



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:41 pm BST

PDB ID : 4LWY  
Title : L(M196)H,H(M202)L Double Mutant Structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV  
Authors : Gabdulkhakov, A.G.  
Deposited on : 2013-07-29  
Resolution : 2.90 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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

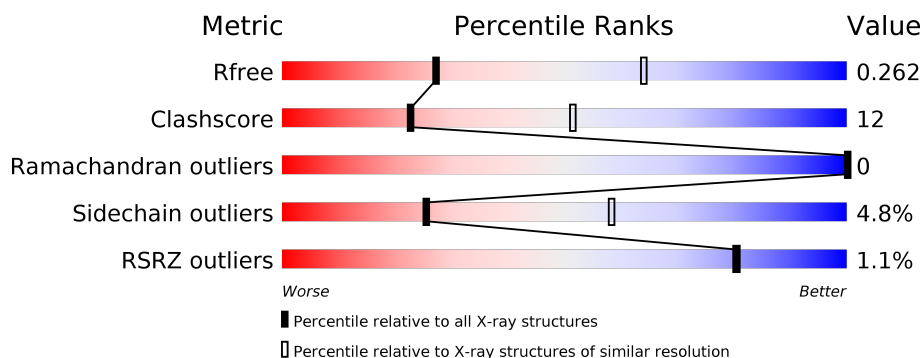
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	H	260	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>8%</div> </div> </div>
2	L	282	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>•</div> </div> </div>
3	M	303	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>•</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	BPH	L	303	X	-	-	-
12	BPH	M	402	X	-	-	-
12	BPH	M	404	X	-	-	-
14	CDL	M	401	-	-	-	X
4	LDA	M	411	-	-	-	X
5	UNL	L	305	-	-	-	X
5	UNL	L	307	-	-	-	X
7	DIO	H	307	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7434 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
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2233	1508	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

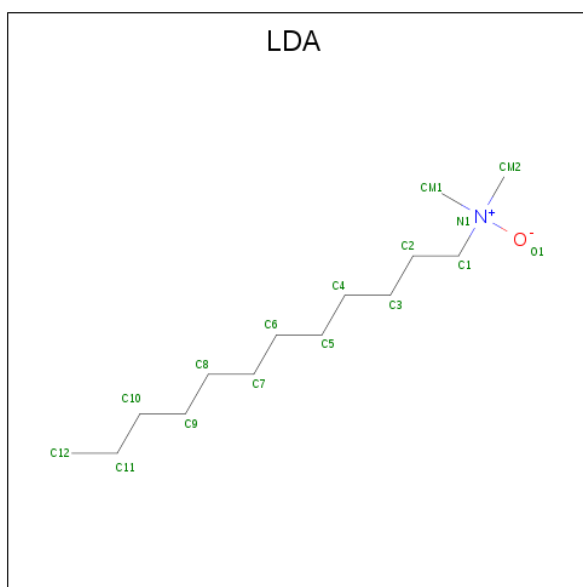
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9
M	196	HIS	LEU	ENGINEERED MUTATION	UNP P0C0Y9
M	202	LEU	HIS	ENGINEERED MUTATION	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



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

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

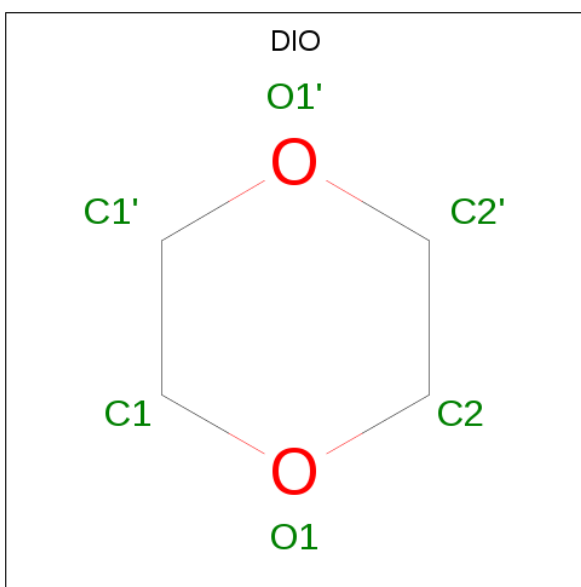
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	4	Total	C	0	0
			48	48		
5	L	4	Total	C	0	0
			46	46		
5	M	3	Total	C	0	0
			36	36		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



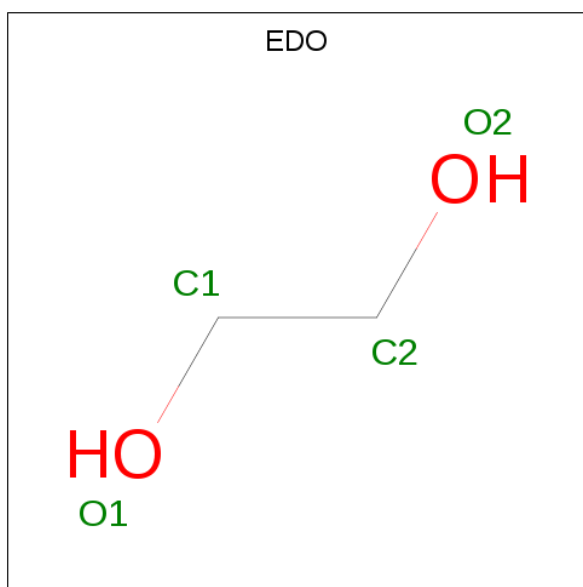
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			6	4	2		

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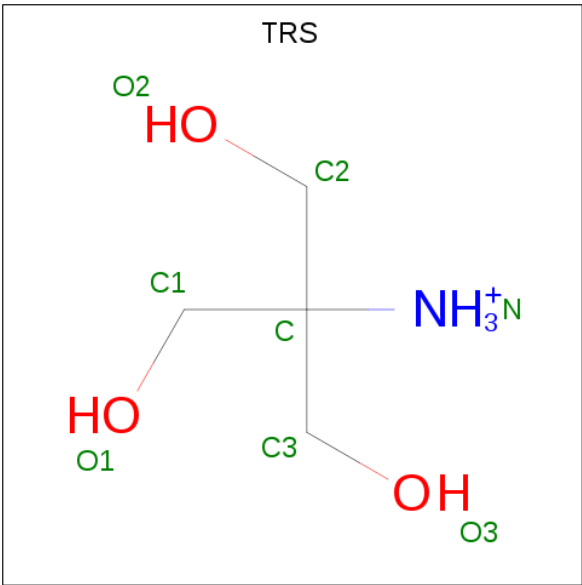
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	4	2		
7	L	1	Total	C	O	0	0
			6	4	2		
7	M	1	Total	C	O	0	0
			6	4	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	L	1	Total	C	O	0	0
			4	2	2		
8	M	1	Total	C	O	0	0
			4	2	2		
8	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).

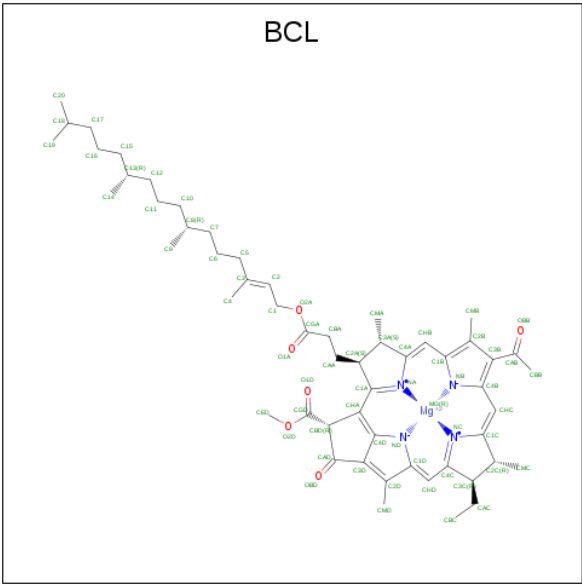


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			8	4	1	3		
9	L	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

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

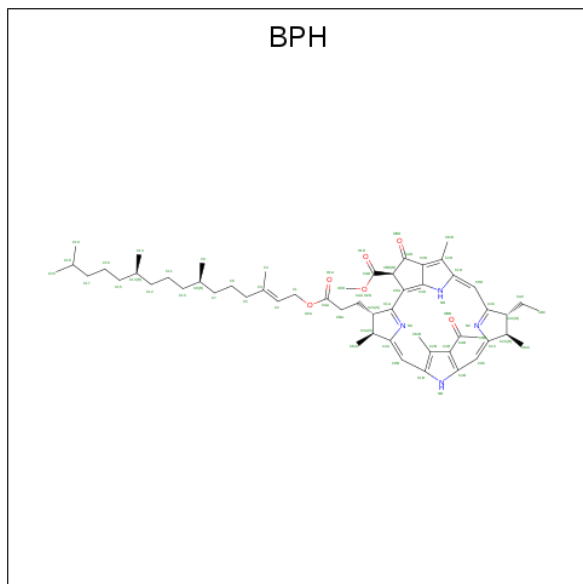
- Molecule 11 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).





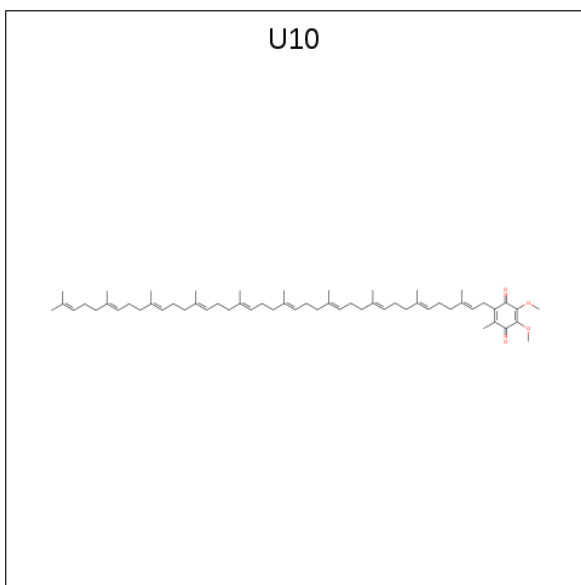
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
11	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 12 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



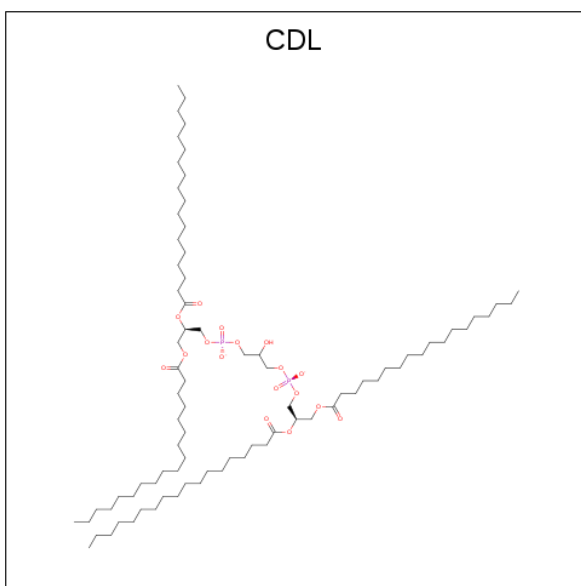
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



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

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).

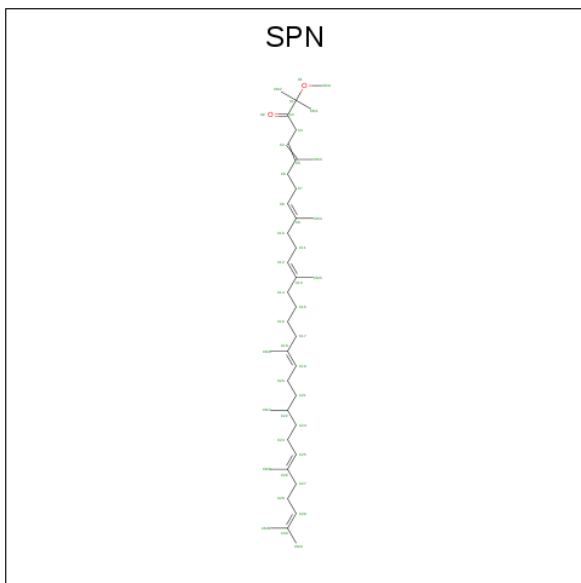


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 15 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 16 is SPEROIDENONE (three-letter code: SPN) (formula: C<sub>41</sub>H<sub>70</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	M	1	Total	C	O	0	0
			43	41	2		

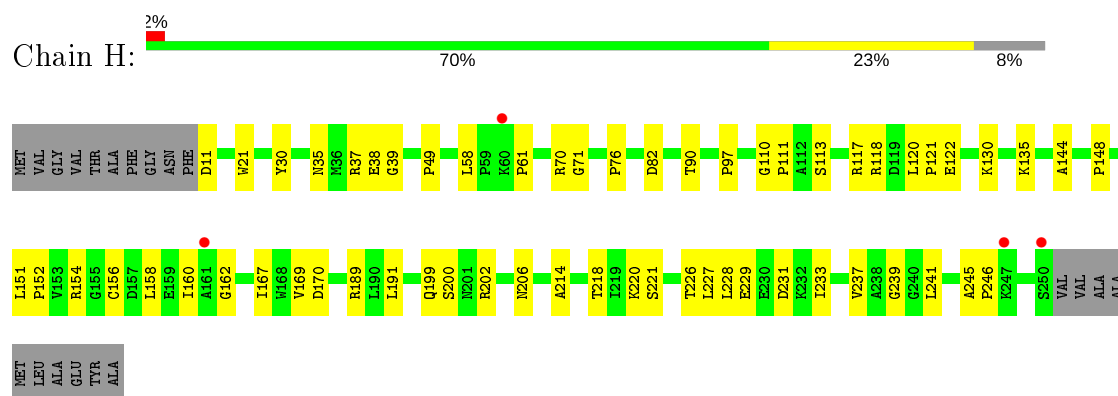
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	11	Total	O	0	0
			11	11		
17	L	10	Total	O	0	0
			10	10		
17	M	18	Total	O	0	0
			18	18		

