



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 02:57 AM EST

PDB ID : 4IN7  
Title : (M)L214N mutant of the Rhodobacter sphaeroides Reaction Center  
Authors : Saer, R.G.; Hardjasa, A.; Murphy, M.E.P.; Beatty, J.T.  
Deposited on : 2013-01-04  
Resolution : 2.85 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)  
Xtriage (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

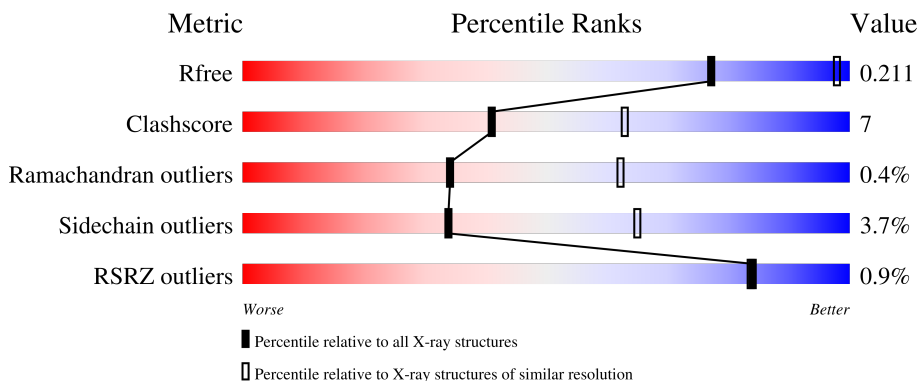
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	266	 2% 77% 11% 10%
2	L	282	 % 89% 10%
3	M	307	 84% 14%

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	HTO	L	309	-	X	-	X
16	PC1	M	410	-	-	-	X
4	GOL	H	303	-	-	-	X
6	GGD	H	307	-	-	-	X
8	LDA	L	302	-	-	-	X
8	LDA	L	303	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7359 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	1849	1183	320	337	9	0	5	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP P0C0Y7
H	-4	HIS	-	expression tag	UNP P0C0Y7
H	-3	HIS	-	expression tag	UNP P0C0Y7
H	-2	HIS	-	expression tag	UNP P0C0Y7
H	-1	HIS	-	expression tag	UNP P0C0Y7
H	0	HIS	-	expression tag	UNP P0C0Y7
H	251	VAL	-	expression tag	UNP P0C0Y7
H	252	VAL	-	expression tag	UNP P0C0Y7
H	253	ALA	-	expression tag	UNP P0C0Y7
H	254	ALA	-	expression tag	UNP P0C0Y7
H	255	MET	-	expression tag	UNP P0C0Y7
H	256	LEU	-	expression tag	UNP P0C0Y7
H	257	ALA	-	expression tag	UNP P0C0Y7
H	258	GLU	-	expression tag	UNP P0C0Y7
H	259	TYR	-	expression tag	UNP P0C0Y7
H	260	ALA	-	expression tag	UNP P0C0Y7

- 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	2239	1513	355	363	8	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	expression tag	UNP P0C0Y8

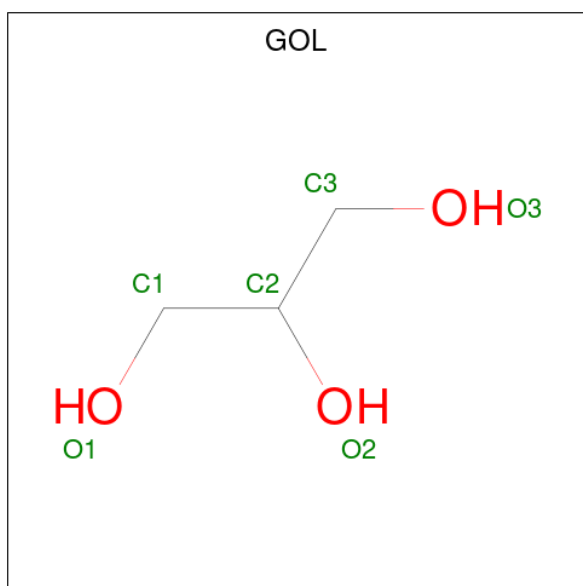
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2410	1605	396	399	10	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	expression tag	UNP P0C0Y9
M	214	ASN	LEU	engineered mutation	UNP P0C0Y9
M	303	MET	-	expression tag	UNP P0C0Y9
M	304	ALA	-	expression tag	UNP P0C0Y9
M	305	PRO	-	expression tag	UNP P0C0Y9
M	306	LEU	-	expression tag	UNP P0C0Y9

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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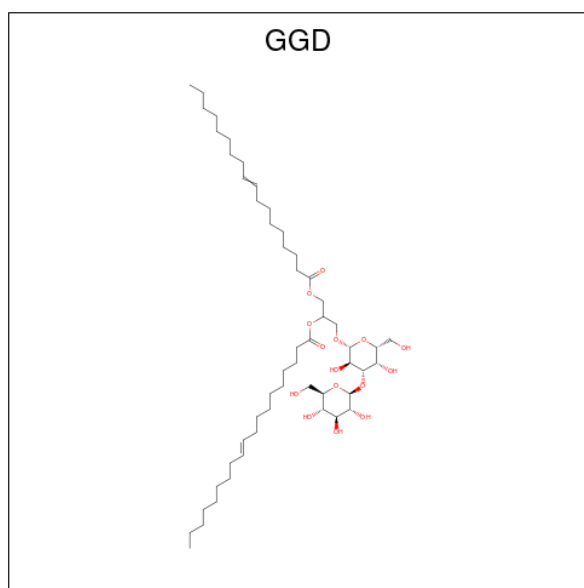
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

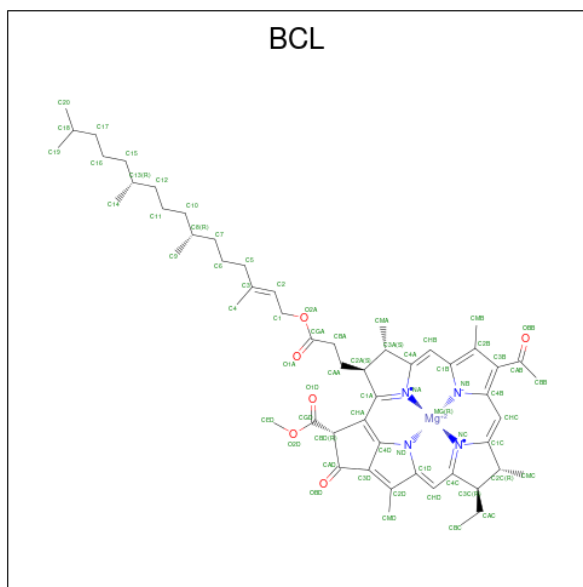
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

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



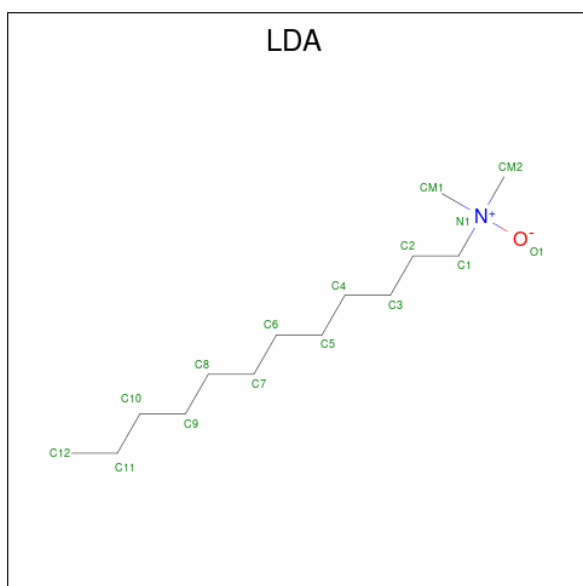
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			57	42	15		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



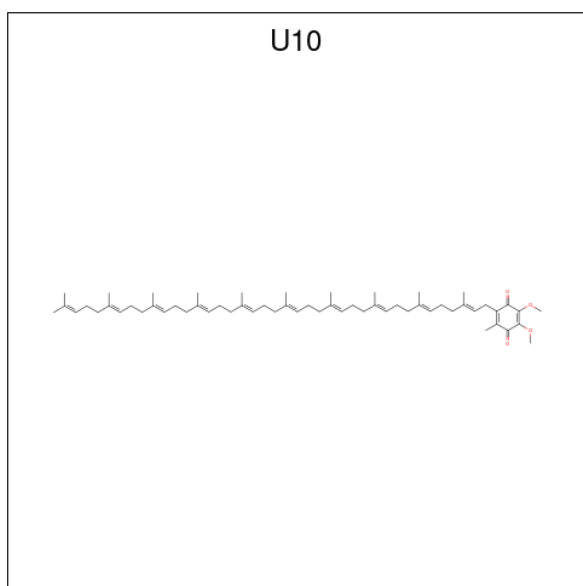
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



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

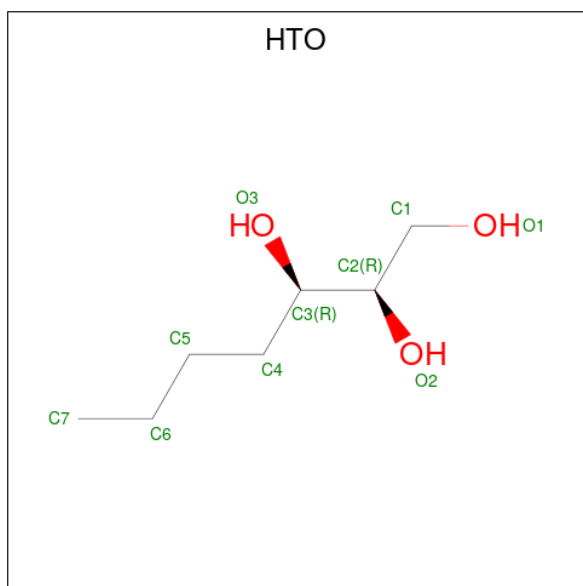
- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





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

- Molecule 11 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).

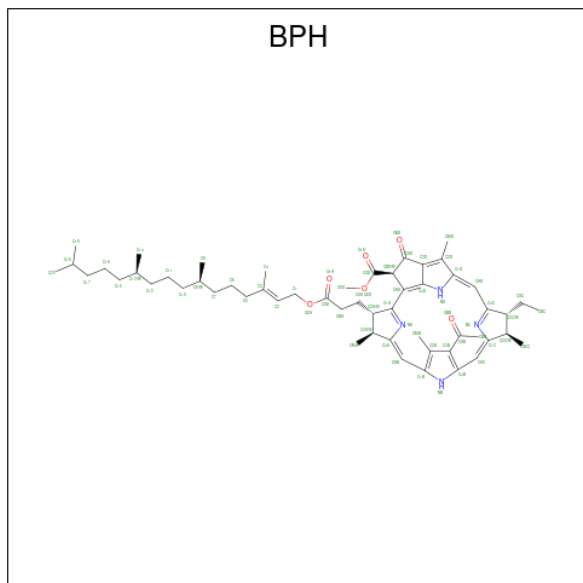


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 10 7 3	0	0
11	L	1	Total C O 10 7 3	0	0

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

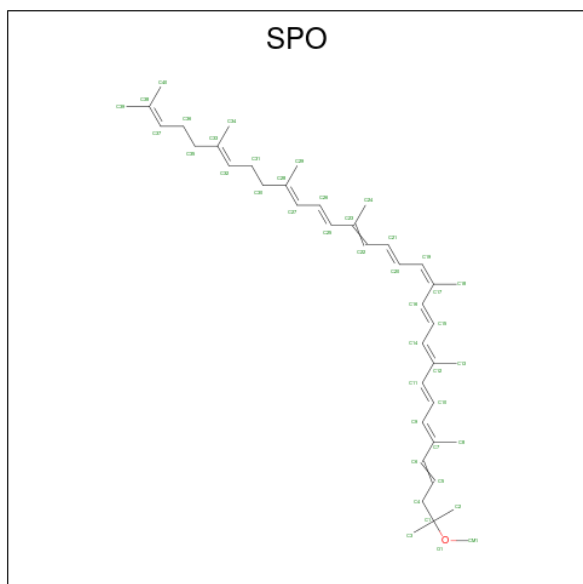
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total Fe 1 1	0	0

- Molecule 13 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



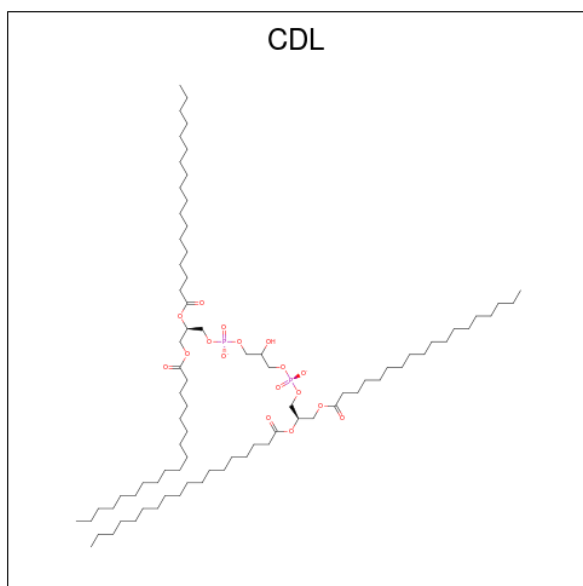
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	M	1	Total 65	C 55	N 4	O 6	0	0
13	M	1	Total 65	C 55	N 4	O 6	0	0

- Molecule 14 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



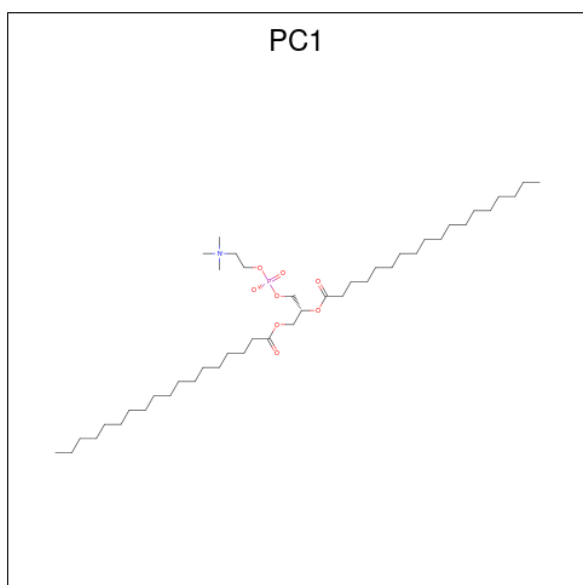
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 16 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



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

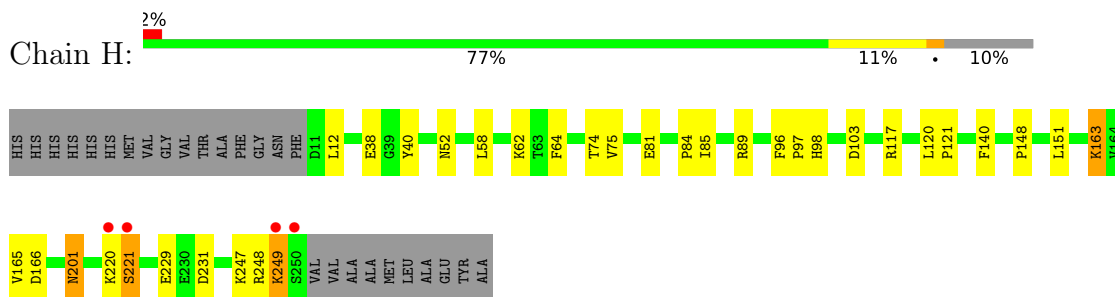
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
17	M	1	1	1	0	0

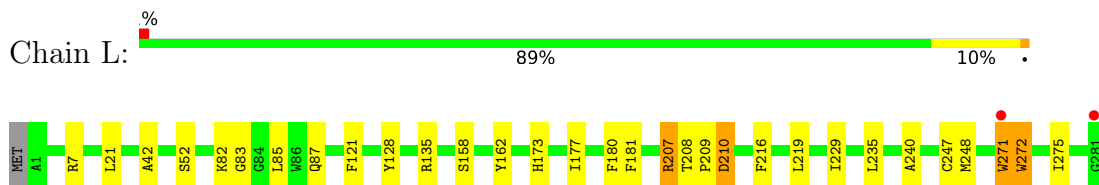
### 3 Residue-property plots [i](#)

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.

