



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 12:48 pm BST

PDB ID : 4N7L  
Title : Zinc Substituted Reaction Center M(L214H) Variant of Rhodobacter sphaeroides  
Authors : Hardjasa, A.; Murphy, M.E.P.  
Deposited on : 2013-10-15  
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

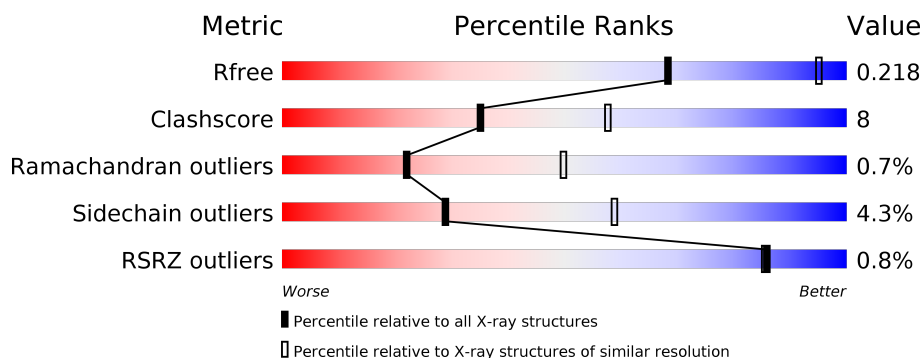
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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 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	241	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>87%</span> <span>12%</span> </div> </div>
2	L	281	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>81%</span> <span>17%</span> </div> </div>
3	M	303	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>85%</span> <span>13%</span> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HTO	L	307	-	-	-	X
10	HTO	L	308	-	-	-	X
14	PC1	M	411	-	-	-	X
4	GOL	H	301	-	-	-	X
4	GOL	H	303	-	-	-	X
4	GOL	H	304	-	-	-	X
4	GOL	L	310	-	-	-	X
5	GGD	H	306	-	-	-	X
6	LDA	L	301	-	-	-	X
6	LDA	L	302	-	-	-	X
6	LDA	L	303	-	-	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7762 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	241	Total	C	N	O	S	0	5	1
			1850	1183	321	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	2	0
			2239	1513	355	363	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	1	1
			2413	1607	398	398	10			

There is a discrepancy between the modelled and reference sequences:

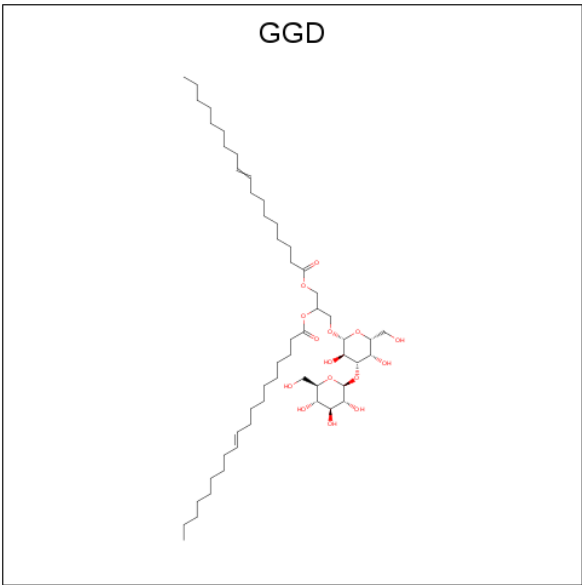
Chain	Residue	Modelled	Actual	Comment	Reference
M	214	HIS	LEU	ENGINEERED MUTATION	UNP P0C0Y9

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



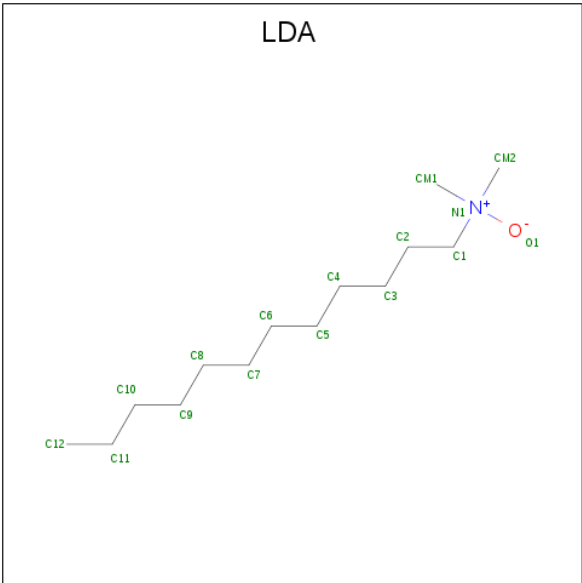
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 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
5	H	1	Total	C	O	0	0
			57	42	15		

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



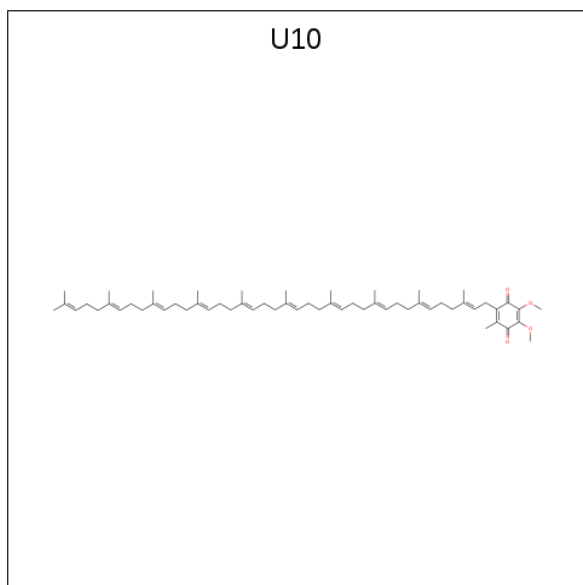
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		

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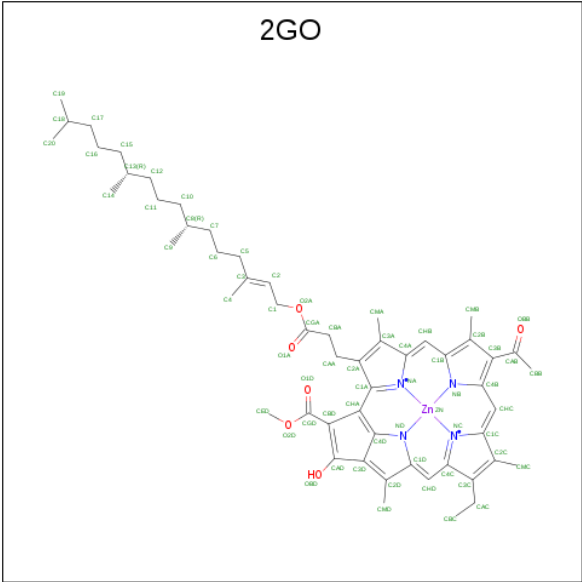
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 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
7	L	1	Total	C	O	0	1
			46	38	8		
7	M	1	Total	C	O	0	0
			48	44	4		

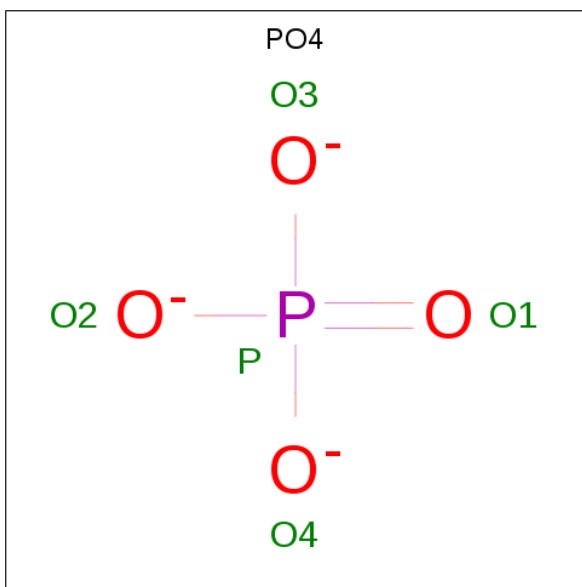
- Molecule 8 is [methyl 9-acetyl-14-ethyl-20-hydroxy-4,8,13,18-tetramethyl-3-{3-oxo-3-[(3,7,11,15-tetramethylhexadec-2-en-1-yl)oxy]propyl}-3,4,20,21-tetradehydrophorbine-21-carboxylato(2-)-kappa 4 N 23 ,N 24 ,N 25 ,N 26 ]zinc (three-letter code: 2GO) (formula: C<sub>55</sub>H<sub>70</sub>N<sub>4</sub>O<sub>6</sub>Zn).



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

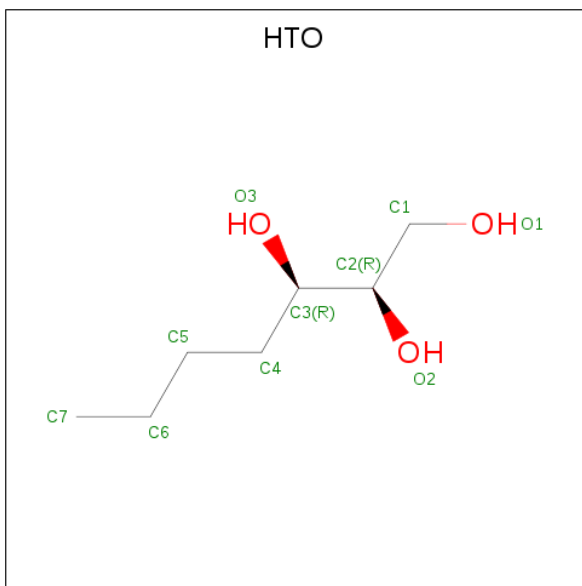
- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





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

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).