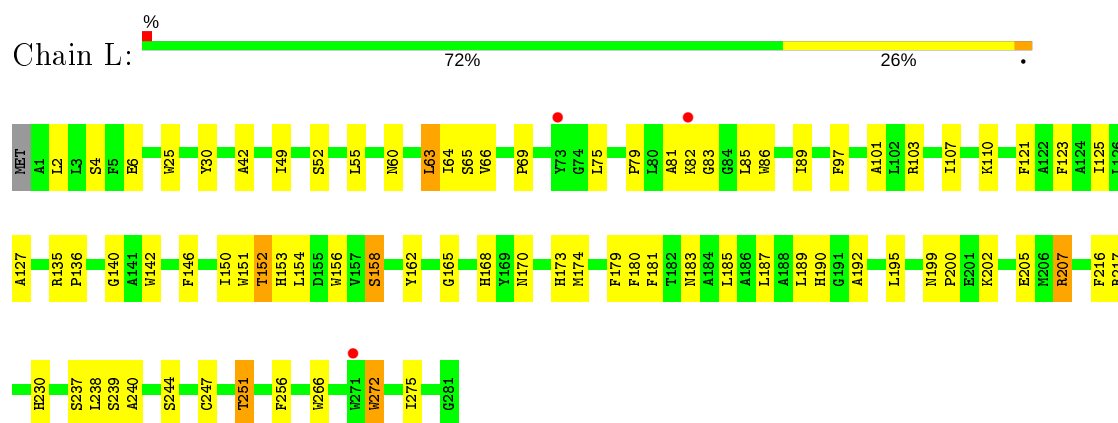
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

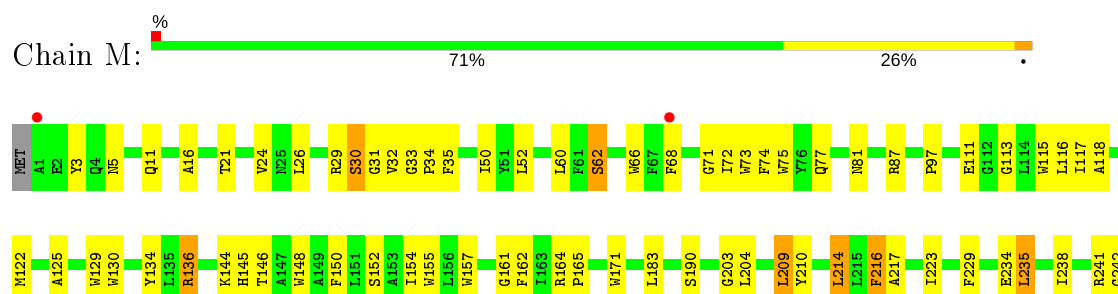
#### • Molecule 1: Reaction center protein H chain



#### • Molecule 2: Reaction center protein L chain



#### • Molecule 3: Reaction center protein M chain



T243	A244	R247	W254	T255	W256	G257	F258	G264	R267	W268	A269	I270	V276	T277	L278	I284	W293	V296	W297	G302
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.04Å 140.04Å 184.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.19 – 2.90 43.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.19-2.90) 99.8 (43.19-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, $R_{free}$	0.214 , 0.262 0.214 , 0.262	Depositor DCC
$R_{free}$ test set	2335 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.066 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: BCL, LDA, DIO, CDL, BPH, K, EDO, FE, SPN, U10, TRS, UNL, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	H	0.43	0/1877	0.63	0/2553
2	L	0.46	0/2321	0.60	0/3177
3	M	0.44	0/2501	0.59	0/3415
All	All	0.44	0/6699	0.60	0/9145

There are no bond length outliers.

There are no bond angle outliers.

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	39	0
2	L	2233	0	2189	63	0
3	M	2409	0	2323	71	0
4	H	16	0	31	2	0
4	M	80	0	155	9	0
5	H	48	0	0	0	0
5	L	46	0	0	0	0
5	M	36	0	0	0	0
6	H	5	0	0	0	0
6	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	6	0	8	0	0
7	L	12	0	16	3	0
7	M	6	0	8	1	0
8	H	16	0	24	3	0
8	L	4	0	6	1	0
8	M	8	0	12	1	0
9	H	8	0	12	1	0
9	L	8	0	12	0	0
10	H	1	0	0	0	0
11	L	132	0	148	11	0
11	M	66	0	74	4	0
12	L	65	0	76	10	0
12	M	130	0	152	11	0
13	L	48	0	63	1	0
13	M	48	0	63	5	0
14	M	81	0	106	6	0
15	M	1	0	0	0	0
16	M	43	0	70	5	0
17	H	11	0	0	0	0
17	L	10	0	0	0	0
17	M	18	0	0	1	0
All	All	7434	0	7384	170	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 12.

All (170) 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)
3:M:34:PRO:HA	4:M:412:LDA:H71	1.55	0.89
2:L:200:PRO:HD2	7:L:309:DIO:H22	1.64	0.80
1:H:202:ARG:HH12	9:H:312:TRS:H21	1.53	0.73
2:L:42:ALA:HA	12:L:303:BPH:H9C3	1.71	0.73
2:L:65:SER:HB2	2:L:152:THR:HG21	1.70	0.72
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.74	0.70
2:L:199:ASN:HA	7:L:309:DIO:H21	1.74	0.70
3:M:21:THR:HG23	3:M:26:LEU:HD11	1.75	0.68
3:M:62:SER:HB2	3:M:125:ALA:HB2	1.73	0.68
2:L:55:LEU:HD13	2:L:81:ALA:HB2	1.74	0.68
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.75	0.68
3:M:35:PHE:H	4:M:412:LDA:H51	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:404:BPH:HHC	12:M:404:BPH:HBB3	1.78	0.66
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.79	0.64
2:L:60:ASN:HB3	2:L:63:LEU:HB2	1.80	0.64
1:H:152:PRO:HB2	1:H:160:ILE:HD12	1.79	0.63
2:L:205:GLU:O	2:L:207:ARG:NH1	2.32	0.63
12:L:303:BPH:H7C2	11:M:403:BCL:H201	1.81	0.63
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.31	0.62
1:H:160:ILE:HG22	1:H:162:GLY:H	1.65	0.62
3:M:75:TRP:HE1	16:M:407:SPN:HMA2	1.65	0.60
2:L:266:TRP:CD2	7:M:418:DIO:H11	2.36	0.60
12:M:402:BPH:H172	12:M:404:BPH:H9C2	1.83	0.60
12:L:303:BPH:H112	11:M:403:BCL:H201	1.84	0.59
1:H:121:PRO:HA	1:H:226:THR:HA	1.84	0.58
1:H:71:GLY:H	8:H:310:EDO:H22	1.68	0.58
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.39	0.58
2:L:2:LEU:HB3	2:L:6:GLU:HB3	1.87	0.57
4:H:301:LDA:H121	4:M:408:LDA:H91	1.86	0.57
3:M:152:SER:O	3:M:155:TRP:HB3	2.05	0.57
1:H:117:ARG:O	1:H:228:LEU:HB2	2.05	0.56
2:L:146:PHE:HA	2:L:156:TRP:CD1	2.40	0.56
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.87	0.56
12:L:303:BPH:HBB2	3:M:210:TYR:HB3	1.87	0.56
2:L:150:ILE:HG22	2:L:151:TRP:CD1	2.40	0.56
12:L:303:BPH:HMA1	13:M:406:U10:H252	1.88	0.56
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.88	0.56
3:M:31:GLY:H	4:M:410:LDA:HM11	1.70	0.55
2:L:170:ASN:HB3	2:L:173:HIS:HB3	1.89	0.55
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.89	0.55
2:L:60:ASN:O	2:L:63:LEU:N	2.39	0.55
1:H:156:CYS:HB3	1:H:206:ASN:O	2.08	0.54
1:H:90:THR:OG1	1:H:97:PRO:O	2.22	0.54
1:H:167:ILE:HG22	1:H:169:VAL:HG12	1.90	0.54
1:H:11:ASP:OD2	3:M:297:TRP:NE1	2.41	0.54
3:M:134:TYR:CE2	3:M:144:LYS:HG3	2.42	0.53
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.88	0.53
3:M:190:SER:HB2	12:M:402:BPH:H3C	1.89	0.53
11:M:403:BCL:HMB1	11:M:403:BCL:HBB2	1.91	0.53
2:L:52:SER:HB2	2:L:85:LEU:HD13	1.90	0.53
2:L:179:PHE:CD2	2:L:239:SER:HB3	2.45	0.52
3:M:148:TRP:HB3	14:M:401:CDL:H761	1.92	0.52
2:L:180:PHE:HB3	3:M:209:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:157:TRP:CZ2	16:M:407:SPN:HM73	2.46	0.51
12:L:303:BPH:H152	11:M:403:BCL:H202	1.92	0.51
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.46	0.51
1:H:21:TRP:HZ2	4:M:408:LDA:HM13	1.75	0.51
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.45	0.50
4:H:301:LDA:H112	13:M:406:U10:H202	1.92	0.50
2:L:127:ALA:HB3	11:L:302:BCL:H43	1.94	0.50
2:L:168:HIS:HB3	3:M:183:LEU:HD13	1.94	0.50
1:H:113:SER:O	3:M:247:ARG:NH1	2.45	0.50
3:M:73:TRP:HE1	3:M:77:GLN:NE2	2.09	0.49
12:L:303:BPH:H3C	3:M:214:LEU:HA	1.93	0.49
1:H:30:TYR:OH	3:M:267:ARG:NH1	2.45	0.49
2:L:181:PHE:CD2	12:M:404:BPH:HBB1	2.48	0.49
11:L:301:BCL:HBB3	11:L:301:BCL:HMB1	1.94	0.49
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.12	0.49
2:L:190:HIS:HA	13:L:304:U10:O2	2.13	0.49
3:M:268:TRP:CD1	13:M:406:U10:H111	2.48	0.49
2:L:153:HIS:CE1	12:L:303:BPH:H201	2.47	0.49
2:L:97:PHE:CE1	11:L:302:BCL:H121	2.48	0.49
3:M:203:GLY:HA3	4:M:408:LDA:HM21	1.95	0.49
3:M:130:TRP:HD1	3:M:150:PHE:HD2	1.61	0.49
3:M:278:LEU:HD11	14:M:401:CDL:H811	1.94	0.49
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.95	0.48
2:L:185:LEU:HD13	12:M:404:BPH:ND	2.28	0.48
1:H:61:PRO:HA	1:H:76:PRO:HD2	1.96	0.48
11:L:301:BCL:H61	12:M:402:BPH:H203	1.95	0.47
2:L:123:PHE:CD1	2:L:238:LEU:HD13	2.48	0.47
2:L:162:TYR:HA	2:L:165:GLY:O	2.13	0.47
3:M:204:LEU:HG	4:M:408:LDA:HM11	1.97	0.47
1:H:189:ARG:NH2	1:H:214:ALA:O	2.40	0.47
2:L:52:SER:OG	8:L:311:EDO:O2	2.29	0.47
3:M:130:TRP:HD1	3:M:150:PHE:CD2	2.32	0.47
1:H:154:ARG:HG2	1:H:158:LEU:HA	1.97	0.47
2:L:60:ASN:O	2:L:64:ILE:HG13	2.15	0.47
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.96	0.47
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.50	0.47
2:L:75:LEU:HD11	2:L:140:GLY:HA2	1.96	0.47
2:L:79:PRO:HB2	2:L:82:LYS:HG3	1.97	0.47
3:M:164:ARG:HD2	3:M:284:ILE:HG22	1.96	0.47
11:L:301:BCL:HHC	12:M:402:BPH:H4C2	1.97	0.46
14:M:401:CDL:H391	14:M:401:CDL:H422	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:157:TRP:CE2	16:M:407:SPN:HM73	2.50	0.46
1:H:199:GLN:OE1	1:H:202:ARG:NH1	2.48	0.46
2:L:69:PRO:HD3	2:L:83:GLY:O	2.16	0.46
1:H:35:ASN:OD1	3:M:264:GLY:HA3	2.16	0.46
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.98	0.46
1:H:220:LYS:HG3	1:H:229:GLU:OE2	2.16	0.45
2:L:97:PHE:HB3	2:L:125:ILE:HD11	1.98	0.45
2:L:199:ASN:HA	7:L:309:DIO:C2	2.46	0.45
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.98	0.45
1:H:118:ARG:HG2	1:H:120:LEU:HG	1.99	0.45
12:L:303:BPH:CBB	3:M:210:TYR:HB3	2.47	0.45
3:M:234:GLU:O	3:M:238:ILE:HG13	2.17	0.45
13:M:406:U10:H322	13:M:406:U10:H28	1.44	0.45
1:H:110:GLY:HA3	1:H:111:PRO:HD2	1.83	0.45
4:M:412:LDA:HM23	4:M:412:LDA:H21	1.61	0.45
3:M:144:LYS:HB2	14:M:401:CDL:HB32	1.98	0.45
1:H:70:ARG:O	1:H:118:ARG:NH2	2.50	0.45
3:M:256:MET:CE	13:M:406:U10:H102	2.47	0.45
11:L:301:BCL:HBB2	12:M:402:BPH:H102	1.98	0.44
11:L:302:BCL:H192	11:L:302:BCL:H161	1.68	0.44
3:M:24:VAL:HG11	3:M:29:ARG:HH11	1.82	0.44
1:H:241:LEU:HD13	8:M:419:EDO:H11	1.98	0.44
2:L:244:SER:OG	11:L:302:BCL:HMA2	2.18	0.44
3:M:35:PHE:N	4:M:412:LDA:H51	2.30	0.44
1:H:245:ALA:N	1:H:246:PRO:HD2	2.32	0.44
2:L:189:LEU:HA	2:L:189:LEU:HD23	1.85	0.44
2:L:237:SER:HB3	3:M:217:ALA:HB2	1.99	0.44
2:L:66:VAL:HG12	2:L:86:TRP:HB2	2.00	0.44
3:M:113:GLY:O	3:M:117:ILE:HG13	2.17	0.43
2:L:101:ALA:HB2	2:L:121:PHE:HD2	1.83	0.43
3:M:60:LEU:HA	12:M:404:BPH:C4	2.48	0.43
1:H:82:ASP:OD2	8:H:311:EDO:H12	2.18	0.43
2:L:25:TRP:CD1	2:L:30:TYR:HA	2.53	0.43
2:L:275:ILE:HG21	3:M:81:ASN:ND2	2.33	0.43
3:M:162:PHE:HD1	16:M:407:SPN:H242	1.84	0.43
2:L:158:SER:HA	11:L:302:BCL:HBC1	2.00	0.43
1:H:144:ALA:HB3	3:M:11:GLN:HG3	2.00	0.43
3:M:32:VAL:HG12	3:M:33:GLY:O	2.18	0.43
1:H:37:ARG:O	1:H:38:GLU:HG2	2.19	0.43
2:L:179:PHE:CE2	2:L:239:SER:HB3	2.54	0.42
2:L:192:ALA:HB1	3:M:146:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:127:ALA:CB	11:L:302:BCL:H43	2.49	0.42
2:L:49:ILE:CG1	2:L:89:ILE:HD13	2.49	0.42
3:M:235:LEU:HD12	17:M:506:HOH:O	2.18	0.42
3:M:209:LEU:N	3:M:276:VAL:HG22	2.35	0.42
3:M:115:TRP:CE3	3:M:116:LEU:HD23	2.55	0.42
3:M:66:TRP:HD1	3:M:118:ALA:O	2.03	0.42
2:L:181:PHE:HB3	12:M:404:BPH:HBB2	2.02	0.41
2:L:217:ARG:O	3:M:50:ILE:HA	2.20	0.41
3:M:68:PHE:O	3:M:72:ILE:HG12	2.20	0.41
1:H:220:LYS:H	1:H:220:LYS:HG3	1.61	0.41
2:L:153:HIS:O	2:L:156:TRP:HB3	2.21	0.41
3:M:161:GLY:HA3	16:M:407:SPN:H201	2.02	0.41
3:M:71:GLY:HA2	3:M:74:PHE:HB2	2.02	0.41
1:H:39:GLY:HA2	2:L:4:SER:OG	2.20	0.41
3:M:30:SER:OG	3:M:31:GLY:N	2.52	0.41
3:M:293:ASN:HB3	3:M:296:VAL:HB	2.03	0.41
1:H:148:PRO:HD2	1:H:167:ILE:HD11	2.03	0.41
2:L:195:LEU:HB3	3:M:145:HIS:CD2	2.56	0.41
2:L:174:MET:SD	11:L:301:BCL:HED3	2.61	0.41
2:L:110:LYS:HD2	3:M:254:TRP:CZ3	2.56	0.41
12:L:303:BPH:HBB1	3:M:210:TYR:CD2	2.55	0.41
2:L:103:ARG:O	2:L:107:ILE:HG13	2.21	0.41
14:M:401:CDL:HB31	14:M:401:CDL:HB21	2.03	0.41
3:M:154:ILE:HG23	3:M:157:TRP:CE3	2.56	0.41
1:H:71:GLY:N	8:H:310:EDO:H22	2.35	0.40
1:H:58:LEU:HA	1:H:58:LEU:HD23	1.85	0.40
1:H:233:ILE:O	1:H:237:VAL:HG23	2.21	0.40
2:L:135:ARG:HH21	2:L:251:THR:HG22	1.86	0.40
3:M:136:ARG:HA	3:M:136:ARG:NH1	2.36	0.40
3:M:148:TRP:NE1	14:M:401:CDL:OB6	2.53	0.40
3:M:129:TRP:CD1	12:M:404:BPH:HBA1	2.56	0.40
2:L:107:ILE:HG23	3:M:254:TRP:HE3	1.86	0.40
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.56	0.40
2:L:272:TRP:CG	3:M:87:ARG:HB2	2.57	0.40
2:L:192:ALA:O	3:M:145:HIS:HB2	2.22	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	H	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
2	L	279/282 (99%)	261 (94%)	18 (6%)	0	100	100
3	M	300/303 (99%)	280 (93%)	20 (7%)	0	100	100
All	All	817/845 (97%)	774 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	H	195/208 (94%)	188 (96%)	7 (4%)	35	69
2	L	220/221 (100%)	208 (94%)	12 (6%)	21	53
3	M	236/237 (100%)	224 (95%)	12 (5%)	24	56
All	All	651/666 (98%)	620 (95%)	31 (5%)	25	58