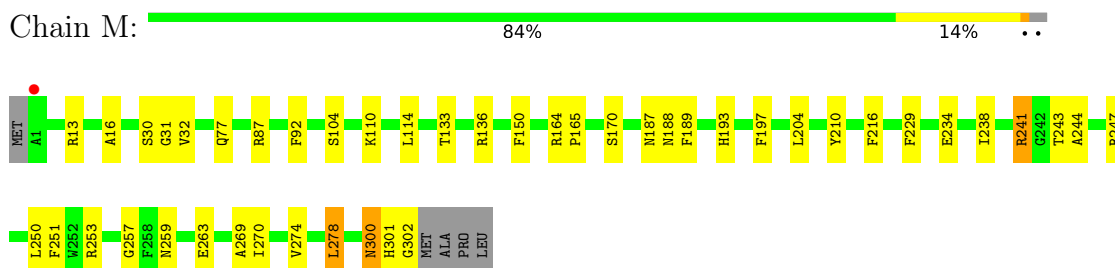
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.14Å 139.14Å 185.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.57 – 2.85 38.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.57-2.85) 99.9 (38.54-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 2.86Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.174 , 0.213 0.179 , 0.211	Depositor DCC
$R_{free}$ test set	2474 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtrriage
Anisotropy	0.042	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: PC1, HTO, K, SPO, GOL, U10, PO4, MG, BCL, CDL, BPH, FE, GGD, LDA

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	0.89	0/1929	1.05	5/2619 (0.2%)
2	L	0.85	0/2339	0.90	5/3203 (0.2%)
3	M	0.86	1/2507 (0.0%)	0.90	3/3422 (0.1%)
All	All	0.86	1/6775 (0.0%)	0.95	13/9244 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	263	GLU	CD-OE1	5.51	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	210	ASP	CB-CG-OD1	7.19	124.77	118.30
2	L	207	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	H	89	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	M	241	ARG	NE-CZ-NH2	6.70	123.65	120.30
3	M	253	ARG	NE-CZ-NH1	-6.66	116.97	120.30
3	M	136	ARG	NE-CZ-NH1	-6.34	117.13	120.30
2	L	207	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	H	117	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	H	89	ARG	NE-CZ-NH1	5.72	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	166	ASP	CB-CG-OD1	5.52	123.27	118.30
1	H	103	ASP	CB-CG-OD2	-5.46	113.38	118.30
2	L	271[A]	TRP	N-CA-CB	5.43	120.37	110.60
2	L	271[B]	TRP	N-CA-CB	5.43	120.37	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1849	0	1873	25	0
2	L	2239	0	2185	24	0
3	M	2410	0	2314	27	0
4	H	30	0	40	0	0
4	L	12	0	16	1	0
5	H	1	0	0	0	0
6	H	57	0	68	3	0
7	L	132	0	148	13	0
7	M	132	0	148	14	0
8	L	48	0	93	2	0
8	M	32	0	62	4	0
9	L	46	0	46	6	0
9	M	48	0	63	1	0
10	L	5	0	0	1	0
11	L	20	0	32	0	0
12	M	1	0	0	0	0
13	M	130	0	150	18	0
14	M	42	0	60	3	0
15	M	81	0	102	1	0
16	M	43	0	60	1	0
17	M	1	0	0	0	0
All	All	7359	0	7460	105	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (105) 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)
13:M:412:BPH:HBB3	13:M:412:BPH:HHC	1.50	0.91
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.63	0.78
13:M:406:BPH:HHC	13:M:406:BPH:HBB3	1.66	0.78
1:H:248:ARG:HA	1:H:249[A]:LYS:HB2	1.68	0.75
1:H:220[B]:LYS:HE2	1:H:221:SER:OG	1.91	0.71
2:L:229:ILE:HD13	9:L:305[B]:U10:H3M2	1.73	0.71
1:H:248:ARG:HA	1:H:249[B]:LYS:HB2	1.73	0.70
7:L:306:BCL:HMB1	7:L:306:BCL:HBB3	1.76	0.68
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.75	0.67
3:M:210:TYR:HB3	13:M:412:BPH:HBB2	1.77	0.67
7:L:306:BCL:HMB1	7:L:306:BCL:CBB	2.24	0.67
1:H:84:PRO:O	1:H:85[A]:ILE:HD13	1.95	0.67
1:H:120:LEU:HB3	1:H:121:PRO:HD2	1.76	0.67
7:M:402:BCL:CBB	7:M:402:BCL:HHC	2.24	0.67
7:L:301:BCL:HBB2	7:L:301:BCL:HHC	1.80	0.63
1:H:201:ASN:H	1:H:201:ASN:HD22	1.45	0.63
7:M:402:BCL:HHC	7:M:402:BCL:HBB2	1.80	0.63
7:M:401:BCL:HBB2	14:M:408:SPO:H243	1.82	0.61
1:H:120:LEU:HB3	1:H:121:PRO:CD	2.30	0.60
3:M:189:PHE:O	3:M:193:HIS:HD2	1.84	0.60
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.84	0.59
1:H:163[A]:LYS:HE2	1:H:165:VAL:HG12	1.83	0.59
13:M:412:BPH:C2	13:M:412:BPH:O1A	2.50	0.59
3:M:31:GLY:N	16:M:410:PC1:O12	2.31	0.57
1:H:220[B]:LYS:HD3	1:H:229:GLU:OE2	2.05	0.57
3:M:270:ILE:O	3:M:274:VAL:HG13	2.03	0.57
2:L:128:TYR:HD1	7:L:301:BCL:HBB1	1.69	0.57
7:M:401:BCL:CBB	7:M:401:BCL:HHC	2.34	0.57
13:M:412:BPH:HHC	13:M:412:BPH:CBB	2.29	0.57
7:M:401:BCL:HBB2	7:M:401:BCL:HHC	1.88	0.55
7:M:401:BCL:H72	7:M:402:BCL:H192	1.89	0.55
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.42	0.55
7:L:306:BCL:C1C	7:M:402:BCL:HBB3	2.38	0.54
2:L:181:PHE:CD2	13:M:406:BPH:HBB1	2.43	0.53
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.91	0.53
2:L:181:PHE:HB3	13:M:406:BPH:HBB2	1.90	0.53
13:M:412:BPH:HBB3	13:M:412:BPH:CHC	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:234:GLU:O	3:M:238:ILE:HG13	2.09	0.52
7:M:401:BCL:C7	7:M:402:BCL:H192	2.40	0.52
7:M:401:BCL:CBB	14:M:408:SPO:H243	2.40	0.52
3:M:300:ASN:O	3:M:302:GLY:N	2.44	0.51
2:L:82:LYS:NZ	10:L:307:PO4:O4	2.40	0.51
9:L:305[B]:U10:H103	8:M:404:LDA:H121	1.93	0.50
2:L:121:PHE:CZ	13:M:412:BPH:HBA2	2.46	0.50
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.45	0.49
1:H:38:GLU:OE1	3:M:241:ARG:NH2	2.46	0.49
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.60	0.49
1:H:52:ASN:ND2	6:H:307:GGD:HA41	2.27	0.49
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.95	0.49
7:M:401:BCL:HMB1	7:M:401:BCL:OBB	2.11	0.49
1:H:62:LYS:HE3	1:H:64:PHE:CZ	2.47	0.49
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.42	0.48
1:H:140:PHE:HA	3:M:13:ARG:O	2.14	0.48
8:L:304:LDA:C12	9:L:305[B]:U10:H1M1	2.43	0.48
7:L:301:BCL:HHC	7:L:301:BCL:CBB	2.43	0.48
2:L:181:PHE:HB3	13:M:406:BPH:CBB	2.44	0.48
2:L:42:ALA:HA	13:M:412:BPH:H9C3	1.95	0.47
3:M:197:PHE:CZ	7:M:402:BCL:HBB2	2.49	0.47
2:L:128:TYR:CD1	7:L:301:BCL:HBB1	2.48	0.47
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.50	0.47
4:L:311:GOL:H12	8:M:403:LDA:O1	2.15	0.47
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.32	0.46
3:M:77:GLN:NE2	3:M:92:PHE:HB3	2.31	0.46
3:M:300:ASN:C	3:M:302:GLY:N	2.69	0.46
13:M:412:BPH:CBB	13:M:412:BPH:CHC	2.91	0.46
1:H:62:LYS:O	1:H:74:THR:HA	2.16	0.45
13:M:406:BPH:HBC2	13:M:406:BPH:HHD	1.99	0.45
3:M:197:PHE:HZ	7:M:402:BCL:HBB2	1.82	0.45
3:M:269:ALA:O	3:M:270:ILE:C	2.55	0.44
1:H:52:ASN:HD21	6:H:307:GGD:HA41	1.83	0.44
7:L:306:BCL:H193	9:M:407:U10:H252	2.00	0.44
3:M:204:LEU:HG	8:M:403:LDA:HM13	1.99	0.44
9:L:305[B]:U10:C10	8:M:404:LDA:H121	2.47	0.44
3:M:251:PHE:CD1	3:M:251:PHE:C	2.90	0.44
7:L:301:BCL:H193	13:M:412:BPH:H7C1	2.00	0.44
1:H:40:TYR:HB3	1:H:58:LEU:HD21	1.98	0.44
2:L:229:ILE:HD13	9:L:305[B]:U10:C3M	2.43	0.44
3:M:243:THR:O	3:M:247:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:402:BCL:HAA2	7:M:402:BCL:HBD	1.98	0.43
3:M:16:ALA:CB	3:M:32:VAL:HG11	2.40	0.43
2:L:83:GLY:O	2:L:87:GLN:HG3	2.19	0.43
7:L:306:BCL:H203	7:L:306:BCL:H161	1.91	0.43
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.54	0.43
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.37	0.43
2:L:52:SER:HB2	2:L:85:LEU:HD13	2.02	0.42
2:L:135:ARG:HD2	2:L:248:MET:O	2.19	0.42
2:L:208:THR:HB	2:L:209:PRO:HD2	2.00	0.42
3:M:274:VAL:O	3:M:278:LEU:HB2	2.19	0.42
13:M:412:BPH:H4C1	13:M:412:BPH:H6C2	1.81	0.42
3:M:150:PHE:N	13:M:406:BPH:HMD3	2.35	0.42
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.00	0.42
13:M:412:BPH:H5C2	13:M:412:BPH:H1C1	1.82	0.42
15:M:409:CDL:C36	15:M:409:CDL:C34	2.97	0.42
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.55	0.41
8:L:304:LDA:H122	9:L:305[B]:U10:H1M1	2.02	0.41
2:L:219:LEU:HD11	3:M:133:THR:HG22	2.03	0.41
1:H:248:ARG:HA	1:H:249[B]:LYS:HB3	1.96	0.41
7:L:301:BCL:HBC1	7:L:306:BCL:CGA	2.51	0.41
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.90	0.41
7:L:301:BCL:C2B	13:M:412:BPH:H202	2.51	0.41
7:L:306:BCL:NC	7:M:402:BCL:HBB3	2.35	0.41
14:M:408:SPO:H181	14:M:408:SPO:H20	1.86	0.40
6:H:307:GGD:HC62	3:M:257:GLY:O	2.21	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	244/266 (92%)	231 (95%)	11 (4%)	2 (1%)	19 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	281/282 (100%)	265 (94%)	16 (6%)	0	100	100
3	M	301/307 (98%)	288 (96%)	11 (4%)	2 (1%)	22	50
All	All	826/855 (97%)	784 (95%)	38 (5%)	4 (0%)	34	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	30	SER
3	M	301	HIS

### 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	200/214 (94%)	192 (96%)	8 (4%)	31	62
2	L	221/221 (100%)	211 (96%)	10 (4%)	27	57
3	M	237/240 (99%)	229 (97%)	8 (3%)	37	67
All	All	658/675 (98%)	632 (96%)	26 (4%)	34	62

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	75	VAL
1	H	163[A]	LYS
1	H	163[B]	LYS
1	H	201	ASN
1	H	221	SER
1	H	231	ASP
1	H	247	LYS
2	L	21	LEU
2	L	158	SER

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Mol	Chain	Res	Type
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	247	CYS
2	L	271[A]	TRP
2	L	271[B]	TRP
2	L	272	TRP
3	M	104	SER
3	M	110	LYS
3	M	114	LEU
3	M	170	SER
3	M	188	ASN
3	M	216	PHE
3	M	259	ASN
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	32	GLN
1	H	98	HIS
1	H	201	ASN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	U10	M	407	-	48,48,63	1.35	5 (10%)	58,61,79	2.29	16 (27%)
4	GOL	H	303	-	5,5,5	0.57	0	5,5,5	0.64	0
10	PO4	L	307	-	4,4,4	1.18	1 (25%)	6,6,6	0.82	0
16	PC1	M	410	-	42,42,53	1.51	4 (9%)	48,50,61	1.49	6 (12%)
13	BPH	M	412	-	51,70,70	1.87	9 (17%)	52,101,101	2.42	18 (34%)
9	U10	L	305[A]	-	23,23,63	1.80	2 (8%)	28,31,79	1.58	6 (21%)
4	GOL	H	306	-	5,5,5	1.13	0	5,5,5	1.02	0
8	LDA	L	304	-	12,15,15	2.17	1 (8%)	14,17,17	0.80	0
11	HTO	L	309	-	9,9,9	1.52	3 (33%)	10,10,10	1.98	4 (40%)
4	GOL	L	310	-	5,5,5	0.46	0	5,5,5	0.51	0
4	GOL	H	304	-	5,5,5	0.80	0	5,5,5	0.75	0
11	HTO	L	308	-	9,9,9	1.32	2 (22%)	10,10,10	1.22	0
6	GGD	H	307	-	58,58,68	1.15	3 (5%)	72,72,82	1.68	14 (19%)
7	BCL	M	402	-	64,74,74	1.63	12 (18%)	78,115,115	2.10	19 (24%)
4	GOL	H	301	-	5,5,5	0.78	0	5,5,5	1.10	0
8	LDA	L	303	-	12,15,15	2.27	1 (8%)	14,17,17	0.79	1 (7%)
7	BCL	L	306	-	64,74,74	1.72	10 (15%)	78,115,115	1.91	21 (26%)
8	LDA	M	404	-	12,15,15	2.10	1 (8%)	14,17,17	0.56	0
9	U10	L	305[B]	-	23,23,63	2.07	2 (8%)	28,31,79	1.47	5 (17%)
14	SPO	M	408	-	40,41,41	0.81	1 (2%)	47,50,50	1.68	11 (23%)
15	CDL	M	409	-	79,79,99	1.52	5 (6%)	84,90,111	1.43	8 (9%)
13	BPH	M	406	-	51,70,70	1.80	9 (17%)	52,101,101	2.16	14 (26%)
4	GOL	H	302	-	5,5,5	0.49	0	5,5,5	0.65	0
8	LDA	M	403	-	12,15,15	2.25	1 (8%)	14,17,17	0.91	1 (7%)
7	BCL	L	301	-	64,74,74	1.60	14 (21%)	78,115,115	2.41	32 (41%)
4	GOL	L	311	-	5,5,5	0.36	0	5,5,5	0.34	0
8	LDA	L	302	-	12,15,15	2.14	1 (8%)	14,17,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BCL	M	401	-	64,74,74	1.75	14 (21%)	78,115,115	2.17	25 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	U10	M	407	-	-	9/45/69/87	0/1/1/1
4	GOL	H	303	-	-	2/4/4/4	-
16	PC1	M	410	-	-	24/46/46/57	-
13	BPH	M	412	-	-	9/37/105/105	0/5/6/6
9	U10	L	305[A]	-	-	1/15/39/87	0/1/1/1
4	GOL	H	306	-	-	2/4/4/4	-
8	LDA	L	304	-	-	8/13/13/13	-
11	HTO	L	309	-	-	5/10/10/10	-
4	GOL	L	310	-	-	4/4/4/4	-
4	GOL	H	304	-	-	2/4/4/4	-
11	HTO	L	308	-	-	5/10/10/10	-
6	GGD	H	307	-	-	20/47/87/97	0/2/2/2
7	BCL	M	402	-	-	6/37/137/137	-
4	GOL	H	301	-	-	2/4/4/4	-
8	LDA	L	303	-	-	7/13/13/13	-
7	BCL	L	306	-	-	4/37/137/137	-
8	LDA	M	404	-	-	7/13/13/13	-
9	U10	L	305[B]	-	-	3/15/39/87	0/1/1/1
14	SPO	M	408	-	-	4/47/47/47	-
15	CDL	M	409	-	-	49/88/88/110	-
13	BPH	M	406	-	-	17/37/105/105	0/5/6/6
4	GOL	H	302	-	-	2/4/4/4	-
8	LDA	M	403	-	-	7/13/13/13	-
7	BCL	L	301	-	-	5/37/137/137	-
4	GOL	L	311	-	-	4/4/4/4	-
8	LDA	L	302	-	-	6/13/13/13	-
7	BCL	M	401	-	-	13/37/137/137	-

