



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 11:09 am BST

PDB ID : 2HHK  
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylglycerol  
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2006-06-28  
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

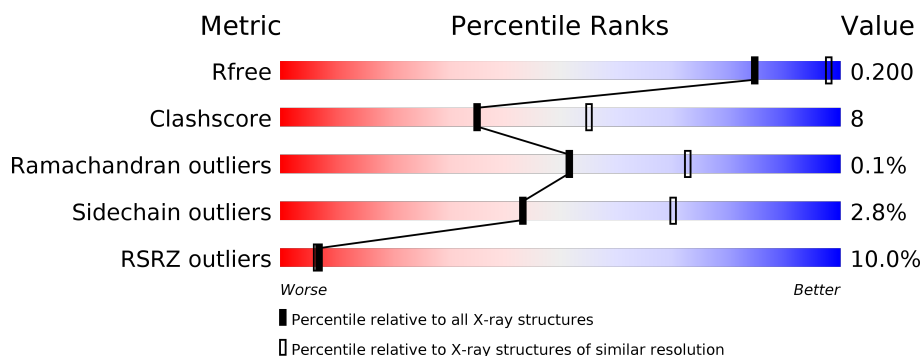
# 1 Overall quality at a glance ⓘ

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>12%</div> <div>94%</div> <div>• •</div> </div>
2	M	307	<div> <div>12%</div> <div>89%</div> <div>9% • •</div> </div>
3	H	260	<div> <div>4%</div> <div>78%</div> <div>13% • 7%</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
11	CDL	M	800	-	-	-	X
12	PGK	M	802	-	-	-	X
13	LDA	H	901	-	-	X	-
13	LDA	H	903	-	-	X	X
13	LDA	H	904	-	-	-	X
13	LDA	M	902	-	-	-	X
13	LDA	M	907	-	-	-	X
13	LDA	M	920	-	-	-	X
15	PGT	H	801[A]	-	-	-	X
15	PGT	H	801[B]	-	-	-	X
6	U10	L	502	-	-	-	X
7	GOL	L	709	-	-	X	X

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7824 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	1	0
			2235	1510	356	361	8			

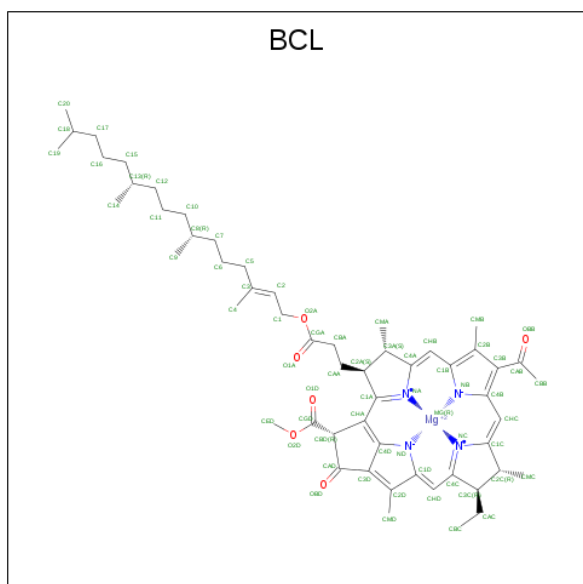
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	10	0
			2448	1633	402	402	11			

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

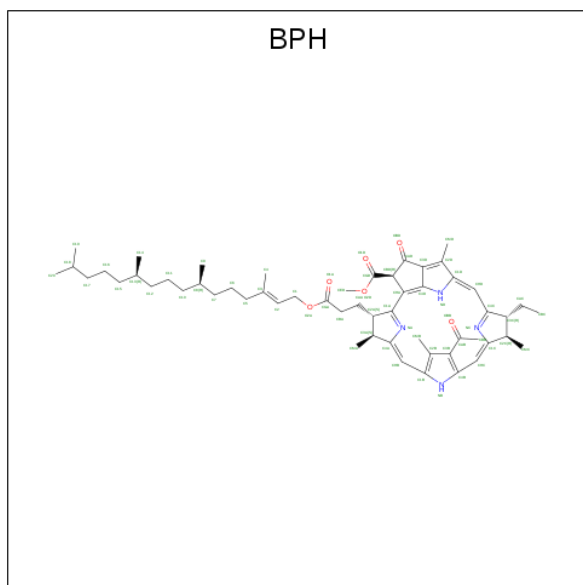
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	8	0
			1862	1189	323	339	11			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



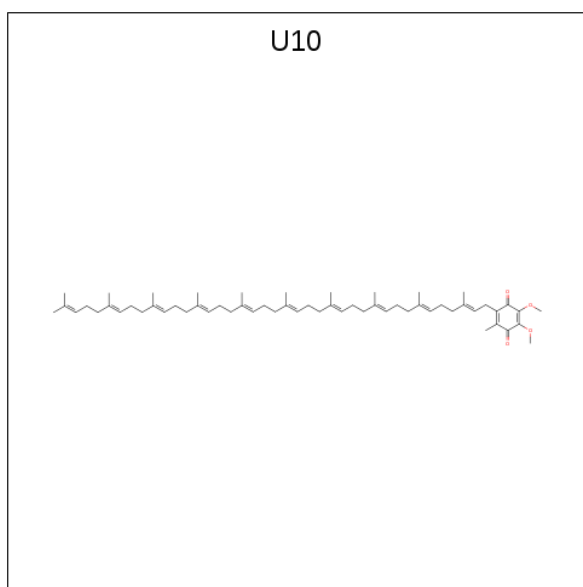
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	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	L	1	Total	C	O	0	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

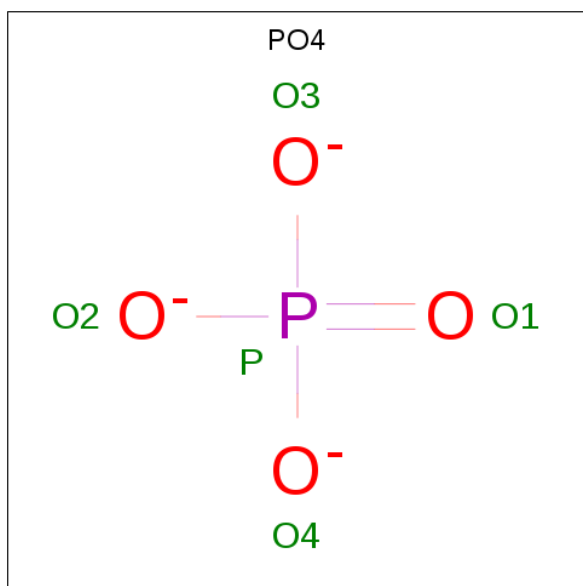
- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



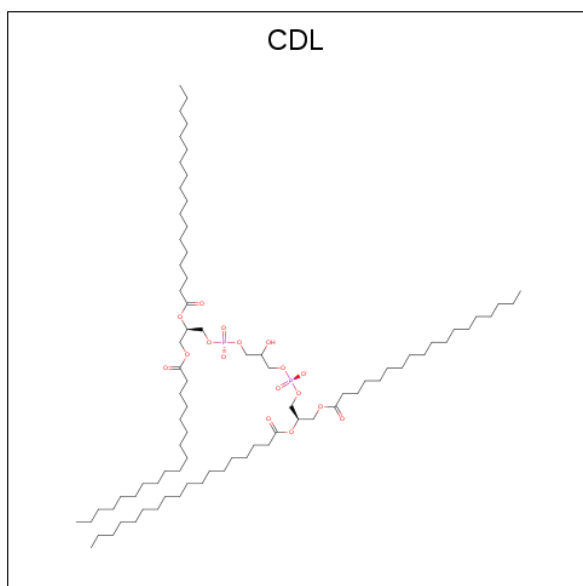
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	O	P	0	0
			5	4	1		

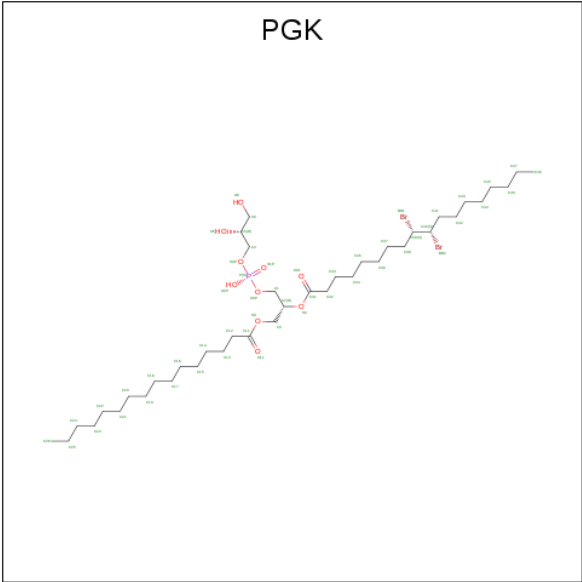
- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

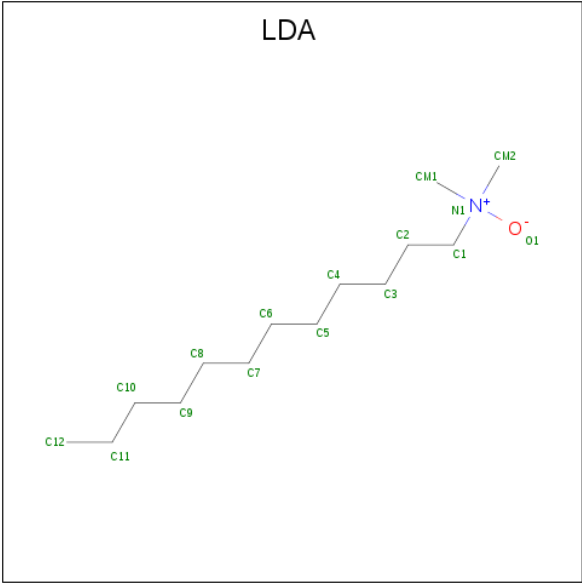
- Molecule 12 is (1R)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (9S,10S)-9,10-DIBROMOOCTADECANOATE (three-letter code: PGK) (formula:  $C_{40}H_{77}Br_2O_{10}P$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	O	P		
12	M	1	53	2	40	10	1	0	0

