



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:34 pm BST

PDB ID : 2HIT  
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylethanolamine  
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2006-06-29  
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

---

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

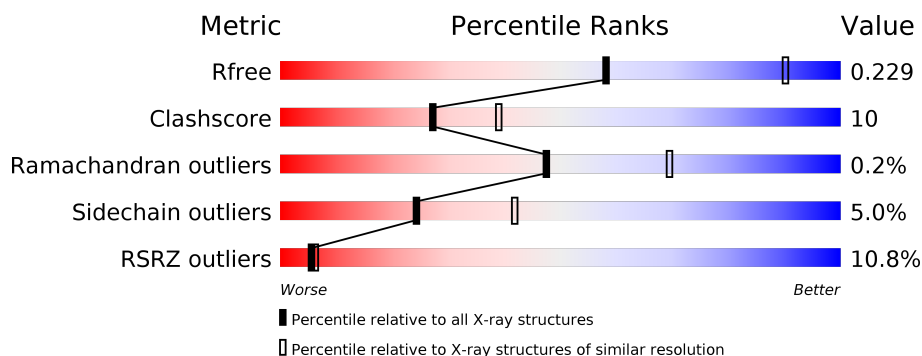
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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>9%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	M	307	<div> <div>14%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
3	H	260	<div> <div>8%</div> <div>77%</div> <div>14%</div> <div>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
10	PO4	M	706	-	-	-	X
11	CDL	M	800	-	-	-	X
12	PEW	M	802	-	-	-	X
13	LDA	H	901	-	-	X	X
13	LDA	H	903	-	-	-	X
13	LDA	H	904	-	-	-	X
13	LDA	M	902	-	-	-	X
13	LDA	M	907	-	-	-	X
13	LDA	M	920	-	-	X	X
15	PEV	H	801[A]	-	-	-	X
15	PEV	H	801[B]	-	-	-	X
6	U10	L	502	-	-	-	X
9	CL	H	703	-	-	-	X

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7851 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
			2256	1523	360	365	8			

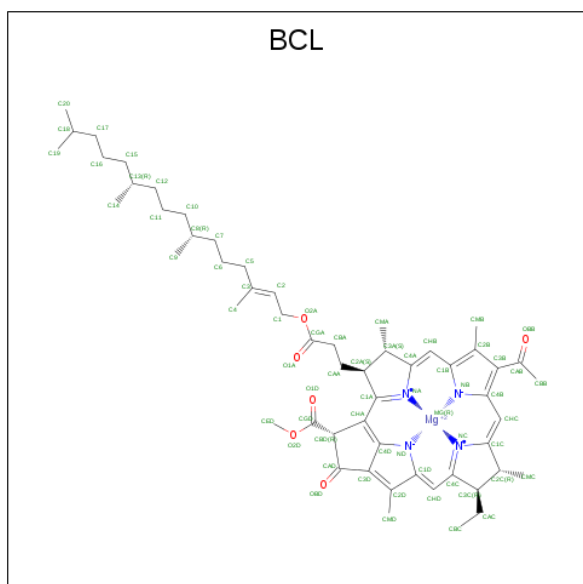
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	12	0
			2477	1650	405	411	11			

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

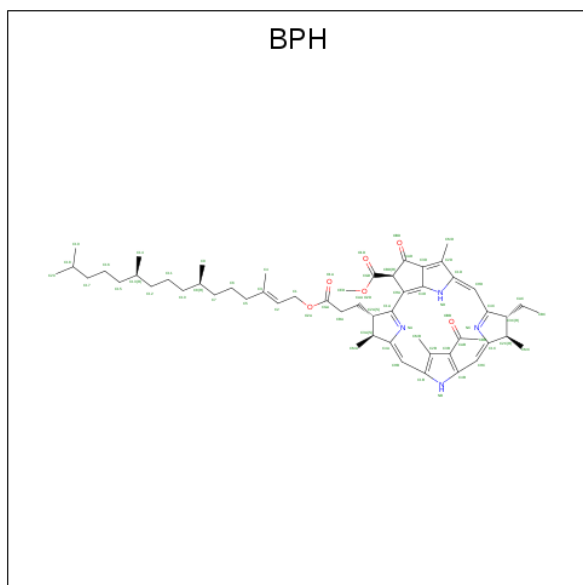
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	243	Total	C	N	O	S	0	6	0
			1876	1199	323	343	11			

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



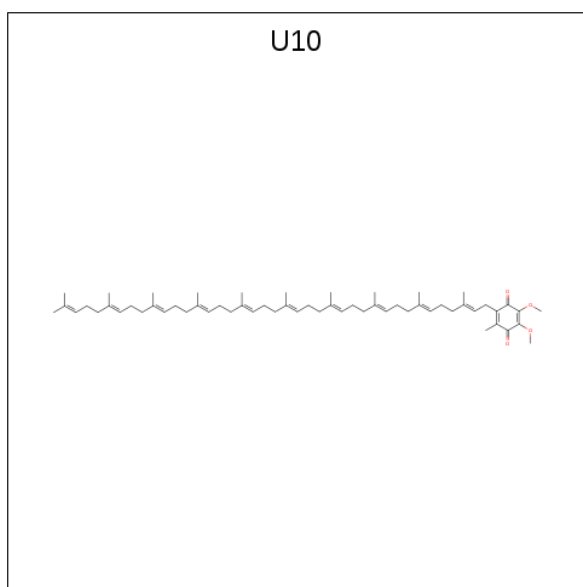
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



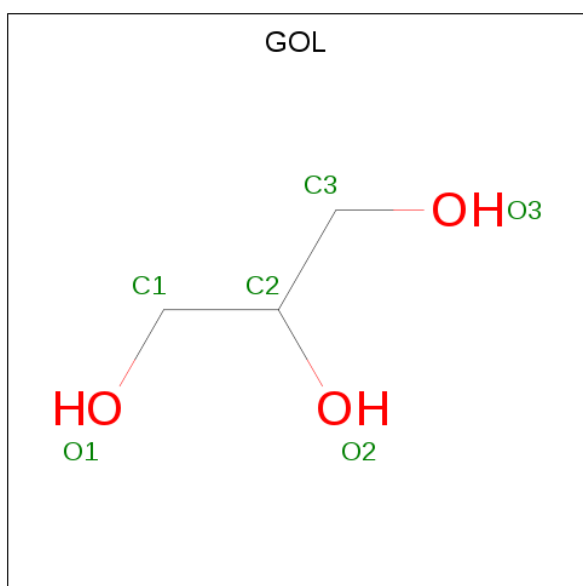
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- 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	H	1	Total	C	O	0	0
			6	3	3		

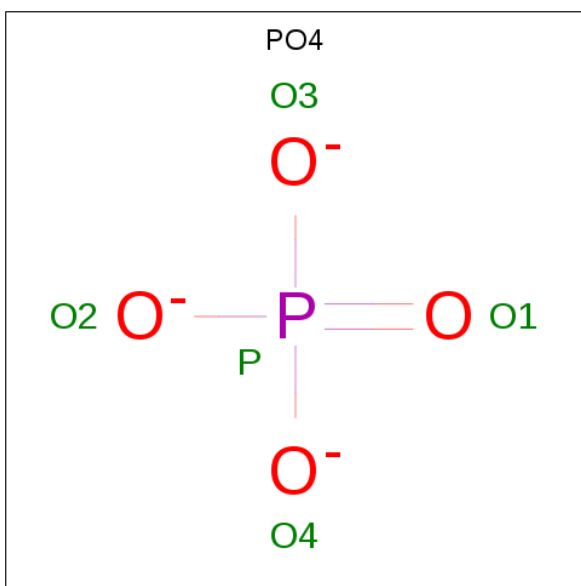
- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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).

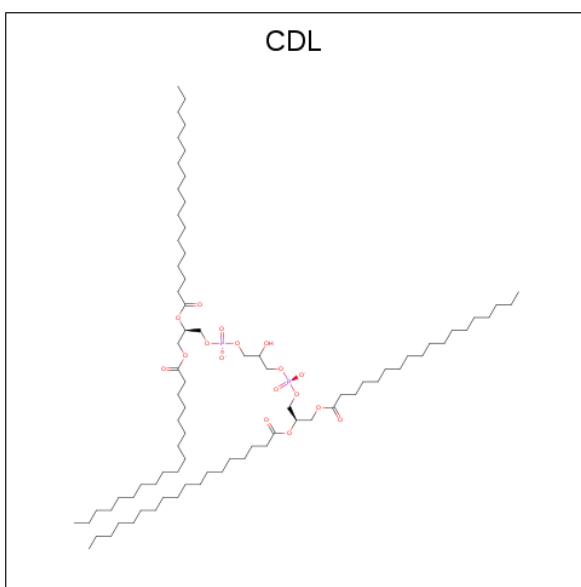
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	Cl	0	0
			1	1		
9	M	2	Total	Cl	0	0
			2	2		

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



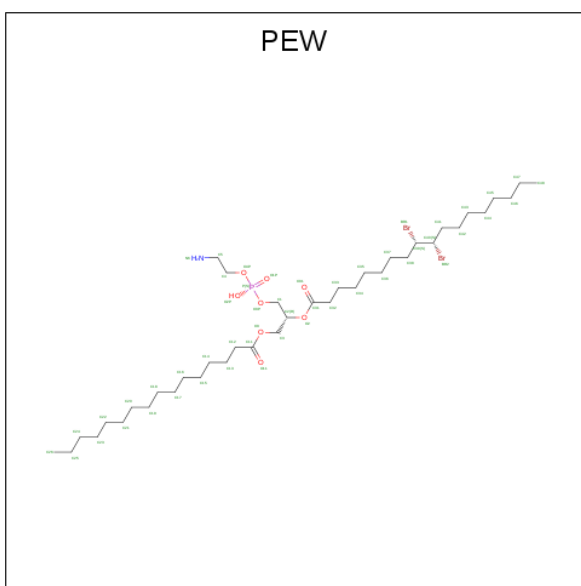
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		
10	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 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
11	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 12 is (1R)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (9S,10S)-9,10-DIBROMOOCTADECANOATE (three-letter code: PEW) (formula:  $C_{39}H_{76}Br_2NO_8P$ ).

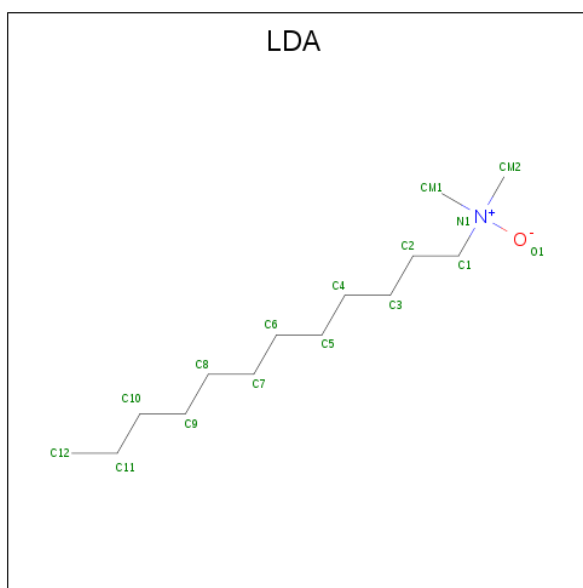


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	M	1	Total	Br	C	N	O	P	0	0
			51	2	39	1	8	1		

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:



C<sub>14</sub>H<sub>31</sub>NO).

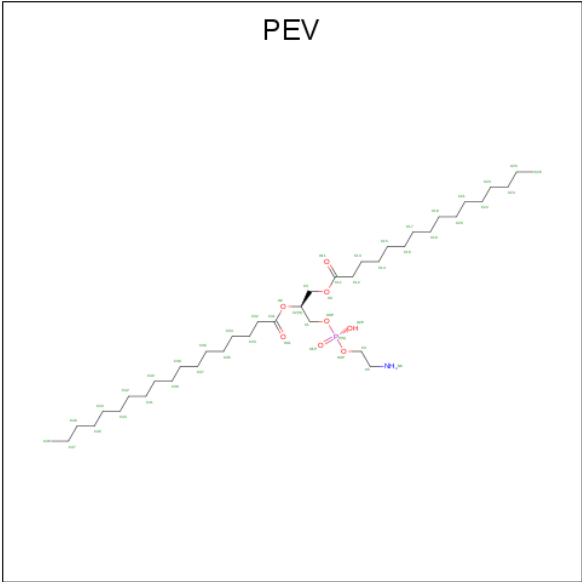


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		

- 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-{{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	C	N	O	P	0	1
			98	78	2	16	2		

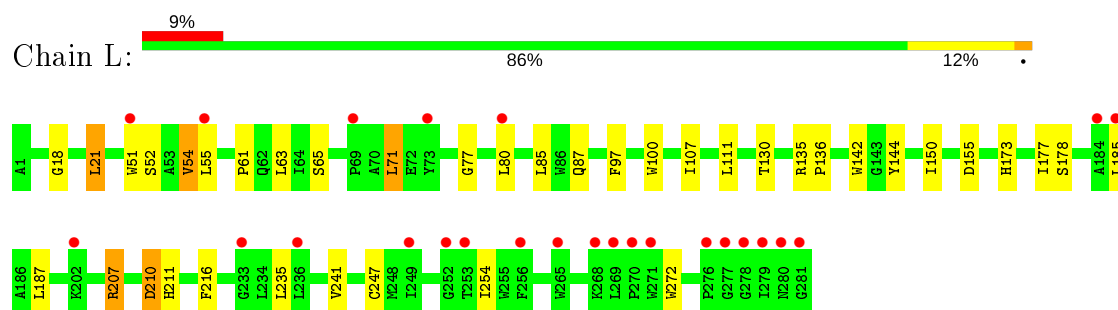
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	91	Total	O	0	0
			91	91		
16	M	118	Total	O	0	0
			118	118		
16	H	185	Total	O	0	0
			185	185		

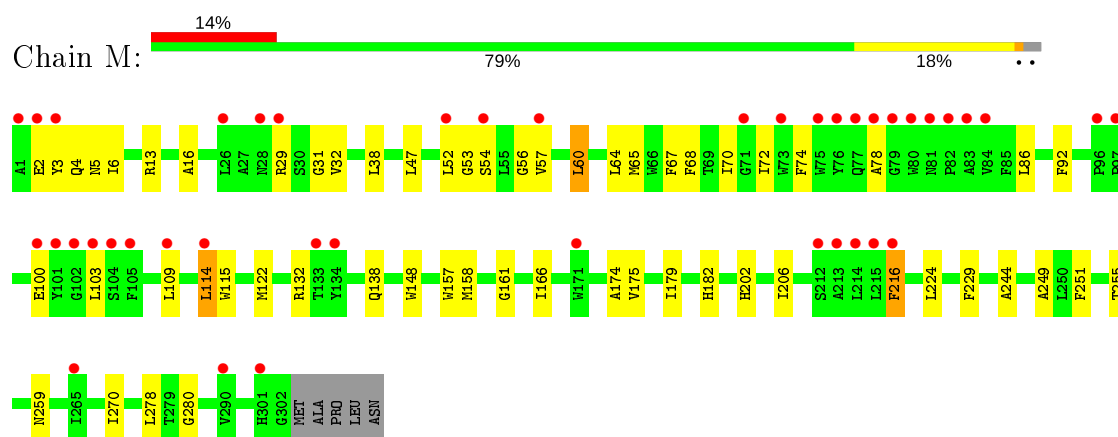
### 3 Residue-property plots [i](#)

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.