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	305[B]	U10	C6-C1	8.47	1.50	1.35
9	L	305[A]	U10	C6-C1	7.66	1.49	1.35
8	L	303	LDA	O1-N1	-7.45	1.24	1.42
8	L	304	LDA	O1-N1	-7.32	1.25	1.42
8	M	403	LDA	O1-N1	-7.12	1.25	1.42
8	M	404	LDA	O1-N1	-7.06	1.25	1.42
8	L	302	LDA	O1-N1	-6.98	1.25	1.42
13	M	412	BPH	C3A-C2A	-6.25	1.49	1.54
13	M	412	BPH	OBD-CAD	6.01	1.30	1.22
16	M	410	PC1	O31-C31	5.94	1.50	1.33
7	L	306	BCL	C1D-ND	-5.83	1.30	1.37
13	M	406	BPH	C2C-C3C	-5.66	1.49	1.54
15	M	409	CDL	OB6-CB5	5.61	1.50	1.34
15	M	409	CDL	OA6-CA5	5.53	1.49	1.34
9	M	407	U10	C6-C1	5.34	1.44	1.35
15	M	409	CDL	OA8-CA7	5.32	1.48	1.33
16	M	410	PC1	O21-C21	5.24	1.49	1.34
7	M	401	BCL	O2A-CGA	5.08	1.48	1.33
7	M	401	BCL	OBD-CAD	4.87	1.30	1.22
13	M	412	BPH	CHA-CBD	-4.85	1.46	1.52
13	M	406	BPH	C3D-C2D	4.83	1.48	1.39
7	M	402	BCL	C1D-ND	-4.76	1.31	1.37
7	L	301	BCL	O2A-CGA	4.69	1.47	1.33
15	M	409	CDL	OB8-CB7	4.66	1.47	1.33
7	L	301	BCL	O2D-CGD	4.65	1.44	1.33
13	M	406	BPH	O2A-CGA	4.42	1.46	1.33
7	L	306	BCL	C3D-C4D	-4.41	1.34	1.44
7	M	402	BCL	C3D-C4D	-4.35	1.34	1.44
7	L	306	BCL	O2D-CGD	4.30	1.43	1.33
6	H	307	GGD	OC6-CC5	4.16	1.46	1.34
13	M	412	BPH	C3D-C2D	4.14	1.46	1.39
7	M	401	BCL	C3B-C2B	4.06	1.46	1.39
7	M	402	BCL	O2D-CGD	4.03	1.43	1.33
7	M	401	BCL	C3D-C4D	-4.01	1.35	1.44
7	L	306	BCL	C3C-C4C	-3.96	1.46	1.51
6	H	307	GGD	OC8-CC7	3.96	1.44	1.33
7	L	301	BCL	C3B-C2B	3.91	1.46	1.39
13	M	406	BPH	CHA-CBD	-3.79	1.47	1.52
7	L	301	BCL	C1D-ND	-3.66	1.33	1.37
7	M	402	BCL	O2A-CGA	3.66	1.44	1.33
13	M	406	BPH	C3B-C2B	3.60	1.45	1.39
7	M	402	BCL	OBD-CAD	3.59	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	306	BCL	C3B-C2B	3.56	1.45	1.39
7	M	401	BCL	O2D-CGD	3.50	1.41	1.33
7	M	402	BCL	C3B-C2B	3.50	1.45	1.39
7	L	306	BCL	O2A-CGA	3.48	1.43	1.33
7	L	306	BCL	OBD-CAD	3.37	1.28	1.22
13	M	412	BPH	O2A-CGA	3.36	1.43	1.33
7	M	401	BCL	C3D-C2D	3.35	1.48	1.39
9	L	305[B]	U10	C4-C3	3.27	1.49	1.36
7	M	402	BCL	CHD-C1D	3.20	1.44	1.38
13	M	406	BPH	O2D-CGD	3.12	1.40	1.33
9	M	407	U10	C31-C29	3.04	1.57	1.51
7	L	306	BCL	MG-ND	-3.04	1.99	2.05
7	M	401	BCL	CHD-C1D	3.01	1.44	1.38
13	M	412	BPH	C3B-C2B	2.97	1.44	1.39
9	M	407	U10	C4-C3	2.90	1.48	1.36
7	L	301	BCL	C3D-C2D	2.89	1.47	1.39
11	L	309	HTO	C4-C3	2.86	1.57	1.52
7	M	401	BCL	C1D-ND	-2.81	1.34	1.37
7	M	401	BCL	C1B-CHB	2.80	1.48	1.41
6	H	307	GGD	OA1-CA1	2.79	1.44	1.40
7	L	301	BCL	C3D-C4D	-2.74	1.38	1.44
7	L	306	BCL	MG-NA	-2.74	1.99	2.06
16	M	410	PC1	C3-C2	2.67	1.58	1.50
7	L	301	BCL	CHD-C4C	2.67	1.46	1.39
9	L	305[A]	U10	C4-C3	2.65	1.47	1.36
11	L	308	HTO	C4-C3	2.61	1.57	1.52
13	M	406	BPH	OBD-CAD	2.58	1.25	1.22
7	M	401	BCL	MG-NA	-2.49	2.00	2.06
7	L	301	BCL	OBD-CAD	2.47	1.26	1.22
7	L	301	BCL	CHD-C1D	2.43	1.43	1.38
14	M	408	SPO	C25-C23	2.43	1.51	1.45
13	M	412	BPH	O2D-CGD	2.39	1.39	1.33
7	L	301	BCL	C1B-CHB	2.39	1.47	1.41
7	M	402	BCL	C2C-C3C	-2.38	1.47	1.54
15	M	409	CDL	CA3-CA4	2.37	1.58	1.50
13	M	406	BPH	C3A-C2A	-2.34	1.52	1.54
9	M	407	U10	C18-C19	2.33	1.38	1.33
7	L	301	BCL	MG-NA	-2.31	2.00	2.06
7	M	401	BCL	CHD-C4C	2.26	1.45	1.39
7	M	401	BCL	C1B-NB	2.26	1.37	1.35
10	L	307	PO4	P-O4	-2.25	1.47	1.54
7	M	402	BCL	C4D-CHA	2.25	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	412	BPH	O1D-CGD	2.24	1.26	1.21
7	L	301	BCL	C2C-C3C	-2.21	1.48	1.54
7	M	401	BCL	CMB-C2B	-2.15	1.47	1.51
11	L	309	HTO	C3-C2	2.11	1.58	1.52
13	M	406	BPH	C1-C2	2.11	1.55	1.49
7	M	402	BCL	MG-NC	-2.11	2.01	2.06
11	L	309	HTO	C1-C2	2.08	1.57	1.52
7	M	401	BCL	MG-NC	-2.05	2.01	2.06
13	M	412	BPH	CBD-CGD	-2.04	1.49	1.52
11	L	308	HTO	C3-C2	2.03	1.58	1.52
9	M	407	U10	C33-C34	2.03	1.37	1.33
7	M	402	BCL	CHD-C4C	2.02	1.44	1.39
16	M	410	PC1	C1-C2	2.02	1.56	1.50
7	L	306	BCL	C3D-C2D	2.01	1.44	1.39
7	L	301	BCL	C4D-CHA	2.01	1.45	1.38
7	L	301	BCL	MG-NC	-2.01	2.01	2.06
7	M	402	BCL	CMB-C2B	-2.00	1.47	1.51

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	407	U10	C30-C29-C31	10.06	132.20	115.27
13	M	412	BPH	O1D-CGD-CBD	8.10	138.23	124.74
7	L	301	BCL	O2D-CGD-CBD	7.66	124.87	111.27
7	L	301	BCL	C2D-C1D-ND	6.59	114.96	110.10
7	M	402	BCL	C1C-NC-C4C	-6.51	103.78	106.71
15	M	409	CDL	OB6-CB5-C51	6.37	125.23	111.50
13	M	412	BPH	CED-O2D-CGD	-6.34	101.60	115.94
9	M	407	U10	C31-C29-C28	-6.17	108.64	121.12
7	L	306	BCL	CMD-C2D-C1D	5.97	135.23	124.71
7	M	402	BCL	CMD-C2D-C1D	5.78	134.91	124.71
13	M	406	BPH	CAC-C3C-C4C	5.35	125.69	113.73
16	M	410	PC1	O21-C21-C22	5.33	122.99	111.50
15	M	409	CDL	OA6-CA5-C11	5.23	122.78	111.50
7	M	401	BCL	CHD-C4C-NC	5.07	130.71	125.08
7	M	401	BCL	CHD-C1D-ND	-5.03	119.83	124.45
7	M	401	BCL	O2A-C1-C2	5.03	121.85	108.64
7	M	402	BCL	C2D-C1D-ND	5.02	113.81	110.10
6	H	307	GGD	OC6-CC5-C14	5.01	122.30	111.50
7	L	306	BCL	C2D-C1D-ND	4.93	113.73	110.10
13	M	406	BPH	O2D-CGD-CBD	4.91	117.22	111.00
7	M	401	BCL	O2D-CGD-CBD	4.91	119.99	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	307	GGD	CA1-OA5-CA5	4.91	123.32	113.69
6	H	307	GGD	OB1-CA3-CA2	4.90	120.30	107.28
7	L	301	BCL	C1C-NC-C4C	-4.80	104.55	106.71
7	M	401	BCL	CMD-C2D-C1D	4.76	133.09	124.71
7	L	306	BCL	CHD-C1D-ND	-4.68	120.16	124.45
7	M	402	BCL	CHD-C1D-ND	-4.60	120.23	124.45
7	L	306	BCL	C3C-C4C-CHD	-4.57	113.62	123.39
13	M	406	BPH	C3D-CAD-CBD	4.57	113.62	107.61
7	M	402	BCL	C3C-C4C-CHD	-4.52	113.73	123.39
13	M	412	BPH	CAC-C3C-C4C	-4.49	103.70	113.73
6	H	307	GGD	CC4-OC6-CC5	-4.45	106.84	117.79
7	M	401	BCL	C3C-C4C-CHD	-4.41	113.97	123.39
7	L	301	BCL	CMD-C2D-C1D	4.39	132.45	124.71
13	M	412	BPH	CAA-CBA-CGA	-4.37	100.48	113.25
7	L	301	BCL	C3D-C2D-C1D	-4.36	99.88	105.83
7	L	301	BCL	O2D-CGD-O1D	-4.35	115.32	123.84
7	L	301	BCL	C3C-C4C-CHD	-4.32	114.17	123.39
9	M	407	U10	C26-C27-C28	-4.31	97.71	111.88
9	M	407	U10	C32-C31-C29	4.30	127.13	112.98
7	M	401	BCL	C1C-NC-C4C	-4.30	104.77	106.71
7	L	301	BCL	CHD-C4C-NC	4.30	129.85	125.08
7	L	301	BCL	OBD-CAD-C3D	-4.29	118.19	128.52
13	M	412	BPH	O2D-CGD-O1D	-4.29	115.45	123.84
13	M	406	BPH	OBD-CAD-CBD	-4.29	119.53	125.82
7	M	402	BCL	C4A-NA-C1A	4.24	108.61	106.71
6	H	307	GGD	CA4-CA3-CA2	-4.22	104.76	110.85
13	M	406	BPH	CMA-C3A-C4A	-4.17	105.23	114.38
16	M	410	PC1	C3-O31-C31	4.07	132.21	117.12
7	L	301	BCL	C4A-NA-C1A	4.02	108.52	106.71
7	M	402	BCL	C3D-C2D-C1D	-4.01	100.36	105.83
7	M	401	BCL	C3D-C4D-ND	3.97	116.67	110.24
14	M	408	SPO	C15-C14-C12	-3.95	121.67	127.31
7	L	306	BCL	C1D-ND-C4D	-3.91	103.56	106.33
13	M	412	BPH	C4-C3-C5	3.87	121.78	115.27
7	M	402	BCL	CHD-C4C-NC	3.81	129.31	125.08
7	M	402	BCL	C1D-ND-C4D	-3.81	103.63	106.33
14	M	408	SPO	C2-C1-C4	-3.80	105.02	110.86
13	M	406	BPH	C1-O2A-CGA	3.78	126.35	116.44
13	M	406	BPH	O2D-CGD-O1D	-3.77	116.47	123.84
13	M	406	BPH	C1A-C2A-C3A	-3.76	99.26	102.84
9	M	407	U10	C7-C8-C9	-3.73	120.58	126.79
13	M	412	BPH	O2D-CGD-CBD	-3.72	106.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	309	HTO	O1-C1-C2	3.70	119.14	111.07
7	M	401	BCL	C1-O2A-CGA	3.69	126.12	116.44
13	M	412	BPH	O2A-C1-C2	3.68	118.30	108.64
7	L	306	BCL	CHD-C4C-NC	3.68	129.16	125.08
7	M	401	BCL	O2D-CGD-O1D	-3.68	116.65	123.84
7	L	301	BCL	CHD-C1D-ND	-3.64	121.11	124.45
13	M	412	BPH	C1-C2-C3	-3.54	119.91	126.04
13	M	406	BPH	CAC-C3C-C2C	-3.51	105.50	114.26
7	M	402	BCL	O2D-CGD-O1D	-3.48	117.03	123.84
7	L	306	BCL	C3D-C4D-ND	3.38	115.71	110.24
14	M	408	SPO	C3-C1-C4	-3.38	105.66	110.86
16	M	410	PC1	O31-C3-C2	3.37	118.25	108.43
9	M	407	U10	C4M-O4-C4	3.37	128.39	116.47
7	L	301	BCL	C1D-ND-C4D	-3.35	103.95	106.33
7	L	306	BCL	C1C-NC-C4C	-3.35	105.20	106.71
7	L	301	BCL	CHB-C4A-NA	3.31	129.09	124.51
7	M	401	BCL	C1D-ND-C4D	-3.30	103.99	106.33
7	L	301	BCL	C5-C3-C2	-3.28	114.48	121.12
7	M	401	BCL	C4B-CHC-C1C	-3.27	123.64	130.12
7	M	402	BCL	CHB-C4A-NA	3.26	129.01	124.51
9	L	305[A]	U10	C8-C7-C6	3.24	120.79	112.05
7	M	402	BCL	O2A-C1-C2	3.24	117.14	108.64
13	M	406	BPH	C4-C3-C2	-3.21	115.44	123.68
13	M	406	BPH	C4C-C3C-C2C	-3.20	99.79	102.84
9	L	305[A]	U10	C16-C14-C15	3.20	121.66	114.60
7	M	401	BCL	C2D-C1D-ND	3.18	112.44	110.10
16	M	410	PC1	O31-C31-C32	3.17	121.85	111.91
7	L	301	BCL	CHC-C1C-NC	3.17	128.89	124.51
13	M	412	BPH	C4C-C3C-C2C	-3.15	99.84	102.84
7	M	401	BCL	O2A-CGA-CBA	3.13	121.72	111.91
9	L	305[B]	U10	C10-C9-C11	3.12	120.51	115.27
15	M	409	CDL	OA8-CA7-C31	3.10	121.64	111.91
11	L	309	HTO	C4-C3-C2	3.10	120.71	113.35
7	M	402	BCL	C3D-C4D-ND	3.09	115.24	110.24
7	L	306	BCL	C4B-CHC-C1C	-3.09	124.01	130.12
7	M	402	BCL	OBD-CAD-C3D	-3.05	121.18	128.52
7	L	301	BCL	OBB-CAB-C3B	3.04	125.39	119.99
7	L	301	BCL	C2A-C1A-CHA	-3.03	118.56	123.86
7	L	301	BCL	C1D-CHD-C4C	-3.03	119.32	126.62
7	L	306	BCL	CHB-C4A-NA	3.01	128.67	124.51
7	L	306	BCL	C1-O2A-CGA	3.00	124.31	116.44
7	L	306	BCL	C3D-C2D-C1D	-2.98	101.76	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	412	BPH	C4-C3-C2	-2.98	116.03	123.68
15	M	409	CDL	OA6-CA5-OA7	-2.98	116.50	123.70
7	L	306	BCL	O2A-CGA-O1A	-2.97	116.11	123.59
7	L	301	BCL	C4-C3-C5	2.97	120.26	115.27
9	L	305[A]	U10	C16-C14-C13	-2.95	114.12	122.65
7	L	301	BCL	O2A-CGA-CBA	2.93	121.11	111.91
7	M	401	BCL	C1-C2-C3	2.93	131.10	126.04
13	M	406	BPH	C6-C5-C3	2.92	121.12	113.45
9	L	305[B]	U10	C16-C14-C15	2.90	121.01	114.60
7	M	402	BCL	C1D-CHD-C4C	-2.89	119.65	126.62
7	L	306	BCL	O2A-CGA-CBA	2.89	120.97	111.91
15	M	409	CDL	OA8-CA7-OA9	-2.88	116.31	123.59
6	H	307	GGD	OC8-CC7-OC9	-2.88	116.33	123.59
7	M	401	BCL	C1B-CHB-C4A	-2.87	124.43	130.12
14	M	408	SPO	C20-C19-C17	-2.86	123.22	127.31
7	L	301	BCL	C3D-C4D-ND	2.82	114.81	110.24
7	M	401	BCL	C1D-CHD-C4C	-2.82	119.81	126.62
7	L	306	BCL	CHC-C1C-NC	2.82	128.41	124.51
7	M	401	BCL	CHC-C1C-NC	2.80	128.39	124.51
9	L	305[B]	U10	O5-C5-C4	-2.79	115.00	120.93
14	M	408	SPO	C27-C26-C25	-2.74	114.67	123.22
7	M	402	BCL	CMB-C2B-C3B	2.70	129.73	124.68
15	M	409	CDL	OB8-CB7-OB9	-2.67	116.86	123.59
13	M	406	BPH	C5-C3-C2	2.66	126.50	121.12
14	M	408	SPO	C6-C7-C9	-2.64	114.89	118.94
13	M	412	BPH	O2A-CGA-O1A	-2.63	116.95	123.59
11	L	309	HTO	C1-C2-C3	2.62	118.79	113.11
13	M	412	BPH	O2A-CGA-CBA	2.59	120.04	111.91
7	L	306	BCL	C2A-C1A-CHA	-2.59	119.33	123.86
6	H	307	GGD	OC8-CC7-C31	2.58	120.01	111.91
7	L	306	BCL	C1D-CHD-C4C	-2.58	120.40	126.62
11	L	309	HTO	C5-C4-C3	2.57	118.41	114.18
7	M	401	BCL	CED-O2D-CGD	-2.57	110.13	115.94
15	M	409	CDL	OB6-CB5-OB7	-2.57	117.50	123.70
9	L	305[A]	U10	O2-C2-C3	-2.54	115.55	120.93
7	M	402	BCL	C1B-CHB-C4A	-2.52	125.12	130.12
6	H	307	GGD	OB5-CB5-CB6	2.52	112.70	106.44
9	M	407	U10	C35-C34-C36	2.52	119.50	115.27
9	M	407	U10	C32-C33-C34	-2.52	121.60	127.66
14	M	408	SPO	C40-C38-C37	-2.52	115.38	122.65
6	H	307	GGD	OA5-CA1-CA2	2.51	115.67	110.35
13	M	412	BPH	CBA-CAA-C2A	2.51	121.14	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	408	SPO	C21-C22-C23	-2.50	123.74	127.31
15	M	409	CDL	CA6-OA8-CA7	2.50	126.38	117.12
7	L	301	BCL	C4B-CHC-C1C	-2.49	125.18	130.12
9	L	305[B]	U10	C1-C6-C5	-2.49	117.24	119.58
7	M	401	BCL	C3D-C2D-C1D	-2.49	102.44	105.83
9	M	407	U10	C6-C1-C2	2.49	121.15	119.18
16	M	410	PC1	O21-C2-C3	2.48	117.38	108.40
7	L	301	BCL	C1B-CHB-C4A	-2.46	125.24	130.12
9	M	407	U10	C17-C18-C19	-2.46	121.73	127.66
7	M	401	BCL	CHB-C4A-NA	2.46	127.91	124.51
7	L	301	BCL	C4D-CHA-C1A	-2.44	118.28	121.25
9	M	407	U10	C41-C39-C40	2.43	119.97	114.60
9	M	407	U10	C25-C24-C26	2.41	119.33	115.27
14	M	408	SPO	C13-C12-C14	-2.41	119.55	122.92
9	L	305[A]	U10	C7-C8-C9	-2.40	122.80	126.79
7	L	301	BCL	C1-O2A-CGA	2.38	122.69	116.44
7	M	401	BCL	C3A-C2A-C1A	-2.38	97.77	101.34
9	L	305[A]	U10	C7-C6-C5	-2.35	115.65	118.48
6	H	307	GGD	OC8-CC6-CC4	2.35	115.28	108.43
9	L	305[B]	U10	C15-C14-C13	-2.35	115.87	122.65
6	H	307	GGD	OA2-CA2-CA3	2.34	116.15	109.94
13	M	412	BPH	C7-C6-C5	2.33	119.69	113.36
7	M	402	BCL	OBB-CAB-C3B	2.33	124.13	119.99
7	L	301	BCL	C16-C15-C13	-2.31	108.47	115.92
9	M	407	U10	C15-C14-C16	2.30	119.15	115.27
7	L	301	BCL	O1D-CGD-CBD	-2.30	119.78	124.48
7	M	402	BCL	O2D-CGD-CBD	2.29	115.34	111.27
9	M	407	U10	C10-C9-C11	2.25	119.06	115.27
6	H	307	GGD	OB1-CA3-CA4	2.25	113.25	107.28
6	H	307	GGD	OC6-CC5-OC7	-2.24	118.29	123.70
7	L	301	BCL	C4B-C3B-CAB	2.23	131.44	127.13
16	M	410	PC1	O21-C21-O22	-2.22	118.33	123.70
7	L	301	BCL	O2A-CGA-O1A	-2.22	117.99	123.59
8	L	303	LDA	CM1-N1-C1	2.20	114.85	110.23
6	H	307	GGD	CB1-OB1-CA3	2.18	123.36	117.96
13	M	412	BPH	C1A-C2A-C3A	2.16	104.90	102.84
7	L	301	BCL	C6-C5-C3	-2.16	107.79	113.45
13	M	412	BPH	CBC-CAC-C3C	-2.16	109.42	113.77
7	L	301	BCL	CED-O2D-CGD	2.15	120.80	115.94
14	M	408	SPO	C13-C12-C11	2.15	121.46	118.08
7	L	306	BCL	O2A-C1-C2	-2.13	103.05	108.64
9	M	407	U10	C26-C24-C23	-2.11	116.85	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	406	BPH	CMB-C2B-C3B	2.09	128.59	124.68
7	L	306	BCL	C3A-C2A-C1A	-2.07	98.23	101.34
7	L	301	BCL	CMB-C2B-C3B	2.05	128.52	124.68
8	M	403	LDA	O1-N1-C1	2.04	114.28	109.27
7	M	401	BCL	CMC-C2C-C3C	-2.03	105.64	113.83
7	M	401	BCL	CMA-C3A-C4A	-2.03	106.32	111.77
9	M	407	U10	C1M-C1-C6	-2.03	121.09	124.40
14	M	408	SPO	C40-C38-C39	2.03	119.08	114.60
7	L	306	BCL	OBD-CAD-C3D	-2.02	123.67	128.52
13	M	412	BPH	C1-O2A-CGA	2.01	121.73	116.44
7	L	306	BCL	CMD-C2D-C3D	-2.01	122.99	127.61
7	M	401	BCL	C4B-C3B-CAB	2.00	130.99	127.13