- Molecule 13 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
			Total	C	N	O		
13	M	1	16	14	1	1	0	0
13	M	1	16	14	1	1	0	0

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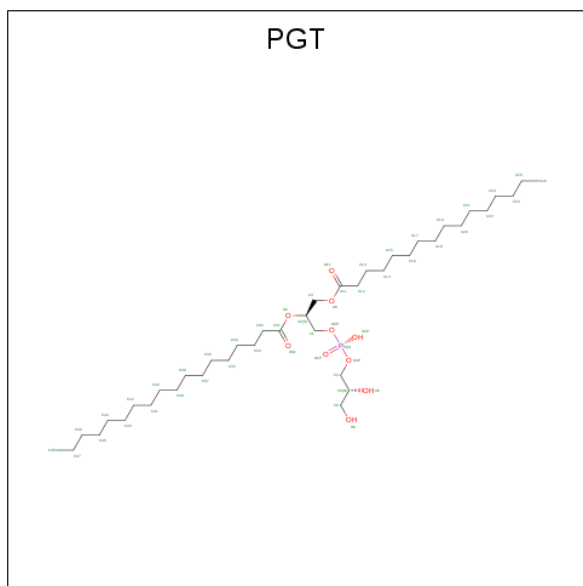
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		

- 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 (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	O	P	0	1
			102	80	20	2		

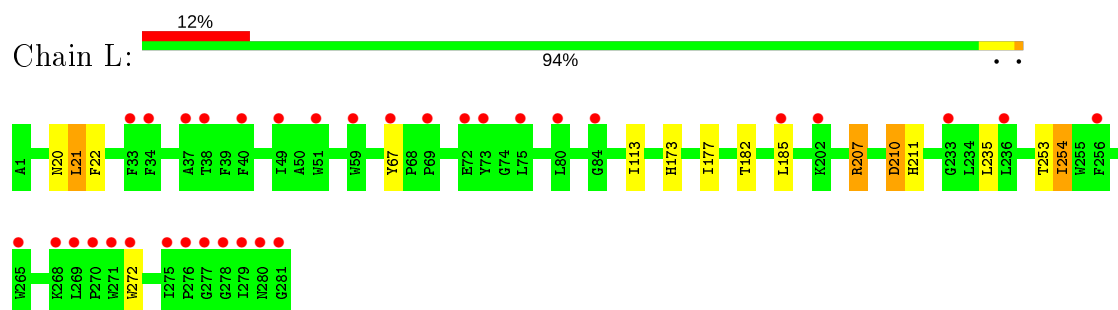
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	92	Total 92	O 92	0	0
16	M	119	Total 119	O 119	0	0
16	H	199	Total 199	O 199	0	0

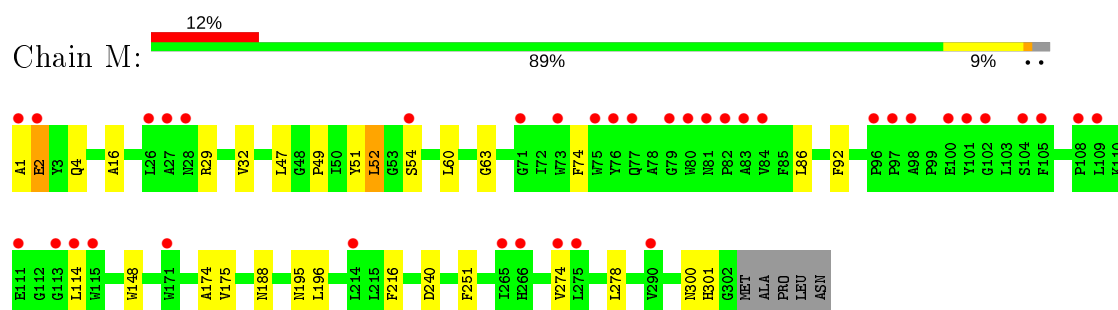
### 3 Residue-property plots [i](#)

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.

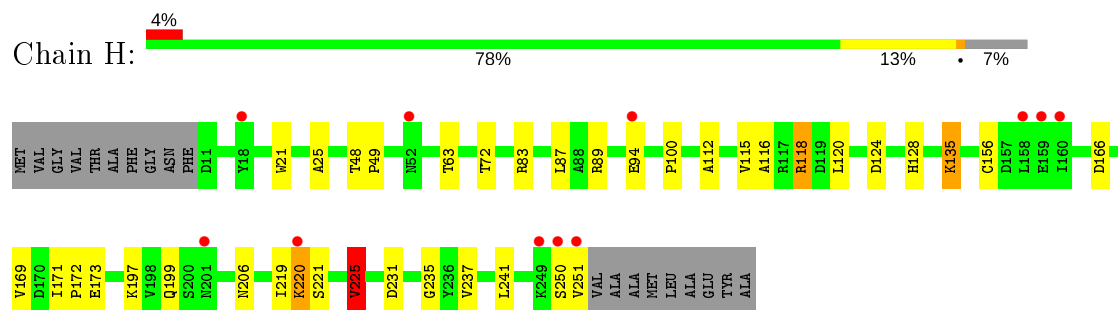
- Molecule 1: Reaction center protein L chain



- 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, $\alpha$ , $\beta$ , $\gamma$	139.42Å 139.42Å 183.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.50 45.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.00-2.50) 99.5 (45.63-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.197 0.177 , 0.200	Depositor DCC
$R_{free}$ test set	3548 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 97.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, CL, CDL, BPH, K, PGK, PGT, 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	0.88	0/2328	0.73	1/3186 (0.0%)
2	M	0.87	0/2592	0.78	1/3536 (0.0%)
3	H	0.93	5/1953 (0.3%)	0.82	4/2652 (0.2%)
All	All	0.89	5/6873 (0.1%)	0.78	6/9374 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	173	GLU	CD-OE2	5.32	1.31	1.25
3	H	237	VAL	CB-CG2	5.12	1.63	1.52
3	H	221[A]	SER	CB-OG	5.07	1.48	1.42
3	H	221[B]	SER	CB-OG	5.07	1.48	1.42
3	H	94	GLU	CG-CD	5.05	1.59	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASP	CB-CG-OD1	6.50	124.15	118.30
3	H	124	ASP	CB-CG-OD1	6.31	123.98	118.30
3	H	225	VAL	CB-CA-C	-5.53	100.90	111.40
3	H	89	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	M	240	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	1	ALA	Peptide

## 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	2235	0	2196	10	0
2	M	2448	0	2367	26	0
3	H	1862	0	1883	25	0
4	L	132	0	148	6	0
4	M	132	0	148	20	0
5	L	65	0	75	0	0
5	M	65	0	76	4	0
6	L	48	0	63	4	0
6	M	48	0	63	1	0
7	H	6	0	8	0	0
7	L	18	0	24	5	0
8	M	1	0	0	0	0
9	M	1	0	0	0	0
10	H	5	0	0	0	0
10	M	15	0	0	1	0
11	M	81	0	106	3	0
12	M	53	0	74	11	0
13	H	48	0	93	25	0
13	M	48	0	93	12	0
14	H	1	0	0	0	0
15	H	102	0	156	20	0
16	H	199	0	0	4	0
16	L	92	0	0	2	0
16	M	119	0	0	2	0
All	All	7824	0	7573	123	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 123 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:301[A]:HIS:HE1	16:M:1031:HOH:O	1.41	1.03
4:M:311:BCL:C9	4:M:311:BCL:H41	1.91	0.99
4:M:311:BCL:C7	4:M:311:BCL:H41	1.92	0.98
13:M:902:LDA:C12	13:H:903:LDA:C12	2.43	0.96
13:M:902:LDA:C12	13:H:903:LDA:H123	1.96	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	280/281 (100%)	274 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	298 (96%)	11 (4%)	1 (0%)	41	61
3	H	247/260 (95%)	242 (98%)	5 (2%)	0	100	100
All	All	837/848 (99%)	814 (97%)	22 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	221/220 (100%)	214 (97%)	7 (3%)	39	65
2	M	246/240 (102%)	240 (98%)	6 (2%)	49	74
3	H	204/208 (98%)	197 (97%)	7 (3%)	37	63
All	All	671/668 (100%)	651 (97%)	20 (3%)	43	68