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	49	PRO
1	H	135	LYS
1	H	191	LEU
1	H	200	SER
1	H	218	THR

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Mol	Chain	Res	Type
1	H	221	SER
1	H	231	ASP
2	L	63	LEU
2	L	152	THR
2	L	154	LEU
2	L	158	SER
2	L	183	ASN
2	L	202	LYS
2	L	207	ARG
2	L	216	PHE
2	L	247	CYS
2	L	251	THR
2	L	256	PHE
2	L	272	TRP
3	M	30	SER
3	M	52	LEU
3	M	62	SER
3	M	111	GLU
3	M	122	MET
3	M	136	ARG
3	M	209	LEU
3	M	214	LEU
3	M	216	PHE
3	M	235	LEU
3	M	258	PHE
3	M	270	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	77	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 11 are unknown and 2 are monoatomic - leaving 32 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	$\# Z  > 2$
11	BCL	L	302	-	58,74,74	1.29	5 (8%)	69,115,115	1.69	14 (20%)
8	EDO	M	420	-	3,3,3	0.52	0	2,2,2	0.20	0
8	EDO	H	308	-	3,3,3	0.47	0	2,2,2	0.28	0
6	PO4	M	417	-	4,4,4	0.87	0	6,6,6	0.35	0
4	LDA	M	412	-	12,15,15	2.04	1 (8%)	14,17,17	0.35	0
12	BPH	L	303	-	64,70,70	1.45	8 (12%)	76,101,101	1.31	8 (10%)
6	PO4	M	416	-	4,4,4	0.84	0	6,6,6	0.43	0
7	DIO	H	307	-	6,6,6	0.86	0	6,6,6	0.76	0
7	DIO	L	309	-	6,6,6	0.81	0	6,6,6	0.80	0
9	TRS	H	312	-	7,7,7	0.30	0	9,9,9	0.34	0
4	LDA	M	409	-	12,15,15	2.04	1 (8%)	14,17,17	0.43	0
16	SPN	M	407	-	40,42,42	1.22	6 (15%)	50,52,52	1.66	13 (26%)
13	U10	M	406	-	48,48,63	2.64	14 (29%)	58,61,79	1.84	14 (24%)
8	EDO	H	310	-	3,3,3	0.46	0	2,2,2	0.48	0
8	EDO	M	419	-	3,3,3	0.51	0	2,2,2	0.28	0
12	BPH	M	402	-	64,70,70	1.37	8 (12%)	76,101,101	1.26	9 (11%)
6	PO4	H	306	-	4,4,4	0.93	0	6,6,6	0.31	0
4	LDA	M	410	-	12,15,15	2.08	1 (8%)	14,17,17	0.60	0
4	LDA	M	408	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
11	BCL	L	301	-	58,74,74	1.31	3 (5%)	69,115,115	1.71	13 (18%)
8	EDO	L	311	-	3,3,3	0.55	0	2,2,2	0.09	0
12	BPH	M	404	-	64,70,70	1.38	7 (10%)	76,101,101	1.44	9 (11%)
7	DIO	M	418	-	6,6,6	0.85	0	6,6,6	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	LDA	M	411	-	12,15,15	2.07	1 (8%)	14,17,17	0.38	0
9	TRS	L	312	-	7,7,7	0.32	0	9,9,9	0.30	0
11	BCL	M	403	-	58,74,74	1.42	6 (10%)	69,115,115	1.84	15 (21%)
13	U10	L	304	-	48,48,63	2.60	13 (27%)	58,61,79	1.84	15 (25%)
14	CDL	M	401	-	80,80,99	0.90	4 (5%)	86,92,111	1.30	7 (8%)
8	EDO	H	311	-	3,3,3	0.54	0	2,2,2	0.17	0
8	EDO	H	309	-	3,3,3	0.44	0	2,2,2	0.55	0
4	LDA	H	301	-	12,15,15	2.03	1 (8%)	14,17,17	0.55	0
7	DIO	L	310	-	6,6,6	0.70	0	6,6,6	1.07	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
11	BCL	L	302	-	-	7/37/137/137	-
8	EDO	M	420	-	-	1/1/1/1	-
8	EDO	H	308	-	-	0/1/1/1	-
4	LDA	M	412	-	-	6/13/13/13	-
12	BPH	L	303	-	2/2/18/22	13/54/105/105	0/5/6/6
7	DIO	H	307	-	-	-	0/1/1/1
7	DIO	L	309	-	-	-	0/1/1/1
9	TRS	H	312	-	-	6/9/9/9	-
4	LDA	M	409	-	-	5/13/13/13	-
16	SPN	M	407	-	-	17/50/51/51	-
13	U10	M	406	-	-	12/45/69/87	0/1/1/1
8	EDO	H	310	-	-	0/1/1/1	-
8	EDO	M	419	-	-	1/1/1/1	-
12	BPH	M	402	-	2/2/18/22	8/54/105/105	0/5/6/6
4	LDA	M	410	-	-	1/13/13/13	-
4	LDA	M	408	-	-	2/13/13/13	-
11	BCL	L	301	-	-	10/37/137/137	-
8	EDO	L	311	-	-	0/1/1/1	-
12	BPH	M	404	-	2/2/18/22	7/54/105/105	0/5/6/6
7	DIO	M	418	-	-	-	0/1/1/1
4	LDA	M	411	-	-	7/13/13/13	-
9	TRS	L	312	-	-	7/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	M	403	-	-	7/37/137/137	-
13	U10	L	304	-	-	11/45/69/87	0/1/1/1
14	CDL	M	401	-	-	44/91/91/110	-
8	EDO	H	311	-	-	0/1/1/1	-
8	EDO	H	309	-	-	0/1/1/1	-
4	LDA	H	301	-	-	8/13/13/13	-
7	DIO	L	310	-	-	-	0/1/1/1

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	408	LDA	O1-N1	-7.13	1.25	1.42
4	M	410	LDA	O1-N1	-7.11	1.25	1.42
4	M	411	LDA	O1-N1	-7.07	1.25	1.42
4	H	301	LDA	O1-N1	-6.97	1.25	1.42
4	M	412	LDA	O1-N1	-6.96	1.25	1.42
4	M	409	LDA	O1-N1	-6.96	1.25	1.42
11	M	403	BCL	C4B-NB	6.87	1.41	1.35
11	L	302	BCL	C4B-NB	6.56	1.41	1.35
13	M	406	U10	C23-C24	6.34	1.48	1.33
13	M	406	U10	C13-C14	6.28	1.48	1.33
13	L	304	U10	C13-C14	6.19	1.47	1.33
13	M	406	U10	C33-C34	6.19	1.47	1.33
13	M	406	U10	C18-C19	6.07	1.47	1.33
13	L	304	U10	C18-C19	6.06	1.47	1.33
11	L	301	BCL	C4B-NB	6.03	1.40	1.35
13	M	406	U10	C28-C29	6.01	1.47	1.33
13	L	304	U10	C33-C34	6.00	1.47	1.33
13	L	304	U10	C23-C24	5.88	1.47	1.33
13	L	304	U10	C28-C29	5.79	1.46	1.33
13	L	304	U10	C38-C39	5.79	1.49	1.32
13	M	406	U10	C8-C9	5.63	1.46	1.33
11	L	301	BCL	C1B-NB	5.46	1.40	1.35
12	L	303	BPH	CHA-C1A	5.45	1.50	1.38
13	L	304	U10	C8-C9	5.28	1.45	1.33
11	M	403	BCL	C1B-NB	5.20	1.39	1.35
13	M	406	U10	C38-C39	5.12	1.47	1.32
12	M	404	BPH	CHA-C1A	4.98	1.49	1.38
12	L	303	BPH	CHD-C4C	4.97	1.50	1.38
13	M	406	U10	O4-C4	-4.97	1.24	1.36
12	M	402	BPH	CHA-C1A	4.78	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	304	U10	O4-C4	-4.75	1.25	1.36
13	L	304	U10	O3-C3	-4.64	1.25	1.36
13	M	406	U10	O3-C3	-4.59	1.25	1.36
11	L	302	BCL	C1B-NB	4.47	1.39	1.35
12	M	402	BPH	CHD-C4C	4.03	1.48	1.38
12	M	404	BPH	C4C-NC	-4.03	1.28	1.37
12	M	404	BPH	CHD-C4C	4.00	1.48	1.38
12	M	402	BPH	C1B-C2B	-3.99	1.37	1.45
12	L	303	BPH	C1B-C2B	-3.75	1.37	1.45
12	M	404	BPH	C1B-C2B	-3.60	1.38	1.45
12	M	402	BPH	C1A-NA	-3.57	1.30	1.37
12	M	402	BPH	C4C-NC	-3.54	1.29	1.37
14	M	401	CDL	OB8-CB7	3.39	1.43	1.33
16	M	407	SPN	C1-C2	-3.33	1.50	1.53
12	L	303	BPH	C1A-NA	-3.33	1.31	1.37
12	M	404	BPH	C1A-NA	-3.24	1.31	1.37
12	L	303	BPH	C4C-NC	-3.06	1.30	1.37
14	M	401	CDL	OA8-CA7	2.93	1.41	1.33
13	M	406	U10	C6-C1	2.92	1.40	1.35
16	M	407	SPN	C25-C26	2.91	1.40	1.33
13	L	304	U10	C4-C5	-2.86	1.40	1.48
13	L	304	U10	C6-C1	2.85	1.40	1.35
14	M	401	CDL	OB6-CB5	2.81	1.42	1.34
16	M	407	SPN	C8-C9	2.67	1.39	1.33
12	M	402	BPH	CHB-C4A	-2.63	1.33	1.40
16	M	407	SPN	C19-C18	2.58	1.39	1.33
11	M	403	BCL	MG-NA	-2.56	2.00	2.06
13	M	406	U10	C4-C5	-2.53	1.41	1.48
13	L	304	U10	C3-C2	-2.50	1.41	1.48
11	M	403	BCL	MG-NC	-2.48	2.00	2.06
11	L	302	BCL	CHD-C4C	-2.38	1.34	1.41
16	M	407	SPN	C29-C30	2.31	1.39	1.32
13	L	304	U10	C6-C5	-2.31	1.40	1.46
12	L	303	BPH	C3D-C2D	-2.30	1.35	1.39
11	L	302	BCL	MG-NA	-2.28	2.00	2.06
12	M	402	BPH	C3D-C2D	-2.26	1.35	1.39
11	M	403	BCL	CHD-C4C	-2.24	1.34	1.41
11	L	301	BCL	C1D-C2D	-2.23	1.37	1.42
14	M	401	CDL	OA6-CA5	2.21	1.40	1.34
12	M	404	BPH	C3D-C2D	-2.19	1.35	1.39
11	L	302	BCL	C1D-C2D	-2.19	1.37	1.42
13	M	406	U10	C6-C5	-2.18	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	303	BPH	CHB-C1B	2.18	1.42	1.38
12	L	303	BPH	CHB-C4A	-2.14	1.34	1.40
13	M	406	U10	C3-C2	-2.13	1.42	1.48
13	M	406	U10	C1-C2	-2.10	1.39	1.47
11	M	403	BCL	C4B-CHC	-2.07	1.35	1.41
12	M	402	BPH	C1D-CHD	-2.07	1.33	1.41
16	M	407	SPN	C12-C13	2.06	1.37	1.33
12	M	404	BPH	CHB-C4A	-2.01	1.35	1.40

