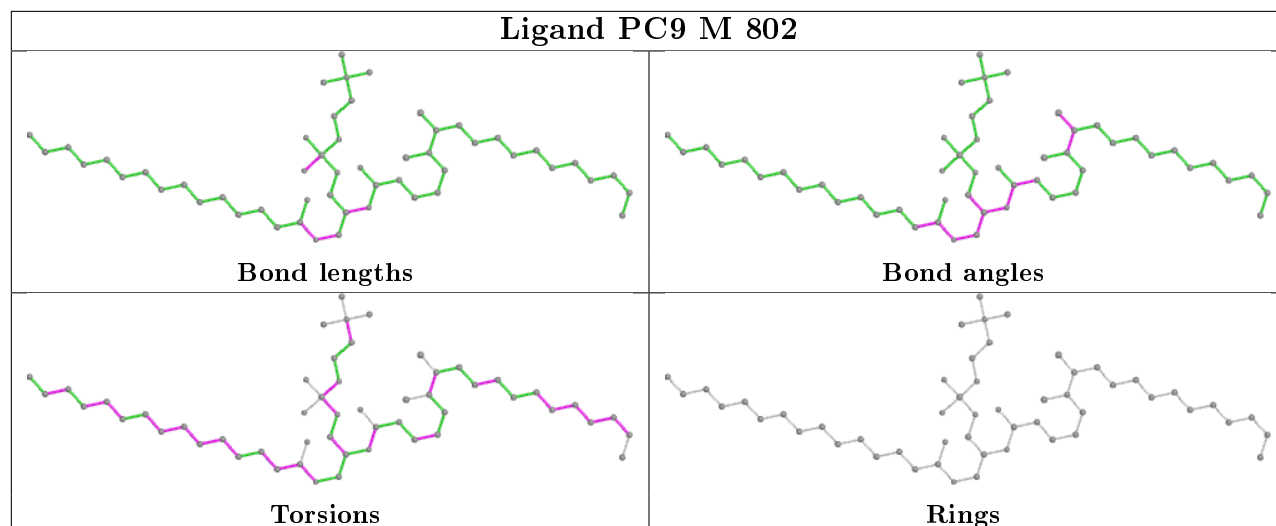
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	314	BCL	3	0
5	M	311	BCL	10	0
9	H	902	LDA	1	0
4	M	703	PO4	2	0
9	L	909	LDA	2	0
5	M	313	BCL	5	0
12	M	800	CDL	3	0
7	M	501	U10	1	0
9	H	904	LDA	2	0
13	M	802	PC9	9	0
9	L	906	LDA	4	0
5	L	312	BCL	3	0
6	M	401	BPH	4	0
9	H	903	LDA	6	0
6	L	402	BPH	3	0
7	L	502	U10	8	0
13	M	801	PC9	14	0
9	M	920	LDA	7	0
9	L	908	LDA	6	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

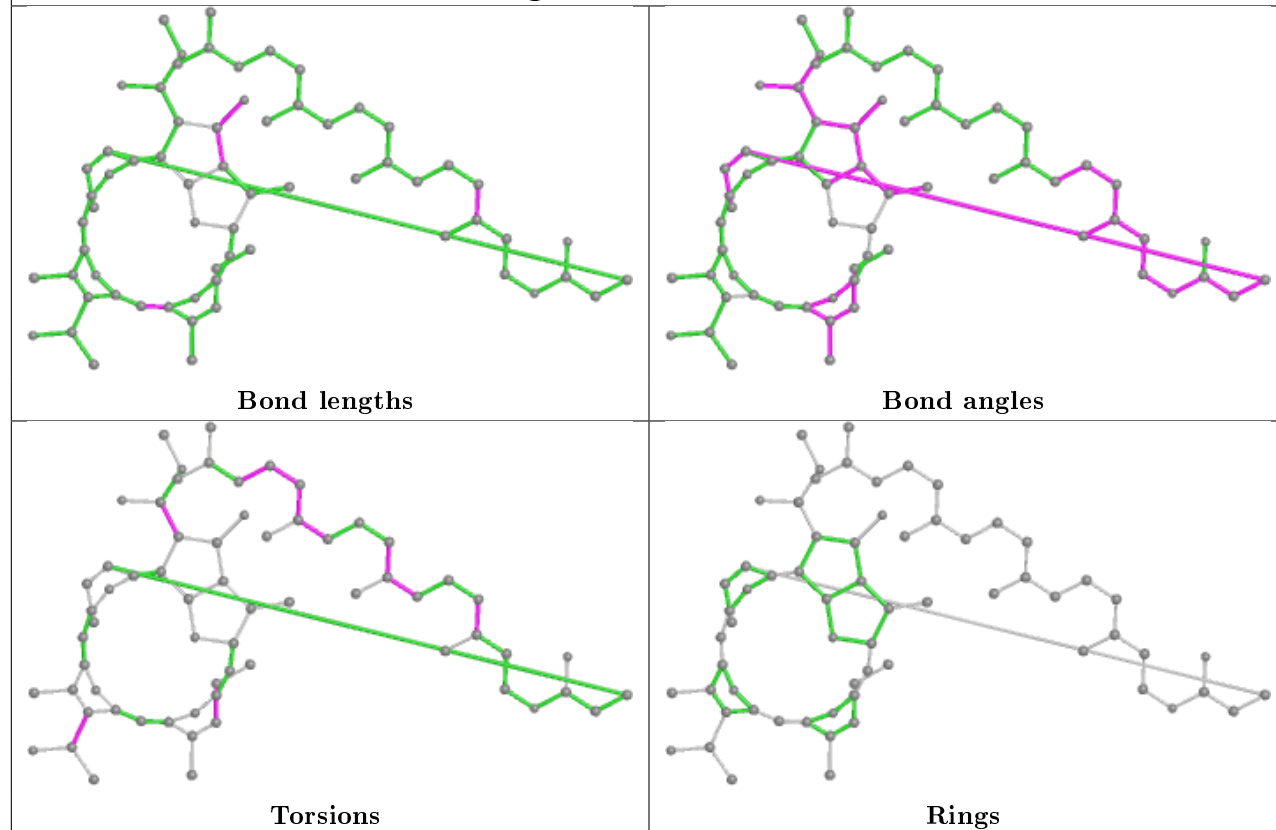
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