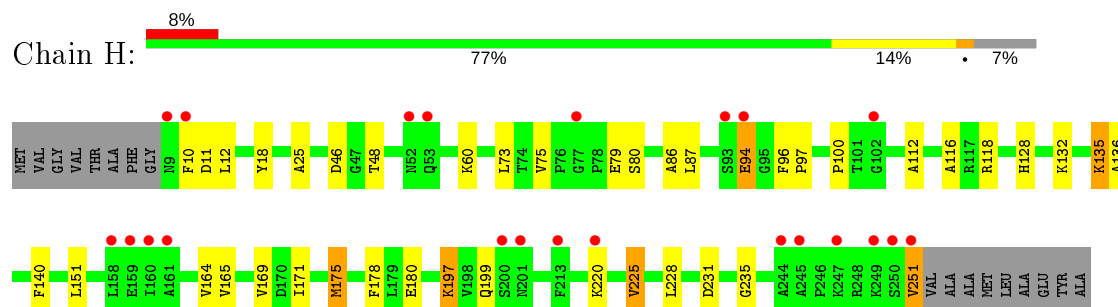
- Molecule 1: Reaction center protein L chain



- 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, $\alpha$ , $\beta$ , $\gamma$	139.29Å 139.29Å 183.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.01 – 2.75 46.01 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.01-2.75) 100.0 (46.01-2.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.182 , 0.222 0.186 , 0.229	Depositor DCC
$R_{free}$ test set	2689 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 106.5	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	0.92	EDS
Total number of atoms	7851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, PEV, PEW, FE, K, 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	0.87	0/2357	0.80	2/3228 (0.1%)
2	M	0.89	0/2617	0.84	2/3569 (0.1%)
3	H	0.92	1/1952 (0.1%)	0.87	3/2653 (0.1%)
All	All	0.89	1/6926 (0.0%)	0.84	7/9450 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	5.10	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASP	CB-CG-OD1	9.16	126.55	118.30
2	M	29	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	M	29	ARG	NE-CZ-NH2	-5.93	117.34	120.30
3	H	118[A]	ARG	NE-CZ-NH1	-5.49	117.55	120.30
3	H	118[B]	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	L	155	ASP	CB-CG-OD1	5.28	123.05	118.30
3	H	225	VAL	CB-CA-C	-5.14	101.62	111.40

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	2256	0	2215	32	0
2	M	2477	0	2381	47	0
3	H	1876	0	1893	28	0
4	L	132	0	148	10	0
4	M	132	0	148	14	0
5	L	65	0	76	3	0
5	M	65	0	76	9	0
6	L	48	0	63	7	0
6	M	48	0	63	0	0
7	H	6	0	8	1	0
7	L	6	0	8	0	0
8	M	1	0	0	0	0
9	H	1	0	0	0	0
9	M	2	0	0	0	0
10	H	5	0	0	1	0
10	M	10	0	0	2	0
11	M	81	0	106	2	0
12	M	51	0	73	11	0
13	H	48	0	93	17	0
13	M	48	0	93	13	0
14	H	1	0	0	0	0
15	H	98	0	154	13	0
16	H	185	0	0	6	0
16	L	91	0	0	1	0
16	M	118	0	0	0	0
All	All	7851	0	7598	152	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 10.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135[B]:ARG:HB3	1:L:136:PRO:HD3	1.18	1.16
11:M:800:CDL:H231	13:H:904:LDA:HM12	1.28	1.15
15:H:801[B]:PEV:H442	13:H:901:LDA:H121	1.10	1.05
1:L:135[B]:ARG:HB3	1:L:136:PRO:CD	1.87	1.02
1:L:135[B]:ARG:HG3	1:L:135[B]:ARG:HH21	1.28	0.95
15:H:801[B]:PEV:C44	13:H:901:LDA:H121	1.97	0.94
15:H:801[B]:PEV:H442	13:H:901:LDA:C12	1.97	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:31:GLY:H	12:M:802:PEW:H11	1.31	0.91
2:M:175:VAL:H	13:M:920:LDA:H122	1.32	0.90
15:H:801[A]:PEV:H442	13:H:901:LDA:C12	2.03	0.88
2:M:47:LEU:HD22	12:M:802:PEW:BR2	2.30	0.86
15:H:801[A]:PEV:H442	13:H:901:LDA:H121	1.55	0.85
1:L:135[B]:ARG:HH21	1:L:135[B]:ARG:CG	1.90	0.83
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.58	0.83
2:M:67[B]:PHE:HD2	2:M:68[B]:PHE:CE1	2.00	0.80
15:H:801[A]:PEV:C44	13:H:901:LDA:H121	2.10	0.80
2:M:70:ILE:HG21	13:M:920:LDA:HM23	1.70	0.74
2:M:67[B]:PHE:HD2	2:M:68[B]:PHE:CD1	2.07	0.73
4:M:313:BCL:C20	12:M:802:PEW:H263	2.19	0.73
3:H:46:ASP:OD1	3:H:48:THR:HG23	1.90	0.72
6:L:502:U10:H351	6:L:502:U10:H38	1.73	0.70
15:H:801[A]:PEV:H431	13:H:901:LDA:H121	1.74	0.69
2:M:70:ILE:HD13	13:M:920:LDA:HM22	1.76	0.67
10:H:705:PO4:P	16:H:1354:HOH:O	2.53	0.67
6:L:502:U10:H4M3	6:L:502:U10:H3M2	1.76	0.66
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.78	0.66
4:M:311:BCL:HBB2	4:M:311:BCL:HMB1	1.77	0.65
4:L:314:BCL:HBB3	5:L:402:BPH:H141	1.79	0.65
15:H:801[A]:PEV:C43	13:H:901:LDA:H121	2.23	0.65
2:M:31:GLY:N	12:M:802:PEW:H11	2.10	0.65
4:M:313:BCL:H203	12:M:802:PEW:H263	1.79	0.64
2:M:67[B]:PHE:CD2	2:M:68[B]:PHE:CE1	2.84	0.64
4:L:314:BCL:HBB2	4:L:314:BCL:HMB1	1.81	0.63
1:L:135[B]:ARG:CB	1:L:136:PRO:CD	2.69	0.62
1:L:77:GLY:HA2	1:L:87:GLN:OE1	2.00	0.62
1:L:71:LEU:HD21	1:L:144:TYR:CZ	2.34	0.61
1:L:61:PRO:O	1:L:150:ILE:HD12	2.00	0.61
1:L:135[B]:ARG:NH2	1:L:135[B]:ARG:CG	2.56	0.60
1:L:135[B]:ARG:CB	1:L:136:PRO:HD3	2.13	0.60
4:M:311:BCL:CBB	4:M:311:BCL:HMB1	2.32	0.60
2:M:70:ILE:HD13	13:M:920:LDA:CM2	2.32	0.59
6:L:502:U10:H351	6:L:502:U10:C38	2.32	0.59
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.84	0.59
1:L:71:LEU:HD13	1:L:71:LEU:O	2.03	0.58
4:M:313:BCL:H201	12:M:802:PEW:H263	1.85	0.58
2:M:67[B]:PHE:CD2	2:M:68[B]:PHE:HE1	2.21	0.58
1:L:97:PHE:CZ	4:L:312:BCL:H112	2.38	0.58
2:M:175:VAL:H	13:M:920:LDA:C12	2.11	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:311:BCL:H192	12:M:802:PEW:H191	1.85	0.57
3:H:128:HIS:HD2	16:H:1245:HOH:O	1.86	0.57
3:H:18:TYR:CD1	13:H:903:LDA:HM12	2.39	0.57
1:L:135[A]:ARG:HB3	1:L:136:PRO:HD3	1.85	0.57
2:M:53:GLY:O	2:M:57:VAL:HG23	2.04	0.57
4:L:312:BCL:CBB	4:L:312:BCL:HMB1	2.35	0.57
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.73	0.57
1:L:216:PHE:CD2	6:L:502:U10:H102	2.40	0.57
3:H:46:ASP:C	3:H:46:ASP:OD1	2.42	0.56
3:H:135:LYS:HG2	3:H:136:ALA:N	2.20	0.56
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.41	0.56
15:H:801[A]:PEV:C44	13:H:901:LDA:C12	2.75	0.55
2:M:70:ILE:HG21	13:M:920:LDA:CM2	2.37	0.55
15:H:801[B]:PEV:C44	13:H:901:LDA:C12	2.69	0.55
2:M:138:GLN:NE2	10:M:706:PO4:O2	2.40	0.55
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.43	0.54
6:L:502:U10:H4M3	6:L:502:U10:C3M	2.38	0.54
2:M:60[A]:LEU:HD12	5:M:401:BPH:H4C1	1.89	0.54
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.44	0.52
1:L:178:SER:HB3	6:L:502:U10:H251	1.92	0.52
2:M:67[B]:PHE:CD2	2:M:68[B]:PHE:CD1	2.95	0.52
5:M:401:BPH:CBC	5:M:401:BPH:HHH	2.39	0.52
4:M:313:BCL:H203	12:M:802:PEW:C26	2.40	0.52
5:M:401:BPH:HBC2	5:M:401:BPH:HHH	1.92	0.51
2:M:56:GLY:O	2:M:60[A]:LEU:HD22	2.10	0.51
2:M:174:ALA:HB1	13:M:920:LDA:C12	2.39	0.51
4:M:311:BCL:H141	5:M:401:BPH:H9C1	1.92	0.51
3:H:135:LYS:CG	3:H:136:ALA:N	2.74	0.51
1:L:52:SER:HA	1:L:55:LEU:CD1	2.41	0.50
1:L:241:VAL:HG21	5:L:402:BPH:H2C	1.93	0.49
1:L:65:SER:O	16:L:1324:HOH:O	2.20	0.49
2:M:74:PHE:CD1	2:M:92:PHE:HB3	2.48	0.49
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.47	0.49
5:M:401:BPH:CBC	5:M:401:BPH:CHD	2.90	0.49
2:M:179:ILE:HG12	13:M:920:LDA:HM13	1.95	0.49
2:M:280:GLY:O	4:M:313:BCL:HED3	2.13	0.48
2:M:78:ALA:HB2	2:M:92:PHE:CZ	2.48	0.47
3:H:135:LYS:HB3	3:H:135:LYS:HE3	1.24	0.47
4:M:313:BCL:HHC	4:M:313:BCL:OBB	2.14	0.47
1:L:80:LEU:HD22	1:L:85:LEU:CD2	2.45	0.47
3:H:135:LYS:HG2	3:H:136:ALA:H	1.80	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:109:LEU:HB3	2:M:114:LEU:HD22	1.97	0.46
5:M:401:BPH:C14	12:M:802:PEW:H182	2.45	0.46
4:L:312:BCL:HMB1	4:L:312:BCL:HBB3	1.97	0.46
13:M:902:LDA:H122	13:H:903:LDA:H121	1.97	0.46
1:L:135[B]:ARG:O	1:L:136:PRO:C	2.54	0.45
3:H:79:GLU:HB2	16:H:1235:HOH:O	2.15	0.45
2:M:249:ALA:HB1	2:M:259:ASN:ND2	2.31	0.45
5:M:401:BPH:CHD	5:M:401:BPH:HBC3	2.47	0.45
3:H:132:LYS:HG3	3:H:171:ILE:HD11	1.98	0.45
3:H:169:VAL:HG23	3:H:171:ILE:HD13	1.99	0.44
13:H:903:LDA:H91	13:H:904:LDA:H72	2.00	0.44
4:L:312:BCL:NA	4:M:313:BCL:HBB2	2.33	0.44
2:M:13:ARG:O	3:H:140:PHE:HA	2.18	0.44
1:L:52:SER:HA	1:L:55:LEU:HD12	1.99	0.44
3:H:112:ALA:HA	3:H:235:GLY:O	2.18	0.44
2:M:175:VAL:N	13:M:920:LDA:H122	2.15	0.44
3:H:175:MET:HE3	16:H:1139:HOH:O	2.17	0.44
1:L:51:TRP:O	1:L:54:VAL:HB	2.18	0.44
2:M:65[A]:MET:HB3	2:M:65[A]:MET:HE3	1.77	0.44
4:L:312:BCL:H52	5:L:402:BPH:HBB2	1.99	0.43
2:M:2[B]:GLU:O	2:M:4:GLN:NE2	2.51	0.43
15:H:801[A]:PEV:O31	15:H:801[A]:PEV:H32	2.18	0.43
15:H:801[A]:PEV:O31	15:H:801[A]:PEV:C3	2.66	0.43
3:H:18:TYR:HD1	13:H:903:LDA:HM12	1.82	0.43
2:M:115:TRP:HZ2	13:M:920:LDA:H121	1.84	0.43
4:L:314:BCL:CBB	4:L:314:BCL:HMB1	2.47	0.43
2:M:157:TRP:CZ3	2:M:158:MET:HG2	2.54	0.43
5:M:401:BPH:H142	12:M:802:PEW:H202	2.01	0.43
3:H:73:LEU:HD11	3:H:75:VAL:HG13	2.02	0.42
2:M:161:GLY:HA2	13:M:920:LDA:H123	2.01	0.42
3:H:116:ALA:HA	3:H:228:LEU:CD1	2.50	0.42
4:L:312:BCL:HHC	4:L:312:BCL:OBB	2.19	0.42
4:L:314:BCL:C4A	4:L:314:BCL:HBA1	2.49	0.42
2:M:6:ILE:HD13	2:M:224:LEU:HD13	2.01	0.42
15:H:801[A]:PEV:H431	13:H:903:LDA:H123	2.02	0.42
1:L:130:THR:O	1:L:135[B]:ARG:HB2	2.18	0.42
3:H:94:GLU:HG2	16:H:1242:HOH:O	2.20	0.42
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.55	0.42
2:M:270:ILE:HD13	11:M:800:CDL:C71	2.49	0.42
3:H:251:VAL:O	3:H:251:VAL:HG12	2.20	0.42
3:H:73:LEU:HD11	3:H:75:VAL:CG1	2.50	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.56	0.41
3:H:135:LYS:NZ	16:H:1306:HOH:O	2.50	0.41
2:M:103:LEU:HD21	2:M:166:ILE:HA	2.00	0.41
1:L:51:TRP:CH2	1:L:80:LEU:HD13	2.54	0.41
1:L:207:ARG:CG	1:L:211:HIS:CG	3.03	0.41
2:M:64:LEU:HD21	5:M:401:BPH:H121	2.02	0.41
13:M:902:LDA:H21	13:M:902:LDA:HM13	1.90	0.41
1:L:216:PHE:CE2	6:L:502:U10:H102	2.55	0.41
2:M:251:PHE:CD1	2:M:251:PHE:C	2.94	0.41
3:H:197[A]:LYS:CD	3:H:199:GLN:CG	2.98	0.41
4:M:313:BCL:HBD	4:M:313:BCL:HAA2	2.02	0.41
3:H:165:VAL:CG2	3:H:180:GLU:HG2	2.51	0.41
3:H:25:ALA:HB1	13:H:904:LDA:HM11	2.03	0.41
1:L:18:GLY:O	1:L:21:LEU:HB2	2.21	0.41
3:H:151:LEU:O	3:H:164:VAL:HG23	2.20	0.40
3:H:178:PHE:CE2	7:H:708:GOL:H11	2.57	0.40
4:M:313:BCL:C20	12:M:802:PEW:C26	2.96	0.40
2:M:122:MET:HE1	4:M:311:BCL:HBB3	2.02	0.40
1:L:107:ILE:HG22	1:L:111:LEU:HD12	2.03	0.40
2:M:54:SER:OG	10:M:704:PO4:O2	2.38	0.40
1:L:100:TRP:CZ2	2:M:255:THR:HG22	2.57	0.40
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.52	0.40