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	86	LEU
2	M	114	LEU
3	H	220[A]	LYS
2	M	2	GLU
2	M	52	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	28	ASN
3	H	199	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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
13	LDA	H	901	-	12,15,15	1.77	1 (8%)	14,17,17	0.86	0
10	PO4	M	702	-	4,4,4	0.63	0	6,6,6	0.66	0
4	BCL	L	314	1	58,74,74	1.17	3 (5%)	69,115,115	1.60	15 (21%)
4	BCL	M	313	2	58,74,74	1.20	3 (5%)	69,115,115	1.86	17 (24%)
13	LDA	H	903	-	12,15,15	1.91	1 (8%)	14,17,17	0.54	0
10	PO4	M	703	-	4,4,4	0.90	0	6,6,6	1.43	1 (16%)
13	LDA	H	904	-	12,15,15	2.02	1 (8%)	14,17,17	0.53	0
7	GOL	L	707	-	5,5,5	0.38	0	5,5,5	0.48	0
11	CDL	M	800	-	80,80,99	1.25	4 (5%)	86,92,111	1.44	12 (13%)
10	PO4	M	705	-	4,4,4	0.85	0	6,6,6	0.78	0
7	GOL	H	706	-	5,5,5	0.27	0	5,5,5	0.85	0
4	BCL	L	312	1	58,74,74	1.23	4 (6%)	69,115,115	1.56	15 (21%)
13	LDA	M	902	-	12,15,15	1.93	1 (8%)	14,17,17	0.54	0
12	PGK	M	802	-	52,52,52	0.88	3 (5%)	55,60,60	1.48	5 (9%)
4	BCL	M	311	2	58,74,74	1.14	3 (5%)	69,115,115	1.83	20 (28%)
5	BPH	L	402	-	64,70,70	0.83	1 (1%)	76,101,101	1.20	11 (14%)
10	PO4	H	704	-	4,4,4	0.90	0	6,6,6	0.68	0
13	LDA	M	920	-	12,15,15	1.87	1 (8%)	14,17,17	0.83	0
13	LDA	M	907	-	12,15,15	2.06	1 (8%)	14,17,17	0.61	0
6	U10	M	501	-	48,48,63	1.15	2 (4%)	58,61,79	1.49	8 (13%)
7	GOL	L	708	-	5,5,5	0.49	0	5,5,5	0.56	0
6	U10	L	502	-	48,48,63	1.10	4 (8%)	58,61,79	1.65	11 (18%)
5	BPH	M	401	-	64,70,70	0.89	1 (1%)	76,101,101	1.56	14 (18%)
15	PGT	H	801[A]	-	50,50,50	0.71	0	53,56,56	0.97	3 (5%)
15	PGT	H	801[B]	-	50,50,50	0.83	1 (2%)	53,56,56	1.10	5 (9%)
7	GOL	L	709	-	5,5,5	0.64	0	5,5,5	0.66	0

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
13	LDA	H	901	-	-	4/13/13/13	-
4	BCL	L	314	1	-	3/37/137/137	-
4	BCL	M	313	2	-	2/37/137/137	-
13	LDA	H	903	-	-	5/13/13/13	-
13	LDA	H	904	-	-	7/13/13/13	-
7	GOL	L	707	-	-	4/4/4/4	-
11	CDL	M	800	-	-	37/91/91/110	-
7	GOL	H	706	-	-	2/4/4/4	-
4	BCL	L	312	1	-	3/37/137/137	-
13	LDA	M	902	-	-	1/13/13/13	-
12	PGK	M	802	-	-	24/60/60/60	-
4	BCL	M	311	2	-	10/37/137/137	-
5	BPH	L	402	-	-	6/54/105/105	0/5/6/6
13	LDA	M	920	-	-	7/13/13/13	-
13	LDA	M	907	-	-	7/13/13/13	-
6	U10	M	501	-	-	5/45/69/87	0/1/1/1
7	GOL	L	708	-	-	4/4/4/4	-
6	U10	L	502	-	-	11/45/69/87	0/1/1/1
5	BPH	M	401	-	-	13/54/105/105	0/5/6/6
15	PGT	H	801[A]	-	-	30/55/55/55	-
15	PGT	H	801[B]	-	-	24/55/55/55	-
7	GOL	L	709	-	-	2/4/4/4	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	907	LDA	O1-N1	-6.96	1.25	1.42
13	H	904	LDA	O1-N1	-6.90	1.26	1.42
13	M	902	LDA	O1-N1	-6.59	1.26	1.42
13	H	903	LDA	O1-N1	-6.53	1.26	1.42
13	M	920	LDA	O1-N1	-6.35	1.27	1.42

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	313	BCL	CMB-C2B-C1B	-5.91	119.38	128.46
11	M	800	CDL	OB6-CB5-C51	5.38	123.09	111.50
12	M	802	PGK	BR1-C39-C40	-5.10	100.39	110.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	313	BCL	CAC-C3C-C2C	-4.71	102.49	114.26
5	M	401	BPH	O2D-CGD-CBD	4.68	119.59	111.27

There are no chirality outliers.

5 of 211 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	H	904	LDA	N1-C1-C2-C3
7	L	707	GOL	O1-C1-C2-C3
11	M	800	CDL	CA2-OA2-PA1-OA3
11	M	800	CDL	CA2-OA2-PA1-OA4
11	M	800	CDL	CA2-OA2-PA1-OA5

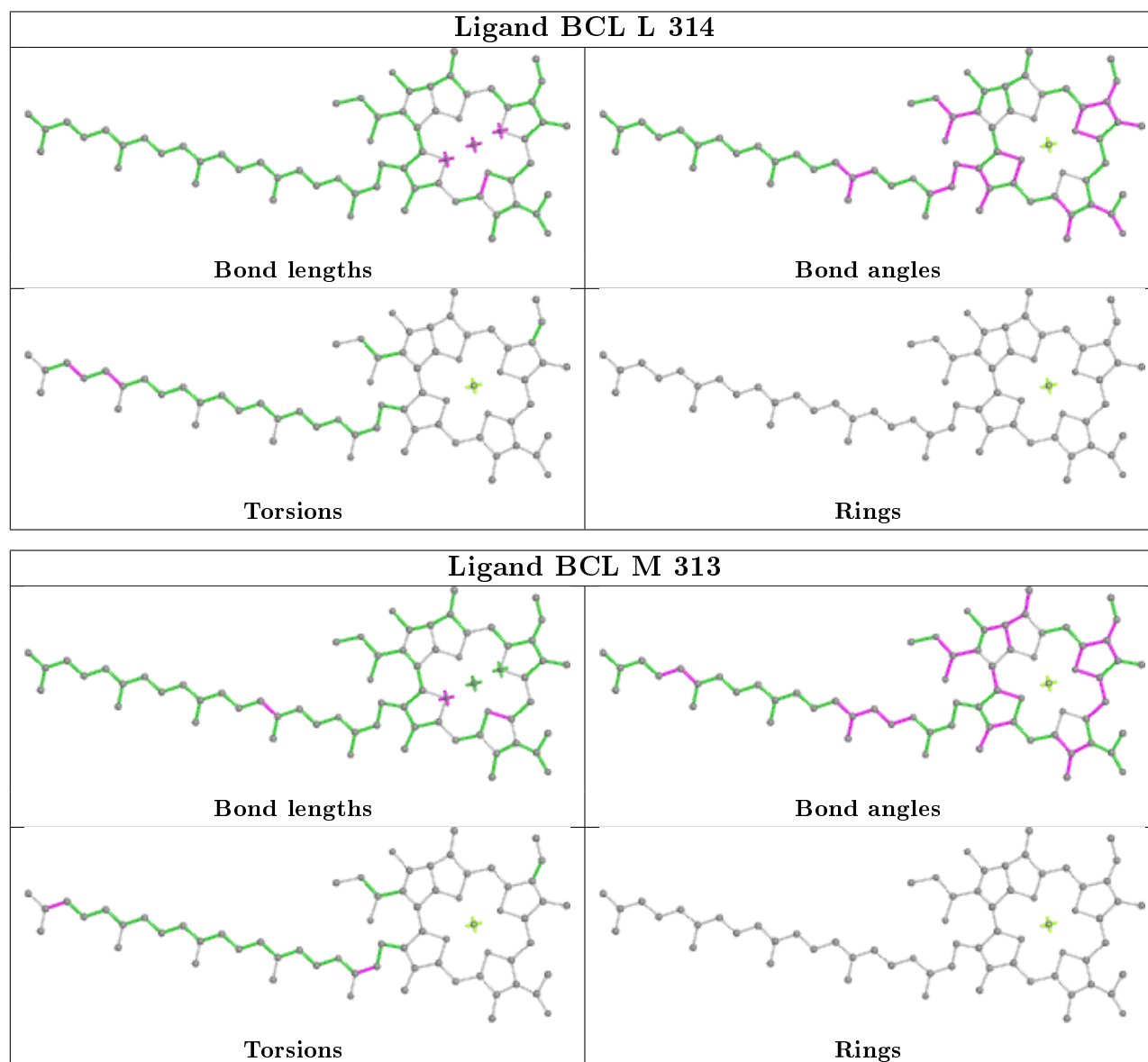
There are no ring outliers.