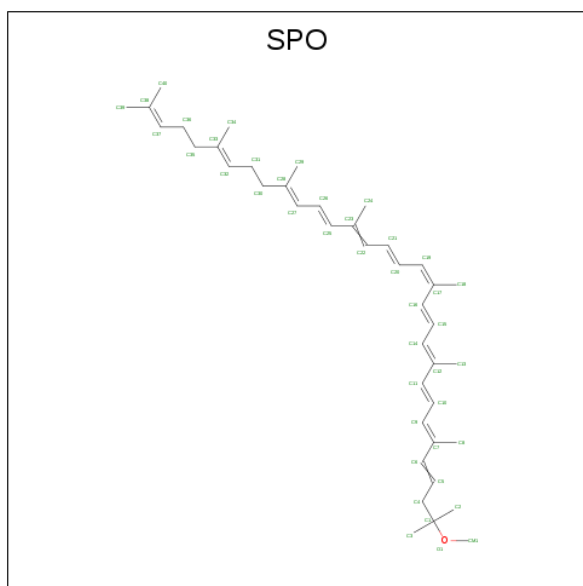


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

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

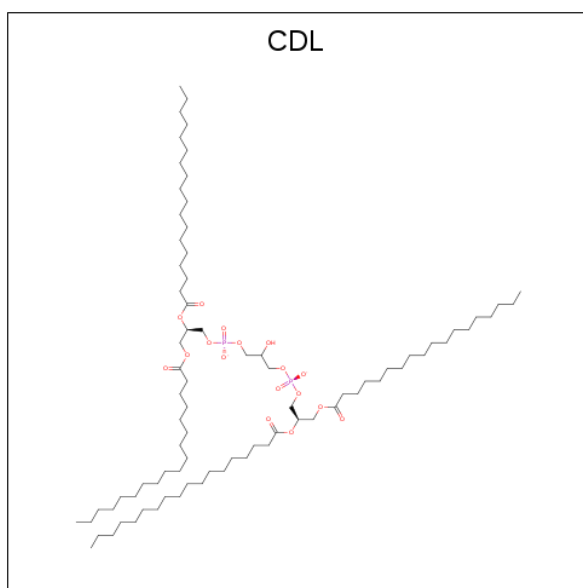
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



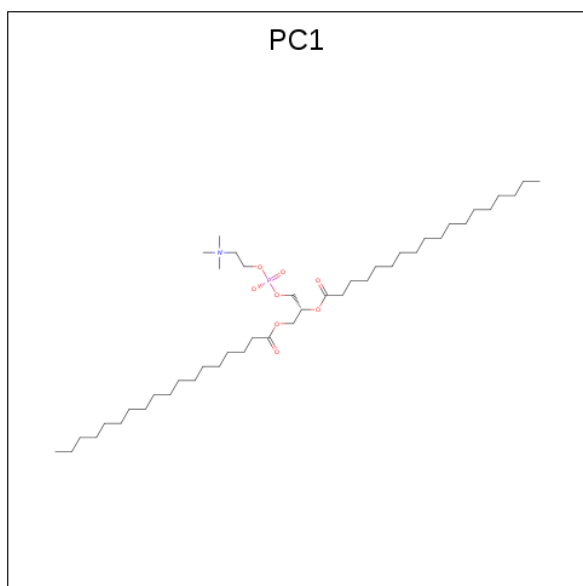
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			42	41	1		

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



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

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



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

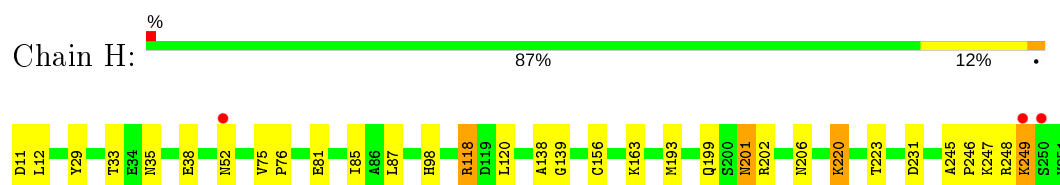
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	156	Total	O	0	0
			156	156		
15	L	114	Total	O	0	0
			114	114		
15	M	129	Total	O	0	0
			129	129		

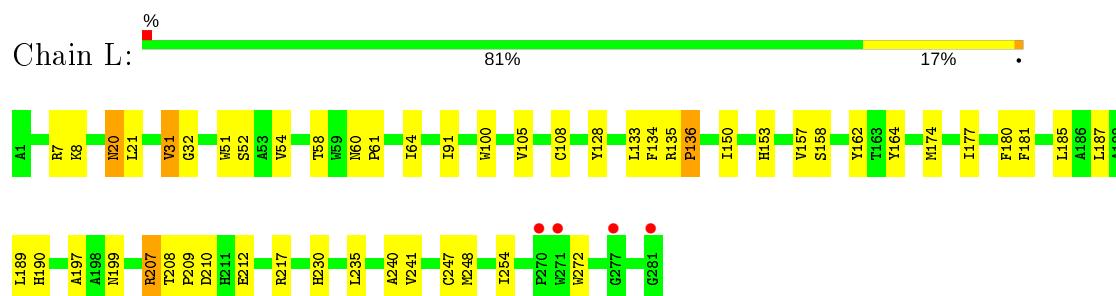
### 3 Residue-property plots [i](#)

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.

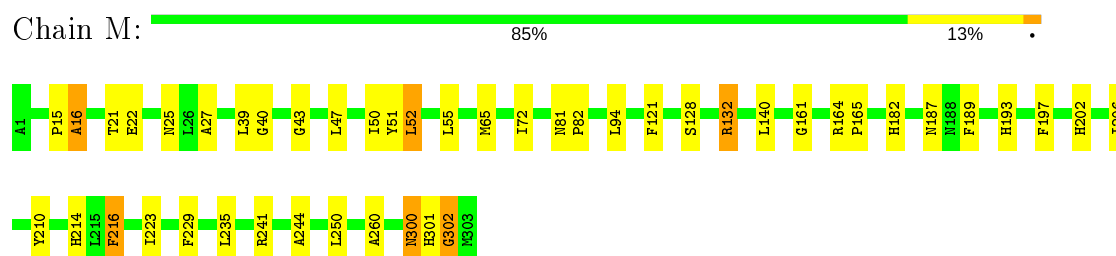
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.59Å 139.59Å 184.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.57 – 2.85 50.52 – 2.85	Depositor EDS
% Data completeness (in resolution range)	87.2 (50.57-2.85) 87.3 (50.52-2.85)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.165 , 0.216 0.171 , 0.218	Depositor DCC
$R_{free}$ test set	2153 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: GOL, LDA, GGD, CDL, PO4, PC1, HTO, FE, SPO, U10, 2GO

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	0.65	0/1930	0.82	0/2621
2	L	0.64	0/2339	0.72	0/3203
3	M	0.64	0/2511	0.74	0/3428
All	All	0.64	0/6780	0.76	0/9252

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

There are no bond length outliers.

There are no bond angle outliers.

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 [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	1850	0	1873	21	0
2	L	2239	0	2185	44	0
3	M	2413	0	2315	43	0
4	H	30	0	40	1	0
4	L	12	0	16	0	0
5	H	57	0	68	1	0
6	L	48	0	93	2	0
6	M	32	0	62	0	0
7	L	46	0	46	13	0
7	M	48	0	63	4	0
8	L	132	0	138	12	0
8	M	264	0	276	29	0
9	L	5	0	0	0	0
10	L	20	0	32	1	0
11	M	1	0	0	0	0
12	M	42	0	60	5	0
13	M	81	0	106	1	0
14	M	43	0	60	1	0
15	H	156	0	0	1	1
15	L	114	0	0	2	0
15	M	129	0	0	5	0
All	All	7762	0	7433	122	1

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 8.

The worst 5 of 122 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:206:ILE:HD13	8:M:401:2GO:H9	1.58	0.84
3:M:210:TYR:HB3	8:M:402:2GO:H21	1.64	0.79
2:L:189:LEU:HD23	8:L:311:2GO:H8	1.64	0.78
8:M:404:2GO:H19	8:M:404:2GO:H22	1.72	0.70
3:M:55:LEU:HB3	15:M:559:HOH:O	1.91	0.70

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:433:HOH:O	15:H:433:HOH:O[4_555]	1.98	0.22

## 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	245/241 (102%)	235 (96%)	8 (3%)	2 (1%)	19	46
2	L	281/281 (100%)	259 (92%)	20 (7%)	2 (1%)	22	50
3	M	302/303 (100%)	280 (93%)	19 (6%)	3 (1%)	15	40
All	All	828/825 (100%)	774 (94%)	47 (6%)	7 (1%)	22	46

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	301	HIS
3	M	16	ALA
3	M	302	GLY
1	H	249[A]	LYS
1	H	249[B]	LYS

### 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	200/196 (102%)	186 (93%)	14 (7%)	15	37
2	L	221/220 (100%)	211 (96%)	10 (4%)	27	57
3	M	237/237 (100%)	229 (97%)	8 (3%)	37	67
All	All	658/653 (101%)	626 (95%)	32 (5%)	29	54

5 of 32 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	L	20	ASN
2	L	158	SER
3	M	132	ARG
2	L	136	PRO
2	L	207	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	20	ASN
3	M	193	HIS
3	M	77	GLN
1	H	206	ASN
2	L	264	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 1 is 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
7	U10	L	304[B]	-	23,23,63	2.03	2 (8%)	28,31,79	1.51	4 (14%)
4	GOL	H	301	-	5,5,5	0.69	0	5,5,5	0.60	0
10	HTO	L	308	-	9,9,9	0.79	0	10,10,10	0.93	1 (10%)
8	2GO	M	403	3	59,74,74	1.99	15 (25%)	52,115,115	2.31	14 (26%)
8	2GO	M	402	3	59,74,74	1.95	16 (27%)	52,115,115	2.41	14 (26%)
8	2GO	L	305	2	59,74,74	1.83	12 (20%)	52,115,115	2.26	11 (21%)
8	2GO	M	401	2	59,74,74	2.14	15 (25%)	52,115,115	2.34	17 (32%)
9	PO4	L	306	-	4,4,4	0.88	0	6,6,6	0.52	0
4	GOL	H	304	-	5,5,5	0.43	0	5,5,5	0.35	0
10	HTO	L	307	-	9,9,9	0.80	0	10,10,10	0.73	0
13	CDL	M	410	-	80,80,99	3.19	5 (6%)	86,92,111	1.33	8 (9%)
6	LDA	M	405	-	12,15,15	1.99	1 (8%)	14,17,17	0.67	1 (7%)
4	GOL	H	302	-	5,5,5	0.69	0	5,5,5	1.08	0
6	LDA	L	302	-	12,15,15	2.09	1 (8%)	14,17,17	0.48	0
5	GGD	H	306	-	58,58,68	1.01	3 (5%)	72,72,82	1.37	10 (13%)
12	SPO	M	409	-	40,41,41	0.78	0	47,50,50	1.74	13 (27%)
4	GOL	H	303	-	5,5,5	0.38	0	5,5,5	0.24	0
4	GOL	L	309	-	5,5,5	0.55	0	5,5,5	0.64	0
14	PC1	M	411	-	42,42,53	1.40	4 (9%)	48,50,61	2.31	10 (20%)
7	U10	M	408	-	48,48,63	1.73	4 (8%)	58,61,79	1.88	13 (22%)
4	GOL	H	305	-	5,5,5	0.70	0	5,5,5	0.92	0
8	2GO	M	404	3	59,74,74	1.97	14 (23%)	52,115,115	2.69	14 (26%)
6	LDA	M	406	-	12,15,15	2.13	1 (8%)	14,17,17	0.73	0
6	LDA	L	303	-	12,15,15	2.07	1 (8%)	14,17,17	0.52	0
4	GOL	L	310	-	5,5,5	0.63	0	5,5,5	0.57	0
7	U10	L	304[A]	-	23,23,63	1.97	2 (8%)	28,31,79	2.36	6 (21%)
8	2GO	L	311	-	59,74,74	2.20	16 (27%)	52,115,115	2.80	17 (32%)
6	LDA	L	301	-	12,15,15	2.08	1 (8%)	14,17,17	0.51	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
7	U10	L	304[B]	-	-	6/15/39/87	0/1/1/1
4	GOL	H	301	-	-	2/4/4/4	-
10	HTO	L	308	-	-	3/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2GO	M	403	3	-	20/37/97/97	-
8	2GO	M	402	3	-	7/37/97/97	-
8	2GO	L	305	2	-	4/37/97/97	-
8	2GO	M	401	2	-	8/37/97/97	-
4	GOL	H	304	-	-	2/4/4/4	-
10	HTO	L	307	-	-	5/10/10/10	-
13	CDL	M	410	-	-	43/91/91/110	-
6	LDA	M	405	-	-	9/13/13/13	-
4	GOL	H	302	-	-	2/4/4/4	-
6	LDA	L	302	-	-	3/13/13/13	-
5	GGD	H	306	-	-	15/47/87/97	0/2/2/2
12	SPO	M	409	-	-	6/47/47/47	-
4	GOL	H	303	-	-	0/4/4/4	-
4	GOL	L	309	-	-	2/4/4/4	-
14	PC1	M	411	-	-	26/46/46/57	-
7	U10	M	408	-	-	10/45/69/87	0/1/1/1
4	GOL	H	305	-	-	2/4/4/4	-
8	2GO	M	404	3	-	8/37/97/97	-
6	LDA	M	406	-	-	7/13/13/13	-
6	LDA	L	303	-	-	6/13/13/13	-
4	GOL	L	310	-	-	1/4/4/4	-
7	U10	L	304[A]	-	-	6/15/39/87	0/1/1/1
8	2GO	L	311	-	-	15/37/97/97	-
6	LDA	L	301	-	-	6/13/13/13	-