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	283/281 (101%)	268 (95%)	14 (5%)	1 (0%)	34	53
2	M	313/307 (102%)	299 (96%)	14 (4%)	0	100	100
3	H	247/260 (95%)	237 (96%)	9 (4%)	1 (0%)	34	53

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	843/848 (99%)	804 (95%)	37 (4%)	2 (0%)	47 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	86	ALA
1	L	54	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%)	214 (96%)	10 (4%)	27 46
2	M	249/240 (104%)	236 (95%)	13 (5%)	23 39
3	H	204/208 (98%)	191 (94%)	13 (6%)	17 31
All	All	677/668 (101%)	641 (95%)	36 (5%)	24 38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	63	LEU
1	L	71	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	247	CYS
1	L	254	ILE
1	L	272	TRP
2	M	38	LEU
2	M	52	LEU
2	M	60[A]	LEU
2	M	60[B]	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	72	ILE
2	M	86	LEU
2	M	100[A]	GLU
2	M	100[B]	GLU
2	M	114	LEU
2	M	132	ARG
2	M	182	HIS
2	M	216	PHE
2	M	278	LEU
3	H	10	PHE
3	H	11	ASP
3	H	12	LEU
3	H	60	LYS
3	H	80	SER
3	H	135	LYS
3	H	175	MET
3	H	197[A]	LYS
3	H	197[B]	LYS
3	H	220	LYS
3	H	225	VAL
3	H	231	ASP
3	H	251	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	4	GLN
2	M	28	ASN
2	M	202	HIS
3	H	9	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 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	M	920	-	12,15,15	1.93	1 (8%)	14,17,17	1.11	1 (7%)
13	LDA	M	902	-	12,15,15	1.86	1 (8%)	14,17,17	0.59	0
4	BCL	M	311	2	58,74,74	1.28	4 (6%)	69,115,115	1.62	17 (24%)
13	LDA	H	901	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
5	BPH	M	401	-	64,70,70	0.86	0	76,101,101	1.86	18 (23%)
6	U10	M	501	-	48,48,63	1.17	3 (6%)	58,61,79	1.55	11 (18%)
13	LDA	M	907	-	12,15,15	2.00	1 (8%)	14,17,17	0.70	0
13	LDA	H	903	-	12,15,15	1.97	1 (8%)	14,17,17	0.56	0
13	LDA	H	904	-	12,15,15	2.00	1 (8%)	14,17,17	0.57	0
7	GOL	L	707	-	5,5,5	0.46	0	5,5,5	0.57	0
7	GOL	H	708	-	5,5,5	0.31	0	5,5,5	0.68	0
5	BPH	L	402	-	64,70,70	0.92	3 (4%)	76,101,101	1.47	13 (17%)
6	U10	L	502	-	48,48,63	1.22	3 (6%)	58,61,79	1.75	13 (22%)
12	PEW	M	802	-	50,50,50	0.96	3 (6%)	53,57,57	1.32	5 (9%)
4	BCL	M	313	2	58,74,74	1.38	4 (6%)	69,115,115	1.73	15 (21%)
4	BCL	L	312	1	58,74,74	1.34	6 (10%)	69,115,115	1.38	10 (14%)
10	PO4	M	704	-	4,4,4	0.64	0	6,6,6	1.71	2 (33%)
10	PO4	M	706	-	4,4,4	0.91	0	6,6,6	0.90	0
11	CDL	M	800	-	80,80,99	1.30	5 (6%)	86,92,111	1.25	9 (10%)
15	PEV	H	801[A]	-	48,48,48	0.91	1 (2%)	51,53,53	1.04	4 (7%)
15	PEV	H	801[B]	-	48,48,48	0.95	2 (4%)	51,53,53	1.05	4 (7%)
4	BCL	L	314	1	58,74,74	1.02	3 (5%)	69,115,115	1.92	20 (28%)
10	PO4	H	705	-	4,4,4	1.05	0	6,6,6	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	M	920	-	-	7/13/13/13	-
13	LDA	M	907	-	-	7/13/13/13	-
13	LDA	H	903	-	-	2/13/13/13	-
4	BCL	L	312	1	-	5/37/137/137	-
13	LDA	M	902	-	-	3/13/13/13	-
13	LDA	H	904	-	-	6/13/13/13	-
5	BPH	L	402	-	-	9/54/105/105	0/5/6/6
7	GOL	L	707	-	-	4/4/4/4	-
7	GOL	H	708	-	-	1/4/4/4	-
11	CDL	M	800	-	-	37/91/91/110	-
13	LDA	H	901	-	-	6/13/13/13	-
6	U10	L	502	-	-	13/45/69/87	0/1/1/1
5	BPH	M	401	-	-	20/54/105/105	0/5/6/6
12	PEW	M	802	-	-	29/57/57/57	-
4	BCL	M	311	2	-	11/37/137/137	-
15	PEV	H	801[A]	-	-	20/52/52/52	-
6	U10	M	501	-	-	6/45/69/87	0/1/1/1
15	PEV	H	801[B]	-	-	28/52/52/52	-
4	BCL	L	314	1	-	6/37/137/137	-
4	BCL	M	313	2	-	8/37/137/137	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	901	LDA	O1-N1	-6.94	1.25	1.42
13	M	907	LDA	O1-N1	-6.83	1.26	1.42
13	H	904	LDA	O1-N1	-6.80	1.26	1.42
13	H	903	LDA	O1-N1	-6.75	1.26	1.42
13	M	920	LDA	O1-N1	-6.63	1.26	1.42
13	M	902	LDA	O1-N1	-6.32	1.27	1.42
4	L	312	BCL	MG-NA	5.77	2.20	2.06
11	M	800	CDL	OA8-CA7	5.48	1.49	1.33
4	M	313	BCL	MG-NA	5.38	2.19	2.06
4	M	311	BCL	C1B-NB	5.07	1.39	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	313	BCL	C4B-NB	5.01	1.39	1.35
6	L	502	U10	O3-C3	4.92	1.48	1.36
11	M	800	CDL	OA6-CA5	4.80	1.47	1.34
11	M	800	CDL	OB6-CB5	4.43	1.46	1.34
11	M	800	CDL	OB8-CB7	4.26	1.45	1.33
4	M	311	BCL	MG-NA	3.96	2.15	2.06
6	M	501	U10	O3-C3	3.90	1.46	1.36
15	H	801[B]	PEV	P-O1P	3.73	1.64	1.50
4	M	313	BCL	C3C-C4C	-3.54	1.47	1.51
4	L	312	BCL	C1B-NB	3.54	1.38	1.35
4	M	313	BCL	C1B-NB	3.43	1.38	1.35
12	M	802	PEW	P-O1P	3.43	1.63	1.50
4	L	312	BCL	C4B-NB	3.27	1.38	1.35
6	M	501	U10	O4-C4	3.21	1.44	1.36
6	L	502	U10	O4-C4	3.18	1.44	1.36
15	H	801[A]	PEV	P-O1P	3.06	1.61	1.50
6	M	501	U10	C31-C29	2.84	1.57	1.51
4	M	311	BCL	OBD-CAD	2.66	1.26	1.22
4	L	314	BCL	MG-NA	2.54	2.12	2.06
4	L	312	BCL	C4-C3	2.50	1.57	1.50
4	L	312	BCL	OBD-CAD	2.47	1.25	1.22
4	M	311	BCL	C4B-NB	2.47	1.37	1.35
6	L	502	U10	C13-C14	2.36	1.38	1.33
12	M	802	PEW	BR1-C39	-2.23	1.92	1.97
11	M	800	CDL	CA3-CA4	2.15	1.57	1.50
15	H	801[B]	PEV	C3-C2	2.14	1.57	1.50
4	L	314	BCL	C2A-C1A	-2.11	1.47	1.52
12	M	802	PEW	P-O4P	2.05	1.67	1.59
5	L	402	BPH	C4C-NC	2.03	1.41	1.37
4	L	314	BCL	O2A-CGA	2.03	1.39	1.33
5	L	402	BPH	C3D-C2D	2.02	1.43	1.39
5	L	402	BPH	O2D-CGD	2.01	1.38	1.33
4	L	312	BCL	MG-NC	2.00	2.11	2.06

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	OBD-CAD-CBD	-7.27	115.51	125.89
6	L	502	U10	C25-C24-C26	6.33	125.93	115.27
12	M	802	PEW	O2-C31-C32	5.37	123.08	111.50
11	M	800	CDL	OA6-CA5-C11	5.01	122.30	111.50
5	M	401	BPH	C4D-C3D-CAD	-4.97	104.72	107.87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	314	BCL	O2D-CGD-CBD	4.82	119.83	111.27
5	L	402	BPH	O2D-CGD-CBD	4.49	119.25	111.27
5	M	401	BPH	O2D-CGD-CBD	4.47	119.22	111.27
4	M	313	BCL	CAC-C3C-C2C	-4.44	103.17	114.26
4	L	314	BCL	O1D-CGD-CBD	-4.40	115.49	124.48
4	M	313	BCL	C1C-NC-C4C	4.39	108.68	106.71
4	M	311	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
4	L	312	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
4	M	313	BCL	C4D-C3D-CAD	-4.10	106.18	108.47
11	M	800	CDL	OB6-CB5-C51	4.10	120.33	111.50
6	M	501	U10	C17-C18-C19	-4.08	117.84	127.66
4	L	314	BCL	CAA-C2A-C3A	-4.01	101.79	112.78
6	L	502	U10	C25-C24-C23	-3.96	113.51	123.68
4	M	313	BCL	CMB-C2B-C1B	-3.95	122.39	128.46
4	M	313	BCL	C4B-C3B-CAB	-3.94	119.51	127.13
15	H	801[A]	PEV	O2-C31-C32	3.88	119.87	111.50
4	L	314	BCL	C4D-C3D-CAD	-3.86	106.32	108.47
5	L	402	BPH	C4D-C3D-CAD	-3.84	105.44	107.87
4	L	314	BCL	CAC-C3C-C4C	-3.83	104.08	112.58
5	M	401	BPH	OBD-CAD-C3D	3.72	134.15	127.98
15	H	801[B]	PEV	O2-C31-C32	3.71	119.50	111.50
5	L	402	BPH	CMD-C2D-C3D	3.59	131.40	124.68
6	M	501	U10	C31-C32-C33	3.57	123.61	111.88
6	M	501	U10	C30-C29-C31	3.53	121.22	115.27
12	M	802	PEW	BR1-C39-C40	-3.53	103.44	110.27
5	L	402	BPH	C1-C2-C3	-3.46	120.06	126.04
4	M	313	BCL	CAC-C3C-C4C	-3.44	104.96	112.58
5	M	401	BPH	C1-C2-C3	-3.42	120.13	126.04
5	M	401	BPH	CAA-C2A-C3A	-3.40	103.46	112.78
4	L	314	BCL	C2C-C3C-C4C	3.39	106.42	101.34
4	M	311	BCL	OBB-CAB-C3B	3.36	125.96	119.99
4	M	311	BCL	C1-O2A-CGA	3.31	125.14	116.44
4	L	314	BCL	CAC-C3C-C2C	-3.27	106.10	114.26
4	M	313	BCL	OBD-CAD-CBD	-3.24	121.26	125.89
12	M	802	PEW	BR2-C40-C39	-3.23	104.02	110.27
4	M	311	BCL	OBD-CAD-C3D	3.17	133.25	127.98
4	L	314	BCL	OBB-CAB-C3B	3.15	125.58	119.99
4	L	314	BCL	C4A-NA-C1A	3.13	108.11	106.71
6	M	501	U10	C22-C23-C24	-3.12	120.16	127.66
4	L	312	BCL	C5-C3-C2	-3.11	114.82	121.12
11	M	800	CDL	OB8-CB7-C71	3.09	121.59	111.91
4	M	313	BCL	CMB-C2B-C3B	3.07	130.43	124.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	311	BCL	O2D-CGD-CBD	3.07	116.73	111.27
6	L	502	U10	C22-C23-C24	-3.05	120.31	127.66
11	M	800	CDL	CA6-OA8-CA7	3.04	128.39	117.12
15	H	801[B]	PEV	O3-C3-C2	3.03	117.24	108.43
6	M	501	U10	C16-C14-C13	-3.02	115.01	121.12
4	L	314	BCL	CAA-CBA-CGA	3.01	122.06	113.25
4	L	314	BCL	C16-C15-C13	-2.99	106.24	115.92
6	L	502	U10	C30-C29-C31	2.98	120.28	115.27
10	M	704	PO4	O4-P-O1	-2.97	100.03	110.89
5	M	401	BPH	CHD-C4C-NC	-2.97	121.68	125.20
4	L	312	BCL	CAA-C2A-C3A	-2.93	104.74	112.78
4	L	314	BCL	C5-C3-C2	-2.92	115.20	121.12
4	M	313	BCL	CHA-C1A-NA	-2.91	119.74	126.40
4	M	311	BCL	CMB-C2B-C3B	2.90	130.11	124.68
4	M	313	BCL	C2C-C3C-C4C	2.90	105.68	101.34
5	M	401	BPH	CMC-C2C-C1C	2.89	120.16	112.09
6	L	502	U10	C1-C6-C5	-2.89	116.87	119.58
11	M	800	CDL	O1-C1-CB2	2.88	119.67	109.56
6	M	501	U10	C26-C27-C28	-2.86	102.49	111.88
6	L	502	U10	O2-C2-C3	-2.85	114.87	120.93
4	M	313	BCL	C4-C3-C5	2.85	120.07	115.27
13	M	920	LDA	CM1-N1-C1	2.84	116.21	110.23
4	L	314	BCL	CMD-C2D-C3D	2.83	129.98	124.68
15	H	801[A]	PEV	O2-C2-C3	2.83	118.65	108.40
6	M	501	U10	C41-C39-C40	2.83	120.85	114.60
4	M	311	BCL	CAA-C2A-C3A	-2.80	105.10	112.78
5	L	402	BPH	CMA-C3A-C2A	-2.80	102.53	113.83
5	M	401	BPH	C1B-NB-C4B	2.79	111.76	106.51
4	L	314	BCL	CMB-C2B-C1B	-2.75	124.24	128.46
4	M	311	BCL	OBD-CAD-CBD	-2.71	122.02	125.89
4	L	312	BCL	CMB-C2B-C3B	2.66	129.66	124.68
15	H	801[A]	PEV	O3-C3-C2	2.64	116.11	108.43
15	H	801[B]	PEV	O3-C11-C12	2.63	120.16	111.91
4	L	314	BCL	OBB-CAB-CBB	-2.62	114.27	120.17
5	M	401	BPH	O2D-CGD-O1D	-2.60	118.75	123.84
5	M	401	BPH	C1-O2A-CGA	2.60	123.26	116.44
4	M	313	BCL	OBD-CAD-C3D	2.59	132.28	127.98
4	M	311	BCL	C4A-NA-C1A	2.58	107.87	106.71
10	M	704	PO4	O4-P-O3	2.58	116.24	107.97
5	L	402	BPH	C1B-NB-C4B	2.58	111.36	106.51
5	M	401	BPH	CAC-C3C-C4C	2.55	119.21	112.67
5	L	402	BPH	O2D-CGD-O1D	-2.54	118.87	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	CAA-C2A-C1A	-2.53	105.78	112.33
6	L	502	U10	C3M-O3-C3	2.52	125.41	116.47
6	M	501	U10	C15-C14-C16	2.52	119.50	115.27
4	L	314	BCL	C4B-C3B-CAB	-2.48	122.34	127.13
12	M	802	PEW	O2-C31-O31	-2.46	117.75	123.70
4	L	312	BCL	C4-C3-C5	2.46	119.41	115.27
6	L	502	U10	C36-C34-C33	2.46	126.10	121.12
4	M	313	BCL	O2A-C1-C2	2.44	115.04	108.64
6	L	502	U10	C12-C13-C14	-2.41	121.85	127.66
6	M	501	U10	C7-C6-C5	-2.40	115.59	118.48
15	H	801[A]	PEV	O3-C11-C12	2.40	119.43	111.91
4	M	311	BCL	CMA-C3A-C4A	-2.39	105.34	111.77
4	L	312	BCL	CHA-C1A-NA	-2.36	120.98	126.40
4	L	312	BCL	C6-C7-C8	-2.36	108.31	115.92
4	M	311	BCL	CED-O2D-CGD	-2.35	110.62	115.94
11	M	800	CDL	OA8-CA7-C31	2.34	119.26	111.91
6	L	502	U10	C7-C8-C9	-2.34	122.90	126.79
4	L	312	BCL	C4B-C3B-CAB	-2.30	122.68	127.13
4	M	311	BCL	CHA-C1A-NA	-2.30	121.14	126.40
4	L	312	BCL	CAC-C3C-C2C	-2.28	108.57	114.26
4	M	311	BCL	O2A-C1-C2	2.25	114.56	108.64
5	M	401	BPH	C2B-C1B-NB	-2.25	106.40	109.79
4	M	313	BCL	O2D-CGD-O1D	-2.24	119.46	123.84
5	L	402	BPH	CMC-C2C-C3C	2.24	122.86	113.83
5	L	402	BPH	CBC-CAC-C3C	2.24	118.45	113.47
4	M	311	BCL	C3D-CAD-CBD	-2.24	104.66	107.61
4	M	313	BCL	C1-C2-C3	-2.22	122.20	126.04
5	M	401	BPH	C2C-C3C-C4C	2.22	104.66	101.34
4	L	314	BCL	C16-C17-C18	-2.22	105.54	115.98
5	L	402	BPH	OBD-CAD-CBD	-2.22	122.73	125.89
6	L	502	U10	C21-C22-C23	-2.21	104.60	111.88
5	L	402	BPH	CED-O2D-CGD	2.21	120.94	115.94
4	L	312	BCL	CAA-C2A-C1A	-2.21	104.73	111.97
4	M	311	BCL	CMD-C2D-C3D	2.21	128.81	124.68
5	M	401	BPH	CMA-C3A-C2A	-2.20	104.96	113.83
12	M	802	PEW	C2-O2-C31	-2.18	112.41	117.79
4	L	314	BCL	CAA-C2A-C1A	-2.18	104.83	111.97
5	L	402	BPH	C4D-CHA-C1A	-2.18	125.13	130.51
4	L	314	BCL	C11-C12-C13	-2.17	108.92	115.92
5	M	401	BPH	C4-C3-C2	-2.12	118.23	123.68
11	M	800	CDL	OB8-CB7-OB9	-2.10	118.29	123.59
6	M	501	U10	C10-C9-C11	2.09	118.79	115.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	C3D-CAD-CBD	2.07	110.33	107.61
5	M	401	BPH	CAC-C3C-C2C	-2.06	109.10	114.26
11	M	800	CDL	OA6-CA5-OA7	-2.06	118.72	123.70
15	H	801[B]	PEV	O2-C31-O31	-2.06	118.72	123.70
6	L	502	U10	C35-C34-C33	-2.06	118.39	123.68
4	M	311	BCL	C1B-CHB-C4A	-2.05	126.06	130.12
11	M	800	CDL	PB2-OB2-CB2	2.03	133.56	121.68
6	L	502	U10	C7-C6-C5	-2.02	116.04	118.48
6	M	501	U10	C31-C29-C28	-2.02	117.03	121.12
4	L	314	BCL	CHB-C4A-NA	2.01	127.30	124.51
4	M	311	BCL	CMC-C2C-C3C	-2.00	105.75	113.83