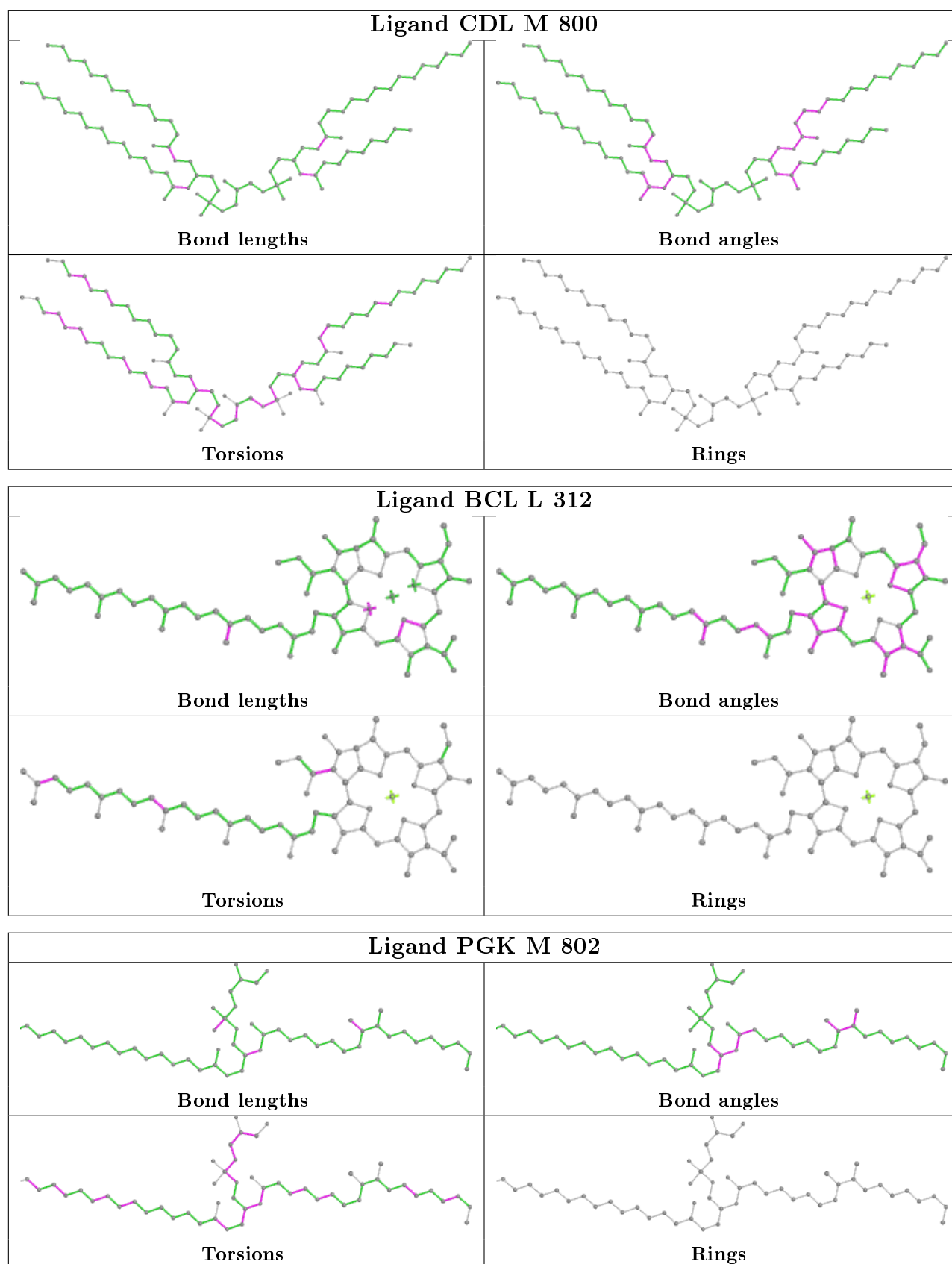
18 monomers are involved in 81 short contacts:

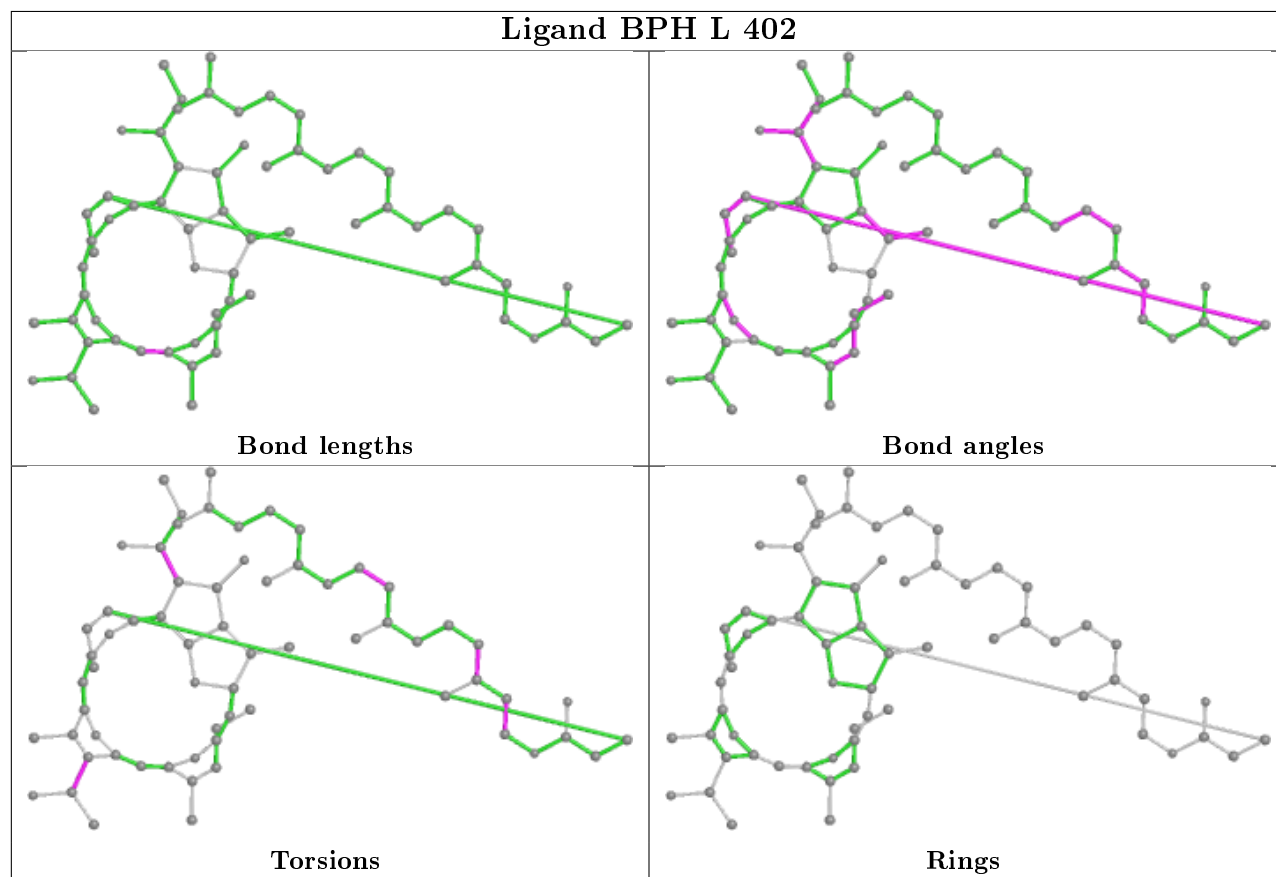
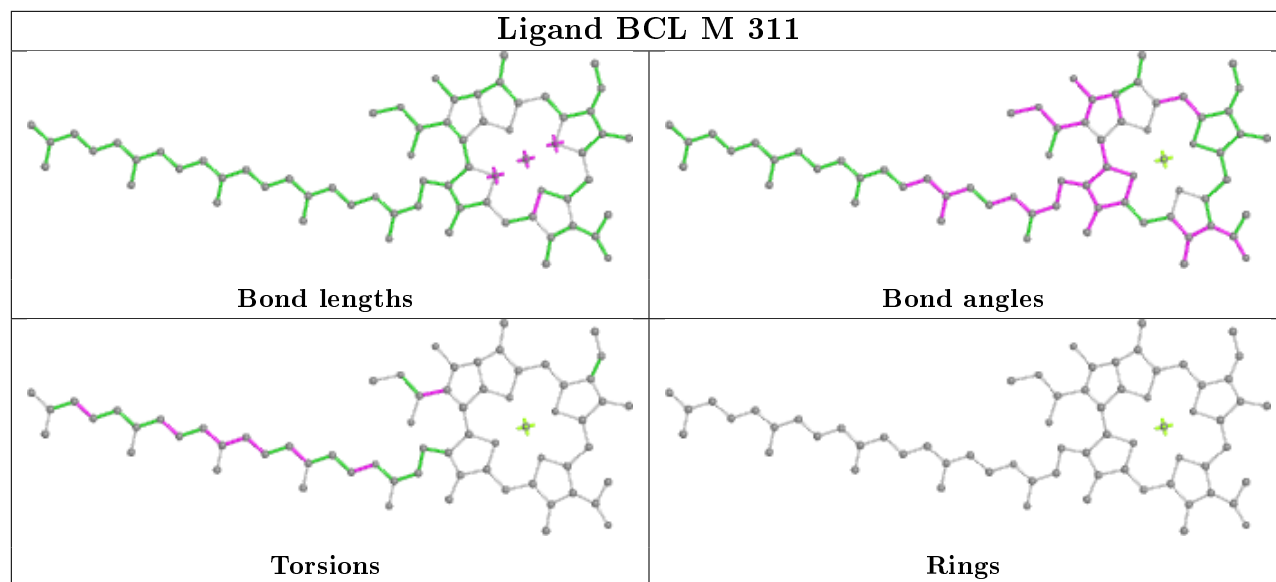
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	901	LDA	11	0
4	L	314	BCL	3	0
4	M	313	BCL	5	0
13	H	903	LDA	12	0
10	M	703	PO4	1	0
13	H	904	LDA	2	0
11	M	800	CDL	3	0
4	L	312	BCL	4	0
13	M	902	LDA	7	0
12	M	802	PGK	11	0
4	M	311	BCL	15	0
13	M	920	LDA	5	0
6	M	501	U10	1	0
6	L	502	U10	4	0
5	M	401	BPH	4	0
15	H	801[A]	PGT	12	0
15	H	801[B]	PGT	8	0
7	L	709	GOL	5	0