There are no chirality outliers.

All (227) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	306	GOL	O1-C1-C2-O2
4	H	306	GOL	O1-C1-C2-C3
4	H	302	GOL	O1-C1-C2-O2
4	H	302	GOL	O1-C1-C2-C3
4	H	303	GOL	C1-C2-C3-O3
4	H	304	GOL	C1-C2-C3-O3
4	L	311	GOL	O1-C1-C2-C3
6	H	307	GGD	OC7-CC5-OC6-CC4
8	L	303	LDA	C2-C1-N1-O1
8	L	303	LDA	C2-C1-N1-CM1
8	L	303	LDA	C2-C1-N1-CM2
8	M	403	LDA	C2-C1-N1-O1
8	M	403	LDA	C2-C1-N1-CM1
8	M	403	LDA	C2-C1-N1-CM2
9	L	305[B]	U10	C9-C11-C12-C13
9	M	407	U10	C24-C26-C27-C28
9	M	407	U10	C30-C29-C31-C32
9	M	407	U10	C29-C31-C32-C33
9	M	407	U10	C34-C36-C37-C38
11	L	308	HTO	C1-C2-C3-O3
11	L	308	HTO	O3-C3-C4-C5
11	L	309	HTO	C1-C2-C3-O3
11	L	309	HTO	C1-C2-C3-C4
11	L	309	HTO	O2-C2-C3-O3
11	L	309	HTO	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
13	M	406	BPH	C4C-C3C-CAC-CBC
13	M	406	BPH	C2C-C3C-CAC-CBC
13	M	412	BPH	C4C-C3C-CAC-CBC
13	M	412	BPH	C2C-C3C-CAC-CBC
13	M	412	BPH	C2-C1-O2A-CGA
13	M	412	BPH	C2-C3-C5-C6
13	M	412	BPH	C4-C3-C5-C6
13	M	412	BPH	C6-C7-C8-C9
14	M	408	SPO	O1-C1-C4-C5
14	M	408	SPO	C2-C1-C4-C5
14	M	408	SPO	C3-C1-C4-C5
15	M	409	CDL	CB2-OB2-PB2-OB3
15	M	409	CDL	CB3-OB5-PB2-OB3
15	M	409	CDL	CB3-OB5-PB2-OB4
16	M	410	PC1	O13-C11-C12-N
6	H	307	GGD	CA2-CA3-OB1-CB1
15	M	409	CDL	OB9-CB7-OB8-CB6
6	H	307	GGD	C14-CC5-OC6-CC4
9	M	407	U10	C28-C29-C31-C32
7	M	401	BCL	C3-C5-C6-C7
6	H	307	GGD	C31-CC7-OC8-CC6
15	M	409	CDL	C71-CB7-OB8-CB6
6	H	307	GGD	OC9-CC7-OC8-CC6
15	M	409	CDL	OA9-CA7-OA8-CA6
6	H	307	GGD	OA5-CA5-CA6-OA6
15	M	409	CDL	O1-C1-CB2-OB2
15	M	409	CDL	C31-CA7-OA8-CA6
15	M	409	CDL	C11-CA5-OA6-CA4
7	M	401	BCL	C11-C12-C13-C14
16	M	410	PC1	O22-C21-O21-C2
16	M	410	PC1	C22-C21-O21-C2
7	L	306	BCL	C15-C16-C17-C18
13	M	406	BPH	C5-C6-C7-C8
7	M	401	BCL	C13-C15-C16-C17
6	H	307	GGD	CC5-C14-C15-C16
15	M	409	CDL	OA7-CA5-OA6-CA4
13	M	406	BPH	C10-C11-C12-C13
16	M	410	PC1	C31-C32-C33-C34
13	M	406	BPH	C11-C12-C13-C15
7	M	401	BCL	C8-C10-C11-C12
9	L	305[A]	U10	C9-C11-C12-C13
8	L	302	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
7	L	301	BCL	C13-C15-C16-C17
15	M	409	CDL	CB3-OB5-PB2-OB2
16	M	410	PC1	C1-O11-P-O13
15	M	409	CDL	C80-C81-C82-C83
8	L	304	LDA	C5-C6-C7-C8
16	M	410	PC1	C3-C2-O21-C21
15	M	409	CDL	C53-C54-C55-C56
15	M	409	CDL	C71-C72-C73-C74
15	M	409	CDL	C11-C12-C13-C14
6	H	307	GGD	CA4-CA5-CA6-OA6
16	M	410	PC1	C2A-C2B-C2C-C2D
15	M	409	CDL	C20-C21-C22-C23
16	M	410	PC1	C22-C23-C24-C25
4	L	310	GOL	O1-C1-C2-C3
4	L	311	GOL	C1-C2-C3-O3
7	M	401	BCL	C16-C17-C18-C20
6	H	307	GGD	C34-C35-C36-C37
8	M	404	LDA	C4-C5-C6-C7
15	M	409	CDL	CB5-C51-C52-C53
15	M	409	CDL	C16-C17-C18-C19
15	M	409	CDL	C38-C39-C40-C41
7	M	401	BCL	O2A-C1-C2-C3
4	H	303	GOL	O2-C2-C3-O3
8	M	404	LDA	C1-C2-C3-C4
16	M	410	PC1	C28-C29-C2A-C2B
6	H	307	GGD	C40-C41-C42-C43
15	M	409	CDL	C52-C53-C54-C55
15	M	409	CDL	CA2-C1-CB2-OB2
8	L	303	LDA	C1-C2-C3-C4
8	L	303	LDA	C4-C5-C6-C7
7	M	401	BCL	C11-C12-C13-C15
13	M	412	BPH	C3-C5-C6-C7
6	H	307	GGD	C31-C32-C33-C34
13	M	412	BPH	C13-C15-C16-C17
8	M	403	LDA	C2-C3-C4-C5
8	L	302	LDA	C3-C4-C5-C6
8	L	302	LDA	C6-C7-C8-C9
15	M	409	CDL	C14-C15-C16-C17
6	H	307	GGD	CC7-C31-C32-C33
8	L	302	LDA	C1-C2-C3-C4
15	M	409	CDL	C15-C16-C17-C18
8	L	302	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	L	304	LDA	C4-C5-C6-C7
13	M	406	BPH	C11-C12-C13-C14
13	M	412	BPH	C5-C6-C7-C8
15	M	409	CDL	C78-C79-C80-C81
15	M	409	CDL	C12-C13-C14-C15
15	M	409	CDL	CB2-OB2-PB2-OB5
15	M	409	CDL	C13-C14-C15-C16
16	M	410	PC1	C27-C28-C29-C2A
8	L	304	LDA	C1-C2-C3-C4
15	M	409	CDL	C31-C32-C33-C34
7	M	401	BCL	C10-C11-C12-C13
15	M	409	CDL	CB7-C71-C72-C73
4	L	311	GOL	O1-C1-C2-O2
4	L	311	GOL	O2-C2-C3-O3
8	L	304	LDA	C9-C10-C11-C12
13	M	406	BPH	C13-C15-C16-C17
11	L	308	HTO	O2-C2-C3-O3
7	M	402	BCL	C15-C16-C17-C18
15	M	409	CDL	CA5-C11-C12-C13
16	M	410	PC1	C33-C34-C35-C36
8	L	304	LDA	N1-C1-C2-C3
8	M	403	LDA	N1-C1-C2-C3
8	M	404	LDA	C9-C10-C11-C12
15	M	409	CDL	C39-C40-C41-C42
16	M	410	PC1	C2-C1-O11-P
15	M	409	CDL	CB3-CB4-CB6-OB8
16	M	410	PC1	C2B-C2C-C2D-C2E
6	H	307	GGD	C17-C18-C19-C20
8	M	404	LDA	C6-C7-C8-C9
15	M	409	CDL	OB5-CB3-CB4-OB6
6	H	307	GGD	C38-C39-C40-C41
8	L	303	LDA	C2-C3-C4-C5
8	M	403	LDA	C11-C10-C9-C8
7	M	401	BCL	C4C-C3C-CAC-CBC
7	M	401	BCL	C16-C17-C18-C19
16	M	410	PC1	O11-C1-C2-C3
7	L	306	BCL	C16-C17-C18-C20
6	H	307	GGD	C41-C42-C43-C44
15	M	409	CDL	CA3-CA4-CA6-OA8
7	M	402	BCL	CHA-CBD-CGD-O1D
8	L	304	LDA	C2-C1-N1-CM1
6	H	307	GGD	OC6-CC4-CC6-OC8

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Mol	Chain	Res	Type	Atoms
4	H	301	GOL	O2-C2-C3-O3
11	L	308	HTO	C2-C3-C4-C5
4	H	301	GOL	C1-C2-C3-O3
4	L	310	GOL	C1-C2-C3-O3
15	M	409	CDL	O1-C1-CA2-OA2
15	M	409	CDL	CB2-OB2-PB2-OB4
16	M	410	PC1	C1-O11-P-O14
8	M	404	LDA	C7-C8-C9-C10
14	M	408	SPO	C1-C4-C5-C6
13	M	406	BPH	CBA-CGA-O2A-C1
6	H	307	GGD	CC3-CC4-CC6-OC8
15	M	409	CDL	OA6-CA4-CA6-OA8
11	L	309	HTO	C3-C4-C5-C6
13	M	406	BPH	O1A-CGA-O2A-C1
15	M	409	CDL	OB5-CB3-CB4-CB6
6	H	307	GGD	CB2-CB1-OB1-CA3
13	M	406	BPH	C2-C1-O2A-CGA
9	M	407	U10	C31-C32-C33-C34
11	L	308	HTO	C4-C5-C6-C7
15	M	409	CDL	CA3-OA5-PA1-OA2
16	M	410	PC1	C11-O13-P-O11
16	M	410	PC1	C32-C33-C34-C35
7	M	402	BCL	C6-C7-C8-C10
8	L	302	LDA	N1-C1-C2-C3
15	M	409	CDL	C40-C41-C42-C43
9	M	407	U10	C25-C24-C26-C27
6	H	307	GGD	OB5-CB1-OB1-CA3
7	M	401	BCL	C12-C13-C15-C16
15	M	409	CDL	C17-C18-C19-C20
4	L	310	GOL	O2-C2-C3-O3
8	L	303	LDA	C5-C6-C7-C8
15	M	409	CDL	OB6-CB4-CB6-OB8
7	L	301	BCL	C3-C5-C6-C7
7	M	402	BCL	CAA-CBA-CGA-O2A
9	M	407	U10	C5-C4-O4-C4M
4	H	304	GOL	O2-C2-C3-O3
9	L	305[B]	U10	C3-C4-O4-C4M
13	M	406	BPH	C2-C3-C5-C6
7	L	301	BCL	CAD-CBD-CGD-O2D
7	L	306	BCL	CAD-CBD-CGD-O2D
7	M	401	BCL	CAD-CBD-CGD-O2D
13	M	406	BPH	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	M	407	U10	C23-C24-C26-C27
15	M	409	CDL	C12-C11-CA5-OA6
8	L	304	LDA	C2-C3-C4-C5
8	M	403	LDA	C7-C8-C9-C10
16	M	410	PC1	C36-C37-C38-C39
16	M	410	PC1	C11-C12-N-C14
13	M	406	BPH	O2A-C1-C2-C3
15	M	409	CDL	C79-C80-C81-C82
7	M	402	BCL	CHA-CBD-CGD-O2D
8	M	404	LDA	C2-C1-N1-CM1
8	M	404	LDA	C2-C1-N1-CM2
15	M	409	CDL	C72-C71-CB7-OB8
15	M	409	CDL	C41-C42-C43-C44
13	M	406	BPH	CHA-CBD-CGD-O2D
8	L	304	LDA	C11-C10-C9-C8
15	M	409	CDL	C81-C82-C83-C84
13	M	406	BPH	C16-C17-C18-C20
7	M	402	BCL	C6-C7-C8-C9
15	M	409	CDL	C12-C11-CA5-OA7
7	L	306	BCL	C16-C17-C18-C19
16	M	410	PC1	O31-C31-C32-C33
6	H	307	GGD	C20-C21-C22-C23
9	L	305[B]	U10	C6-C7-C8-C9
16	M	410	PC1	C11-O13-P-O14
16	M	410	PC1	C11-C12-N-C13
16	M	410	PC1	C11-C12-N-C15
15	M	409	CDL	C72-C71-CB7-OB9
7	L	301	BCL	C14-C13-C15-C16
7	M	401	BCL	C14-C13-C15-C16
4	L	310	GOL	O1-C1-C2-O2
16	M	410	PC1	O32-C31-C32-C33
7	L	301	BCL	C12-C13-C15-C16
13	M	406	BPH	C12-C13-C15-C16
13	M	406	BPH	C4-C3-C5-C6

There are no ring outliers.

