



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 02:18 PM EST

PDB ID : 8VTK  
Title : Crystal structure of R.sphaeroides Photosynthetic Reaction Center variant Y (M210)2-chlorophenylalanine  
Authors : Tran, K.; Mathews, I.; Boxer, S.G.  
Deposited on : 2024-01-26  
Resolution : 3.07 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

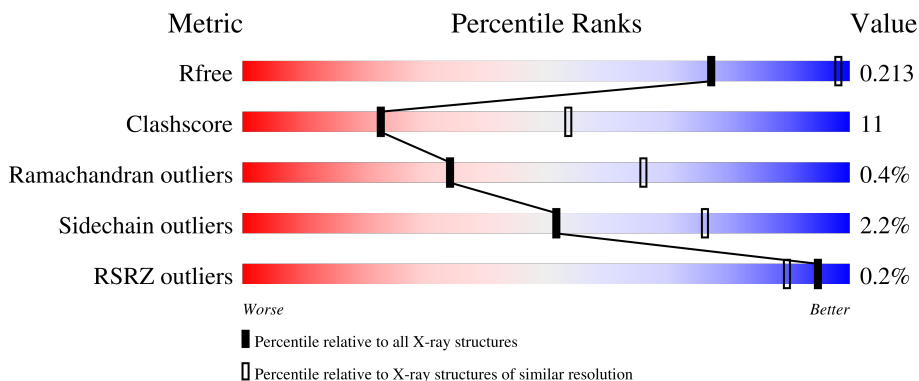
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 of 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	H	240	 81% 18% .
2	L	281	 78% 22%
3	M	301	 77% 22% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CDL	M	405	X	-	-	-
7	U10	L	305	-	-	-	X
8	CL	L	307	-	-	X	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7024 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	240	1829	1169	314	337	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2248	1517	357	366	8	0	2	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	Cl	N	O	S			
3	M	301	2396	1598	1	392	395	10	0	0	0

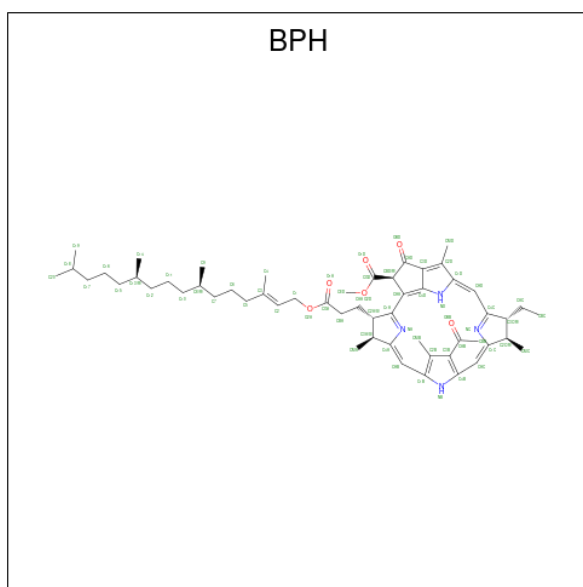
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	210	2L5	TYR	conflict	UNP P0C0Y9
M	252	VAL	TRP	conflict	UNP P0C0Y9

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

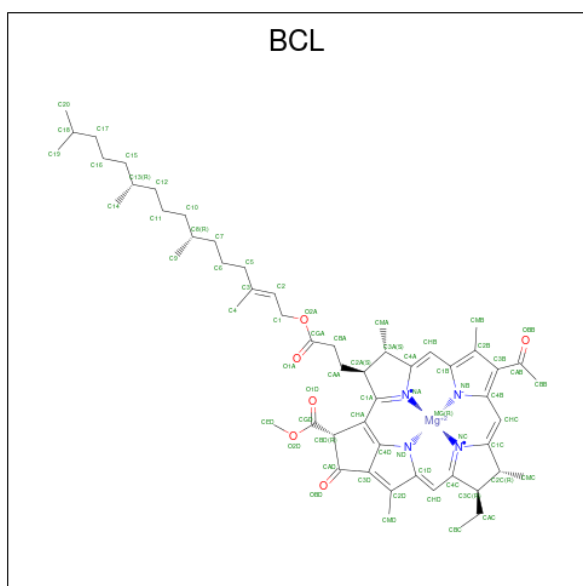
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
5	L	1	Total	55	45	4	6	0	0
5	L	1	Total	65	55	4	6	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



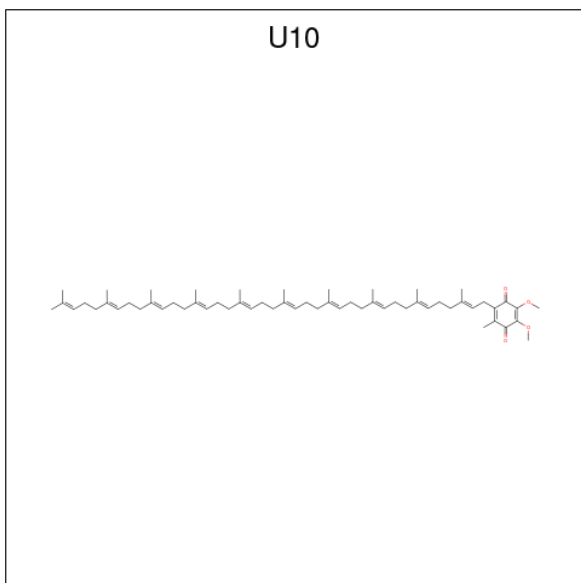
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	Mg	N			O	
6	L	1	Total	66	55	1	4	6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			51	40	1	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).

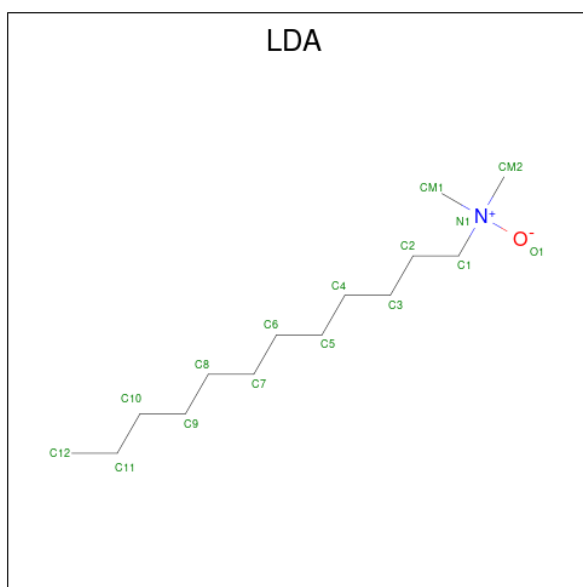


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			18	14	4		

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

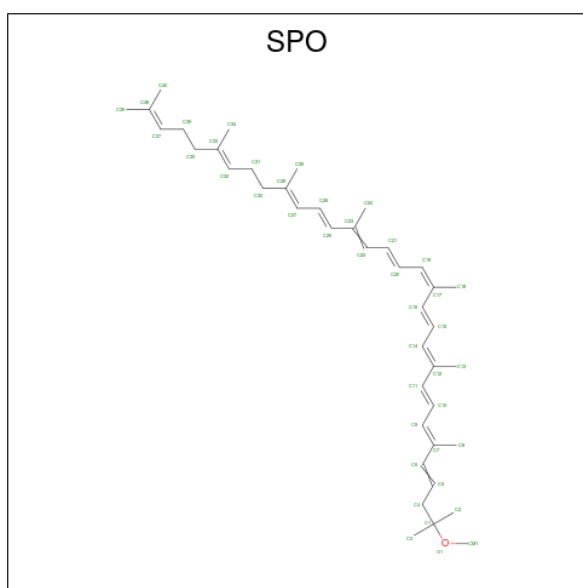
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total	Cl	0	0
			1	1		

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



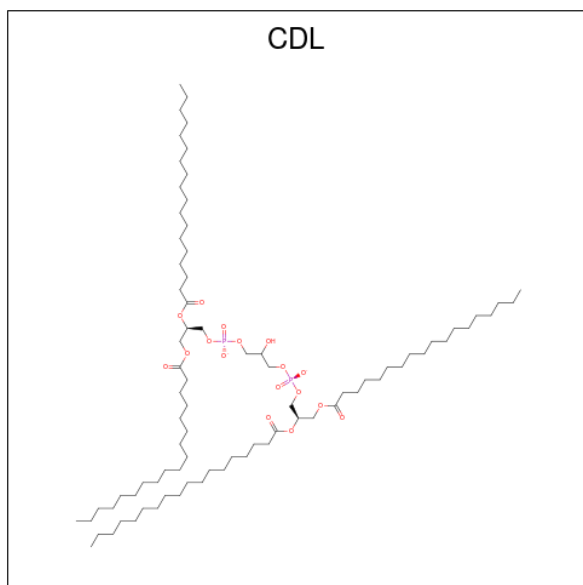
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
11	M	1	69	50	17	2	0	0

- Molecule 12 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	5	Total	O	0	0
			5	5		
12	L	4	Total	O	0	0
			4	4		
12	M	10	Total	O	0	0
			10	10		

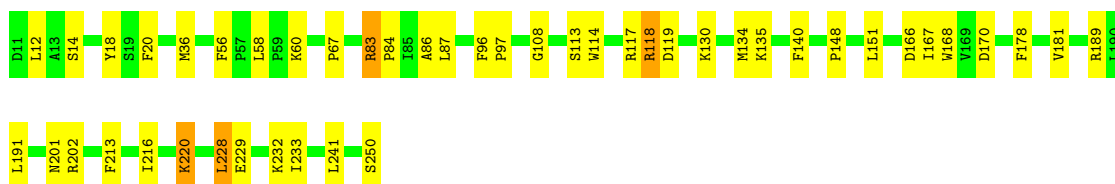


### 3 Residue-property plots [i](#)


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.

