



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:52 pm BST

PDB ID : 1PPR  
Title : PERIDININ-CHLOROPHYLL-PROTEIN OF AMPHIDINIUM CARTERAE  
Authors : Hofmann, E.; Welte, W.; Diederichs, K.  
Deposited on : 1996-03-06  
Resolution : 2.00 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

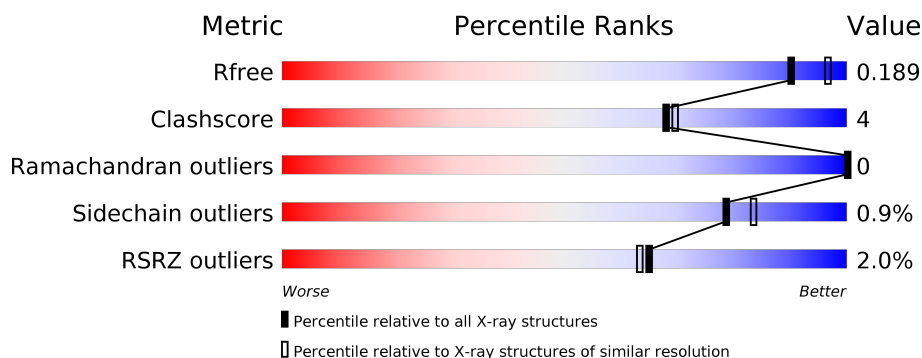
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	M	312	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>96%</span> <span>.</span> </div> </div>
1	N	312	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>3%</span> <span>96%</span> <span>.</span> </div> </div>
1	O	312	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>2%</span> <span>95%</span> <span>5%</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
2	CLA	M	601	X	-	-	-
2	CLA	M	602	X	-	-	-
2	CLA	N	601	X	-	-	-
2	CLA	N	602	X	-	-	-
2	CLA	O	601	X	-	-	-
2	CLA	O	602	X	-	-	-
3	PID	M	613	X	-	-	-
3	PID	N	613	X	-	-	-
3	PID	O	613	X	-	-	-
4	DGD	M	615	X	-	-	-
4	DGD	N	615	X	-	-	-
4	DGD	O	615	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9152 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.

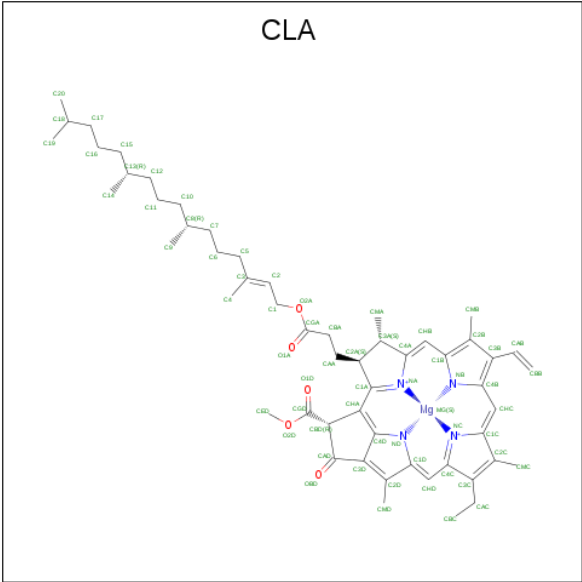
- Molecule 1 is a protein called PERIDININ-CHLOROPHYLL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	312	Total	C	N	O	S	0	0	0
			2282	1445	382	444	11			
1	N	312	Total	C	N	O	S	0	0	0
			2282	1445	382	444	11			
1	O	312	Total	C	N	O	S	0	0	0
			2282	1445	382	444	11			

There are 9 discrepancies between the modelled and reference sequences:

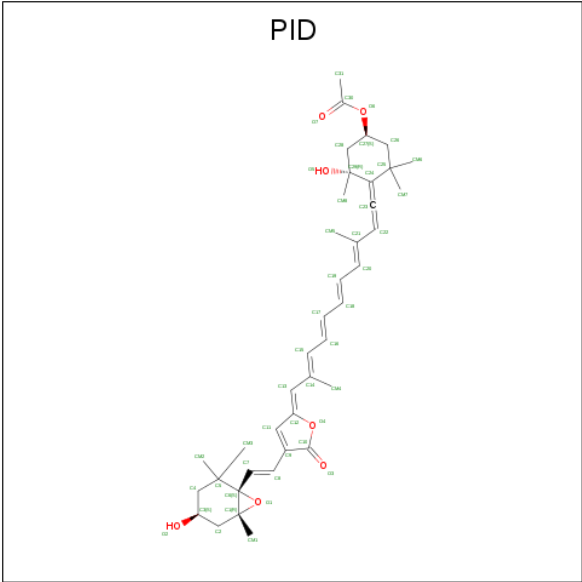
Chain	Residue	Modelled	Actual	Comment	Reference
M	73	ILE	VAL	CONFLICT	UNP P80484
M	128	ASN	SER	CONFLICT	UNP P80484
M	276	VAL	ALA	CONFLICT	UNP P80484
N	73	ILE	VAL	CONFLICT	UNP P80484
N	128	ASN	SER	CONFLICT	UNP P80484
N	276	VAL	ALA	CONFLICT	UNP P80484
O	73	ILE	VAL	CONFLICT	UNP P80484
O	128	ASN	SER	CONFLICT	UNP P80484
O	276	VAL	ALA	CONFLICT	UNP P80484

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	M	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	O	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	O	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 3 is PERIDININ (three-letter code: PID) (formula: C<sub>39</sub>H<sub>50</sub>O<sub>7</sub>).



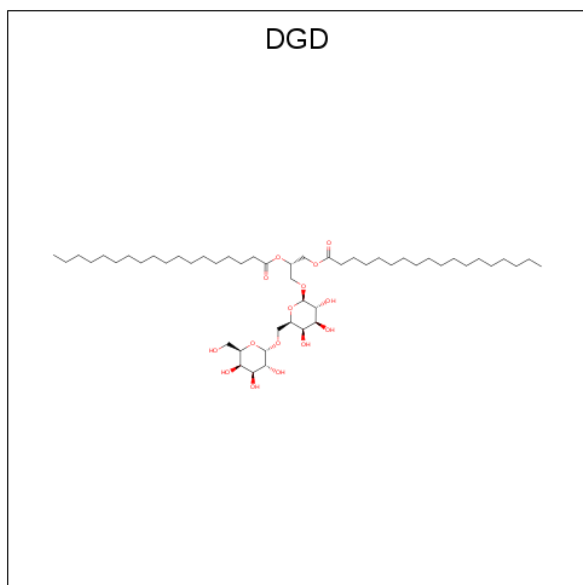
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	N	1	Total	C	O	0	0
			46	39	7		
3	N	1	Total	C	O	0	0
			46	39	7		
3	N	1	Total	C	O	0	0
			46	39	7		
3	N	1	Total	C	O	0	0
			46	39	7		
3	N	1	Total	C	O	0	0
			46	39	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	N	1	Total	C	O	0	0
			46	39	7		
3	N	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		

- Molecule 4 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	0
			66	51	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	0
			66	51	15		
4	N	1	Total	C	O	0	0
			66	51	15		
4	N	1	Total	C	O	0	0
			66	51	15		
4	O	1	Total	C	O	0	0
			66	51	15		
4	O	1	Total	C	O	0	0
			66	51	15		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	139	Total	O	0	0
			139	139		
5	N	137	Total	O	0	0
			137	137		
5	O	140	Total	O	0	0
			140	140		



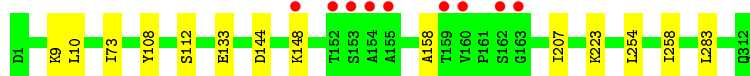
### 3 Residue-property plots [i](#)

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.

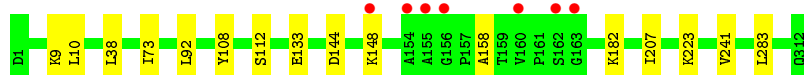
- Molecule 1: PERIDININ-CHLOROPHYLL PROTEIN



- Molecule 1: PERIDININ-CHLOROPHYLL PROTEIN



- Molecule 1: PERIDININ-CHLOROPHYLL PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.43 Å   116.30 Å   67.03 Å 90.00°   94.89°   90.00°	Depositor
Resolution (Å)	40.00 – 2.00 33.84 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.5 (40.00-2.00) 89.5 (33.84-1.99)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.77 (at 2.00 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.179   ,   0.201 0.168   ,   0.189	Depositor DCC
$R_{free}$ test set	2325 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: PID, CLA, DGD

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	M	0.58	0/2323	0.60	0/3154
1	N	0.56	0/2323	0.58	0/3154
1	O	0.59	0/2323	0.60	0/3154
All	All	0.58	0/6969	0.59	0/9462

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2282	0	2300	9	0
1	N	2282	0	2300	10	0
1	O	2282	0	2300	12	0
2	M	130	0	144	3	0
2	N	130	0	144	2	0
2	O	130	0	144	4	0
3	M	368	0	400	9	0
3	N	368	0	400	9	0
3	O	368	0	400	9	0
4	M	132	0	192	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	132	0	192	10	0
4	O	132	0	192	11	0
5	M	139	0	0	0	0
5	N	137	0	0	0	0
5	O	140	0	0	0	0
All	All	9152	0	9108	67	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 4.

The worst 5 of 67 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:73:ILE:HD11	3:O:614:PID:HM72	1.27	1.15
1:M:73:ILE:HD11	3:M:614:PID:HM72	1.30	1.07
1:N:73:ILE:HD11	3:N:614:PID:HM72	1.31	1.06
1:O:73:ILE:HD11	3:O:614:PID:CM7	2.12	0.75
2:M:602:CLA:HBB1	2:M:602:CLA:HHC	1.71	0.72

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	M	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
1	N	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
1	O	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
All	All	930/936 (99%)	921 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	M	233 / 233 (100%)	231 (99%)	2 (1%)	78	83
1	N	233 / 233 (100%)	231 (99%)	2 (1%)	78	83
1	O	233 / 233 (100%)	231 (99%)	2 (1%)	78	83
All	All	699 / 699 (100%)	693 (99%)	6 (1%)	78	83

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	10	LEU
1	O	283	LEU
1	N	283	LEU
1	M	283	LEU
1	O	10	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	216	GLN
1	N	216	GLN
1	O	216	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](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PID	M	623	-	41,49,49	1.76	10 (24%)	49,76,76	2.13	15 (30%)
3	PID	N	613	-	41,49,49	1.84	10 (24%)	49,76,76	2.18	16 (32%)
3	PID	M	624	-	41,49,49	1.76	9 (21%)	49,76,76	1.92	12 (24%)
3	PID	N	622	-	41,49,49	1.95	11 (26%)	49,76,76	2.20	14 (28%)
3	PID	N	614	-	41,49,49	1.89	12 (29%)	49,76,76	2.31	16 (32%)
2	CLA	M	602	5	59,73,73	1.60	8 (13%)	67,113,113	1.87	12 (17%)
3	PID	M	621	-	41,49,49	1.86	11 (26%)	49,76,76	2.08	13 (26%)
3	PID	N	612	-	41,49,49	1.84	11 (26%)	49,76,76	2.17	19 (38%)
3	PID	M	612	-	41,49,49	1.91	10 (24%)	49,76,76	2.15	19 (38%)
3	PID	O	622	-	41,49,49	1.90	10 (24%)	49,76,76	2.17	14 (28%)
3	PID	M	622	-	41,49,49	1.83	10 (24%)	49,76,76	2.18	15 (30%)
2	CLA	M	601	5	59,73,73	1.58	11 (18%)	67,113,113	1.76	10 (14%)
3	PID	N	624	-	41,49,49	1.87	11 (26%)	49,76,76	2.16	17 (34%)
4	DGD	M	625	-	67,67,67	0.73	0	81,81,81	0.89	4 (4%)
4	DGD	N	615	-	67,67,67	0.77	1 (1%)	81,81,81	1.39	7 (8%)
3	PID	O	621	-	41,49,49	1.62	7 (17%)	49,76,76	1.88	15 (30%)
3	PID	O	611	-	41,49,49	1.79	10 (24%)	49,76,76	2.12	17 (34%)
4	DGD	M	615	-	67,67,67	0.85	2 (2%)	81,81,81	1.39	7 (8%)
2	CLA	O	601	5	59,73,73	1.62	11 (18%)	67,113,113	1.75	10 (14%)
3	PID	M	614	-	41,49,49	1.90	11 (26%)	49,76,76	2.22	13 (26%)
3	PID	M	613	-	41,49,49	1.77	10 (24%)	49,76,76	2.19	14 (28%)
3	PID	O	623	-	41,49,49	1.68	7 (17%)	49,76,76	1.97	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PID	O	613	-	41,49,49	1.67	9 (21%)	49,76,76	2.25	16 (32%)
3	PID	O	612	-	41,49,49	1.76	12 (29%)	49,76,76	2.17	17 (34%)
3	PID	O	624	-	41,49,49	1.75	10 (24%)	49,76,76	1.99	16 (32%)
2	CLA	N	602	5	59,73,73	1.63	9 (15%)	67,113,113	1.89	13 (19%)
4	DGD	N	625	-	67,67,67	0.78	1 (1%)	81,81,81	0.97	5 (6%)
2	CLA	O	602	5	59,73,73	1.58	8 (13%)	67,113,113	1.77	15 (22%)
3	PID	N	623	-	41,49,49	1.81	8 (19%)	49,76,76	2.13	15 (30%)
3	PID	O	614	-	41,49,49	1.83	11 (26%)	49,76,76	2.21	15 (30%)
2	CLA	N	601	5	59,73,73	1.54	11 (18%)	67,113,113	1.69	11 (16%)
3	PID	M	611	-	41,49,49	1.90	13 (31%)	49,76,76	2.17	15 (30%)
4	DGD	O	625	-	67,67,67	0.76	1 (1%)	81,81,81	0.96	5 (6%)
3	PID	N	611	-	41,49,49	1.85	10 (24%)	49,76,76	2.17	18 (36%)
3	PID	N	621	-	41,49,49	1.77	9 (21%)	49,76,76	2.12	15 (30%)
4	DGD	O	615	-	67,67,67	0.85	1 (1%)	81,81,81	1.39	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PID	M	623	-	-	0/24/93/93	0/4/4/4
3	PID	N	613	-	1/1/14/25	1/24/93/93	0/4/4/4
3	PID	M	624	-	-	0/24/93/93	0/4/4/4
3	PID	N	622	-	-	1/24/93/93	0/4/4/4
3	PID	N	614	-	-	0/24/93/93	0/4/4/4
2	CLA	M	602	5	3/3/20/25	1/37/135/135	-
3	PID	M	621	-	-	1/24/93/93	0/4/4/4
3	PID	N	612	-	-	1/24/93/93	0/4/4/4
3	PID	M	612	-	-	1/24/93/93	0/4/4/4
3	PID	O	622	-	-	1/24/93/93	0/4/4/4
4	DGD	M	615	-	3/3/13/13	33/55/95/95	0/2/2/2
2	CLA	M	601	5	4/4/20/25	3/37/135/135	-
3	PID	N	624	-	-	1/24/93/93	0/4/4/4
3	PID	N	623	-	-	1/24/93/93	0/4/4/4
4	DGD	M	625	-	-	25/55/95/95	0/2/2/2
4	DGD	N	615	-	3/3/13/13	33/55/95/95	0/2/2/2
3	PID	O	621	-	-	1/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PID	O	611	-	-	1/24/93/93	0/4/4/4
3	PID	M	622	-	-	1/24/93/93	0/4/4/4
2	CLA	O	601	5	4/4/20/25	4/37/135/135	-
3	PID	M	614	-	-	0/24/93/93	0/4/4/4
3	PID	M	613	-	1/1/14/25	1/24/93/93	0/4/4/4
3	PID	O	623	-	-	0/24/93/93	0/4/4/4
3	PID	O	613	-	1/1/14/25	1/24/93/93	0/4/4/4
3	PID	O	612	-	-	1/24/93/93	0/4/4/4
3	PID	O	624	-	-	0/24/93/93	0/4/4/4
2	CLA	N	602	5	3/3/20/25	2/37/135/135	-
4	DGD	N	625	-	-	25/55/95/95	0/2/2/2
2	CLA	O	602	5	3/3/20/25	2/37/135/135	-
4	DGD	O	615	-	3/3/13/13	33/55/95/95	0/2/2/2
3	PID	O	614	-	-	0/24/93/93	0/4/4/4
2	CLA	N	601	5	4/4/20/25	3/37/135/135	-
3	PID	M	611	-	-	1/24/93/93	0/4/4/4
4	DGD	O	625	-	-	24/55/95/95	0/2/2/2
3	PID	N	611	-	-	1/24/93/93	0/4/4/4
3	PID	N	621	-	-	1/24/93/93	0/4/4/4

