



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:36 AM BST

PDB ID : 4IN6  
Title : (M)L214A mutant of the Rhodobacter sphaeroides Reaction Center  
Authors : Saer, R.G.; Hardjasa, A.; Murphy, M.E.P.; Beatty, J.T.  
Deposited on : 2013-01-04  
Resolution : 2.70 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.

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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 : 2.13.1  
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) : 2.13.1

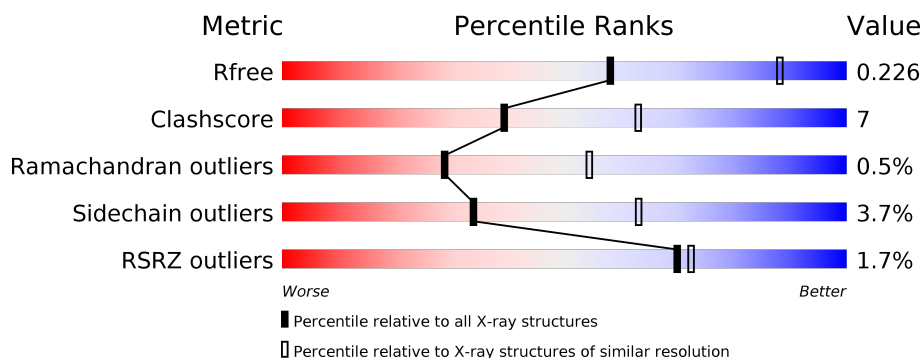
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 89%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>89%</span> <span>10%</span> </div> </div>
2	M	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 18%, green 82%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>82%</span> <span>18%</span> </div> </div>
3	H	266	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 14%, green 74%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>74%</span> <span>14%</span> <span>10%</span> </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
7	PO4	H	304	-	-	X	-
7	PO4	L	310	-	-	-	X
8	HTO	L	305	-	X	-	-

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7418 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
			2230	1505	354	363	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	1	0
			2407	1604	395	398	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	214	ALA	LEU	ENGINEERED MUTATION	UNP P0C0Y9

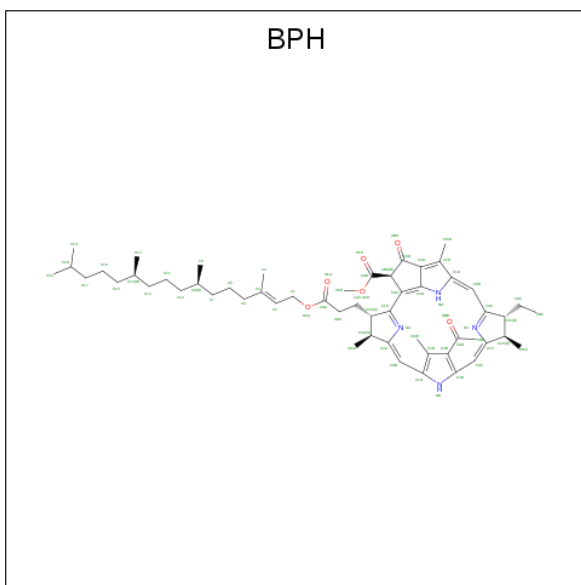
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	2	0
			1840	1178	316	337	9			

There are 6 discrepancies between the modelled and reference sequences:

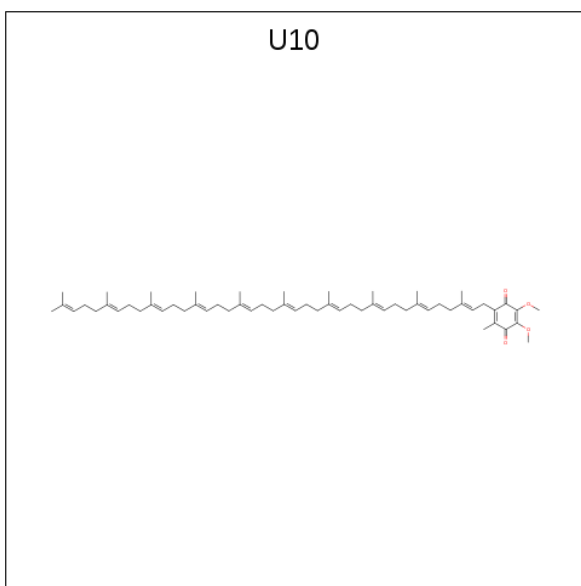
Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-4	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-3	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-2	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-1	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	0	HIS	-	EXPRESSION TAG	UNP P0C0Y7

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



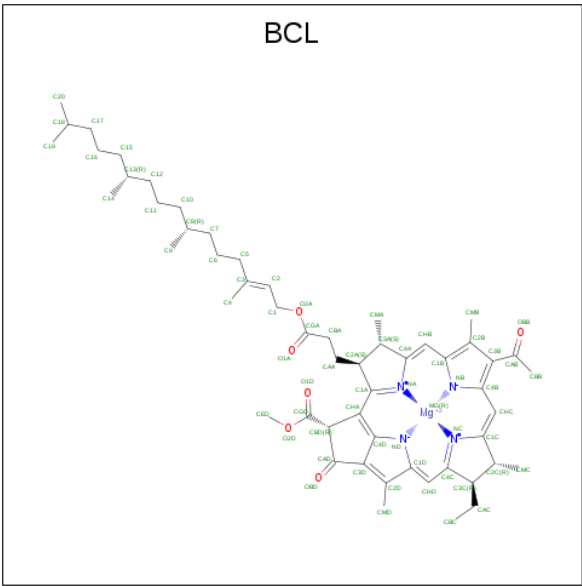
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			65	55	4	6		
4	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 5 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



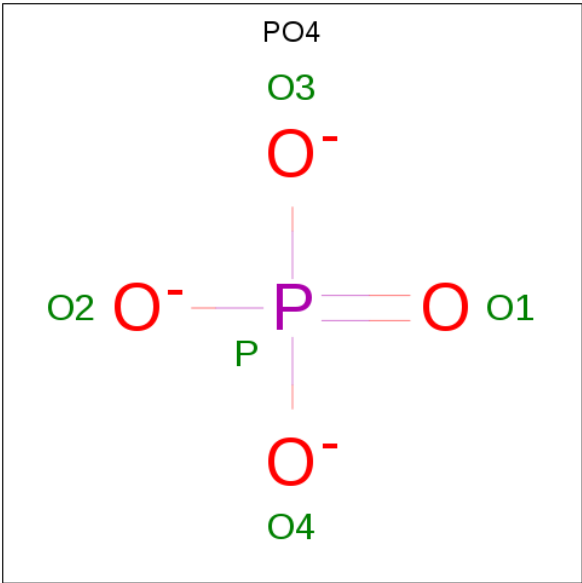
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	1
			46	38	8		
5	M	1	Total	C	O	0	0
			48	44	4		

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



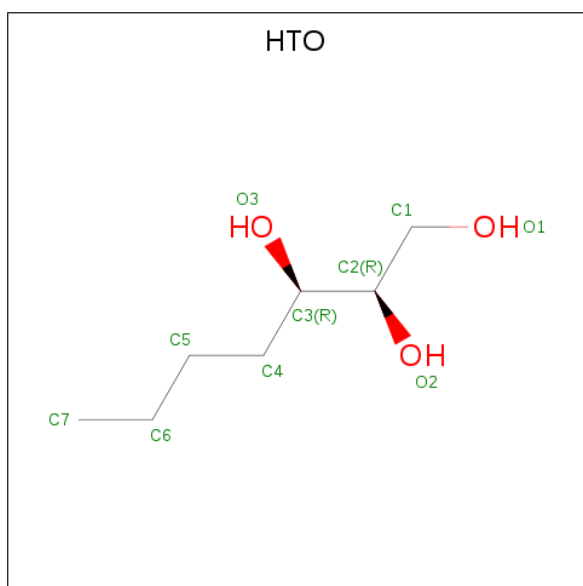
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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



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

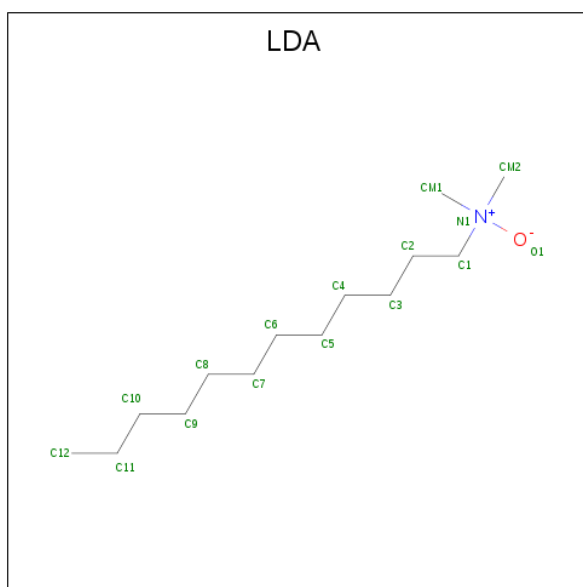
- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



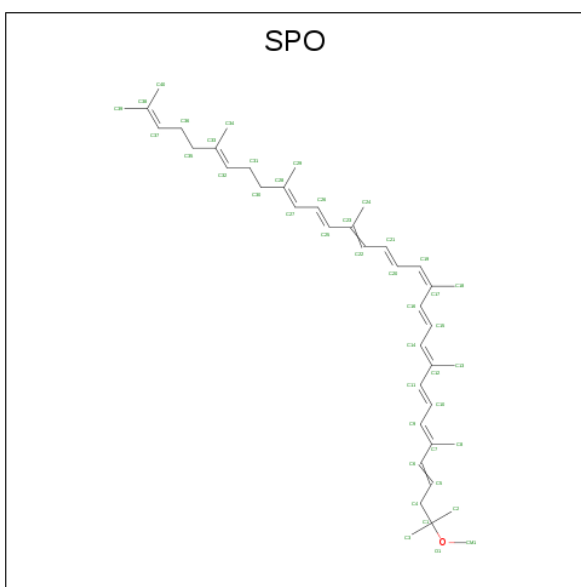


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		

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

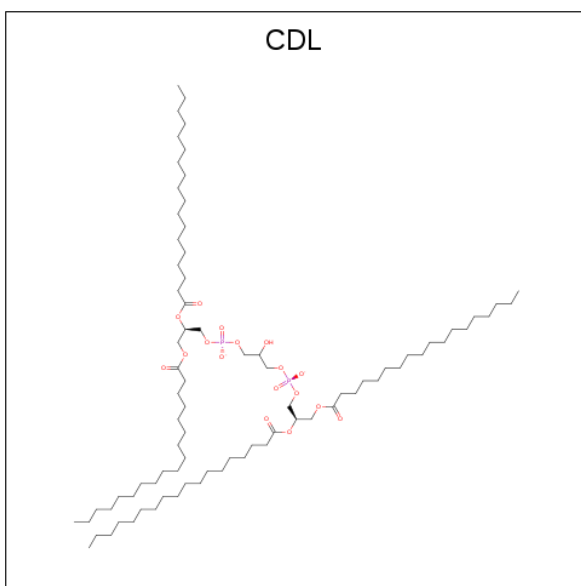
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O).



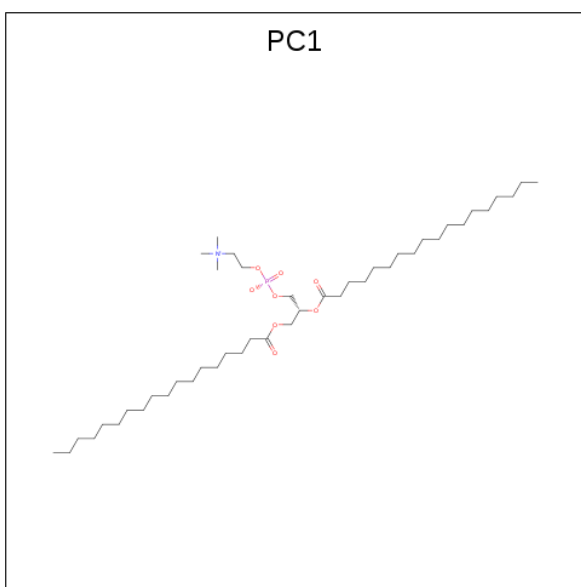
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



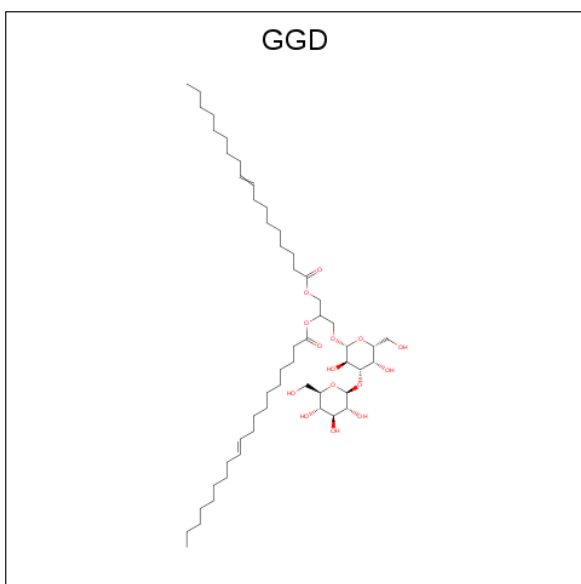
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	M	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

- Molecule 15 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-L-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY]-1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (three-letter code: GGD) (formula: C<sub>52</sub>H<sub>94</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	H	1	Total	C	O	0	0
			57	42	15		

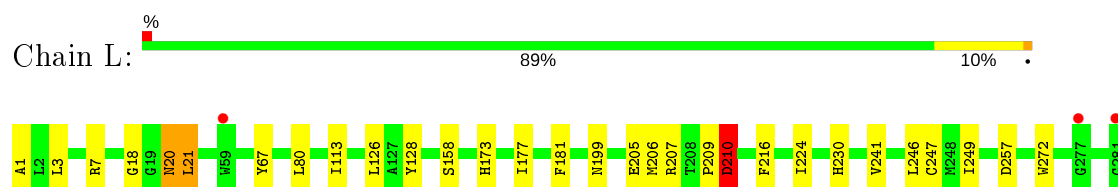
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	28	Total 28	O 28	0	0
16	M	22	Total 22	O 22	0	0
16	H	30	Total 30	O 30	0	0

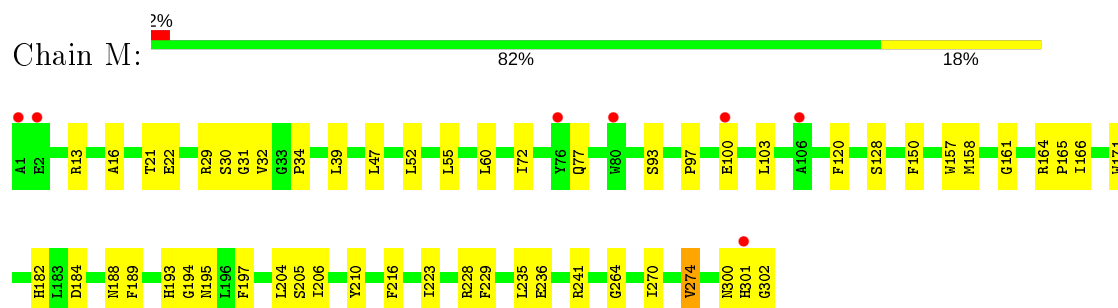
### 3 Residue-property plots

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

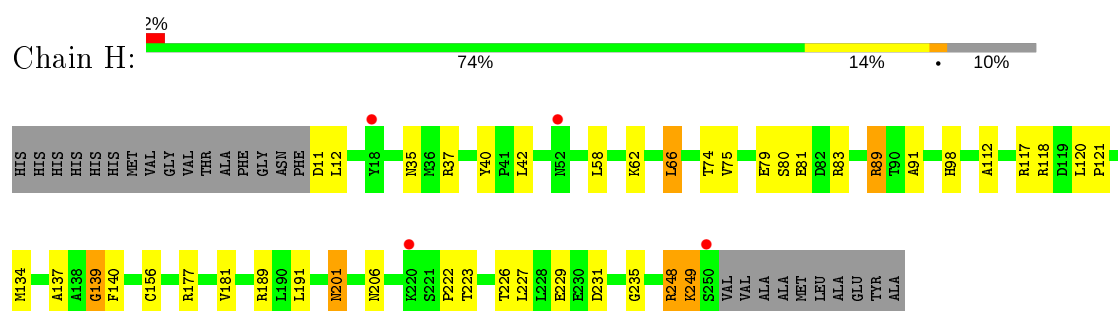
- Molecule 1: Reaction center protein L chain