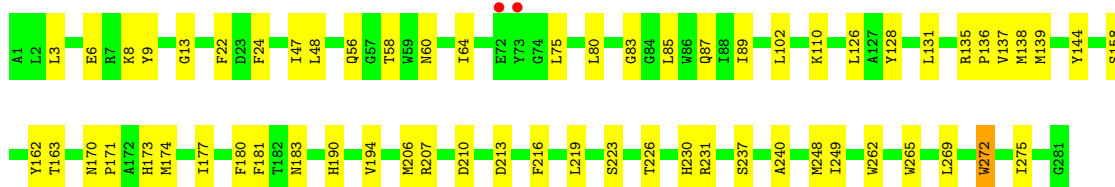
- Molecule 1: Reaction center protein H chain

Chain H:  81% 18%



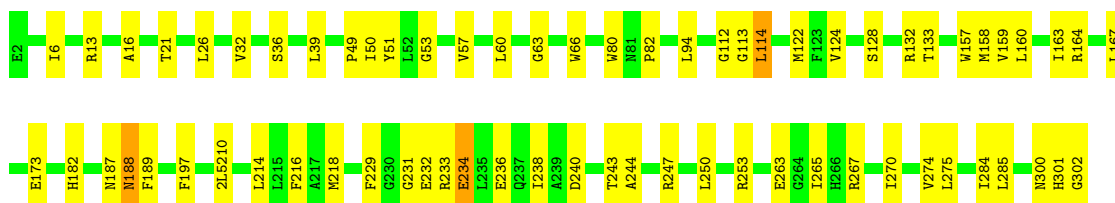
- Molecule 2: Reaction center protein L chain

Chain L:  78% 22%



- Molecule 3: Reaction center protein M chain

Chain M:  77% 22%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.95Å 140.95Å 186.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.76 – 3.07 39.76 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.76-3.07) 91.1 (39.76-3.07)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 3.06Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.177 , 0.213 0.181 , 0.213	Depositor DCC
$R_{free}$ test set	2036 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.8	Xtrriage
Anisotropy	0.185	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, 2L5, CDL, FE, BCL, CL, LDA, U10, BPH

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	H	0.60	0/1877	0.73	0/2553
2	L	0.60	0/2336	0.68	0/3197
3	M	0.59	0/2472	0.70	1/3372 (0.0%)
All	All	0.60	0/6685	0.70	1/9122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	234	GLU	OE1-CD-OE2	-7.75	114.00	123.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1836	49	0
2	L	2248	0	2200	45	0
3	M	2396	0	2307	55	0
4	L	1	0	0	0	0
5	L	120	0	129	12	0
6	L	132	0	148	10	0
6	M	117	0	115	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	18	0	15	3	0
8	L	1	0	0	2	0
9	M	32	0	62	3	0
10	M	42	0	60	1	0
11	M	69	0	82	3	0
12	H	5	0	0	0	0
12	L	4	0	0	1	0
12	M	10	0	0	1	0
All	All	7024	0	6954	160	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 11.

All (160) 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:H:119:ASP:OD2	1:H:220:LYS:NZ	1.68	1.26
2:L:230:HIS:NE2	3:M:234:GLU:OE2	1.72	1.22
1:H:83:ARG:NH2	1:H:108:GLY:O	1.75	1.19
1:H:229:GLU:O	1:H:233:ILE:HD12	1.59	1.02
1:H:117:ARG:O	1:H:228:LEU:HD12	1.62	0.99
1:H:118:ARG:HG3	1:H:118:ARG:HH11	1.24	0.99
1:H:118:ARG:HH12	3:M:240:ASP:HB2	1.35	0.88
3:M:112:GLY:O	3:M:114:LEU:N	2.07	0.87
11:M:405:CDL:HB4	11:M:405:CDL:HA61	1.55	0.86
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.57	0.85
1:H:117:ARG:O	1:H:228:LEU:CD1	2.26	0.83
3:M:238:ILE:HD13	3:M:263:GLU:HB2	1.61	0.82
1:H:118:ARG:HG3	1:H:118:ARG:NH1	1.94	0.81
1:H:119:ASP:CG	1:H:220:LYS:NZ	2.35	0.79
2:L:162:TYR:OH	3:M:187:ASN:OD1	2.00	0.79
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.63	0.79
1:H:119:ASP:CG	1:H:220:LYS:HZ2	1.86	0.78
6:L:303:BCL:HBB3	6:L:306:BCL:H52	1.63	0.78
2:L:56:GLN:HG2	2:L:58:THR:HG22	1.67	0.77
11:M:405:CDL:H312	11:M:405:CDL:H511	1.66	0.76
1:H:118:ARG:NH1	3:M:240:ASP:HB2	2.03	0.74
3:M:265:ILE:O	3:M:265:ILE:HG13	1.87	0.74
1:H:148:PRO:HD2	1:H:167:ILE:HD11	1.70	0.74
2:L:219:LEU:O	3:M:132:ARG:NH2	2.21	0.74
1:H:83:ARG:NH1	1:H:114:TRP:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:304:BPH:HHC	5:L:304:BPH:HBB3	1.70	0.72
1:H:189:ARG:HD2	1:H:216:ILE:HB	1.72	0.71
3:M:197:PHE:HZ	6:M:401:BCL:HBB2	1.54	0.71
1:H:60:LYS:H	1:H:60:LYS:HD2	1.56	0.69
2:L:230:HIS:CE1	3:M:234:GLU:OE2	2.46	0.67
1:H:229:GLU:O	1:H:233:ILE:CD1	2.40	0.67
6:L:303:BCL:HHC	6:L:303:BCL:HBB2	1.80	0.64
1:H:14:SER:O	1:H:18:TYR:HD1	1.81	0.63
3:M:300:ASN:C	3:M:302:GLY:H	2.02	0.63
1:H:118:ARG:HH12	3:M:240:ASP:CB	2.12	0.62
5:L:302:BPH:H6C1	6:M:401:BCL:H192	1.81	0.61
3:M:231:GLY:C	3:M:233:ARG:H	2.02	0.61
1:H:220:LYS:HE3	1:H:229:GLU:OE2	2.01	0.61
5:L:302:BPH:H5C1	3:M:63:GLY:HA3	1.84	0.59
1:H:83:ARG:HH12	1:H:114:TRP:H	1.50	0.59
2:L:85:LEU:O	2:L:89:ILE:HG13	2.02	0.58
5:L:302:BPH:H4C1	3:M:60:LEU:HD12	1.85	0.58
5:L:302:BPH:HBC3	5:L:302:BPH:HHD	1.86	0.57
3:M:197:PHE:CZ	6:M:401:BCL:HBB2	2.39	0.56
6:M:406:BCL:HBB2	6:M:406:BCL:HHC	1.88	0.55
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.89	0.55
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.89	0.54
3:M:231:GLY:C	3:M:233:ARG:N	2.61	0.54
1:H:220:LYS:CE	1:H:229:GLU:OE2	2.56	0.54
2:L:171:PRO:HA	2:L:174:MET:HG3	1.89	0.53
8:L:307:CL:CL	12:L:404:HOH:O	2.56	0.53
1:H:140:PHE:HA	3:M:13:ARG:O	2.09	0.53
3:M:36:SER:HB3	3:M:39:LEU:HB2	1.90	0.52
7:L:305:U10:H4M3	9:M:403:LDA:H122	1.91	0.52
6:M:401:BCL:HBB2	6:M:401:BCL:HHC	1.92	0.51
3:M:160:LEU:HD23	3:M:284:ILE:HG21	1.93	0.51
3:M:53:GLY:O	3:M:57:VAL:HG23	2.11	0.51
2:L:177:ILE:HD11	6:L:306:BCL:C1B	2.41	0.51
2:L:190:HIS:NE2	3:M:234:GLU:OE2	2.42	0.51
2:L:272:TRP:HA	2:L:275:ILE:HG13	1.93	0.51
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.46	0.51
1:H:113:SER:HB3	2:L:8:LYS:HD2	1.92	0.51
2:L:262:TRP:O	2:L:265:TRP:HD1	1.94	0.51
7:L:305:U10:H71	9:M:402:LDA:H121	1.93	0.50
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.93	0.50
2:L:181:PHE:HB3	5:L:302:BPH:HBB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:75:LEU:HD21	2:L:137:VAL:HA	1.92	0.50
3:M:267:ARG:NH1	12:M:501:HOH:O	2.44	0.50
7:L:305:U10:C11	8:L:307:CL:CL	2.97	0.50
3:M:167:LEU:HD12	3:M:285:LEU:HD11	1.94	0.49
2:L:8:LYS:HE2	2:L:9:TYR:CE2	2.48	0.49
3:M:94:LEU:HD11	3:M:114:LEU:HB3	1.95	0.49
2:L:83:GLY:O	2:L:87:GLN:HG3	2.13	0.48
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.95	0.48
3:M:231:GLY:O	3:M:233:ARG:N	2.46	0.48
3:M:300:ASN:O	3:M:302:GLY:N	2.46	0.48
2:L:60:ASN:O	2:L:64:ILE:HG13	2.13	0.48
6:L:306:BCL:HMB2	6:M:401:BCL:HMB2	1.95	0.48
1:H:20:PHE:HD2	11:M:405:CDL:H401	1.78	0.48
2:L:163:THR:O	2:L:163:THR:HG22	2.12	0.48
5:L:302:BPH:HBB3	5:L:302:BPH:HHC	1.95	0.48
1:H:134:MET:CE	1:H:167:ILE:HB	2.44	0.48
2:L:170:ASN:HB3	2:L:173:HIS:HB2	1.95	0.47
1:H:118:ARG:NH1	3:M:240:ASP:CB	2.76	0.47
2:L:13:GLY:O	2:L:110:LYS:NZ	2.29	0.47
6:M:406:BCL:HHC	6:M:406:BCL:CBB	2.44	0.47
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.80	0.47
1:H:118:ARG:NH1	1:H:118:ARG:CG	2.72	0.47
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.15	0.47
2:L:138:MET:HE3	2:L:249:ILE:HD11	1.97	0.47
2:L:47:ILE:HG22	2:L:48:LEU:HD23	1.97	0.47
3:M:300:ASN:C	3:M:302:GLY:N	2.68	0.47
1:H:228:LEU:HD23	1:H:232:LYS:HE3	1.95	0.47
2:L:216:PHE:HB2	2:L:223:SER:HB2	1.97	0.47
2:L:269:LEU:HB2	2:L:272:TRP:NE1	2.30	0.47
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.50	0.46
6:L:306:BCL:C1C	6:M:401:BCL:HBB3	2.46	0.46
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.50	0.46
1:H:117:ARG:O	1:H:118:ARG:C	2.51	0.46
1:H:213:PHE:O	1:H:216:ILE:HG13	2.15	0.46
3:M:188:ASN:O	3:M:189:PHE:C	2.53	0.46
6:L:306:BCL:OBB	6:L:306:BCL:HHC	2.16	0.46
1:H:36:MET:HE2	1:H:58:LEU:HD23	1.98	0.45
3:M:236:GLU:O	3:M:236:GLU:HG3	2.16	0.45
6:M:401:BCL:HAA2	6:M:401:BCL:HBD	1.99	0.45
3:M:50:ILE:HG12	3:M:51:TYR:N	2.32	0.45
2:L:226:THR:O	2:L:230:HIS:ND1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:243:THR:O	3:M:247:ARG:HG3	2.17	0.45
1:H:67:PRO:HG3	2:L:206:MET:O	2.17	0.44
9:M:402:LDA:HM13	9:M:402:LDA:H21	1.79	0.44
5:L:304:BPH:HHC	5:L:304:BPH:CBB	2.44	0.44
3:M:124:VAL:O	3:M:128:SER:OG	2.29	0.44
3:M:275:LEU:HD23	3:M:275:LEU:HA	1.87	0.44
1:H:135:LYS:HB3	1:H:135:LYS:HE2	1.76	0.44
2:L:181:PHE:HB3	5:L:302:BPH:CBB	2.48	0.43
2:L:219:LEU:HD11	3:M:133:THR:HG22	2.00	0.43
10:M:404:SPO:H243	6:M:406:BCL:CBB	2.48	0.43
2:L:190:HIS:O	2:L:194:VAL:HG23	2.19	0.43
1:H:12:LEU:HD23	1:H:12:LEU:O	2.18	0.43
5:L:304:BPH:ND	3:M:214:LEU:HD13	2.33	0.43
1:H:134:MET:HE3	1:H:167:ILE:HB	2.00	0.43
1:H:135:LYS:HE2	1:H:166:ASP:OD2	2.17	0.43
2:L:158:SER:HA	6:L:306:BCL:HBC1	2.01	0.43
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.53	0.43
2:L:102:LEU:HD23	2:L:102:LEU:HA	1.71	0.43
3:M:80:TRP:O	3:M:82:PRO:HD3	2.19	0.42
3:M:159:VAL:HA	3:M:163:ILE:HB	2.01	0.42
3:M:164:ARG:NH1	3:M:173:GLU:OE1	2.49	0.42
3:M:167:LEU:CD1	3:M:285:LEU:HD11	2.49	0.42
2:L:131:LEU:HD21	2:L:248:MET:HG2	2.00	0.42
3:M:32:VAL:HG12	3:M:49:PRO:HD3	2.01	0.42
3:M:218:MET:HE3	3:M:218:MET:HB3	1.88	0.42
1:H:118:ARG:HG3	3:M:240:ASP:OD2	2.19	0.42
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.89	0.42
1:H:86:ALA:O	1:H:87:LEU:HD23	2.20	0.42
2:L:131:LEU:HD23	2:L:131:LEU:HA	1.85	0.42
1:H:201:ASN:OD1	1:H:201:ASN:N	2.53	0.41
3:M:253:ARG:HH11	3:M:253:ARG:HG3	1.85	0.41
3:M:270:ILE:O	3:M:274:VAL:HG13	2.20	0.41
2:L:3:LEU:HB2	2:L:6:GLU:HB2	2.02	0.41
3:M:32:VAL:H	3:M:32:VAL:HG22	1.66	0.41
3:M:51:TYR:O	3:M:132:ARG:NH1	2.38	0.41
2:L:128:TYR:HD1	6:L:303:BCL:HBB1	1.84	0.41
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.51	0.41
2:L:181:PHE:CD2	5:L:302:BPH:HBB1	2.55	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.01	0.41
2:L:183:ASN:OD1	2:L:237:SER:HB3	2.20	0.41
2:L:139:MET:HB3	2:L:144:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:231:ARG:HD3	3:M:6:ILE:O	2.20	0.41
1:H:241:LEU:HD23	1:H:241:LEU:HA	1.95	0.41
2:L:80:LEU:HD22	2:L:85:LEU:HD23	2.03	0.41
6:M:401:BCL:HHC	6:M:401:BCL:CBB	2.51	0.41
2:L:269:LEU:HD23	2:L:269:LEU:HA	1.70	0.41
1:H:201:ASN:HD21	1:H:202:ARG:NH2	2.19	0.40
6:L:306:BCL:NC	6:M:401:BCL:HBB3	2.36	0.40
1:H:83:ARG:HA	1:H:84:PRO:HD3	1.90	0.40
5:L:302:BPH:H3A	5:L:302:BPH:HBA2	1.79	0.40
2:L:213:ASP:OD1	2:L:223:SER:OG	2.32	0.40
1:H:119:ASP:OD1	1:H:220:LYS:NZ	2.45	0.40
6:L:303:BCL:HHC	6:L:303:BCL:CBB	2.49	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	H	238/240 (99%)	228 (96%)	10 (4%)	0	100	100
2	L	281/281 (100%)	271 (96%)	10 (4%)	0	100	100
3	M	298/301 (99%)	280 (94%)	15 (5%)	3 (1%)	15	47
All	All	817/822 (99%)	779 (95%)	35 (4%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	113	GLY
3	M	301	HIS
3	M	232	GLU