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	403	BCL	C1C-NC-C4C	6.48	109.62	106.71
11	L	301	BCL	C1C-NC-C4C	5.95	109.38	106.71
13	L	304	U10	C7-C8-C9	-5.69	117.32	126.79
11	L	302	BCL	CMB-C2B-C1B	-4.99	120.80	128.46
11	L	301	BCL	O2D-CGD-CBD	4.89	119.96	111.27
11	M	403	BCL	O2D-CGD-CBD	4.89	119.95	111.27
11	M	403	BCL	CHD-C4C-NC	4.87	130.49	125.08
12	M	404	BPH	C4D-CHA-C1A	-4.63	119.10	130.51
13	M	406	U10	C30-C29-C31	4.59	123.00	115.27
12	M	404	BPH	C4D-C3D-CAD	-4.25	105.18	107.87
12	L	303	BPH	C4D-CHA-C1A	-4.23	120.09	130.51
12	M	402	BPH	C4D-CHA-C1A	-4.20	120.16	130.51
14	M	401	CDL	OB8-CB6-CB4	4.01	120.09	108.43
11	L	302	BCL	C1C-NC-C4C	3.94	108.48	106.71
11	L	302	BCL	CHD-C4C-NC	3.87	129.38	125.08
13	L	304	U10	C10-C9-C11	3.85	121.74	115.27
14	M	401	CDL	OB6-CB5-C51	3.71	119.49	111.50
13	L	304	U10	C17-C18-C19	-3.70	118.75	127.66
13	M	406	U10	C15-C14-C16	3.67	121.44	115.27
13	M	406	U10	C22-C23-C24	-3.57	119.06	127.66
11	L	301	BCL	C1B-CHB-C4A	-3.57	123.05	130.12
13	M	406	U10	C10-C9-C11	3.54	121.23	115.27
11	L	302	BCL	CMB-C2B-C3B	3.51	131.25	124.68
16	M	407	SPN	C3-C4-C5	-3.49	120.98	126.79
11	M	403	BCL	CHB-C4A-NA	3.46	129.30	124.51
12	M	404	BPH	C4-C3-C5	-3.45	109.47	115.27
12	M	404	BPH	CMD-C2D-C3D	3.44	131.11	124.68
16	M	407	SPN	C24-C25-C26	-3.43	119.40	127.66
13	M	406	U10	C35-C34-C36	3.42	121.02	115.27
14	M	401	CDL	OA8-CA6-CA4	3.42	118.38	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	301	BCL	C1-C2-C3	-3.41	120.14	126.04
14	M	401	CDL	OA6-CA5-C11	3.39	118.80	111.50
13	M	406	U10	C17-C18-C19	-3.34	119.61	127.66
11	M	403	BCL	C4D-C3D-CAD	-3.33	106.61	108.47
11	L	301	BCL	CHD-C4C-NC	3.31	128.76	125.08
12	M	404	BPH	C5-C3-C2	3.27	127.74	121.12
16	M	407	SPN	C6-C5-C4	-3.25	114.53	121.12
11	L	301	BCL	CMB-C2B-C1B	-3.25	123.48	128.46
11	L	302	BCL	C1D-CHD-C4C	-3.24	121.10	125.88
13	M	406	U10	C41-C39-C40	3.24	121.76	114.60
11	M	403	BCL	C1-C2-C3	-3.23	120.46	126.04
12	L	303	BPH	C4D-C3D-CAD	-3.23	105.83	107.87
12	M	404	BPH	C1C-NC-C4C	-3.22	107.71	110.54
13	M	406	U10	C27-C28-C29	-3.20	119.96	127.66
11	L	302	BCL	O2A-CGA-CBA	3.19	121.91	111.91
16	M	407	SPN	C7-C8-C9	-3.17	120.04	127.66
13	L	304	U10	C25-C24-C26	3.16	120.59	115.27
12	M	402	BPH	OBB-CAB-CBB	-3.14	112.77	119.73
13	L	304	U10	C22-C23-C24	-3.11	120.18	127.66
12	M	402	BPH	C1-C2-C3	3.06	131.34	126.04
13	M	406	U10	C32-C33-C34	-3.06	120.30	127.66
13	L	304	U10	C20-C19-C21	3.05	120.40	115.27
13	L	304	U10	C32-C33-C34	-3.01	120.42	127.66
14	M	401	CDL	CB4-OB6-CB5	3.00	125.17	117.79
11	L	302	BCL	C4-C3-C5	2.97	120.27	115.27
11	L	302	BCL	CED-O2D-CGD	2.97	122.65	115.94
13	L	304	U10	C12-C13-C14	-2.96	120.52	127.66
14	M	401	CDL	OB8-CB7-C71	2.96	121.20	111.91
13	L	304	U10	C30-C29-C31	2.96	120.25	115.27
16	M	407	SPN	CM3-C5-C6	2.93	120.20	115.27
12	M	404	BPH	C1-C2-C3	2.91	131.07	126.04
13	L	304	U10	C35-C34-C36	2.89	120.14	115.27
16	M	407	SPN	C20-C19-C18	-2.89	120.69	127.66
12	L	303	BPH	C1B-NB-C4B	2.87	111.92	106.51
11	L	301	BCL	CED-O2D-CGD	2.85	122.39	115.94
11	L	301	BCL	O1D-CGD-CBD	-2.84	118.68	124.48
13	M	406	U10	C20-C19-C21	2.80	119.99	115.27
13	L	304	U10	C27-C28-C29	-2.77	120.99	127.66
11	M	403	BCL	C1D-CHD-C4C	-2.77	121.80	125.88
12	L	303	BPH	CMD-C2D-C3D	2.70	129.73	124.68
12	L	303	BPH	C2B-C1B-NB	-2.70	105.72	109.79
12	M	402	BPH	CMD-C2D-C3D	2.69	129.71	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	403	BCL	C4-C3-C5	2.67	119.76	115.27
11	L	301	BCL	C4-C3-C5	2.65	119.73	115.27
16	M	407	SPN	C11-C12-C13	-2.64	121.31	127.66
12	L	303	BPH	O2D-CGD-O1D	2.61	128.94	123.84
11	L	302	BCL	C4D-C3D-CAD	-2.59	107.03	108.47
11	M	403	BCL	CMB-C2B-C1B	-2.55	124.54	128.46
11	L	302	BCL	C1B-CHB-C4A	-2.52	125.12	130.12
11	L	301	BCL	C1D-CHD-C4C	-2.52	122.16	125.88
11	M	403	BCL	C2A-C1A-CHA	-2.51	119.47	123.86
11	M	403	BCL	C3C-C4C-CHD	-2.51	118.03	123.39
16	M	407	SPN	CM8-C26-C27	2.49	119.45	115.27
11	L	301	BCL	C6-C5-C3	-2.48	106.94	113.45
13	M	406	U10	C37-C38-C39	-2.46	119.36	127.75
12	M	402	BPH	C6-C5-C3	2.45	119.88	113.45
12	M	402	BPH	CMB-C2B-C1B	-2.44	121.30	125.06
12	L	303	BPH	C6-C5-C3	2.44	119.84	113.45
14	M	401	CDL	OA8-CA7-C31	2.43	119.53	111.91
11	M	403	BCL	O1D-CGD-CBD	-2.43	119.52	124.48
16	M	407	SPN	CM6-C18-C17	2.42	119.35	115.27
11	L	302	BCL	O2D-CGD-CBD	2.42	115.57	111.27
13	M	406	U10	C7-C8-C9	-2.42	122.76	126.79
13	L	304	U10	C35-C34-C33	-2.42	117.48	123.68
13	M	406	U10	C25-C24-C26	2.41	119.33	115.27
11	L	302	BCL	CHB-C4A-NA	2.38	127.81	124.51
13	L	304	U10	C15-C14-C16	2.33	119.19	115.27
11	L	302	BCL	C3C-C4C-CHD	-2.30	118.47	123.39
12	M	402	BPH	C2A-C1A-NA	2.30	114.50	111.86
11	L	301	BCL	CMB-C2B-C3B	2.27	128.92	124.68
12	M	402	BPH	C4D-C3D-CAD	-2.25	106.44	107.87
16	M	407	SPN	C7-C6-C5	2.23	120.32	112.98
11	M	403	BCL	CHC-C1C-NC	2.19	127.54	124.51
12	M	404	BPH	C1B-NB-C4B	2.16	110.59	106.51
12	L	303	BPH	OBB-CAB-C3B	2.12	124.33	120.41
16	M	407	SPN	CM5-C13-C14	2.12	118.83	115.27
16	M	407	SPN	C27-C28-C29	2.12	118.84	111.88
13	L	304	U10	C10-C9-C8	-2.12	118.25	123.68
16	M	407	SPN	CM4-C9-C10	2.11	118.81	115.27
11	M	403	BCL	C1B-CHB-C4A	-2.10	125.95	130.12
13	M	406	U10	C26-C27-C28	-2.08	105.05	111.88
11	L	301	BCL	C4D-C3D-CAD	-2.03	107.34	108.47
12	M	402	BPH	C1B-NB-C4B	2.03	110.33	106.51
12	M	404	BPH	OBB-CAB-C3B	2.03	124.16	120.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	403	BCL	O2A-CGA-CBA	2.02	118.26	111.91
13	L	304	U10	C1M-C1-C6	-2.02	121.10	124.40
11	L	302	BCL	O2A-CGA-O1A	-2.02	118.49	123.59

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	L	303	BPH	C8
12	L	303	BPH	C13
12	M	402	BPH	C8
12	M	402	BPH	C13
12	M	404	BPH	C8
12	M	404	BPH	C13