The worst 5 of 306 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	602	CLA	MG-NA	7.58	2.24	2.06
2	N	602	CLA	MG-NA	7.11	2.23	2.06
2	O	602	CLA	MG-NA	6.92	2.22	2.06
2	O	601	CLA	MG-NA	6.23	2.21	2.06
2	M	601	CLA	MG-NA	5.54	2.19	2.06

The worst 5 of 478 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	602	CLA	C4A-NA-C1A	9.74	111.09	106.71
2	N	602	CLA	C4A-NA-C1A	9.72	111.08	106.71
2	M	601	CLA	C4A-NA-C1A	9.41	110.94	106.71
3	N	613	PID	O3-C10-C9	-8.65	120.89	130.74
2	O	602	CLA	C4A-NA-C1A	8.36	110.46	106.71

5 of 33 chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
3	N	613	PID	C3
2	M	602	CLA	NC
2	M	602	CLA	ND
2	M	602	CLA	NA
2	M	601	CLA	C8

5 of 205 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	615	DGD	O2G-C2G-C3G-O3G
4	N	615	DGD	O6D-C1D-O3G-C3G
4	N	615	DGD	C4D-C5D-C6D-O5D
4	M	615	DGD	O2G-C2G-C3G-O3G
4	M	615	DGD	O6D-C1D-O3G-C3G

There are no ring outliers.

29 monomers are involved in 55 short contacts:

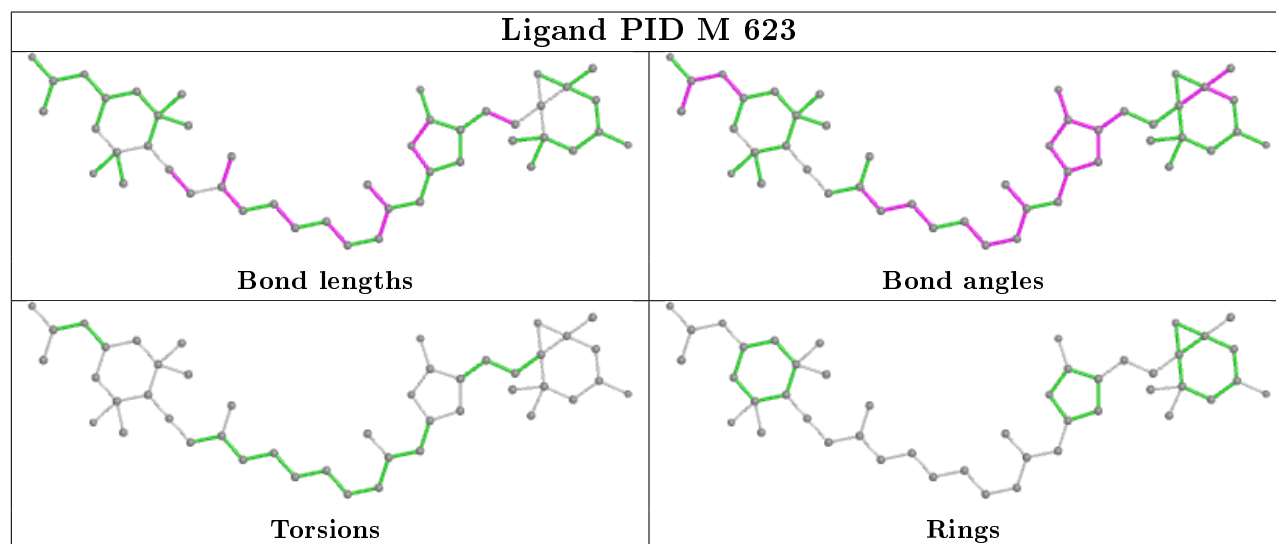
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	623	PID	1	0
3	N	622	PID	1	0
3	N	614	PID	2	0
2	M	602	CLA	2	0
3	M	621	PID	1	0
3	N	612	PID	2	0
3	M	612	PID	1	0
3	O	622	PID	1	0
3	M	622	PID	1	0
2	M	601	CLA	1	0
3	N	624	PID	1	0
4	M	625	DGD	1	0
4	N	615	DGD	9	0
3	O	621	PID	2	0
3	O	611	PID	3	0
4	M	615	DGD	11	0
2	O	601	CLA	2	0
3	M	614	PID	2	0
3	O	613	PID	1	0
2	N	602	CLA	1	0
4	N	625	DGD	1	0
2	O	602	CLA	2	0
3	O	614	PID	2	0
2	N	601	CLA	1	0