17 monomers are involved in 56 short contacts:

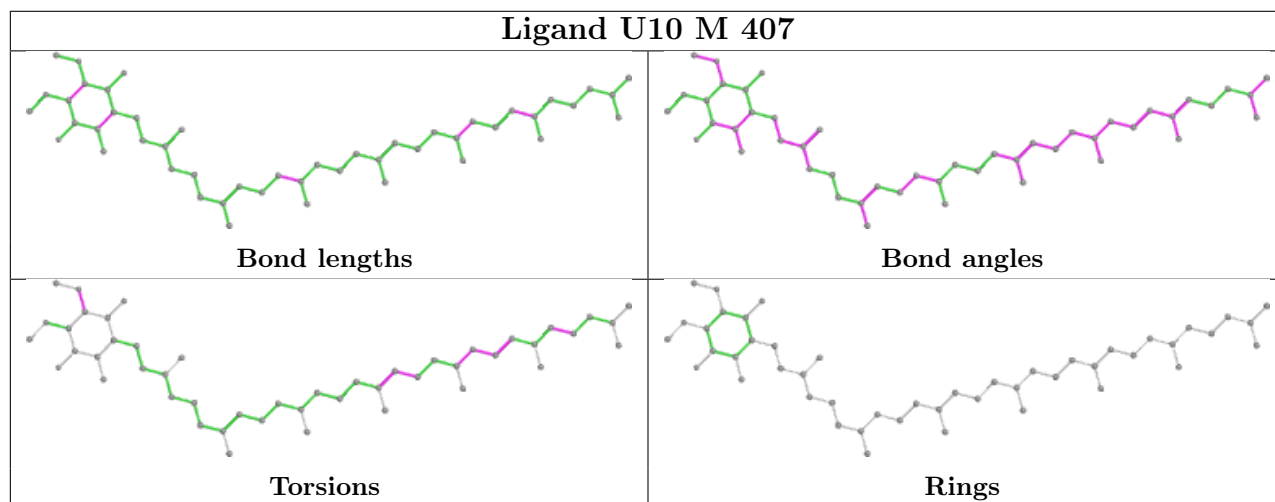
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	407	U10	1	0
10	L	307	PO4	1	0
16	M	410	PC1	1	0

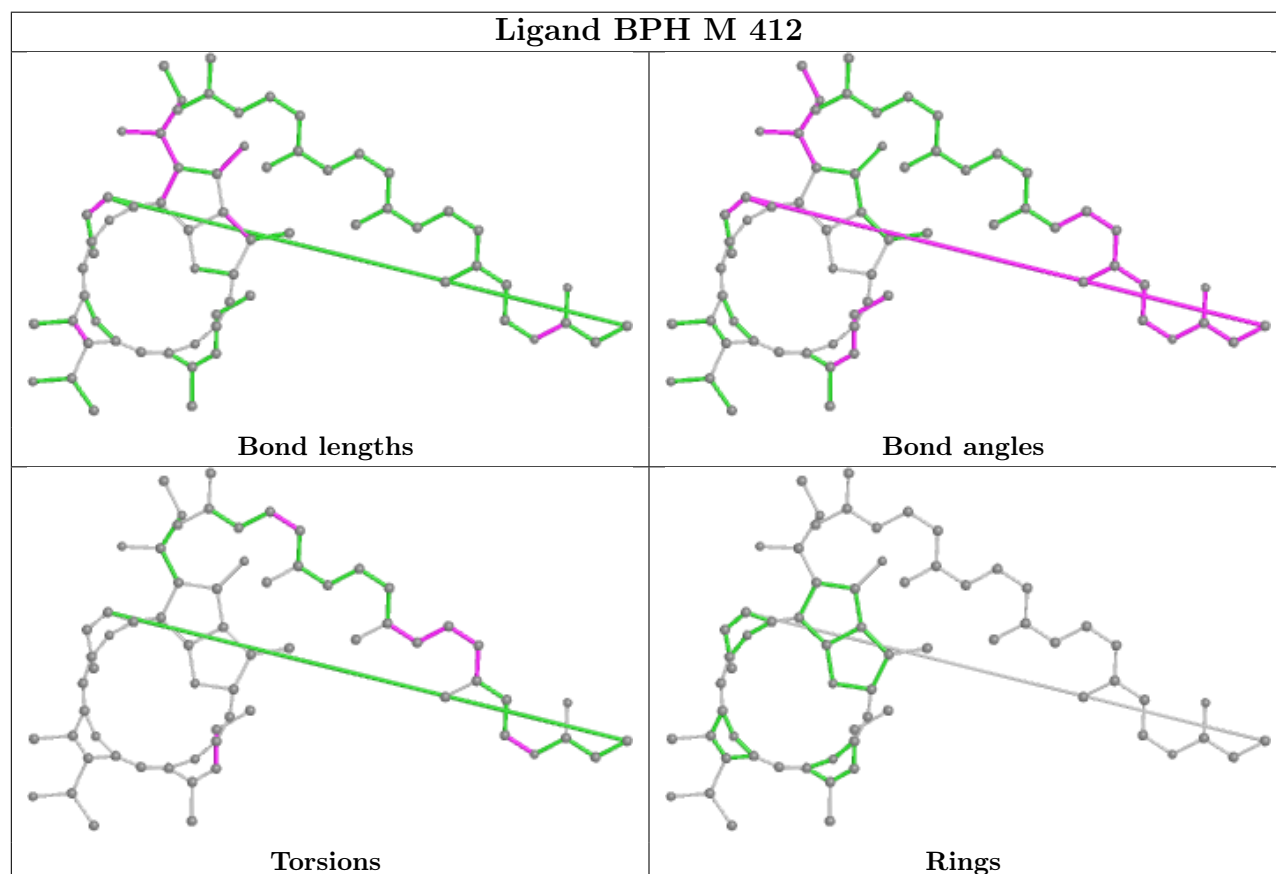
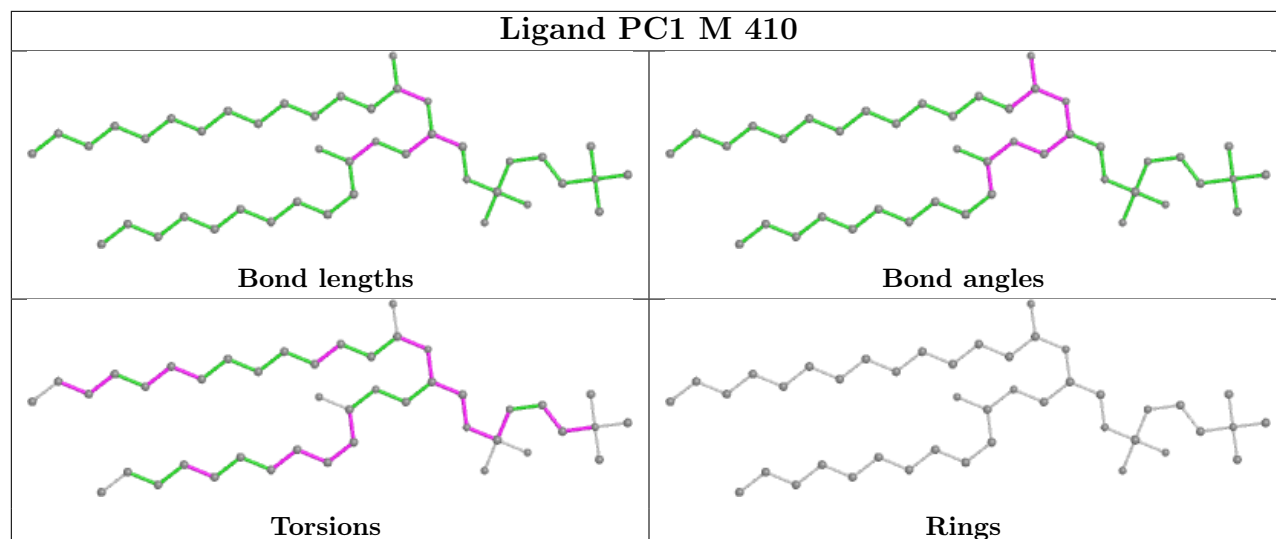
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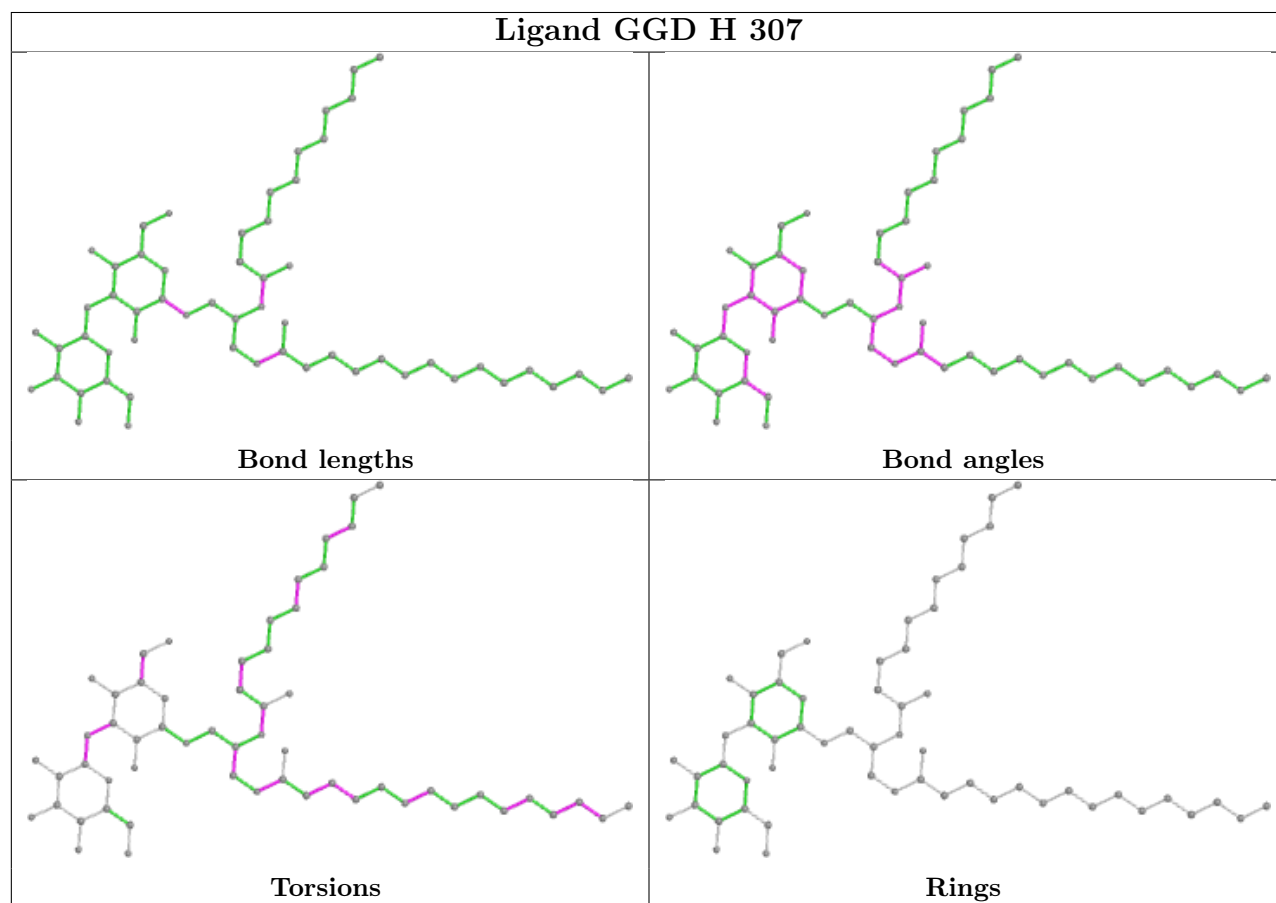
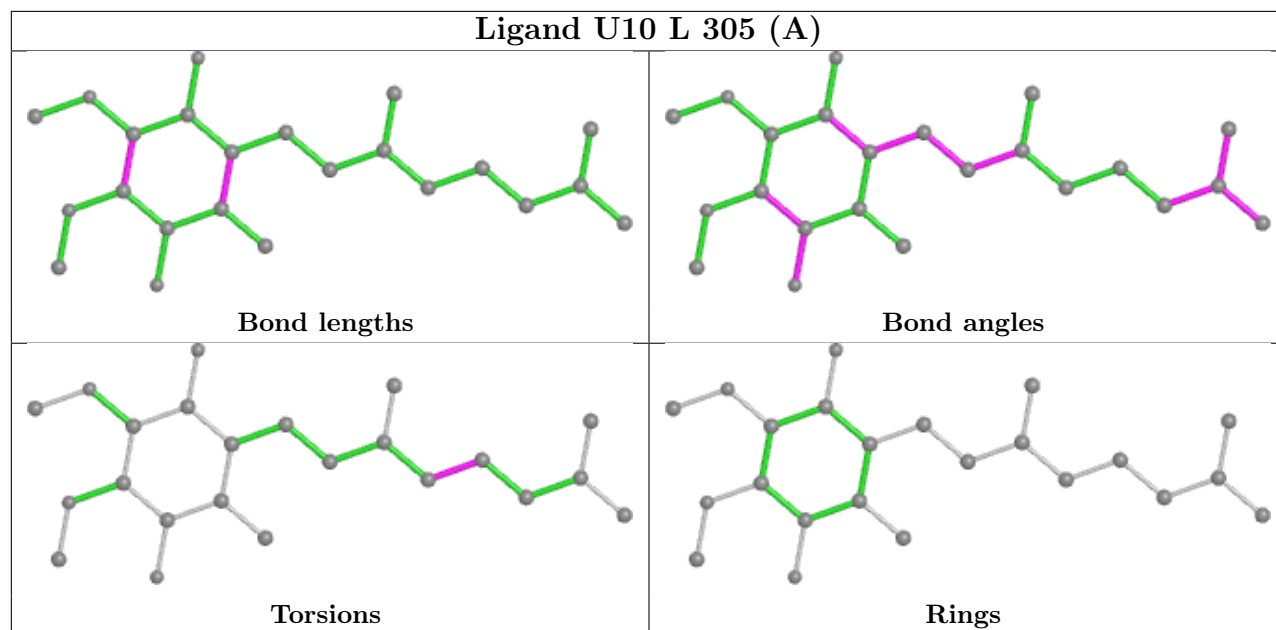
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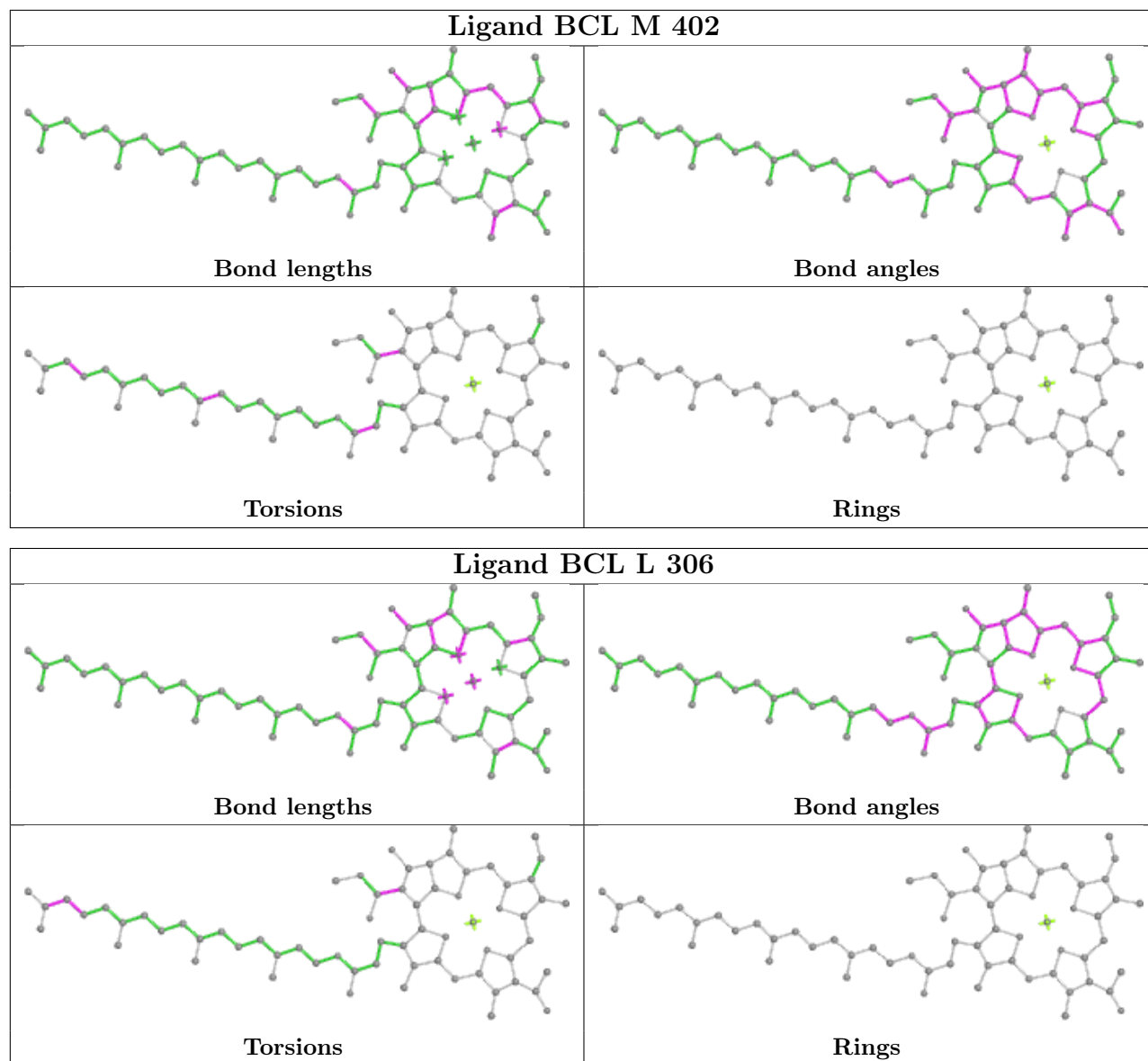
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	412	BPH	12	0
8	L	304	LDA	2	0
6	H	307	GGD	3	0
7	M	402	BCL	9	0
7	L	306	BCL	7	0
8	M	404	LDA	2	0
9	L	305[B]	U10	6	0
14	M	408	SPO	3	0
15	M	409	CDL	1	0
13	M	406	BPH	6	0
8	M	403	LDA	2	0
7	L	301	BCL	7	0
4	L	311	GOL	1	0
7	M	401	BCL	7	0