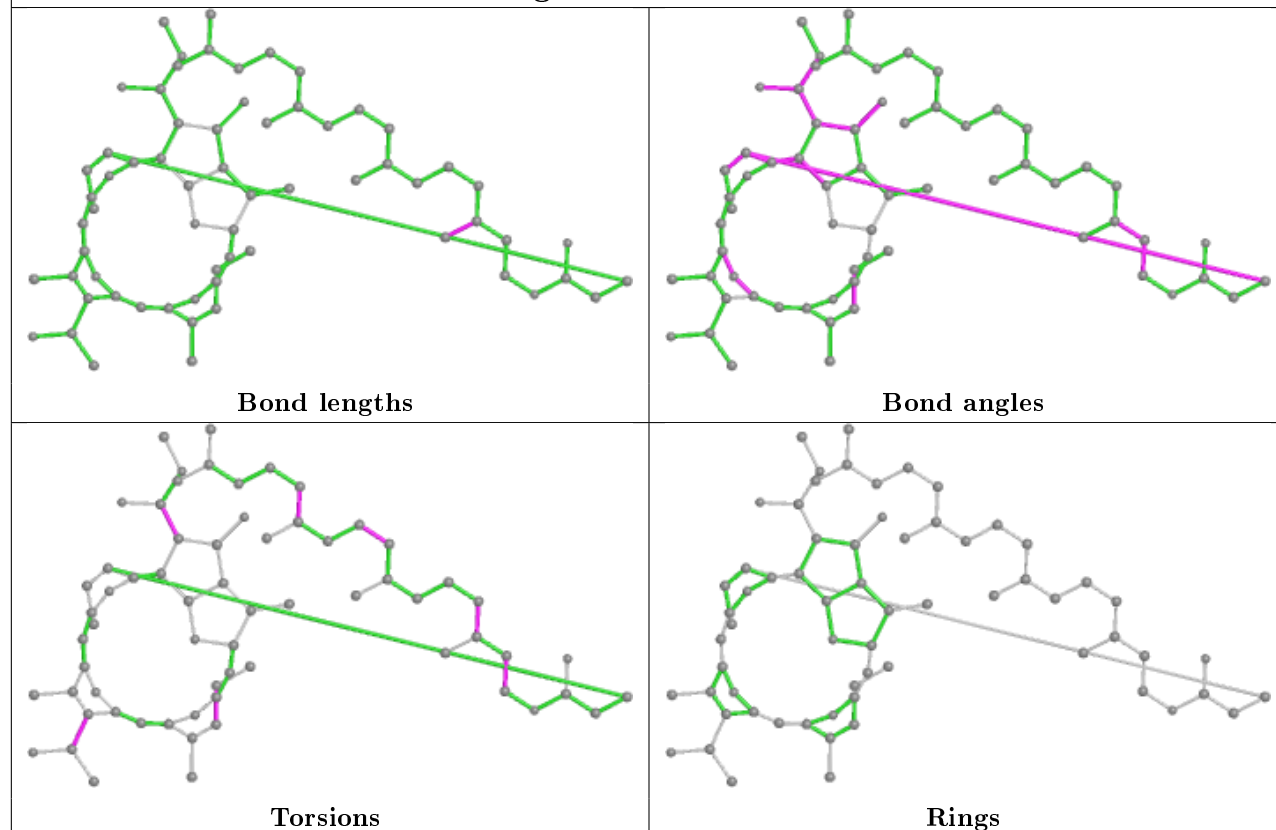


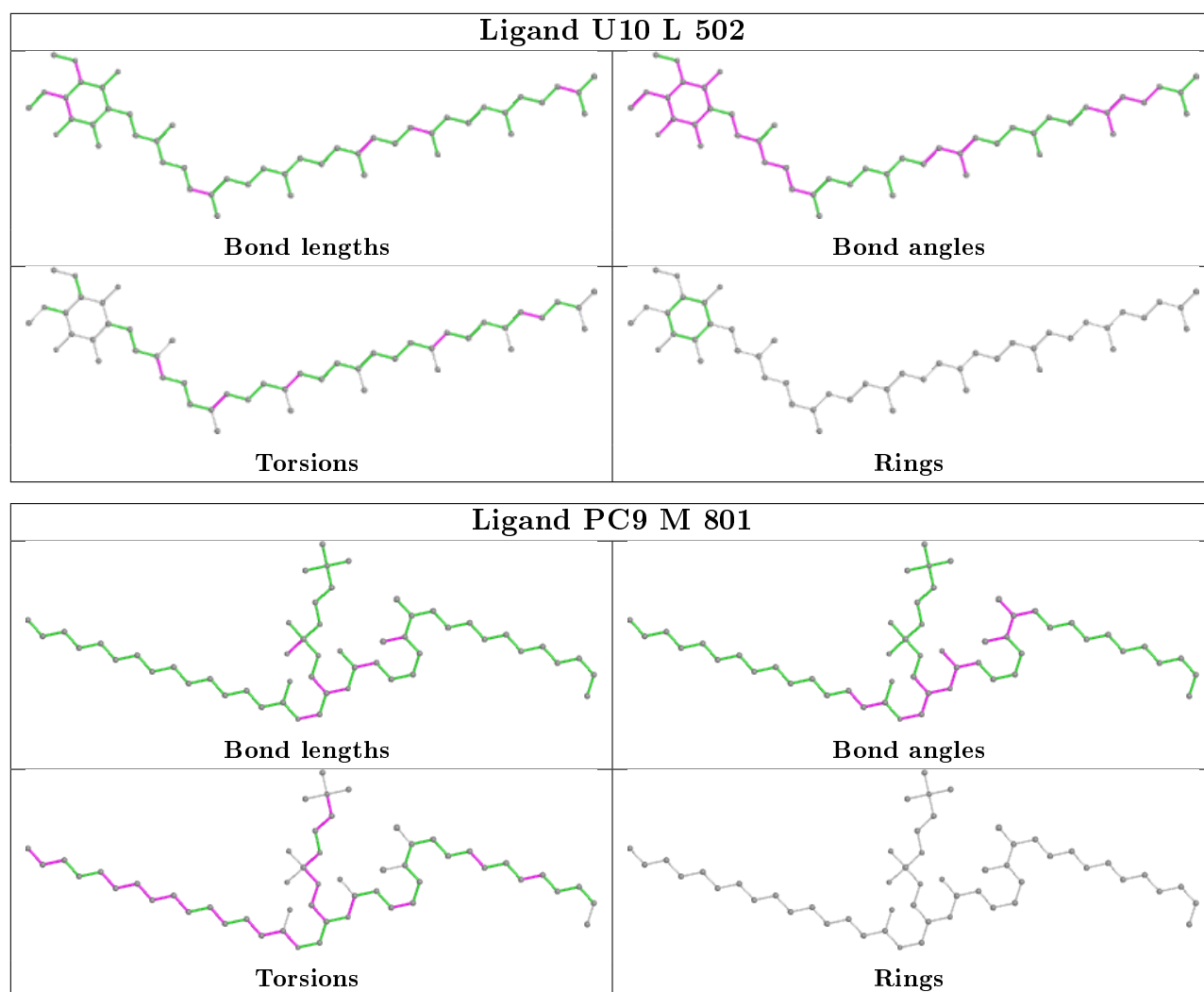


## Ligand BPH M 401



## Ligand BPH L 402





## 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%)	-0.45	9 (3%) 47 48	42, 51, 63, 72	0
2	M	302/307 (98%)	-0.15	13 (4%) 35 33	40, 51, 61, 88	1 (0%)
3	H	240/260 (92%)	-0.29	6 (2%) 57 59	39, 51, 59, 83	0
All	All	823/848 (97%)	-0.30	28 (3%) 45 45	39, 51, 62, 88	1 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	4.7
1	L	271	TRP	4.2
2	M	1	ALA	3.8
1	L	270	PRO	3.6
1	L	269	LEU	3.1