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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/195 (100%)	189 (97%)	6 (3%)	40	69
2	L	222/220 (101%)	217 (98%)	5 (2%)	50	75
3	M	235/235 (100%)	231 (98%)	4 (2%)	60	82
All	All	652/650 (100%)	637 (98%)	15 (2%)	52	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	56	PHE
1	H	83	ARG
1	H	118	ARG
1	H	220	LYS
1	H	228	LEU
1	H	250	SER
2	L	126[A]	LEU
2	L	126[B]	LEU
2	L	207	ARG
2	L	210	ASP
2	L	272	TRP
3	M	114	LEU
3	M	182	HIS
3	M	188	ASN
3	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
3	2L5	M	210	3	11,12,13	0.92	1 (9%)	11,15,17	0.53	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
3	2L5	M	210	3	-	2/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	210	2L5	O-C	2.99	1.31	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	2L5	CA-C13-C14-C15
3	M	210	2L5	CA-C13-C14-C16

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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
6	BCL	M	406	-	49,59,74	1.93	11 (22%)	60,97,115	1.84	15 (25%)
6	BCL	L	306	-	64,74,74	1.44	7 (10%)	78,115,115	1.59	13 (16%)
9	LDA	M	402	-	12,15,15	2.05	1 (8%)	14,17,17	0.53	0
11	CDL	M	405	-	68,68,99	1.26	11 (16%)	74,80,111	1.01	6 (8%)
5	BPH	L	304	-	51,70,70	0.98	1 (1%)	52,101,101	1.36	8 (15%)
6	BCL	M	401	-	64,74,74	1.42	7 (10%)	78,115,115	1.52	11 (14%)
7	U10	L	305	-	18,18,63	2.45	7 (38%)	22,25,79	1.66	4 (18%)
9	LDA	M	403	-	12,15,15	1.92	1 (8%)	14,17,17	0.71	0
10	SPO	M	404	-	40,41,41	0.56	1 (2%)	47,50,50	0.71	1 (2%)
5	BPH	L	302	-	41,60,70	0.95	2 (4%)	40,89,101	1.72	9 (22%)
6	BCL	L	303	-	64,74,74	1.65	11 (17%)	78,115,115	1.62	15 (19%)

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
6	BCL	M	406	-	-	1/19/119/137	-
6	BCL	L	306	-	-	4/37/137/137	-
11	CDL	M	405	-	1/1/9/9	33/79/79/110	-
9	LDA	M	402	-	-	6/13/13/13	-
5	BPH	L	304	-	-	5/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	M	401	-	-	1/37/137/137	-
7	U10	L	305	-	-	2/9/33/87	0/1/1/1
9	LDA	M	403	-	-	6/13/13/13	-
10	SPO	M	404	-	-	6/47/47/47	-
5	BPH	L	302	-	-	5/25/93/105	0/5/6/6
6	BCL	L	303	-	-	3/37/137/137	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	402	LDA	O1-N1	-6.98	1.25	1.42
6	M	406	BCL	C1B-NB	6.62	1.41	1.35
9	M	403	LDA	O1-N1	-6.58	1.26	1.42
6	L	303	BCL	C1B-NB	5.62	1.40	1.35
6	M	401	BCL	C1B-NB	5.46	1.40	1.35
6	L	306	BCL	C1B-NB	5.41	1.40	1.35
6	M	406	BCL	MG-NA	5.10	2.18	2.06
6	L	306	BCL	MG-NA	5.07	2.18	2.06
7	L	305	U10	C8-C9	4.94	1.46	1.32
7	L	305	U10	O3-C3	-4.91	1.24	1.36
6	L	303	BCL	MG-NA	4.76	2.17	2.06
5	L	304	BPH	CBD-CGD	-4.74	1.46	1.52
6	M	401	BCL	MG-NA	4.73	2.17	2.06
7	L	305	U10	O4-C4	-4.70	1.25	1.36
6	L	303	BCL	C4B-NB	4.19	1.38	1.35
6	L	303	BCL	MG-NC	4.16	2.16	2.06
6	M	406	BCL	C4B-NB	3.88	1.38	1.35
6	M	406	BCL	C1-C2	3.73	1.60	1.49
6	M	401	BCL	MG-NC	3.63	2.14	2.06
6	L	303	BCL	O1A-CGA	-3.57	1.12	1.22
6	M	406	BCL	MG-NC	3.43	2.14	2.06
11	M	405	CDL	PA1-OA5	3.43	1.73	1.59
6	M	406	BCL	O2A-CGA	3.35	1.43	1.33
6	M	401	BCL	C4B-NB	3.30	1.38	1.35
6	M	406	BCL	OBD-CAD	3.24	1.28	1.22
11	M	405	CDL	PA1-OA4	-3.08	1.40	1.55
6	L	306	BCL	MG-NC	3.07	2.13	2.06
11	M	405	CDL	PB2-OB5	3.06	1.71	1.59
7	L	305	U10	C6-C1	2.92	1.40	1.35
11	M	405	CDL	PA1-OA3	-2.91	1.40	1.50
6	L	306	BCL	C4B-NB	2.88	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	404	SPO	C27-C28	-2.87	1.31	1.34
11	M	405	CDL	PB2-OB4	-2.76	1.42	1.55
6	L	303	BCL	CHD-C1D	2.76	1.43	1.38
11	M	405	CDL	PB2-OB3	-2.64	1.41	1.50
11	M	405	CDL	CA3-CA4	2.62	1.58	1.50
6	M	406	BCL	CHD-C1D	2.62	1.43	1.38
7	L	305	U10	C4-C5	-2.61	1.41	1.48
5	L	302	BPH	CBD-CGD	-2.56	1.49	1.52
11	M	405	CDL	OB8-CB7	2.42	1.40	1.33
6	M	406	BCL	C1D-ND	2.40	1.40	1.37
6	M	401	BCL	C3D-C4D	-2.36	1.38	1.44
7	L	305	U10	C3-C2	-2.33	1.42	1.48
6	L	303	BCL	C1D-ND	2.30	1.40	1.37
7	L	305	U10	C6-C5	-2.29	1.40	1.46
6	L	303	BCL	C1D-C2D	-2.26	1.40	1.45
11	M	405	CDL	OB6-CB5	2.22	1.40	1.34
6	L	303	BCL	OBD-CAD	2.22	1.26	1.22
6	L	306	BCL	CMB-C2B	2.22	1.56	1.51
6	M	401	BCL	OBD-CAD	2.21	1.26	1.22
6	M	401	BCL	C1D-C2D	-2.18	1.41	1.45
11	M	405	CDL	OA6-CA5	2.15	1.40	1.34
6	L	303	BCL	CAC-C3C	2.13	1.58	1.54
6	L	306	BCL	C3D-C4D	-2.11	1.39	1.44
6	M	406	BCL	C3B-C2B	2.11	1.43	1.39
6	L	306	BCL	C5-C3	2.10	1.55	1.51
6	L	303	BCL	C5-C3	2.10	1.55	1.51
5	L	302	BPH	CHA-CBD	2.10	1.54	1.52
6	M	406	BCL	CAA-CBA	2.08	1.59	1.52
11	M	405	CDL	CB3-CB4	2.02	1.56	1.50