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	302	BCL	C4-C3-C5-C6
12	L	303	BPH	C4B-C3B-CAB-CBB
12	L	303	BPH	C4B-C3B-CAB-OB
4	M	409	LDA	N1-C1-C2-C3
16	M	407	SPN	C7-C8-C9-C10
16	M	407	SPN	C11-C10-C9-C8
13	M	406	U10	C14-C16-C17-C18
9	H	312	TRS	C2-C-C1-O1
9	H	312	TRS	C3-C-C1-O1
9	H	312	TRS	N-C-C1-O1
9	H	312	TRS	C1-C-C2-O2
9	H	312	TRS	N-C-C2-O2
12	M	402	BPH	C4C-C3C-CAC-CBC
12	M	402	BPH	C2C-C3C-CAC-CBC
9	L	312	TRS	N-C-C2-O2
12	M	404	BPH	C4B-C3B-CAB-CBB
12	M	404	BPH	C4B-C3B-CAB-OB
13	L	304	U10	C14-C16-C17-C18
14	M	401	CDL	O1-C1-CB2-OB2
14	M	401	CDL	CA2-OA2-PA1-OA3
4	H	301	LDA	C2-C1-N1-O1
4	H	301	LDA	C2-C1-N1-CM1
4	H	301	LDA	C2-C1-N1-CM2
11	M	403	BCL	CBD-CGD-O2D-CED
13	M	406	U10	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
16	M	407	SPN	CM3-C5-C6-C7
11	L	302	BCL	C2-C3-C5-C6
16	M	407	SPN	C12-C13-C14-C15
14	M	401	CDL	C31-CA7-OA8-CA6
14	M	401	CDL	OA9-CA7-OA8-CA6
14	M	401	CDL	O1-C1-CA2-OA2
14	M	401	CDL	OB9-CB7-OB8-CB6
16	M	407	SPN	C14-C15-C16-C17
14	M	401	CDL	C71-CB7-OB8-CB6
13	M	406	U10	C37-C38-C39-C41
13	M	406	U10	C29-C31-C32-C33
11	M	403	BCL	O1D-CGD-O2D-CED
11	L	302	BCL	C15-C16-C17-C18
12	M	402	BPH	C15-C16-C17-C18
16	M	407	SPN	C16-C17-C18-C19
12	L	303	BPH	C14-C13-C15-C16
11	L	301	BCL	C10-C11-C12-C13
16	M	407	SPN	C28-C29-C30-CM9
13	M	406	U10	C32-C33-C34-C35
16	M	407	SPN	C26-C27-C28-C29
14	M	401	CDL	CA2-OA2-PA1-OA5
14	M	401	CDL	C39-C40-C41-C42
14	M	401	CDL	CB7-C71-C72-C73
14	M	401	CDL	C19-C20-C21-C22
4	M	411	LDA	C5-C6-C7-C8
14	M	401	CDL	C37-C38-C39-C40
12	L	303	BPH	C11-C12-C13-C14
11	L	301	BCL	C6-C7-C8-C9
4	M	411	LDA	C7-C8-C9-C10
14	M	401	CDL	C79-C80-C81-C82
4	M	409	LDA	C2-C3-C4-C5
14	M	401	CDL	C72-C73-C74-C75
12	L	303	BPH	C10-C11-C12-C13
13	M	406	U10	C25-C24-C26-C27
4	M	412	LDA	C4-C5-C6-C7
14	M	401	CDL	C14-C15-C16-C17
14	M	401	CDL	C35-C36-C37-C38
4	H	301	LDA	C1-C2-C3-C4
4	M	409	LDA	C1-C2-C3-C4
4	M	412	LDA	C1-C2-C3-C4
14	M	401	CDL	C20-C21-C22-C23
13	M	406	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
11	L	301	BCL	C6-C7-C8-C10
13	L	304	U10	C18-C19-C21-C22
12	L	303	BPH	C8-C10-C11-C12
4	M	412	LDA	C7-C8-C9-C10
14	M	401	CDL	C17-C18-C19-C20
4	M	410	LDA	C4-C5-C6-C7
12	M	404	BPH	C5-C6-C7-C8
13	L	304	U10	C20-C19-C21-C22
11	L	301	BCL	C11-C10-C8-C9
9	L	312	TRS	C1-C-C2-O2
4	M	412	LDA	C3-C4-C5-C6
4	M	411	LDA	C4-C5-C6-C7
14	M	401	CDL	C80-C81-C82-C83
14	M	401	CDL	CA2-C1-CB2-OB2
14	M	401	CDL	C36-C37-C38-C39
14	M	401	CDL	CB3-CB4-CB6-OB8
4	M	411	LDA	C2-C3-C4-C5
14	M	401	CDL	C13-C14-C15-C16
4	M	411	LDA	C9-C10-C11-C12
4	M	409	LDA	C4-C5-C6-C7
13	M	406	U10	C30-C29-C31-C32
12	M	402	BPH	C13-C15-C16-C17
4	M	412	LDA	C2-C3-C4-C5
4	M	411	LDA	C1-C2-C3-C4
12	M	404	BPH	C11-C12-C13-C15
14	M	401	CDL	OA5-CA3-CA4-CA6
14	M	401	CDL	OB5-CB3-CB4-CB6
13	L	304	U10	C24-C26-C27-C28
16	M	407	SPN	CM1-C1-C2-O2
16	M	407	SPN	CM1-C1-C2-C3
14	M	401	CDL	CB5-C51-C52-C53
14	M	401	CDL	C78-C79-C80-C81
4	H	301	LDA	C7-C8-C9-C10
4	H	301	LDA	C9-C10-C11-C12
13	M	406	U10	C32-C33-C34-C36
16	M	407	SPN	C28-C29-C30-CMB
12	M	404	BPH	C15-C16-C17-C18
16	M	407	SPN	C9-C10-C11-C12
13	L	304	U10	C9-C11-C12-C13
14	M	401	CDL	CB2-C1-CA2-OA2
14	M	401	CDL	C38-C39-C40-C41
12	L	303	BPH	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
12	L	303	BPH	C12-C13-C15-C16
13	M	406	U10	C28-C29-C31-C32
14	M	401	CDL	C18-C19-C20-C21
11	L	301	BCL	CBA-CGA-O2A-C1
11	L	301	BCL	CAD-CBD-CGD-O2D
13	L	304	U10	C5-C4-O4-C4M
12	M	402	BPH	CHA-CBD-CGD-O1D
11	M	403	BCL	CHA-CBD-CGD-O1D
11	M	403	BCL	CHA-CBD-CGD-O2D
12	L	303	BPH	C3-C5-C6-C7
11	L	301	BCL	O1A-CGA-O2A-C1
16	M	407	SPN	O1-C1-C2-O2
9	H	312	TRS	C3-C-C2-O2
9	L	312	TRS	C3-C-C1-O1
9	L	312	TRS	N-C-C1-O1
9	L	312	TRS	N-C-C3-O3
14	M	401	CDL	C73-C74-C75-C76
14	M	401	CDL	CA2-OA2-PA1-OA4
4	M	412	LDA	C9-C10-C11-C12
12	M	402	BPH	CAD-CBD-CGD-O1D
14	M	401	CDL	CA5-C11-C12-C13
11	L	302	BCL	C16-C17-C18-C19
16	M	407	SPN	C21-C22-C23-C24
11	L	301	BCL	C11-C12-C13-C15
14	M	401	CDL	C76-C77-C78-C79
16	M	407	SPN	CM7-C22-C23-C24
12	M	402	BPH	O1A-CGA-O2A-C1
14	M	401	CDL	C11-C12-C13-C14
4	H	301	LDA	C4-C5-C6-C7
14	M	401	CDL	OA5-CA3-CA4-OA6
12	M	402	BPH	CBA-CGA-O2A-C1
11	L	301	BCL	C11-C10-C8-C7
16	M	407	SPN	C16-C17-C18-CM6
14	M	401	CDL	C53-C54-C55-C56
11	M	403	BCL	C15-C16-C17-C18
9	L	312	TRS	C1-C-C3-O3
9	L	312	TRS	C2-C-C3-O3
11	L	302	BCL	C16-C17-C18-C20
12	L	303	BPH	O2A-C1-C2-C3
13	L	304	U10	C28-C29-C31-C32
14	M	401	CDL	OB6-CB4-CB6-OB8
13	L	304	U10	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
12	L	303	BPH	C2-C1-O2A-CGA
8	M	420	EDO	O1-C1-C2-O2
4	M	408	LDA	C4-C5-C6-C7
13	L	304	U10	C30-C29-C31-C32
13	M	406	U10	C5-C4-O4-C4M
13	L	304	U10	C3-C4-O4-C4M
12	M	404	BPH	C11-C12-C13-C14
11	L	302	BCL	CAD-CBD-CGD-O2D
12	L	303	BPH	CAD-CBD-CGD-O2D
12	M	404	BPH	CAD-CBD-CGD-O2D
11	L	301	BCL	C5-C6-C7-C8
11	M	403	BCL	CBA-CGA-O2A-C1
13	L	304	U10	C33-C34-C36-C37
16	M	407	SPN	C13-C14-C15-C16
14	M	401	CDL	OA6-CA4-CA6-OA8
4	M	408	LDA	C9-C10-C11-C12
4	H	301	LDA	C6-C7-C8-C9
11	L	302	BCL	C2-C1-O2A-CGA
14	M	401	CDL	C40-C41-C42-C43
4	M	409	LDA	C9-C10-C11-C12
14	M	401	CDL	C81-C82-C83-C84
14	M	401	CDL	CA3-OA5-PA1-OA3
8	M	419	EDO	O1-C1-C2-O2
14	M	401	CDL	C52-C51-CB5-OB7
4	M	411	LDA	C11-C10-C9-C8
12	L	303	BPH	C6-C7-C8-C9
11	M	403	BCL	O1A-CGA-O2A-C1
13	M	406	U10	C3-C4-O4-C4M
14	M	401	CDL	C12-C11-CA5-OA7

There are no ring outliers.

21 monomers are involved in 65 short contacts:

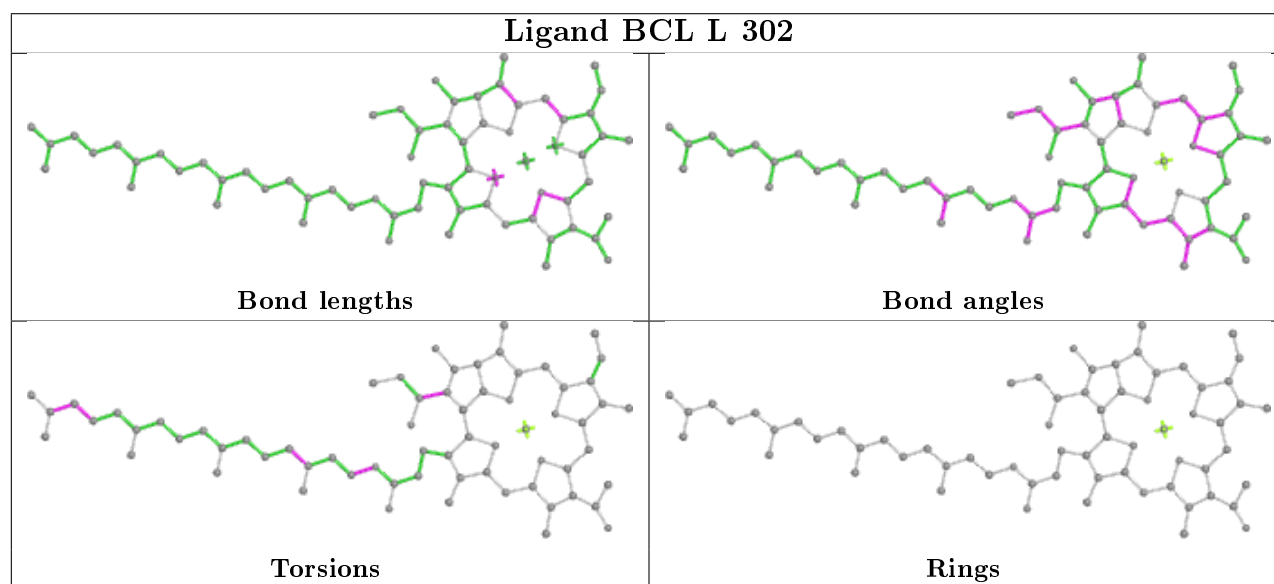
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	302	BCL	6	0
4	M	412	LDA	4	0
12	L	303	BPH	10	0
7	L	309	DIO	3	0
9	H	312	TRS	1	0
16	M	407	SPN	5	0
13	M	406	U10	5	0
8	H	310	EDO	2	0

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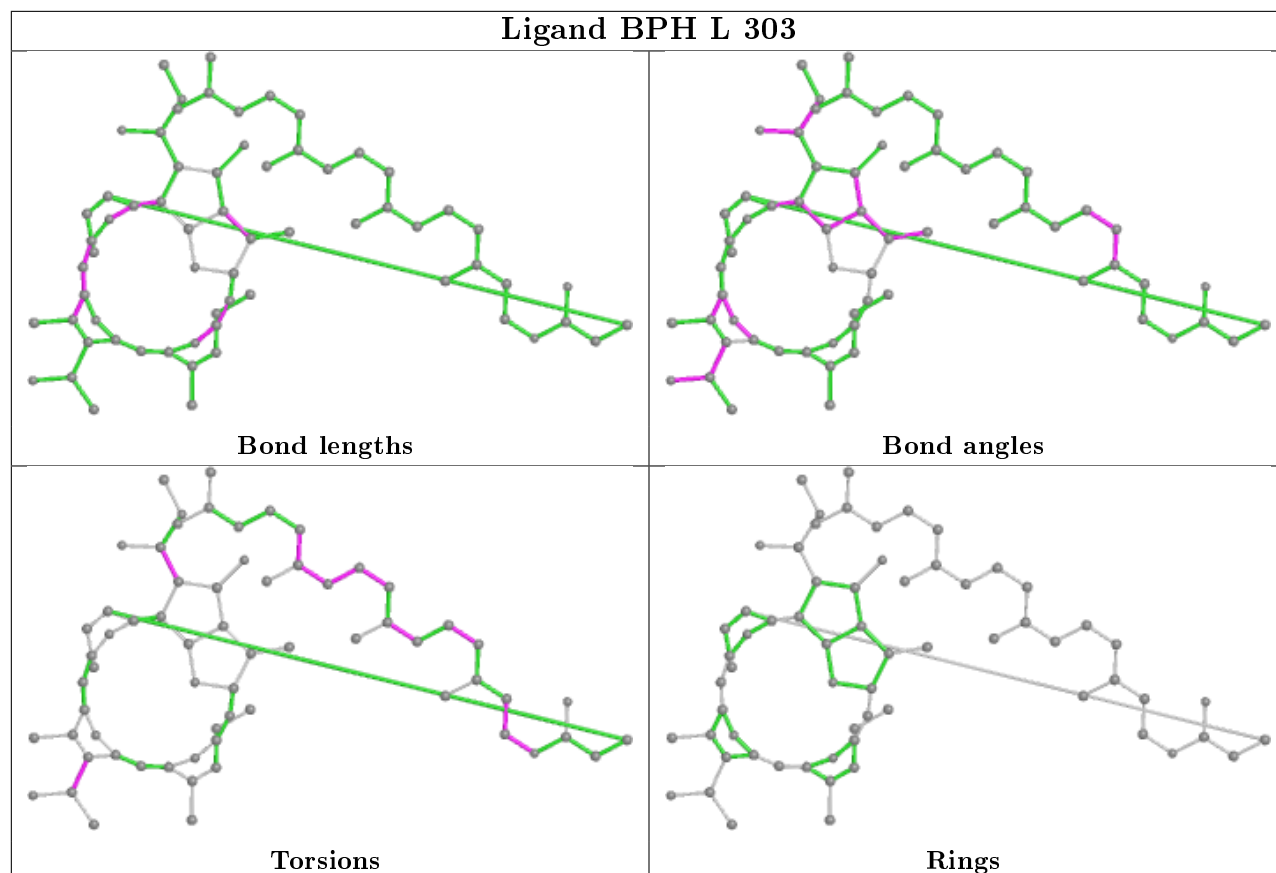
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	419	EDO	1	0
12	M	402	BPH	5	0
4	M	410	LDA	1	0
4	M	408	LDA	4	0
11	L	301	BCL	5	0
8	L	311	EDO	1	0
12	M	404	BPH	7	0
7	M	418	DIO	1	0
11	M	403	BCL	4	0
13	L	304	U10	1	0
14	M	401	CDL	6	0
8	H	311	EDO	1	0
4	H	301	LDA	2	0

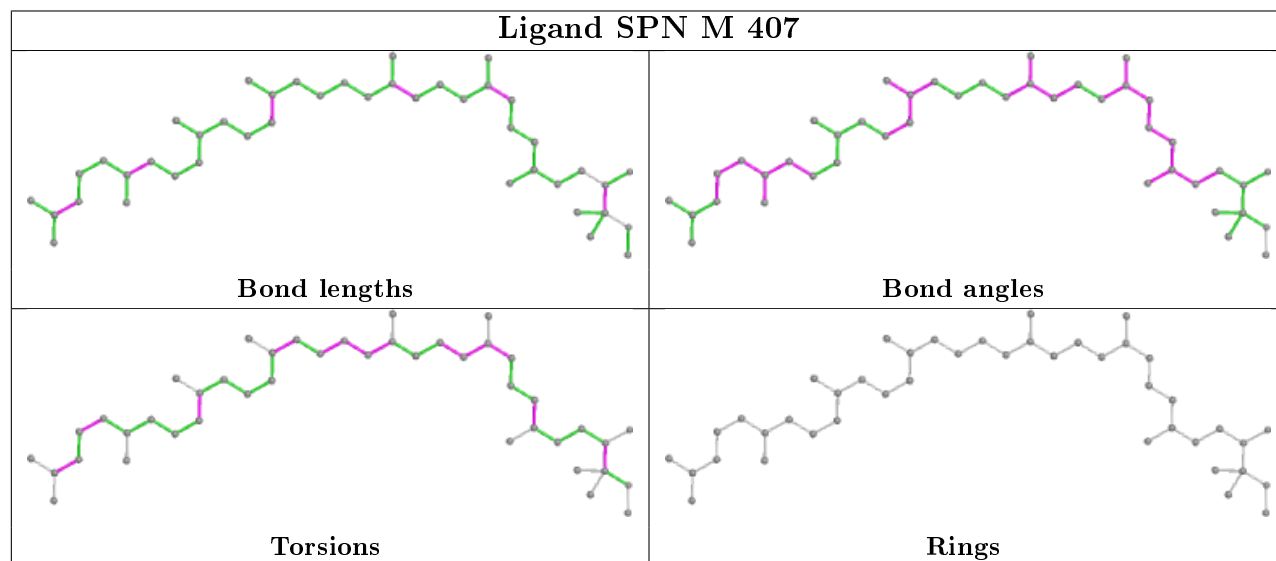
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