### 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 [i](#)

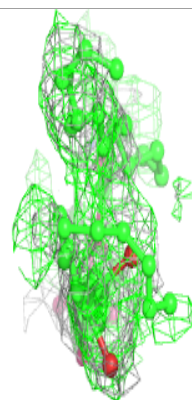
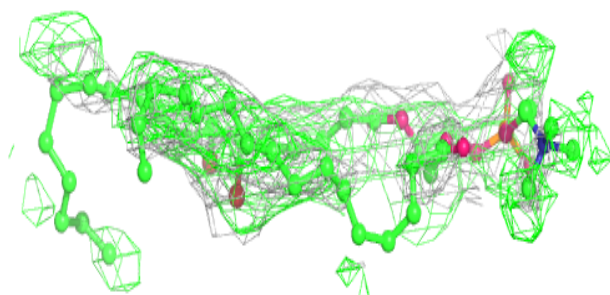
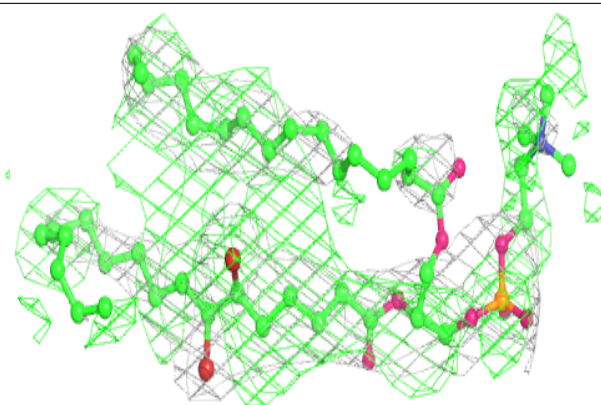
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
9	LDA	L	905	16/16	0.26	1.20	61,66,70,71	16
9	LDA	L	909	16/16	0.50	0.45	50,54,71,73	16
9	LDA	H	903	16/16	0.54	0.47	49,55,63,63	16
9	LDA	H	902	16/16	0.56	0.59	64,66,72,72	16
9	LDA	H	901	16/16	0.57	0.49	52,55,66,66	16
13	PC9	M	802	54/54	0.66	0.52	42,54,70,73	54
9	LDA	M	920	16/16	0.66	0.70	49,53,65,66	16
13	PC9	M	801	54/54	0.71	0.48	30,52,79,80	54
10	GOL	H	709	6/6	0.71	0.23	50,51,52,53	6
9	LDA	L	906	16/16	0.72	0.45	51,55,69,70	16
7	U10	L	502	48/63	0.73	0.45	37,56,66,67	48
12	CDL	M	800	81/100	0.74	0.37	50,69,80,87	81
4	PO4	M	703	5/5	0.75	0.38	64,65,66,67	5
9	LDA	L	908	16/16	0.75	0.44	51,59,72,73	16
9	LDA	H	904	16/16	0.80	0.44	60,62,66,66	16
9	LDA	M	907	16/16	0.81	0.30	60,64,70,71	16
10	GOL	L	707	6/6	0.85	0.28	58,61,62,66	6
4	PO4	L	701	5/5	0.88	0.32	65,65,66,67	5
8	HTO	L	705	10/10	0.88	0.41	56,60,62,65	10
6	BPH	M	401	65/65	0.90	0.20	44,52,96,97	0
7	U10	M	501	48/63	0.91	0.22	46,54,80,83	0
4	PO4	L	702	5/5	0.93	0.16	64,65,66,68	5
10	GOL	H	706	6/6	0.95	0.45	59,62,63,65	6
10	GOL	L	708	6/6	0.95	0.27	49,57,59,60	0
5	BCL	M	311	66/66	0.96	0.21	41,51,103,104	0
4	PO4	M	704	5/5	0.96	0.19	54,54,56,58	5
6	BPH	L	402	65/65	0.97	0.12	42,49,55,56	0
5	BCL	M	313	66/66	0.97	0.14	41,48,72,80	0
5	BCL	L	312	66/66	0.97	0.12	40,48,55,59	0
14	K	H	700	1/1	0.98	0.13	52,52,52,52	0
5	BCL	L	314	66/66	0.98	0.11	38,46,66,73	0
11	FE	M	500	1/1	1.00	0.14	52,52,52,52	0