- 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, $\alpha$ , $\beta$ , $\gamma$	139.03Å 139.03Å 184.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.62 – 2.70 33.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (33.62-2.70) 98.1 (33.60-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.182 , 0.223 0.188 , 0.226	Depositor DCC
$R_{free}$ test set	2836 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, GGD, CDL, BPH, PO4, PC1, HTO, FE, SPO, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	L	0.87	0/2323	0.86	4/3180 (0.1%)
2	M	0.85	0/2504	0.90	4/3418 (0.1%)
3	H	0.87	0/1903	0.97	7/2586 (0.3%)
All	All	0.86	0/6730	0.91	15/9184 (0.2%)

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
3	H	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	228	ARG	NE-CZ-NH2	-7.29	116.66	120.30
2	M	228	ARG	NE-CZ-NH1	6.95	123.78	120.30
3	H	189	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	L	210	ASP	CB-CG-OD1	6.47	124.12	118.30
2	M	241	ARG	NE-CZ-NH2	6.21	123.41	120.30
2	M	184	ASP	CB-CG-OD1	6.21	123.89	118.30
1	L	126	LEU	CB-CG-CD2	5.78	120.83	111.00
3	H	89	ARG	NE-CZ-NH2	-5.75	117.43	120.30
3	H	139	GLY	N-CA-C	-5.59	99.11	113.10
3	H	189	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	L	210	ASP	CB-CG-OD2	-5.34	113.50	118.30
3	H	177	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	L	3	LEU	CB-CG-CD1	-5.27	102.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	37	ARG	NE-CZ-NH2	5.26	122.93	120.30
3	H	89	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	248	ARG	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	2230	0	2179	24	0
2	M	2407	0	2313	33	0
3	H	1840	0	1855	26	0
4	L	65	0	76	7	0
4	M	65	0	76	9	0
5	L	46	0	46	9	0
5	M	48	0	63	1	0
6	L	132	0	148	12	0
6	M	132	0	148	10	0
7	H	5	0	0	3	0
7	L	10	0	0	0	0
7	M	10	0	0	0	0
8	L	10	0	16	0	0
9	H	30	0	40	1	0
9	L	36	0	48	3	0
10	M	48	0	93	0	0
11	M	1	0	0	0	0
12	M	42	0	60	6	0
13	M	81	0	102	0	0
14	M	43	0	60	2	0
15	H	57	0	68	0	0
16	H	30	0	0	1	0
16	L	28	0	0	3	0
16	M	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7418	0	7391	109	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 7.

All (109) 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)
5:L:302[B]:U10:C3M	5:L:302[B]:U10:H4M3	1.34	1.54
5:L:302[B]:U10:C4M	5:L:302[B]:U10:H3M3	1.38	1.54
4:M:406:BPH:HHC	4:M:406:BPH:HBB3	1.55	0.89
3:H:134:MET:O	7:H:304:PO4:O1	1.96	0.84
4:L:301:BPH:HBB3	4:L:301:BPH:HHC	1.59	0.84
1:L:199:ASN:HA	9:L:306:GOL:H31	1.63	0.81
4:M:406:BPH:HHB	4:M:406:BPH:HBC3	1.65	0.78
5:L:302[B]:U10:C3M	5:L:302[B]:U10:C4M	2.21	0.78
2:M:300:ASN:O	2:M:302:GLY:N	2.21	0.73
4:L:301:BPH:HBB2	2:M:210:TYR:HB3	1.71	0.72
6:L:308:BCL:HBB2	6:L:308:BCL:HHC	1.73	0.71
3:H:201:ASN:HD22	3:H:201:ASN:H	1.39	0.68
2:M:270:ILE:O	2:M:274:VAL:HG13	1.95	0.67
6:L:303:BCL:HMB1	6:L:303:BCL:HBB3	1.81	0.62
3:H:79:GLU:O	3:H:80:SER:HB3	2.01	0.60
3:H:140:PHE:O	7:H:304:PO4:O4	2.20	0.59
2:M:77:GLN:HE22	2:M:93:SER:H	1.49	0.59
3:H:66:LEU:HD23	3:H:66:LEU:N	2.17	0.59
3:H:81:GLU:O	3:H:83:ARG:HG2	2.03	0.58
6:M:402:BCL:CBB	6:M:402:BCL:HHC	2.34	0.58
4:M:406:BPH:CHD	4:M:406:BPH:HBC3	2.32	0.58
2:M:197:PHE:HZ	6:M:402:BCL:HBB2	1.68	0.57
1:L:224:ILE:HG22	5:L:302[B]:U10:H3M2	1.87	0.57
6:M:401:BCL:HBB2	6:M:401:BCL:HHC	1.87	0.57
2:M:197:PHE:CZ	6:M:402:BCL:HBB2	2.39	0.57
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.85	0.57
6:M:401:BCL:CBB	6:M:401:BCL:HHC	2.34	0.57
9:L:313:GOL:H32	16:L:424:HOH:O	2.05	0.57
6:M:402:BCL:HHC	6:M:402:BCL:HBB3	1.86	0.57
1:L:128:TYR:HD1	6:L:308:BCL:HBB1	1.69	0.56
1:L:224:ILE:H	5:L:302[B]:U10:H4M1	1.70	0.56
6:M:402:BCL:HBD	6:M:402:BCL:HAA2	1.87	0.56
1:L:246:LEU:HA	1:L:249:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:189:PHE:O	2:M:193:HIS:HD2	1.90	0.55
1:L:1:ALA:HB1	3:H:42:LEU:HB3	1.88	0.55
6:M:401:BCL:HBB2	12:M:408:SPO:H243	1.89	0.55
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.89	0.54
3:H:139:GLY:HA2	9:H:307:GOL:O2	2.08	0.54
2:M:300:ASN:C	2:M:302:GLY:N	2.62	0.53
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.09	0.53
1:L:181:PHE:CD2	4:M:406:BPH:HBB1	2.45	0.52
2:M:16:ALA:CB	2:M:32:VAL:HG11	2.39	0.52
4:M:406:BPH:CHC	4:M:406:BPH:HBB3	2.36	0.52
2:M:31:GLY:N	14:M:410:PC1:O14	2.43	0.52
4:L:301:BPH:HBB1	2:M:210:TYR:CD2	2.45	0.52
2:M:34:PRO:O	2:M:47:LEU:HB2	2.10	0.52
6:M:401:BCL:HBB3	6:M:402:BCL:H41	1.92	0.52
5:M:407:U10:H312	5:M:407:U10:H352	1.91	0.51
2:M:55:LEU:HD22	2:M:128:SER:HB2	1.91	0.51
1:L:181:PHE:HB3	4:M:406:BPH:HBB2	1.92	0.50
2:M:13:ARG:O	3:H:140:PHE:HA	2.11	0.50
2:M:161:GLY:HA3	12:M:408:SPO:H292	1.94	0.50
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.94	0.50
6:L:308:BCL:HHC	6:L:308:BCL:CBB	2.39	0.50
6:M:401:BCL:CBB	12:M:408:SPO:H243	2.43	0.49
1:L:67:TYR:HE1	16:L:416:HOH:O	1.95	0.49
2:M:120:PHE:CD1	12:M:408:SPO:H402	2.48	0.49
4:M:406:BPH:HHH	4:M:406:BPH:CBC	2.40	0.48
4:L:301:BPH:CBB	2:M:210:TYR:HB3	2.43	0.48
4:L:301:BPH:HHC	4:L:301:BPH:CBB	2.40	0.48
3:H:137:ALA:O	7:H:304:PO4:O1	2.32	0.48
1:L:20:ASN:C	1:L:20:ASN:HD22	2.16	0.47
1:L:241:VAL:HG21	4:L:301:BPH:HAC1	1.97	0.47
1:L:80:LEU:HD23	9:L:307:GOL:H11	1.96	0.47
2:M:194:GLY:O	2:M:195:ASN:HB3	2.15	0.46
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.98	0.46
6:L:308:BCL:HMB1	6:L:308:BCL:OBB	2.16	0.46
6:L:303:BCL:CBB	6:L:303:BCL:HMB1	2.46	0.45
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.52	0.45
1:L:181:PHE:HB3	4:M:406:BPH:CBB	2.47	0.45
3:H:117:ARG:NH1	3:H:227:LEU:HD22	2.31	0.45
3:H:248:ARG:HA	3:H:249:LYS:CB	2.46	0.45
6:L:308:BCL:HMD1	2:M:206:ILE:HD13	1.98	0.45
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:222:PRO:HG2	3:H:223:THR:HG23	1.99	0.45
12:M:408:SPO:H15	12:M:408:SPO:H131	1.83	0.44
3:H:89:ARG:HD3	3:H:91:ALA:O	2.17	0.44
12:M:408:SPO:H20	12:M:408:SPO:H181	1.70	0.44
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.18	0.44
1:L:7:ARG:HE	3:H:98:HIS:CD2	2.35	0.44
5:L:302[B]:U10:H1M1	5:L:302[B]:U10:H71	1.75	0.43
2:M:150:PHE:N	4:M:406:BPH:HMD3	2.33	0.43
3:H:40:TYR:CB	3:H:58:LEU:HD21	2.47	0.43
5:L:302[B]:U10:H121	5:L:302[B]:U10:H101	1.46	0.43
3:H:120:LEU:HB3	3:H:121:PRO:CD	2.48	0.43
4:L:301:BPH:H202	6:L:308:BCL:C2B	2.48	0.43
2:M:204:LEU:O	2:M:205:SER:C	2.56	0.43
1:L:205:GLU:O	1:L:206:MET:C	2.58	0.43
5:L:302[A]:U10:H153	14:M:410:PC1:C2E	2.48	0.43
6:L:303:BCL:H52	6:L:308:BCL:HBB3	2.00	0.42
1:L:7:ARG:HH21	3:H:98:HIS:HD2	1.68	0.42
2:M:21:THR:O	2:M:22:GLU:C	2.58	0.42
1:L:257:ASP:HB3	16:L:407:HOH:O	2.18	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.20	0.42
2:M:103:LEU:HD11	2:M:166:ILE:HA	2.00	0.41
3:H:62:LYS:O	3:H:74:THR:HA	2.20	0.41
1:L:18:GLY:O	1:L:21:LEU:HB2	2.21	0.41
1:L:128:TYR:CD1	6:L:308:BCL:HBB1	2.52	0.41
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.54	0.41
1:L:210:ASP:OD1	1:L:210:ASP:N	2.54	0.41
1:L:209:PRO:HD3	2:M:235:LEU:HD12	2.02	0.41
6:L:303:BCL:H41	6:L:308:BCL:HBB3	2.02	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.21	0.41
6:L:308:BCL:CMD	2:M:206:ILE:HD13	2.52	0.40
1:L:113:ILE:HG22	2:M:229:PHE:HE1	1.85	0.40
5:L:302[B]:U10:H101	5:L:302[B]:U10:C13	2.43	0.40
2:M:236:GLU:HB3	16:H:427:HOH:O	2.20	0.40
3:H:201:ASN:HD22	3:H:201:ASN:N	2.07	0.40
3:H:181:VAL:CG2	3:H:191:LEU:HD23	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	280/281 (100%)	274 (98%)	6 (2%)	0	100	100
2	M	301/302 (100%)	287 (95%)	11 (4%)	3 (1%)	15	37
3	H	241/266 (91%)	231 (96%)	9 (4%)	1 (0%)	34	60
All	All	822/849 (97%)	792 (96%)	26 (3%)	4 (0%)	29	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
3	H	249	LYS
2	M	30	SER
2	M	100	GLU

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	212 (96%)	8 (4%)	35	64
2	M	236/235 (100%)	227 (96%)	9 (4%)	33	62
3	H	198/214 (92%)	191 (96%)	7 (4%)	36	65
All	All	654/669 (98%)	630 (96%)	24 (4%)	34	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	21	LEU
1	L	158	SER
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	247	CYS
1	L	272	TRP
2	M	29	ARG
2	M	39	LEU
2	M	52	LEU
2	M	60	LEU
2	M	72	ILE
2	M	182	HIS
2	M	188	ASN
2	M	216	PHE
2	M	274	VAL
3	H	11	ASP
3	H	12	LEU
3	H	66	LEU
3	H	75	VAL
3	H	118	ARG
3	H	201	ASN
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	159	ASN
1	L	183	ASN
1	L	264	GLN
2	M	77	GLN
2	M	187	ASN
2	M	193	HIS
2	M	300	ASN
3	H	98	HIS
3	H	201	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 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$
9	GOL	L	312	-	5,5,5	0.65	0	5,5,5	0.81	0
5	U10	L	302[B]	-	23,23,63	2.29	4 (17%)	28,31,79	1.88	8 (28%)
12	SPO	M	408	-	40,41,41	0.94	2 (5%)	47,50,50	1.81	13 (27%)
15	GGD	H	301	-	58,58,68	1.13	3 (5%)	72,72,82	1.60	11 (15%)
7	PO4	M	412	-	4,4,4	1.16	0	6,6,6	0.72	0
9	GOL	L	307	-	5,5,5	0.54	0	5,5,5	0.91	0
9	GOL	L	309	-	5,5,5	0.60	0	5,5,5	0.66	0
6	BCL	L	308	-	58,74,74	1.53	10 (17%)	69,115,115	2.22	23 (33%)
6	BCL	L	303	-	58,74,74	1.63	8 (13%)	69,115,115	1.72	14 (20%)
7	PO4	M	411	-	4,4,4	0.53	0	6,6,6	0.81	0
7	PO4	L	310	-	4,4,4	0.86	0	6,6,6	0.62	0
7	PO4	H	304	-	4,4,4	1.47	1 (25%)	6,6,6	1.51	2 (33%)
7	PO4	L	304	-	4,4,4	0.41	0	6,6,6	0.98	0
6	BCL	M	401	-	58,74,74	1.68	10 (17%)	69,115,115	1.98	14 (20%)
9	GOL	H	302	-	5,5,5	0.45	0	5,5,5	0.23	0
4	BPH	M	406	-	64,70,70	1.99	13 (20%)	76,101,101	1.92	21 (27%)
6	BCL	M	402	-	58,74,74	1.57	10 (17%)	69,115,115	1.86	17 (24%)
9	GOL	H	306	-	5,5,5	0.56	0	5,5,5	0.72	0
14	PC1	M	410	-	42,42,53	1.48	4 (9%)	48,50,61	1.46	6 (12%)
8	HTO	L	305	-	9,9,9	1.19	1 (11%)	10,10,10	1.67	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	GOL	L	313	-	5,5,5	0.49	0	5,5,5	0.67	0
10	LDA	M	403	-	12,15,15	2.25	1 (8%)	14,17,17	0.91	1 (7%)
10	LDA	M	404	-	12,15,15	2.06	1 (8%)	14,17,17	0.73	0
4	BPH	L	301	-	64,70,70	2.01	13 (20%)	76,101,101	1.80	14 (18%)
10	LDA	M	413	-	12,15,15	2.20	1 (8%)	14,17,17	0.60	0
9	GOL	L	311	-	5,5,5	0.56	0	5,5,5	0.59	0
9	GOL	H	305	-	5,5,5	0.47	0	5,5,5	0.32	0
9	GOL	L	306	-	5,5,5	0.68	0	5,5,5	1.30	0
9	GOL	H	303	-	5,5,5	0.16	0	5,5,5	0.82	0
5	U10	M	407	-	48,48,63	1.47	4 (8%)	58,61,79	1.68	14 (24%)
9	GOL	H	307	-	5,5,5	0.48	0	5,5,5	0.59	0
5	U10	L	302[A]	-	23,23,63	1.78	2 (8%)	28,31,79	1.92	9 (32%)
13	CDL	M	409	-	79,79,99	1.44	4 (5%)	84,90,111	1.42	8 (9%)