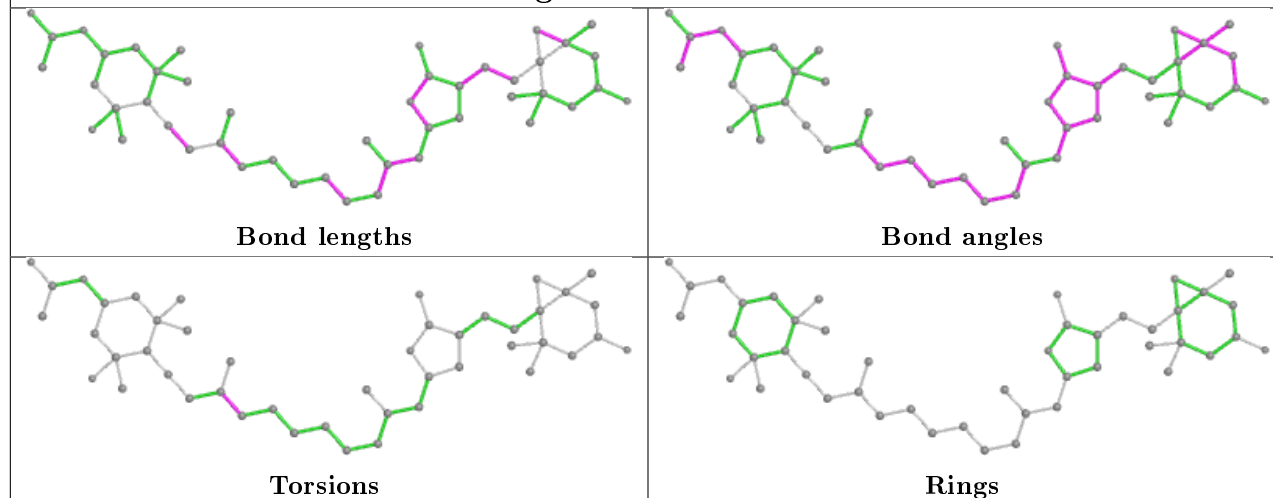
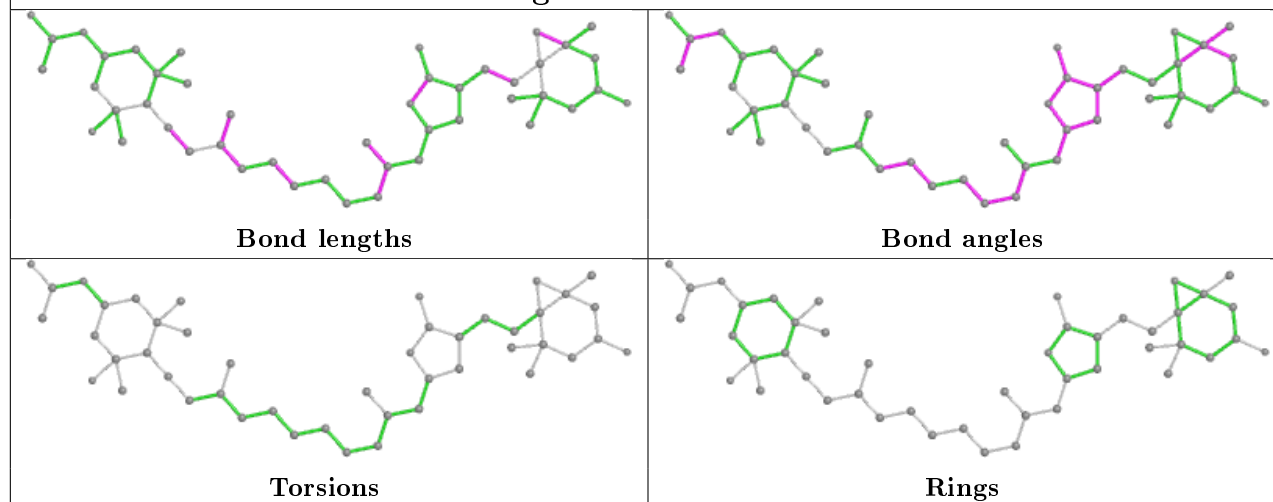
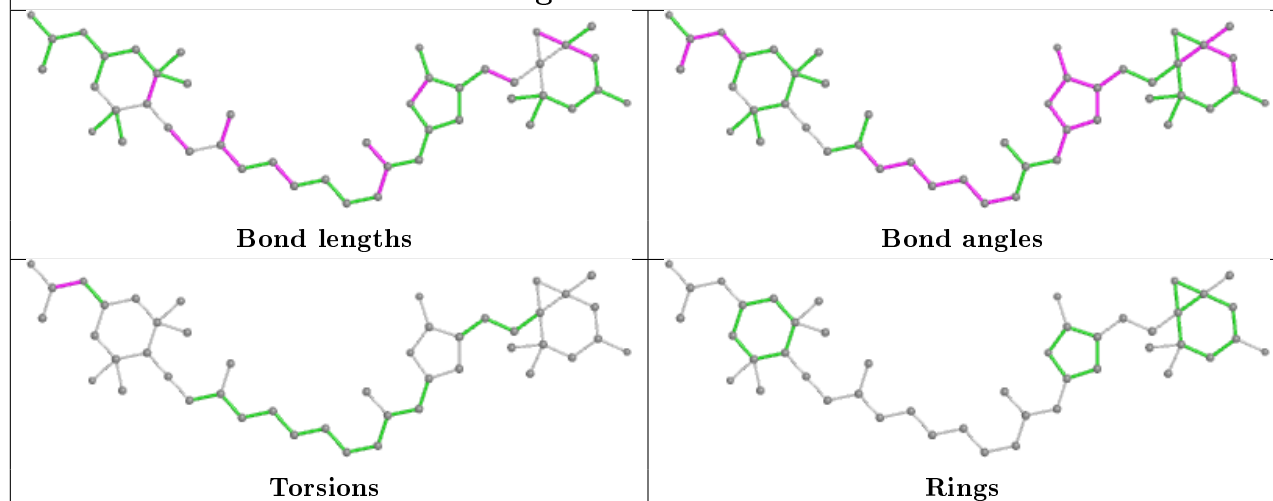
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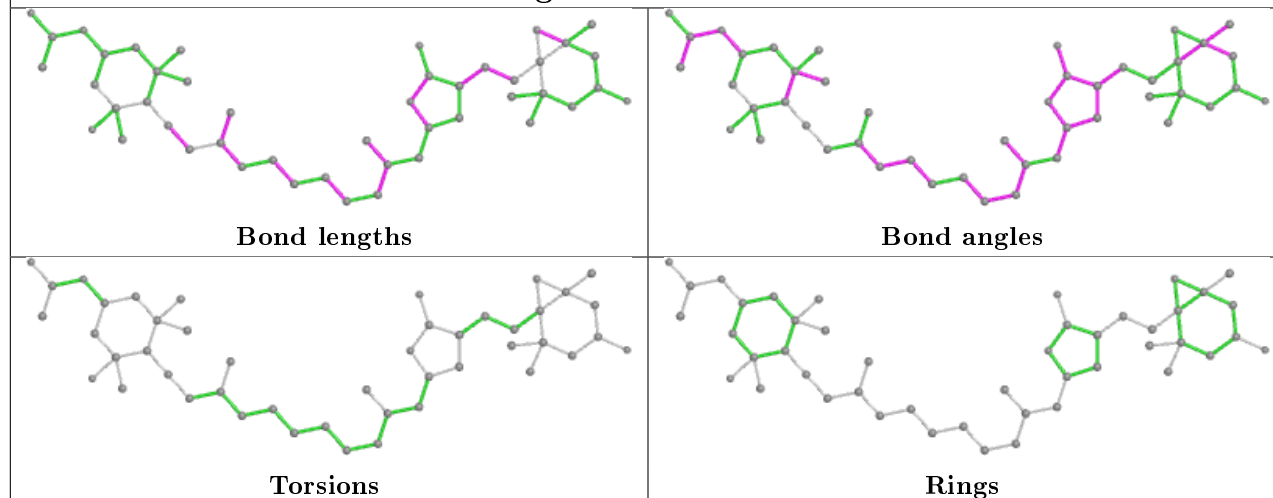
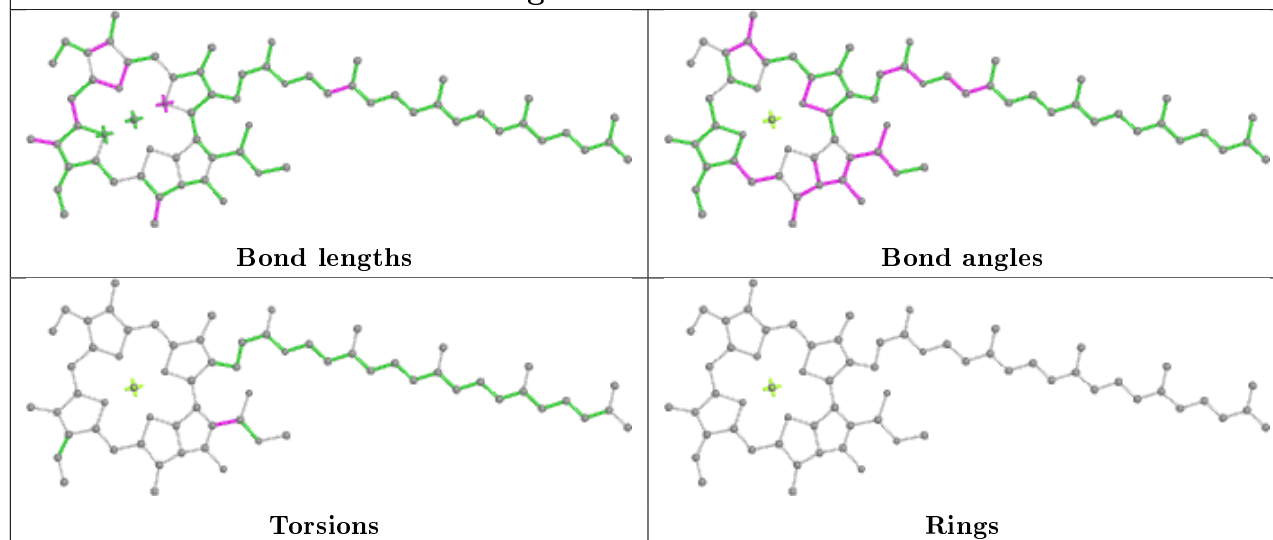
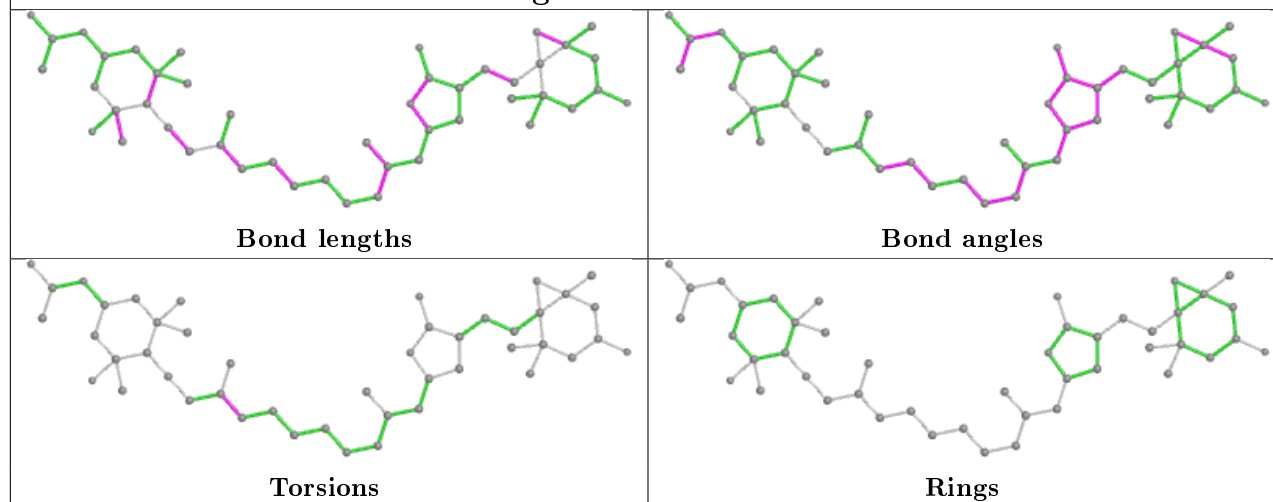
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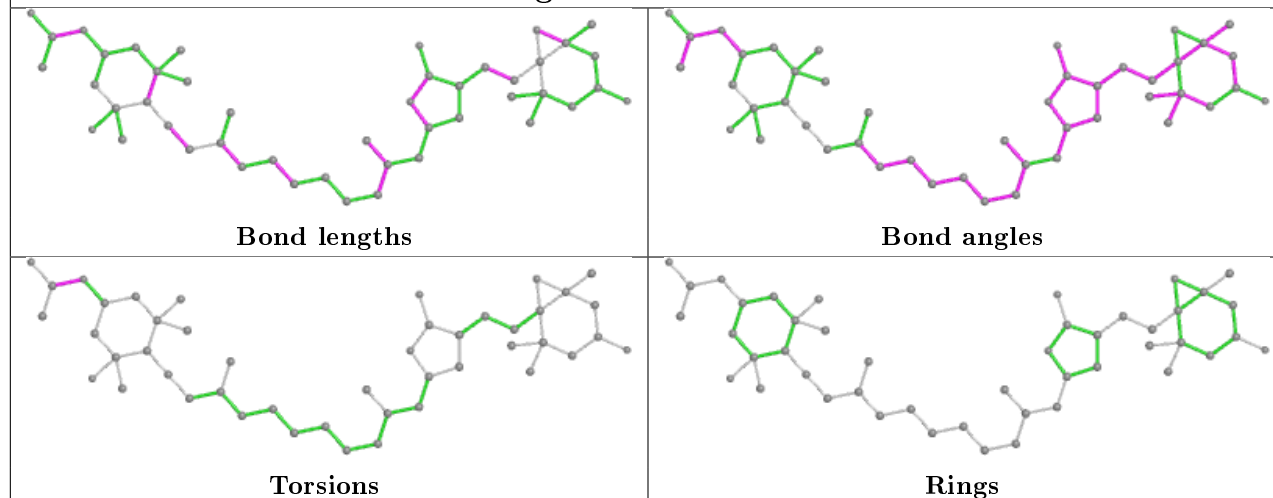
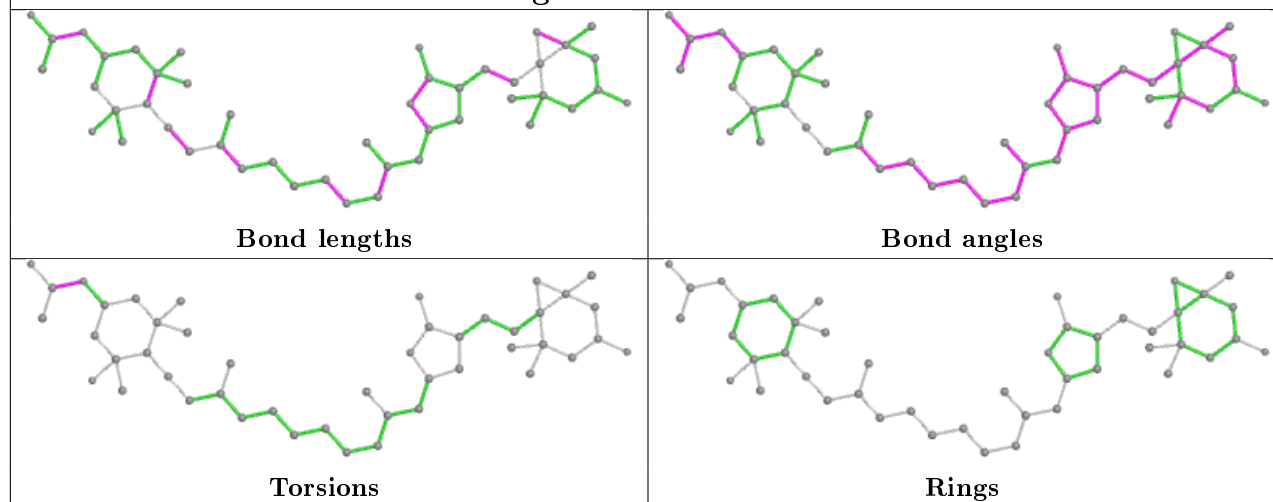
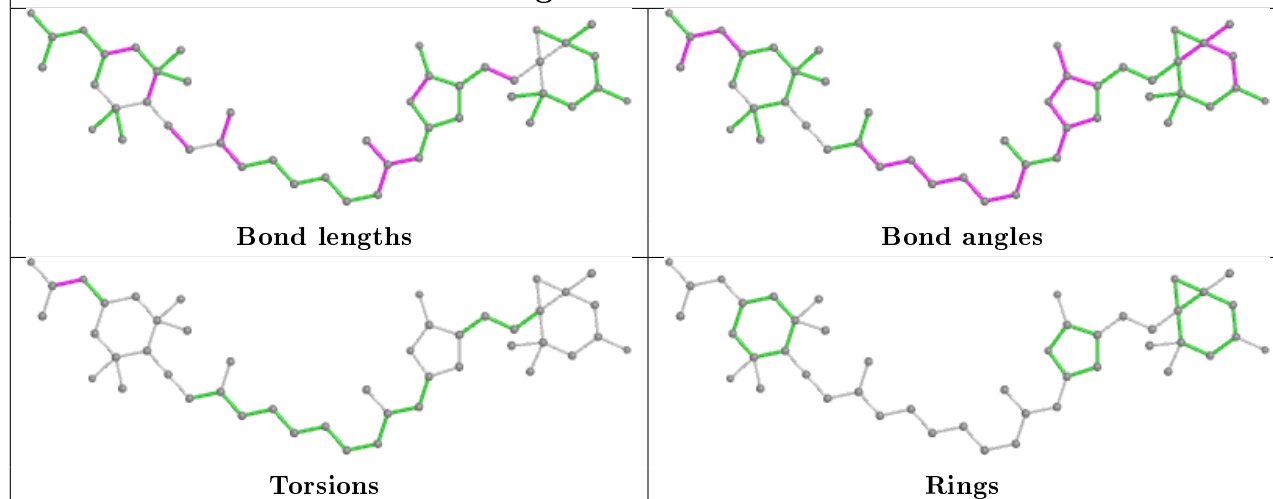
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	611	PID	3	0
4	O	625	DGD	2	0
3	N	611	PID	2	0
3	N	621	PID	1	0
4	O	615	DGD	9	0