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.

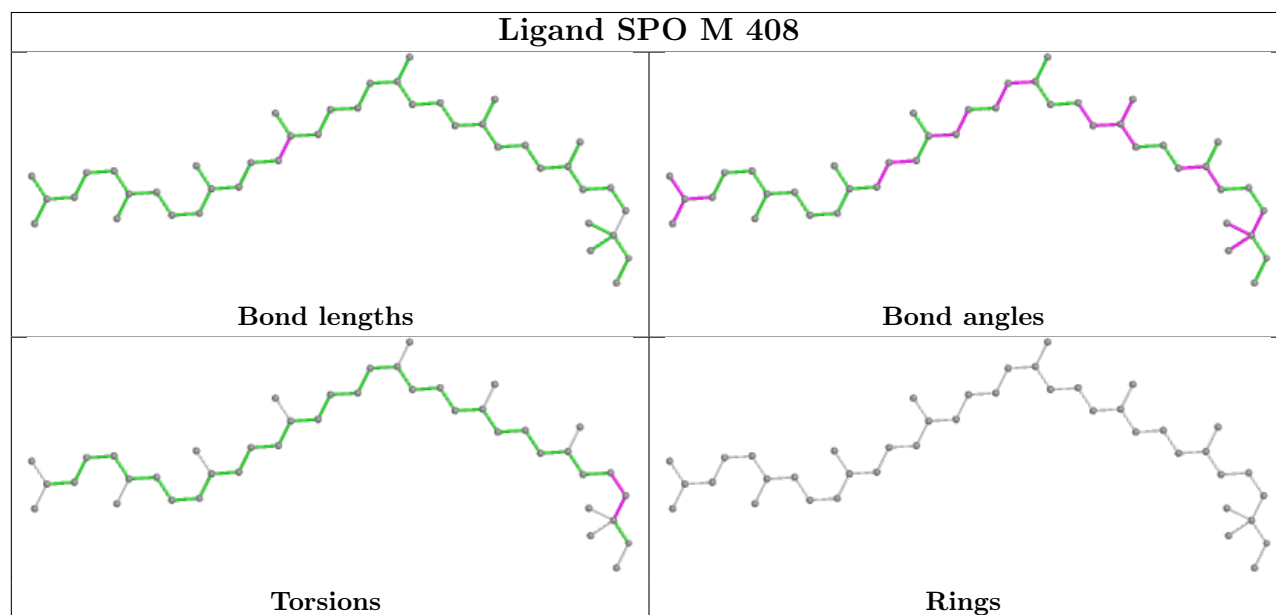
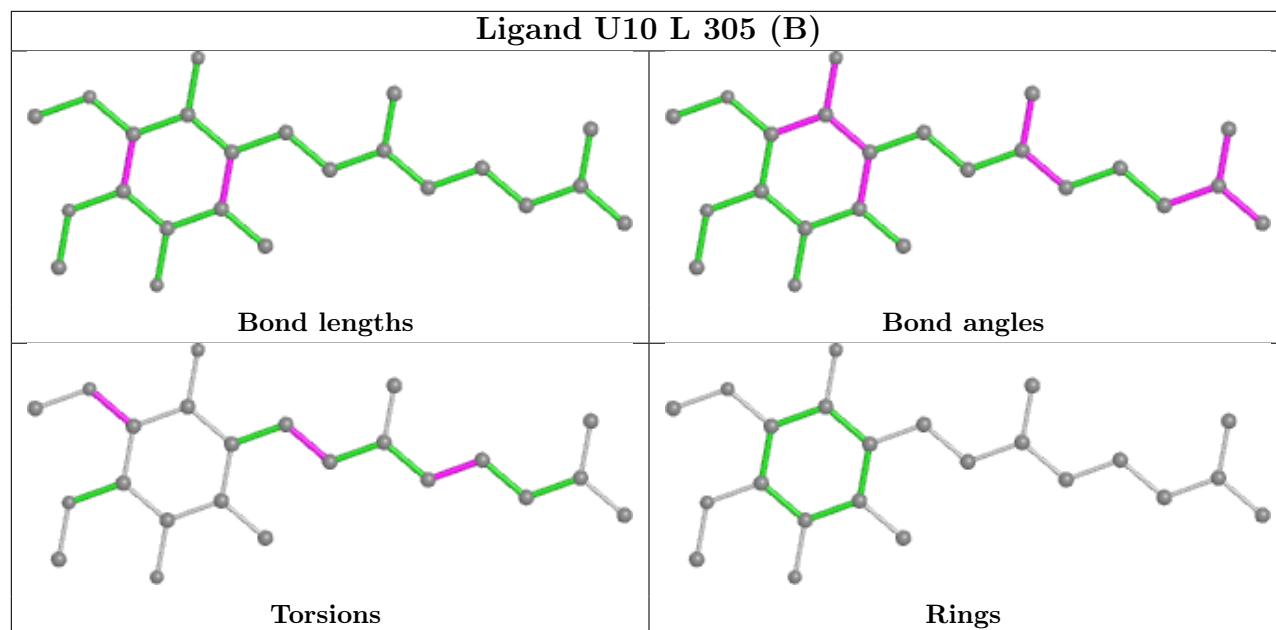


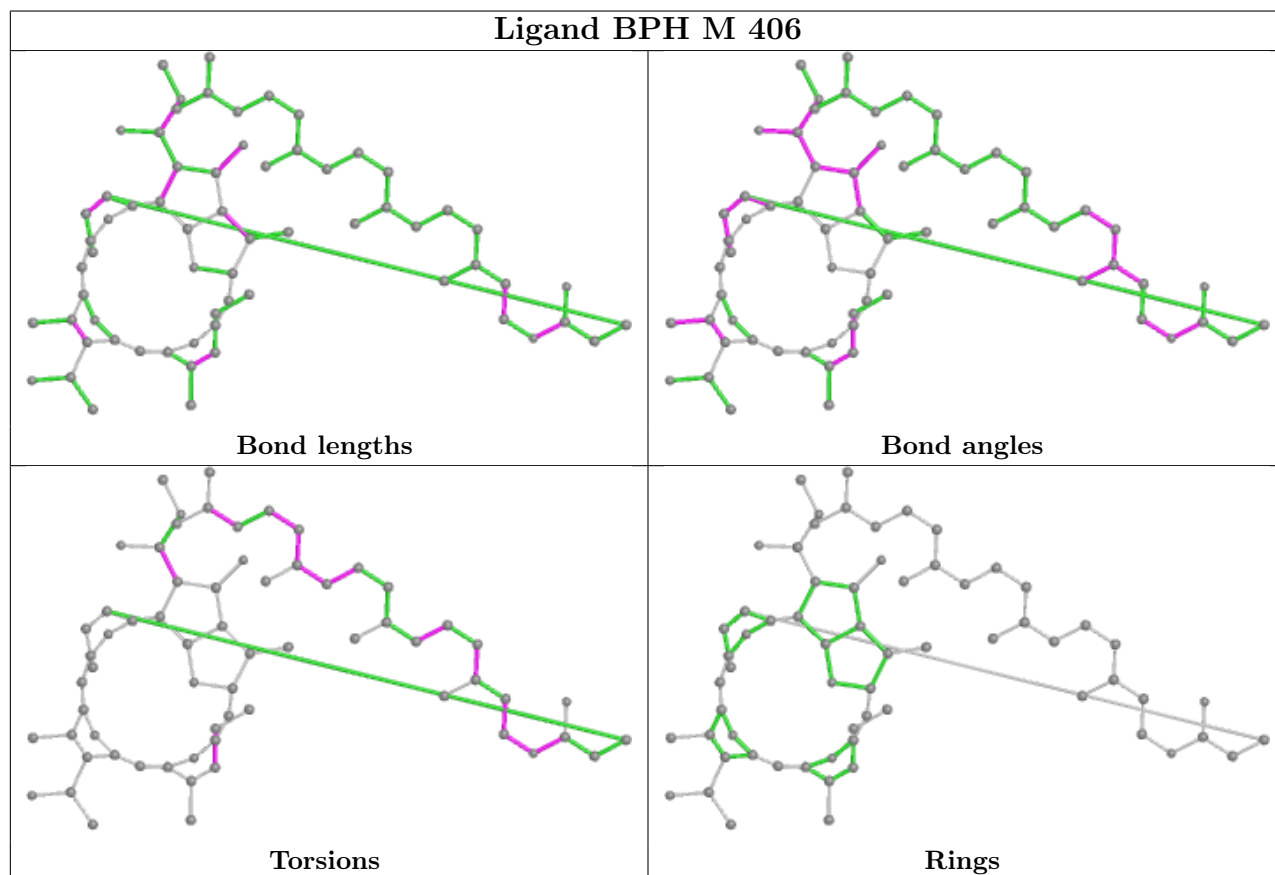
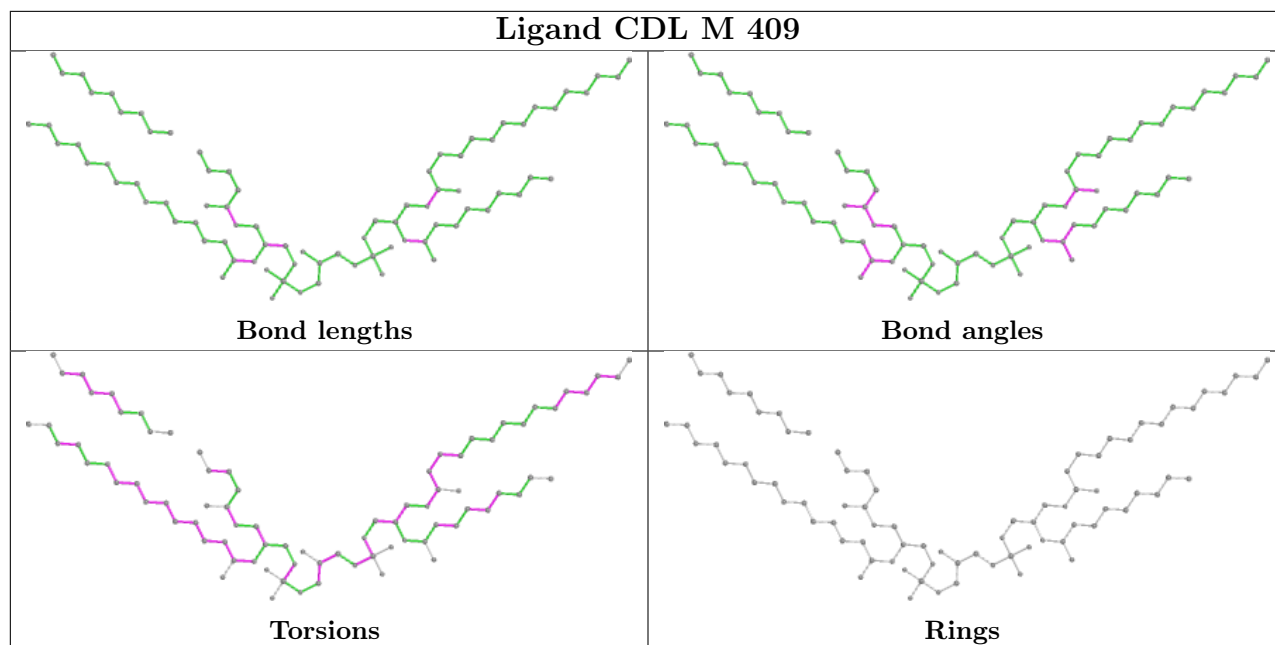