The worst 5 of 113 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	410	CDL	C75-C74	26.18	2.98	1.51
7	L	304[B]	U10	C6-C1	8.73	1.51	1.35
7	M	408	U10	C6-C1	8.66	1.51	1.35
7	L	304[A]	U10	C6-C1	7.94	1.49	1.35
6	M	406	LDA	O1-N1	-7.24	1.25	1.42

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	304[A]	U10	C7-C6-C5	8.46	128.66	118.48
8	M	404	2GO	CMA-C3A-C2A	-8.36	109.19	124.94
8	M	403	2GO	CMA-C3A-C2A	-8.14	109.59	124.94
14	M	411	PC1	C15-N-C13	-7.96	88.51	108.97
8	L	305	2GO	CMA-C3A-C2A	-7.88	110.08	124.94

There are no chirality outliers.

5 of 224 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	GOL	O1-C1-C2-C3
8	M	403	2GO	C1A-C2A-CAA-CBA
8	M	402	2GO	C1A-C2A-CAA-CBA
8	M	402	2GO	O2A-C1-C2-C3
8	L	305	2GO	C4C-C3C-CAC-CBC

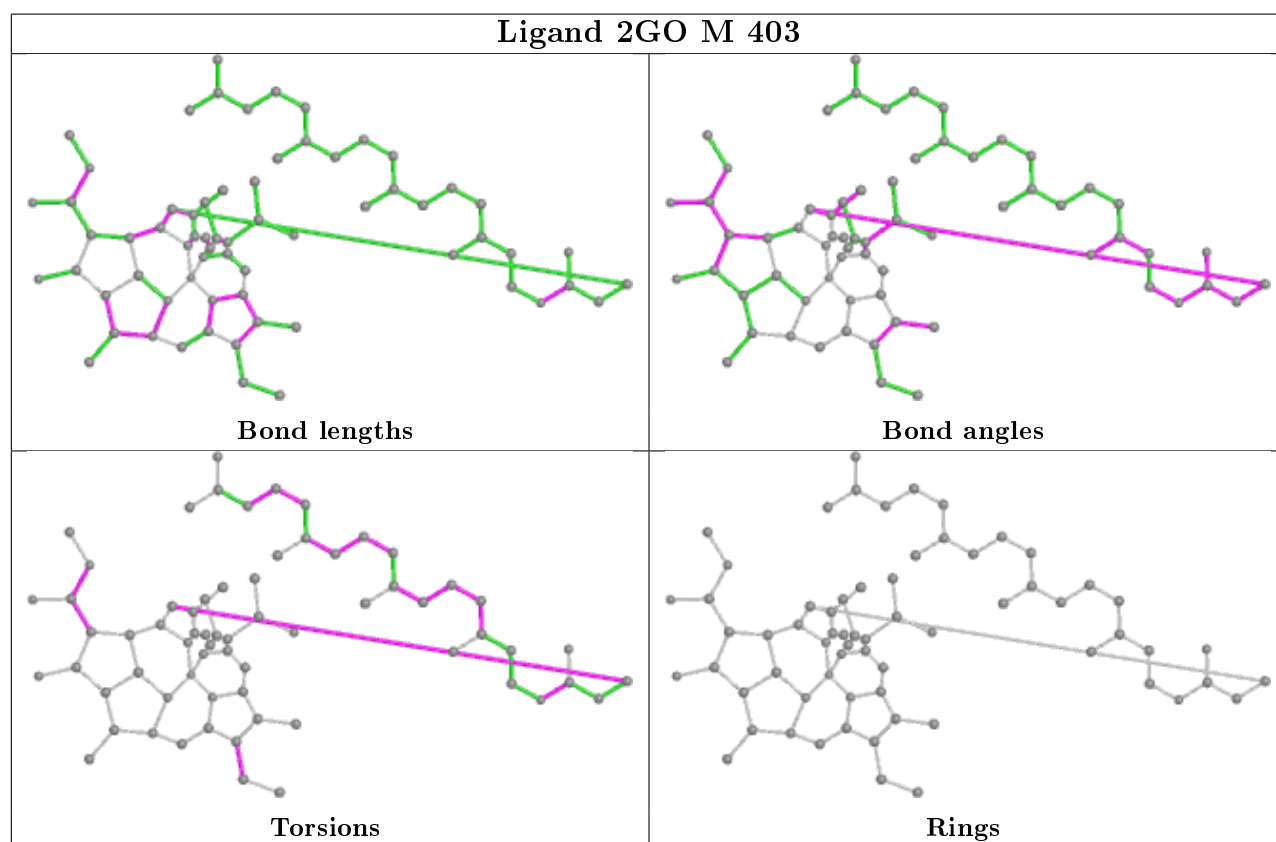
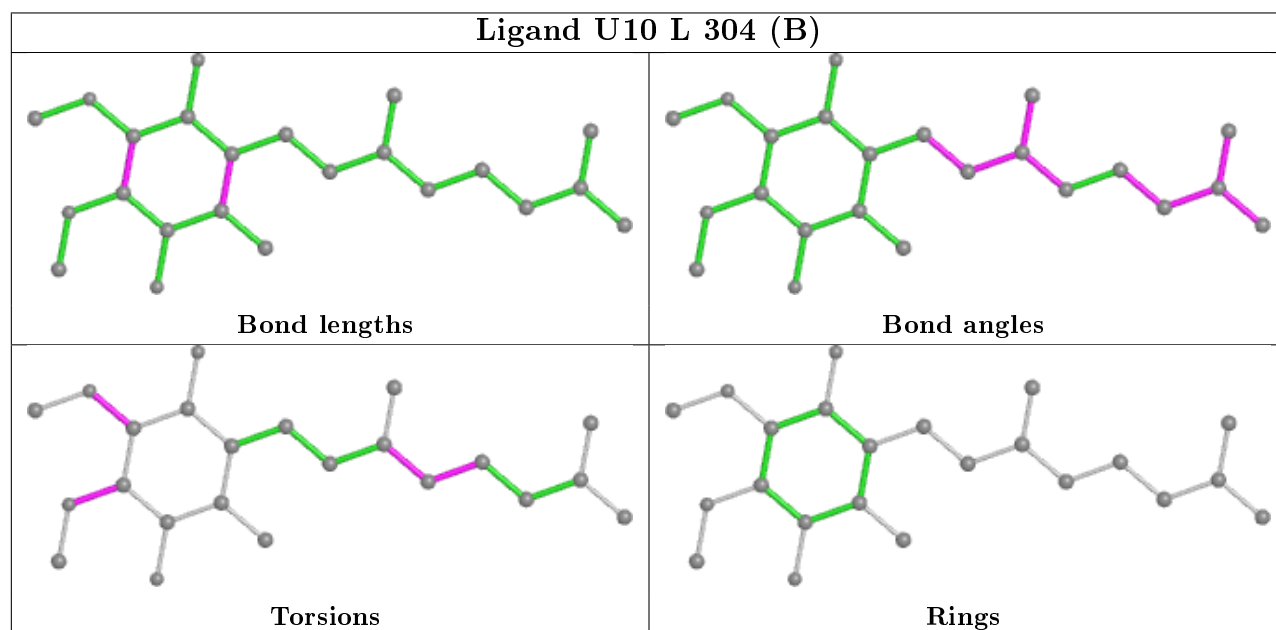
There are no ring outliers.