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
9	GOL	L	312	-	-	2/4/4/4	-
5	U10	L	302[B]	-	-	4/15/39/87	0/1/1/1
12	SPO	M	408	-	-	6/47/47/47	-
15	GGD	H	301	-	-	27/47/87/97	0/2/2/2
9	GOL	L	307	-	-	3/4/4/4	-
9	GOL	L	309	-	-	3/4/4/4	-
6	BCL	L	308	-	-	5/37/137/137	-
6	BCL	L	303	-	-	5/37/137/137	-
9	GOL	H	302	-	-	0/4/4/4	-
6	BCL	M	401	-	-	11/37/137/137	-
4	BPH	M	406	-	-	17/54/105/105	0/5/6/6
6	BCL	M	402	-	-	4/37/137/137	-
9	GOL	H	306	-	-	0/4/4/4	-
14	PC1	M	410	-	-	19/46/46/57	-
8	HTO	L	305	-	-	8/10/10/10	-
9	GOL	L	313	-	-	2/4/4/4	-
10	LDA	M	403	-	-	4/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LDA	M	404	-	-	9/13/13/13	-
4	BPH	L	301	-	-	7/54/105/105	0/5/6/6
10	LDA	M	413	-	-	3/13/13/13	-
9	GOL	L	311	-	-	2/4/4/4	-
9	GOL	H	305	-	-	0/4/4/4	-
9	GOL	L	306	-	-	2/4/4/4	-
9	GOL	H	303	-	-	2/4/4/4	-
5	U10	M	407	-	-	6/45/69/87	0/1/1/1
9	GOL	H	307	-	-	2/4/4/4	-
5	U10	L	302[A]	-	-	2/15/39/87	0/1/1/1
13	CDL	M	409	-	-	54/88/88/110	-

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302[B]	U10	C6-C1	8.82	1.51	1.35
10	M	413	LDA	O1-N1	-7.48	1.24	1.42
5	L	302[A]	U10	C6-C1	7.40	1.48	1.35
10	M	403	LDA	O1-N1	-7.31	1.25	1.42
10	M	404	LDA	O1-N1	-6.81	1.26	1.42
4	L	301	BPH	OBD-CAD	6.81	1.31	1.22
5	M	407	U10	C6-C1	6.49	1.47	1.35
13	M	409	CDL	OB6-CB5	5.90	1.50	1.34
4	L	301	BPH	CHB-C1B	5.55	1.49	1.38
13	M	409	CDL	OA6-CA5	5.47	1.49	1.34
14	M	410	PC1	O21-C21	5.47	1.49	1.34
6	M	401	BCL	OBD-CAD	5.44	1.29	1.22
14	M	410	PC1	O31-C31	5.43	1.49	1.33
4	M	406	BPH	C1A-NA	-5.39	1.27	1.37
4	L	301	BPH	C1A-NA	-5.27	1.27	1.37
6	M	402	BCL	O2D-CGD	5.24	1.46	1.33
4	M	406	BPH	CHB-C1B	5.24	1.48	1.38
13	M	409	CDL	OA8-CA7	5.20	1.48	1.33
4	M	406	BPH	CHA-C1A	5.20	1.49	1.38
4	M	406	BPH	C4C-NC	-4.80	1.27	1.37
6	L	303	BCL	C3B-C2B	4.79	1.48	1.39
13	M	409	CDL	OB8-CB7	4.70	1.47	1.33
4	M	406	BPH	O2A-CGA	4.69	1.47	1.33
4	M	406	BPH	O2D-CGD	4.63	1.44	1.33
6	M	401	BCL	O2A-CGA	4.51	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	406	BPH	C3D-C2D	4.49	1.47	1.39
4	L	301	BPH	O2A-CGA	4.42	1.46	1.33
4	L	301	BPH	CHA-C1A	4.39	1.47	1.38
6	L	303	BCL	O2D-CGD	4.35	1.43	1.33
6	L	303	BCL	O2A-CGA	4.19	1.45	1.33
6	L	308	BCL	OBD-CAD	4.14	1.28	1.22
15	H	301	GGD	OC8-CC7	4.14	1.45	1.33
6	M	401	BCL	C3B-C2B	3.97	1.46	1.39
6	M	402	BCL	OBD-CAD	3.93	1.27	1.22
6	L	303	BCL	C3D-C2D	3.92	1.46	1.39
6	M	402	BCL	O2A-CGA	3.89	1.44	1.33
4	L	301	BPH	O2D-CGD	3.88	1.42	1.33
6	M	401	BCL	C3D-C2D	3.85	1.46	1.39
6	L	308	BCL	O2A-CGA	3.85	1.44	1.33
4	L	301	BPH	C3D-C2D	3.83	1.46	1.39
6	L	308	BCL	O2D-CGD	3.81	1.42	1.33
6	L	308	BCL	C3D-C2D	3.79	1.46	1.39
6	M	401	BCL	O2D-CGD	3.77	1.42	1.33
4	M	406	BPH	CHC-C4B	3.68	1.49	1.40
6	L	303	BCL	OBD-CAD	3.66	1.27	1.22
6	M	402	BCL	C3B-C2B	3.59	1.45	1.39
15	H	301	GGD	OC6-CC5	3.56	1.44	1.34
6	L	303	BCL	C3C-C4C	-3.55	1.47	1.51
4	L	301	BPH	CHC-C4B	3.54	1.48	1.40
5	L	302[B]	U10	C4-C3	3.39	1.50	1.36
6	M	402	BCL	C3D-C2D	3.37	1.45	1.39
4	M	406	BPH	OBD-CAD	3.29	1.26	1.22
5	M	407	U10	C31-C29	3.05	1.57	1.51
6	L	308	BCL	C3B-C2B	3.02	1.44	1.39
6	L	308	BCL	C1B-CHB	2.96	1.49	1.41
4	L	301	BPH	C1B-NB	-2.94	1.32	1.38
6	M	401	BCL	CBD-CGD	-2.92	1.43	1.52
6	L	308	BCL	C2C-C3C	-2.91	1.46	1.54
6	M	401	BCL	C1B-CHB	2.80	1.48	1.41
5	M	407	U10	C4-C3	2.80	1.47	1.36
4	L	301	BPH	C4C-NC	-2.80	1.31	1.37
6	M	402	BCL	C1D-C2D	2.75	1.48	1.42
5	L	302[B]	U10	C7-C8	2.74	1.54	1.50
4	L	301	BPH	CHD-C4C	2.73	1.45	1.38
7	H	304	PO4	P-O4	-2.67	1.46	1.54
4	M	406	BPH	CHD-C4C	2.58	1.44	1.38
6	L	303	BCL	CMD-C2D	-2.56	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	402	BCL	C3C-C4C	-2.54	1.48	1.51
6	L	308	BCL	CBD-CGD	-2.54	1.44	1.52
15	H	301	GGD	OB5-CB1	2.49	1.48	1.41
6	M	402	BCL	C4B-CHC	2.48	1.47	1.41
6	L	303	BCL	MG-NA	-2.46	2.00	2.06
5	M	407	U10	C33-C34	2.46	1.38	1.33
5	L	302[B]	U10	C7-C6	2.35	1.55	1.51
6	M	401	BCL	C3C-C4C	-2.35	1.48	1.51
14	M	410	PC1	C1-C2	2.33	1.57	1.50
5	L	302[A]	U10	C4-C3	2.30	1.45	1.36
6	L	308	BCL	MG-NA	-2.20	2.01	2.06
12	M	408	SPO	C11-C12	2.18	1.50	1.45
6	L	308	BCL	C4B-NB	-2.16	1.33	1.35
8	L	305	HTO	C4-C3	2.15	1.56	1.52
4	L	301	BPH	CBB-CAB	-2.15	1.45	1.50
6	M	401	BCL	C1-C2	2.12	1.55	1.49
14	M	410	PC1	P-O11	2.09	1.67	1.59
4	L	301	BPH	OBB-CAB	2.09	1.27	1.23
6	M	402	BCL	C2C-C3C	-2.09	1.48	1.54
12	M	408	SPO	C16-C17	2.06	1.50	1.45
4	M	406	BPH	CAC-C3C	-2.06	1.49	1.54
6	M	402	BCL	C1B-CHB	2.05	1.46	1.41
4	M	406	BPH	C2-C3	2.05	1.37	1.33
6	M	401	BCL	MG-NA	-2.03	2.01	2.06
4	M	406	BPH	C3B-C2B	2.03	1.44	1.39

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	402	BCL	C1C-NC-C4C	-7.45	103.36	106.71
4	L	301	BPH	C4A-NA-C1A	7.12	113.89	108.14
6	L	308	BCL	C1C-NC-C4C	-7.01	103.56	106.71
13	M	409	CDL	OB6-CB5-C51	6.39	125.27	111.50
6	M	401	BCL	O2D-CGD-CBD	6.11	122.13	111.27
14	M	410	PC1	O21-C21-C22	6.10	124.64	111.50
4	M	406	BPH	O2D-CGD-CBD	5.97	121.88	111.27
15	H	301	GGD	OC6-CC5-C14	5.83	124.07	111.50
6	M	401	BCL	C1D-CHD-C4C	-5.81	117.31	125.88
12	M	408	SPO	C2-C1-C4	-5.33	102.68	110.86
6	L	308	BCL	O2D-CGD-CBD	5.25	120.60	111.27
6	M	401	BCL	CHD-C4C-NC	5.07	130.71	125.08
6	M	401	BCL	C3C-C4C-CHD	-5.03	112.64	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	408	SPO	C20-C19-C17	-4.96	120.22	127.31
5	M	407	U10	C30-C29-C31	4.90	123.51	115.27
6	L	303	BCL	C3C-C4C-CHD	-4.84	113.05	123.39
4	M	406	BPH	CMB-C2B-C1B	4.84	132.51	125.06
15	H	301	GGD	OB5-CB5-CB6	4.79	118.34	106.44
6	M	401	BCL	O2A-C1-C2	4.74	121.08	108.64
6	L	308	BCL	OBD-CAD-C3D	-4.71	120.17	127.98
6	L	308	BCL	C1D-CHD-C4C	-4.67	118.99	125.88
15	H	301	GGD	OB1-CB1-OB5	4.64	123.64	110.67
6	M	402	BCL	OBD-CAD-C3D	-4.64	120.28	127.98
6	M	402	BCL	C3C-C4C-CHD	-4.63	113.50	123.39
6	L	303	BCL	C1C-NC-C4C	-4.56	104.66	106.71
5	L	302[B]	U10	C7-C8-C9	-4.50	119.31	126.79
13	M	409	CDL	OA6-CA5-C11	4.49	121.17	111.50
15	H	301	GGD	CB1-OB1-CA3	4.47	129.01	117.96
6	L	303	BCL	C1D-CHD-C4C	-4.41	119.37	125.88
4	L	301	BPH	CBB-CAB-C3B	-4.39	111.05	120.43
13	M	409	CDL	OA8-CA7-C31	4.38	125.65	111.91
5	L	302[A]	U10	C1M-C1-C6	-4.32	117.35	124.40
6	L	308	BCL	C3C-C4C-CHD	-4.30	114.20	123.39
4	L	301	BPH	CMB-C2B-C1B	4.28	131.66	125.06
4	M	406	BPH	O2D-CGD-O1D	-4.27	115.48	123.84
6	L	308	BCL	C4A-NA-C1A	4.09	108.54	106.71
4	M	406	BPH	C4A-NA-C1A	4.05	111.41	108.14
4	M	406	BPH	C1-O2A-CGA	4.02	126.98	116.44
6	L	308	BCL	C4-C3-C5	3.99	121.98	115.27
4	L	301	BPH	C1-C2-C3	-3.92	119.27	126.04
4	L	301	BPH	OBB-CAB-C3B	3.91	127.64	120.41
6	L	308	BCL	C1-O2A-CGA	3.91	126.70	116.44
13	M	409	CDL	OA8-CA7-OA9	-3.89	113.78	123.59
5	L	302[B]	U10	C7-C6-C5	3.87	123.14	118.48
4	L	301	BPH	CHC-C1C-NC	3.78	129.70	125.20
6	M	401	BCL	C1-O2A-CGA	3.75	126.29	116.44
6	M	402	BCL	O2A-C1-C2	3.72	118.40	108.64
5	L	302[A]	U10	C8-C7-C6	3.71	122.04	112.05
4	M	406	BPH	C3D-CAD-CBD	3.64	112.39	107.61
6	L	303	BCL	CHD-C4C-NC	3.62	129.09	125.08
15	H	301	GGD	OC6-CC5-OC7	-3.56	115.09	123.70
5	M	407	U10	C30-C29-C28	-3.53	114.61	123.68
6	L	303	BCL	CHB-C4A-NA	3.49	129.34	124.51
5	L	302[A]	U10	O5-C5-C6	-3.46	115.47	121.55
6	L	308	BCL	CHC-C1C-NC	3.46	129.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	406	BPH	CAC-C3C-C2C	-3.46	105.62	114.26
6	L	308	BCL	CHD-C4C-NC	3.45	128.91	125.08
15	H	301	GGD	CA3-CA4-CA5	3.39	116.89	109.66
14	M	410	PC1	O31-C31-C32	3.39	122.54	111.91
6	M	401	BCL	C1C-NC-C4C	-3.37	105.19	106.71
6	L	308	BCL	C5-C3-C2	-3.36	114.33	121.12
6	L	303	BCL	CHC-C1C-NC	3.33	129.11	124.51
5	M	407	U10	C25-C24-C26	3.31	120.83	115.27
4	M	406	BPH	C3B-C2B-C1B	-3.26	101.12	105.87
13	M	409	CDL	OB8-CB7-OB9	-3.18	115.57	123.59
6	M	402	BCL	OBB-CAB-C3B	3.12	125.53	119.99
12	M	408	SPO	C3-C1-C2	3.11	116.23	110.37
6	M	401	BCL	O1D-CGD-CBD	-3.11	118.12	124.48
8	L	305	HTO	O2-C2-C1	-3.11	101.86	109.14
6	L	308	BCL	CHB-C4A-NA	3.09	128.78	124.51
6	M	401	BCL	O2A-CGA-CBA	3.09	121.59	111.91
6	L	303	BCL	O2A-CGA-CBA	3.07	121.54	111.91
12	M	408	SPO	C40-C38-C39	3.05	121.34	114.60
6	M	401	BCL	CHC-C1C-NC	3.03	128.71	124.51
5	L	302[B]	U10	C1M-C1-C6	-3.03	119.46	124.40
4	M	406	BPH	CHC-C1C-NC	3.03	128.80	125.20
5	M	407	U10	C41-C39-C40	3.01	121.25	114.60
4	L	301	BPH	C7-C6-C5	-3.00	105.22	113.36
6	M	402	BCL	OBD-CAD-CBD	3.00	130.18	125.89
12	M	408	SPO	C6-C7-C9	-2.98	114.37	118.94
12	M	408	SPO	C13-C12-C14	-2.96	118.78	122.92
4	L	301	BPH	C3A-C4A-NA	-2.92	108.07	113.05
5	L	302[A]	U10	O2-C2-C3	-2.87	114.84	120.93
5	M	407	U10	C32-C31-C29	2.86	122.38	112.98
6	L	303	BCL	OBD-CAD-C3D	-2.85	123.25	127.98
13	M	409	CDL	OB6-CB5-OB7	-2.85	116.82	123.70
4	M	406	BPH	CBB-CAB-C3B	-2.85	114.35	120.43
4	L	301	BPH	CMD-C2D-C3D	-2.83	119.39	124.68
14	M	410	PC1	C3-O31-C31	2.82	127.56	117.12
4	M	406	BPH	C4-C3-C2	-2.80	116.48	123.68
14	M	410	PC1	C2-O21-C21	2.75	124.57	117.79
5	M	407	U10	C17-C18-C19	-2.75	121.04	127.66
4	M	406	BPH	C2B-C1B-NB	2.74	113.93	109.79
5	M	407	U10	C31-C32-C33	2.72	120.83	111.88
5	L	302[B]	U10	C1-C6-C5	-2.72	117.02	119.58
5	L	302[B]	U10	C6-C1-C2	2.71	121.33	119.18
6	L	308	BCL	C4B-CHC-C1C	-2.71	124.74	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	301	BPH	O2D-CGD-CBD	2.71	116.09	111.27
6	L	308	BCL	C1-C2-C3	-2.70	121.36	126.04
6	M	402	BCL	C1-C2-C3	-2.68	121.40	126.04
5	L	302[A]	U10	C16-C14-C13	-2.67	114.92	122.65
5	M	407	U10	C1M-C1-C6	-2.67	120.04	124.40
6	M	402	BCL	O2D-CGD-O1D	-2.66	118.63	123.84
4	M	406	BPH	C11-C12-C13	2.66	124.52	115.92
6	L	308	BCL	OBD-CAD-CBD	2.66	129.69	125.89
5	L	302[B]	U10	C8-C7-C6	2.63	119.14	112.05
4	M	406	BPH	C1C-NC-C4C	-2.62	108.23	110.54
5	L	302[B]	U10	C11-C9-C8	2.62	126.42	121.12
14	M	410	PC1	O31-C31-O32	-2.60	117.03	123.59
8	L	305	HTO	C1-C2-C3	2.59	118.73	113.11
6	L	303	BCL	C2A-C1A-CHA	-2.57	119.36	123.86
6	L	308	BCL	C6-C5-C3	-2.57	106.71	113.45
5	M	407	U10	C15-C14-C16	2.56	119.58	115.27
6	L	303	BCL	C4B-CHC-C1C	-2.56	125.05	130.12
6	M	401	BCL	C4B-CHC-C1C	-2.55	125.06	130.12
6	M	402	BCL	CHD-C4C-NC	2.54	127.89	125.08
13	M	409	CDL	OB8-CB7-C71	2.52	119.81	111.91
4	M	406	BPH	C4D-C3D-CAD	-2.50	106.29	107.87
12	M	408	SPO	C35-C36-C37	-2.50	103.68	111.88
4	L	301	BPH	C2B-C1B-NB	2.49	113.55	109.79
12	M	408	SPO	C18-C17-C19	-2.48	119.44	122.92
6	M	402	BCL	C4B-CHC-C1C	-2.44	125.28	130.12
4	L	301	BPH	CHB-C4A-NA	2.43	129.12	124.94
4	M	406	BPH	C4D-CHA-C1A	-2.43	124.52	130.51
5	M	407	U10	C4M-O4-C4	2.42	125.04	116.47
4	L	301	BPH	C4D-CHA-C1A	-2.40	124.58	130.51
6	L	308	BCL	O1D-CGD-CBD	-2.40	119.57	124.48
7	H	304	PO4	O4-P-O1	-2.34	102.34	110.89
5	M	407	U10	C17-C16-C14	-2.33	105.30	112.98
6	L	303	BCL	CMA-C3A-C4A	-2.33	105.50	111.77
6	M	402	BCL	C1D-CHD-C4C	-2.33	122.44	125.88
5	L	302[A]	U10	C3M-O3-C3	2.32	124.70	116.47
14	M	410	PC1	O21-C21-O22	-2.31	118.12	123.70
15	H	301	GGD	OC8-CC7-C31	2.29	119.09	111.91
8	L	305	HTO	O3-C3-C2	2.28	114.42	109.72
6	L	303	BCL	CAC-C3C-C4C	-2.27	107.54	112.58
6	M	401	BCL	CMB-C2B-C3B	2.27	128.92	124.68
6	L	308	BCL	C16-C15-C13	-2.27	108.59	115.92
6	L	303	BCL	O2A-CGA-O1A	-2.26	117.88	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	408	SPO	C40-C38-C37	-2.24	116.17	122.65
6	M	402	BCL	CBB-CAB-C3B	-2.24	113.69	120.34
12	M	408	SPO	C13-C12-C11	2.23	121.60	118.08
5	M	407	U10	C7-C8-C9	-2.23	123.08	126.79
6	M	402	BCL	CAC-C3C-C4C	-2.21	107.67	112.58
6	M	401	BCL	C1B-CHB-C4A	-2.20	125.75	130.12
6	M	402	BCL	C2A-C1A-CHA	-2.20	120.01	123.86
6	L	303	BCL	C3A-C2A-C1A	-2.19	98.06	101.34
13	M	409	CDL	CB4-OB6-CB5	2.17	123.14	117.79
6	L	308	BCL	C4B-C3B-CAB	2.17	131.31	127.13
6	L	308	BCL	O2A-C1-C2	-2.15	102.98	108.64
4	M	406	BPH	OBD-CAD-C3D	-2.15	124.41	127.98
4	M	406	BPH	C3A-C4A-NA	-2.15	109.39	113.05
5	L	302[A]	U10	O4-C4-C3	-2.13	115.60	123.64
5	M	407	U10	C27-C28-C29	-2.13	122.53	127.66
10	M	403	LDA	CM1-N1-C1	2.13	114.70	110.23
6	M	402	BCL	CHC-C1C-NC	2.12	127.44	124.51
6	L	308	BCL	O2A-CGA-O1A	-2.11	118.26	123.59
15	H	301	GGD	CA6-CA5-CA4	2.11	117.94	113.00
6	M	402	BCL	CHB-C4A-NA	2.11	127.43	124.51
4	M	406	BPH	CHD-C4C-NC	-2.10	122.70	125.20
5	L	302[A]	U10	O3-C3-C2	2.10	123.66	116.56
6	M	401	BCL	O2D-CGD-O1D	-2.09	119.75	123.84
4	L	301	BPH	C4-C3-C5	2.09	118.79	115.27
5	L	302[A]	U10	C7-C6-C5	-2.09	115.96	118.48
12	M	408	SPO	C27-C26-C25	-2.07	116.77	123.22
6	L	308	BCL	O2D-CGD-O1D	-2.06	119.81	123.84
15	H	301	GGD	OC8-CC7-OC9	-2.06	118.40	123.59
7	H	304	PO4	O3-P-O2	2.05	114.54	107.97
12	M	408	SPO	C25-C23-C22	-2.05	115.80	118.94
5	M	407	U10	C41-C39-C38	-2.04	116.74	122.65
5	L	302[B]	U10	C3M-O3-C3	2.03	123.67	116.47
4	M	406	BPH	C5-C3-C2	2.03	125.23	121.12
6	L	308	BCL	C1B-CHB-C4A	-2.03	126.09	130.12
12	M	408	SPO	C18-C17-C16	2.03	121.27	118.08
15	H	301	GGD	CC6-OC8-CC7	2.01	124.56	117.12
15	H	301	GGD	CB1-OB5-CB5	-2.01	109.75	113.69
6	M	402	BCL	CMB-C2B-C3B	2.01	128.43	124.68
4	M	406	BPH	C6-C5-C3	2.00	118.70	113.45