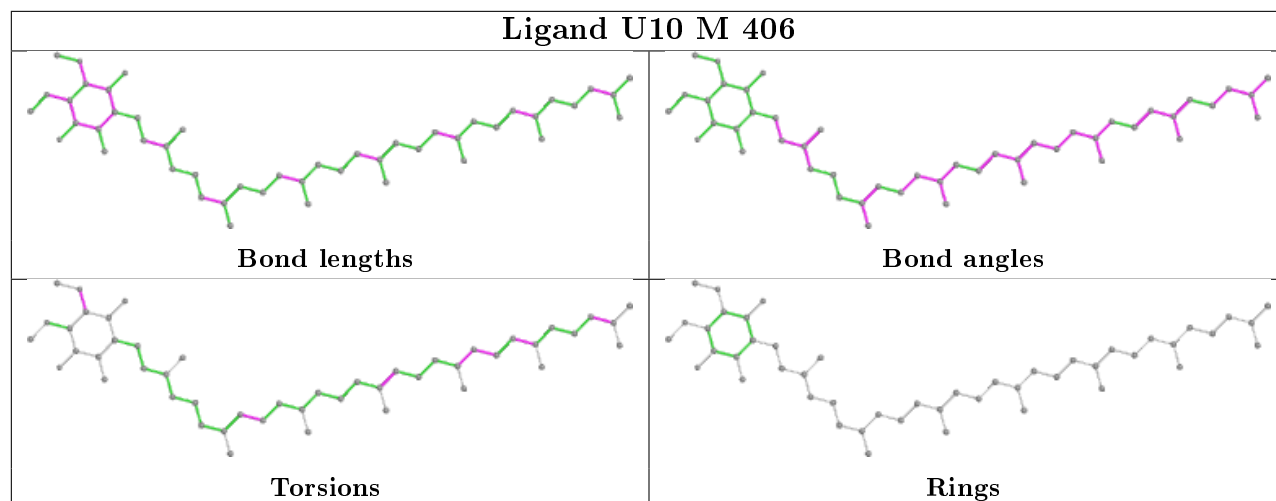
## Ligand BPH L 303



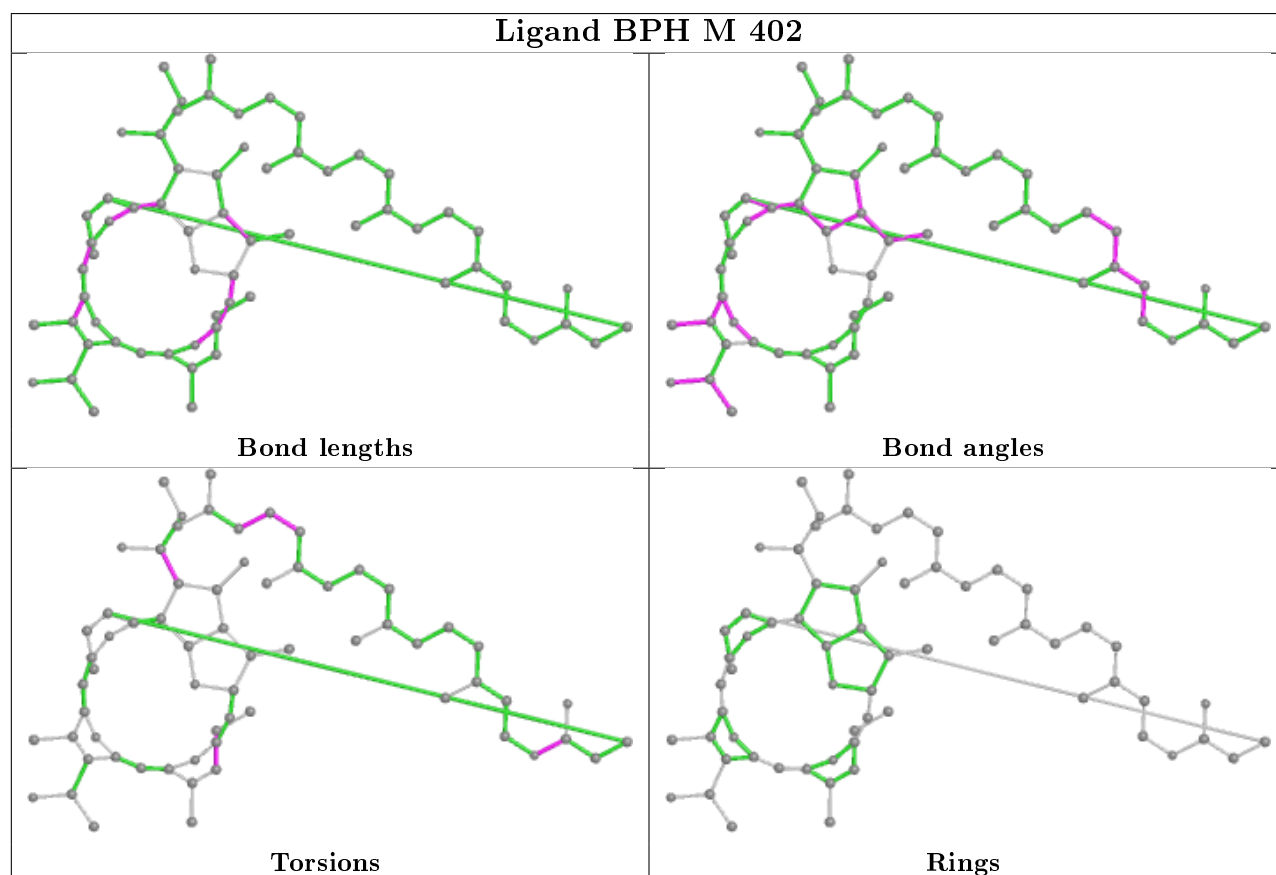
## Ligand SPN M 407

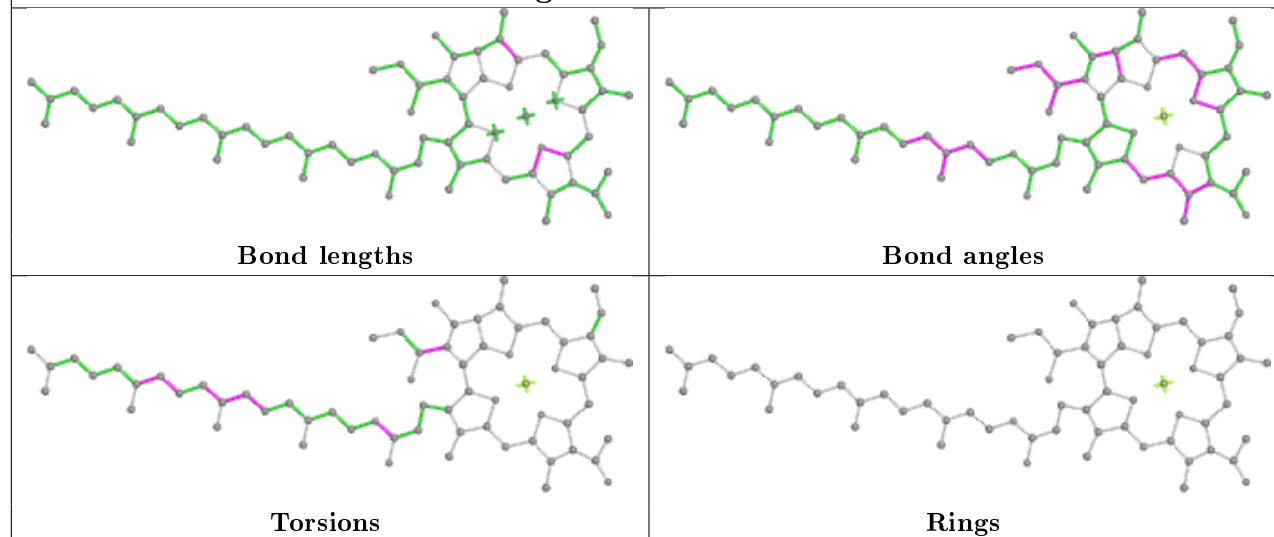
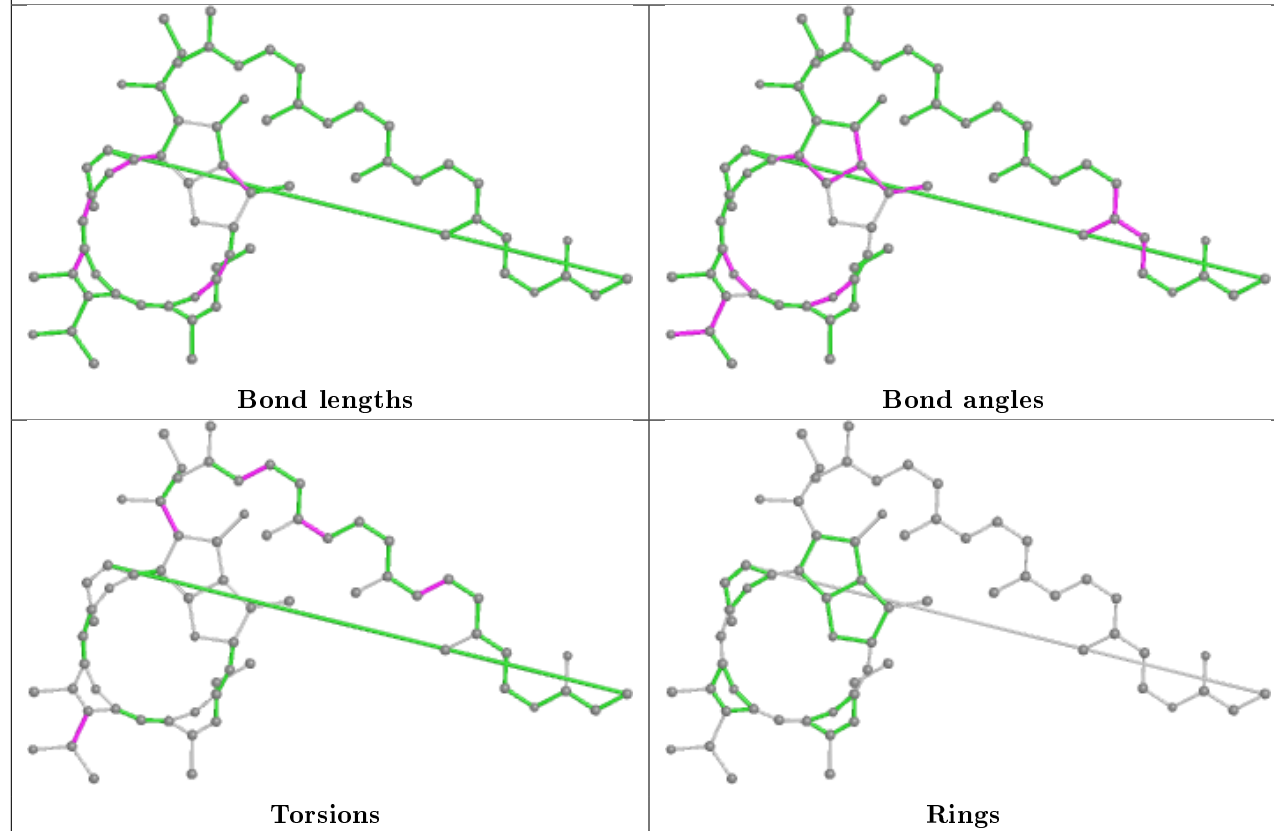