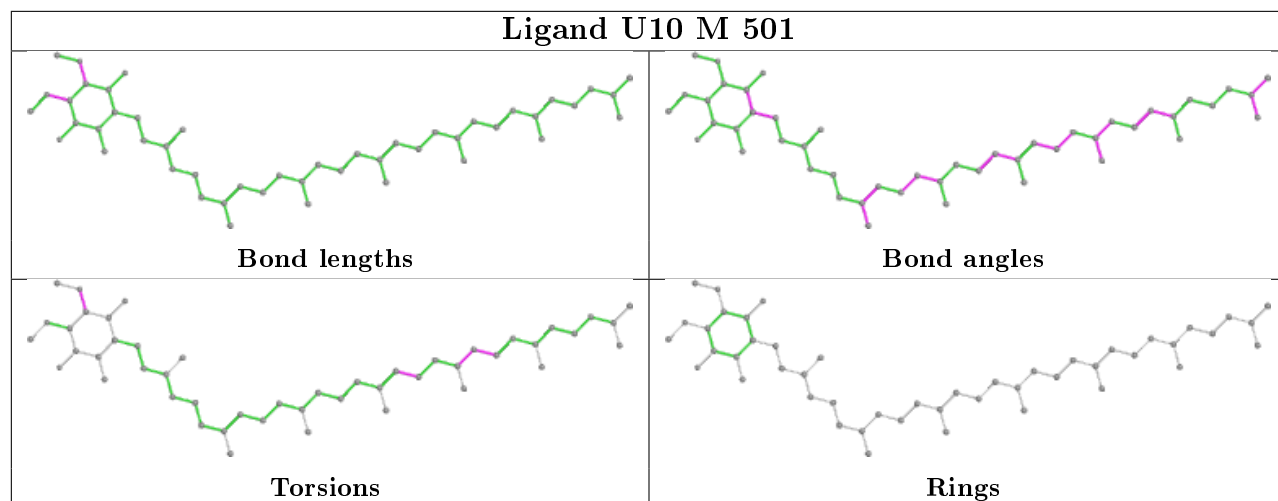
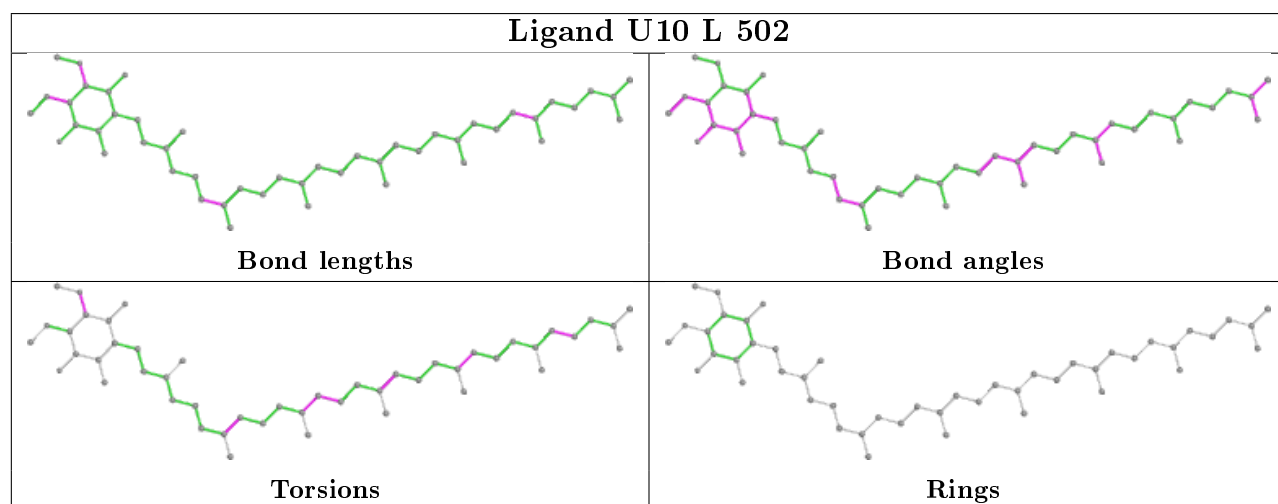
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

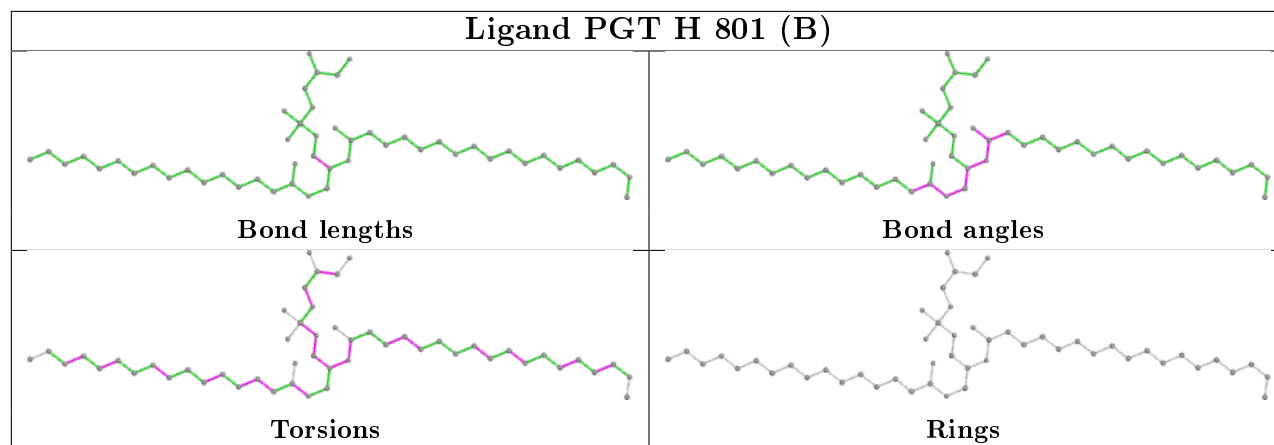
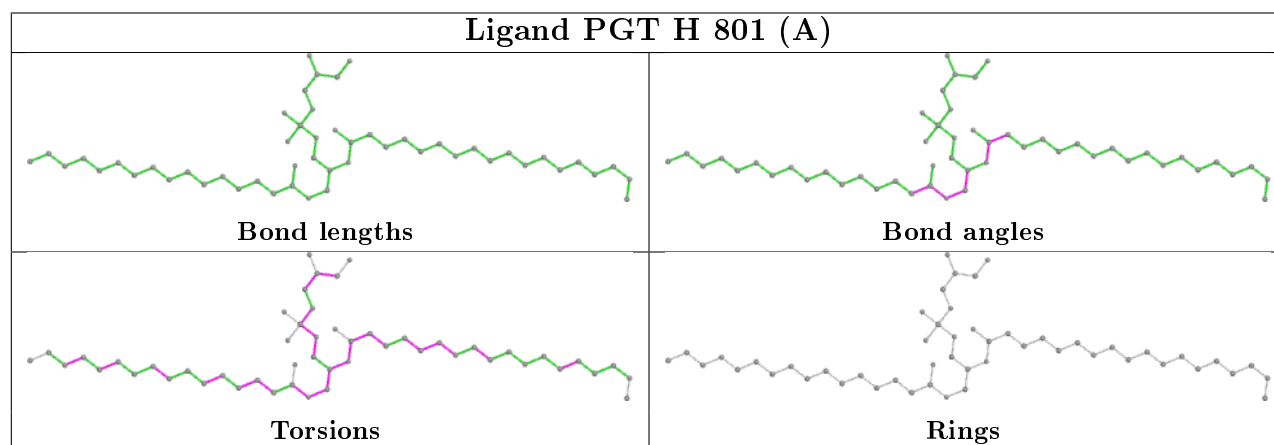
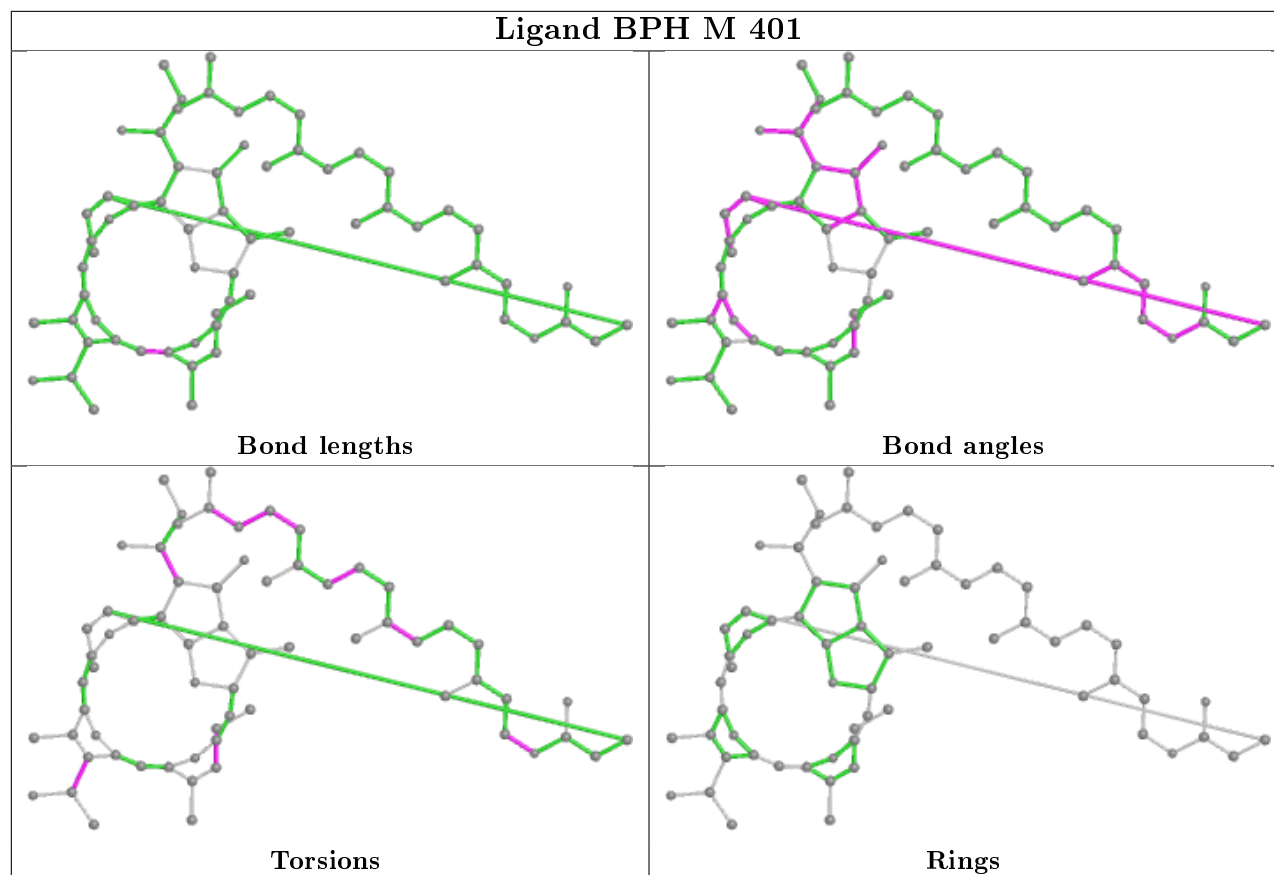