There are no chirality outliers.

All (228) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	920	LDA	C2-C1-N1-O1
13	M	920	LDA	C2-C1-N1-CM1
4	M	311	BCL	C11-C12-C13-C14
5	M	401	BPH	C4C-C3C-CAC-CBC
5	M	401	BPH	C2C-C3C-CAC-CBC
5	M	401	BPH	C4B-C3B-CAB-CBB
5	M	401	BPH	C4B-C3B-CAB-OB
5	M	401	BPH	C2B-C3B-CAB-CBB
5	M	401	BPH	C2B-C3B-CAB-OB
13	H	904	LDA	N1-C1-C2-C3
7	L	707	GOL	O1-C1-C2-C3
5	L	402	BPH	C4C-C3C-CAC-CBC
12	M	802	PEW	C40-C41-C42-C43
12	M	802	PEW	BR1-C39-C40-C41
12	M	802	PEW	C38-C39-C40-C41
12	M	802	PEW	C38-C39-C40-BR2
12	M	802	PEW	C1-O3P-P-O1P
12	M	802	PEW	C1-O3P-P-O2P
12	M	802	PEW	C4-O4P-P-O1P
12	M	802	PEW	C4-O4P-P-O2P
12	M	802	PEW	O11-C11-O3-C3
11	M	800	CDL	CA2-C1-CB2-OB2
11	M	800	CDL	CA2-OA2-PA1-OA3
11	M	800	CDL	CA2-OA2-PA1-OA4
11	M	800	CDL	CA2-OA2-PA1-OA5
11	M	800	CDL	C1-CB2-OB2-PB2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
11	M	800	CDL	CB3-OB5-PB2-OB2
11	M	800	CDL	CB3-OB5-PB2-OB3
11	M	800	CDL	CB3-OB5-PB2-OB4
11	M	800	CDL	OB6-CB4-CB6-OB8
15	H	801[A]	PEV	C1-O3P-P-O1P
15	H	801[A]	PEV	O4P-C4-C5-N6
15	H	801[B]	PEV	C32-C31-O2-C2
15	H	801[B]	PEV	C1-O3P-P-O1P
15	H	801[B]	PEV	C4-O4P-P-O1P
15	H	801[B]	PEV	C4-O4P-P-O2P
12	M	802	PEW	C12-C11-O3-C3
15	H	801[B]	PEV	C12-C11-O3-C3
15	H	801[B]	PEV	O31-C31-O2-C2
11	M	800	CDL	O1-C1-CB2-OB2
15	H	801[B]	PEV	O11-C11-O3-C3
11	M	800	CDL	C36-C37-C38-C39
5	M	401	BPH	C11-C12-C13-C14
11	M	800	CDL	C38-C39-C40-C41
11	M	800	CDL	CB7-C71-C72-C73
15	H	801[B]	PEV	C31-C32-C33-C34
5	M	401	BPH	C8-C10-C11-C12
4	M	313	BCL	C13-C15-C16-C17
15	H	801[A]	PEV	C11-C12-C13-C14
5	M	401	BPH	C12-C13-C15-C16
12	M	802	PEW	C1-O3P-P-O4P
12	M	802	PEW	C4-O4P-P-O3P
15	H	801[B]	PEV	C4-O4P-P-O3P
13	H	901	LDA	C11-C10-C9-C8
4	M	311	BCL	C16-C17-C18-C20
12	M	802	PEW	C19-C20-C21-C22
11	M	800	CDL	C18-C19-C20-C21
13	H	901	LDA	C5-C6-C7-C8
15	H	801[A]	PEV	C19-C20-C21-C22
15	H	801[B]	PEV	C37-C38-C39-C40
13	M	920	LDA	C7-C8-C9-C10
15	H	801[B]	PEV	C21-C22-C23-C24
5	L	402	BPH	C4-C3-C5-C6
13	H	904	LDA	C7-C8-C9-C10
12	M	802	PEW	C15-C16-C17-C18
11	M	800	CDL	C78-C79-C80-C81
4	M	313	BCL	C6-C7-C8-C9
4	L	314	BCL	C14-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	H	708	GOL	O1-C1-C2-C3
5	L	402	BPH	C8-C10-C11-C12
12	M	802	PEW	C32-C31-O2-C2
13	M	920	LDA	C4-C5-C6-C7
13	M	920	LDA	C5-C6-C7-C8
13	H	901	LDA	C6-C7-C8-C9
15	H	801[A]	PEV	C36-C37-C38-C39
15	H	801[B]	PEV	C43-C44-C45-C46
5	M	401	BPH	C16-C17-C18-C20
12	M	802	PEW	C34-C35-C36-C37
7	L	707	GOL	O1-C1-C2-O2
11	M	800	CDL	C20-C21-C22-C23
13	M	902	LDA	C1-C2-C3-C4
13	H	901	LDA	C1-C2-C3-C4
13	H	904	LDA	C2-C3-C4-C5
12	M	802	PEW	O31-C31-O2-C2
15	H	801[B]	PEV	C16-C17-C18-C19
15	H	801[A]	PEV	C2-C1-O3P-P
13	H	904	LDA	C1-C2-C3-C4
13	M	907	LDA	C11-C10-C9-C8
15	H	801[B]	PEV	C11-C12-C13-C14
11	M	800	CDL	C71-C72-C73-C74
15	H	801[A]	PEV	C37-C38-C39-C40
5	L	402	BPH	C2-C3-C5-C6
15	H	801[A]	PEV	O31-C31-O2-C2
15	H	801[A]	PEV	C32-C33-C34-C35
11	M	800	CDL	C72-C73-C74-C75
15	H	801[B]	PEV	C14-C15-C16-C17
15	H	801[A]	PEV	C32-C31-O2-C2
11	M	800	CDL	C17-C18-C19-C20
15	H	801[B]	PEV	C17-C18-C19-C20
4	M	311	BCL	C16-C17-C18-C19
13	H	903	LDA	C7-C8-C9-C10
15	H	801[A]	PEV	C15-C16-C17-C18
11	M	800	CDL	OA5-CA3-CA4-CA6
11	M	800	CDL	C13-C14-C15-C16
11	M	800	CDL	C19-C20-C21-C22
15	H	801[B]	PEV	C18-C19-C20-C21
11	M	800	CDL	CB3-CB4-CB6-OB8
13	H	901	LDA	C9-C10-C11-C12
12	M	802	PEW	C11-C12-C13-C14
15	H	801[B]	PEV	C19-C20-C21-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	M	907	LDA	C2-C3-C4-C5
5	L	402	BPH	C2B-C3B-CAB-OBB
6	M	501	U10	C33-C34-C36-C37
15	H	801[A]	PEV	C3-C2-O2-C31
15	H	801[B]	PEV	C1-C2-O2-C31
13	M	907	LDA	C1-C2-C3-C4
13	M	920	LDA	C3-C4-C5-C6
13	M	907	LDA	C6-C7-C8-C9
13	M	907	LDA	C9-C10-C11-C12
5	M	401	BPH	C15-C16-C17-C18
15	H	801[A]	PEV	C44-C45-C46-C47
6	M	501	U10	C35-C34-C36-C37
5	M	401	BPH	C11-C12-C13-C15
15	H	801[A]	PEV	C12-C13-C14-C15
12	M	802	PEW	C39-C40-C41-C42
6	L	502	U10	C20-C19-C21-C22
4	L	312	BCL	C15-C16-C17-C18
12	M	802	PEW	C12-C13-C14-C15
11	M	800	CDL	CA3-CA4-CA6-OA8
12	M	802	PEW	C14-C15-C16-C17
11	M	800	CDL	C74-C75-C76-C77
15	H	801[A]	PEV	C1-O3P-P-O4P
11	M	800	CDL	OA5-CA3-CA4-OA6
11	M	800	CDL	C55-C56-C57-C58
13	H	904	LDA	C6-C7-C8-C9
6	M	501	U10	C24-C26-C27-C28
13	M	907	LDA	C7-C8-C9-C10
5	M	401	BPH	C16-C17-C18-C19
4	M	311	BCL	C11-C12-C13-C15
6	L	502	U10	C18-C19-C21-C22
4	M	313	BCL	C6-C7-C8-C10
5	L	402	BPH	C4B-C3B-CAB-OBB
5	M	401	BPH	C10-C11-C12-C13
11	M	800	CDL	C79-C80-C81-C82
11	M	800	CDL	C31-CA7-OA8-CA6
5	M	401	BPH	CAD-CBD-CGD-O2D
11	M	800	CDL	OA9-CA7-OA8-CA6
12	M	802	PEW	O3P-C1-C2-O2
15	H	801[A]	PEV	C13-C14-C15-C16
13	M	920	LDA	C2-C1-N1-CM2
11	M	800	CDL	OA6-CA4-CA6-OA8
7	L	707	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	L	502	U10	C15-C14-C16-C17
11	M	800	CDL	C51-C52-C53-C54
13	H	903	LDA	C6-C7-C8-C9
12	M	802	PEW	O3P-C1-C2-C3
5	M	401	BPH	C6-C7-C8-C10
13	M	902	LDA	C4-C5-C6-C7
15	H	801[B]	PEV	C36-C37-C38-C39
4	L	312	BCL	C4-C3-C5-C6
15	H	801[A]	PEV	C18-C19-C20-C21
5	M	401	BPH	C6-C7-C8-C9
5	M	401	BPH	C14-C13-C15-C16
12	M	802	PEW	C22-C23-C24-C25
15	H	801[B]	PEV	C32-C33-C34-C35
6	L	502	U10	C5-C4-O4-C4M
6	L	502	U10	C13-C14-C16-C17
15	H	801[B]	PEV	C12-C13-C14-C15
15	H	801[B]	PEV	C1-O3P-P-O4P
15	H	801[B]	PEV	C1-C2-C3-O3
4	L	314	BCL	C12-C13-C15-C16
4	M	311	BCL	C3-C5-C6-C7
5	M	401	BPH	C3-C5-C6-C7
4	L	314	BCL	C15-C16-C17-C18
6	M	501	U10	C31-C32-C33-C34
13	M	902	LDA	C5-C6-C7-C8
4	M	311	BCL	C13-C15-C16-C17
15	H	801[B]	PEV	C23-C24-C25-C26
12	M	802	PEW	BR2-C40-C41-C42
11	M	800	CDL	C14-C15-C16-C17
13	H	901	LDA	C2-C3-C4-C5
11	M	800	CDL	C40-C41-C42-C43
11	M	800	CDL	OB7-CB5-OB6-CB4
4	M	311	BCL	C12-C13-C15-C16
6	M	501	U10	C5-C4-O4-C4M
13	M	907	LDA	C4-C5-C6-C7
13	H	904	LDA	C11-C10-C9-C8
6	L	502	U10	C12-C11-C9-C10
12	M	802	PEW	O2-C31-C32-C33
7	L	707	GOL	C1-C2-C3-O3
4	M	311	BCL	C4C-C3C-CAC-CBC
6	L	502	U10	C34-C36-C37-C38
15	H	801[B]	PEV	C34-C35-C36-C37
4	L	314	BCL	C16-C17-C18-C19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	L	502	U10	C3-C4-O4-C4M
15	H	801[A]	PEV	O2-C31-C32-C33
11	M	800	CDL	C15-C16-C17-C18
4	M	313	BCL	C4-C3-C5-C6
4	M	311	BCL	CAD-CBD-CGD-O2D
5	L	402	BPH	CAD-CBD-CGD-O2D
4	M	313	BCL	CAD-CBD-CGD-O2D
4	L	312	BCL	CAD-CBD-CGD-O2D
15	H	801[A]	PEV	C16-C17-C18-C19
5	M	401	BPH	O2A-C1-C2-C3
5	L	402	BPH	O2A-C1-C2-C3
4	L	314	BCL	CHA-CBD-CGD-O1D
4	L	314	BCL	CHA-CBD-CGD-O2D
6	L	502	U10	C12-C11-C9-C8
4	M	311	BCL	C15-C16-C17-C18
6	L	502	U10	C28-C29-C31-C32
4	M	313	BCL	C2-C3-C5-C6
4	L	312	BCL	C2-C3-C5-C6
12	M	802	PEW	O3-C11-C12-C13
4	M	313	BCL	CAA-CBA-CGA-O2A
6	L	502	U10	C9-C11-C12-C13
15	H	801[B]	PEV	C41-C42-C43-C44
6	L	502	U10	C11-C12-C13-C14
15	H	801[A]	PEV	O31-C31-C32-C33
5	L	402	BPH	C2B-C3B-CAB-CBB
6	L	502	U10	C31-C32-C33-C34
12	M	802	PEW	O4P-C4-C5-N6
6	M	501	U10	C25-C24-C26-C27
12	M	802	PEW	C5-C4-O4P-P
4	M	313	BCL	CAD-CBD-CGD-O1D
15	H	801[B]	PEV	C5-C4-O4P-P
4	M	311	BCL	C14-C13-C15-C16
4	L	312	BCL	C11-C10-C8-C9
11	M	800	CDL	C72-C71-CB7-OB8