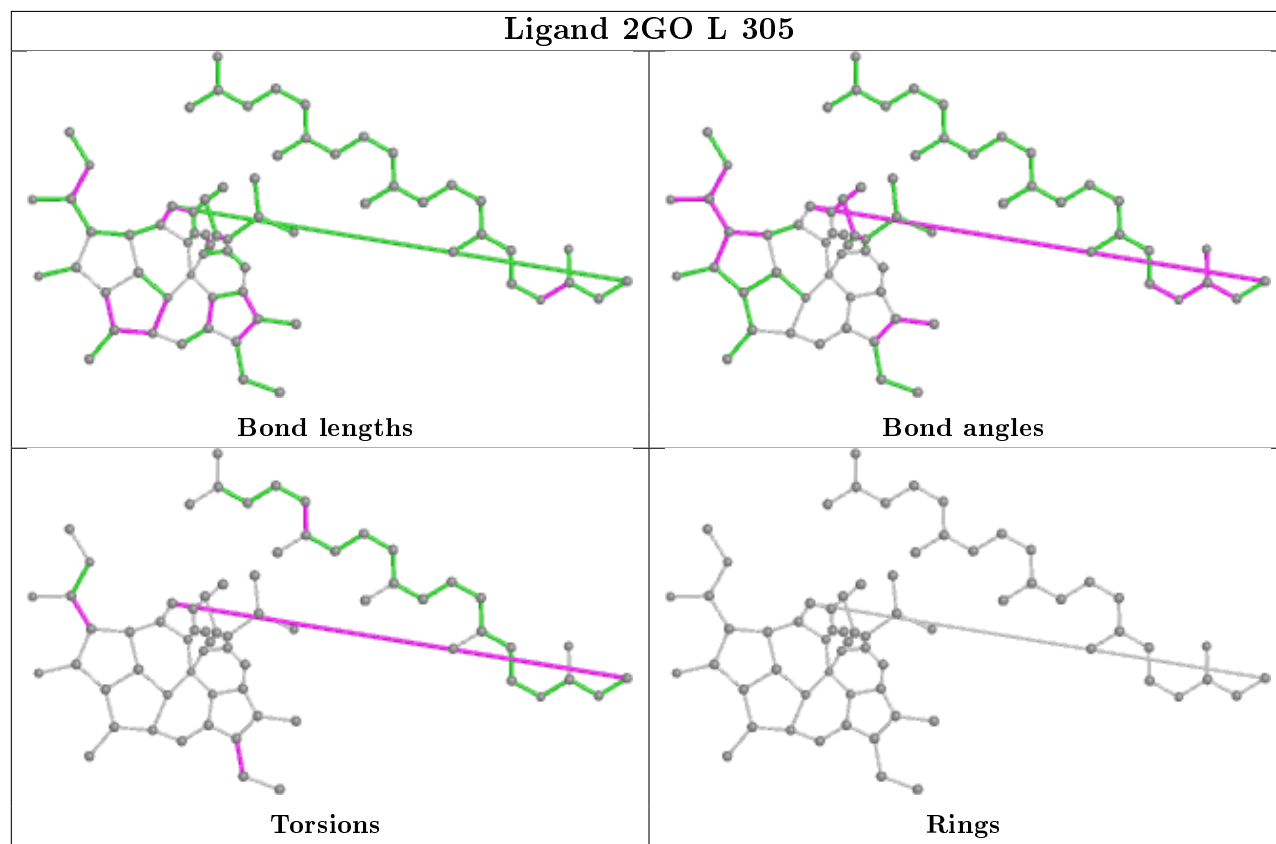
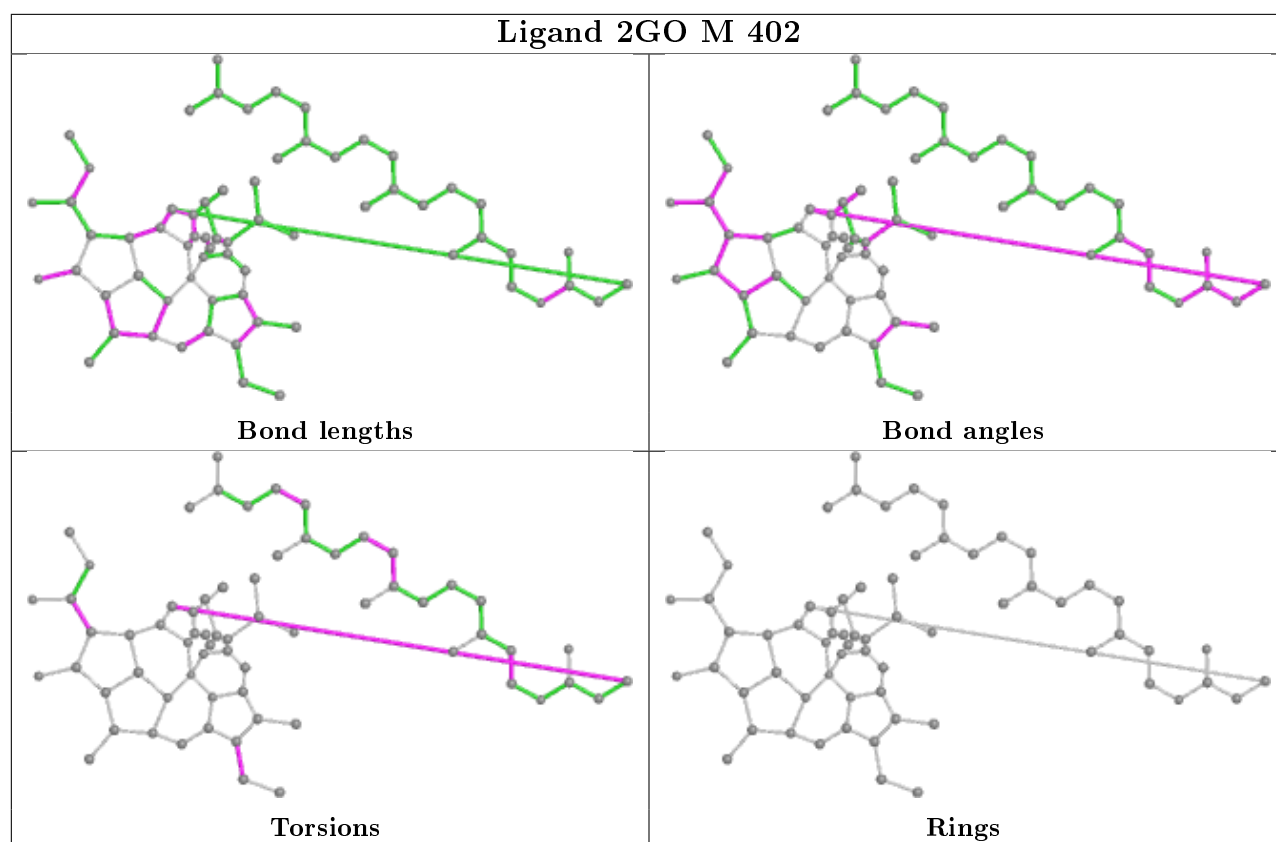
16 monomers are involved in 60 short contacts:

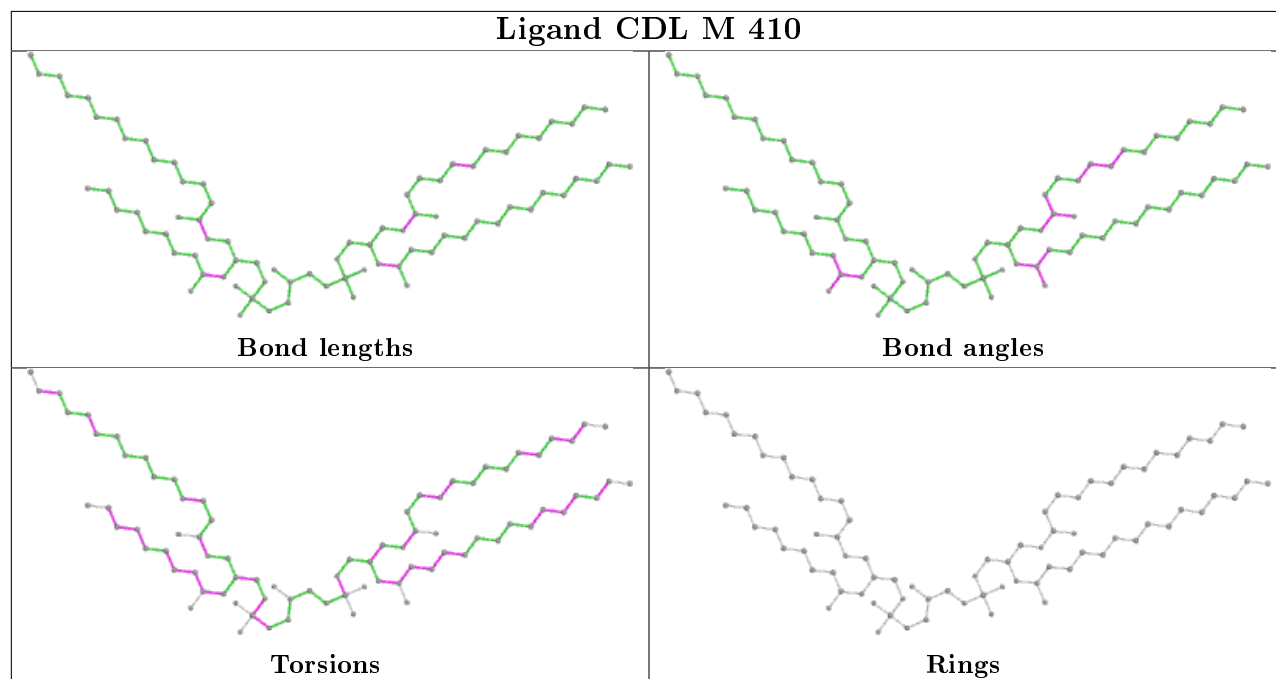
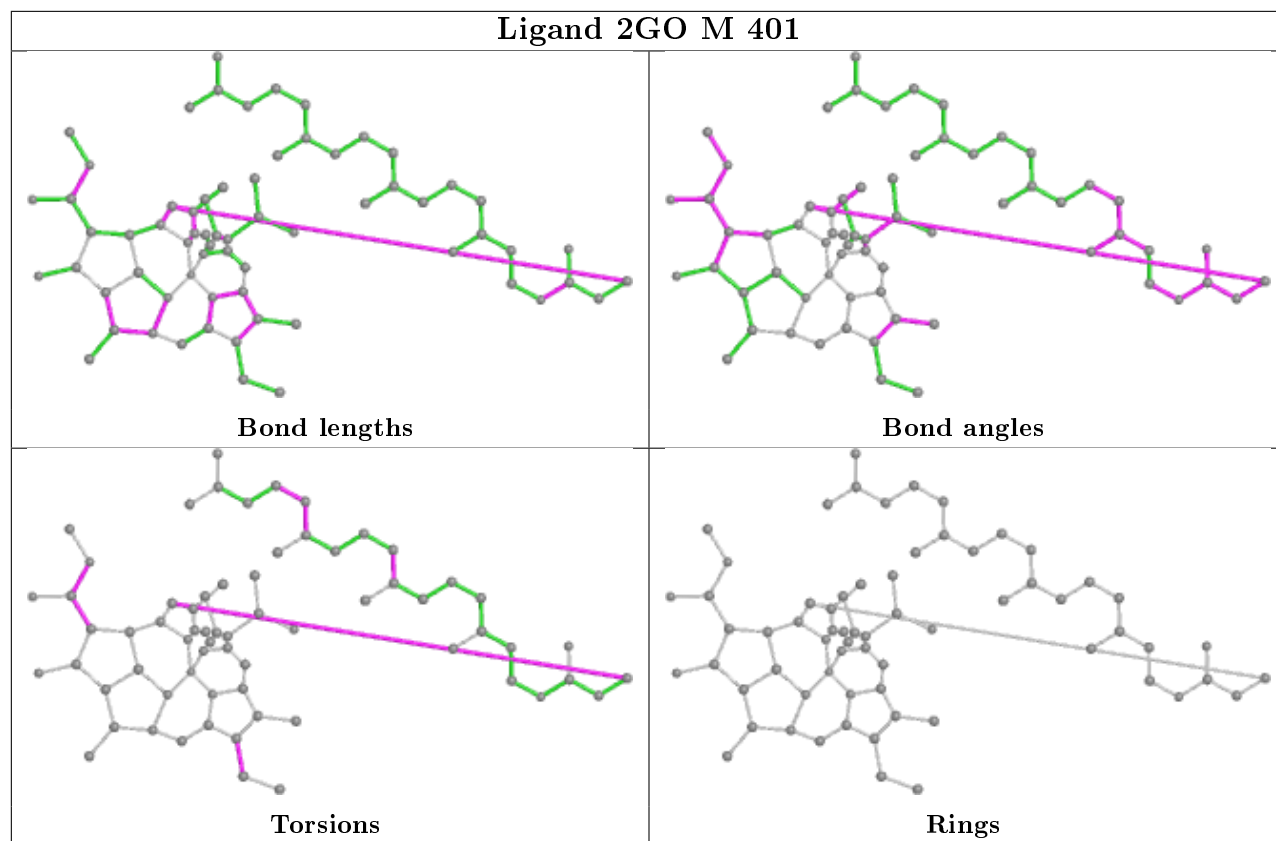
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	304[B]	U10	8	0
8	M	403	2GO	8	0
8	M	402	2GO	11	0
8	L	305	2GO	2	0
8	M	401	2GO	6	0
10	L	307	HTO	1	0
13	M	410	CDL	1	0
5	H	306	GGD	1	0
12	M	409	SPO	5	0
14	M	411	PC1	1	0
7	M	408	U10	4	0
4	H	305	GOL	1	0
8	M	404	2GO	6	0
6	L	303	LDA	2	0
7	L	304[A]	U10	5	0
8	L	311	2GO	10	0