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

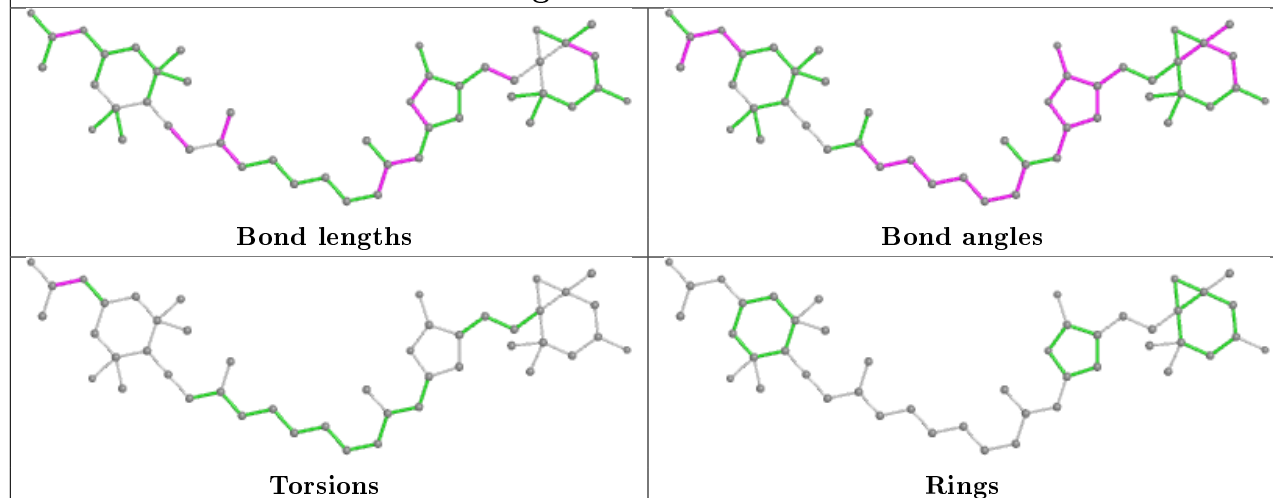


**Ligand PID N 613****Ligand PID M 624****Ligand PID N 622**

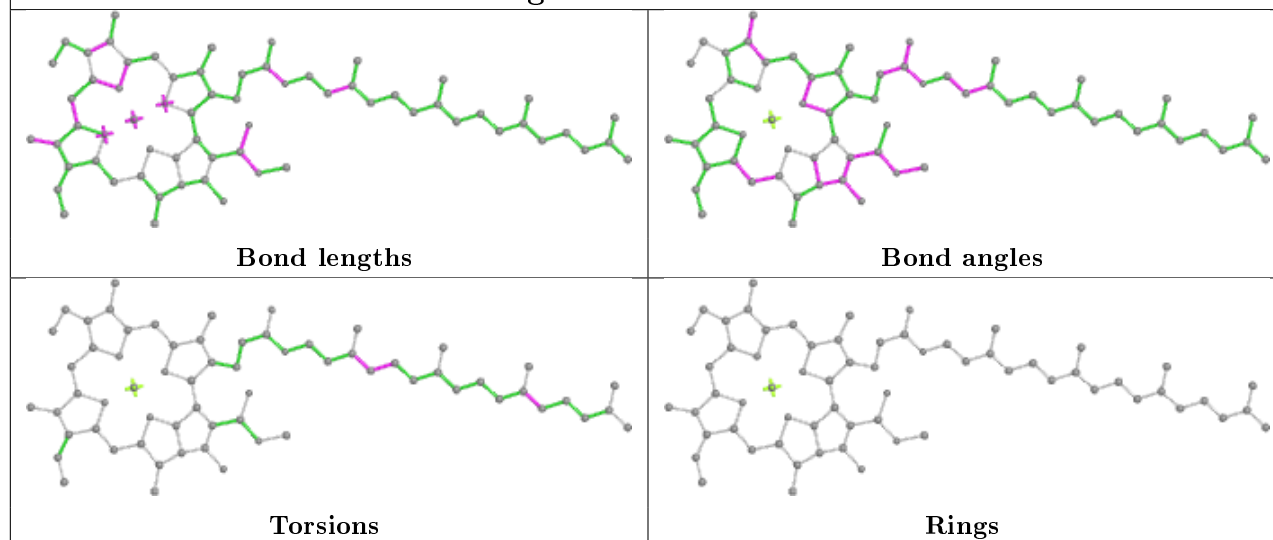
**Ligand PID N 614****Ligand CLA M 602****Ligand PID M 621**

**Ligand PID N 612****Ligand PID M 612****Ligand PID O 622**

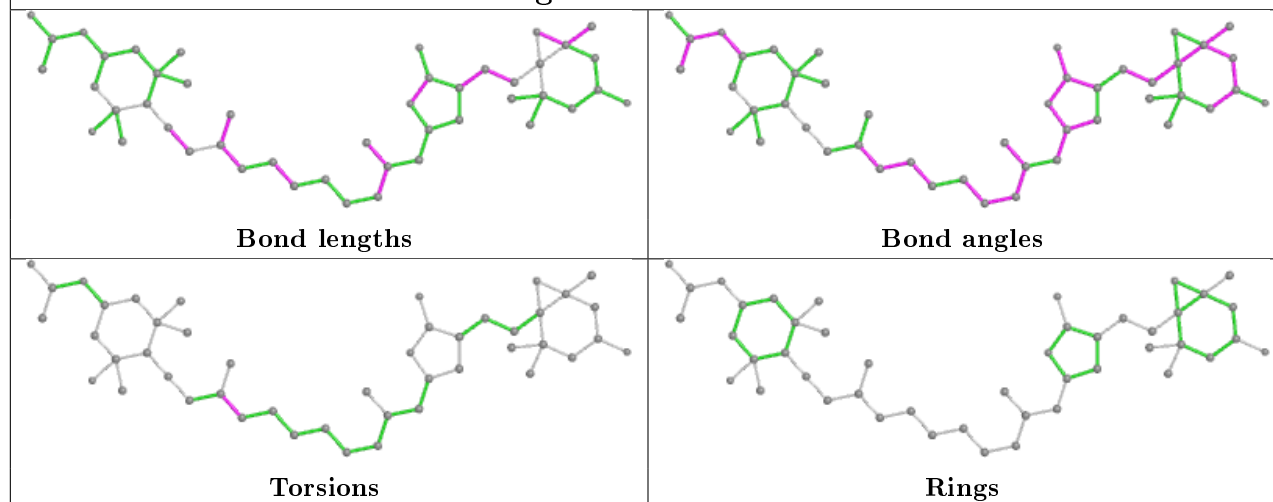
## Ligand PID M 622

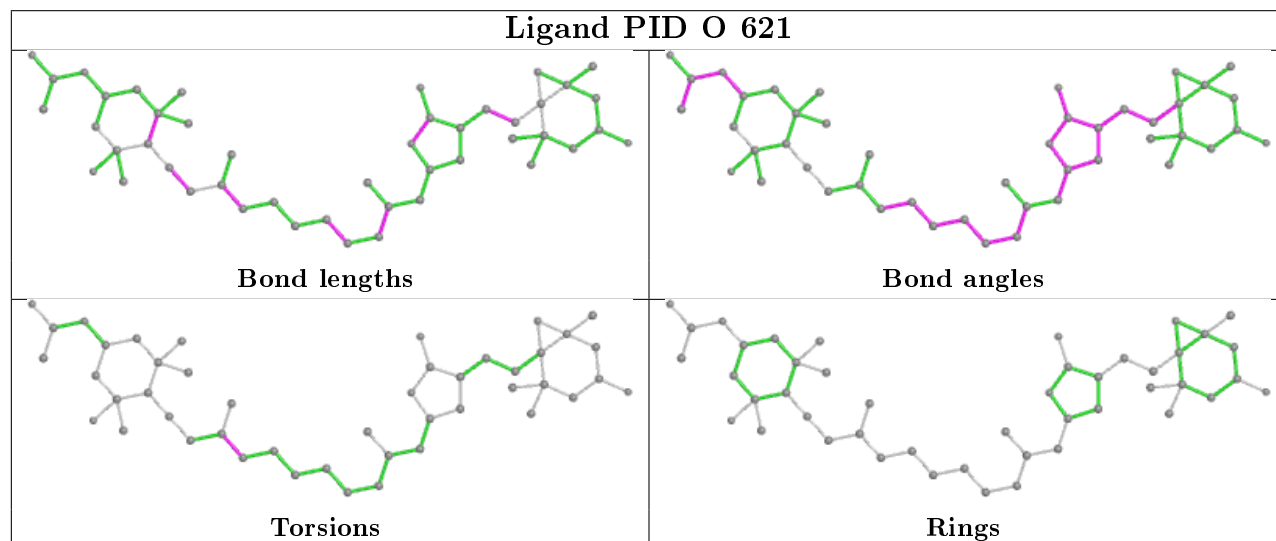
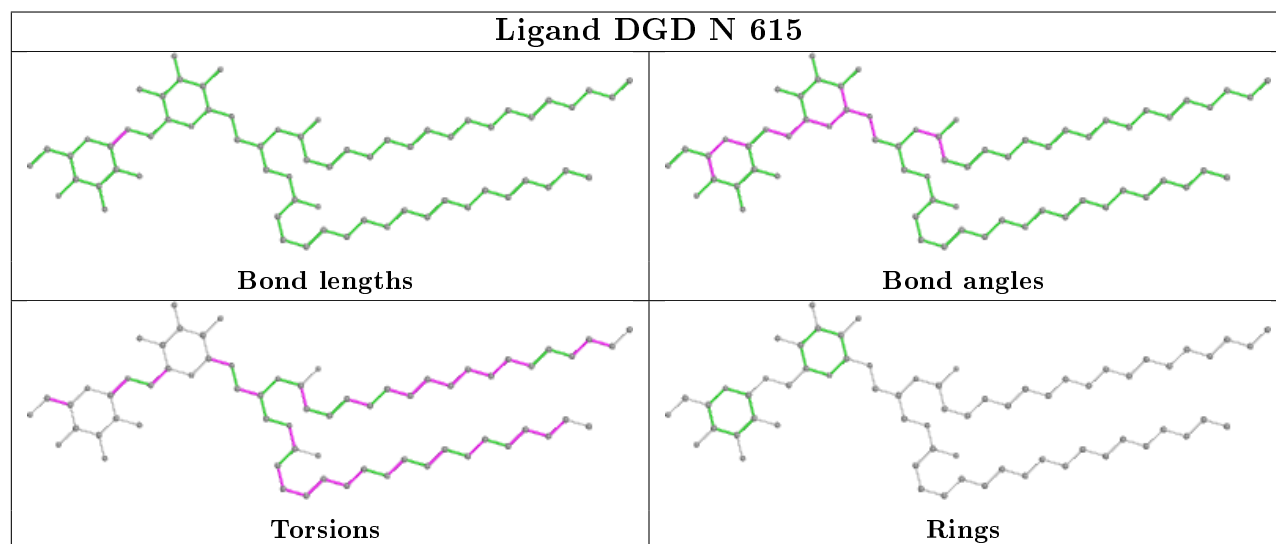
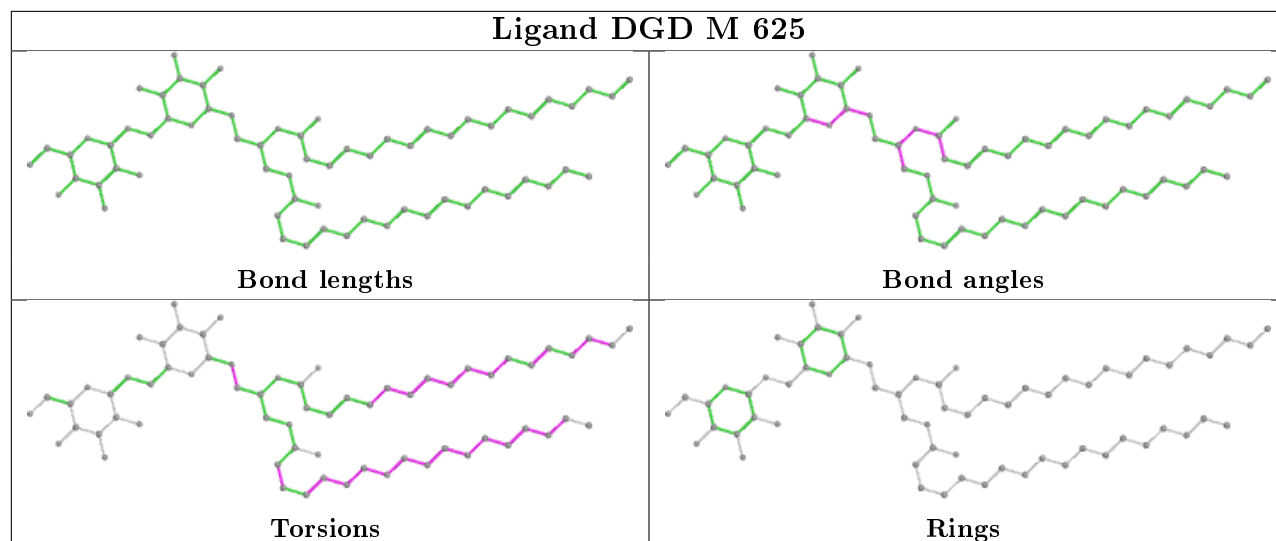