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	BPH	C1-C2-C3	-5.72	116.15	126.04
6	M	406	BCL	CHD-C1D-ND	-5.66	119.26	124.45
6	M	401	BCL	CHD-C1D-ND	-5.19	119.68	124.45
6	L	303	BCL	CHD-C1D-ND	-5.04	119.82	124.45
6	L	306	BCL	CHD-C1D-ND	-4.97	119.89	124.45
6	M	406	BCL	C4D-CHA-C1A	4.89	127.20	121.25
6	M	406	BCL	C1-O2A-CGA	4.76	128.94	116.44
6	M	401	BCL	C4D-CHA-C1A	4.72	127.00	121.25
6	L	303	BCL	C1D-ND-C4D	-4.59	103.07	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	306	BCL	C4D-CHA-C1A	4.39	126.59	121.25
6	M	406	BCL	C1D-ND-C4D	-4.19	103.36	106.33
6	L	306	BCL	C16-C15-C13	-4.00	102.99	115.92
6	L	303	BCL	C4D-CHA-C1A	3.94	126.04	121.25
6	L	306	BCL	C1D-ND-C4D	-3.92	103.55	106.33
6	L	306	BCL	C15-C13-C12	-3.91	91.55	112.13
6	L	303	BCL	O2D-CGD-CBD	3.85	118.11	111.27
6	M	401	BCL	C1D-ND-C4D	-3.73	103.69	106.33
5	L	304	BPH	C11-C10-C8	-3.65	104.11	115.92
7	L	305	U10	C11-C9-C10	3.60	122.56	114.60
5	L	302	BPH	OBD-CAD-CBD	-3.56	120.60	125.82
6	L	303	BCL	CMB-C2B-C1B	-3.51	123.07	128.46
7	L	305	U10	C7-C8-C9	-3.43	116.50	127.26
6	L	303	BCL	C16-C17-C18	-3.35	100.18	115.98
6	M	406	BCL	CMB-C2B-C1B	-3.26	123.45	128.46
5	L	302	BPH	CBA-CAA-C2A	-3.24	104.33	113.81
6	L	303	BCL	CED-O2D-CGD	3.22	123.23	115.94
6	M	401	BCL	CHA-C1A-NA	-3.12	119.25	126.40
10	M	404	SPO	C2-C1-C4	-3.11	106.08	110.86
6	L	306	BCL	CHA-C1A-NA	-3.06	119.40	126.40
6	M	401	BCL	C11-C10-C8	-3.03	106.11	115.92
7	L	305	U10	O5-C5-C6	-3.01	116.27	121.55
5	L	304	BPH	OBD-CAD-CBD	-2.97	121.46	125.82
6	M	406	BCL	CHA-C1A-NA	-2.94	119.66	126.40
6	L	303	BCL	C2A-C1A-CHA	2.86	128.86	123.86
6	L	303	BCL	CHA-C1A-NA	-2.85	119.86	126.40
6	L	306	BCL	CMB-C2B-C1B	-2.83	124.11	128.46
6	L	303	BCL	C2D-C1D-ND	2.79	112.16	110.10
5	L	304	BPH	OBB-CAB-CBB	-2.78	113.91	120.17
5	L	304	BPH	C1-C2-C3	-2.77	121.25	126.04
6	L	306	BCL	C2A-C1A-CHA	2.77	128.70	123.86
11	M	405	CDL	OA4-PA1-OA3	2.75	125.83	112.24
7	L	305	U10	C1M-C1-C6	-2.74	119.93	124.40
6	L	306	BCL	C11-C10-C8	-2.69	107.24	115.92
6	M	401	BCL	CMB-C2B-C1B	-2.68	124.35	128.46
11	M	405	CDL	CB4-OB6-CB5	2.63	124.27	117.79
5	L	302	BPH	O2D-CGD-CBD	2.60	114.29	111.00
6	M	406	BCL	O2D-CGD-CBD	2.59	115.87	111.27
6	L	306	BCL	CED-O2D-CGD	2.58	121.77	115.94
5	L	302	BPH	CAC-C3C-C2C	-2.54	107.92	114.26
5	L	302	BPH	CMD-C2D-C3D	2.53	129.41	124.68
5	L	304	BPH	CMD-C2D-C3D	2.52	129.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	306	BCL	CMB-C2B-C3B	2.51	129.37	124.68
11	M	405	CDL	OA6-CA5-C11	2.51	116.90	111.50
6	M	406	BCL	O2D-CGD-O1D	-2.49	118.97	123.84
6	M	406	BCL	C2D-C1D-ND	2.49	111.94	110.10
6	M	406	BCL	C2A-C1A-CHA	2.48	128.20	123.86
11	M	405	CDL	OB4-PB2-OB3	2.48	124.52	112.24
6	L	303	BCL	C4A-NA-C1A	2.47	107.82	106.71
11	M	405	CDL	OA6-CA5-OA7	-2.44	117.80	123.70
5	L	304	BPH	C16-C15-C13	-2.43	108.08	115.92
6	M	401	BCL	CHC-C1C-NC	-2.42	121.17	124.51
5	L	304	BPH	C4C-C3C-C2C	-2.41	100.54	102.84
5	L	302	BPH	CAC-C3C-C4C	2.38	119.06	113.73
11	M	405	CDL	OB8-CB6-CB4	2.37	115.32	108.43
6	M	406	BCL	O2A-C1-C2	-2.36	102.44	108.64
6	M	406	BCL	C4-C3-C2	2.33	129.39	122.65
6	M	401	BCL	C2A-C1A-CHA	2.33	127.92	123.86
6	M	406	BCL	C5-C3-C4	-2.30	109.53	114.60
6	L	303	BCL	O2D-CGD-O1D	-2.28	119.38	123.84
6	L	306	BCL	C4B-C3B-CAB	-2.26	122.76	127.13
6	L	303	BCL	OBB-CAB-CBB	-2.26	115.09	120.17
5	L	302	BPH	O2A-C1-C2	-2.23	102.77	108.64
6	L	306	BCL	C17-C16-C15	2.21	123.40	113.24
6	L	303	BCL	CMB-C2B-C3B	2.19	128.78	124.68
6	M	401	BCL	CMB-C2B-C3B	2.19	128.77	124.68
6	L	303	BCL	O2A-C1-C2	-2.18	102.89	108.64
6	M	406	BCL	CMB-C2B-C3B	2.16	128.71	124.68
6	M	401	BCL	C2D-C1D-ND	2.15	111.69	110.10
5	L	304	BPH	CMB-C2B-C3B	2.15	128.71	124.68
6	M	401	BCL	OBB-CAB-CBB	-2.09	115.46	120.17
5	L	302	BPH	CMA-C3A-C4A	-2.04	109.91	114.38
6	M	406	BCL	OBB-CAB-CBB	-2.04	115.59	120.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	405	CDL	CA4

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	403	LDA	C2-C1-N1-O1
9	M	403	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
11	M	405	CDL	CA3-OA5-PA1-OA4
11	M	405	CDL	CB2-OB2-PB2-OB4
11	M	405	CDL	CB3-OB5-PB2-OB3
11	M	405	CDL	OB5-CB3-CB4-OB6
7	L	305	U10	C7-C8-C9-C11
7	L	305	U10	C7-C8-C9-C10
11	M	405	CDL	C51-CB5-OB6-CB4
11	M	405	CDL	C71-CB7-OB8-CB6
5	L	302	BPH	C5-C6-C7-C8
11	M	405	CDL	O1-C1-CA2-OA2
10	M	404	SPO	C5-C6-C7-C8
6	L	303	BCL	C15-C16-C17-C18
11	M	405	CDL	OB7-CB5-OB6-CB4
5	L	304	BPH	C15-C16-C17-C18
11	M	405	CDL	OB9-CB7-OB8-CB6
11	M	405	CDL	CB2-OB2-PB2-OB5
11	M	405	CDL	CB3-OB5-PB2-OB2
11	M	405	CDL	O1-C1-CB2-OB2
11	M	405	CDL	C31-CA7-OA8-CA6
5	L	304	BPH	C4-C3-C5-C6
5	L	302	BPH	C2-C3-C5-C6
9	M	403	LDA	C5-C6-C7-C8
11	M	405	CDL	C51-C52-C53-C54
9	M	403	LDA	C6-C7-C8-C9
9	M	403	LDA	C2-C3-C4-C5
11	M	405	CDL	C39-C40-C41-C42
5	L	302	BPH	C4-C3-C5-C6
5	L	304	BPH	C2-C3-C5-C6
11	M	405	CDL	C11-CA5-OA6-CA4
9	M	402	LDA	C1-C2-C3-C4
11	M	405	CDL	OA7-CA5-OA6-CA4
11	M	405	CDL	OA9-CA7-OA8-CA6
6	L	306	BCL	C13-C15-C16-C17
11	M	405	CDL	OA6-CA4-CA6-OA8
11	M	405	CDL	C76-C77-C78-C79
9	M	403	LDA	C1-C2-C3-C4
10	M	404	SPO	C2-C1-C4-C5
9	M	402	LDA	C4-C5-C6-C7
9	M	402	LDA	N1-C1-C2-C3
11	M	405	CDL	C14-C15-C16-C17
5	L	302	BPH	C2-C1-O2A-CGA
10	M	404	SPO	C5-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
11	M	405	CDL	OB5-CB3-CB4-CB6
11	M	405	CDL	C34-C35-C36-C37
5	L	304	BPH	CAD-CBD-CGD-O2D
6	L	306	BCL	CAD-CBD-CGD-O2D
6	M	406	BCL	CAD-CBD-CGD-O2D
6	L	306	BCL	C15-C16-C17-C18
11	M	405	CDL	CA3-OA5-PA1-OA2
11	M	405	CDL	CB2-OB2-PB2-OB3
11	M	405	CDL	CB3-OB5-PB2-OB4
9	M	402	LDA	C9-C10-C11-C12
11	M	405	CDL	C12-C13-C14-C15
11	M	405	CDL	CA3-CA4-CA6-OA8
11	M	405	CDL	CB3-CB4-CB6-OB8
10	M	404	SPO	C29-C28-C30-C31
11	M	405	CDL	C72-C73-C74-C75
6	L	303	BCL	C16-C17-C18-C19
6	L	306	BCL	C2A-CAA-CBA-CGA
11	M	405	CDL	CB2-C1-CA2-OA2
9	M	402	LDA	C7-C8-C9-C10
10	M	404	SPO	C34-C33-C35-C36
10	M	404	SPO	C27-C28-C30-C31
9	M	402	LDA	C5-C6-C7-C8
5	L	302	BPH	CAD-CBD-CGD-O2D
5	L	304	BPH	O2A-C1-C2-C3
6	L	303	BCL	CHA-CBD-CGD-O2D
6	M	401	BCL	CAA-CBA-CGA-O2A
11	M	405	CDL	CA3-OA5-PA1-OA3
11	M	405	CDL	CB7-C71-C72-C73

There are no ring outliers.