**Ligand U10 M 501****Ligand U10 L 502**





## 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%)	0.48	33 (11%) 4 4	54, 62, 73, 80	0
2	M	302/307 (98%)	0.59	38 (12%) 3 3	54, 62, 73, 94	0
3	H	241/260 (92%)	0.16	11 (4%) 32 34	54, 62, 73, 100	0
All	All	824/848 (97%)	0.42	82 (9%) 7 6	54, 62, 73, 100	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	6.7
2	M	80	TRP	6.5
3	H	250	SER	6.2
3	H	251	VAL	5.7
1	L	277	GLY	5.0

### 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](#)

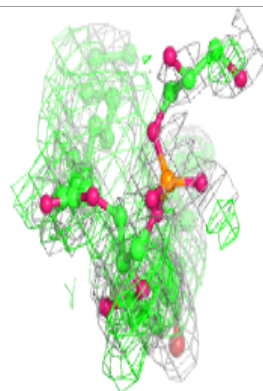
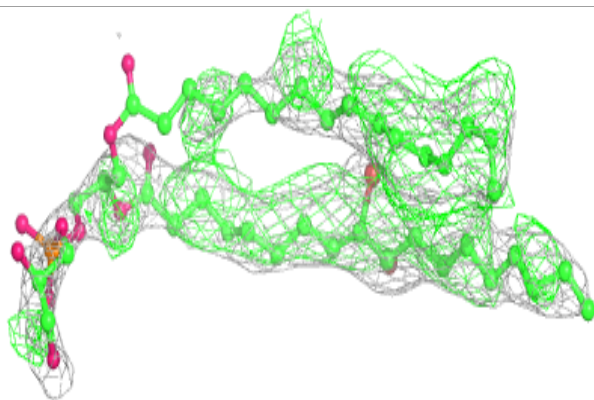
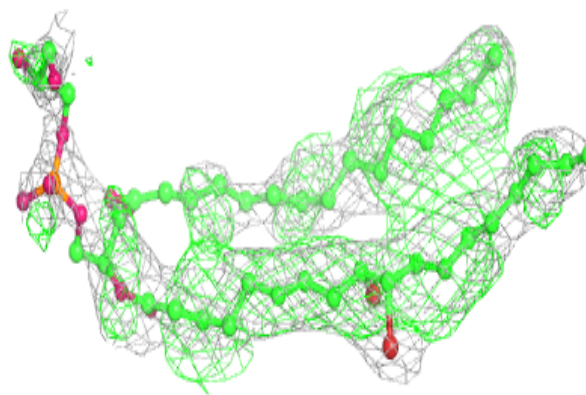
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
13	LDA	H	903	16/16	-0.13	1.34	73,75,78,78	16
12	PGK	M	802	53/53	0.19	0.75	61,67,76,77	53
13	LDA	M	902	16/16	0.22	0.93	66,71,75,79	16
15	PGT	H	801[A]	51/51	0.41	1.25	45,73,81,82	51
15	PGT	H	801[B]	51/51	0.41	1.25	47,76,84,85	51
13	LDA	H	904	16/16	0.44	0.74	76,79,86,86	16
13	LDA	M	920	16/16	0.61	0.62	41,60,78,80	16
11	CDL	M	800	81/100	0.64	0.49	49,74,88,90	81
7	GOL	L	707	6/6	0.65	0.35	65,67,68,68	6
10	PO4	H	704	5/5	0.68	0.26	61,61,63,63	5
13	LDA	M	907	16/16	0.75	0.47	69,72,77,77	16
7	GOL	L	709	6/6	0.75	0.46	65,66,68,70	6
6	U10	L	502	48/63	0.76	0.59	53,68,86,90	48
10	PO4	M	705	5/5	0.78	0.25	63,64,65,65	5
7	GOL	L	708	6/6	0.81	0.32	60,66,68,68	6
13	LDA	H	901	16/16	0.83	0.41	72,77,86,88	16
6	U10	M	501	48/63	0.84	0.31	56,69,90,93	0
5	BPH	M	401	65/65	0.90	0.20	56,62,116,118	0
7	GOL	H	706	6/6	0.91	0.39	72,72,73,74	6
4	BCL	L	312	66/66	0.93	0.17	49,59,70,78	0
5	BPH	L	402	65/65	0.93	0.17	50,62,66,68	0
4	BCL	L	314	66/66	0.93	0.19	50,59,75,80	0
9	CL	M	701	1/1	0.93	0.32	73,73,73,73	1
4	BCL	M	313	66/66	0.94	0.20	51,59,84,95	0
10	PO4	M	702	5/5	0.95	0.21	69,71,74,77	5
10	PO4	M	703	5/5	0.95	0.21	59,59,63,64	5
4	BCL	M	311	66/66	0.95	0.20	55,62,119,120	0
14	K	H	700	1/1	0.96	0.10	58,58,58,58	0
8	FE	M	500	1/1	1.00	0.18	59,59,59,59	0

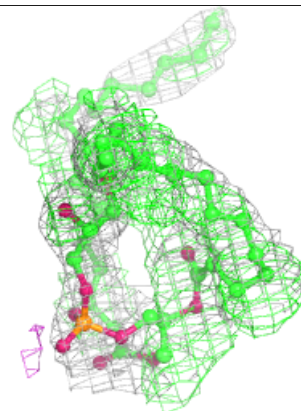
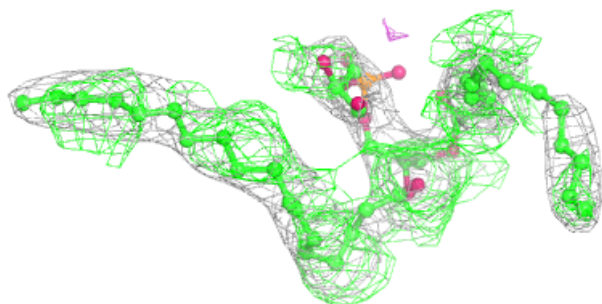
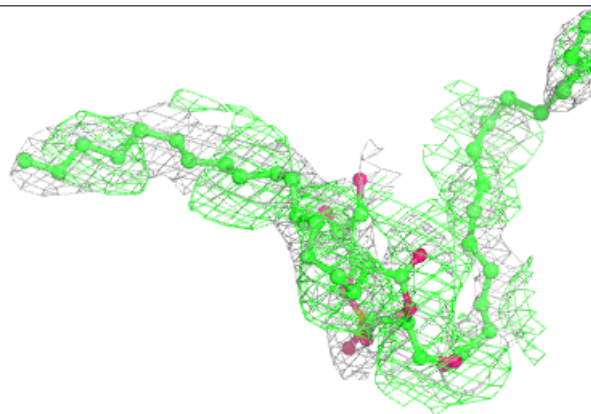
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PGK 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)

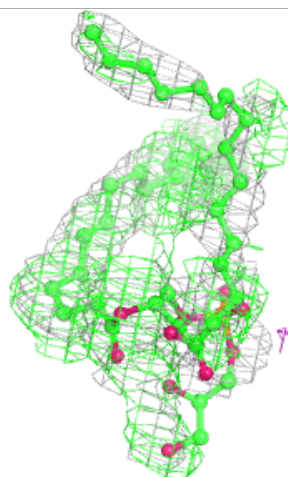
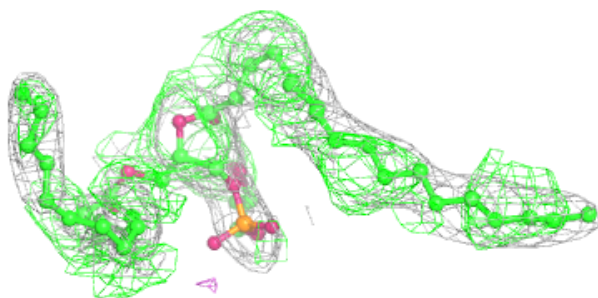
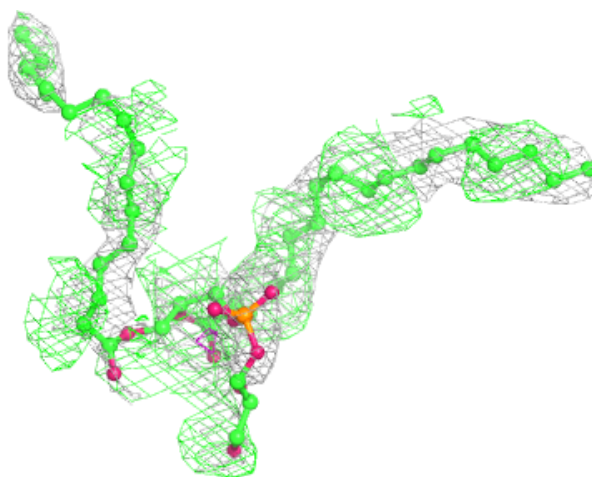
**Electron density around PGT H 801 (A):**