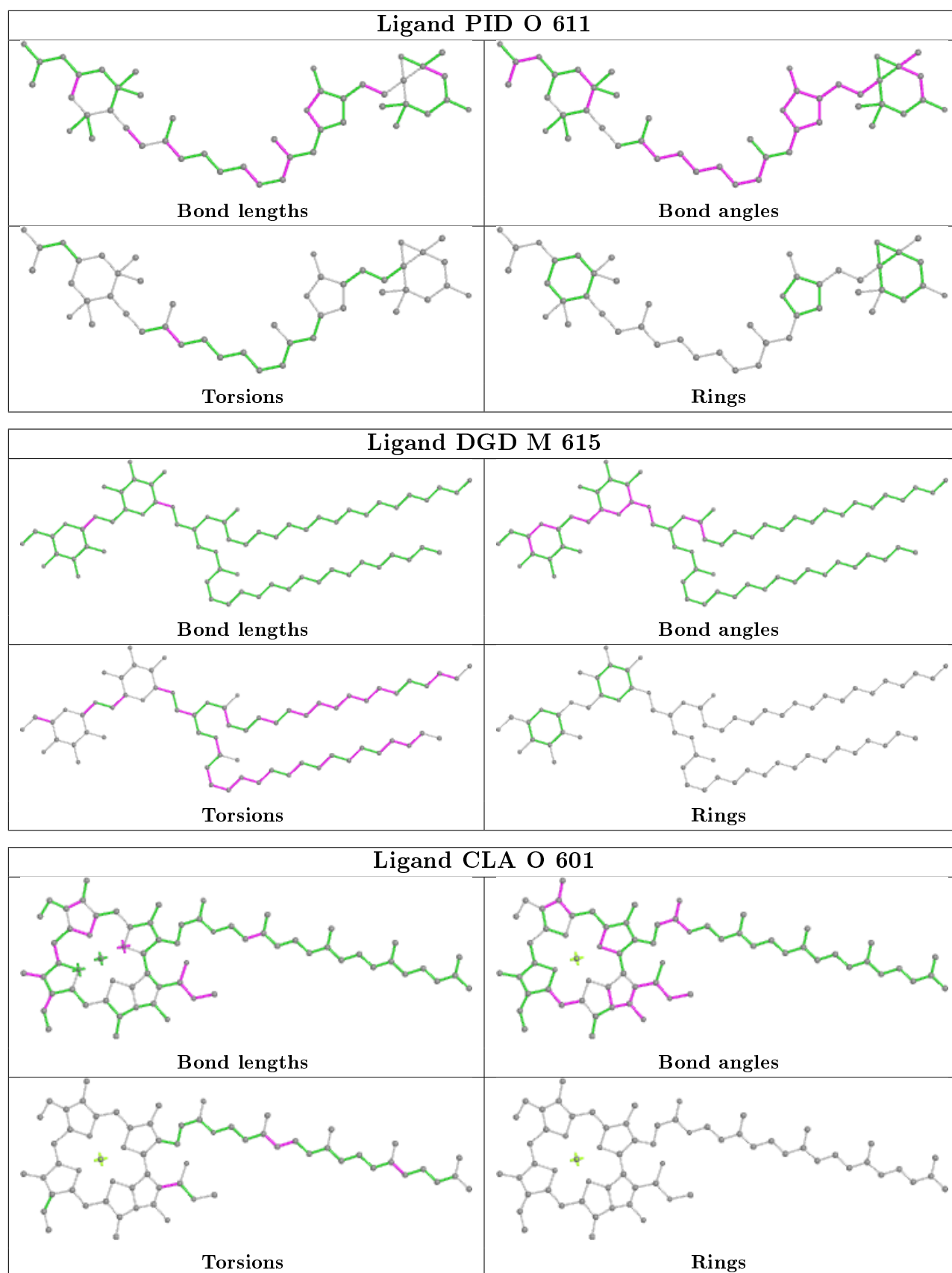
## Ligand CLA M 601



## Ligand PID N 624

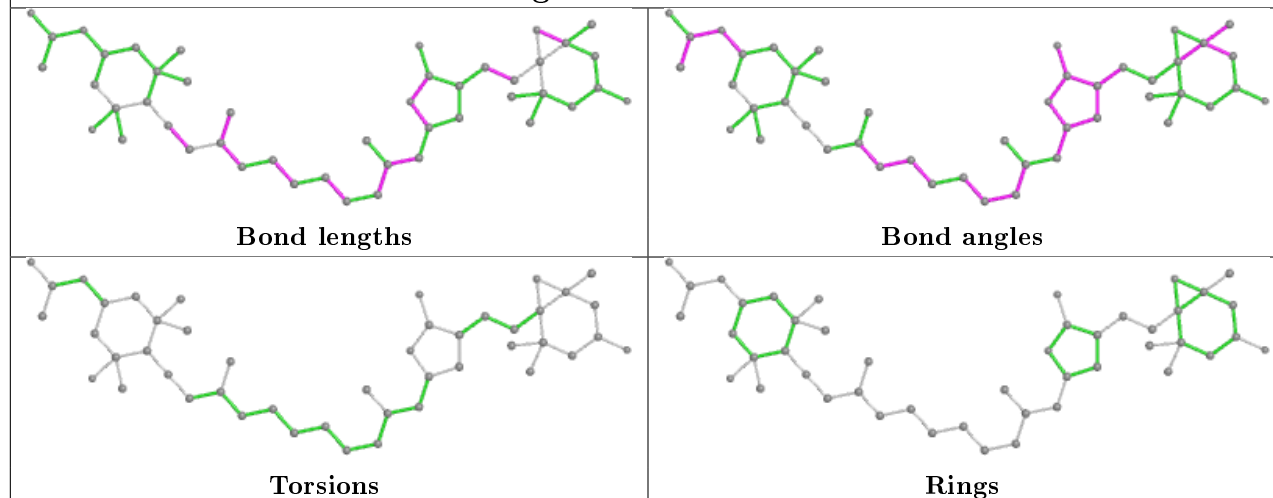




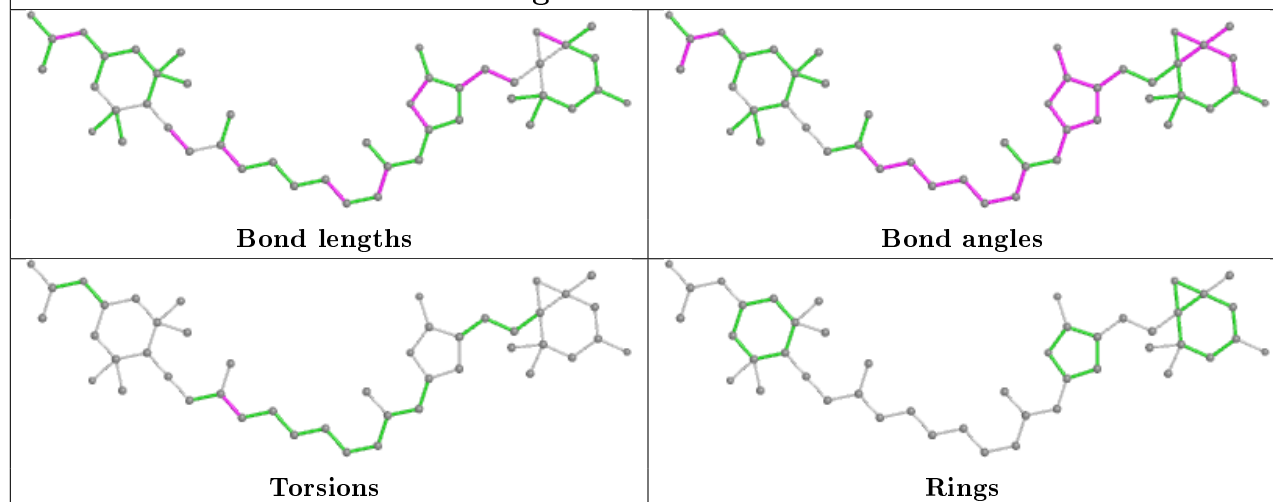




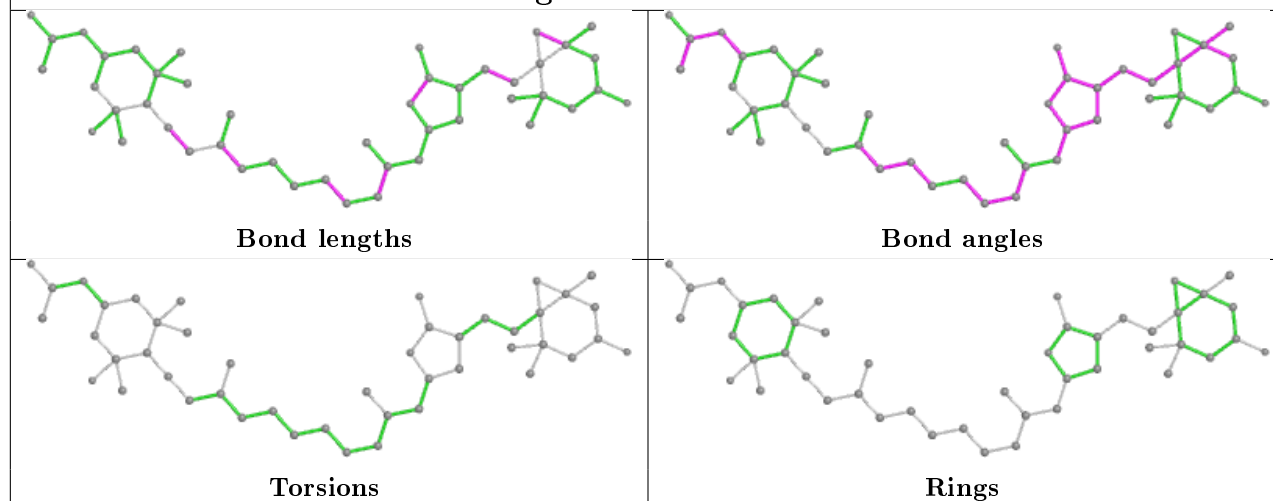
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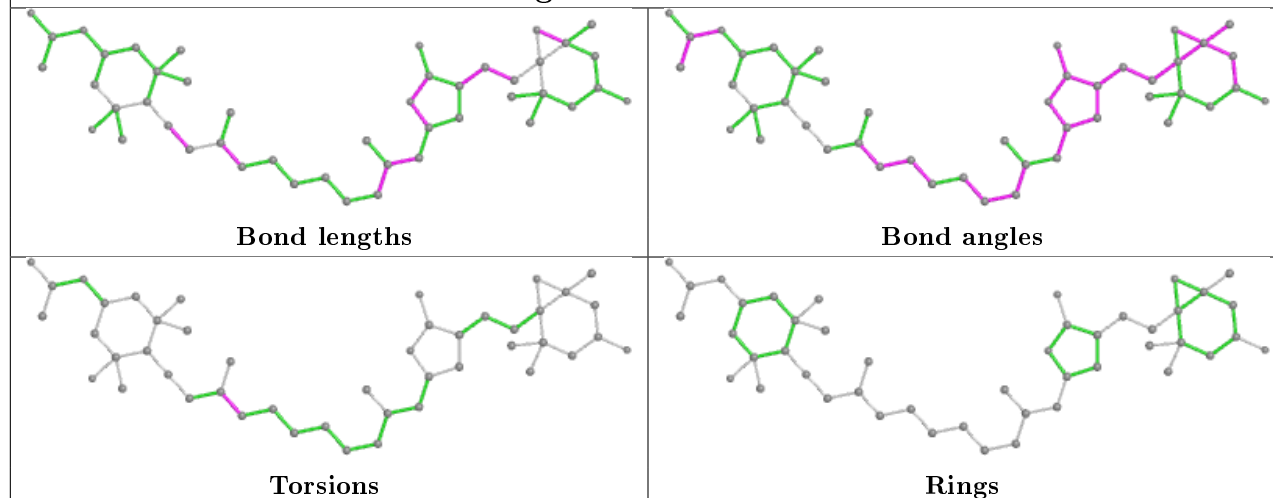
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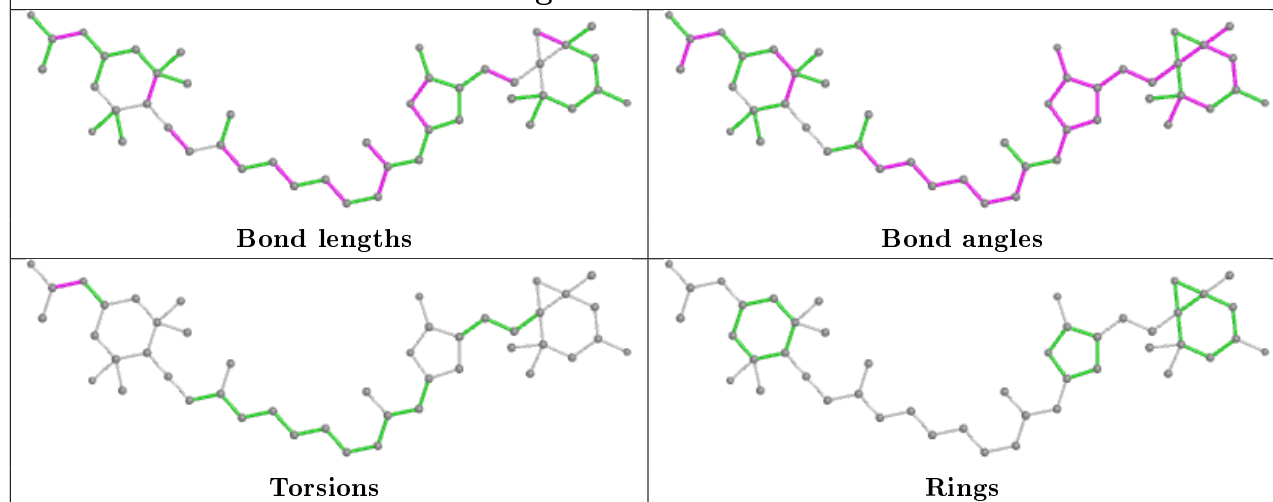