11 monomers are involved in 37 short contacts:

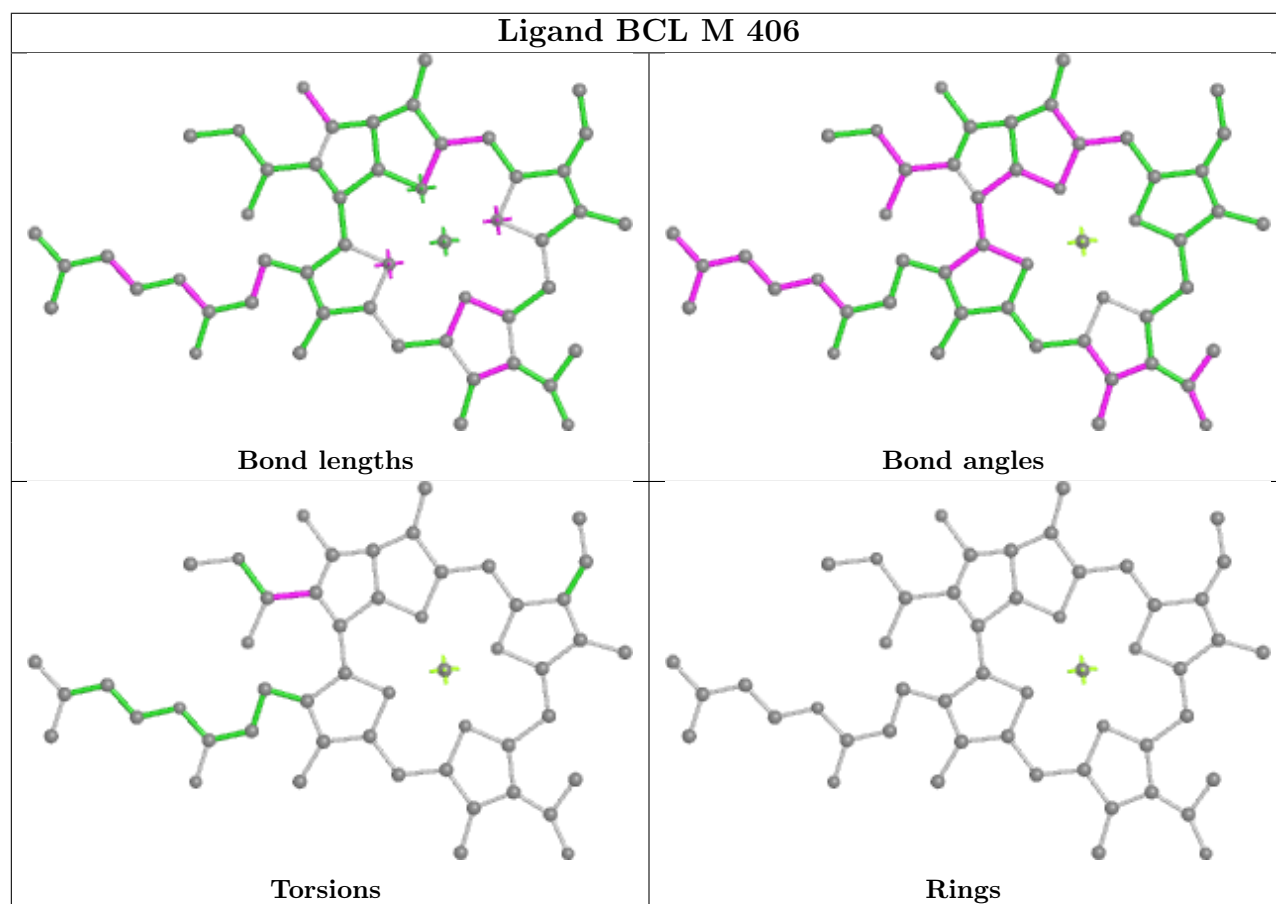
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	406	BCL	3	0
6	L	306	BCL	7	0
9	M	402	LDA	2	0
11	M	405	CDL	3	0
5	L	304	BPH	3	0
6	M	401	BCL	9	0
7	L	305	U10	3	0
9	M	403	LDA	1	0
10	M	404	SPO	1	0