There are no ring outliers.

20 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	920	LDA	11	0
13	M	902	LDA	2	0
4	M	311	BCL	5	0

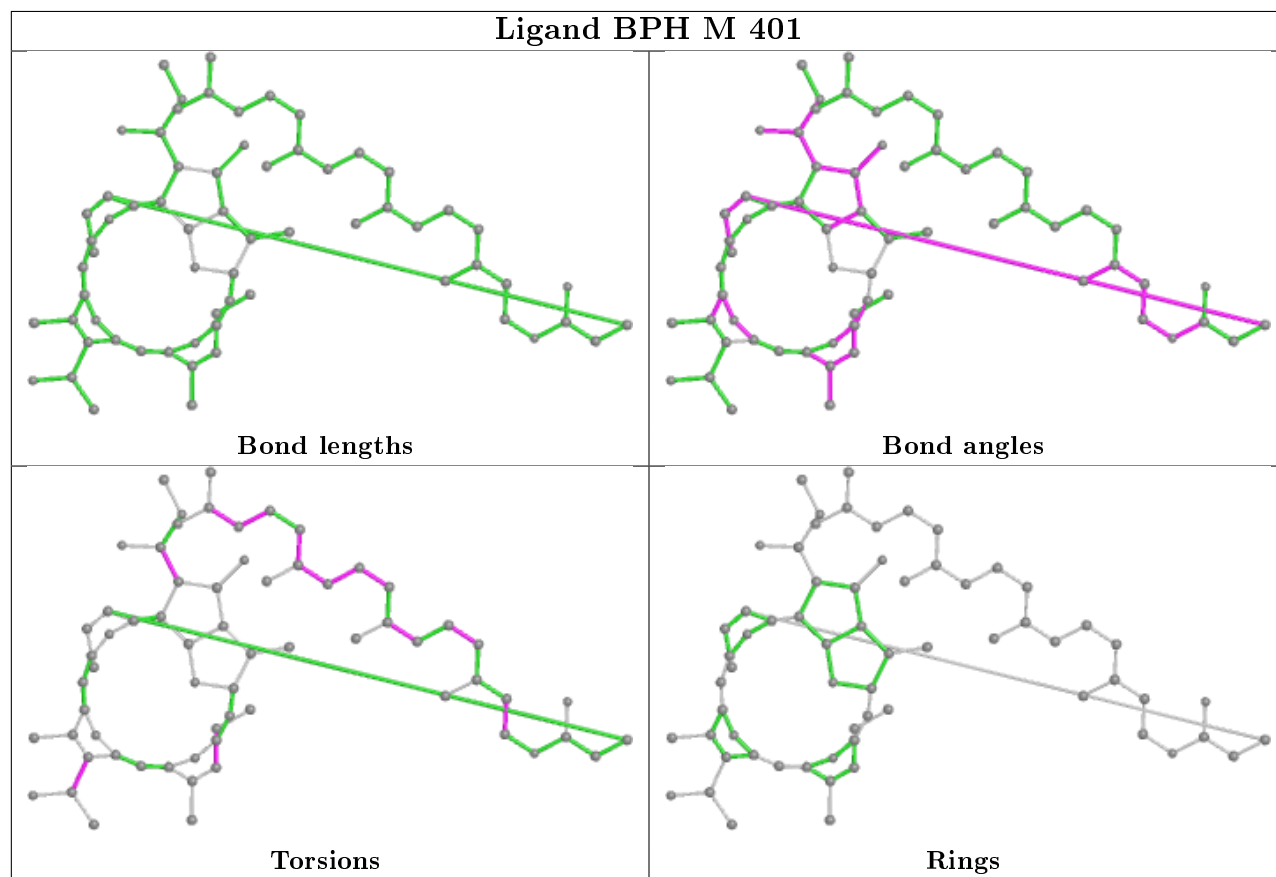
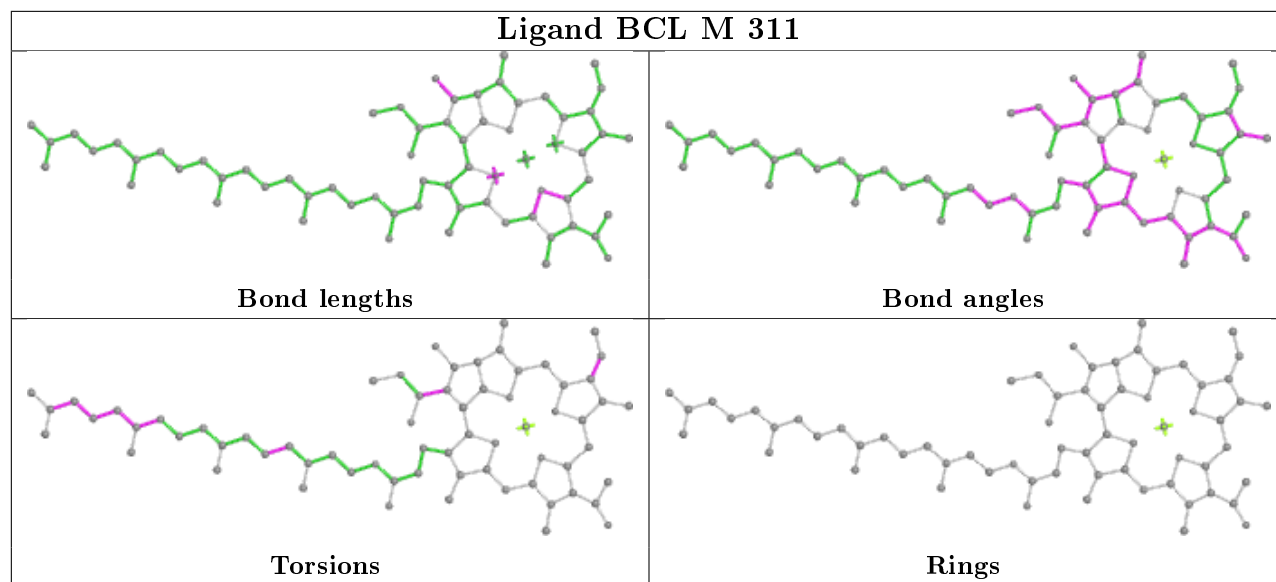
*Continued on next page...*



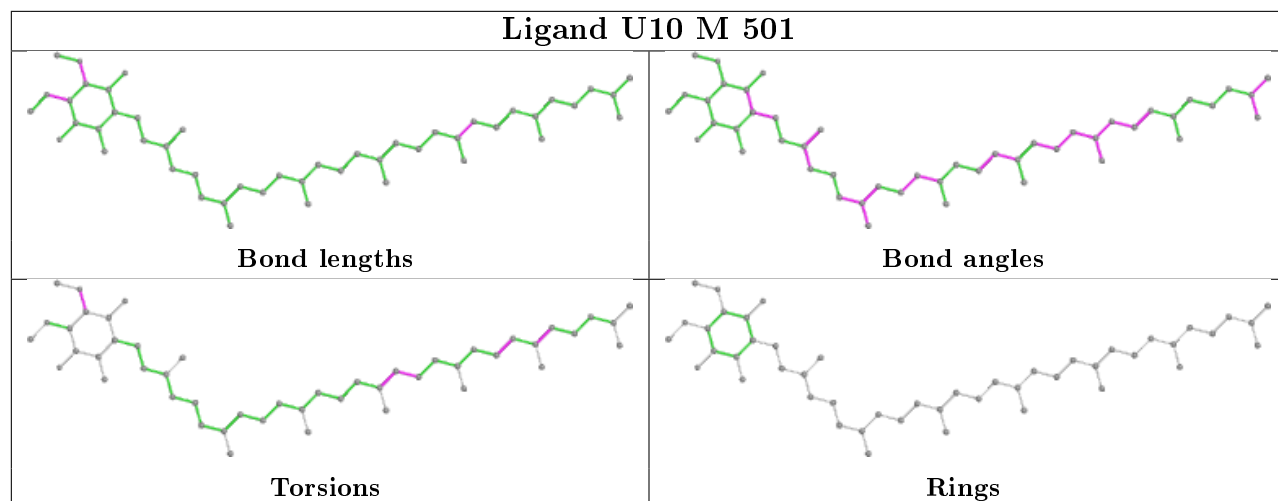
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	901	LDA	10	0
5	M	401	BPH	9	0
13	H	903	LDA	5	0
13	H	904	LDA	3	0
7	H	708	GOL	1	0
5	L	402	BPH	3	0
6	L	502	U10	7	0
12	M	802	PEW	11	0
4	M	313	BCL	9	0
4	L	312	BCL	6	0
10	M	704	PO4	1	0
10	M	706	PO4	1	0
11	M	800	CDL	2	0
15	H	801[A]	PEV	9	0
15	H	801[B]	PEV	4	0
4	L	314	BCL	4	0
10	H	705	PO4	1	0

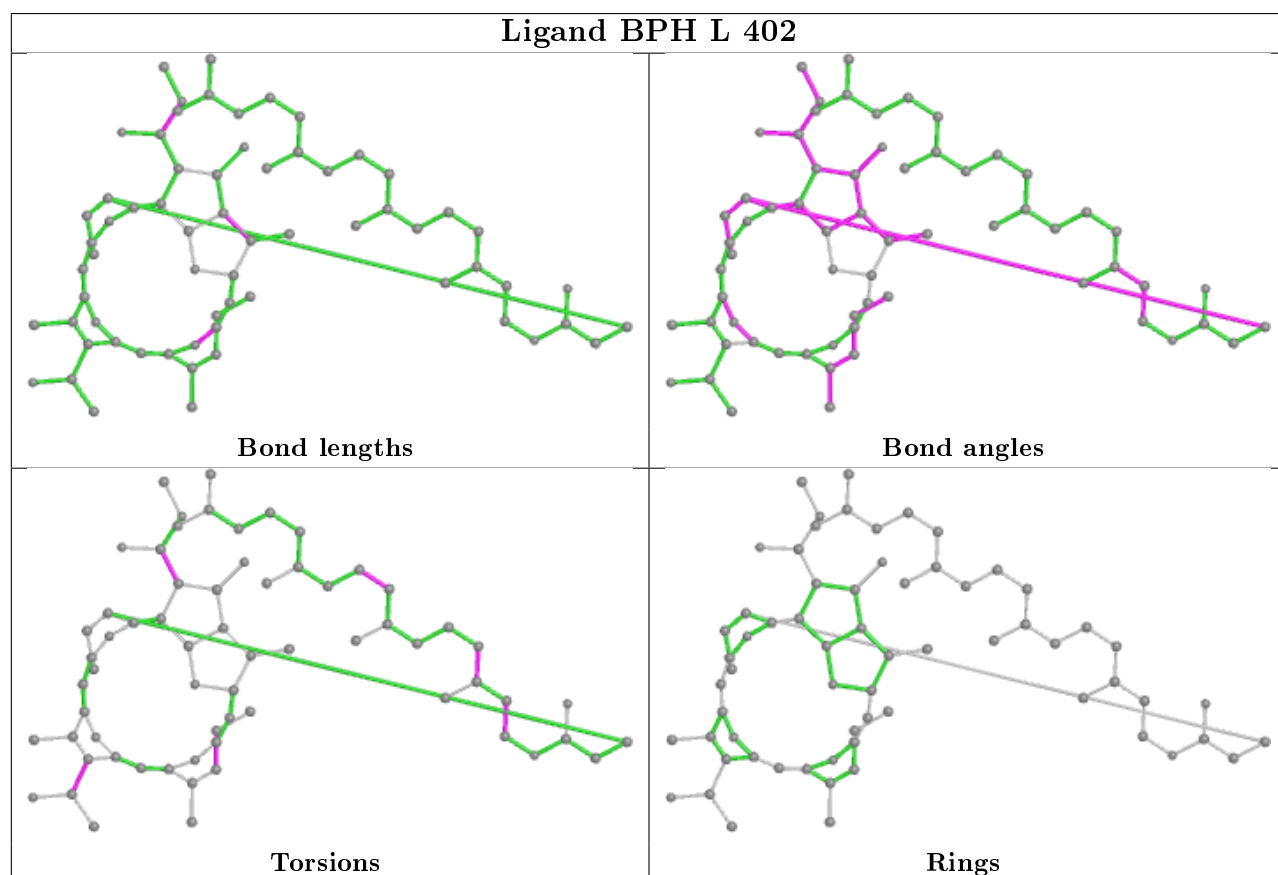
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