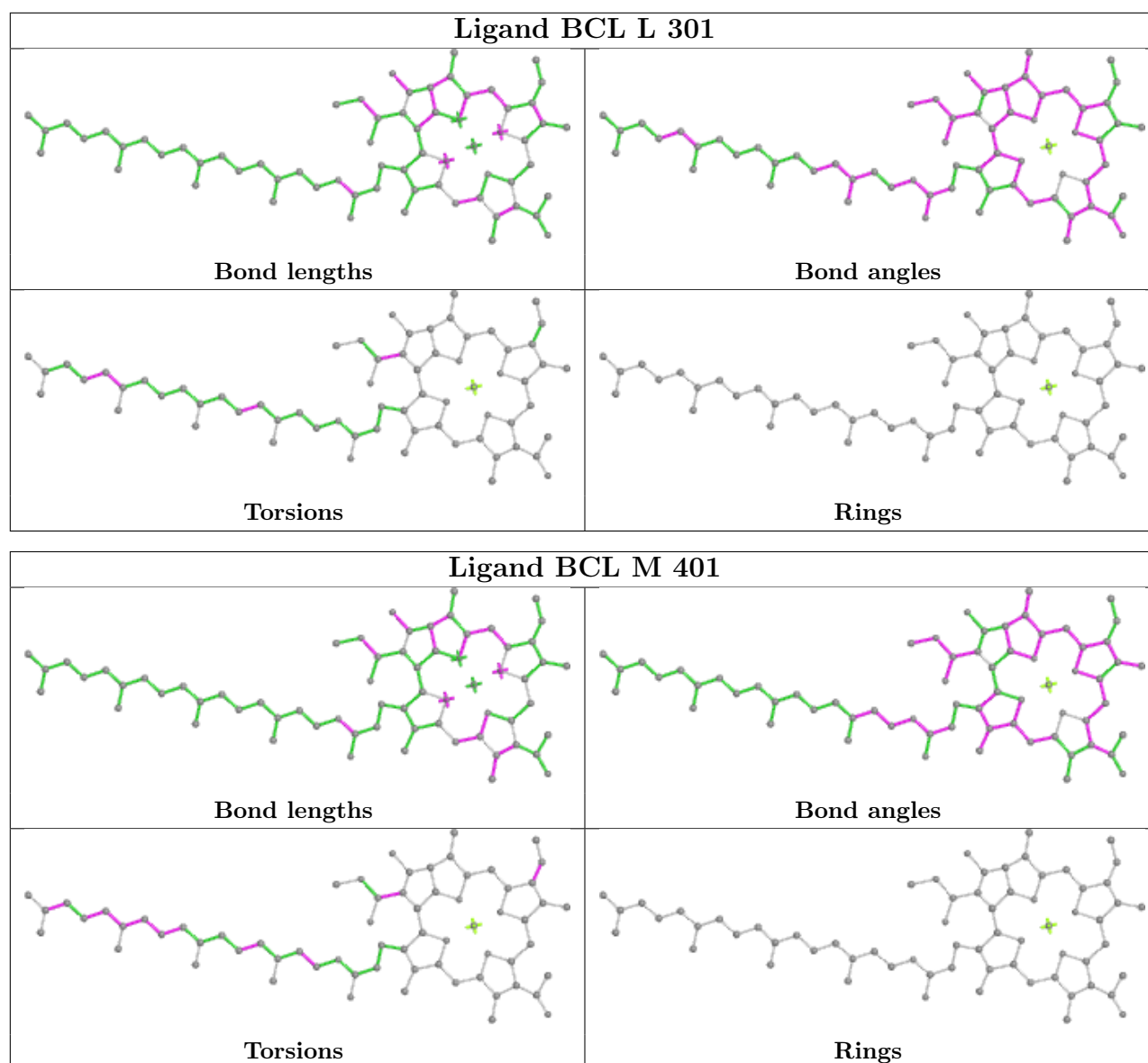












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	H	240/266 (90%)	-0.48	4 (1%) 70 68	33, 43, 61, 133	3 (1%)
2	L	281/282 (99%)	-0.63	2 (0%) 87 87	30, 41, 64, 89	0
3	M	302/307 (98%)	-0.46	1 (0%) 94 94	31, 45, 66, 99	6 (1%)
All	All	823/855 (96%)	-0.52	7 (0%) 84 84	30, 43, 64, 133	9 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	7.1
1	H	249[A]	LYS	3.2
3	M	1	ALA	3.1
2	L	281	GLY	2.5
1	H	220[A]	LYS	2.4
2	L	271[A]	TRP	2.3
1	H	221	SER	2.3

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

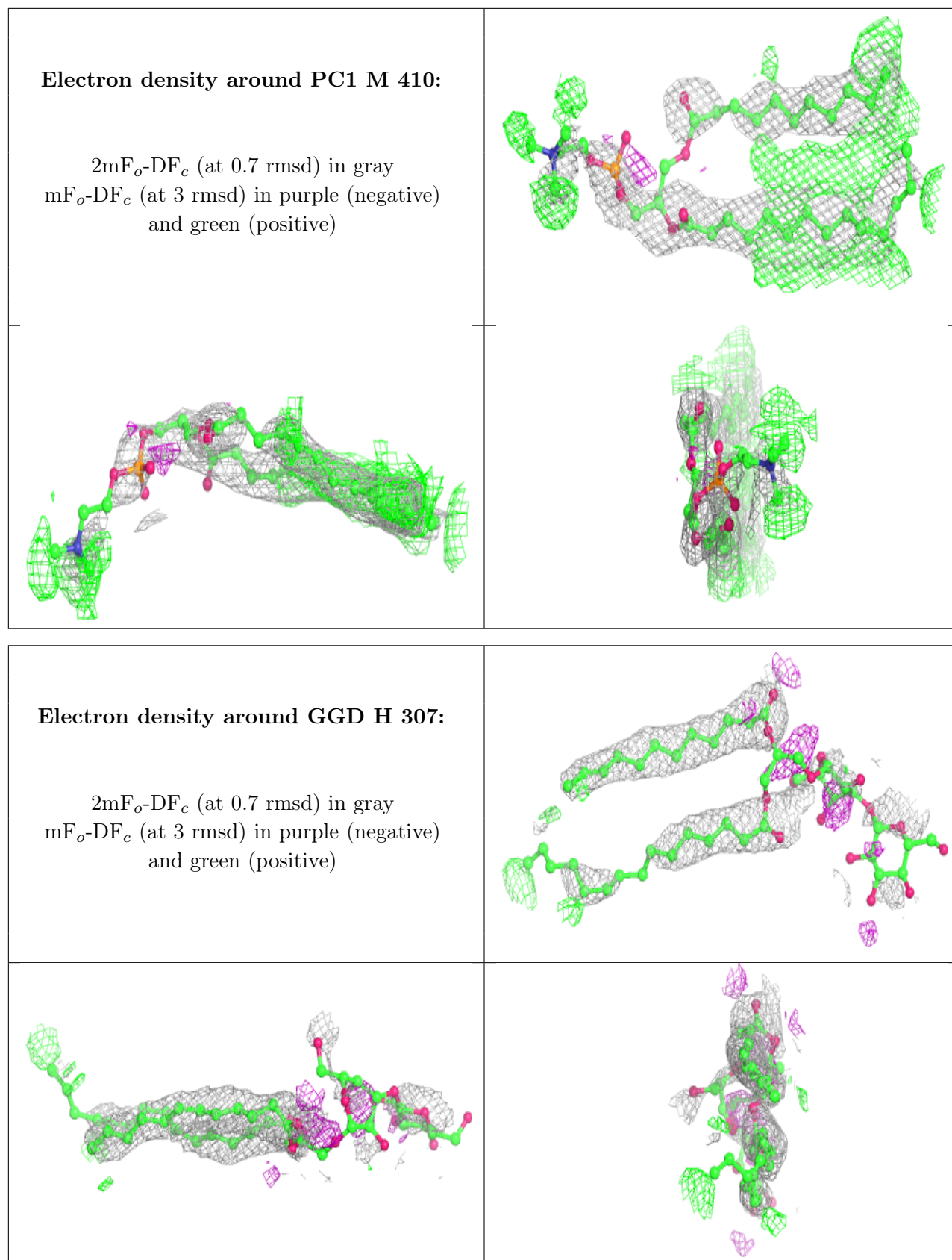
### 6.4 Ligands [i](#)

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.

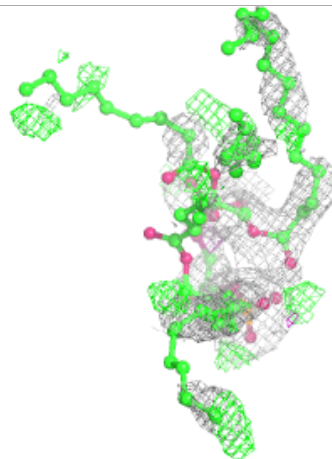
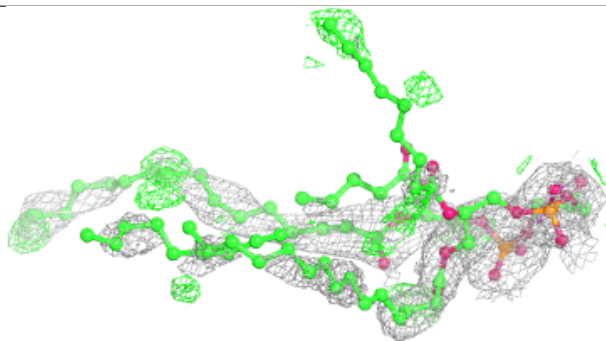
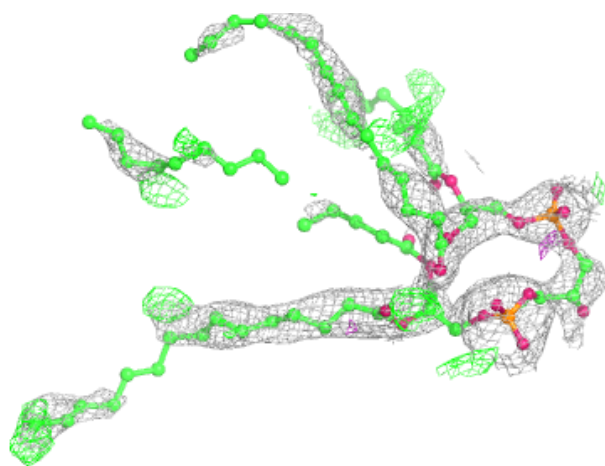
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
16	PC1	M	410	43/54	0.47	0.45	61,99,145,170	0
8	LDA	L	303	16/16	0.57	0.54	80,90,108,114	0
8	LDA	L	304	16/16	0.58	0.40	71,98,123,128	0
8	LDA	L	302	16/16	0.67	0.57	47,125,153,155	0
11	HTO	L	309	10/10	0.70	0.87	72,96,120,121	0
6	GGD	H	307	57/67	0.75	0.41	51,108,185,203	0
4	GOL	H	303	6/6	0.76	0.42	85,89,92,95	0
4	GOL	H	306	6/6	0.78	0.37	69,76,89,90	0
4	GOL	L	311	6/6	0.83	0.33	83,88,91,94	0
11	HTO	L	308	10/10	0.84	0.50	66,87,102,105	0
15	CDL	M	409	81/100	0.85	0.40	53,96,139,153	0
4	GOL	H	302	6/6	0.85	0.34	81,82,85,90	0
4	GOL	L	310	6/6	0.87	0.47	73,81,85,86	0
4	GOL	H	301	6/6	0.90	0.39	59,65,69,80	0
8	LDA	M	404	16/16	0.91	0.33	59,69,92,96	0
8	LDA	M	403	16/16	0.92	0.20	52,68,77,78	0
4	GOL	H	304	6/6	0.92	0.32	40,52,63,71	0
9	U10	L	305[A]	23/63	0.92	0.26	33,37,65,71	23
9	U10	L	305[B]	23/63	0.92	0.26	35,50,60,62	23
13	BPH	M	406	65/65	0.93	0.23	35,47,119,134	0
9	U10	M	407	48/63	0.94	0.24	33,46,91,110	0
14	SPO	M	408	42/42	0.94	0.21	33,47,80,92	0
5	K	H	305	1/1	0.95	0.12	50,50,50,50	0
10	PO4	L	307	5/5	0.96	0.11	60,62,66,67	0
17	MG	M	411	1/1	0.96	0.15	39,39,39,39	0
7	BCL	L	306	66/66	0.97	0.15	28,39,49,65	0
7	BCL	M	401	66/66	0.97	0.21	28,38,95,105	0
7	BCL	L	301	66/66	0.97	0.13	26,34,56,61	0
7	BCL	M	402	66/66	0.98	0.20	33,40,51,75	0
13	BPH	M	412	65/65	0.98	0.15	30,39,48,57	0
12	FE	M	405	1/1	0.99	0.16	36,36,36,36	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.



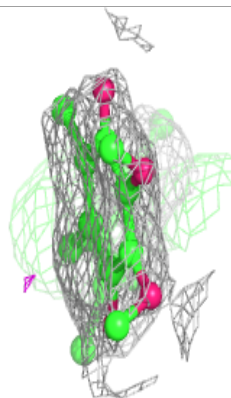
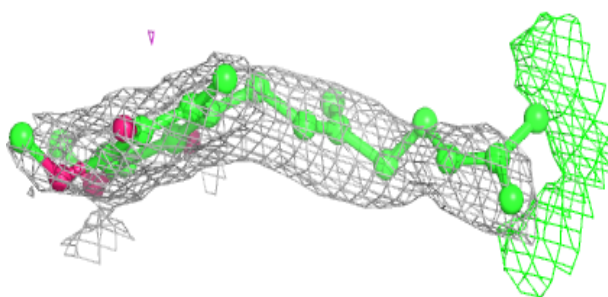
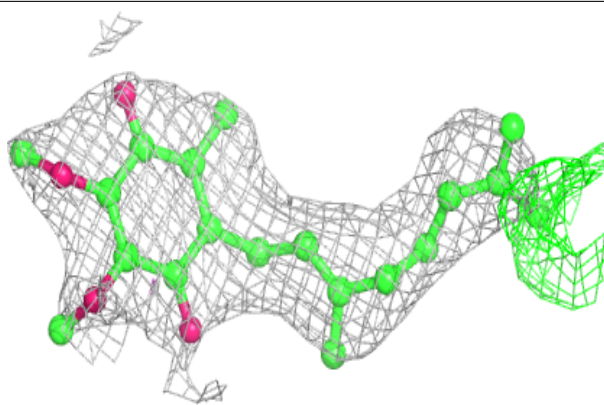
**Electron density around CDL M 409:**

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

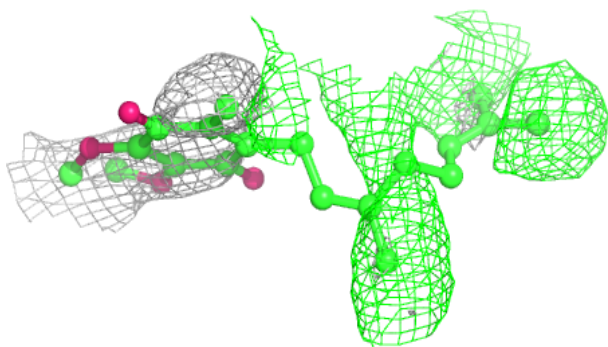
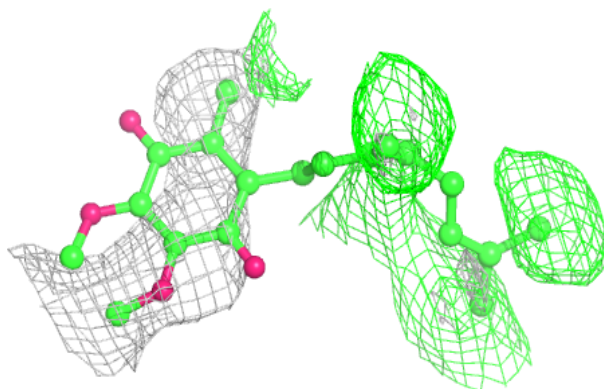


**Electron density around U10 L 305 (A):**

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

**Electron density around U10 L 305 (B):**

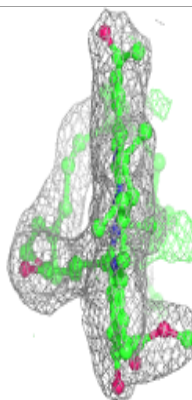
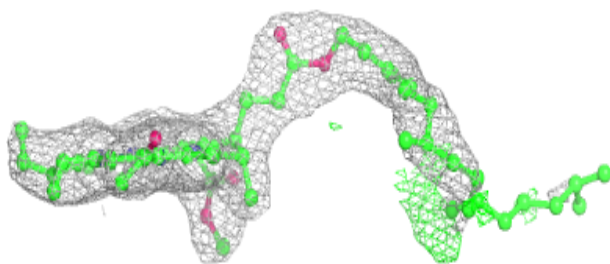
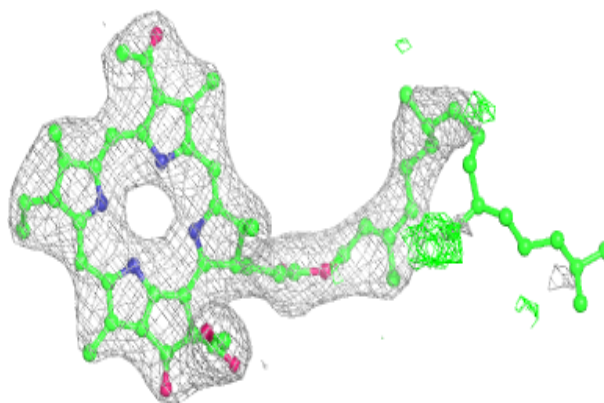
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