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



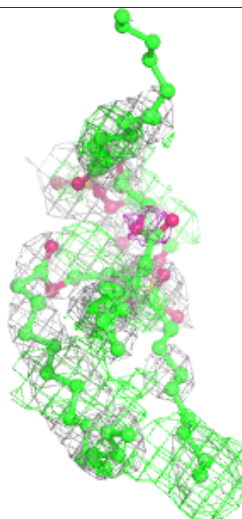
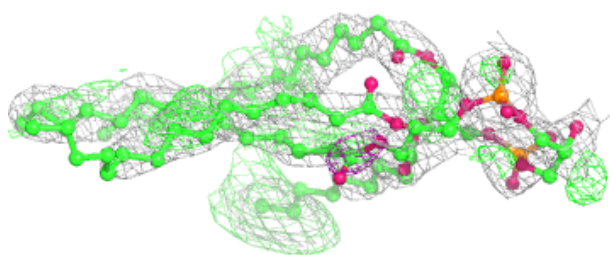
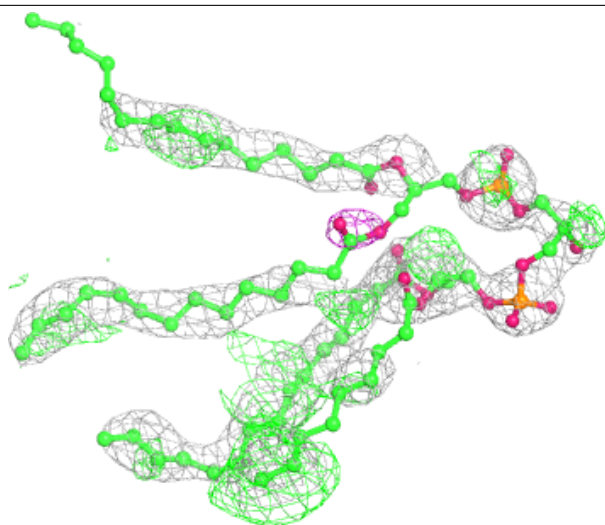
**Electron density around PGT H 801 (B):**

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



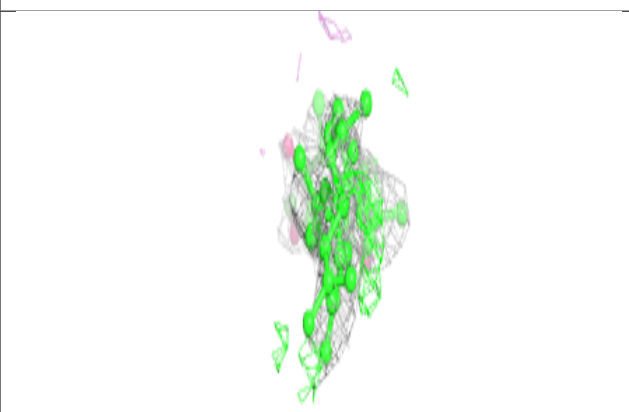
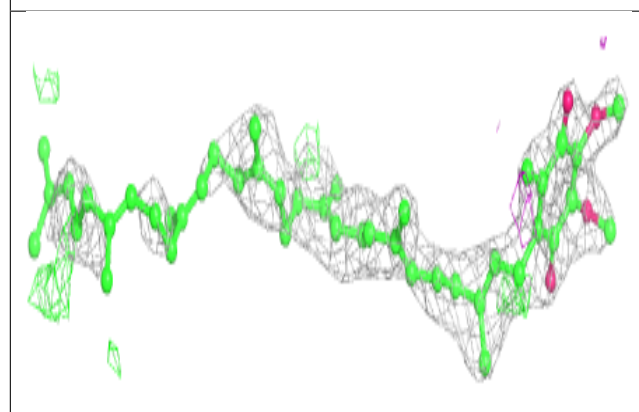
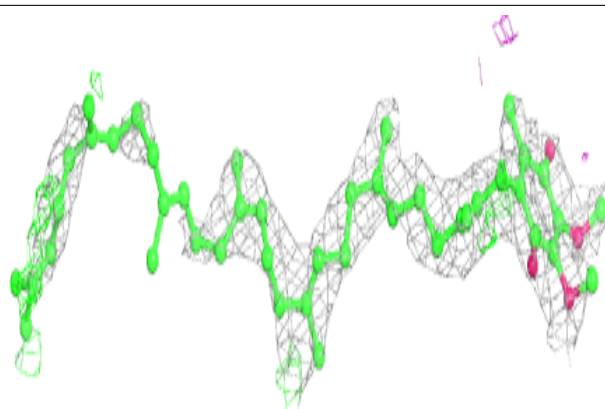
**Electron density around CDL M 800:**

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

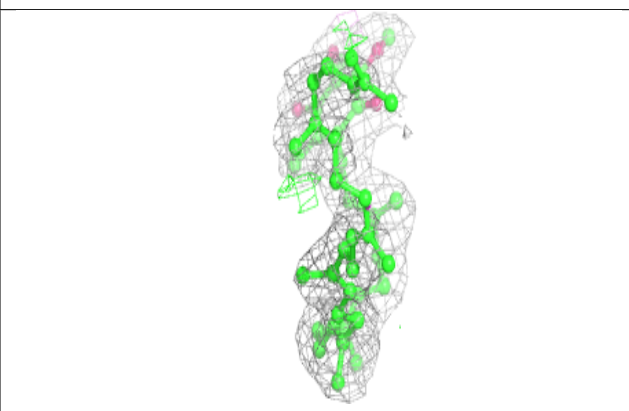
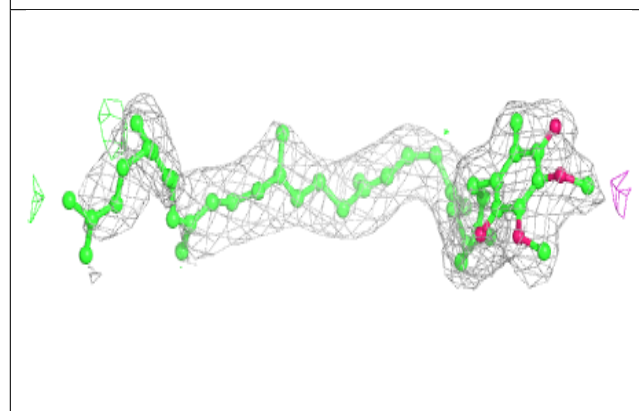
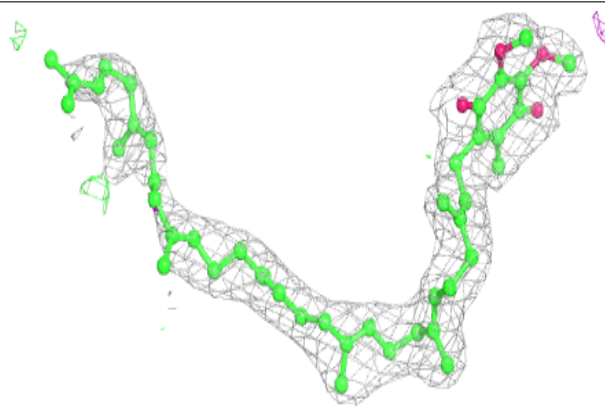


**Electron density around U10 L 502:**

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

**Electron density around U10 M 501:**

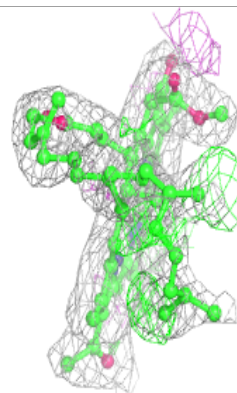
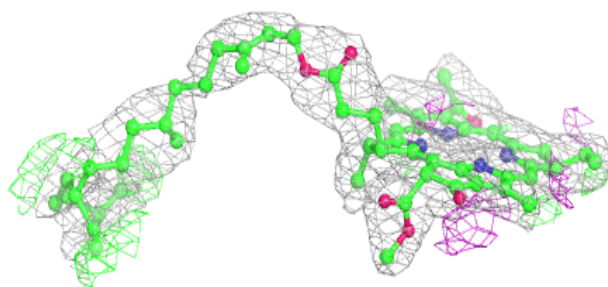
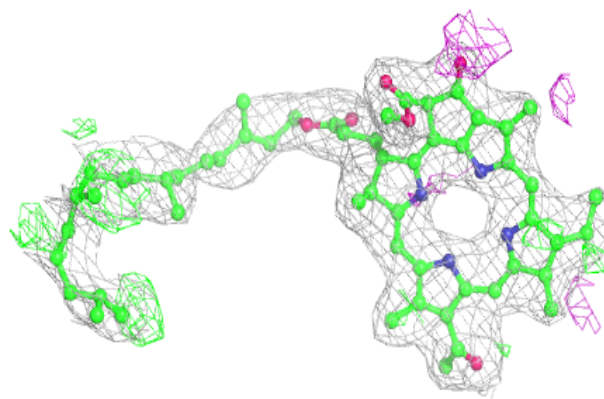
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



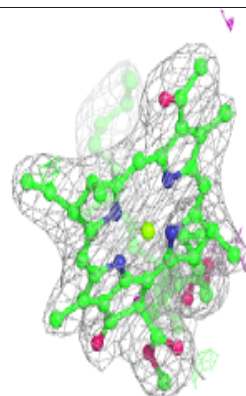
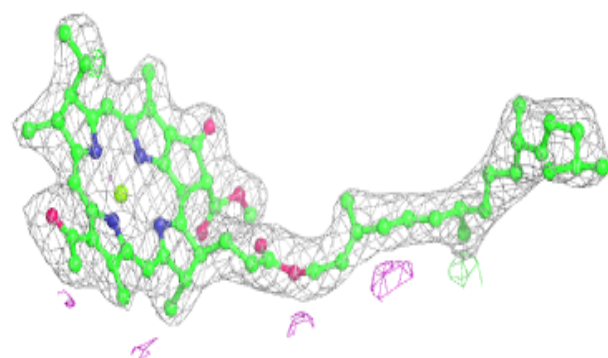
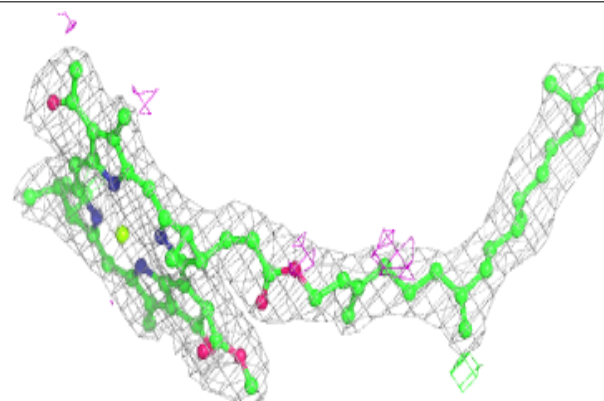