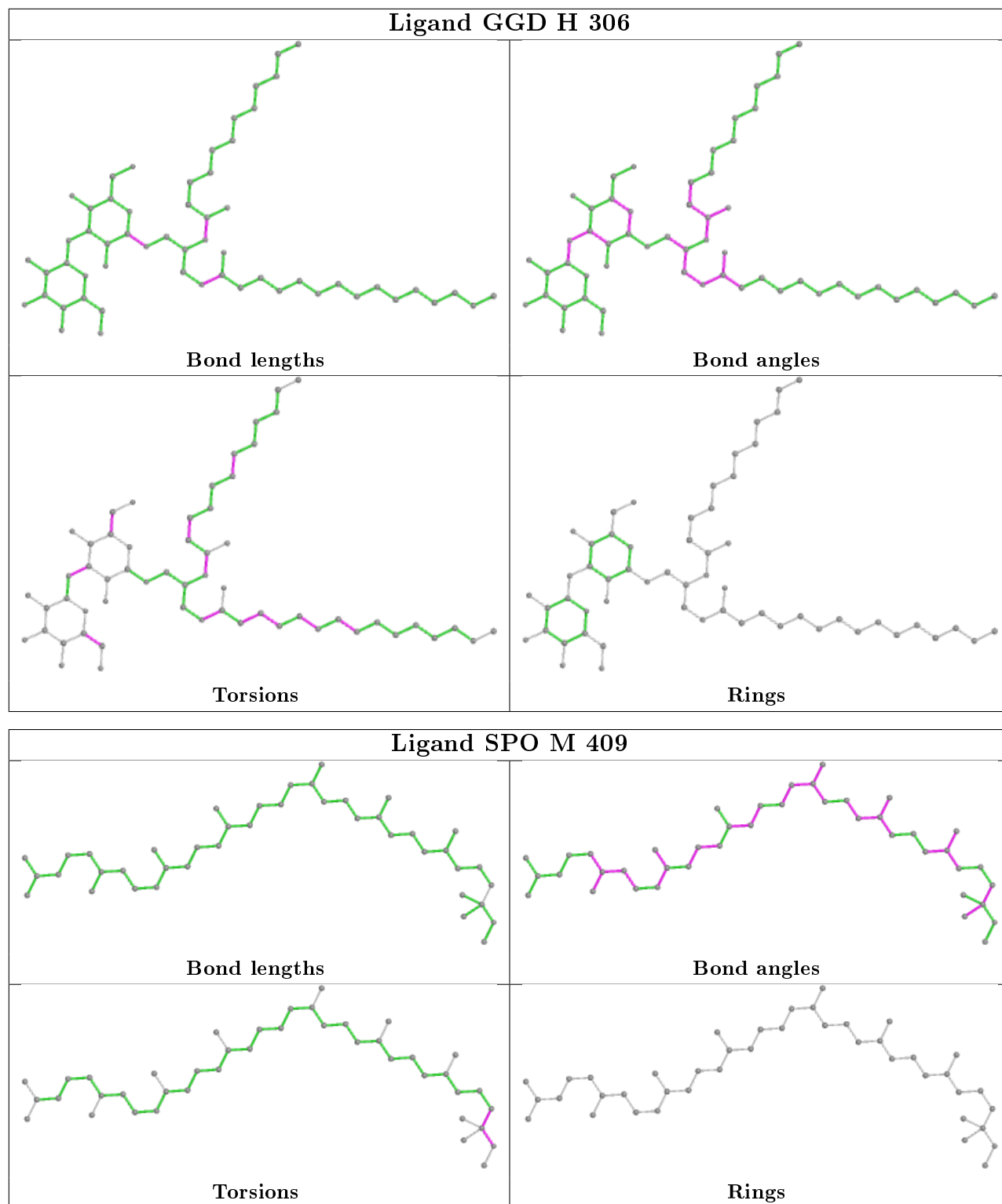
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

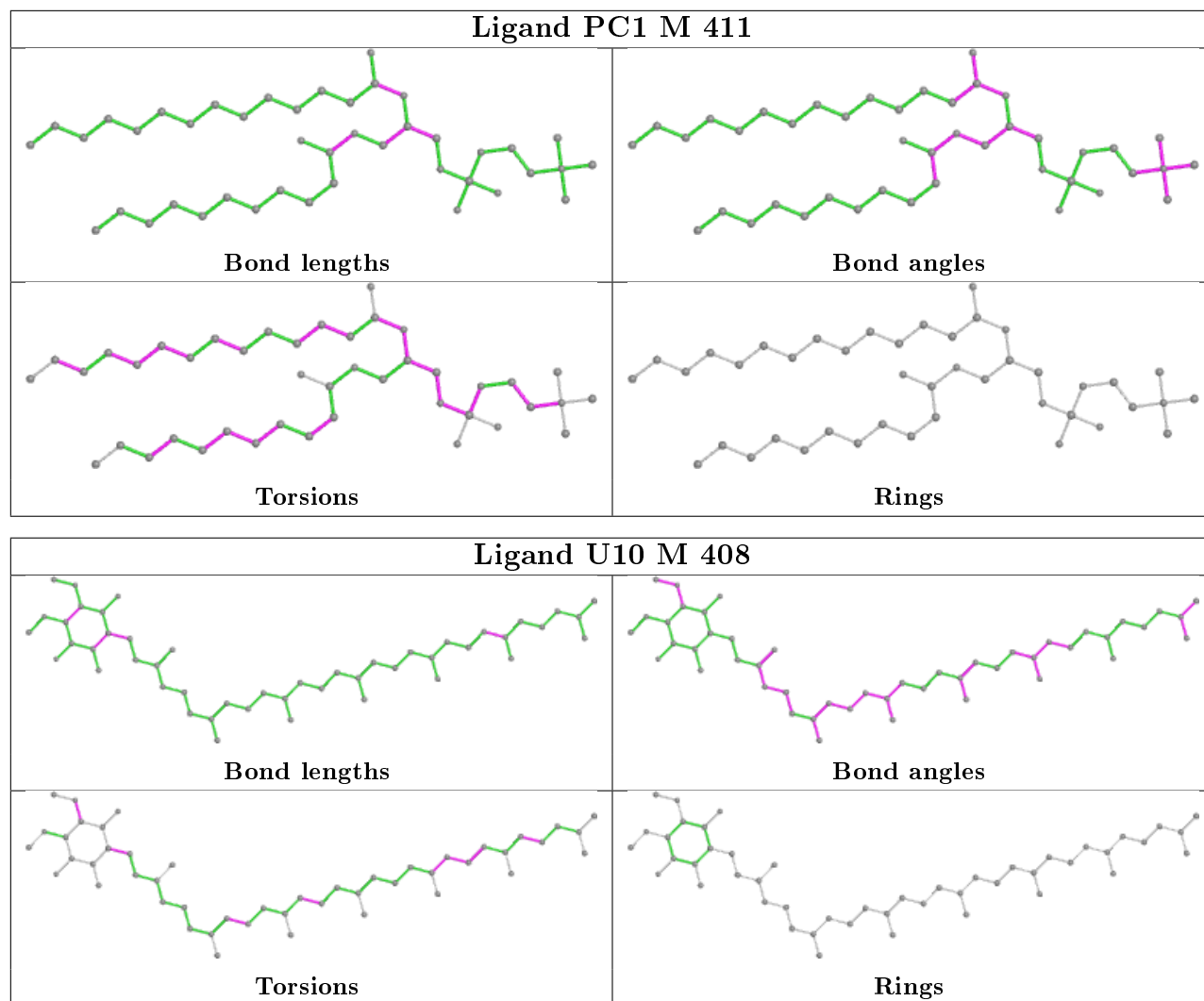


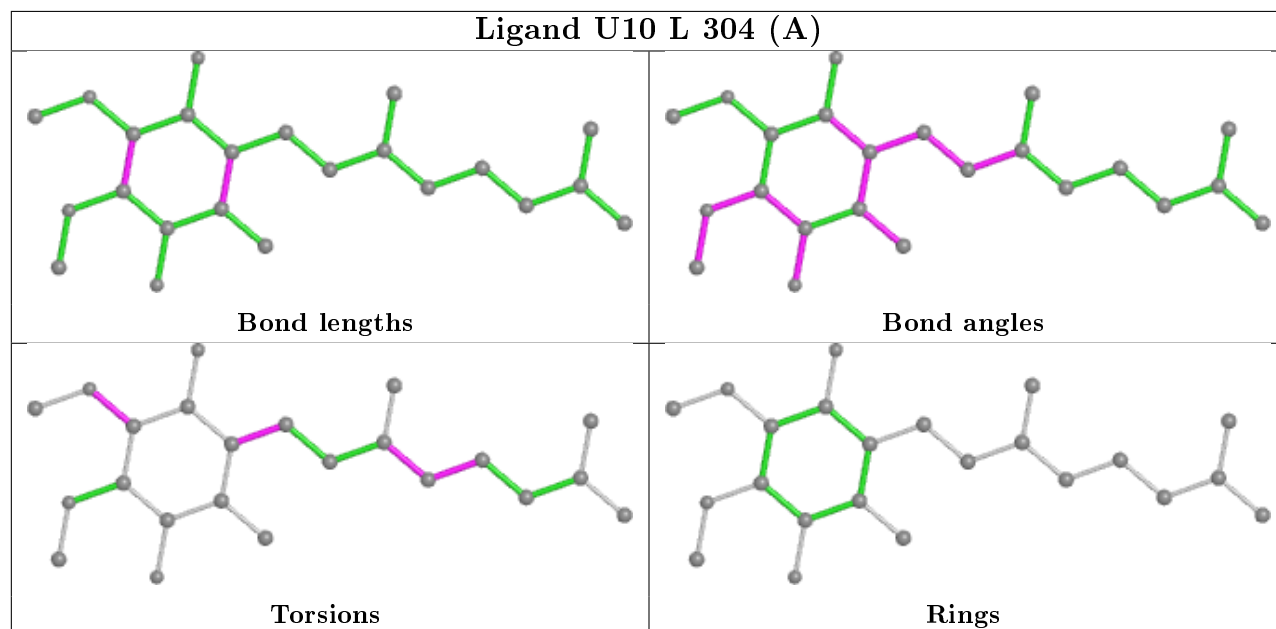
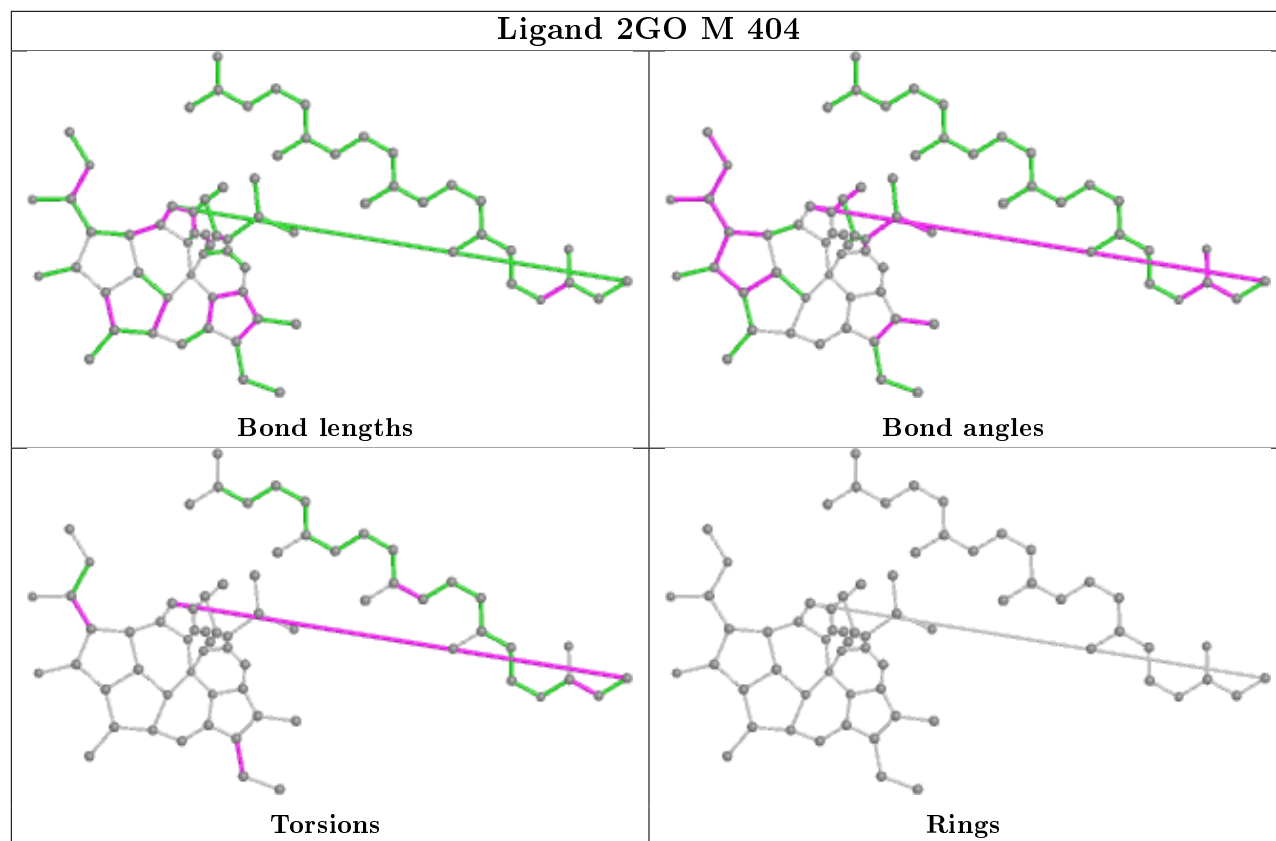