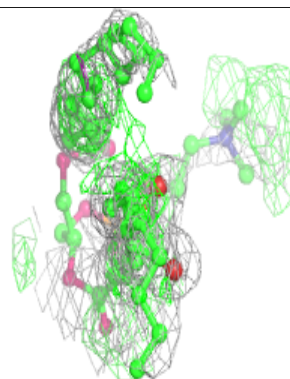
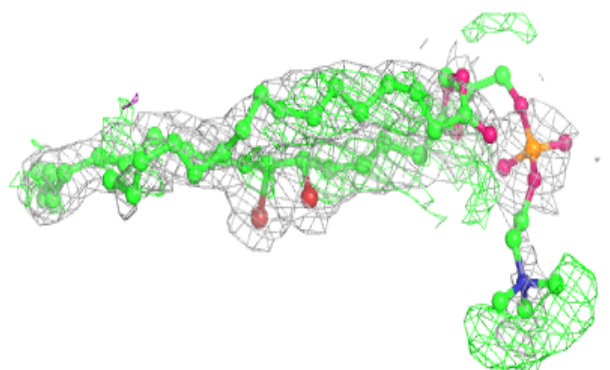
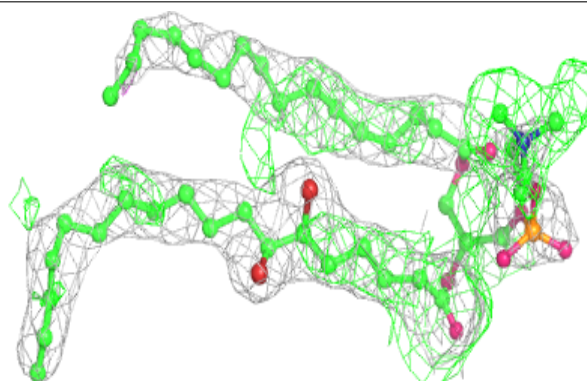
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PC9 M 802:**

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

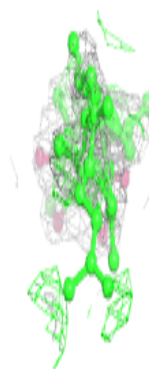
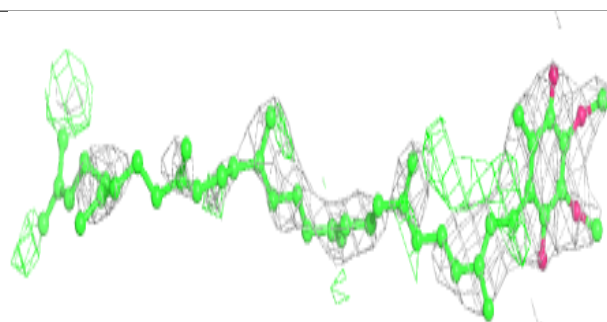
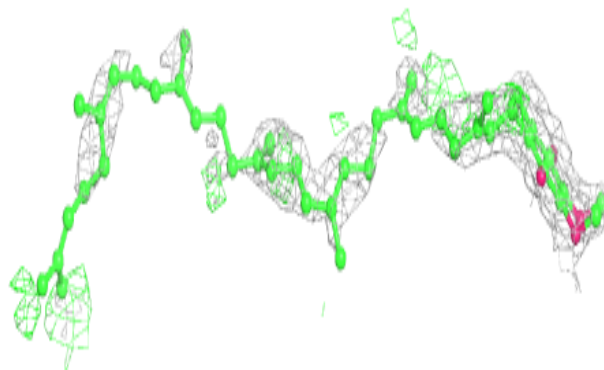
**Electron density around PC9 M 801:**

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



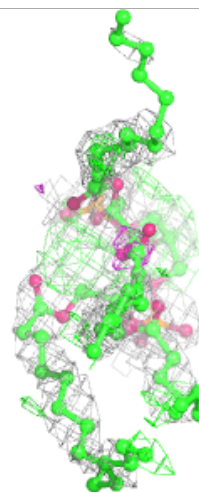
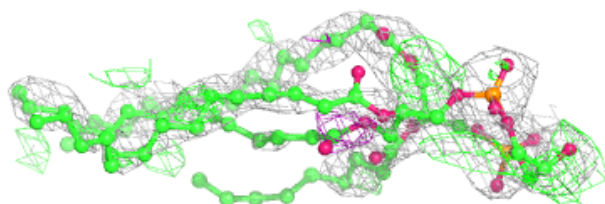
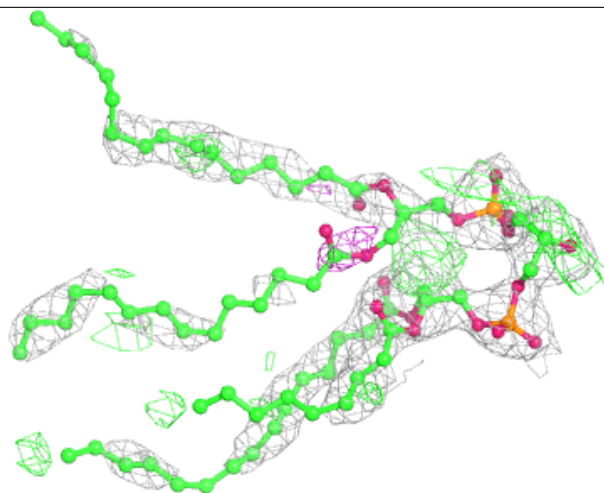
**Electron density around U10 L 502:**