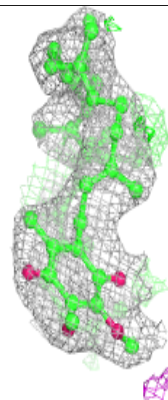
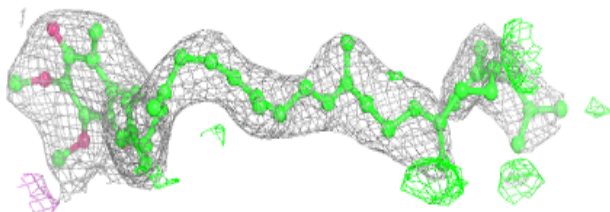
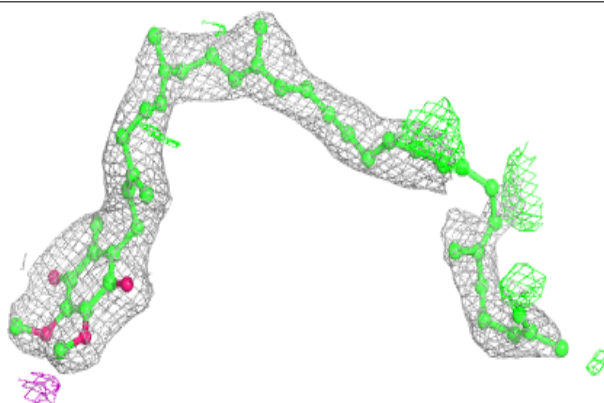


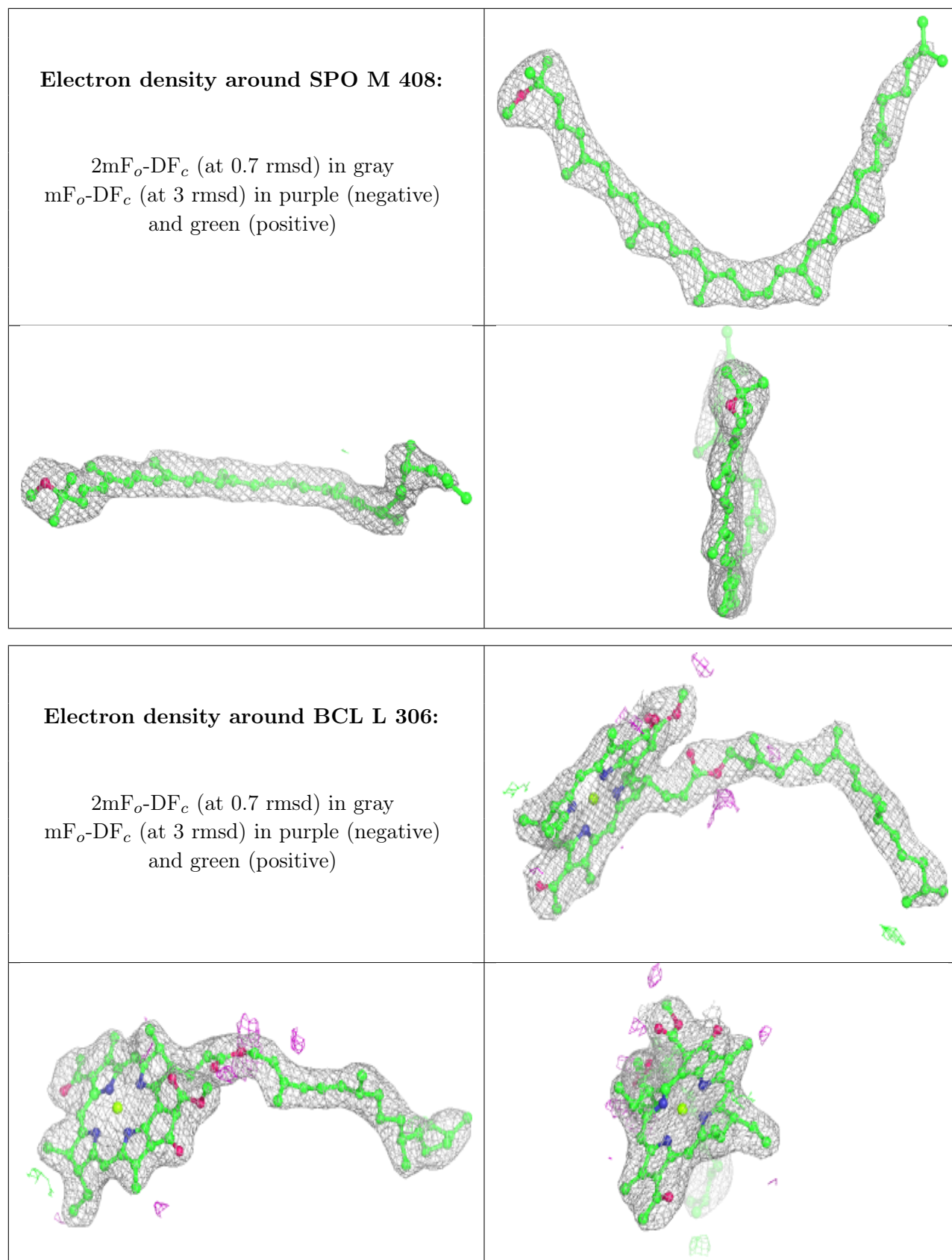
**Electron density around BPH M 406:**

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

**Electron density around U10 M 407:**

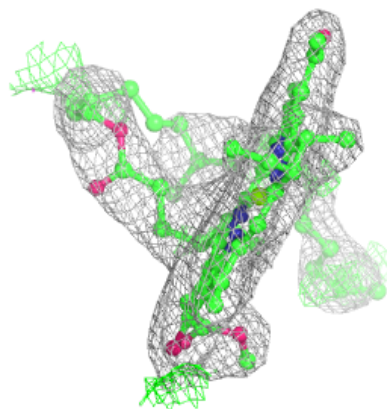
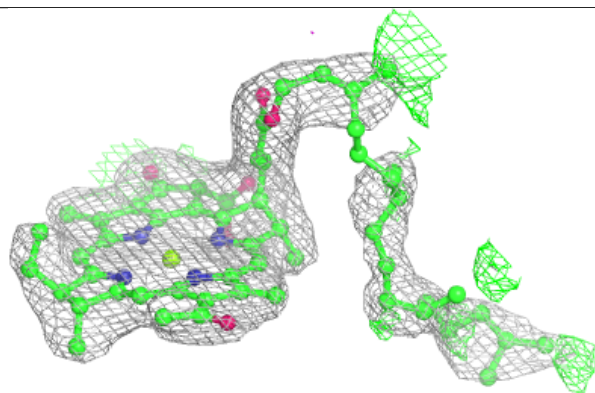
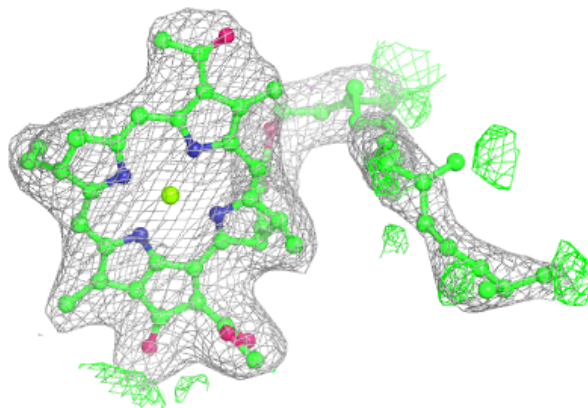
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





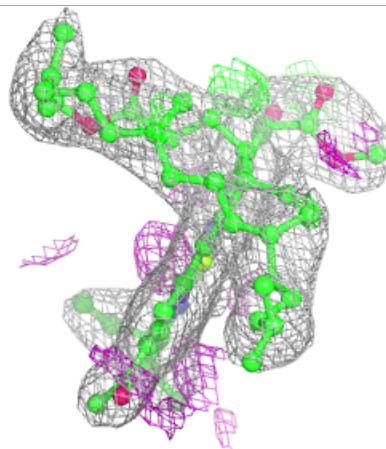
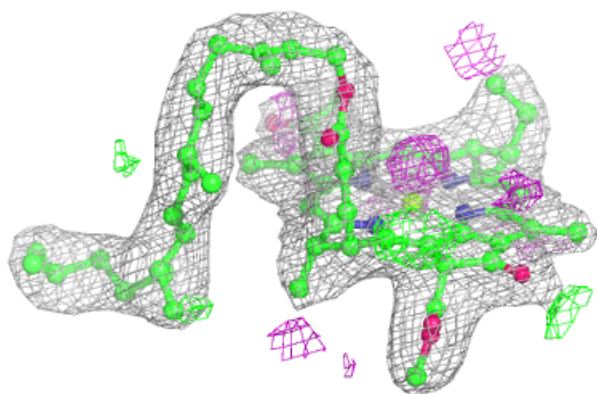
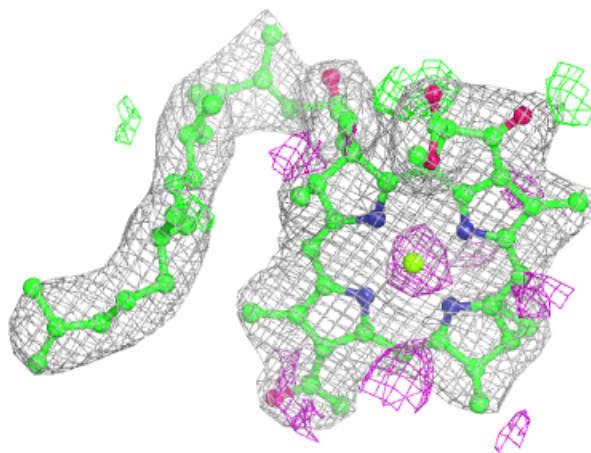
**Electron density around BCL M 401:**

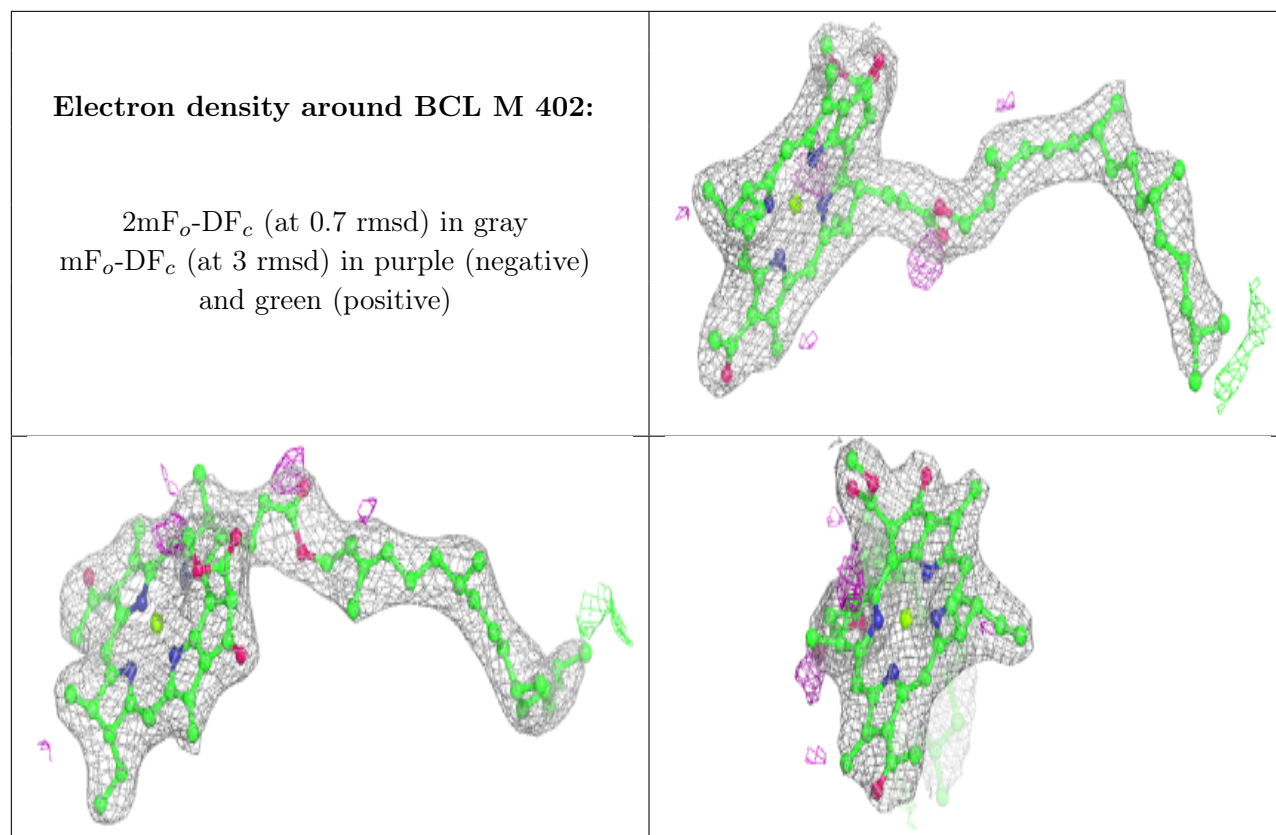
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

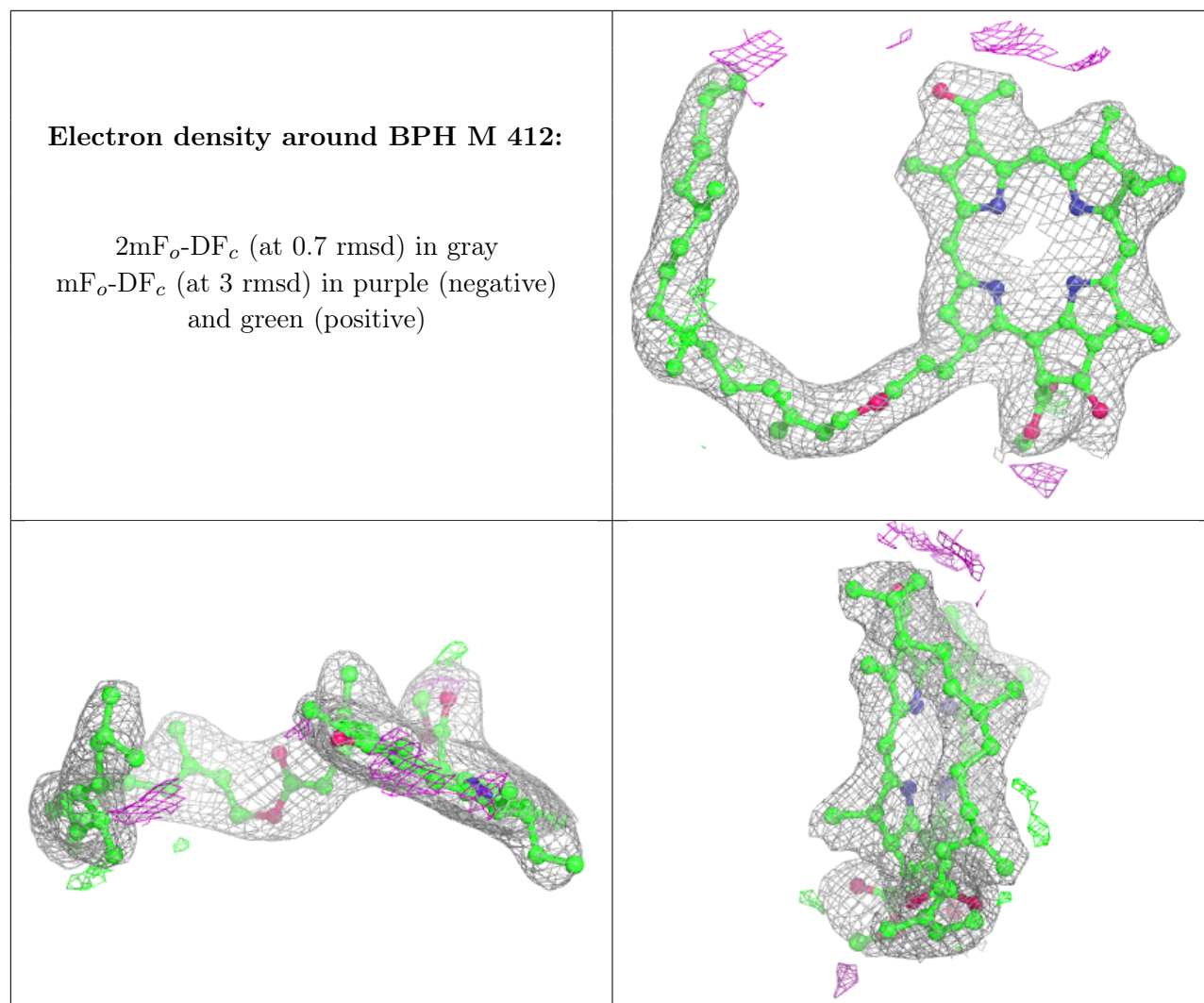


**Electron density around BCL L 301:**

$2mF_o-DF_c$  (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.