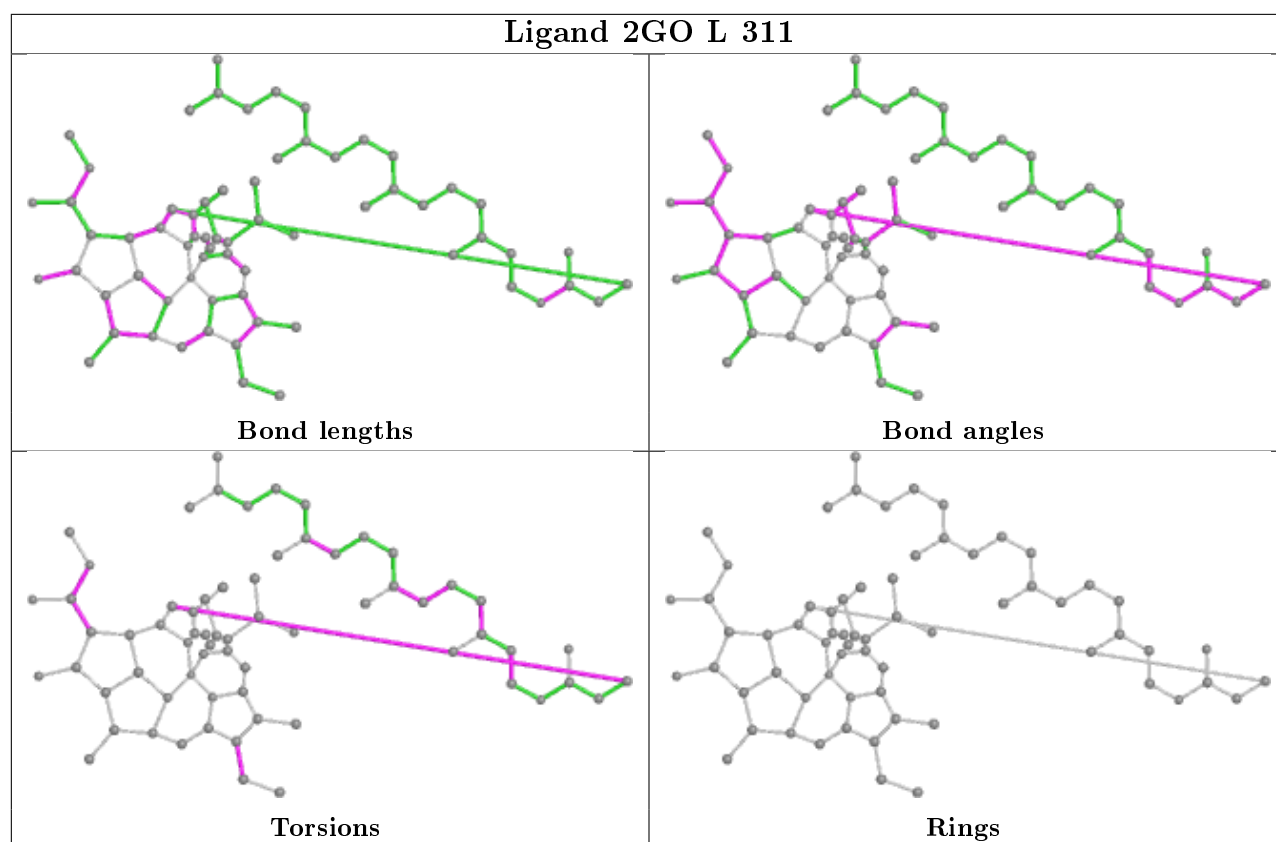












## 5.7 Other polymers [i](#)

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	241/241 (100%)	-0.64	3 (1%) 79 78	33, 47, 67, 141	3 (1%)
2	L	281/281 (100%)	-0.58	4 (1%) 75 74	34, 48, 82, 109	0
3	M	303/303 (100%)	-0.49	0 100 100	31, 50, 77, 92	6 (1%)
All	All	825/825 (100%)	-0.57	7 (0%) 86 85	31, 48, 78, 141	9 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	249[A]	LYS	3.2
2	L	281	GLY	2.8
2	L	277	GLY	2.8
1	H	250	SER	2.3
2	L	271[A]	TRP	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

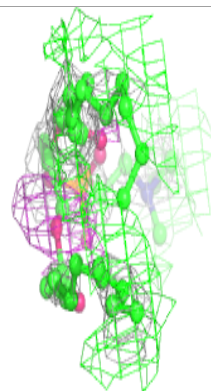
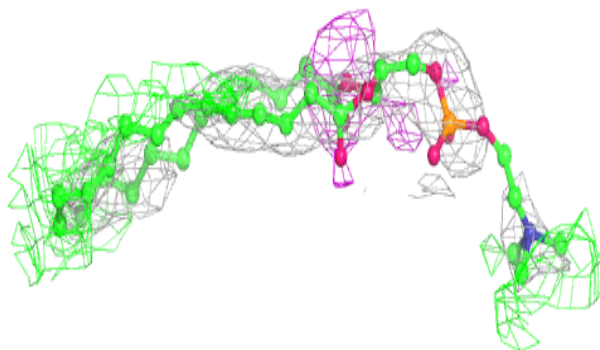
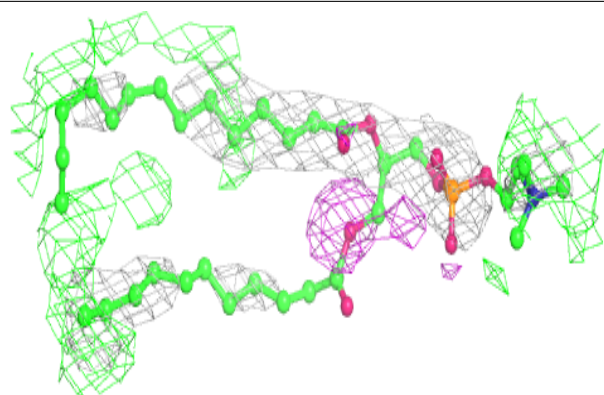
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	LDA	L	302	16/16	0.50	0.54	74,96,139,142	0
14	PC1	M	411	43/54	0.59	0.49	79,115,160,164	0
4	GOL	L	310	6/6	0.61	0.46	88,103,108,112	0
5	GGD	H	306	57/67	0.62	0.56	67,132,184,197	0
6	LDA	L	303	16/16	0.65	0.50	70,118,144,144	0
4	GOL	H	304	6/6	0.69	0.41	86,95,99,102	0
4	GOL	H	303	6/6	0.70	0.65	97,113,117,118	0
6	LDA	L	301	16/16	0.70	0.62	63,114,151,153	0
4	GOL	H	301	6/6	0.76	0.41	90,106,116,120	0
10	HTO	L	308	10/10	0.77	0.93	89,100,116,127	0
7	U10	L	304[A]	23/63	0.78	0.35	69,80,92,94	23
7	U10	L	304[B]	23/63	0.78	0.35	38,44,49,52	23
10	HTO	L	307	10/10	0.79	0.75	84,101,113,113	0
4	GOL	H	302	6/6	0.81	0.47	66,78,82,86	0
8	2GO	L	311	66/66	0.84	0.32	75,108,133,143	0
7	U10	M	408	48/63	0.85	0.26	61,76,91,94	0
4	GOL	L	309	6/6	0.86	0.40	75,83,84,89	0
13	CDL	M	410	81/100	0.89	0.35	64,96,144,149	0
6	LDA	M	405	16/16	0.89	0.38	65,86,92,93	0
6	LDA	M	406	16/16	0.90	0.26	62,79,106,106	0
12	SPO	M	409	42/42	0.95	0.24	41,59,96,117	0
4	GOL	H	305	6/6	0.95	0.21	49,63,73,78	0
9	PO4	L	306	5/5	0.97	0.15	84,87,95,99	0
8	2GO	M	401	66/66	0.98	0.16	28,39,65,78	0
8	2GO	M	403	66/66	0.98	0.15	33,41,128,145	0
8	2GO	M	402	66/66	0.98	0.16	34,42,55,62	0
8	2GO	M	404	66/66	0.98	0.17	39,48,98,121	0
8	2GO	L	305	66/66	0.98	0.18	37,44,61,77	0
11	FE	M	407	1/1	0.99	0.16	40,40,40,40	0