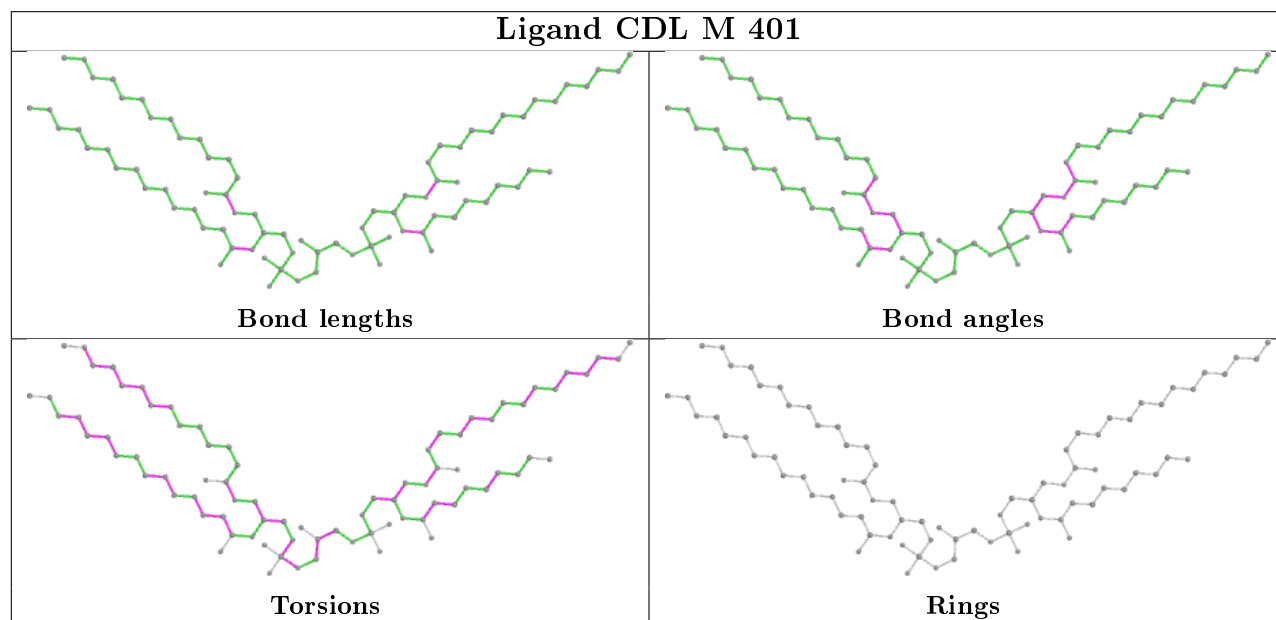
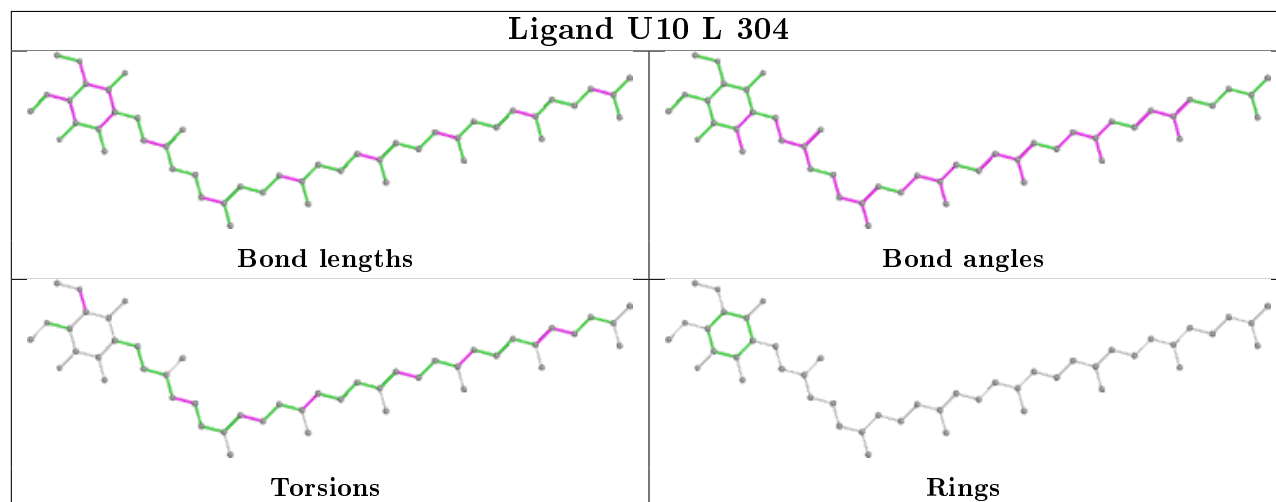
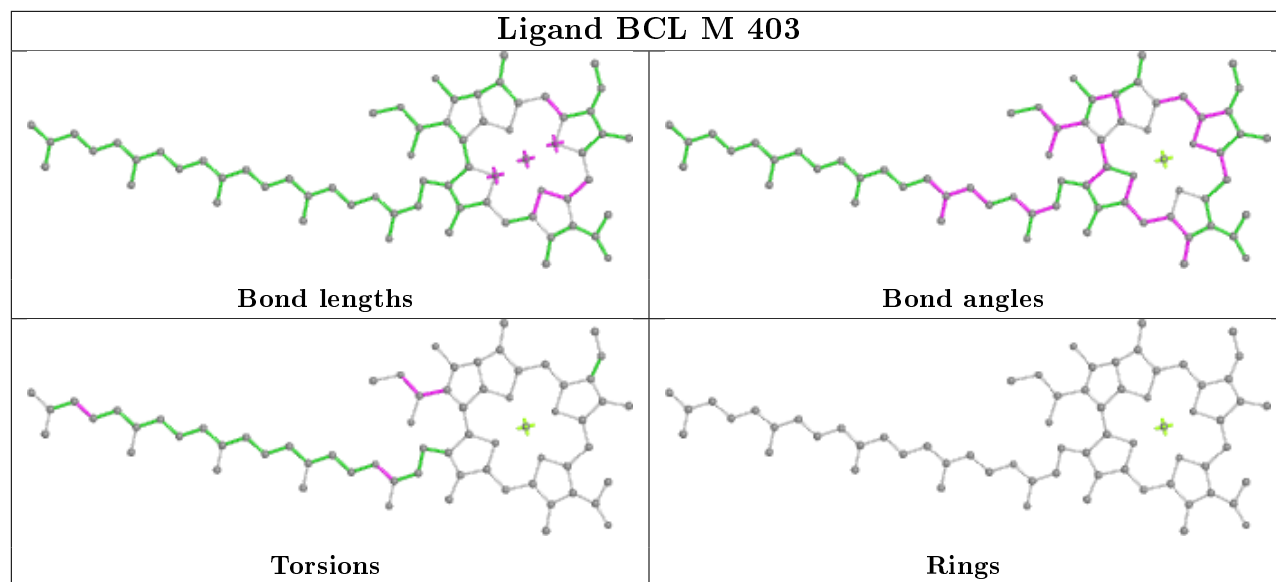
## Ligand U10 M 406



## Ligand BPH M 402



**Ligand BCL L 301****Ligand BPH M 404**



## 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	H	240/260 (92%)	-0.41	4 (1%) 70 69	19, 45, 74, 127	0
2	L	281/282 (99%)	-0.32	3 (1%) 80 80	13, 42, 83, 130	0
3	M	302/303 (99%)	-0.30	2 (0%) 87 87	18, 45, 84, 118	0
All	All	823/845 (97%)	-0.34	9 (1%) 80 80	13, 44, 82, 130	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	4.5
1	H	247	LYS	3.1
3	M	1	ALA	2.7
2	L	82	LYS	2.2
3	M	68	PHE	2.2
2	L	271	TRP	2.2
1	H	161	ALA	2.2
1	H	60	LYS	2.2
2	L	73	TYR	2.1

### 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 carbohydrates 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.

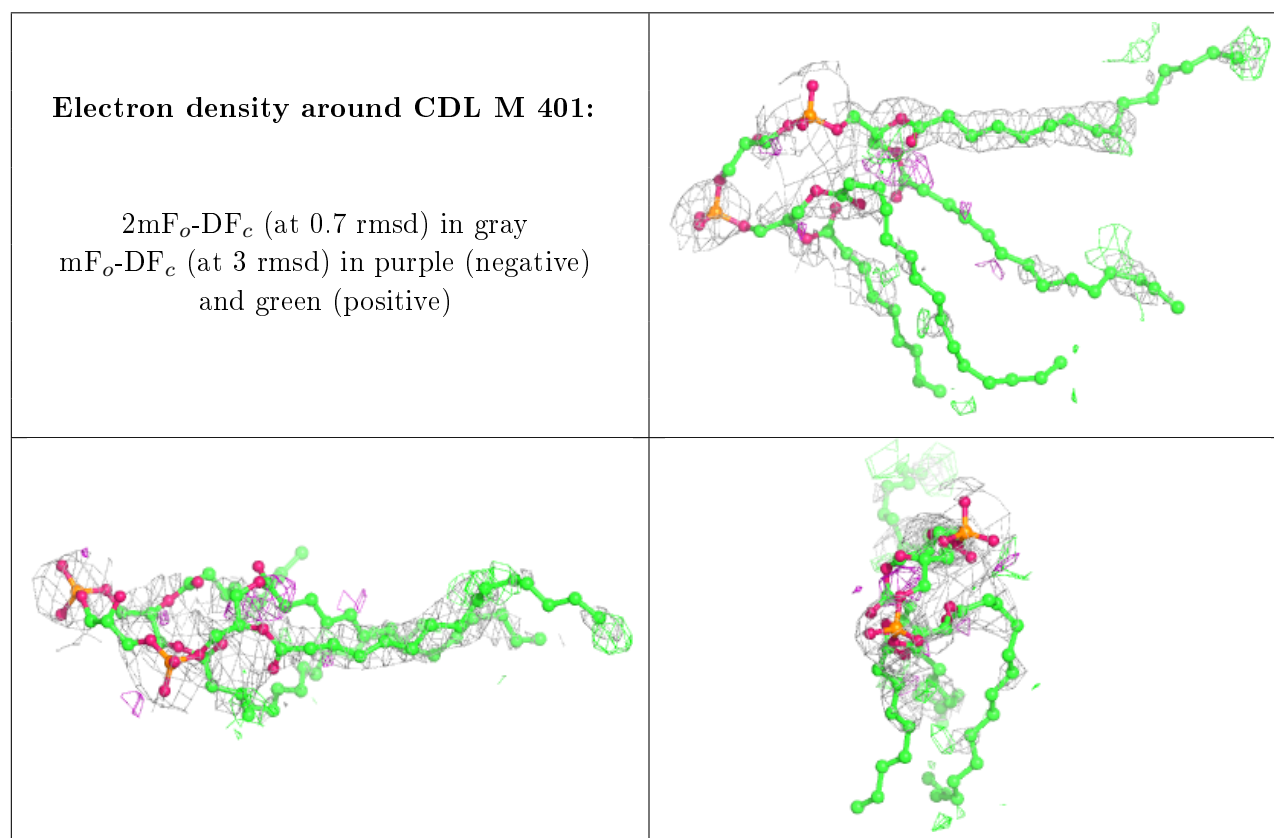
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	LDA	M	411	16/16	0.63	0.93	63,106,135,139	0
8	EDO	H	311	4/4	0.71	0.37	58,60,62,63	0
5	UNL	L	308	12/-	0.73	0.36	39,70,76,79	0
7	DIO	H	307	6/6	0.75	0.60	100,102,102,102	0
5	UNL	L	305	12/-	0.76	0.83	67,78,91,94	0
5	UNL	L	307	10/-	0.76	0.91	53,79,104,107	0
5	UNL	M	414	12/-	0.79	0.32	45,66,80,85	0
4	LDA	M	412	16/16	0.80	0.34	63,87,99,105	0
14	CDL	M	401	81/100	0.80	0.48	58,97,140,158	0
5	UNL	H	304	12/-	0.81	0.51	39,53,80,83	0
5	UNL	M	415	12/-	0.82	0.69	70,82,90,92	0
9	TRS	H	312	8/8	0.83	0.26	76,84,92,102	0
8	EDO	M	419	4/4	0.84	0.29	60,73,77,78	0
9	TRS	L	312	8/8	0.85	0.39	73,77,88,89	0
5	UNL	L	306	12/-	0.85	0.38	35,54,67,68	0
6	PO4	M	416	5/5	0.85	0.13	95,108,121,134	0
5	UNL	M	413	12/-	0.85	0.25	32,47,55,58	0
5	UNL	H	303	12/-	0.85	0.55	43,54,70,73	0
4	LDA	M	410	16/16	0.85	0.29	48,66,88,98	0
6	PO4	M	417	5/5	0.86	0.22	94,102,115,118	0
5	UNL	H	305	12/-	0.86	0.38	54,66,81,82	0
4	LDA	M	409	16/16	0.86	0.46	34,45,80,83	0
7	DIO	L	310	6/6	0.87	0.23	64,68,73,82	0
5	UNL	H	302	12/-	0.87	0.41	53,59,78,82	0
13	U10	L	304	48/63	0.88	0.24	53,70,84,90	0
8	EDO	H	310	4/4	0.88	0.34	61,65,68,70	0
10	K	H	313	1/1	0.88	0.15	64,64,64,64	0
8	EDO	H	308	4/4	0.89	0.18	79,79,82,86	0
6	PO4	H	306	5/5	0.89	0.16	94,105,115,120	0
8	EDO	L	311	4/4	0.90	0.20	68,73,73,81	0
7	DIO	M	418	6/6	0.91	0.36	99,104,105,112	0
13	U10	M	406	48/63	0.91	0.24	28,39,57,64	0
12	BPH	M	404	65/65	0.92	0.26	39,54,101,113	0
16	SPN	M	407	43/43	0.92	0.40	30,52,74,78	0
7	DIO	L	309	6/6	0.93	0.32	34,36,40,46	6
4	LDA	H	301	16/16	0.94	0.18	48,58,63,69	0
12	BPH	L	303	65/65	0.95	0.18	25,31,44,51	0

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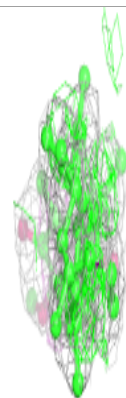
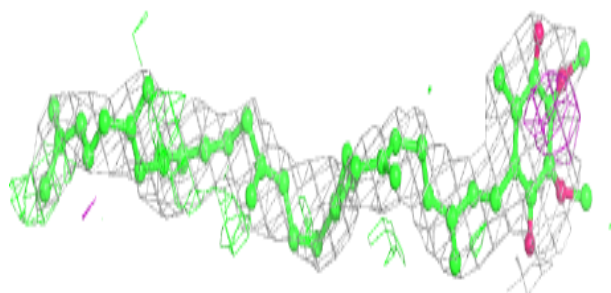
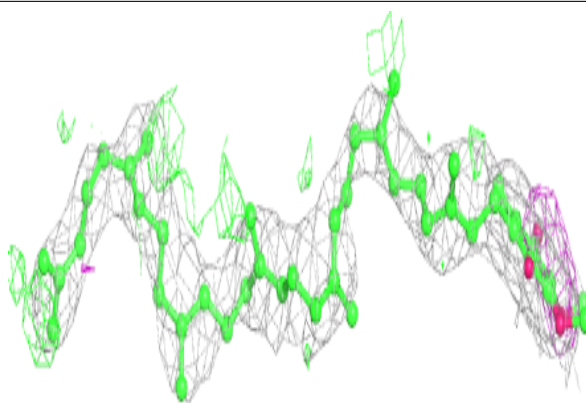
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EDO	H	309	4/4	0.95	0.17	55,56,59,61	0
4	LDA	M	408	16/16	0.95	0.18	45,55,64,66	0
8	EDO	M	420	4/4	0.96	0.19	37,40,46,47	0
11	BCL	L	302	66/66	0.97	0.16	24,32,42,46	0
11	BCL	M	403	66/66	0.97	0.16	19,24,37,41	0
12	BPH	M	402	65/65	0.97	0.16	27,33,55,67	0
11	BCL	L	301	66/66	0.97	0.17	21,34,65,72	0
15	FE	M	405	1/1	1.00	0.15	25,25,25,25	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.