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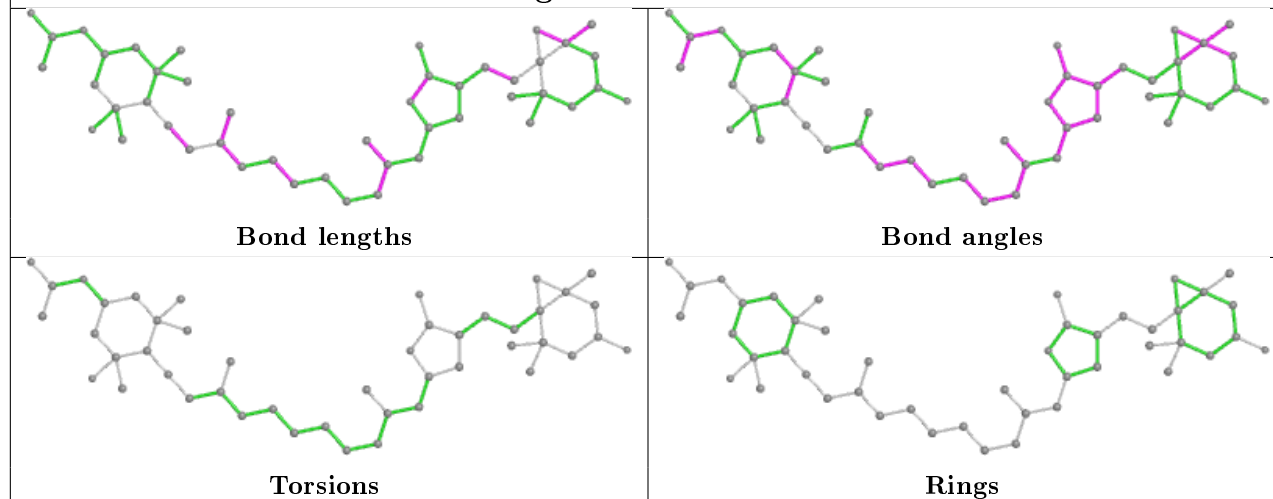
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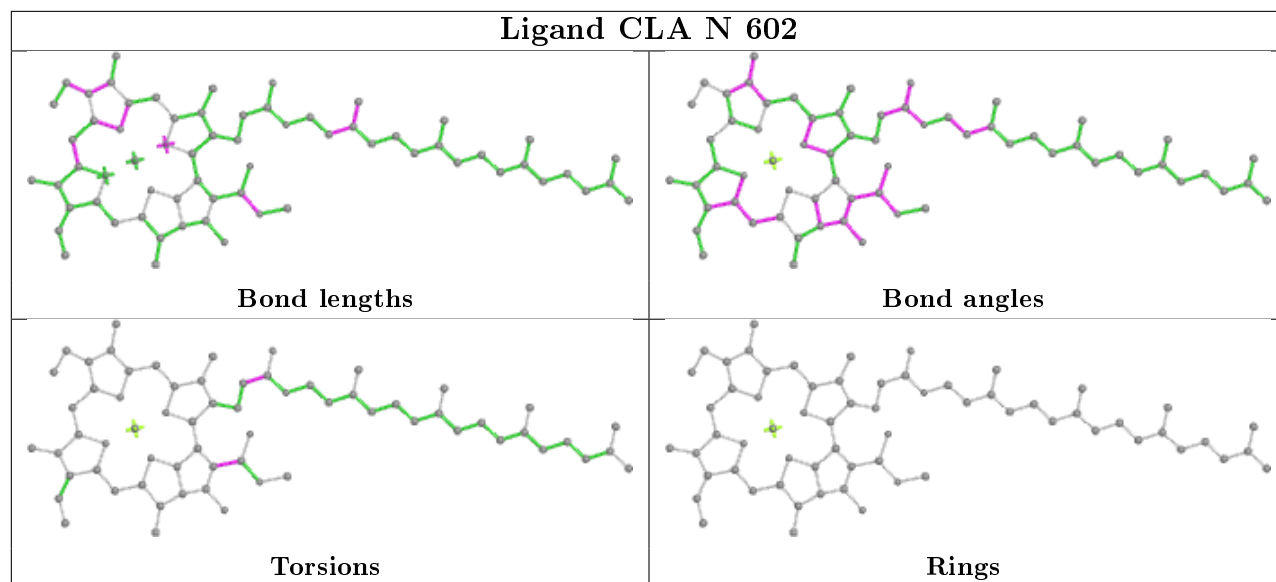
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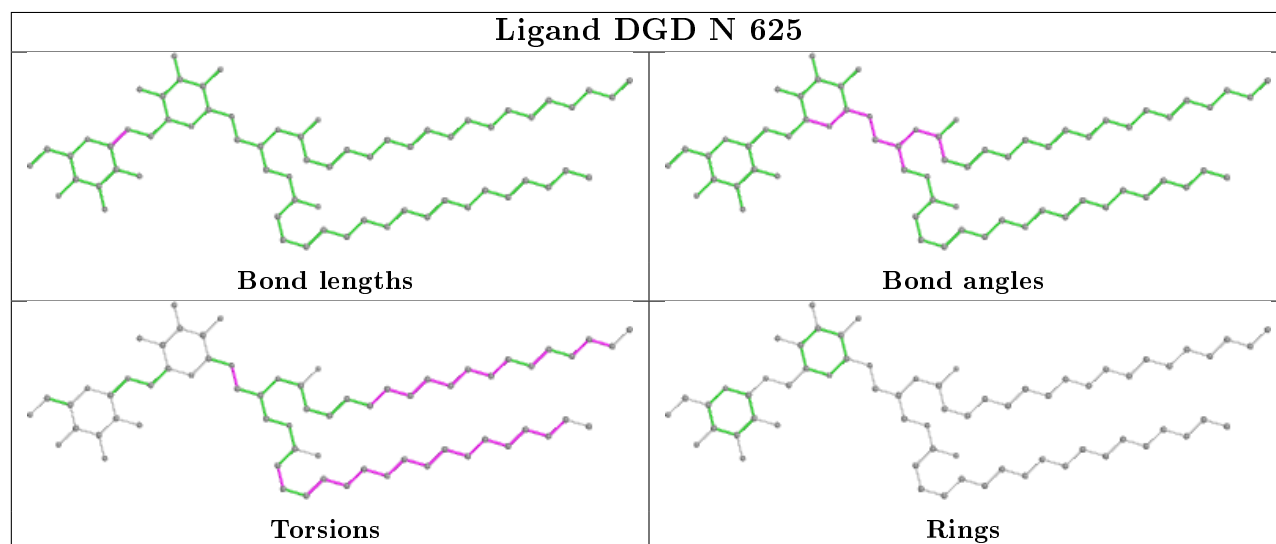
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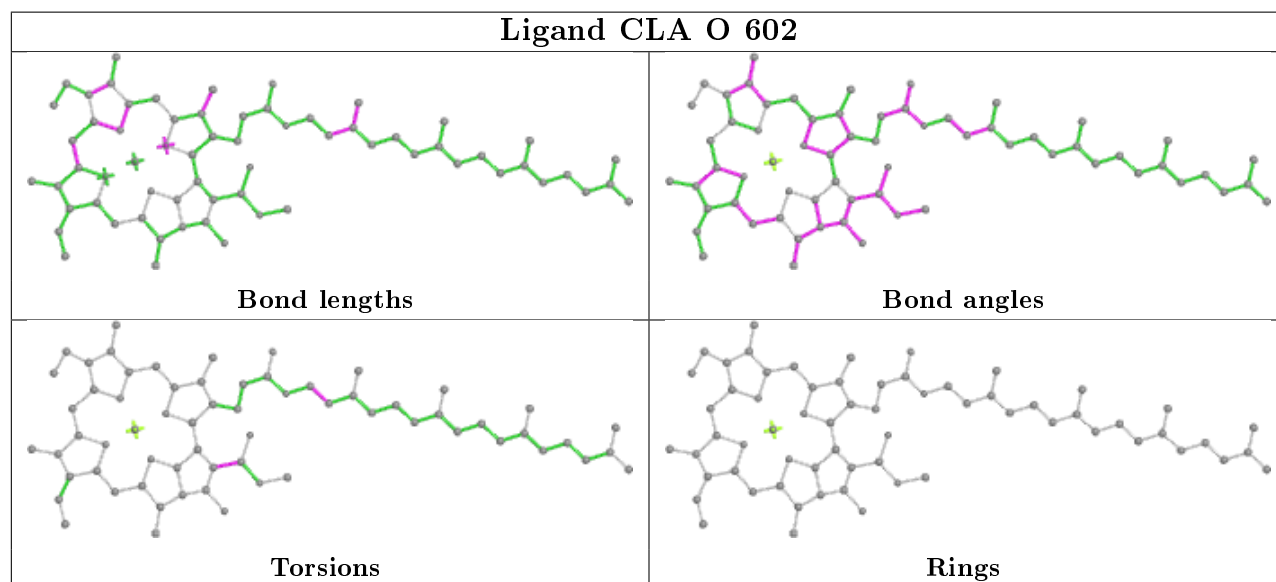
## Ligand CLA N 602