There are no chirality outliers.

All (209) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	312	GOL	C1-C2-C3-O3
12	M	408	SPO	C2-C1-C4-C5
12	M	408	SPO	C3-C1-C4-C5
15	H	301	GGD	OA5-CA1-OA1-CC3
15	H	301	GGD	C14-CC5-OC6-CC4
4	M	406	BPH	C4B-C3B-CAB-CBB
4	M	406	BPH	C4B-C3B-CAB-OB
8	L	305	HTO	O1-C1-C2-O2
8	L	305	HTO	O1-C1-C2-C3
8	L	305	HTO	C1-C2-C3-O3
8	L	305	HTO	C1-C2-C3-C4
8	L	305	HTO	O2-C2-C3-O3
8	L	305	HTO	O2-C2-C3-C4
8	L	305	HTO	O3-C3-C4-C5
9	L	313	GOL	O1-C1-C2-C3
10	M	403	LDA	N1-C1-C2-C3
10	M	404	LDA	C2-C1-N1-O1
10	M	404	LDA	C2-C1-N1-CM1
10	M	404	LDA	C2-C1-N1-CM2
9	L	311	GOL	C1-C2-C3-O3
9	L	306	GOL	C1-C2-C3-O3
9	H	303	GOL	C1-C2-C3-O3
5	M	407	U10	C29-C31-C32-C33
5	M	407	U10	C31-C32-C33-C34
13	M	409	CDL	CA2-OA2-PA1-OA3
13	M	409	CDL	CA2-OA2-PA1-OA4
13	M	409	CDL	CA2-OA2-PA1-OA5
13	M	409	CDL	CA3-OA5-PA1-OA3
13	M	409	CDL	CA3-OA5-PA1-OA4
13	M	409	CDL	C11-CA5-OA6-CA4
13	M	409	CDL	CB2-OB2-PB2-OB3
13	M	409	CDL	CB3-OB5-PB2-OB3
13	M	409	CDL	CB3-OB5-PB2-OB4
13	M	409	CDL	OB9-CB7-OB8-CB6
13	M	409	CDL	C71-CB7-OB8-CB6
15	H	301	GGD	OB5-CB1-OB1-CA3
15	H	301	GGD	OC7-CC5-OC6-CC4
14	M	410	PC1	O22-C21-O21-C2
13	M	409	CDL	OA7-CA5-OA6-CA4
4	M	406	BPH	C10-C11-C12-C13
14	M	410	PC1	C22-C21-O21-C2
15	H	301	GGD	OA5-CA5-CA6-OA6
5	L	302[B]	U10	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
5	M	407	U10	C30-C29-C31-C32
5	L	302[B]	U10	C12-C11-C9-C8
5	M	407	U10	C28-C29-C31-C32
13	M	409	CDL	CB2-C1-CA2-OA2
14	M	410	PC1	C32-C31-O31-C3
13	M	409	CDL	CB5-C51-C52-C53
15	H	301	GGD	CA4-CA5-CA6-OA6
14	M	410	PC1	C2A-C2B-C2C-C2D
15	H	301	GGD	CA2-CA1-OA1-CC3
6	M	401	BCL	C11-C12-C13-C14
15	H	301	GGD	CB4-CB5-CB6-OB6
4	M	406	BPH	C13-C15-C16-C17
13	M	409	CDL	CA5-C11-C12-C13
5	M	407	U10	C34-C36-C37-C38
15	H	301	GGD	OB5-CB5-CB6-OB6
14	M	410	PC1	O32-C31-O31-C3
4	M	406	BPH	C5-C6-C7-C8
14	M	410	PC1	C11-O13-P-O11
13	M	409	CDL	CA3-OA5-PA1-OA2
13	M	409	CDL	CB3-OB5-PB2-OB2
4	M	406	BPH	C8-C10-C11-C12
13	M	409	CDL	C38-C39-C40-C41
10	M	404	LDA	C6-C7-C8-C9
13	M	409	CDL	C14-C15-C16-C17
13	M	409	CDL	C12-C13-C14-C15
6	M	401	BCL	C11-C10-C8-C9
14	M	410	PC1	C28-C29-C2A-C2B
9	L	309	GOL	C1-C2-C3-O3
15	H	301	GGD	C31-C32-C33-C34
13	M	409	CDL	C71-C72-C73-C74
6	L	303	BCL	C16-C17-C18-C19
13	M	409	CDL	C40-C41-C42-C43
14	M	410	PC1	C27-C28-C29-C2A
13	M	409	CDL	C16-C17-C18-C19
15	H	301	GGD	C14-C15-C16-C17
9	L	313	GOL	O1-C1-C2-O2
9	L	311	GOL	O2-C2-C3-O3
9	L	306	GOL	O2-C2-C3-O3
15	H	301	GGD	C35-C36-C37-C38
15	H	301	GGD	C39-C40-C41-C42
10	M	413	LDA	C3-C4-C5-C6
4	L	301	BPH	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	M	401	BCL	C11-C10-C8-C7
6	M	401	BCL	C11-C12-C13-C15
4	L	301	BPH	C2-C3-C5-C6
10	M	404	LDA	C11-C10-C9-C8
13	M	409	CDL	C11-C12-C13-C14
13	M	409	CDL	C17-C18-C19-C20
10	M	404	LDA	C4-C5-C6-C7
14	M	410	PC1	C22-C23-C24-C25
13	M	409	CDL	CB2-OB2-PB2-OB5
13	M	409	CDL	OA5-CA3-CA4-CA6
6	L	308	BCL	C3-C5-C6-C7
12	M	408	SPO	C1-C4-C5-C6
15	H	301	GGD	CC3-CC4-CC6-OC8
13	M	409	CDL	C81-C82-C83-C84
12	M	408	SPO	C4-C1-O1-CM1
10	M	404	LDA	C1-C2-C3-C4
9	H	303	GOL	O2-C2-C3-O3
15	H	301	GGD	CC3-CC4-OC6-CC5
14	M	410	PC1	C21-C22-C23-C24
12	M	408	SPO	C3-C1-O1-CM1
6	M	402	BCL	C14-C13-C15-C16
13	M	409	CDL	C78-C79-C80-C81
10	M	413	LDA	N1-C1-C2-C3
15	H	301	GGD	C34-C35-C36-C37
5	L	302[B]	U10	C9-C11-C12-C13
13	M	409	CDL	CB3-CB4-CB6-OB8
6	L	303	BCL	C16-C17-C18-C20
6	M	401	BCL	C13-C15-C16-C17
15	H	301	GGD	C33-C34-C35-C36
9	L	307	GOL	O1-C1-C2-O2
9	H	307	GOL	O1-C1-C2-O2
13	M	409	CDL	OB5-CB3-CB4-OB6
15	H	301	GGD	C32-C31-CC7-OC8
15	H	301	GGD	C15-C16-C17-C18
13	M	409	CDL	C13-C14-C15-C16
4	M	406	BPH	C2-C1-O2A-CGA
6	M	401	BCL	C6-C7-C8-C9
10	M	403	LDA	C11-C10-C9-C8
10	M	413	LDA	C4-C5-C6-C7
4	L	301	BPH	C4C-C3C-CAC-CBC
13	M	409	CDL	C18-C19-C20-C21
4	L	301	BPH	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	M	409	CDL	C52-C53-C54-C55
6	L	308	BCL	C12-C13-C15-C16
6	M	401	BCL	C6-C7-C8-C10
14	M	410	PC1	C26-C27-C28-C29
10	M	403	LDA	C1-C2-C3-C4
6	L	308	BCL	CAD-CBD-CGD-O2D
6	M	401	BCL	CAD-CBD-CGD-O2D
6	M	401	BCL	C8-C10-C11-C12
15	H	301	GGD	OC6-CC4-CC6-OC8
9	L	312	GOL	O2-C2-C3-O3
9	L	307	GOL	O2-C2-C3-O3
14	M	410	PC1	C31-C32-C33-C34
9	H	307	GOL	O1-C1-C2-C3
15	H	301	GGD	C40-C41-C42-C43
14	M	410	PC1	C33-C34-C35-C36
14	M	410	PC1	C11-O13-P-O12
13	M	409	CDL	CB2-OB2-PB2-OB4
4	M	406	BPH	C4-C3-C5-C6
4	M	406	BPH	C2-C3-C5-C6
4	M	406	BPH	C12-C13-C15-C16
10	M	404	LDA	C7-C8-C9-C10
13	M	409	CDL	C54-C55-C56-C57
14	M	410	PC1	O13-C11-C12-N
13	M	409	CDL	OB6-CB4-CB6-OB8
15	H	301	GGD	C18-C19-C20-C21
6	L	308	BCL	C14-C13-C15-C16
4	M	406	BPH	C16-C17-C18-C20
13	M	409	CDL	C19-C20-C21-C22
5	L	302[A]	U10	C5-C6-C7-C8
13	M	409	CDL	OA9-CA7-OA8-CA6
14	M	410	PC1	C3-C2-O21-C21
13	M	409	CDL	OB5-CB3-CB4-CB6
13	M	409	CDL	OA5-CA3-CA4-OA6
15	H	301	GGD	CB2-CB1-OB1-CA3
13	M	409	CDL	C31-CA7-OA8-CA6
10	M	404	LDA	C9-C10-C11-C12
12	M	408	SPO	C2-C1-O1-CM1
14	M	410	PC1	C25-C26-C27-C28
14	M	410	PC1	C1-O11-P-O13
4	M	406	BPH	C14-C13-C15-C16
15	H	301	GGD	C41-C42-C43-C44
4	L	301	BPH	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	H	301	GGD	C36-C37-C38-C39
6	L	303	BCL	C2A-CAA-CBA-CGA
13	M	409	CDL	C1-CB2-OB2-PB2
6	M	402	BCL	CAA-CBA-CGA-O2A
4	L	301	BPH	C8-C10-C11-C12
13	M	409	CDL	O1-C1-CA2-OA2
13	M	409	CDL	C39-C40-C41-C42
6	L	303	BCL	C15-C16-C17-C18
6	M	401	BCL	C12-C13-C15-C16
13	M	409	CDL	CA2-C1-CB2-OB2
8	L	305	HTO	C2-C3-C4-C5
13	M	409	CDL	C36-C37-C38-C39
9	L	307	GOL	C1-C2-C3-O3
5	L	302[B]	U10	C5-C4-O4-C4M
5	M	407	U10	C5-C4-O4-C4M
15	H	301	GGD	C20-C21-C22-C23
13	M	409	CDL	C20-C21-C22-C23
6	L	303	BCL	CAD-CBD-CGD-O2D
4	M	406	BPH	CAD-CBD-CGD-O2D
6	M	402	BCL	CAD-CBD-CGD-O2D
13	M	409	CDL	C12-C11-CA5-OA6
6	M	401	BCL	O2A-C1-C2-C3
4	L	301	BPH	O2A-C1-C2-C3
13	M	409	CDL	C80-C81-C82-C83
15	H	301	GGD	C32-C31-CC7-OC9
9	L	309	GOL	O2-C2-C3-O3
6	M	402	BCL	C12-C13-C15-C16
13	M	409	CDL	O1-C1-CB2-OB2
4	M	406	BPH	C16-C17-C18-C19
10	M	403	LDA	C2-C3-C4-C5
13	M	409	CDL	C12-C11-CA5-OA7
6	L	308	BCL	C13-C15-C16-C17
14	M	410	PC1	C1-O11-P-O14
9	L	309	GOL	O1-C1-C2-O2
13	M	409	CDL	CA4-CA3-OA5-PA1
5	L	302[A]	U10	C12-C11-C9-C10
4	M	406	BPH	C6-C7-C8-C10
4	M	406	BPH	C11-C10-C8-C7
13	M	409	CDL	C52-C51-CB5-OB6
4	M	406	BPH	O1A-CGA-O2A-C1