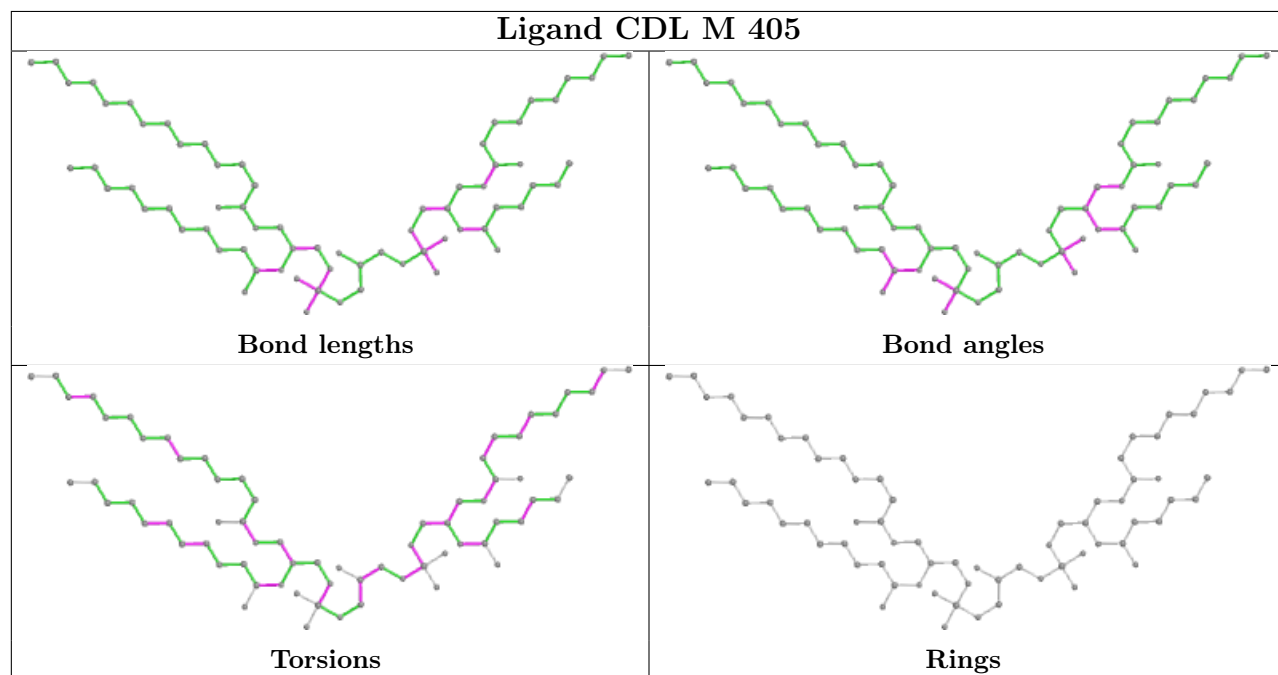
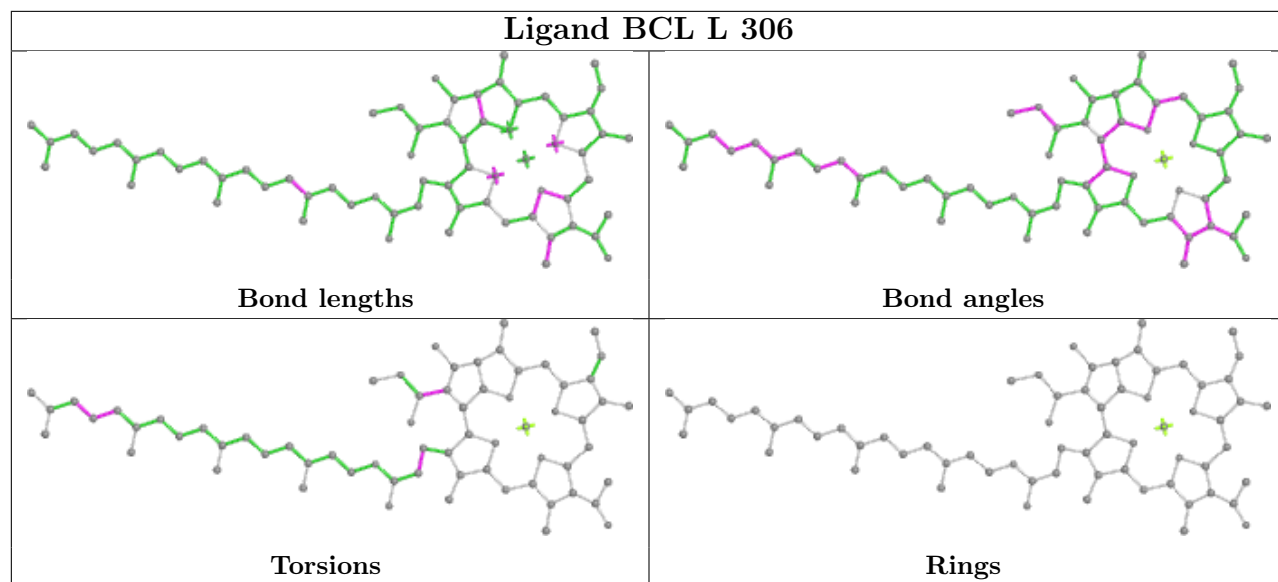
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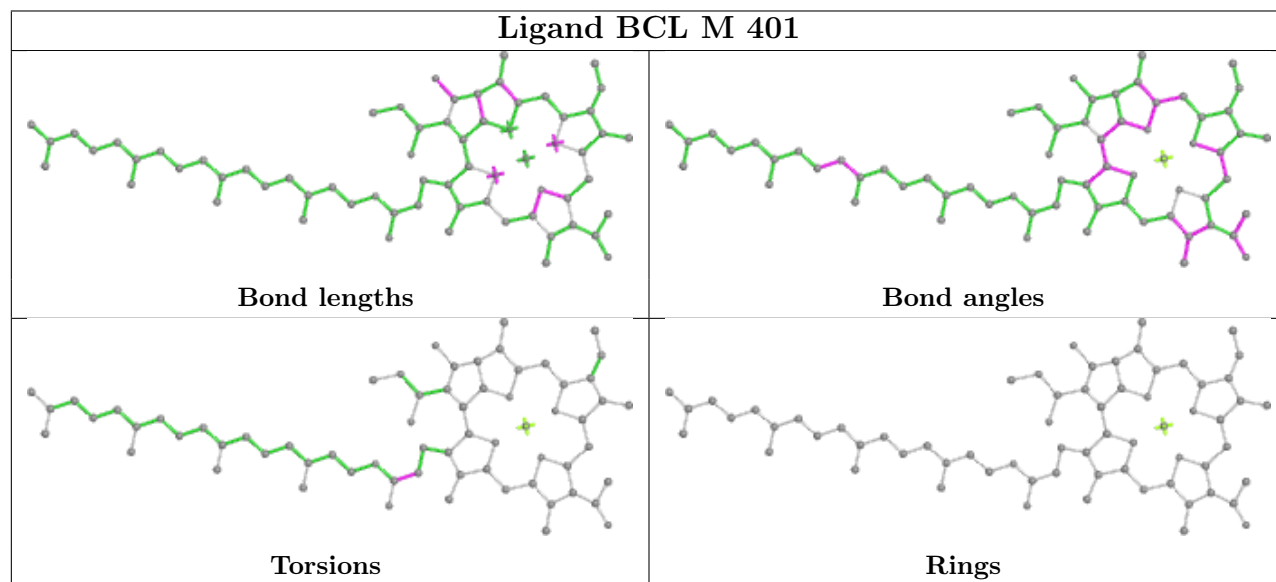
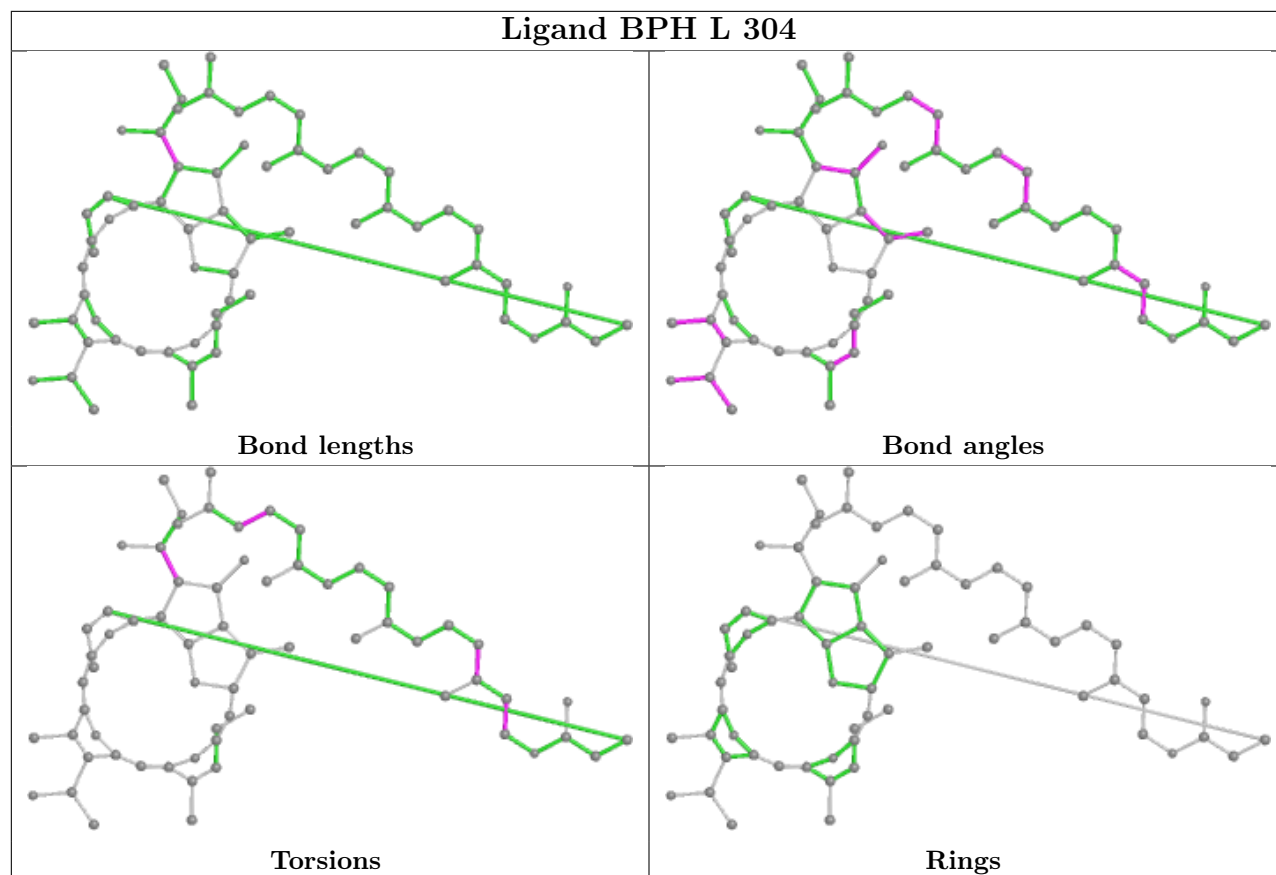
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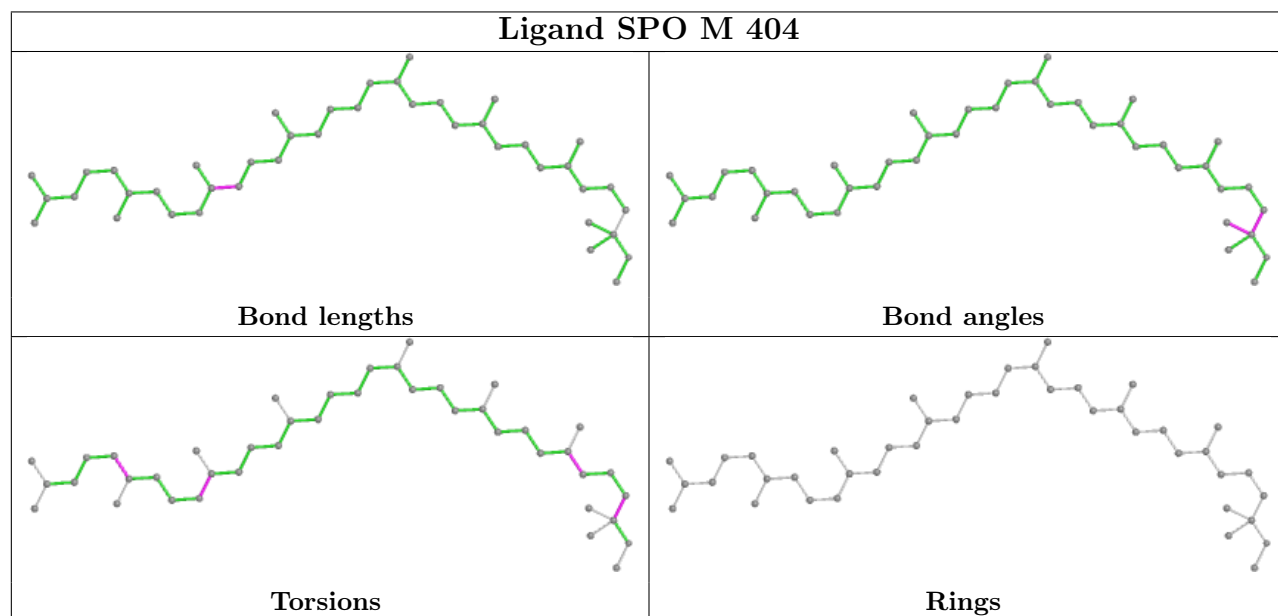
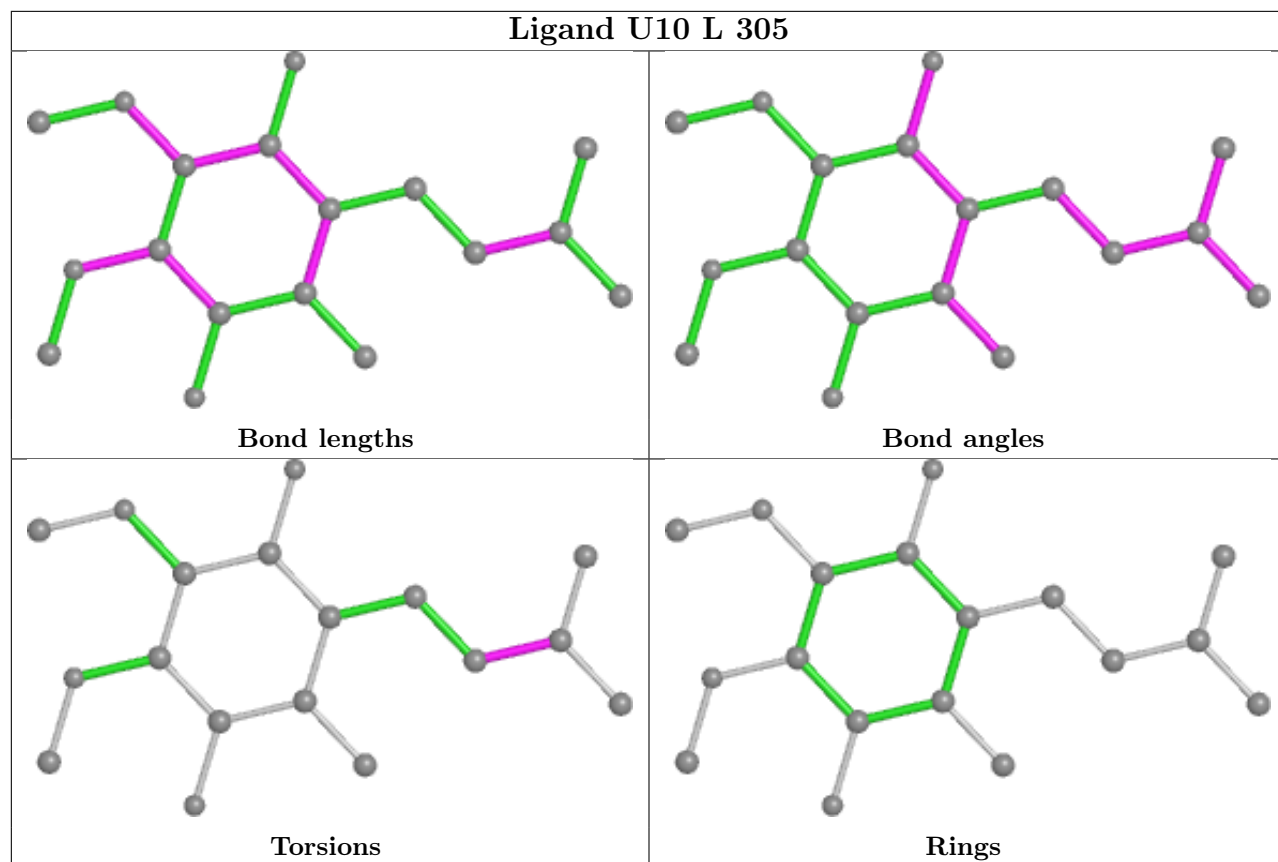
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302	BPH	9	0
6	L	303	BCL	4	0