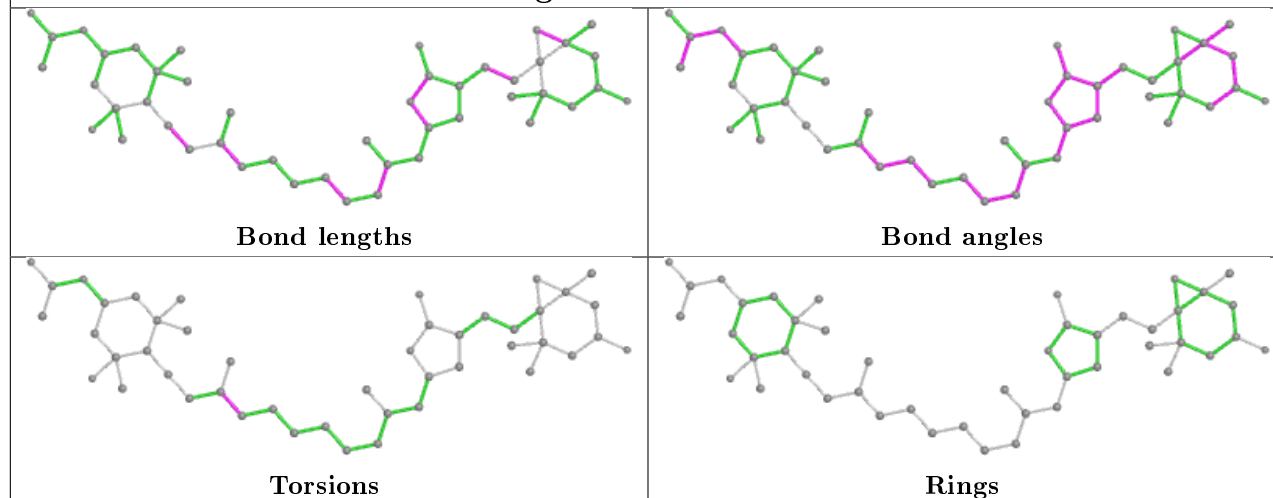
## Ligand DGD N 625



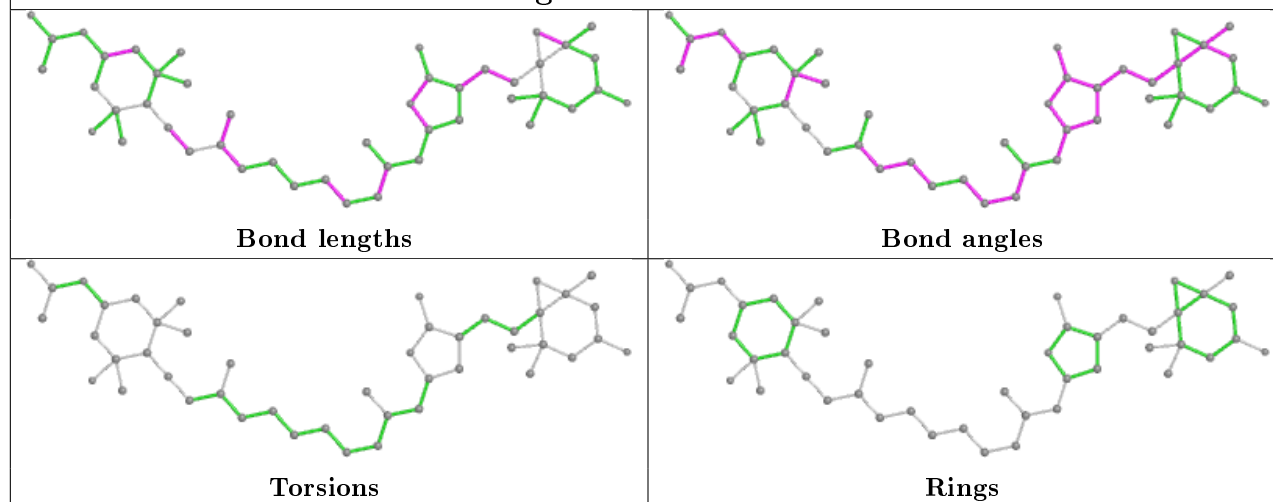
## Ligand CLA O 602



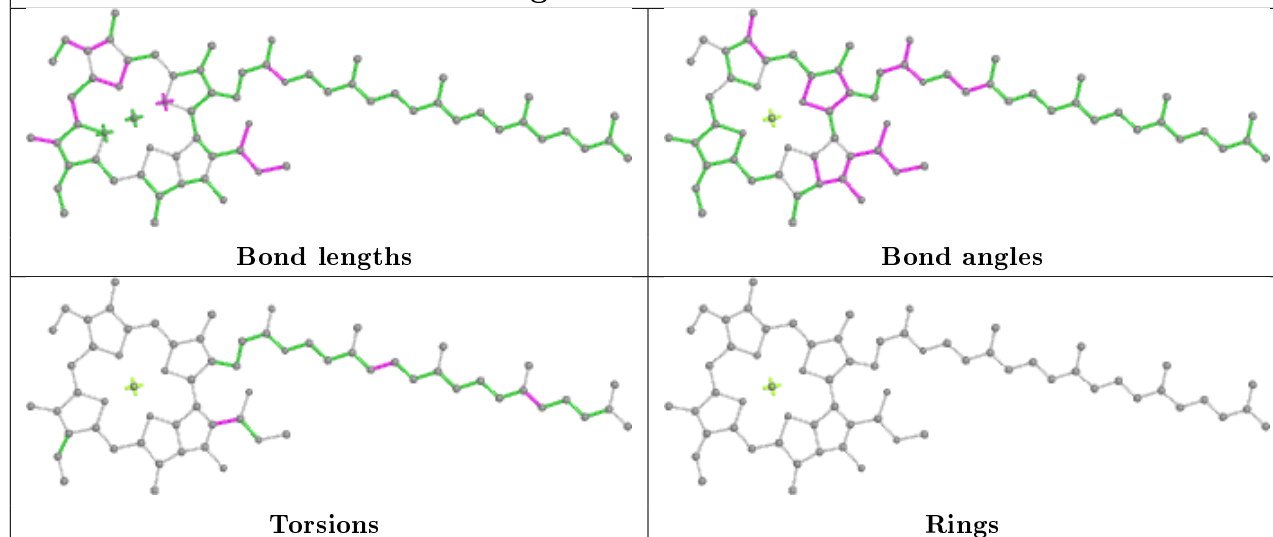
## Ligand PID N 623



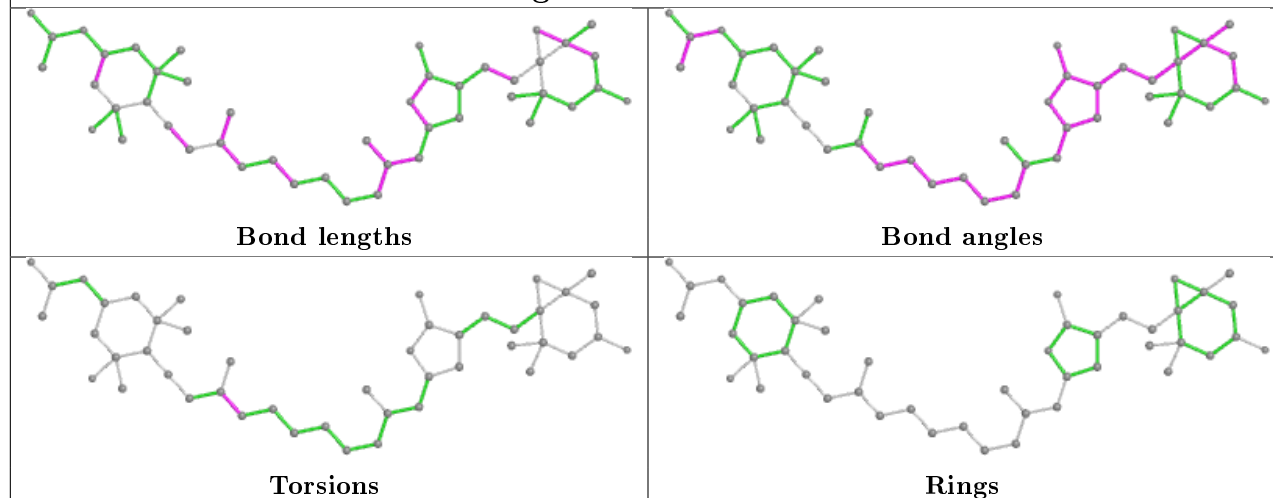
## Ligand PID O 614



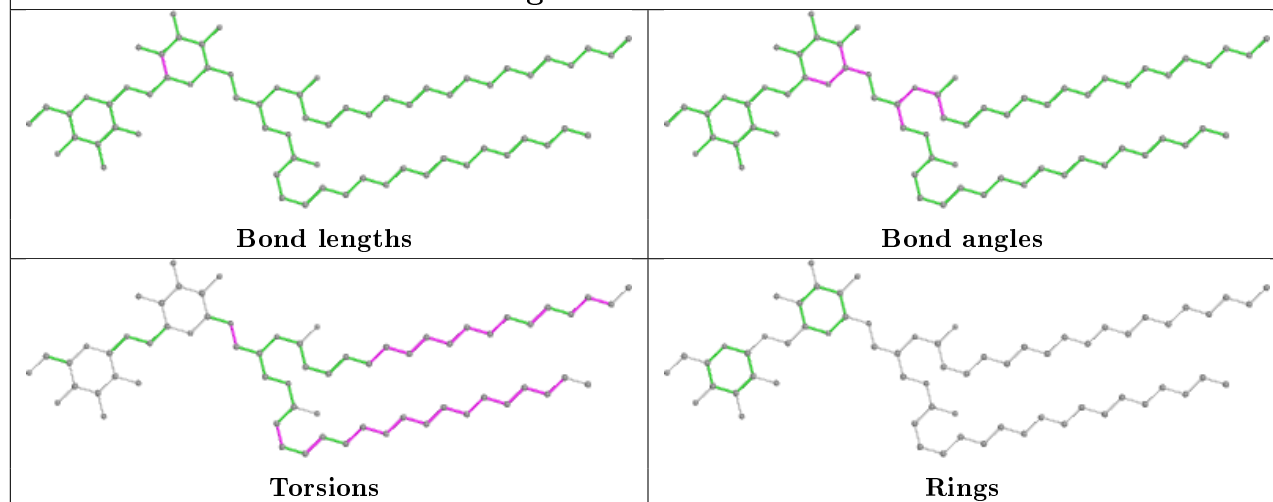
## Ligand CLA N 601



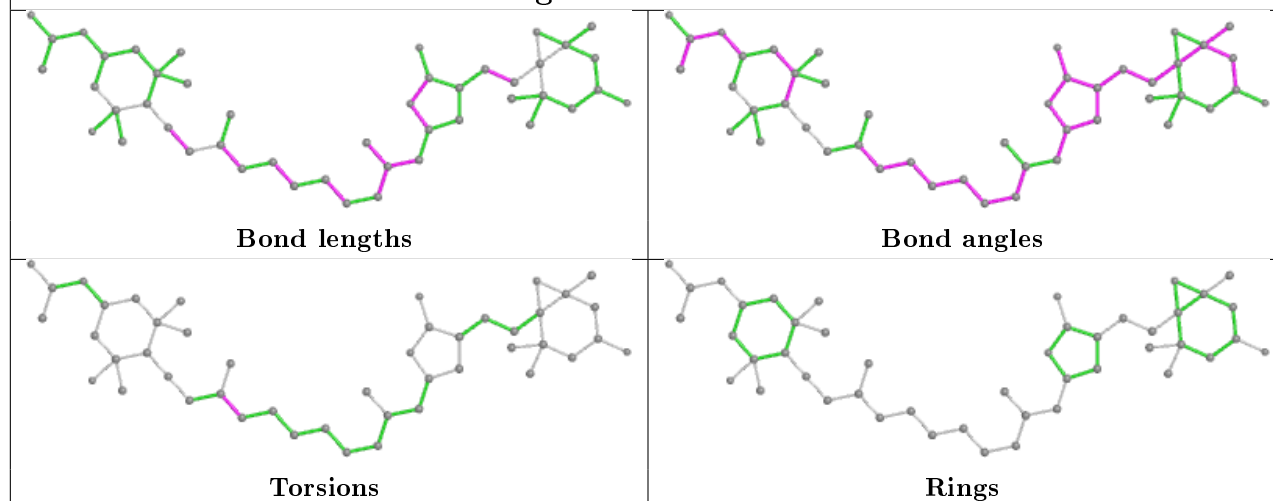
## Ligand PID M 611

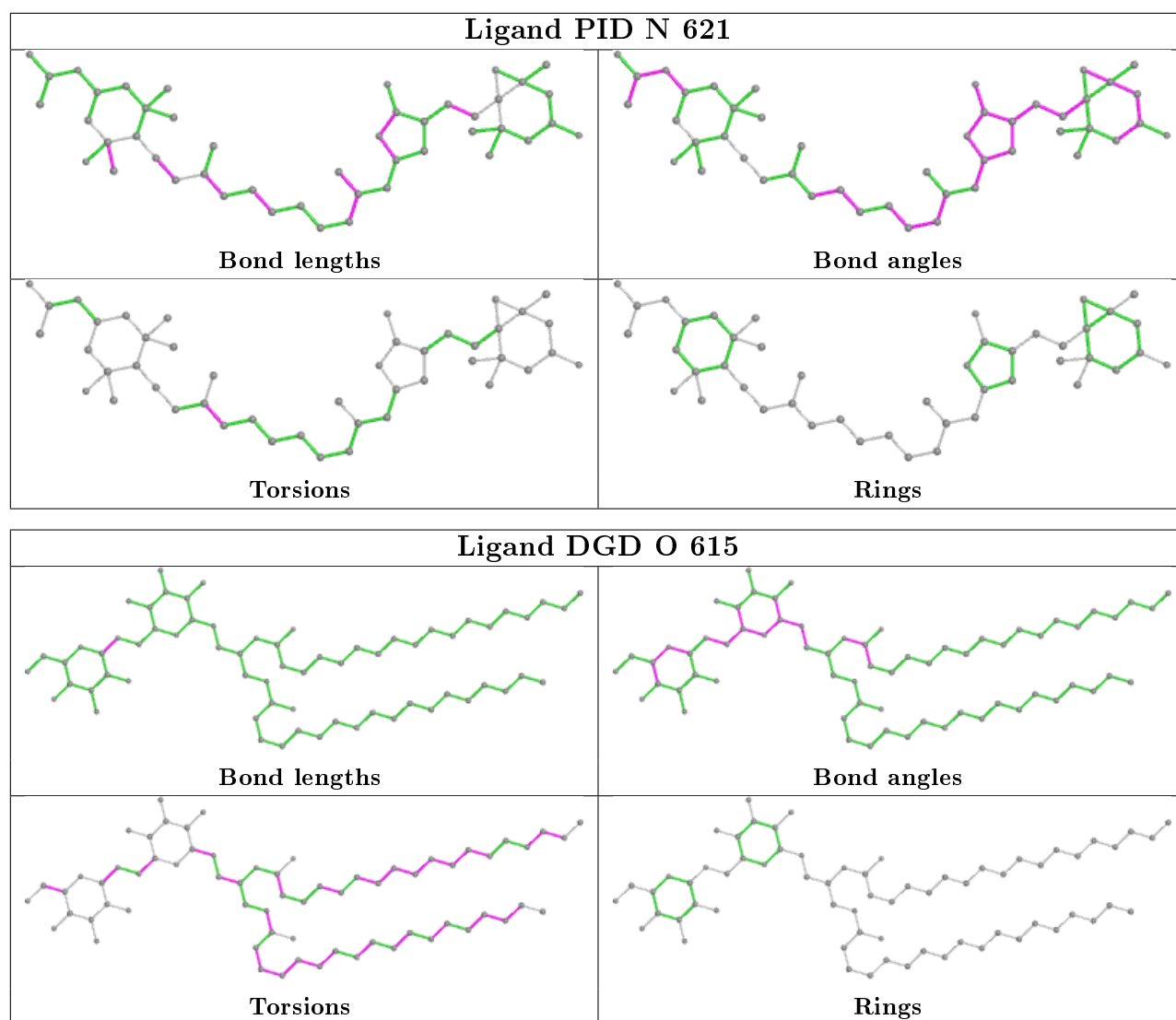


## Ligand DGD O 625



## Ligand PID N 611





## 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	M	312/312 (100%)	-0.66	3 (0%) 82 81	20, 31, 53, 63	0
1	N	312/312 (100%)	-0.51	9 (2%) 51 50	22, 34, 57, 66	0
1	O	312/312 (100%)	-0.68	7 (2%) 62 60	21, 29, 51, 64	0
All	All	936/936 (100%)	-0.62	19 (2%) 65 63	20, 31, 53, 66	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	159	THR	3.7
1	M	162	SER	3.5
1	N	163	GLY	3.2
1	O	163	GLY	3.2
1	N	153	SER	3.1