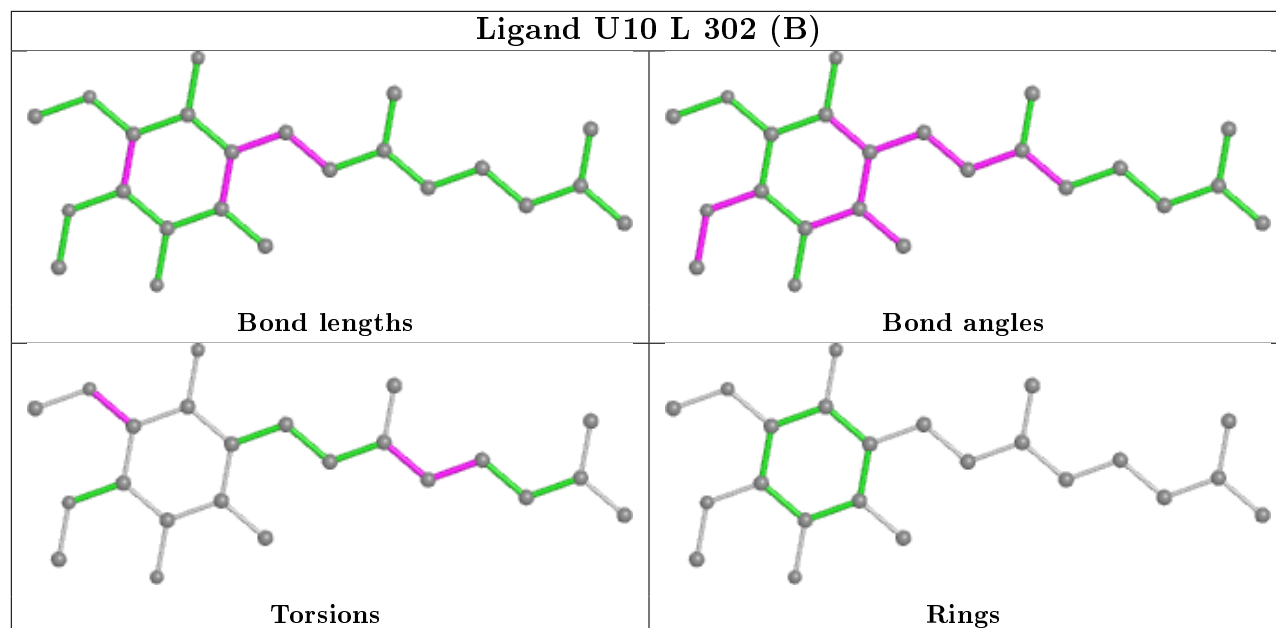
There are no ring outliers.

16 monomers are involved in 59 short contacts:

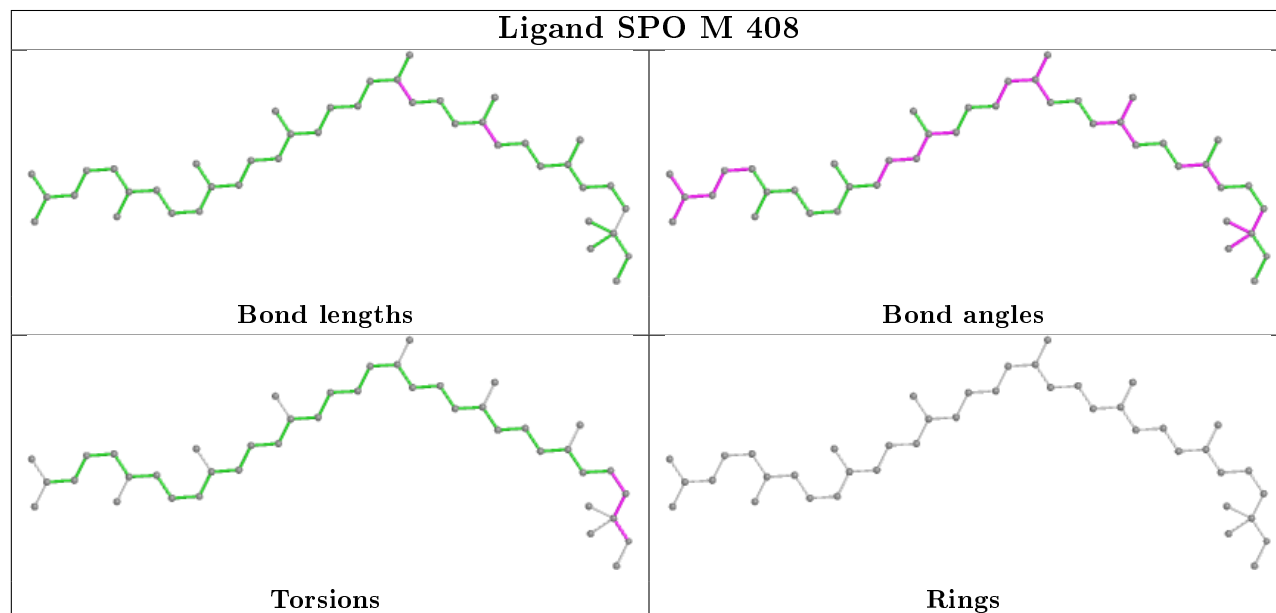
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302[B]	U10	8	0
12	M	408	SPO	6	0
9	L	307	GOL	1	0
6	L	308	BCL	10	0
6	L	303	BCL	4	0
7	H	304	PO4	3	0
6	M	401	BCL	5	0
4	M	406	BPH	9	0
6	M	402	BCL	6	0
14	M	410	PC1	2	0
9	L	313	GOL	1	0
4	L	301	BPH	7	0
9	L	306	GOL	1	0
5	M	407	U10	1	0
9	H	307	GOL	1	0
5	L	302[A]	U10	1	0

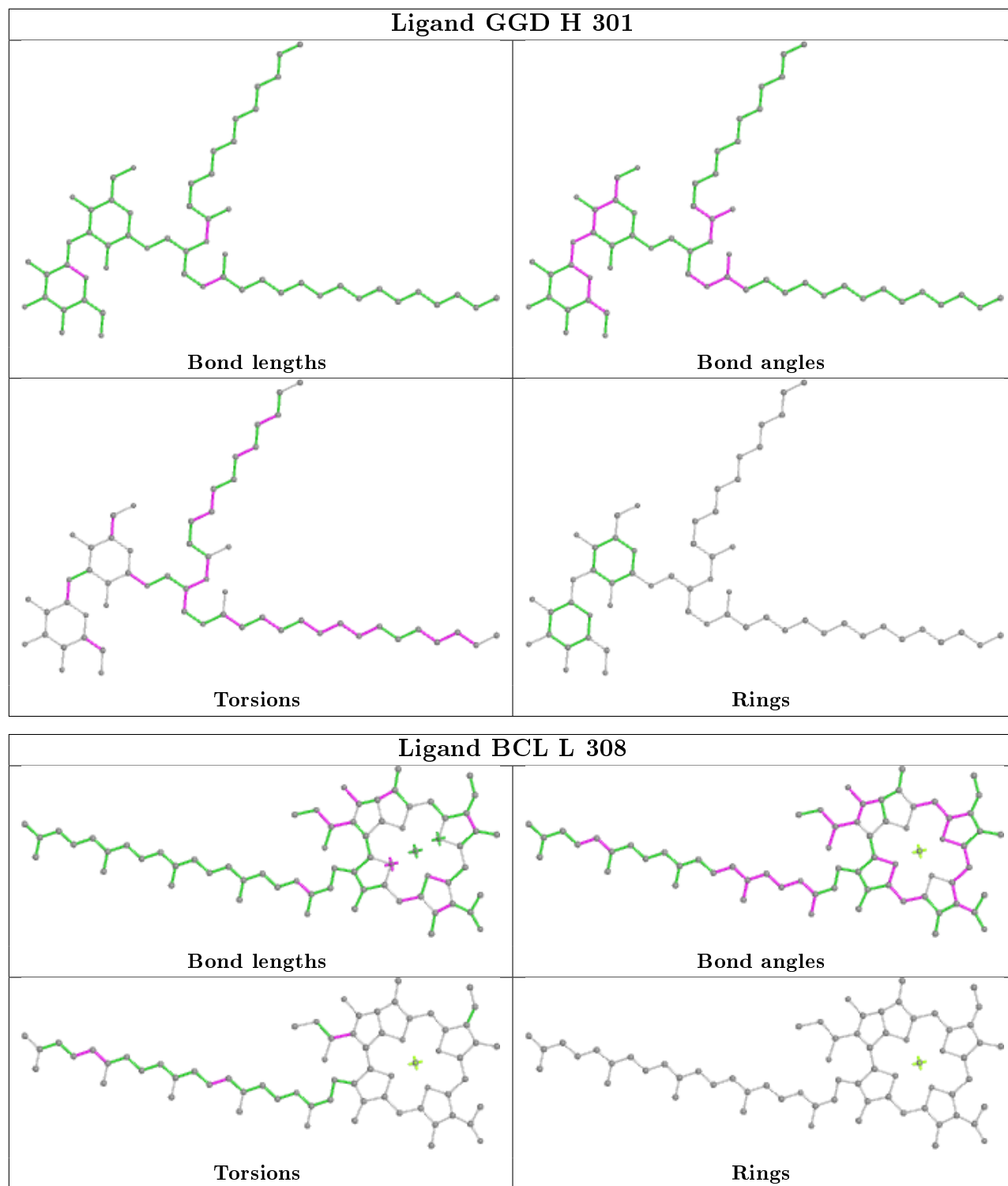
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

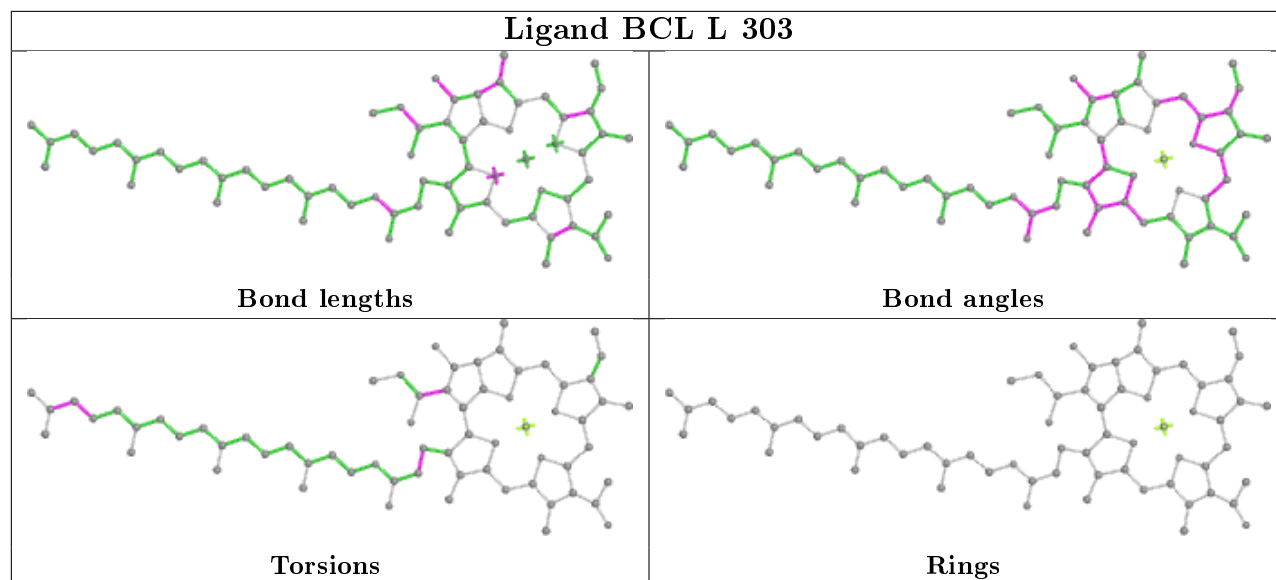
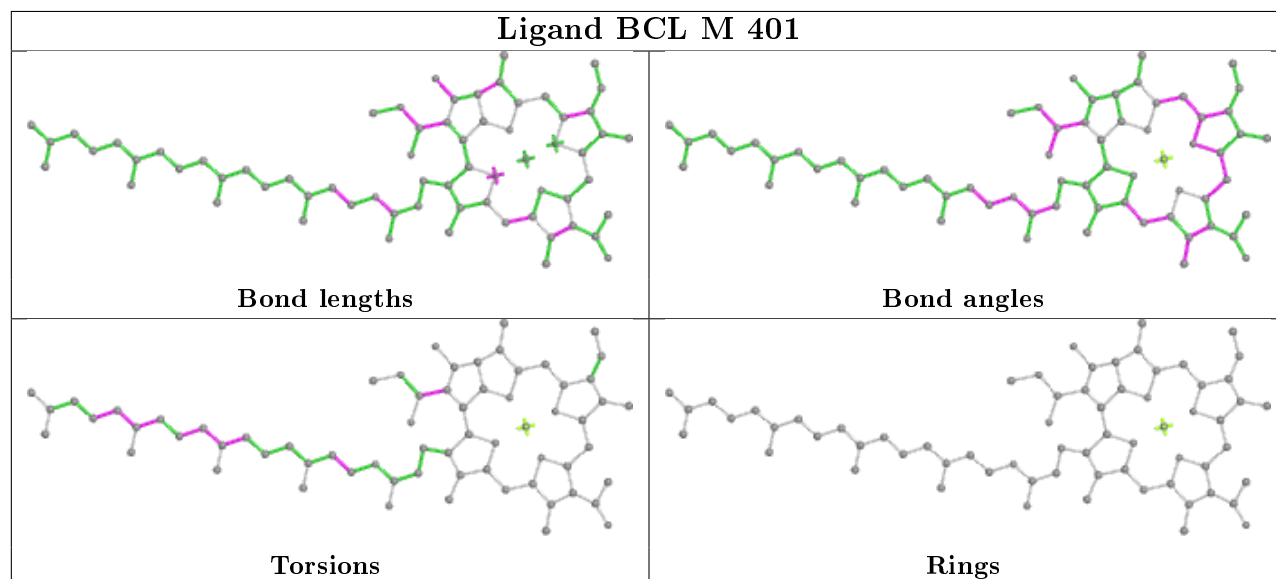
## Ligand U10 L 302 (B)