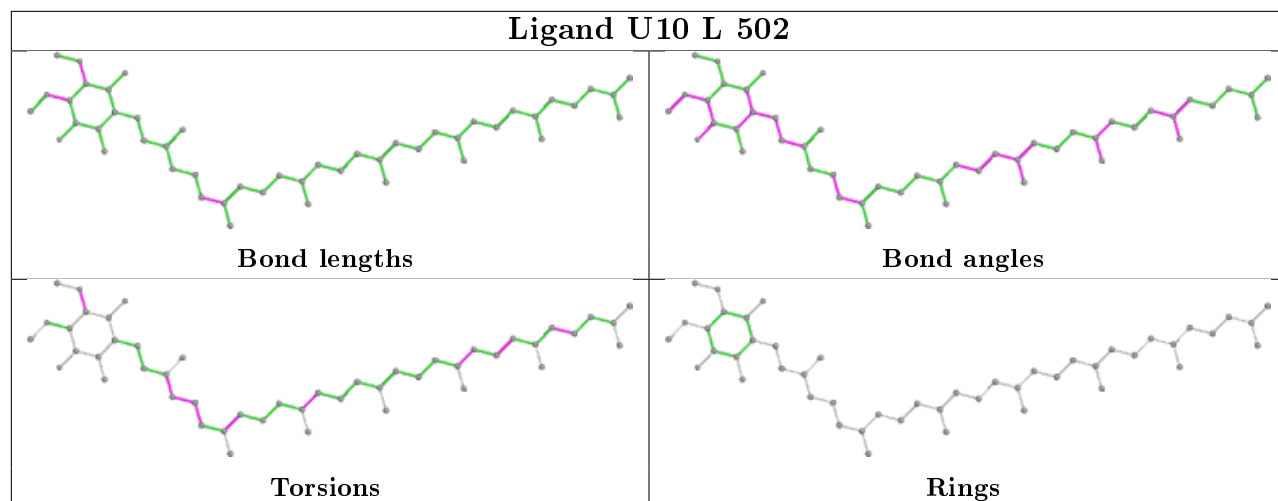
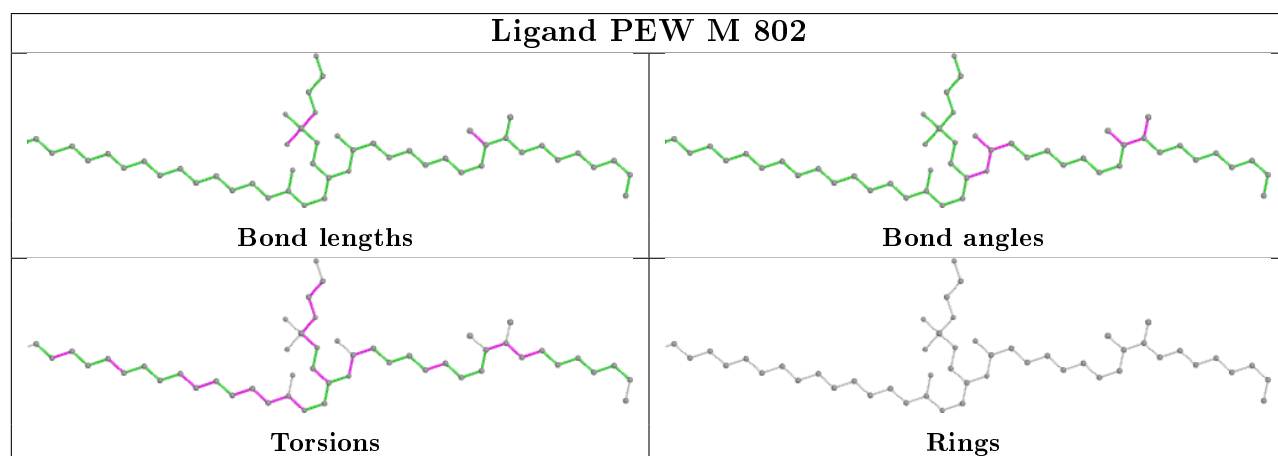
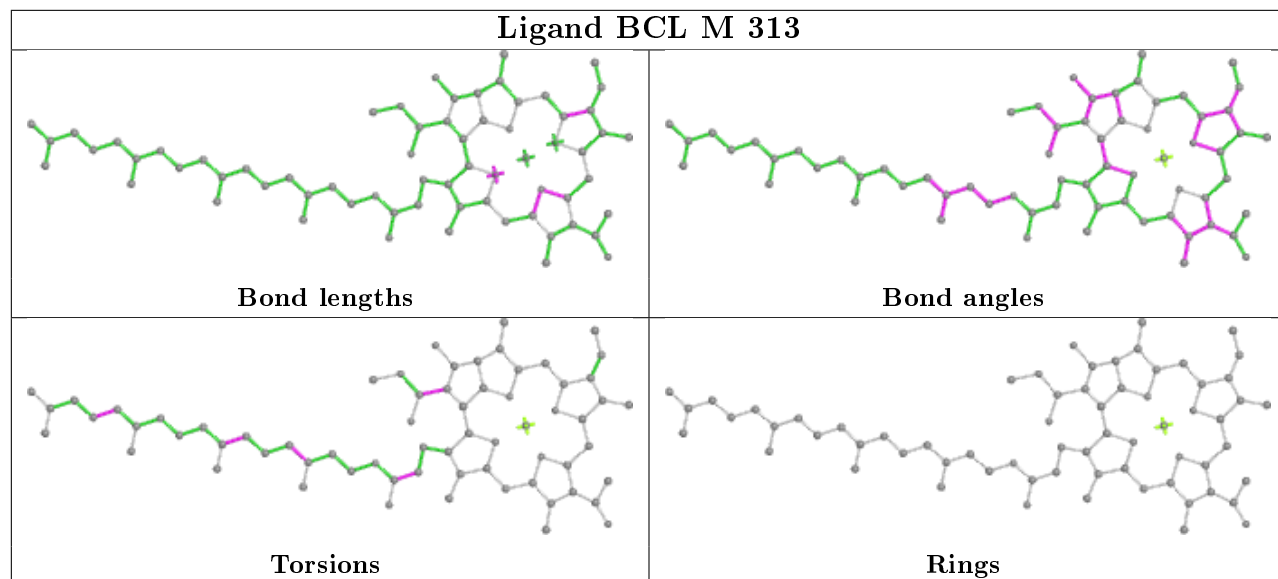


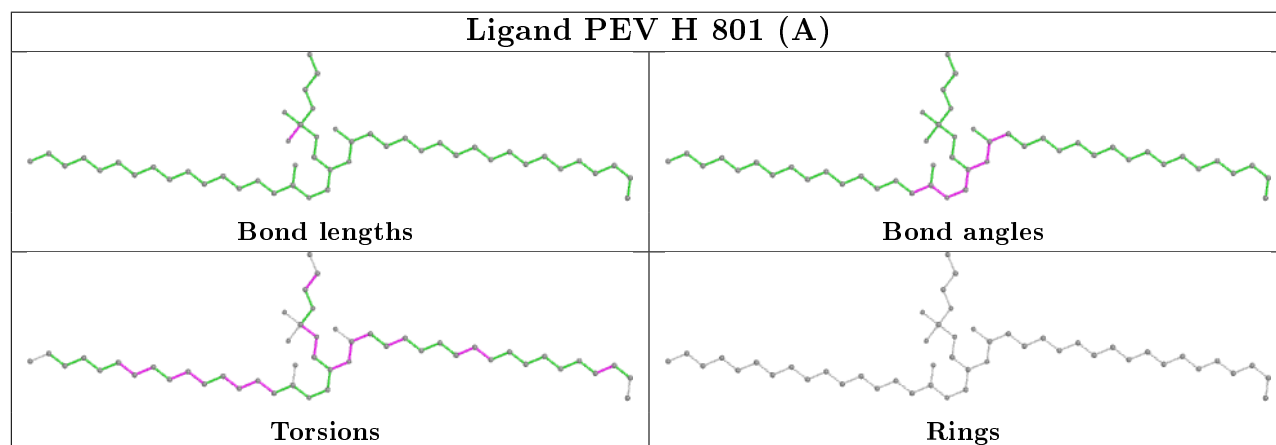
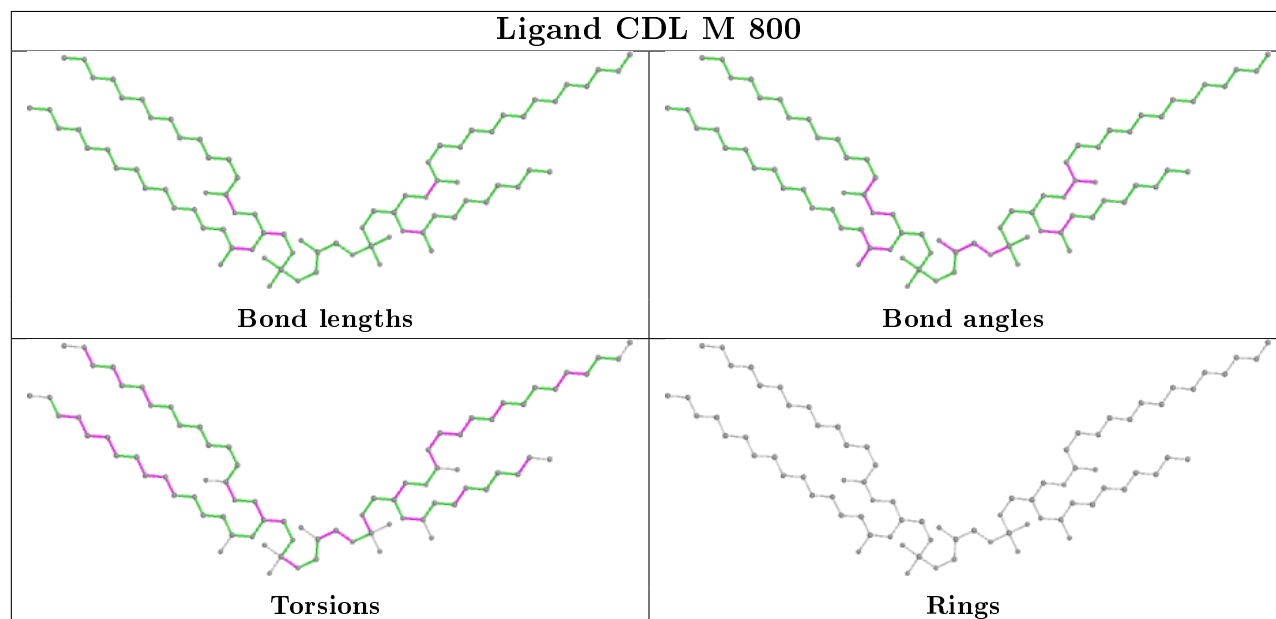
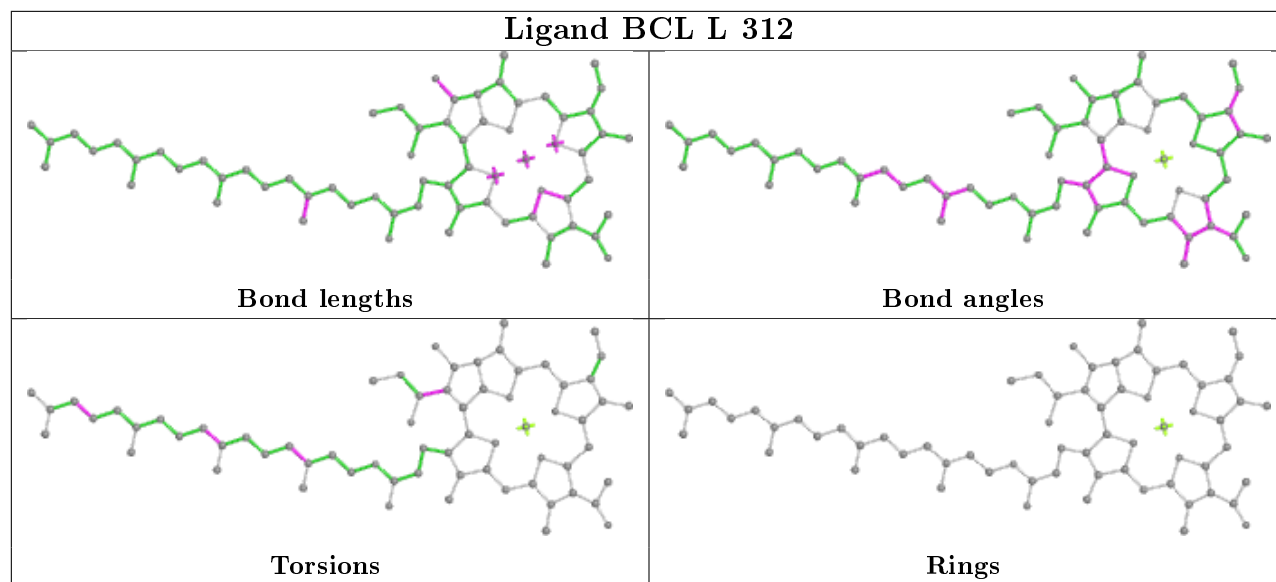
## Ligand U10 M 501