**Electron density around BPH M 401:**

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

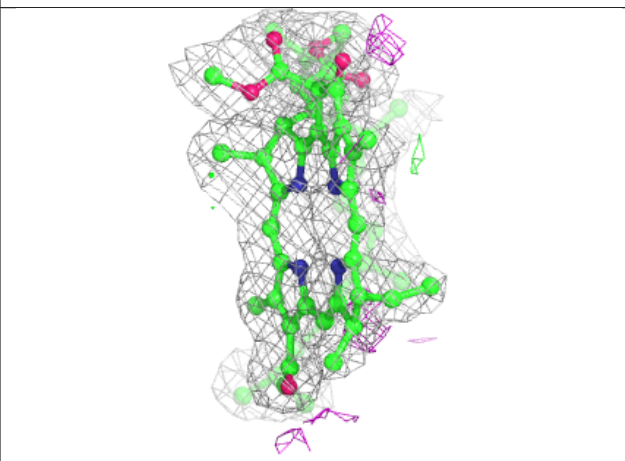
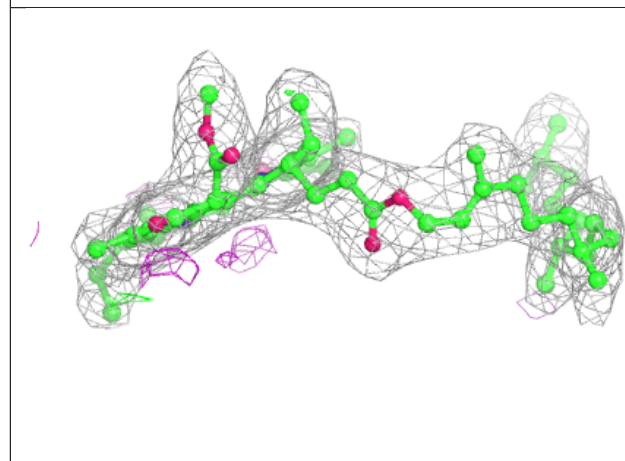
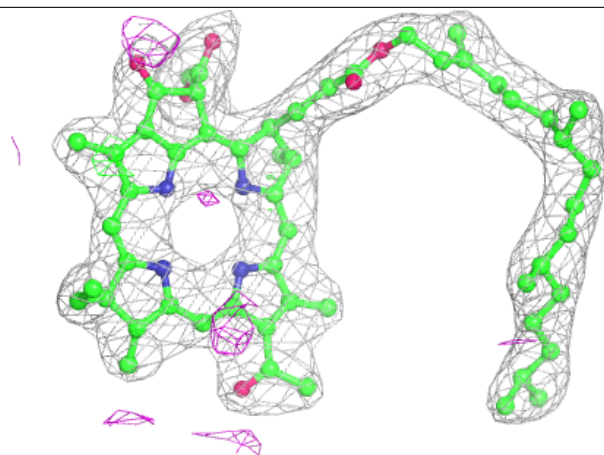
**Electron density around BCL L 312:**

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



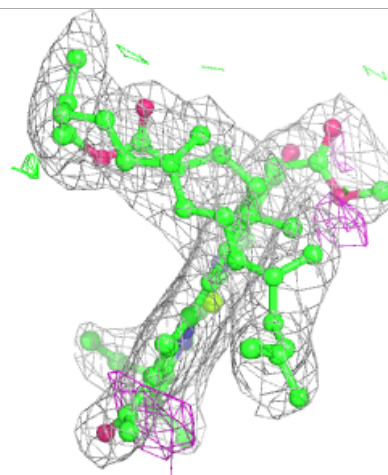
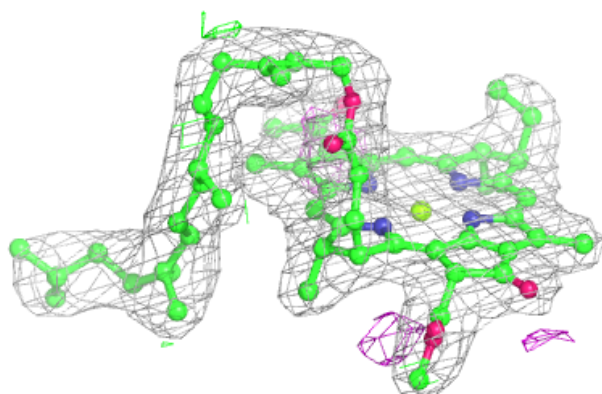
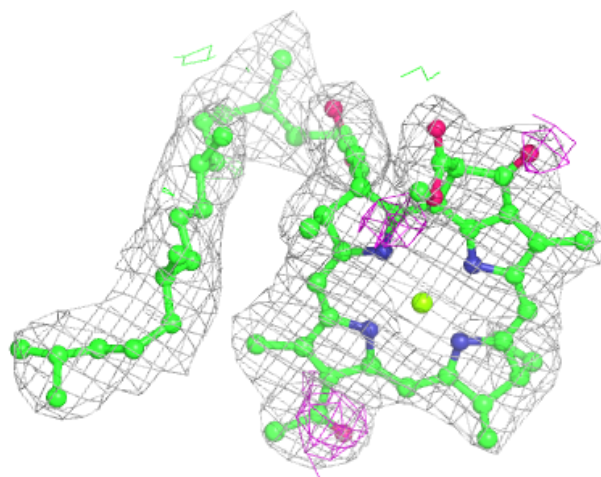
**Electron density around BPH L 402:**

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



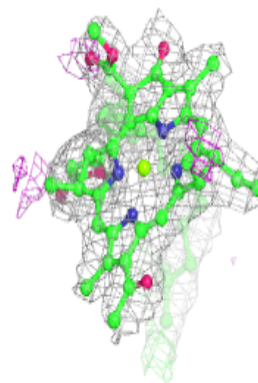
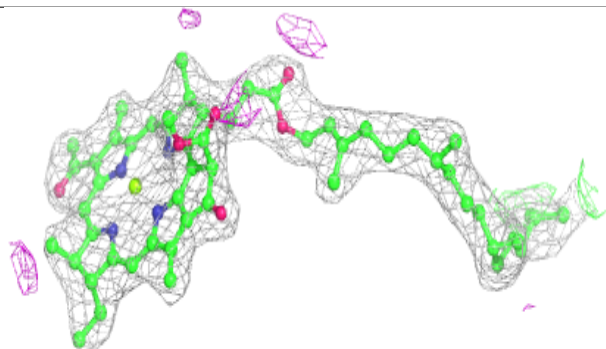
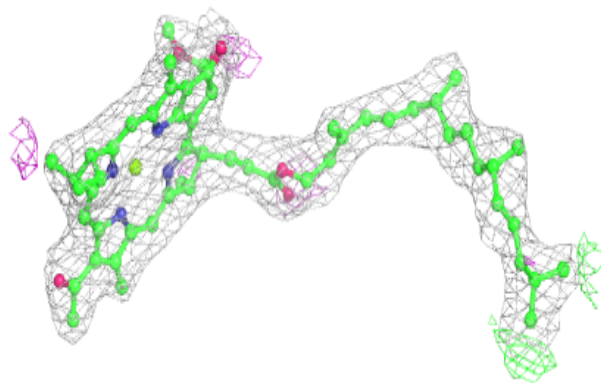
**Electron density around BCL L 314:**

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

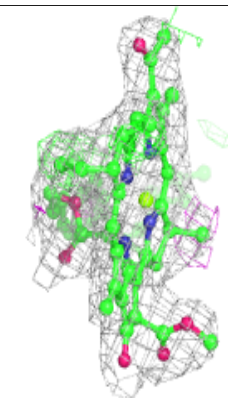
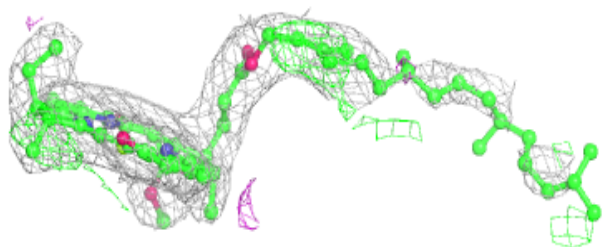
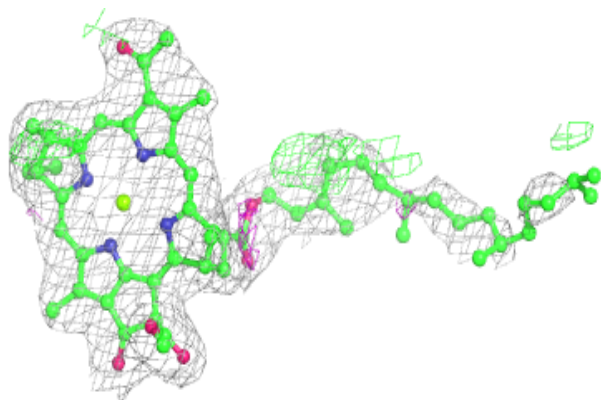


**Electron density around BCL M 313:**

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

**Electron density around BCL 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.