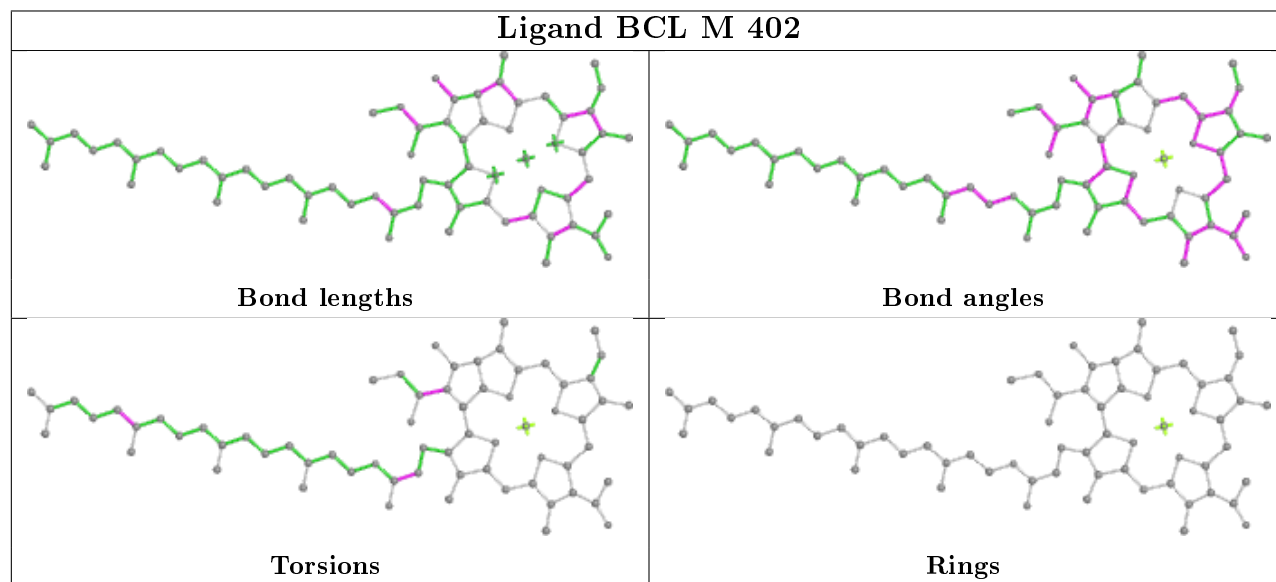
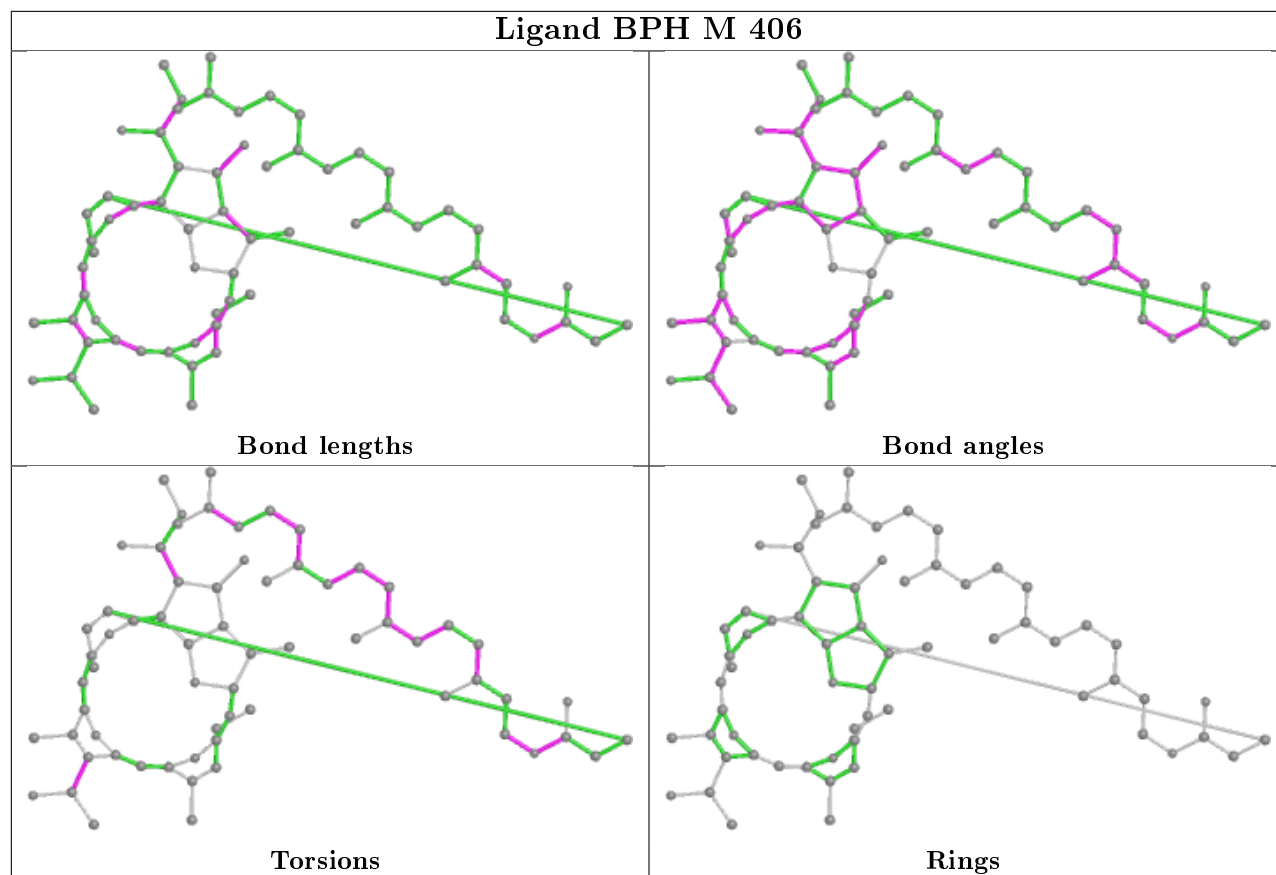