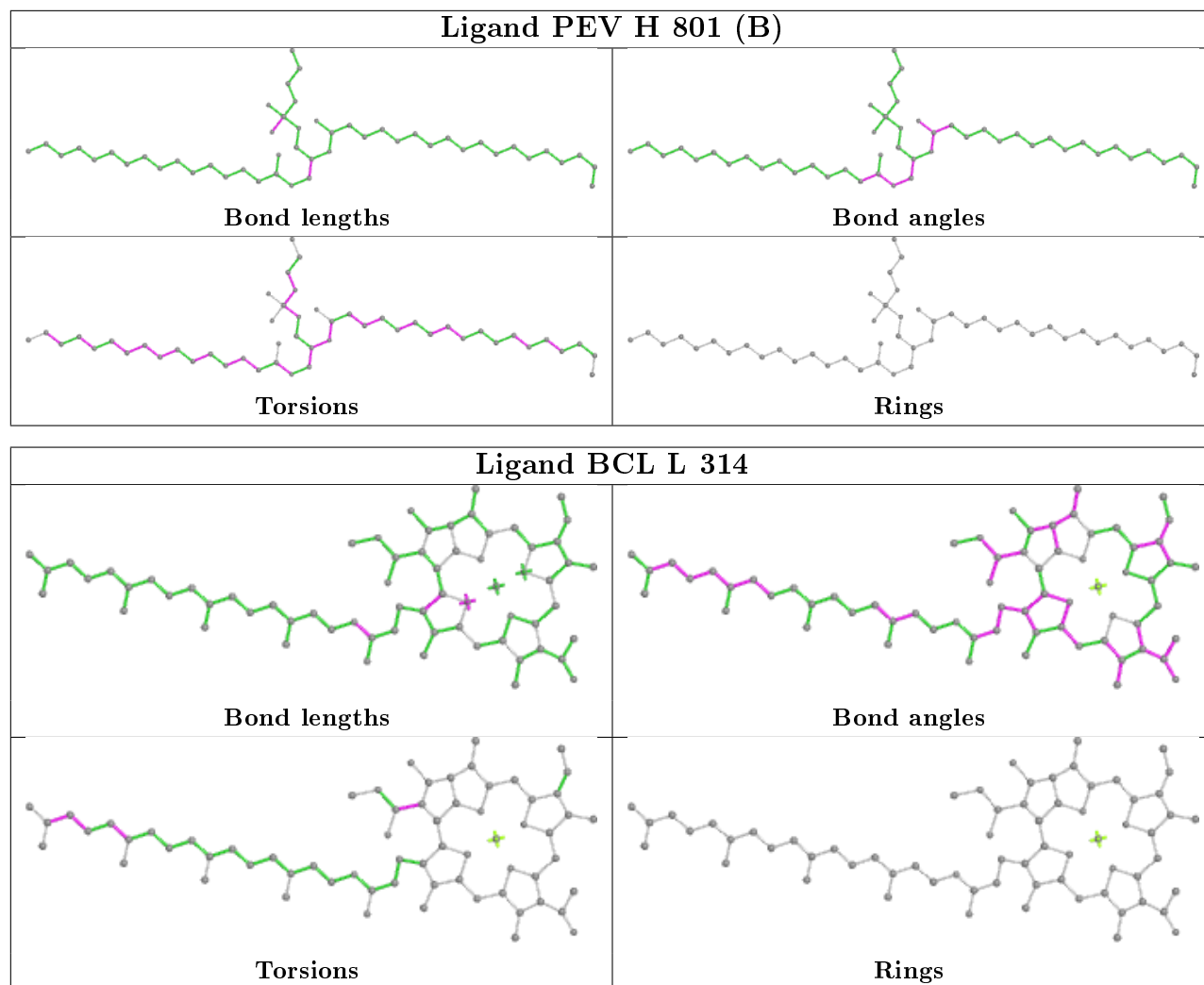


## Ligand BPH L 402



**Ligand U10 L 502****Ligand PEW M 802****Ligand BCL M 313**





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)	0.35	25 (8%) 9 11	63, 73, 81, 90	0
2	M	302/307 (98%)	0.64	42 (13%) 2 3	63, 72, 82, 106	0
3	H	243/260 (93%)	0.37	22 (9%) 9 10	61, 72, 86, 111	0
All	All	826/848 (97%)	0.46	89 (10%) 5 6	61, 73, 83, 111	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	8.5
3	H	9	ASN	8.4
2	M	80	TRP	6.1
2	M	102	GLY	6.0
2	M	2[A]	GLU	5.2
3	H	251	VAL	5.0
3	H	250	SER	5.0
2	M	3	TYR	4.7
2	M	103	LEU	4.7
3	H	10	PHE	4.5
1	L	73	TYR	4.5
2	M	75	TRP	4.4
2	M	104	SER	4.4
2	M	28	ASN	4.3
3	H	159	GLU	4.2
3	H	161	ALA	4.1
3	H	52	ASN	4.1
1	L	281	GLY	4.0
2	M	171	TRP	4.0
2	M	84	VAL	3.8
1	L	270	PRO	3.6
3	H	53	GLN	3.6
2	M	101	TYR	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	M	79	GLY	3.5
2	M	82	PRO	3.5
3	H	160	ILE	3.5
1	L	202	LYS	3.4
1	L	280	ASN	3.3
1	L	277	GLY	3.3
3	H	93	SER	3.2
2	M	81	ASN	3.2
1	L	265	TRP	3.2
3	H	247	LYS	3.1
1	L	279	ILE	3.1
2	M	105	PHE	3.1
3	H	220	LYS	3.1
2	M	114	LEU	3.1
2	M	73	TRP	3.0
2	M	83	ALA	3.0
1	L	269	LEU	3.0
2	M	54	SER	3.0
3	H	200	SER	3.0
1	L	278	GLY	3.0
3	H	158	LEU	3.0
2	M	100[A]	GLU	2.9
1	L	249	ILE	2.9
2	M	26	LEU	2.9
2	M	214	LEU	2.8
3	H	213	PHE	2.8
3	H	249	LYS	2.7
2	M	265	ILE	2.7
3	H	201	ASN	2.7
2	M	76	TYR	2.6
2	M	290	VAL	2.6
1	L	253	THR	2.6
2	M	52	LEU	2.6
3	H	102	GLY	2.6
1	L	268	LYS	2.5
2	M	212	SER	2.5
2	M	29	ARG	2.5
2	M	97	PRO	2.4
3	H	245	ALA	2.4
2	M	71	GLY	2.4
1	L	80	LEU	2.4
2	M	134	TYR	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	69	PRO	2.4
1	L	185	LEU	2.4
1	L	51	TRP	2.4
2	M	109	LEU	2.3
1	L	256	PHE	2.3
2	M	77	GLN	2.3
2	M	78	ALA	2.3
3	H	94	GLU	2.3
1	L	55	LEU	2.3
3	H	244	ALA	2.3
1	L	276[A]	PRO	2.3
3	H	77	GLY	2.2
1	L	271	TRP	2.2
2	M	213	ALA	2.2
2	M	57	VAL	2.2
2	M	133	THR	2.2
1	L	252	GLY	2.1
2	M	301[A]	HIS	2.1
1	L	233	GLY	2.1
1	L	236	LEU	2.0
1	L	184	ALA	2.0
2	M	216	PHE	2.0
2	M	215	LEU	2.0
2	M	96	PRO	2.0

## 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](#)

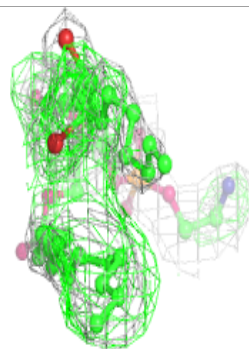
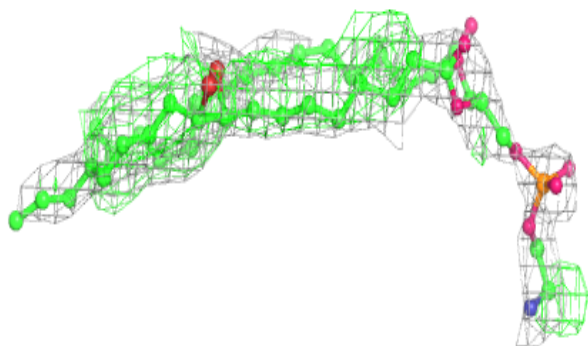
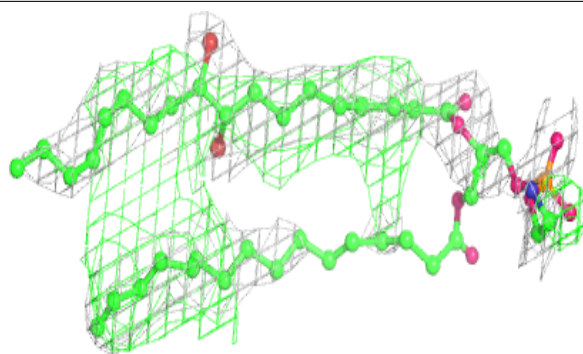
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	0.11	1.17	76,79,84,84	16
13	LDA	H	904	16/16	0.27	0.87	75,78,87,87	16
12	PEW	M	802	51/51	0.31	0.72	62,74,82,84	51
13	LDA	M	902	16/16	0.46	0.79	73,77,87,88	16
10	PO4	M	706	5/5	0.61	0.47	73,73,75,75	5
11	CDL	M	800	81/100	0.68	0.57	51,71,89,91	81
15	PEV	H	801[A]	49/49	0.68	0.96	50,72,79,80	49
15	PEV	H	801[B]	49/49	0.68	0.96	48,75,85,85	49
6	U10	L	502	48/63	0.69	0.58	60,69,77,78	48
13	LDA	M	920	16/16	0.70	0.53	52,61,74,75	16
13	LDA	H	901	16/16	0.73	0.51	74,77,85,86	16
10	PO4	H	705	5/5	0.75	0.39	80,80,80,81	5
9	CL	H	703	1/1	0.78	0.89	72,72,72,72	1
13	LDA	M	907	16/16	0.79	0.42	74,80,85,87	16
6	U10	M	501	48/63	0.84	0.33	64,76,99,100	0
7	GOL	L	707	6/6	0.85	0.53	69,78,79,79	6
10	PO4	M	704	5/5	0.90	0.31	69,69,75,76	5
9	CL	M	702	1/1	0.91	0.40	66,66,66,66	1
7	GOL	H	708	6/6	0.91	0.51	75,75,76,76	6
5	BPH	M	401	65/65	0.91	0.21	63,75,122,124	0
4	BCL	M	311	66/66	0.94	0.22	64,73,127,128	0
4	BCL	L	312	66/66	0.94	0.19	58,70,77,84	0
4	BCL	L	314	66/66	0.94	0.22	56,68,80,86	0
5	BPH	L	402	65/65	0.94	0.22	59,71,75,75	0
4	BCL	M	313	66/66	0.96	0.19	61,69,90,101	0
9	CL	M	701	1/1	0.97	0.23	71,71,71,71	1
14	K	H	700	1/1	0.99	0.10	66,66,66,66	0
8	FE	M	500	1/1	1.00	0.19	72,72,72,72	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.

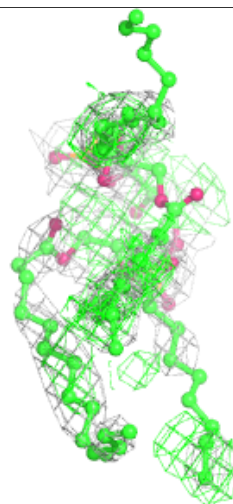
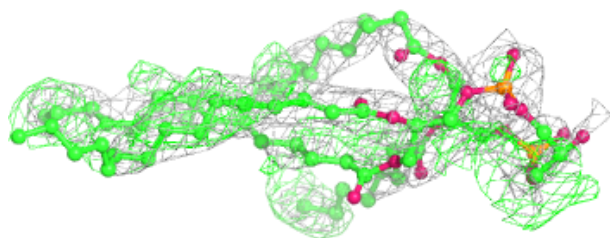
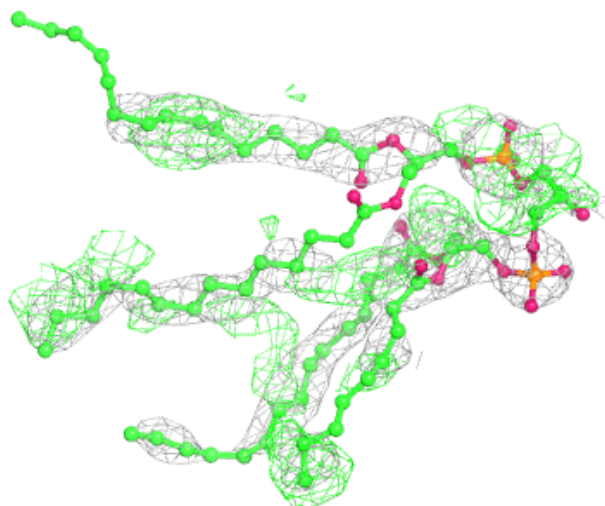
**Electron density around PEW M 802:**

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



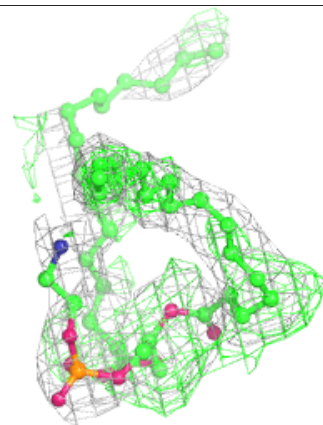
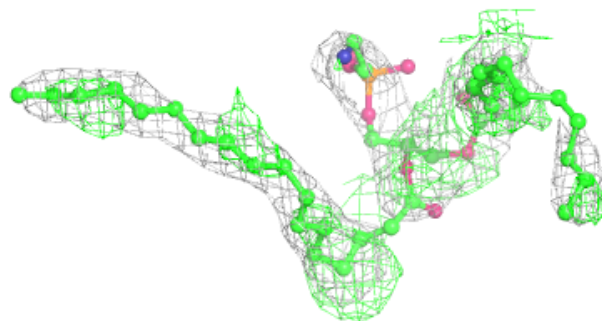
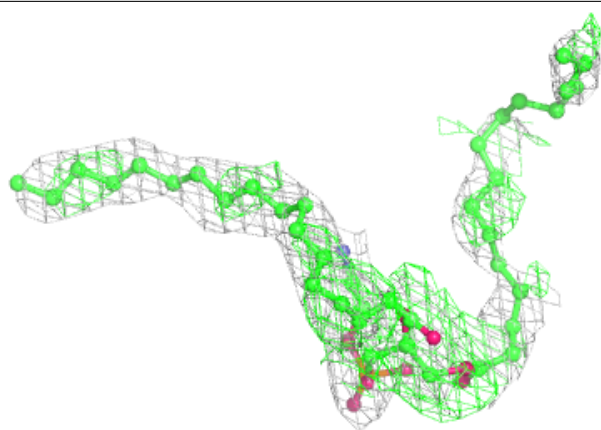
**Electron density around CDL M 800:**

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



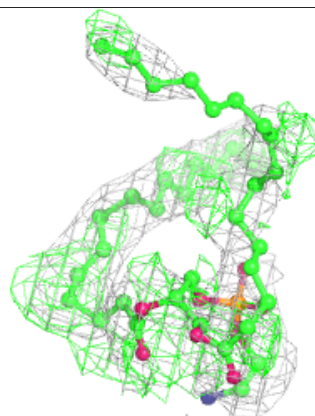
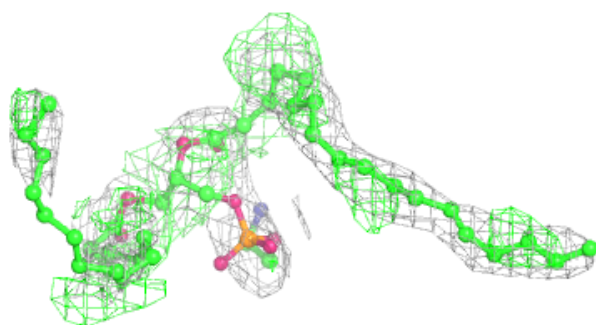
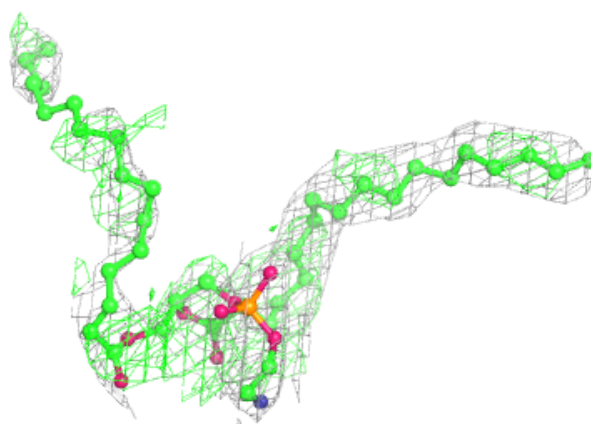
**Electron density around PEV H 801 (A):**

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

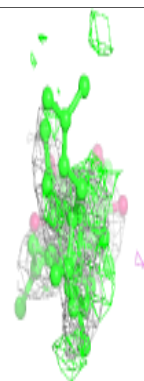
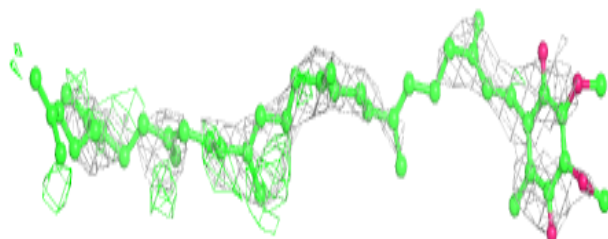
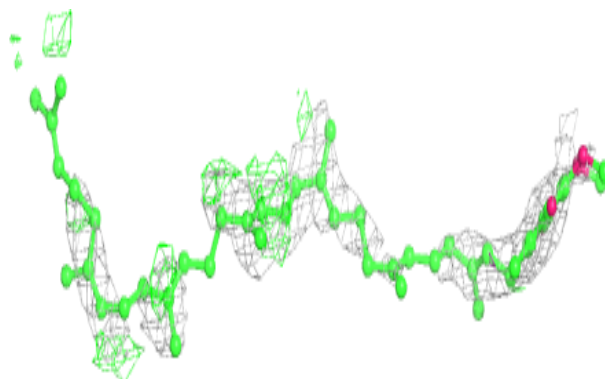