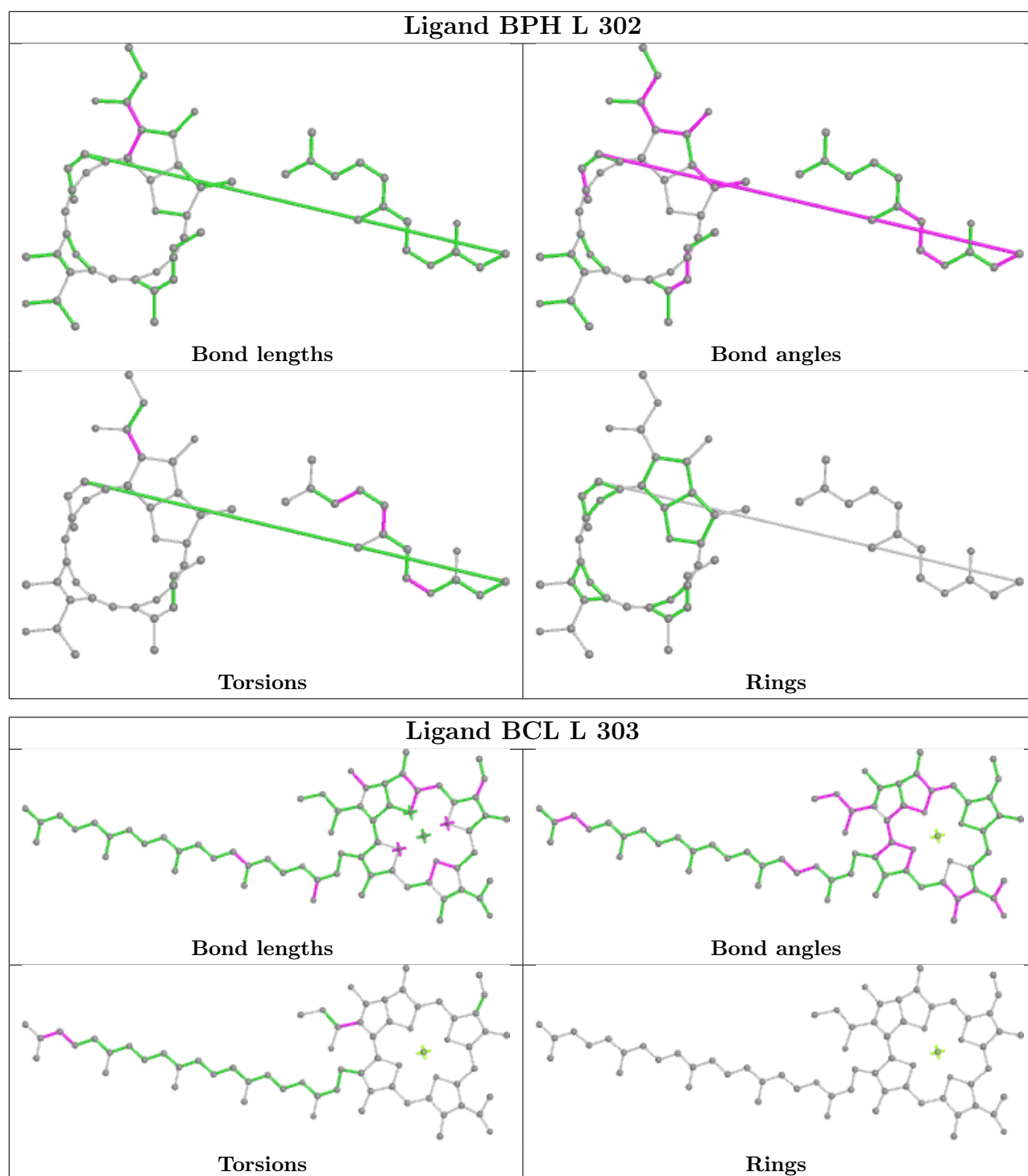
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [\(i\)](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	H	240/240 (100%)	-0.54	0 <a href="#">100</a>   <a href="#">100</a>	50, 62, 89, 132	0
2	L	281/281 (100%)	-0.71	2 (0%) <a href="#">87</a>   <a href="#">74</a>	42, 57, 93, 117	0
3	M	300/301 (99%)	-0.75	0 <a href="#">100</a>   <a href="#">100</a>	43, 62, 91, 120	0
All	All	821/822 (99%)	-0.67	2 (0%) <a href="#">95</a>   <a href="#">89</a>	42, 60, 91, 132	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	72	GLU	2.4
2	L	73	TYR	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
3	2L5	M	210	12/13	0.98	0.13	44,49,52,53	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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,



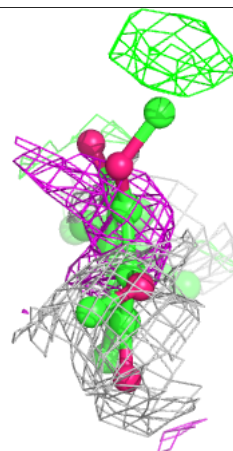
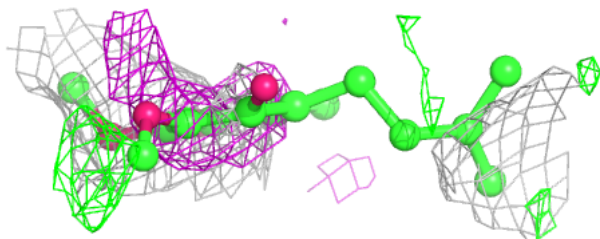
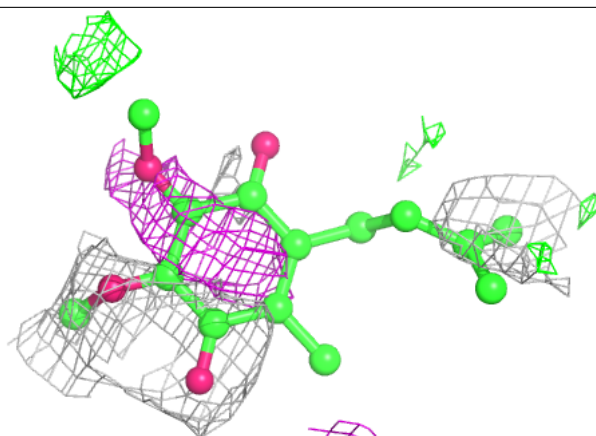
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	U10	L	305	18/63	0.60	0.49	117,136,151,152	0
9	LDA	M	402	16/16	0.85	0.45	82,86,103,105	0
9	LDA	M	403	16/16	0.85	0.27	66,86,111,111	0
8	CL	L	307	1/1	0.86	0.22	109,109,109,109	0
4	FE	L	301	1/1	0.90	0.16	130,130,130,130	0
11	CDL	M	405	69/100	0.90	0.35	64,93,116,123	0
10	SPO	M	404	42/42	0.96	0.29	49,66,82,92	0
5	BPH	L	302	55/65	0.97	0.16	36,54,71,85	0
6	BCL	M	401	66/66	0.97	0.18	36,49,66,83	0
5	BPH	L	304	65/65	0.98	0.14	36,50,59,64	0
6	BCL	M	406	51/66	0.98	0.15	41,50,66,71	0
6	BCL	L	303	66/66	0.98	0.14	42,49,66,68	0
6	BCL	L	306	66/66	0.98	0.16	42,50,59,66	0

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

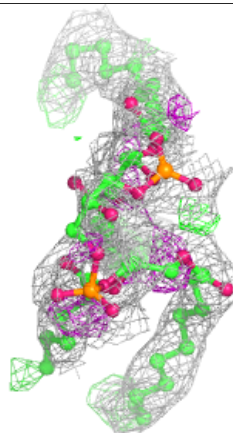
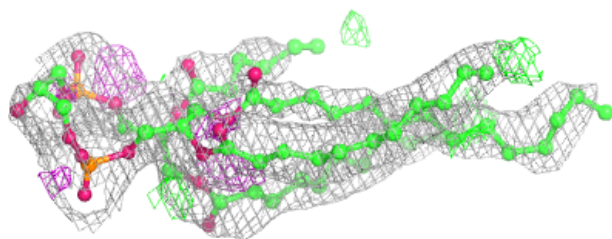
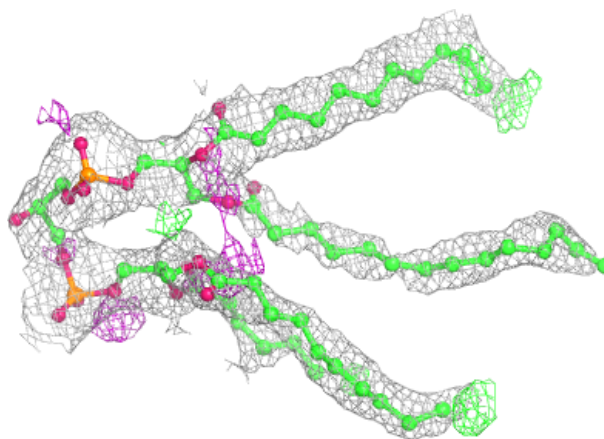
**Electron density around U10 L 305:**

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

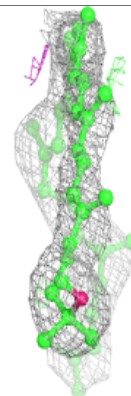
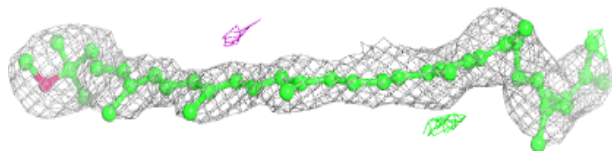
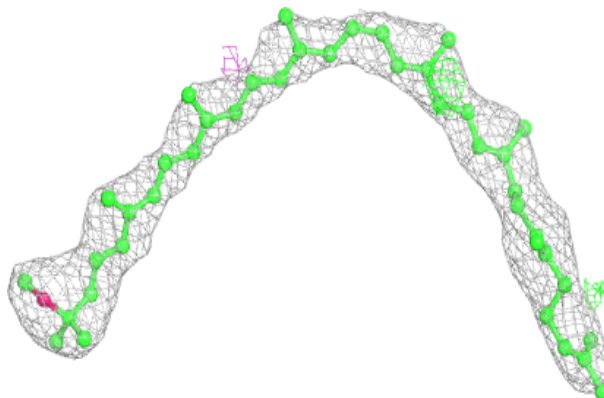


**Electron density around CDL M 405:**

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

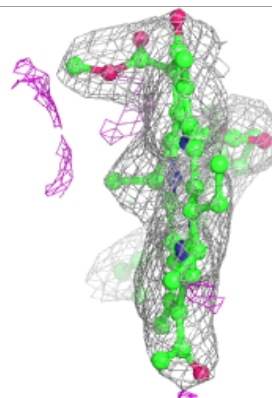
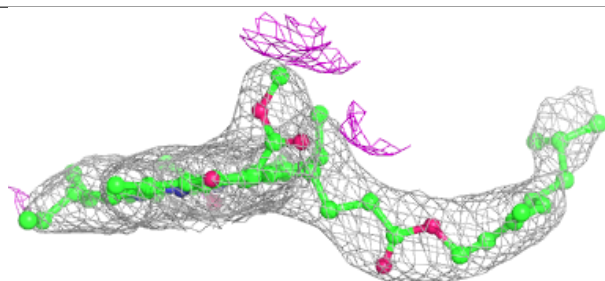
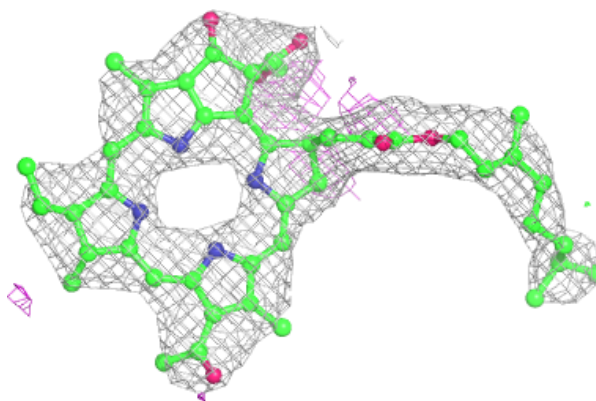
**Electron density around SPO M 404:**