## Ligand SPO M 408



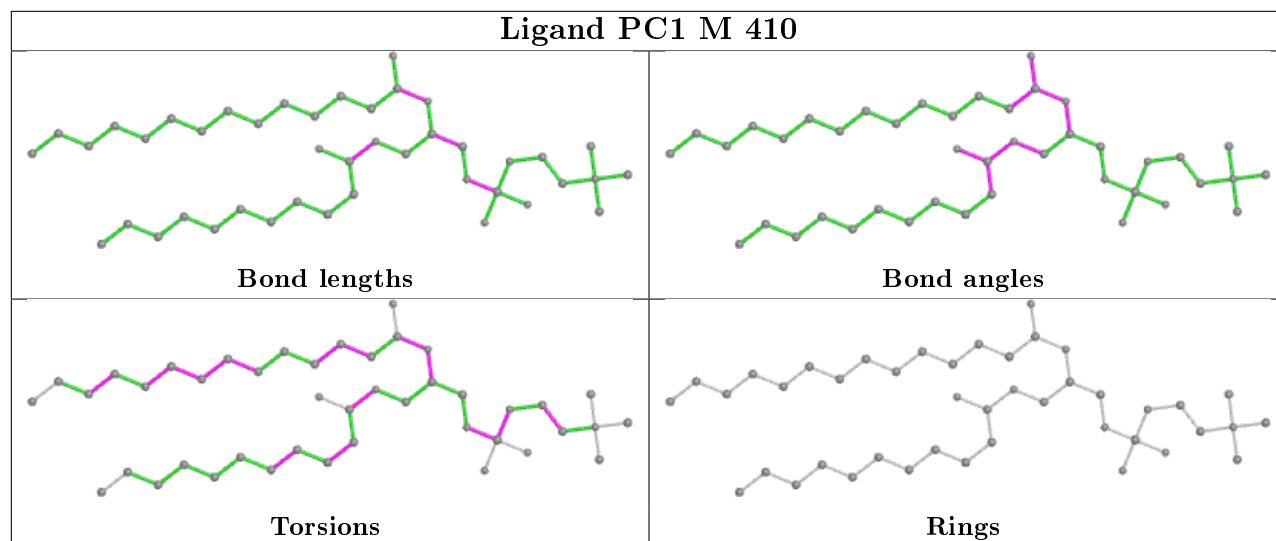


**Ligand BCL L 303****Ligand BCL M 401**

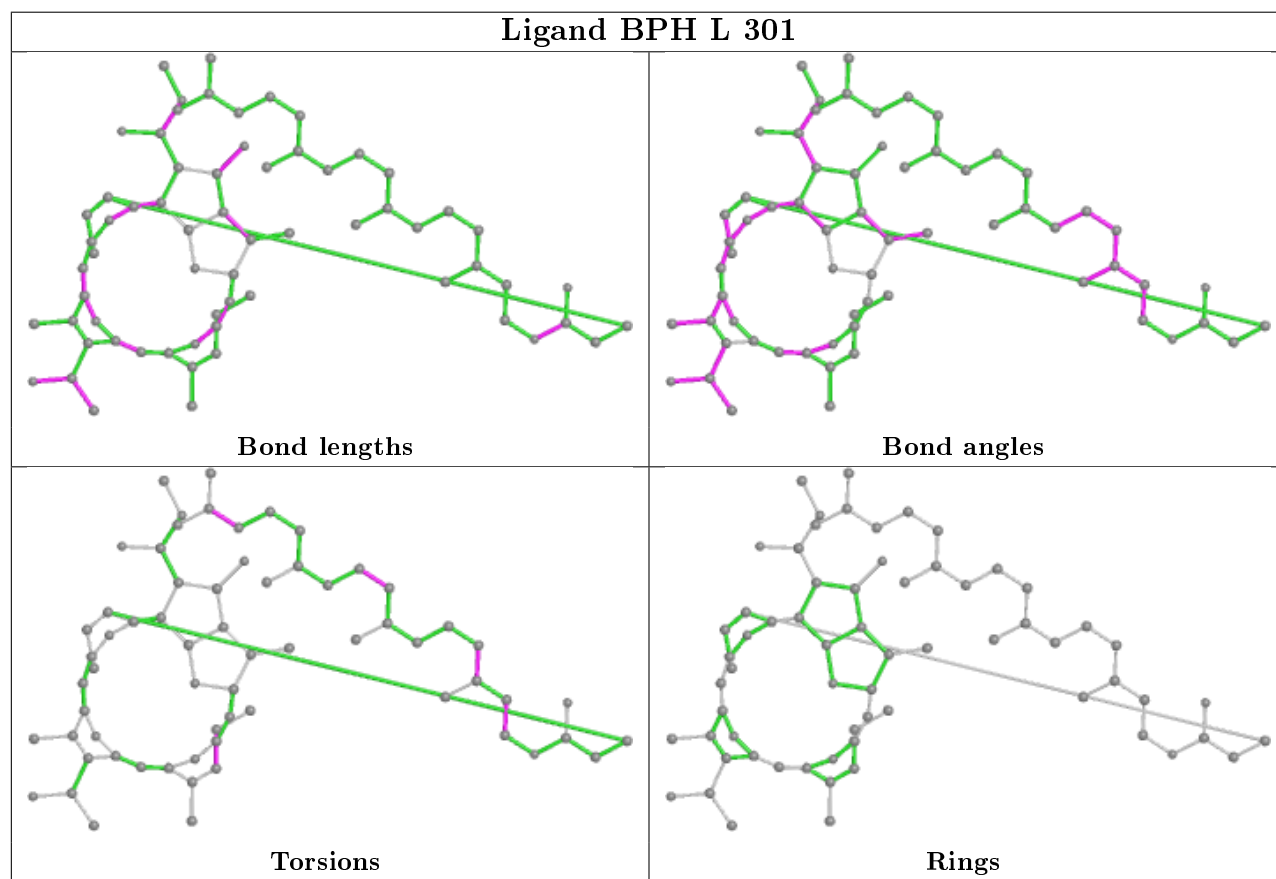




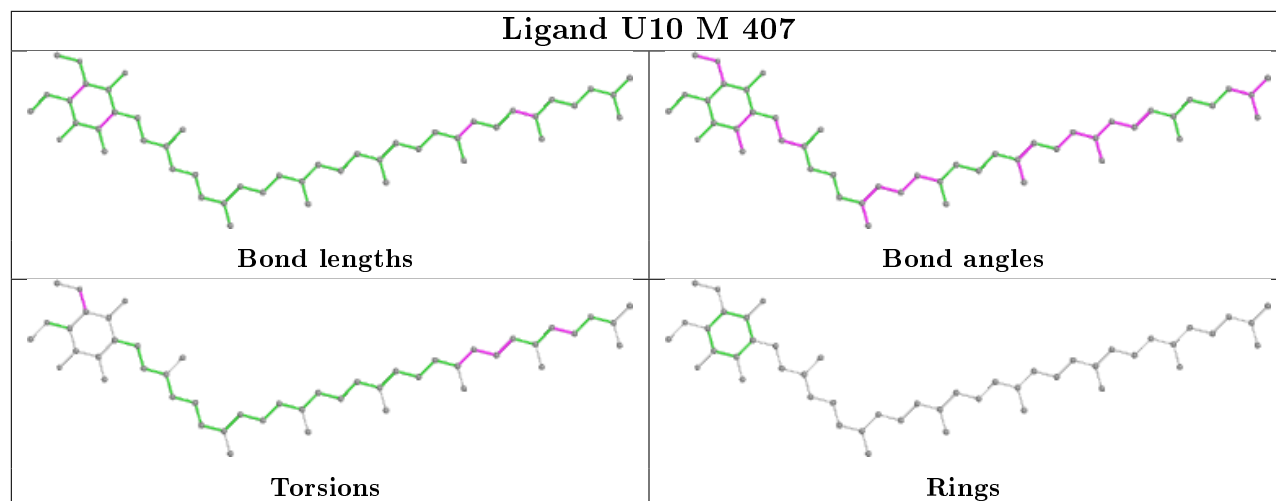
## Ligand PC1 M 410



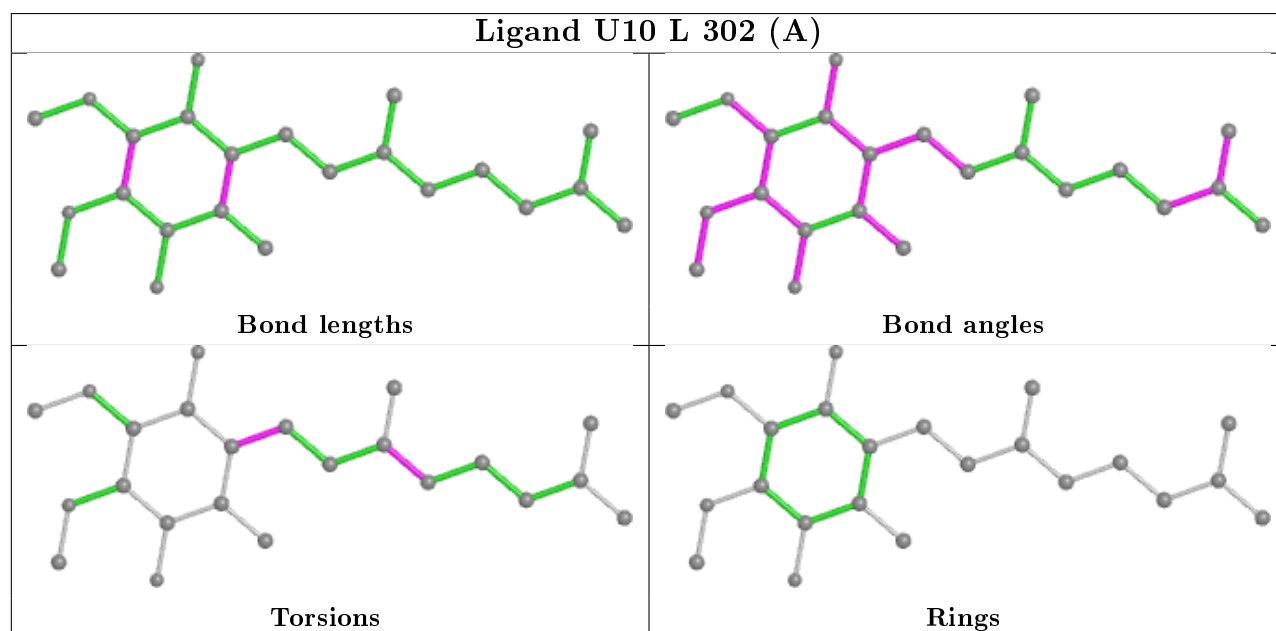
## Ligand BPH L 301



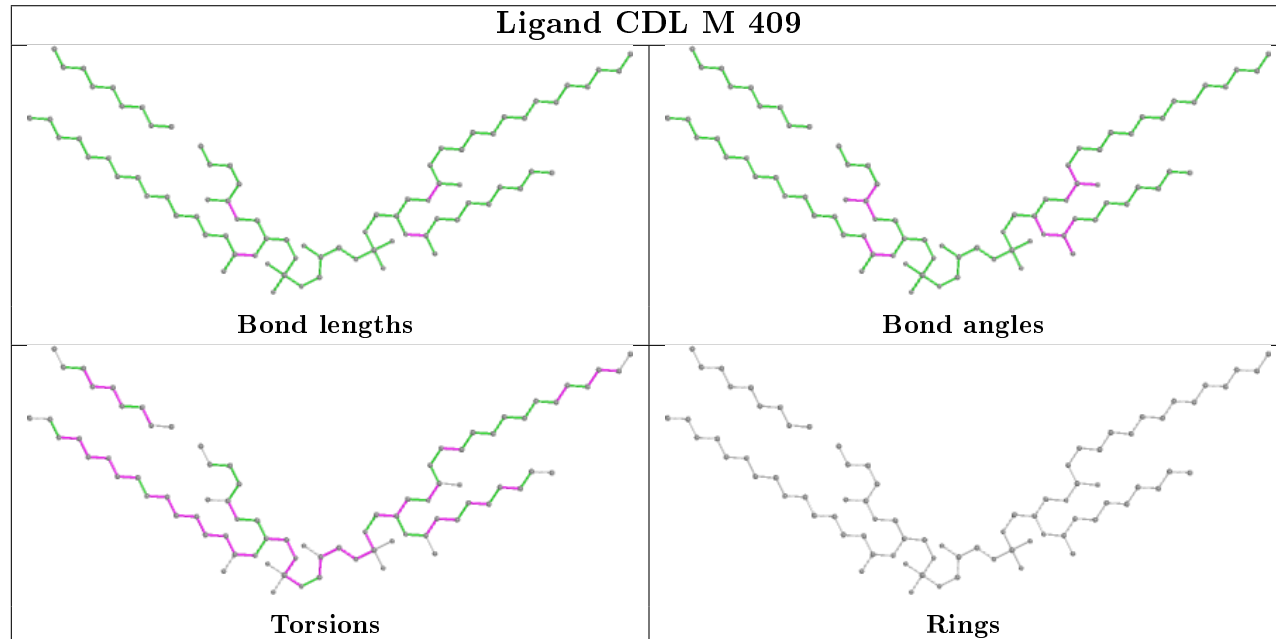
## Ligand U10 M 407



## Ligand U10 L 302 (A)



## Ligand CDL M 409



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)	-0.72	3 (1%) 80 82	30, 39, 60, 78	0
2	M	302/302 (100%)	-0.35	7 (2%) 60 62	29, 43, 64, 104	6 (1%)
3	H	240/266 (90%)	-0.47	4 (1%) 70 72	33, 43, 58, 95	3 (1%)
All	All	823/849 (96%)	-0.51	14 (1%) 70 72	29, 42, 62, 104	9 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	7.7
3	H	250	SER	4.5
2	M	301	HIS	3.2
3	H	220[A]	LYS	2.8
1	L	281	GLY	2.7
2	M	80	TRP	2.5
3	H	52	ASN	2.4
2	M	2	GLU	2.4
2	M	106	ALA	2.2
1	L	59	TRP	2.2
2	M	100	GLU	2.1
3	H	18	TYR	2.1
1	L	277	GLY	2.0
2	M	76	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

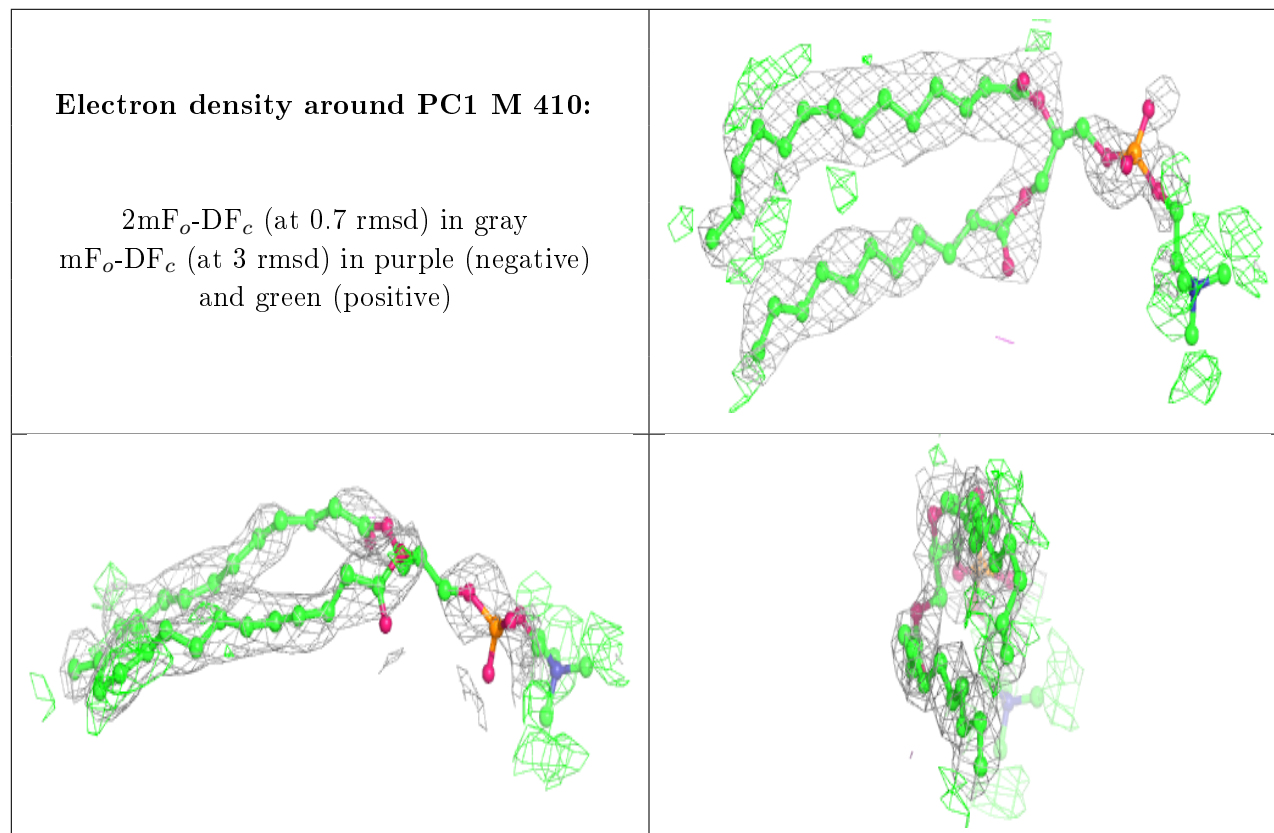
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	PC1	M	410	43/54	0.52	0.37	64,94,167,184	0
15	GGD	H	301	57/67	0.62	0.39	56,100,200,209	0
7	PO4	L	310	5/5	0.77	1.05	129,132,166,171	0
9	GOL	H	305	6/6	0.79	0.24	62,73,83,87	0
9	GOL	L	309	6/6	0.80	0.28	74,81,83,83	0
7	PO4	M	412	5/5	0.81	0.32	73,121,129,134	0
9	GOL	H	303	6/6	0.83	0.23	71,77,78,80	0
10	LDA	M	413	16/16	0.86	0.34	61,77,118,135	0
9	GOL	H	302	6/6	0.86	0.42	71,92,101,107	0
8	HTO	L	305	10/10	0.86	0.40	64,79,90,97	0
5	U10	L	302[B]	23/63	0.87	0.31	20,34,40,41	23
5	U10	L	302[A]	23/63	0.87	0.31	33,42,71,75	23
13	CDL	M	409	81/100	0.87	0.28	48,79,111,124	0
10	LDA	M	404	16/16	0.90	0.36	61,66,89,91	0
9	GOL	L	307	6/6	0.91	0.19	58,60,69,74	0
9	GOL	L	312	6/6	0.91	0.19	53,61,64,80	0
9	GOL	L	313	6/6	0.91	0.25	58,79,88,90	0
4	BPH	M	406	65/65	0.92	0.24	33,39,116,120	0
9	GOL	H	307	6/6	0.92	0.15	57,65,67,67	0
7	PO4	M	411	5/5	0.92	0.24	65,71,79,87	0
10	LDA	M	403	16/16	0.92	0.24	50,69,92,94	0
7	PO4	H	304	5/5	0.93	0.16	52,72,89,90	0
5	U10	M	407	48/63	0.93	0.22	32,51,92,101	0
9	GOL	L	311	6/6	0.93	0.15	49,59,63,63	0
12	SPO	M	408	42/42	0.93	0.17	36,49,77,91	0
9	GOL	L	306	6/6	0.93	0.27	44,59,64,68	0
9	GOL	H	306	6/6	0.96	0.24	49,56,60,65	0
6	BCL	M	401	66/66	0.97	0.17	29,36,82,94	0
6	BCL	M	402	66/66	0.97	0.17	30,38,54,79	0
4	BPH	L	301	65/65	0.97	0.14	28,34,46,49	0
6	BCL	L	308	66/66	0.97	0.17	23,32,58,62	0
6	BCL	L	303	66/66	0.98	0.13	33,37,52,66	0

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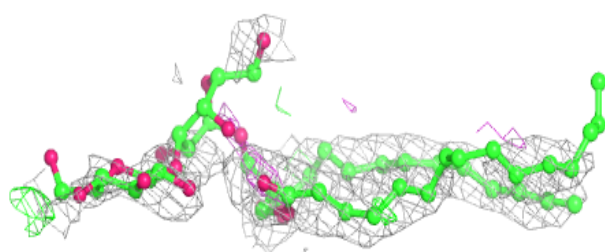
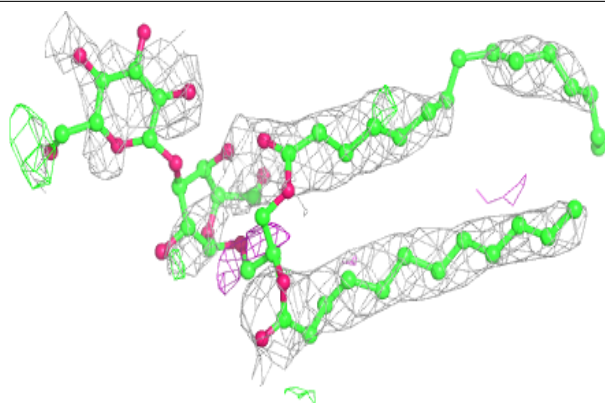
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PO4	L	304	5/5	0.98	0.16	53,60,60,61	0
11	FE	M	405	1/1	1.00	0.14	34,34,34,34	0

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.

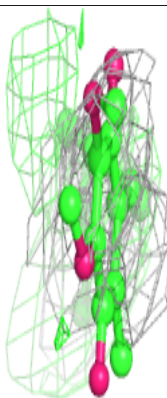
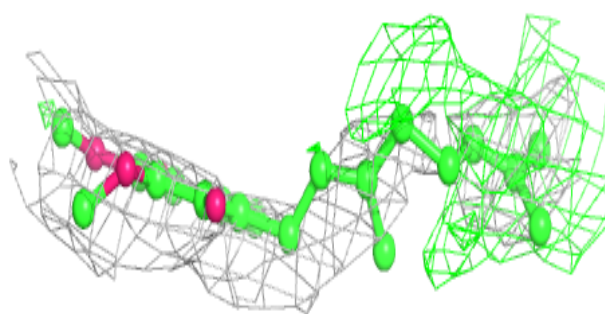
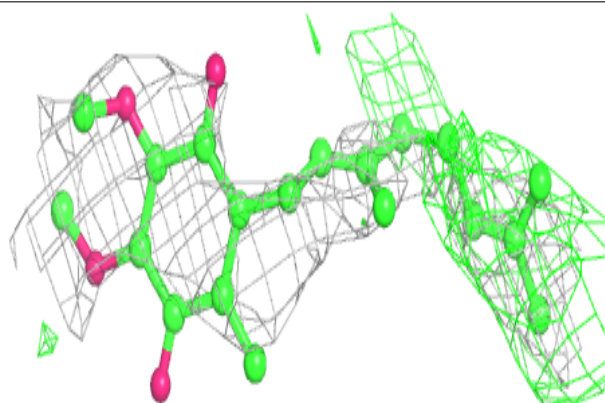


**Electron density around GGD H 301:**

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

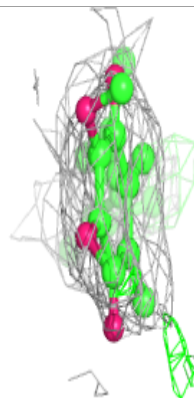
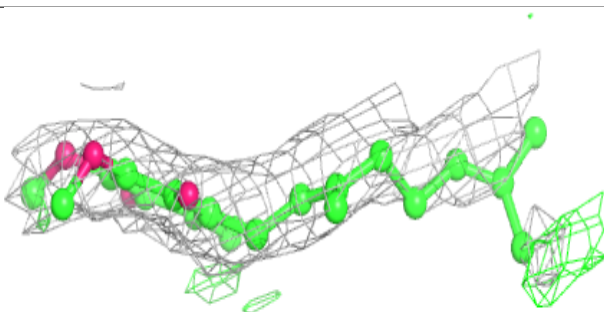
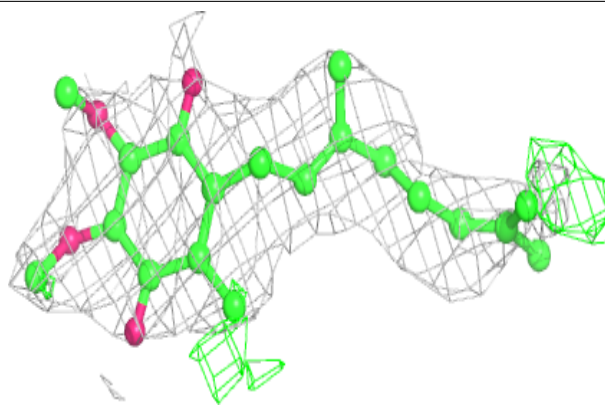
**Electron density around U10 L 302 (B):**

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



**Electron density around U10 L 302 (A):**

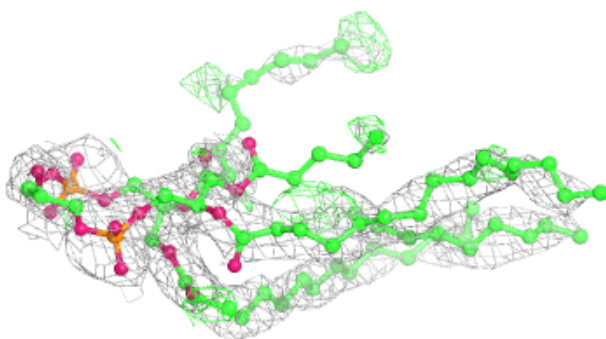
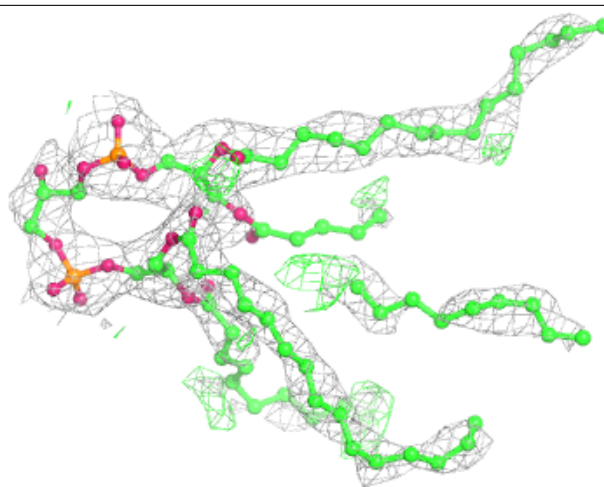
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