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



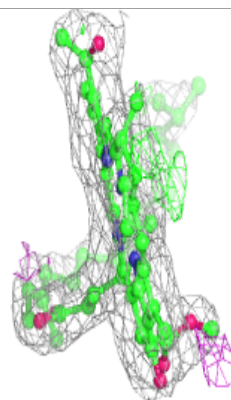
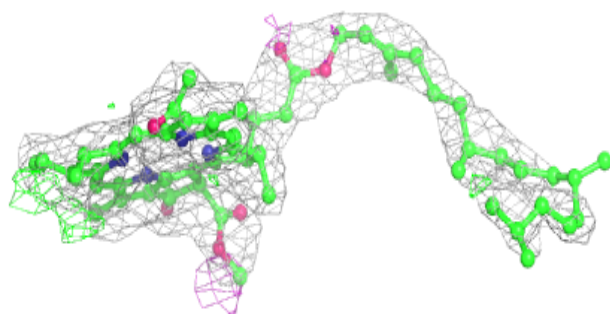
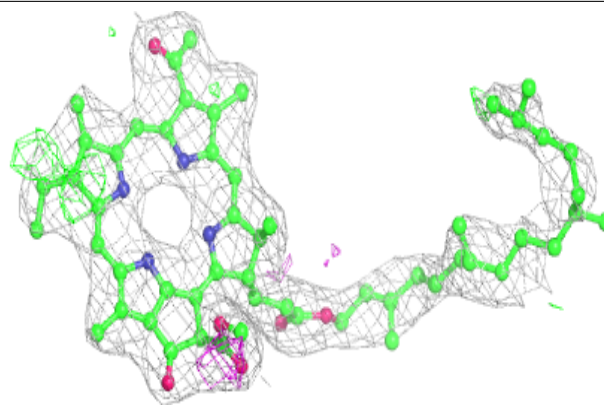
**Electron density around CDL M 800:**

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

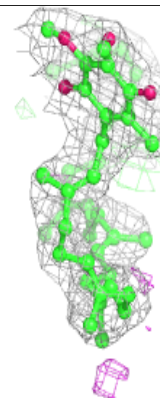
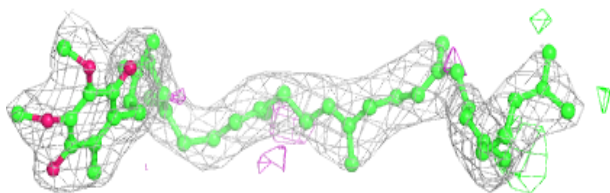
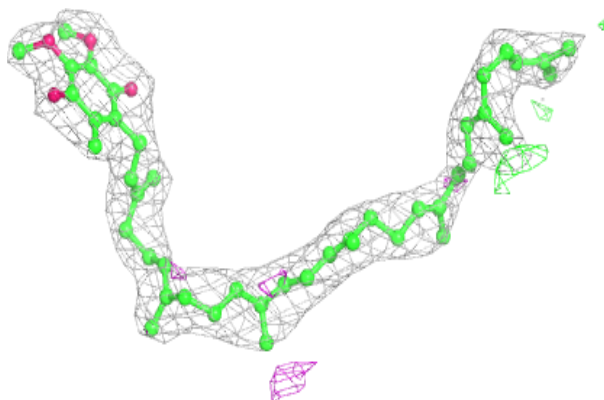


**Electron density around BPH M 401:**

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and green (positive)