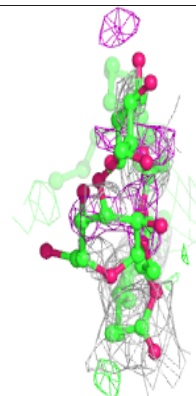
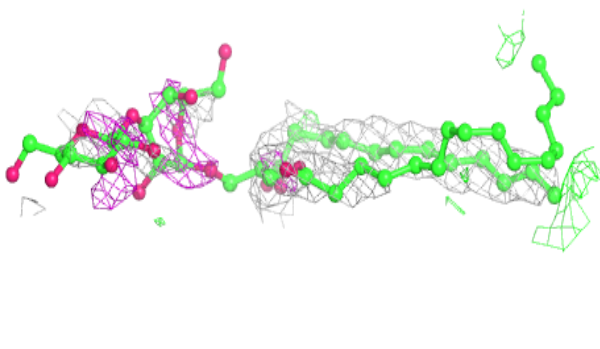
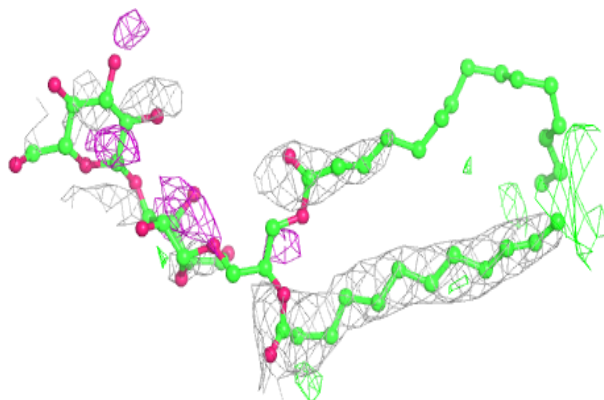
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PC1 M 411:**

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

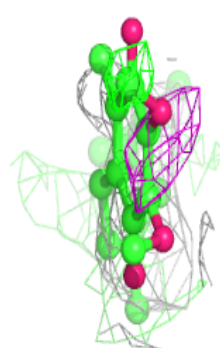
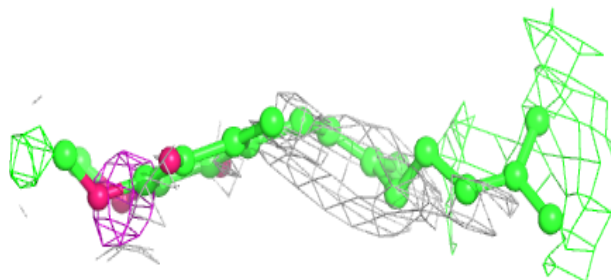
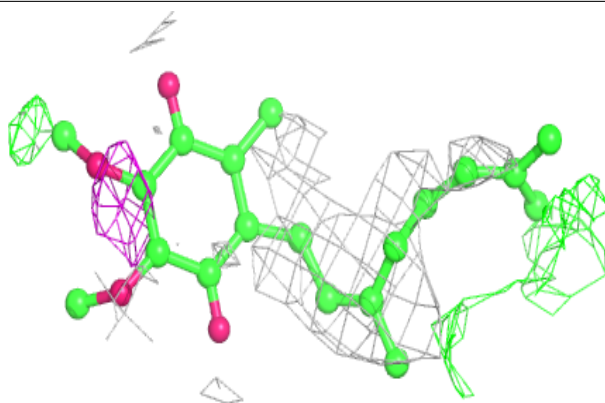
**Electron density around GGD H 306:**

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

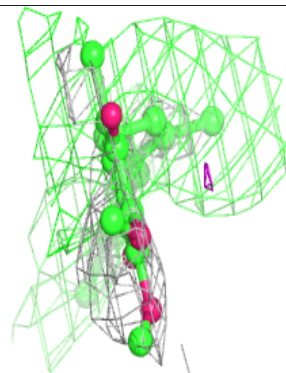
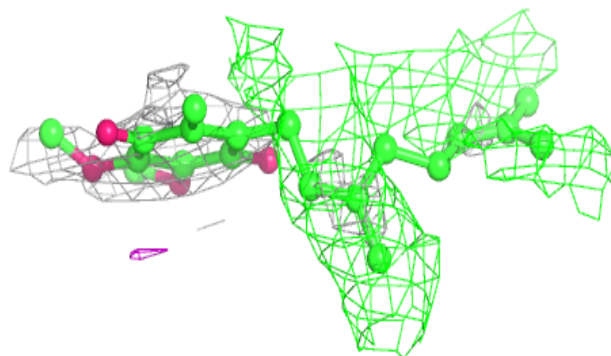
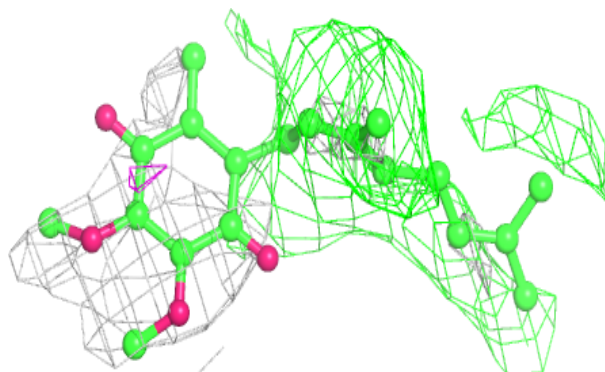


**Electron density around U10 L 304 (A):**

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

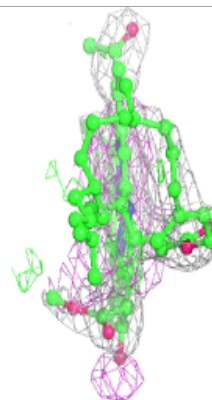
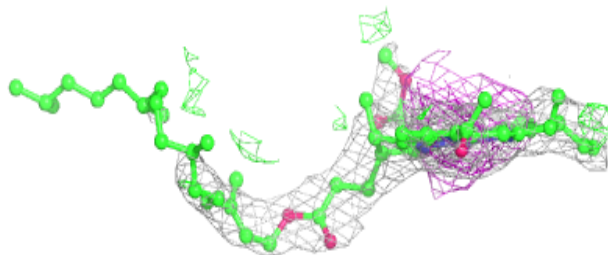
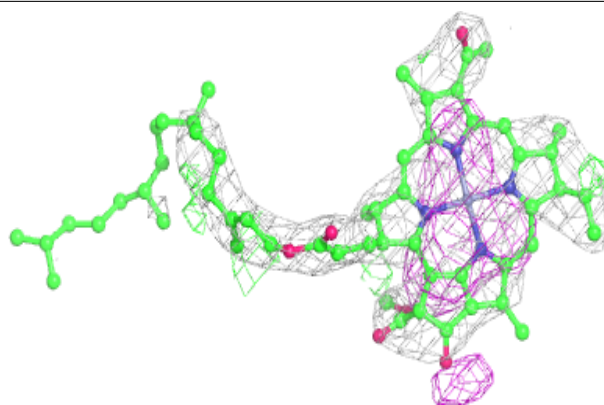
**Electron density around U10 L 304 (B):**

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

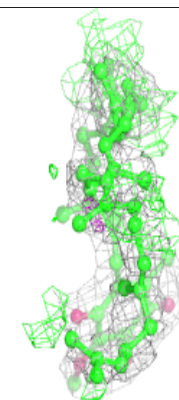
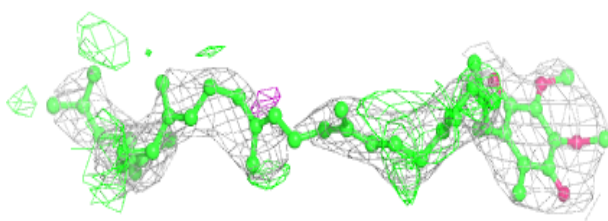
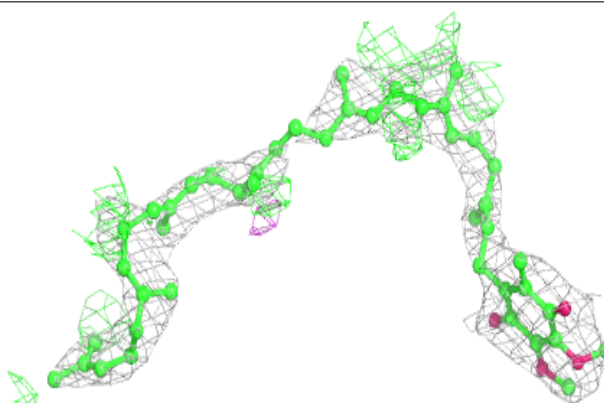


**Electron density around 2GO L 311:**

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

**Electron density around U10 M 408:**

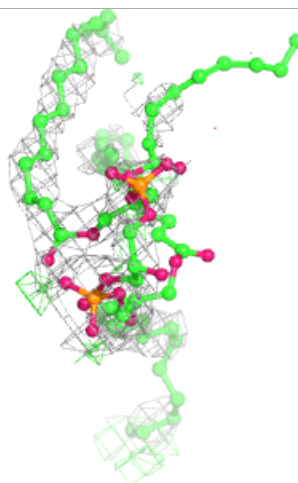
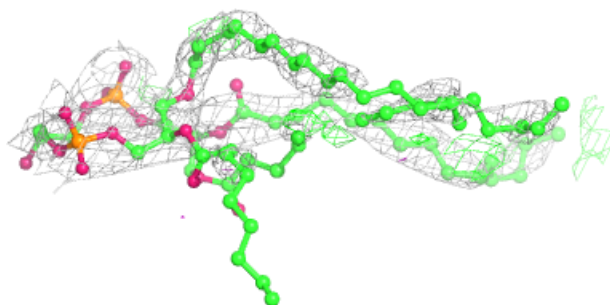
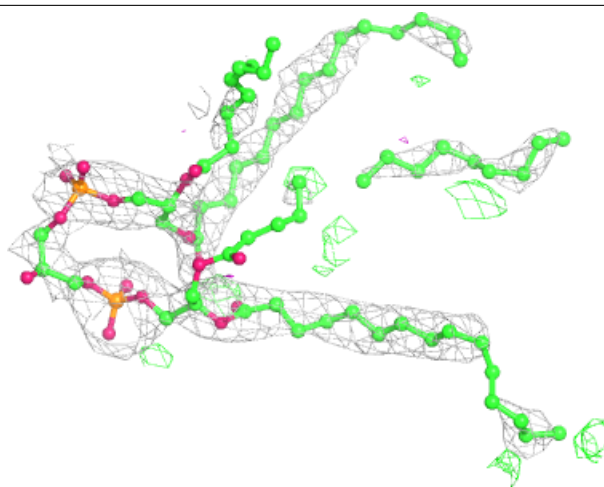
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