**Electron density around PEV H 801 (B):**

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

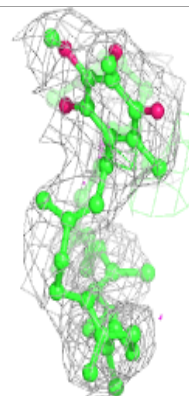
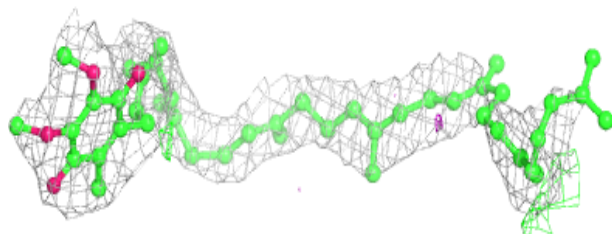
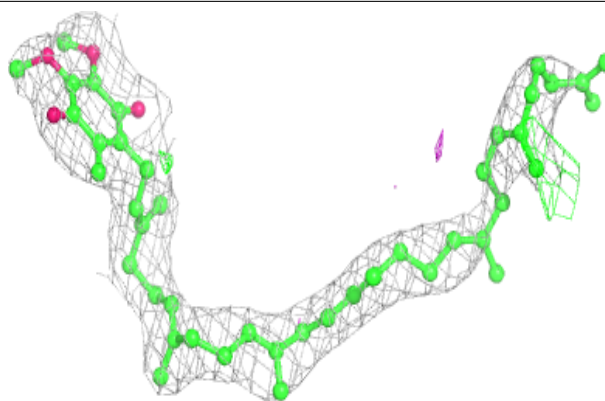
**Electron density around U10 L 502:**

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

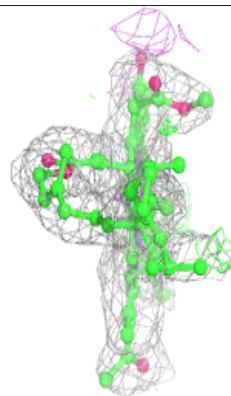
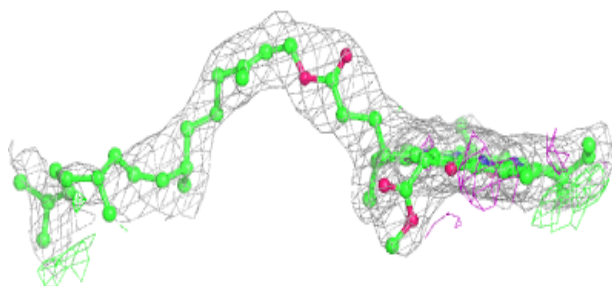
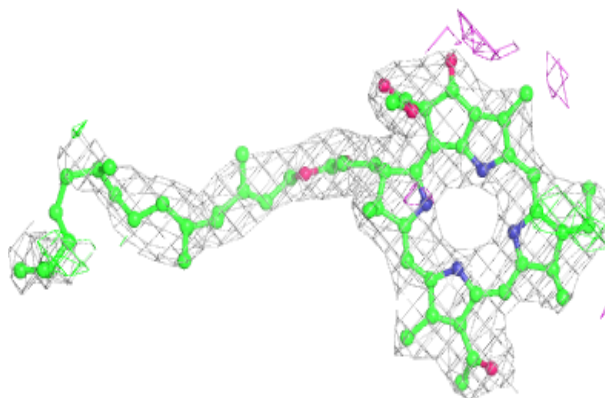


**Electron density around U10 M 501:**

$2mF_o-DF_c$  (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:**

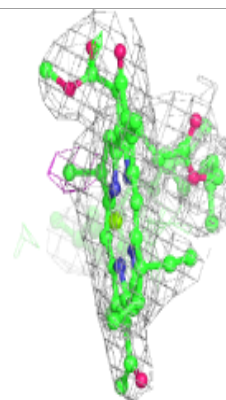
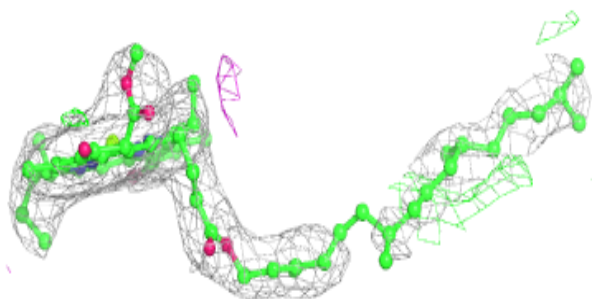
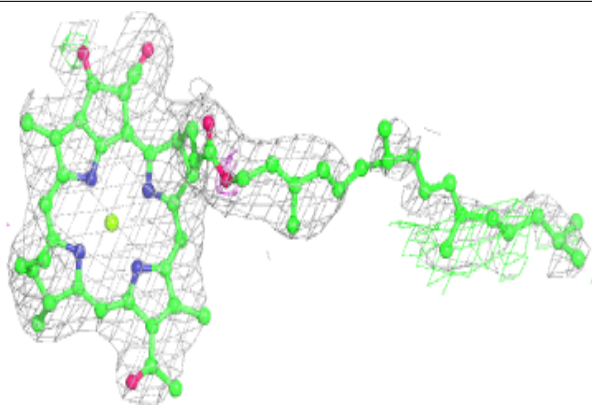
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



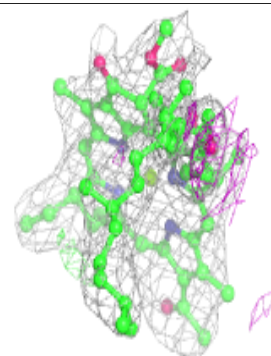
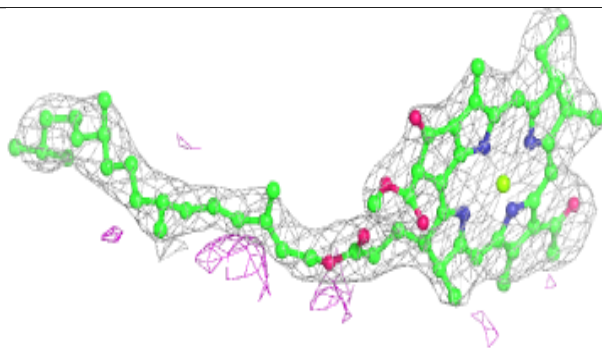
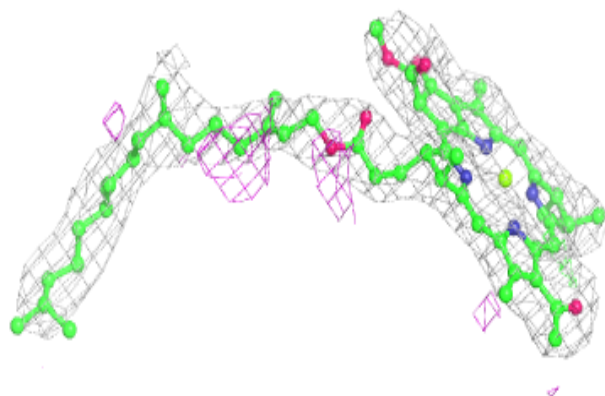


**Electron density around BCL M 311:**

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

**Electron density around BCL L 312:**

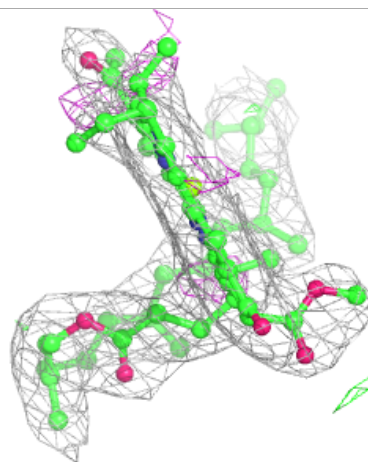
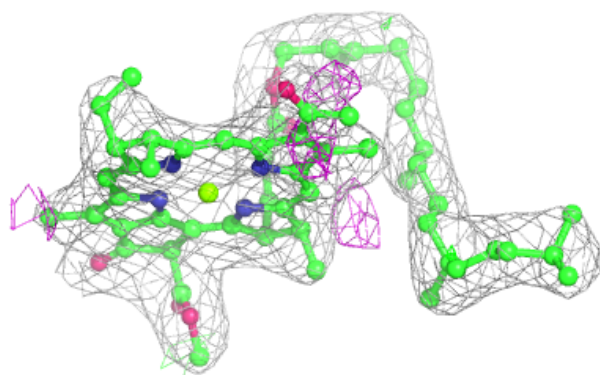
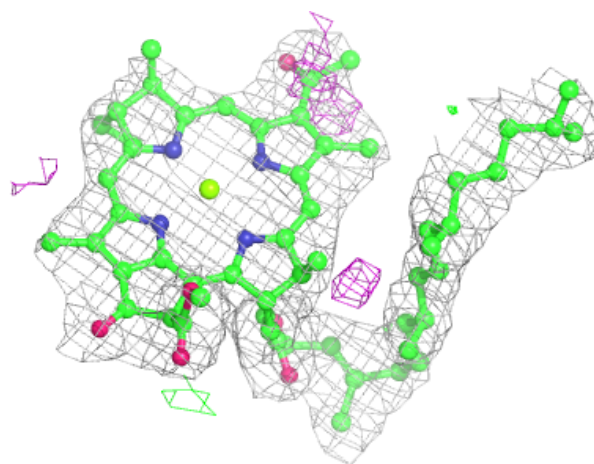
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





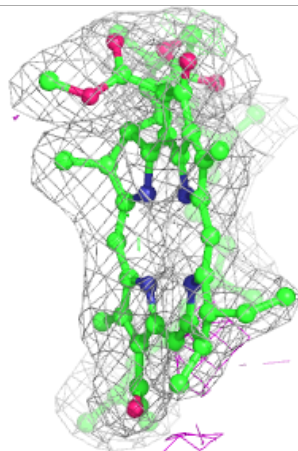
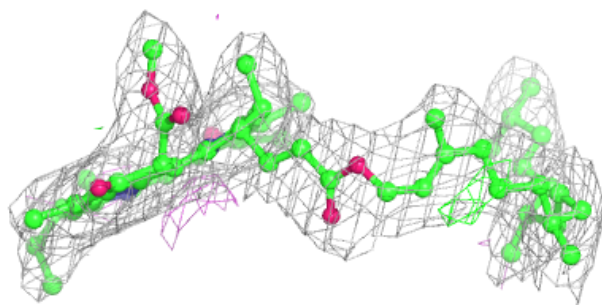
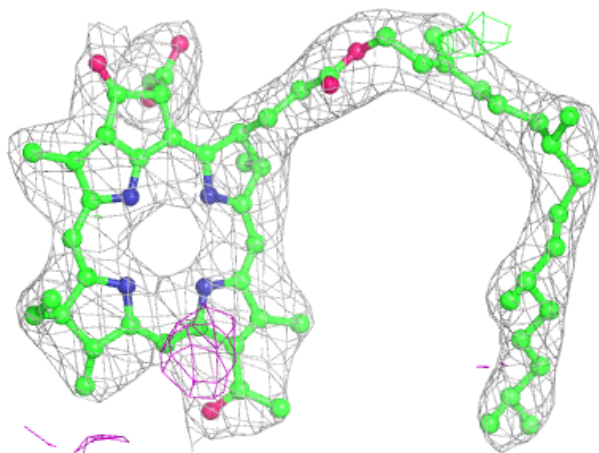
**Electron density around BCL L 314:**

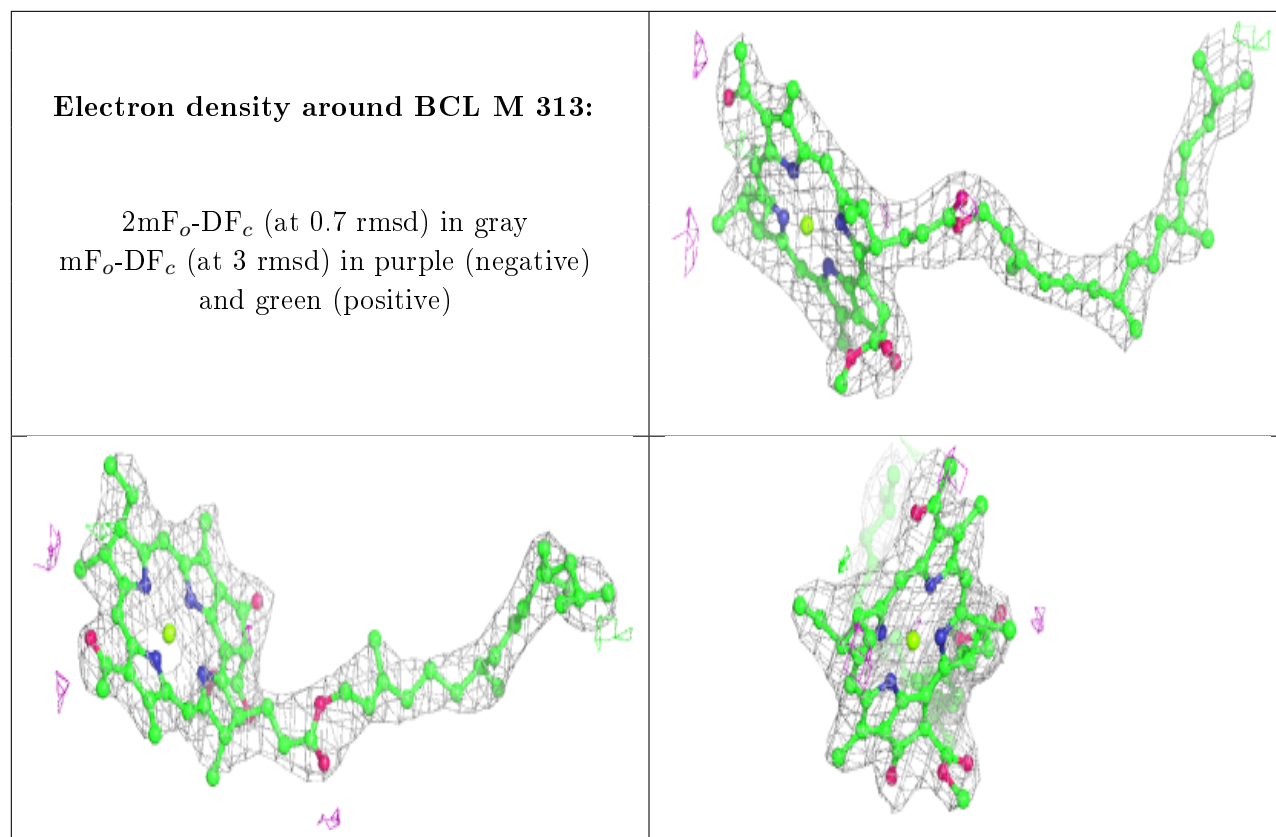
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.