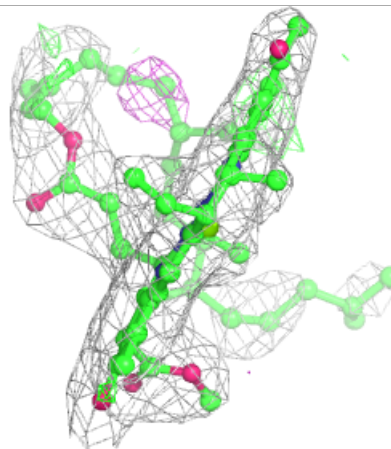
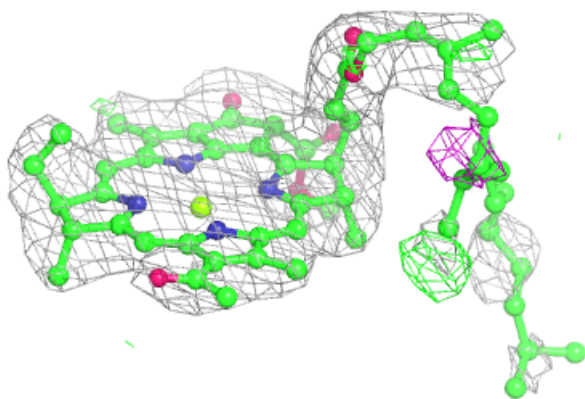
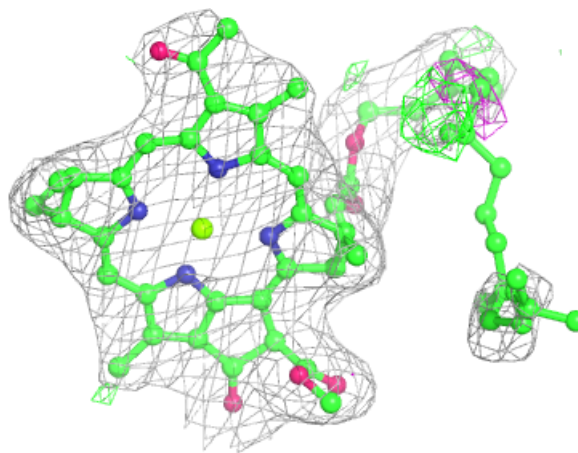
**Electron density around U10 M 501:**

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



**Electron density around BCL M 311:**

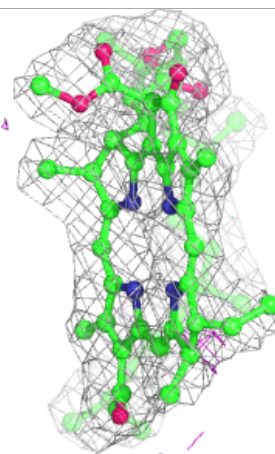
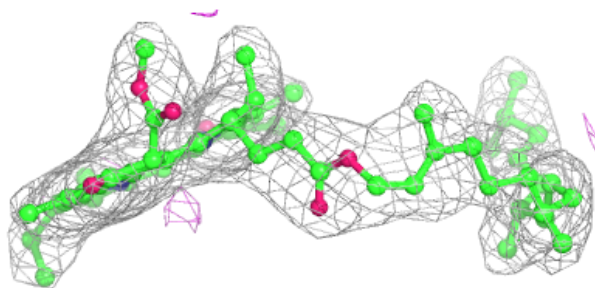
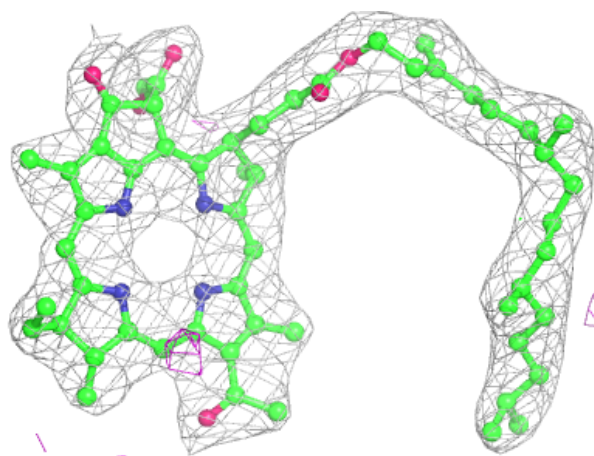
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BPH L 402:**