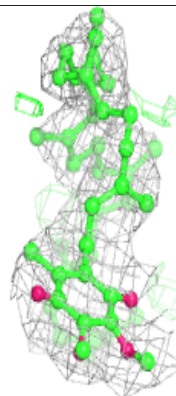
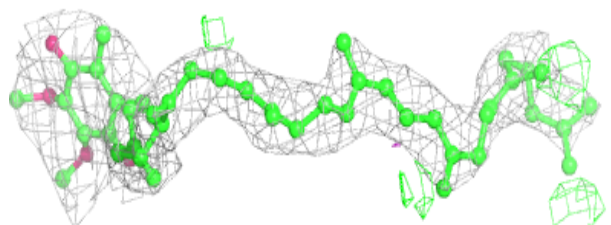
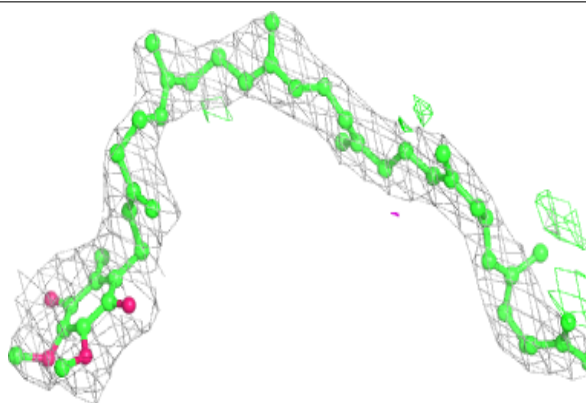


**Electron density around U10 L 304:**

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

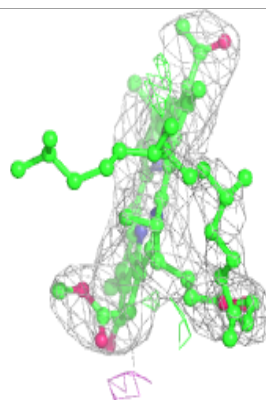
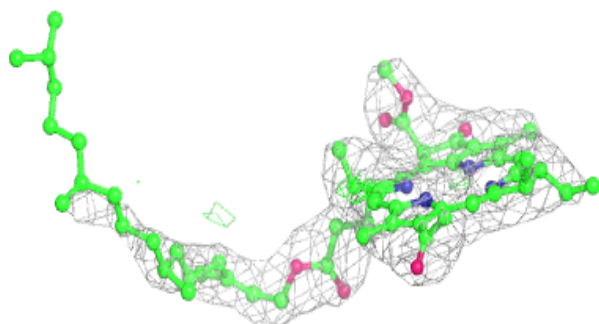
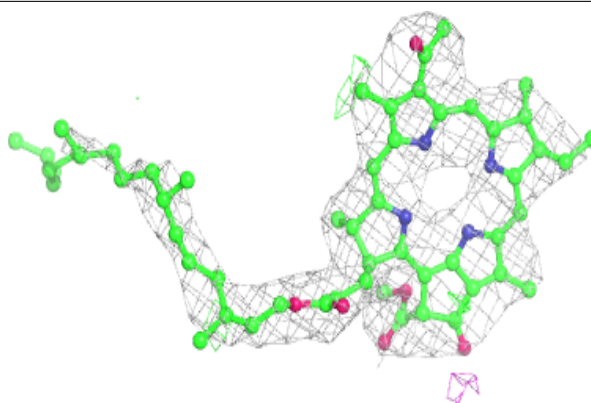
**Electron density around U10 M 406:**

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

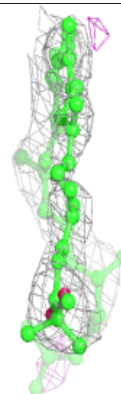
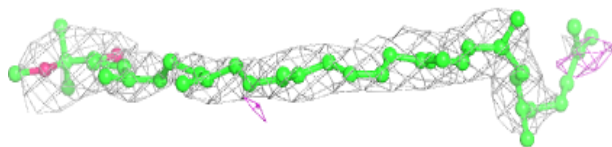
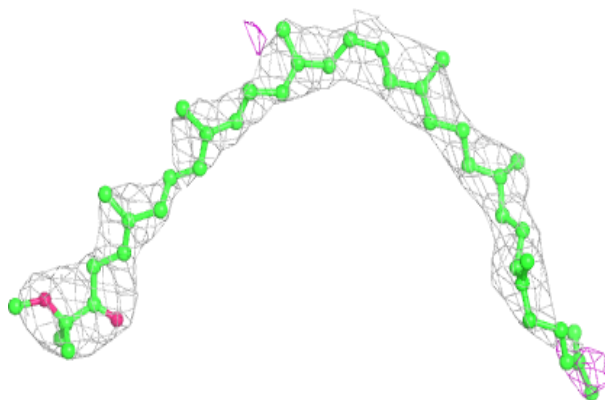


**Electron density around BPH M 404:**

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

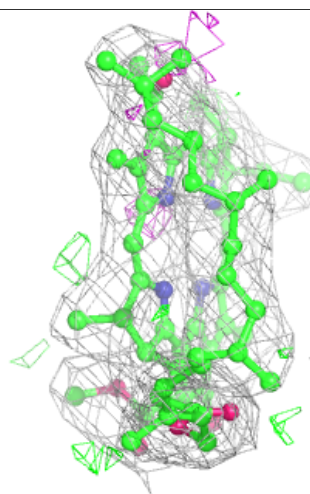
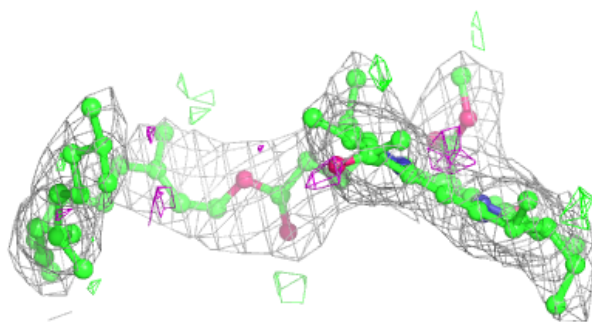
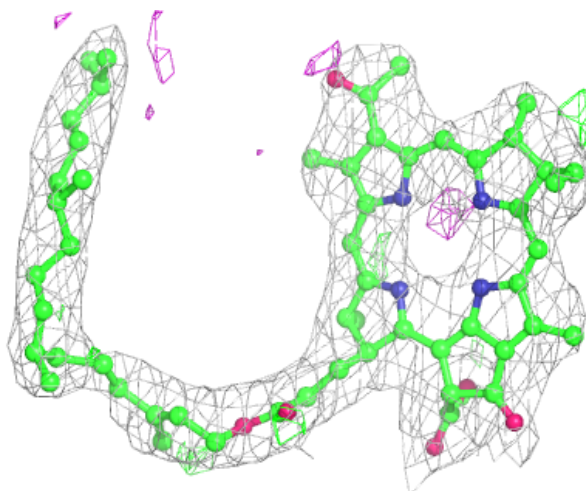
**Electron density around SPN M 407:**

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



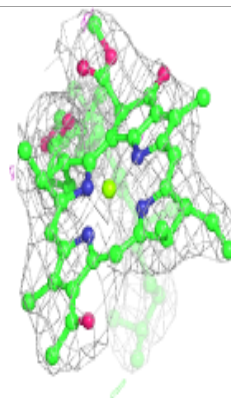
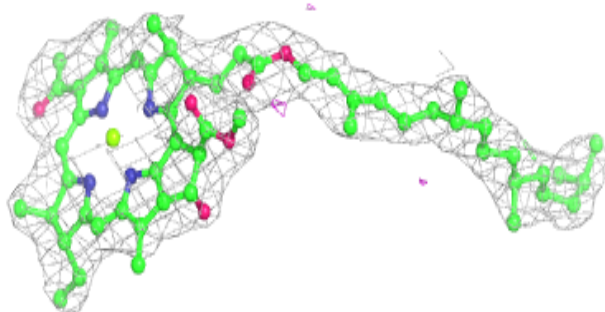
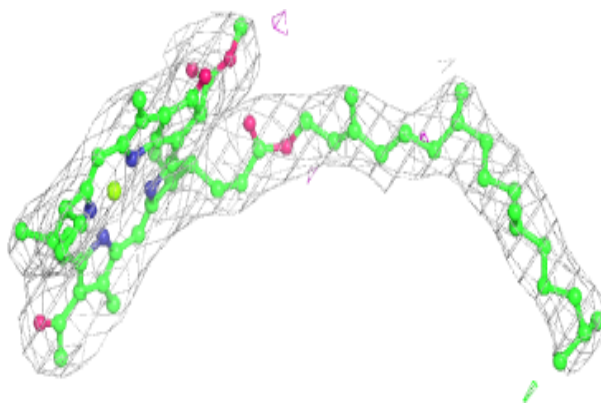
**Electron density around BPH L 303:**

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



**Electron density around BCL L 302:**

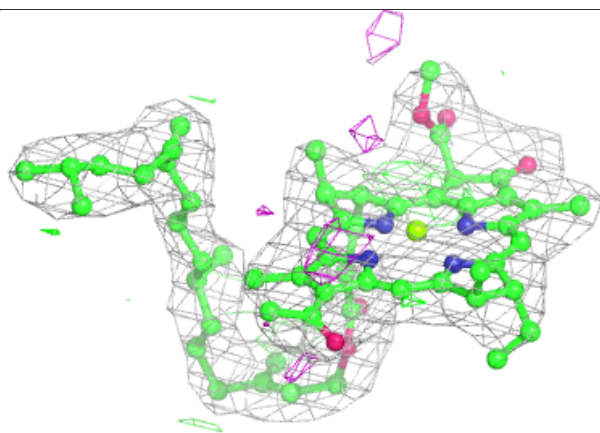
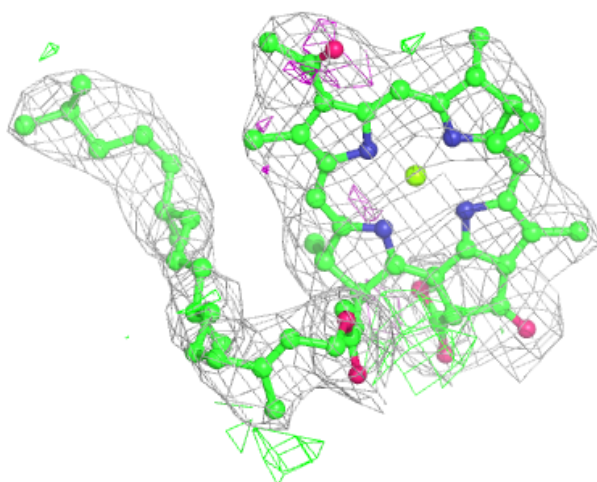
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BCL M 403:**

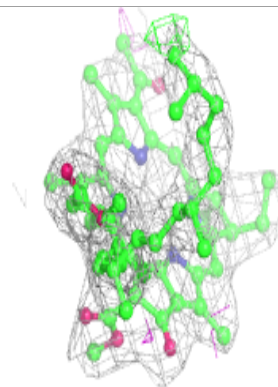
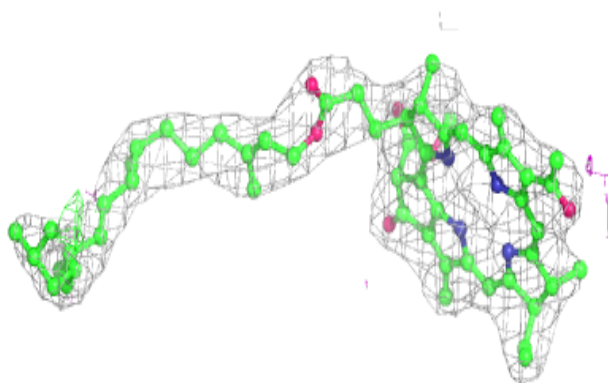
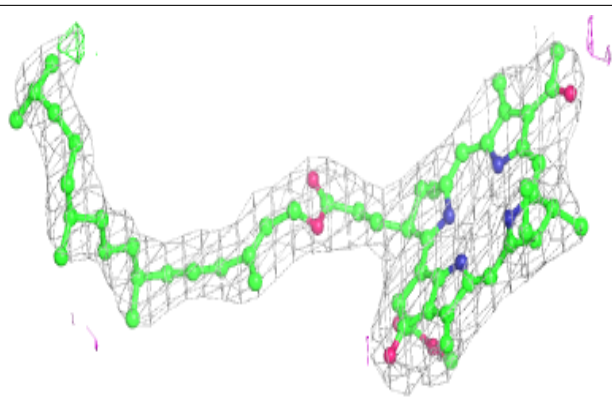
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





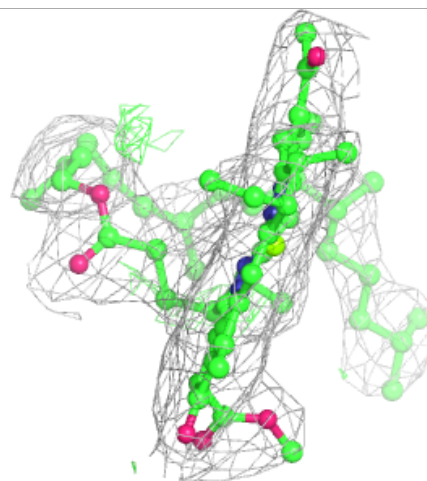
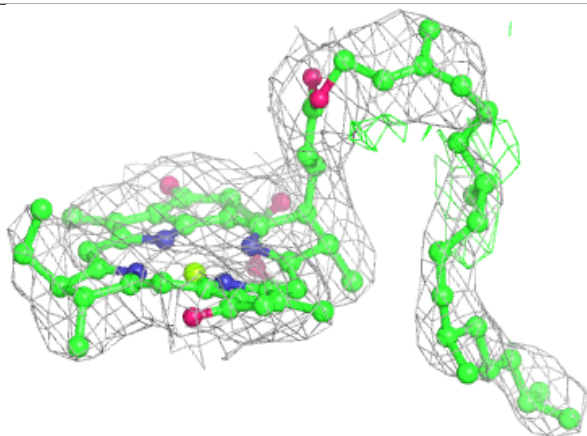
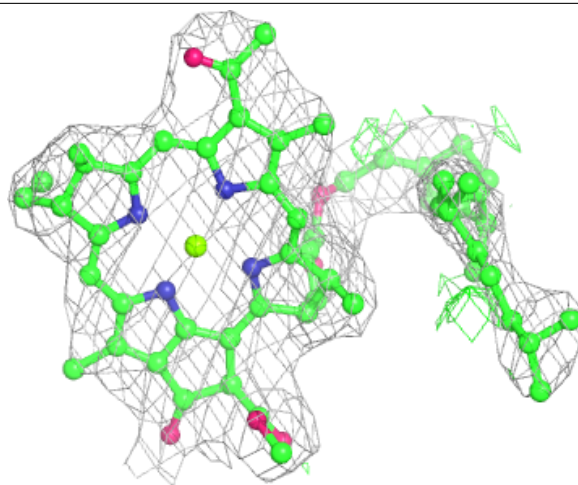
**Electron density around BPH M 402:**

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



**Electron density around BCL L 301:**

$2mF_o-DF_c$  (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.