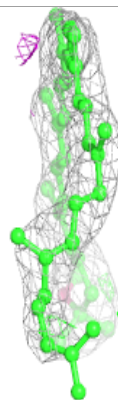
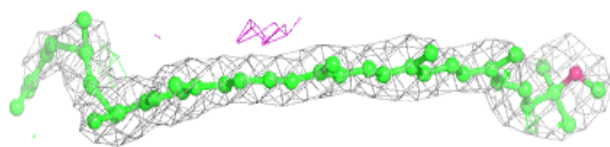
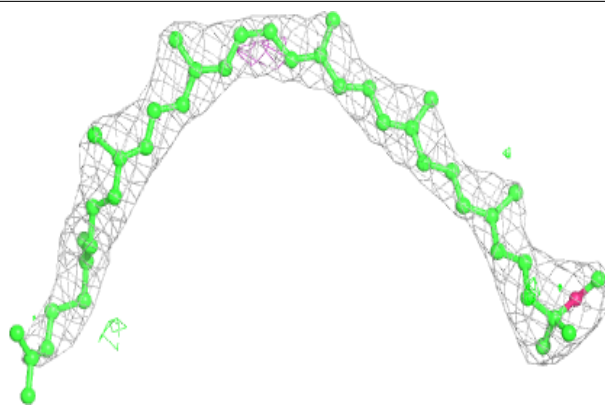
**Electron density around CDL M 410:**

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and green (positive)



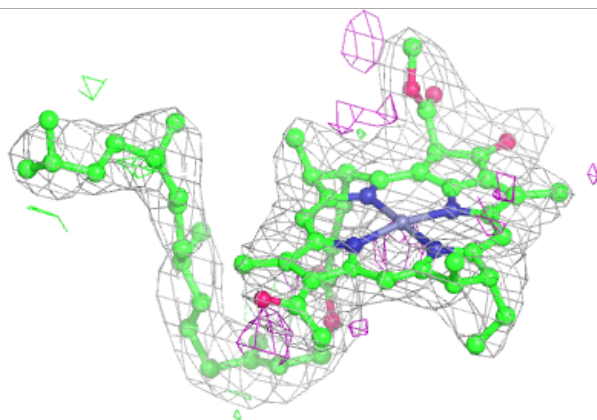
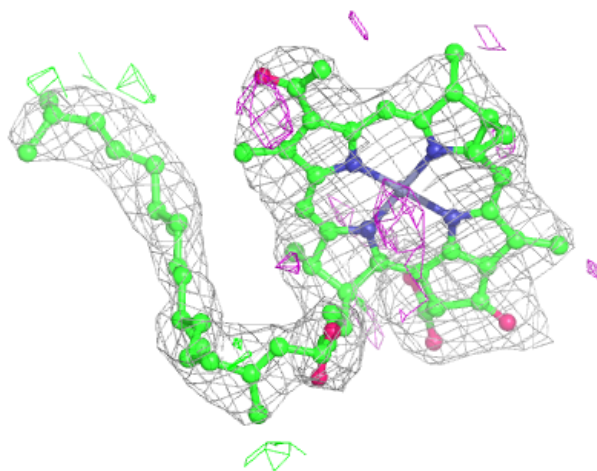
**Electron density around SPO M 409:**

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



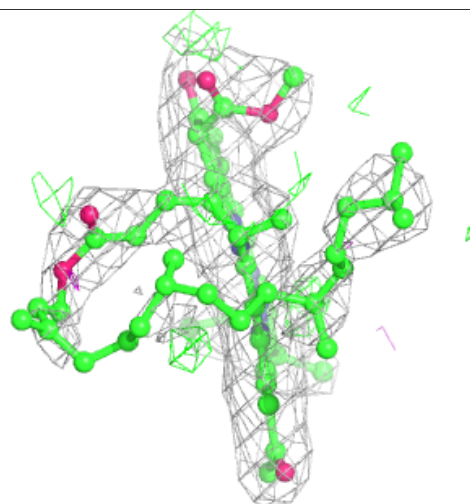
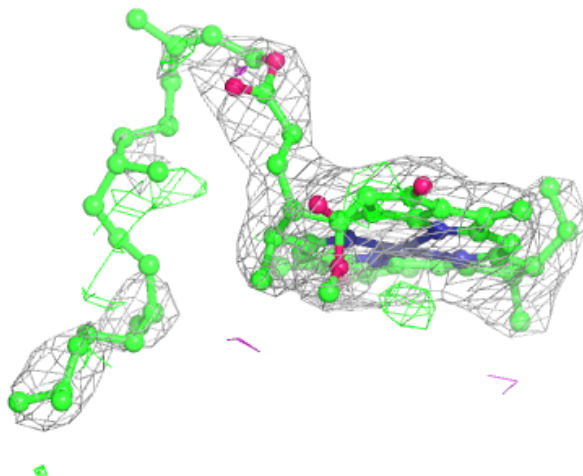
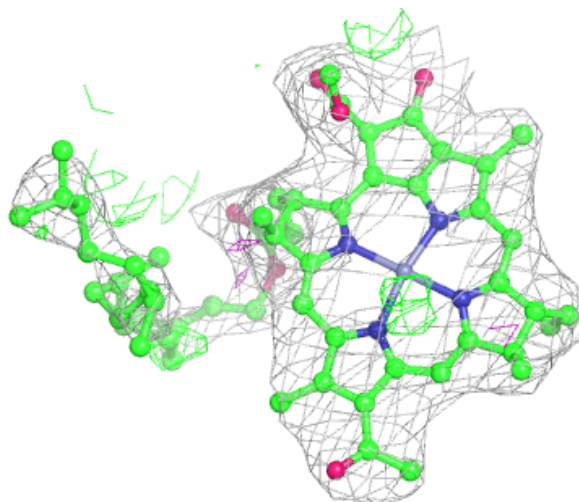
**Electron density around 2GO M 401:**

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



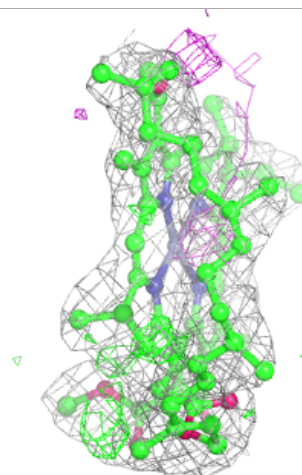
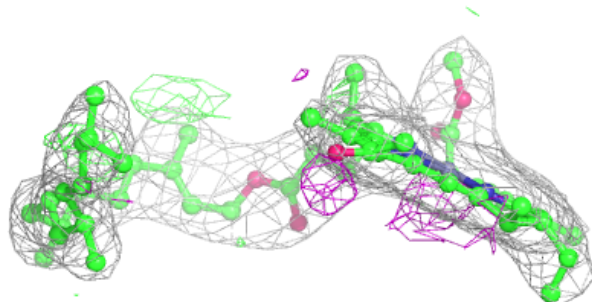
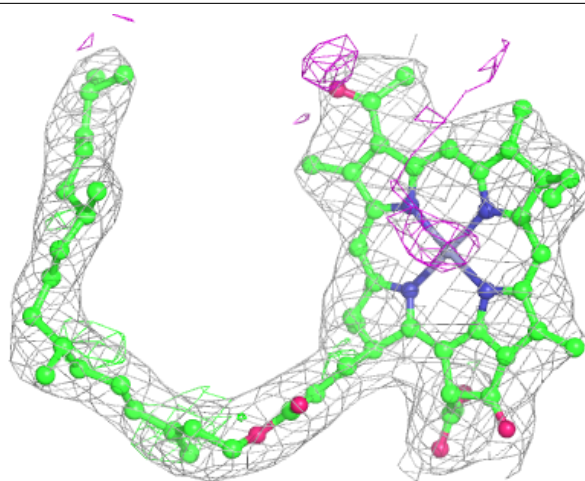
**Electron density around 2GO M 403:**

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



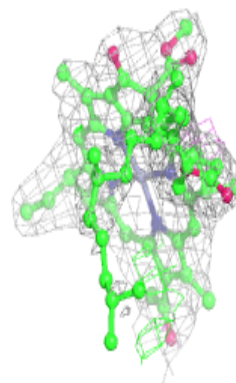
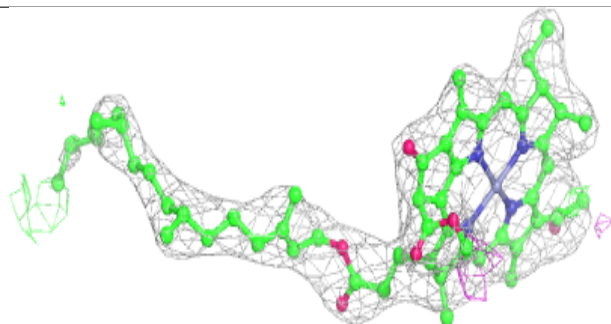
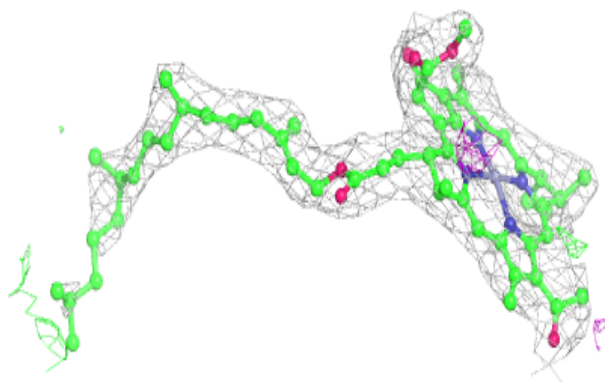
**Electron density around 2GO M 402:**

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

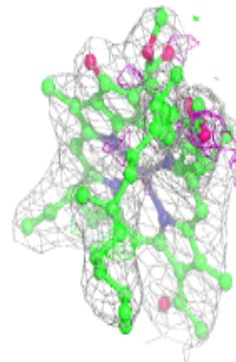
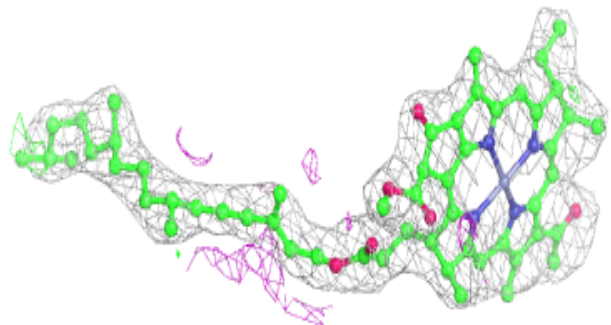
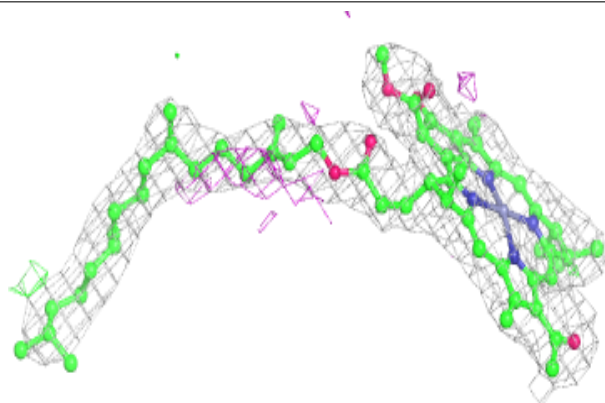


**Electron density around 2GO M 404:**

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

**Electron density around 2GO L 305:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.