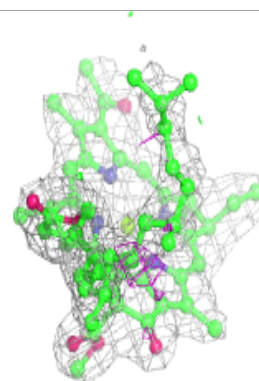
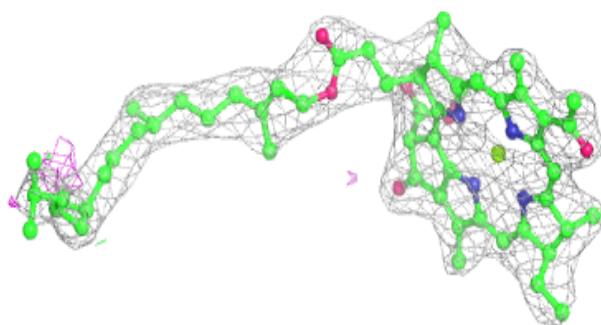
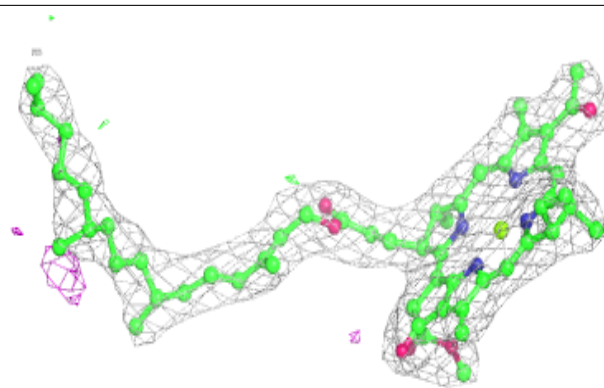
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



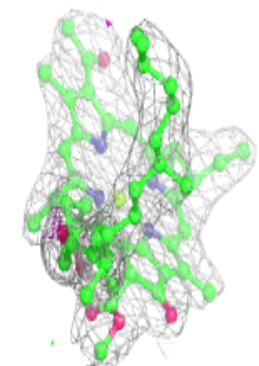
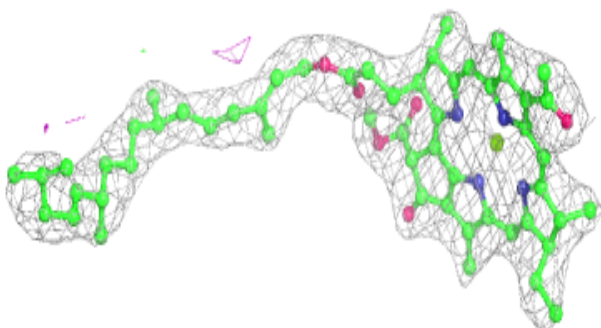
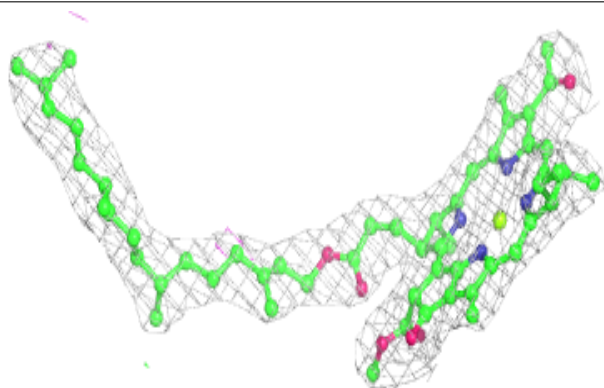


**Electron density around BCL M 313:**

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

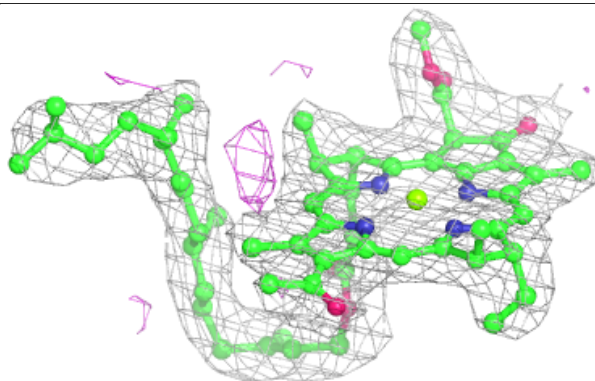
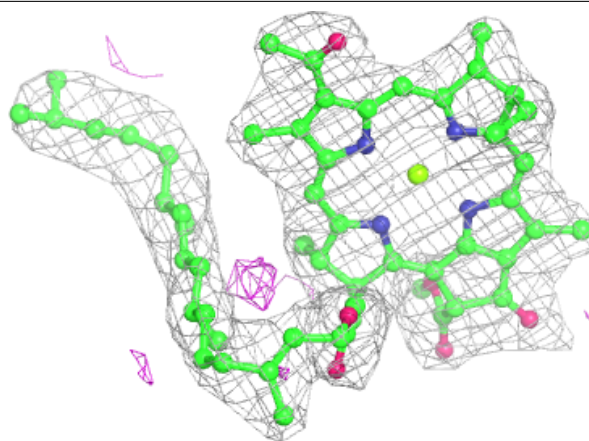
**Electron density around BCL L 312:**

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



**Electron density around BCL L 314:**

$2mF_o-DF_c$  (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.