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

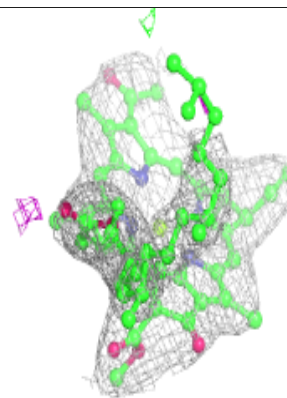
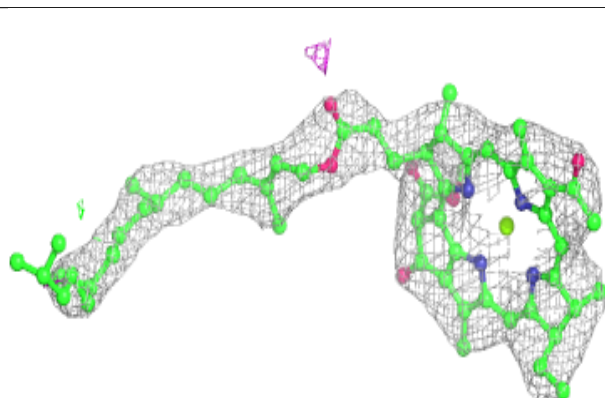
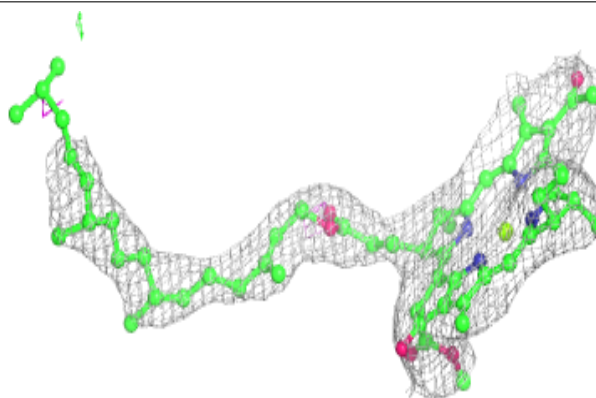


**Electron density around BPH L 302:**

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

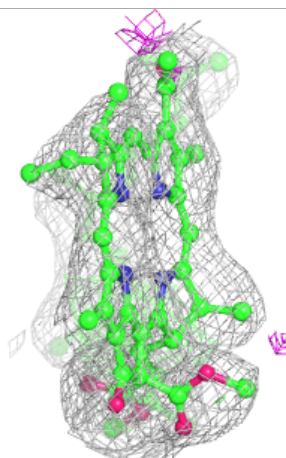
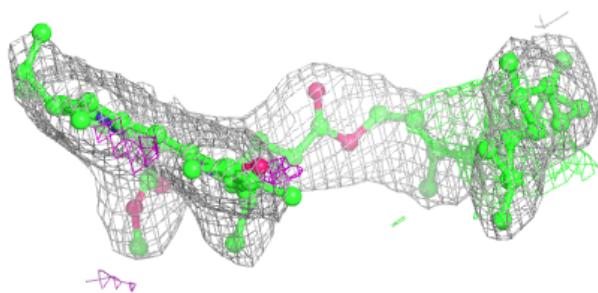
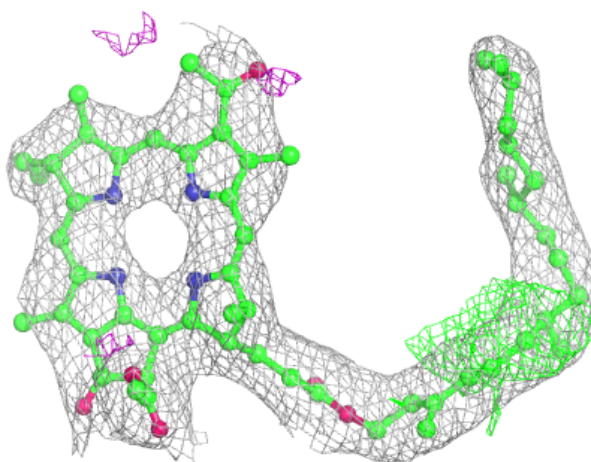
**Electron density around BCL M 401:**

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



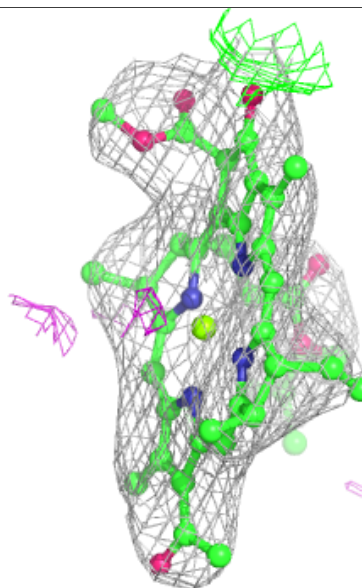
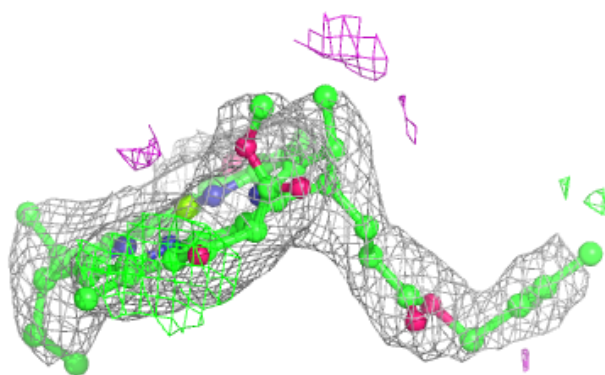
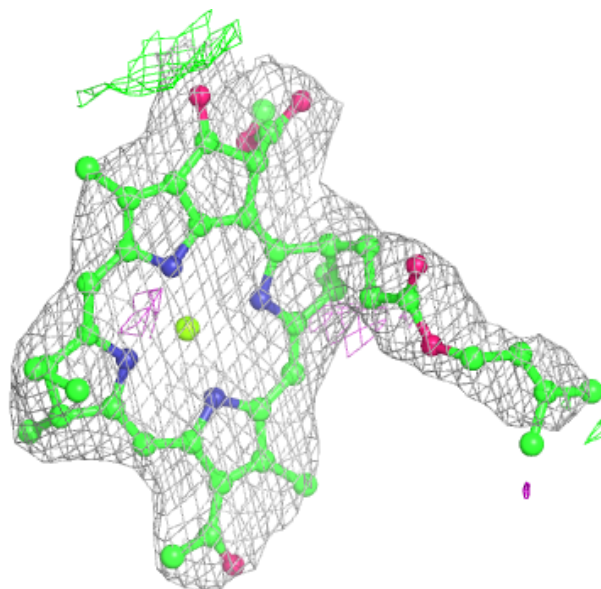
**Electron density around BPH L 304:**

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



**Electron density around BCL M 406:**

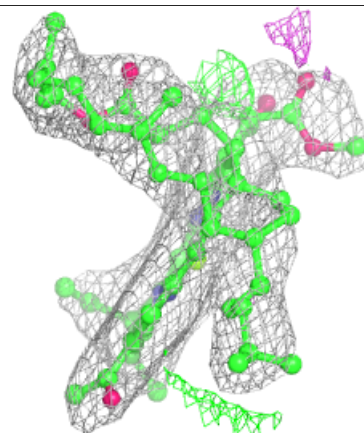
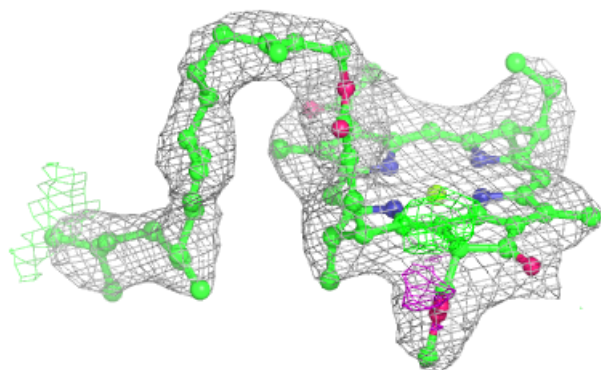
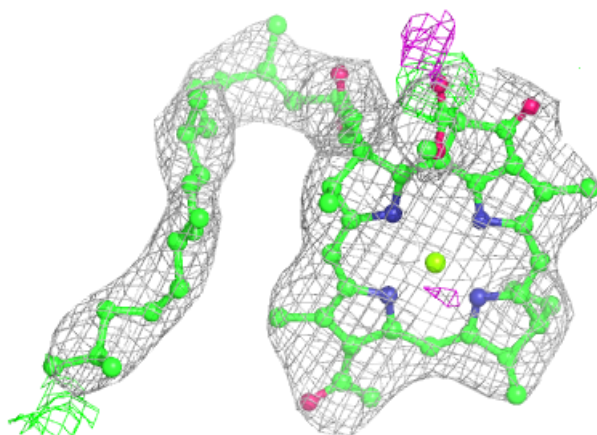
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



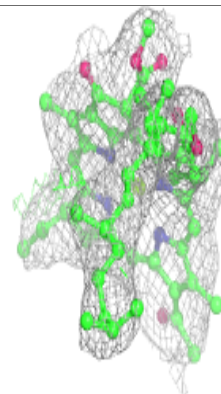
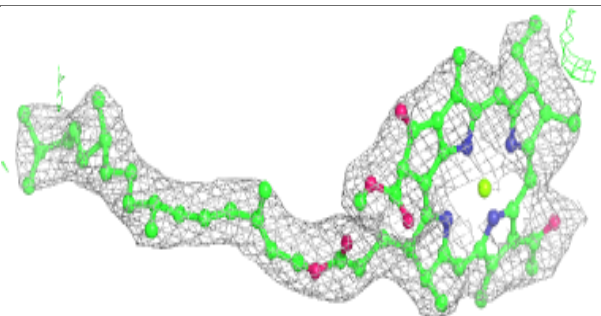
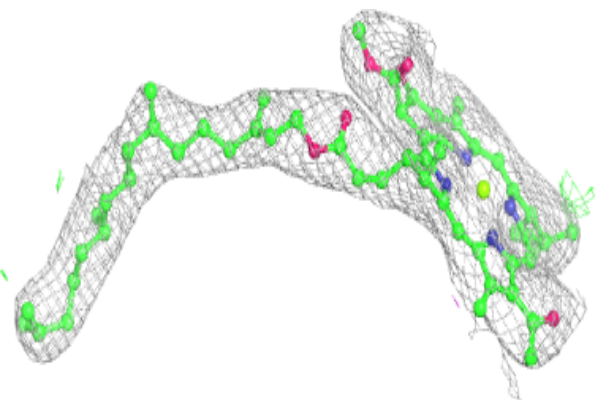


**Electron density around BCL L 303:**

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

**Electron density around BCL L 306:**

$2mF_o-DF_c$  (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.