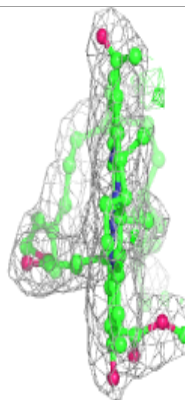
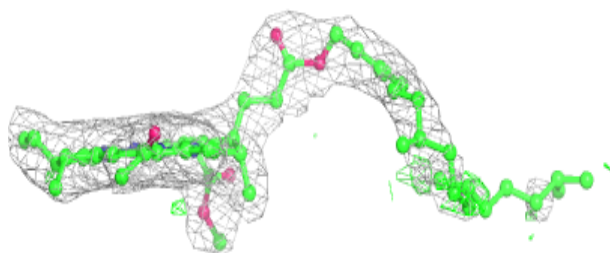
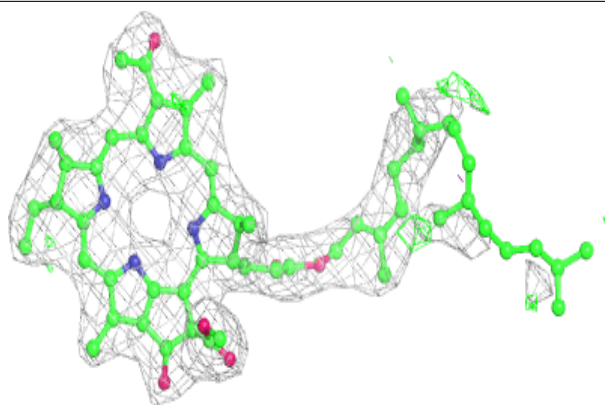
**Electron density around CDL M 409:**

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

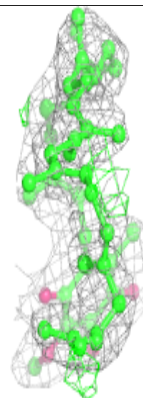
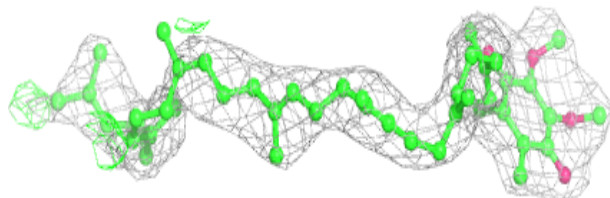
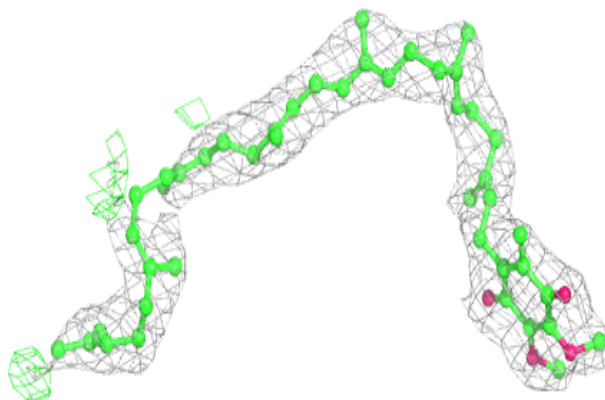


**Electron density around BPH M 406:**

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

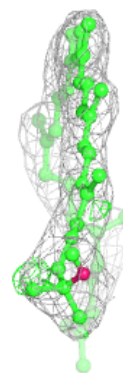
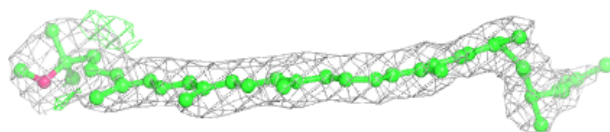
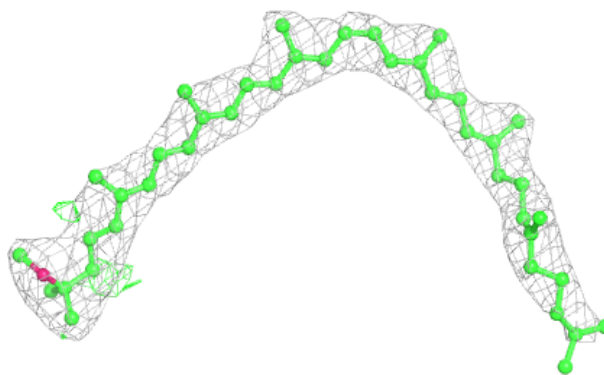
**Electron density around U10 M 407:**

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

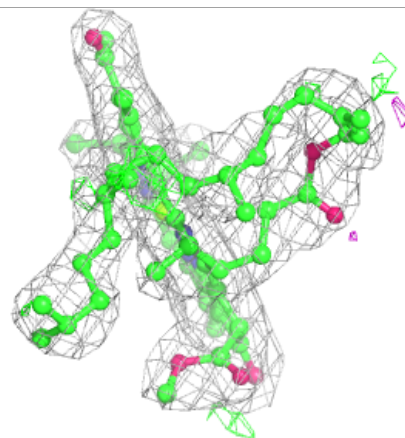
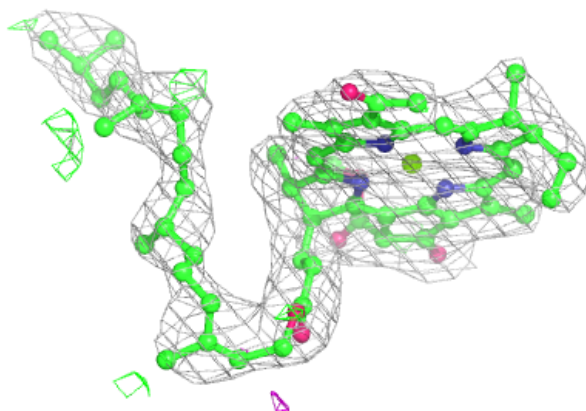
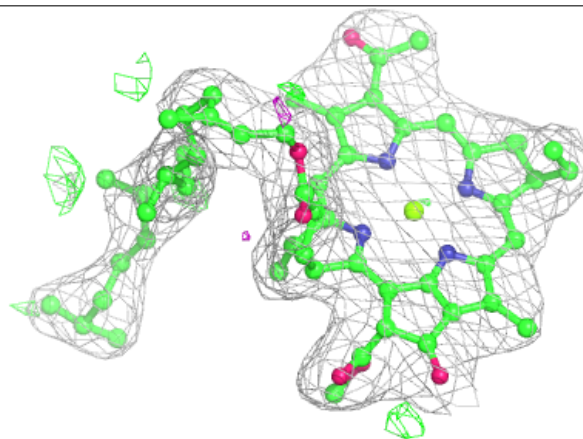


**Electron density around SPO M 408:**

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

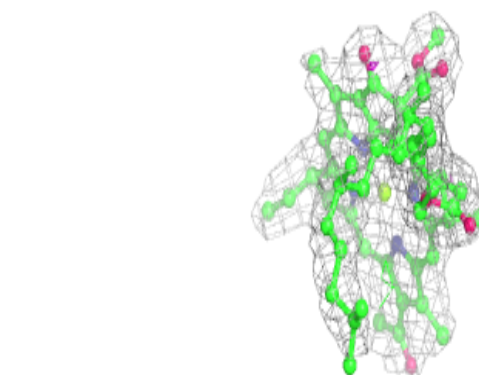
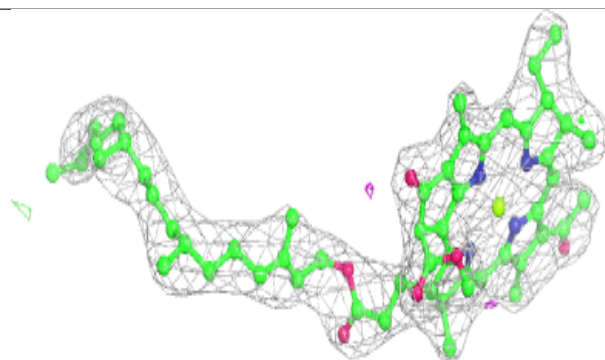
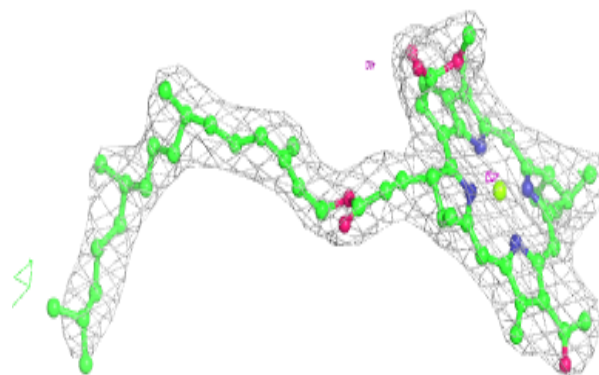
**Electron density around BCL M 401:**

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

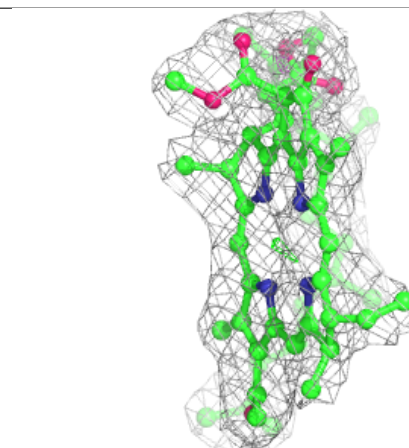
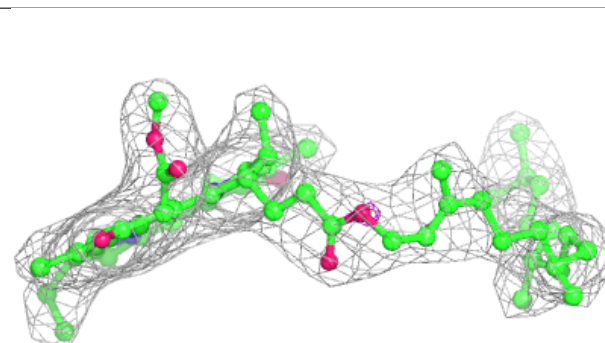
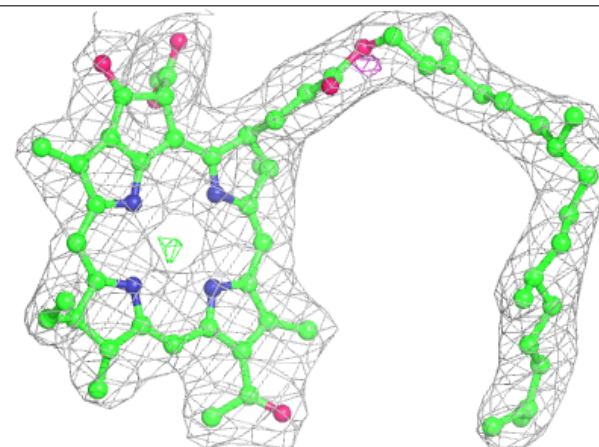


**Electron density around BCL M 402:**

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

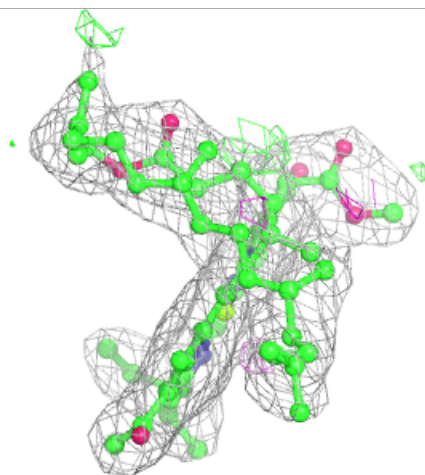
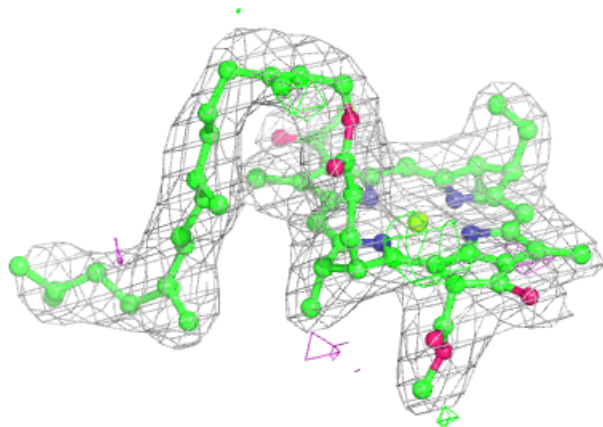
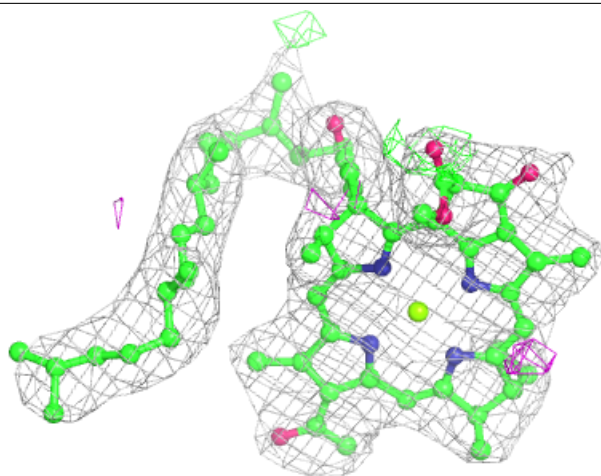
**Electron density around BPH L 301:**

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

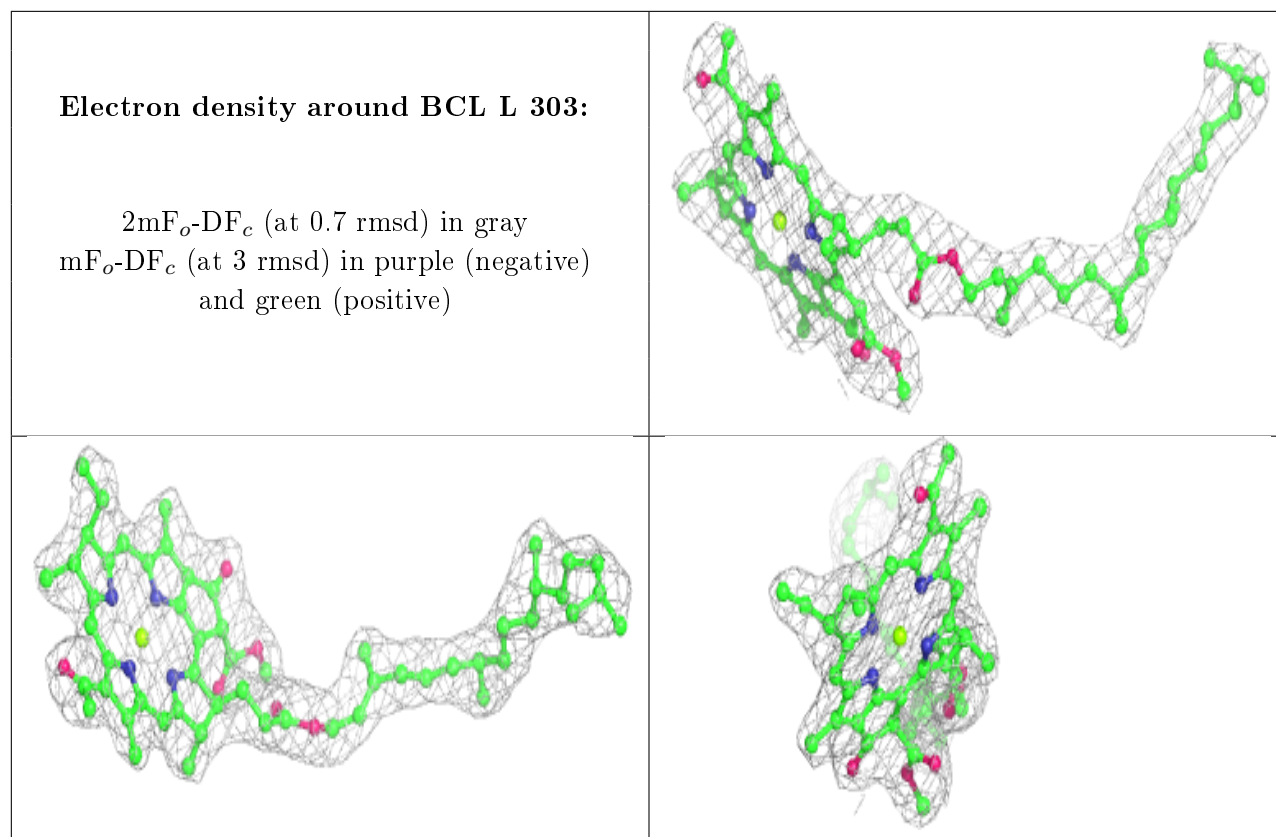


**Electron density around BCL L 308:**

$2mF_o-DF_c$  (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.