### 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.

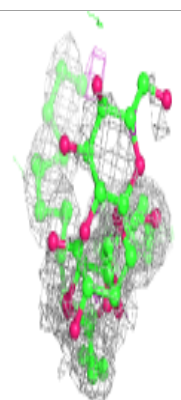
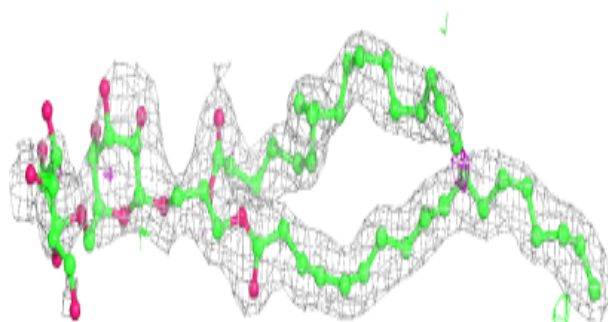
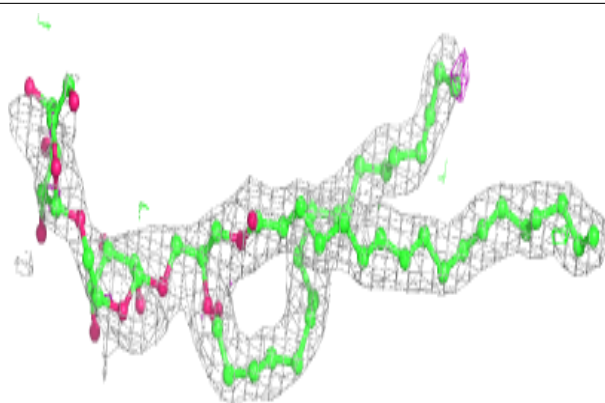
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DGD	N	615	66/66	0.61	0.25	42,51,105,106	0
4	DGD	O	615	66/66	0.64	0.25	37,49,104,104	0
4	DGD	M	615	66/66	0.66	0.24	38,50,105,105	0
3	PID	N	613	46/46	0.86	0.15	30,40,57,61	0
3	PID	O	613	46/46	0.89	0.13	23,34,54,60	0
3	PID	M	613	46/46	0.89	0.15	25,36,56,61	0
3	PID	N	612	46/46	0.91	0.14	26,29,40,51	0
3	PID	M	612	46/46	0.92	0.13	24,27,37,47	0
3	PID	N	611	46/46	0.92	0.11	21,30,41,45	0
3	PID	O	611	46/46	0.92	0.12	19,26,36,43	0
3	PID	M	611	46/46	0.93	0.12	20,28,39,41	0
3	PID	O	612	46/46	0.93	0.14	20,25,35,48	0
3	PID	N	623	46/46	0.93	0.13	22,30,38,42	0
3	PID	M	614	46/46	0.94	0.10	24,34,41,44	0
3	PID	N	614	46/46	0.94	0.10	25,38,44,49	0
3	PID	O	623	46/46	0.94	0.12	18,24,34,42	0
3	PID	O	614	46/46	0.95	0.10	20,30,38,41	0
3	PID	M	622	46/46	0.95	0.12	18,25,29,33	0
4	DGD	N	625	66/66	0.95	0.11	19,24,38,41	0
3	PID	M	623	46/46	0.95	0.11	18,26,33,38	0
3	PID	O	622	46/46	0.96	0.11	18,24,29,32	0
3	PID	N	622	46/46	0.96	0.11	21,26,33,37	0
2	CLA	N	601	65/65	0.96	0.15	26,32,46,47	0
2	CLA	M	601	65/65	0.96	0.14	22,29,43,46	0
4	DGD	O	625	66/66	0.96	0.10	19,24,39,41	0
2	CLA	O	601	65/65	0.96	0.14	21,26,43,45	0
4	DGD	M	625	66/66	0.96	0.11	22,25,41,43	0
3	PID	M	624	46/46	0.97	0.08	19,22,26,34	0
3	PID	O	621	46/46	0.97	0.09	17,21,25,26	0
3	PID	O	624	46/46	0.97	0.08	19,23,28,32	0
2	CLA	N	602	65/65	0.97	0.11	19,26,34,37	0
3	PID	N	624	46/46	0.97	0.08	22,26,31,35	0
2	CLA	M	602	65/65	0.97	0.11	19,23,33,35	0
2	CLA	O	602	65/65	0.98	0.11	18,22,31,34	0
3	PID	N	621	46/46	0.98	0.08	20,22,28,29	0
3	PID	M	621	46/46	0.98	0.09	17,21,26,28	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.

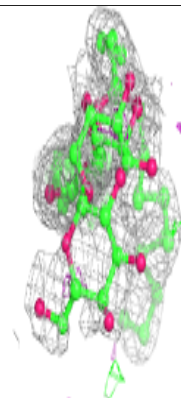
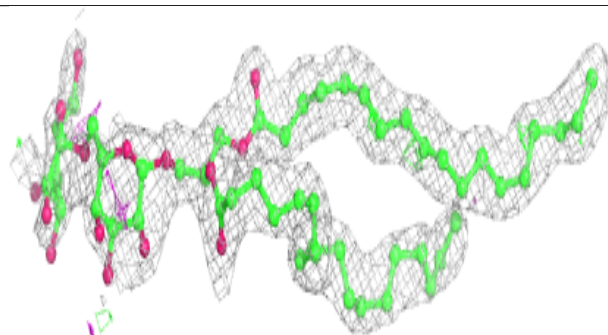
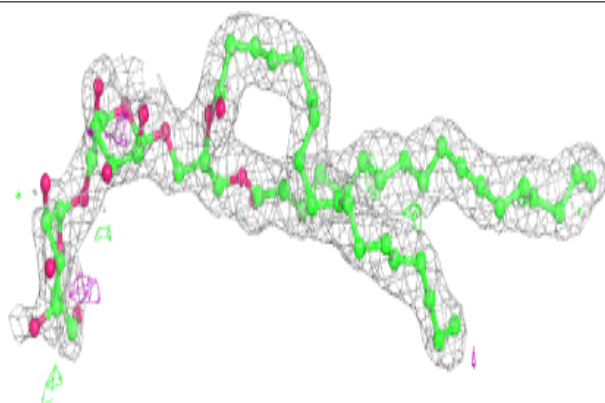


**Electron density around DGD N 615:**

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

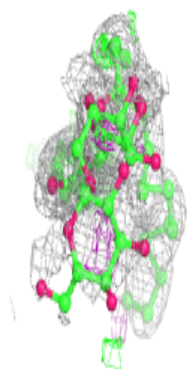
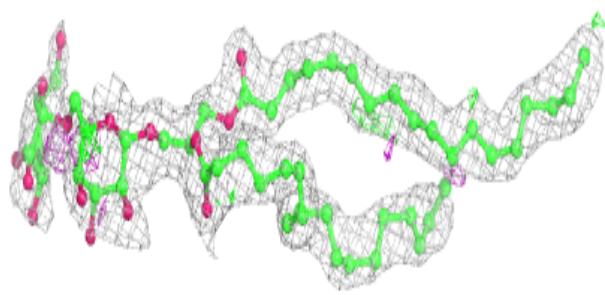
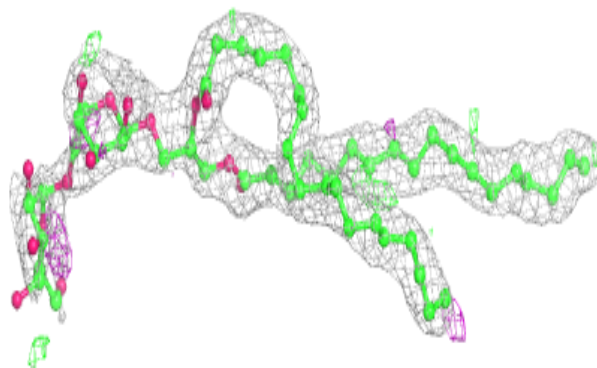
**Electron density around DGD O 615:**

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

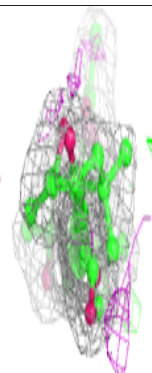
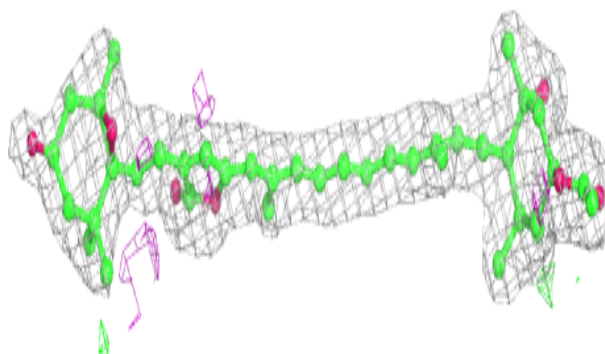
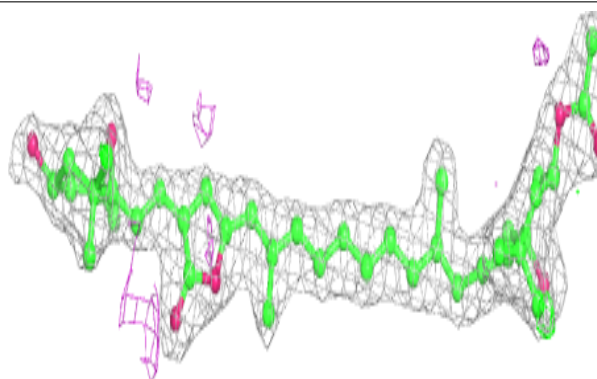


**Electron density around DGD M 615:**

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

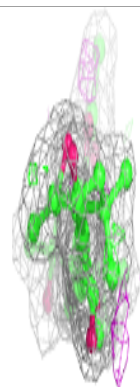
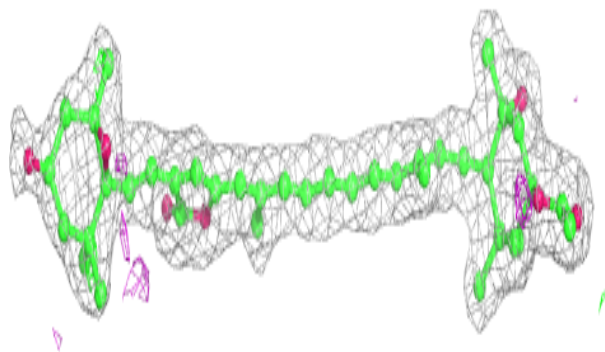
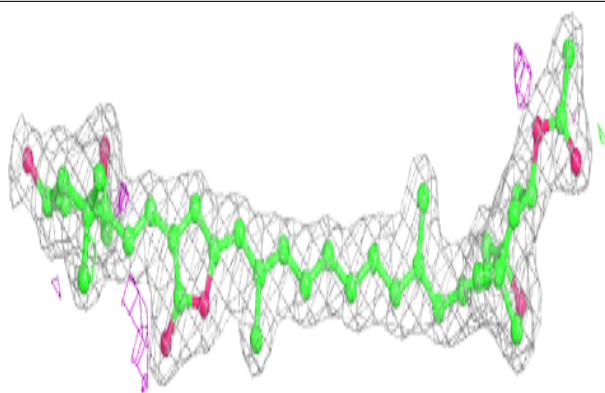
**Electron density around PID N 613:**

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

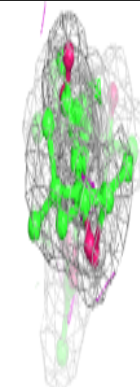
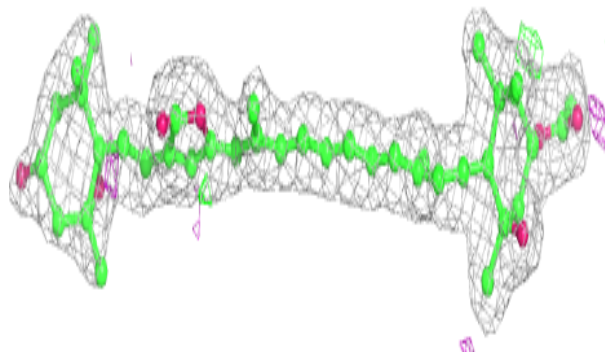
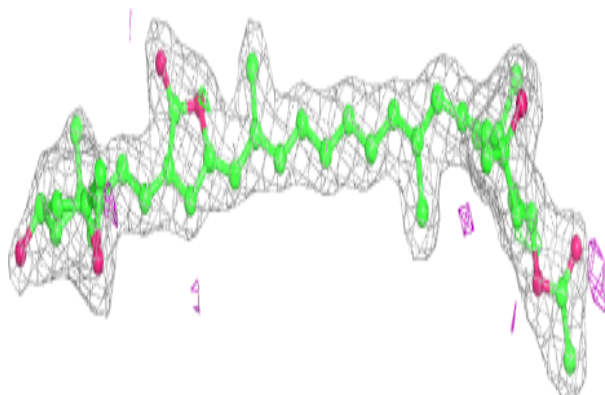


**Electron density around PID O 613:**

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

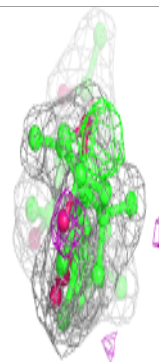
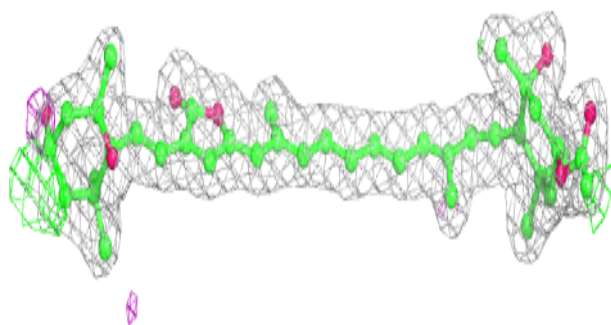
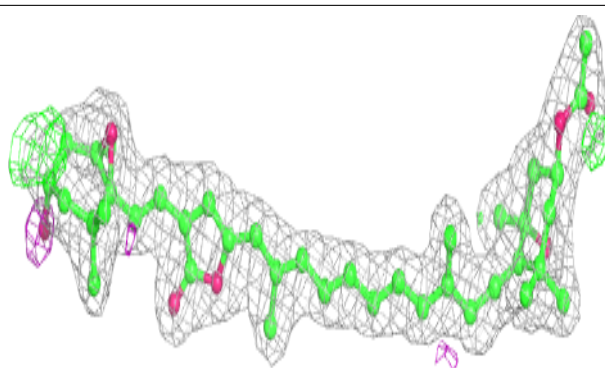
**Electron density around PID M 613:**

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

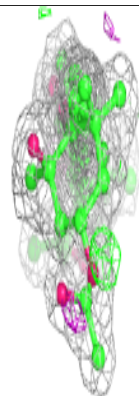
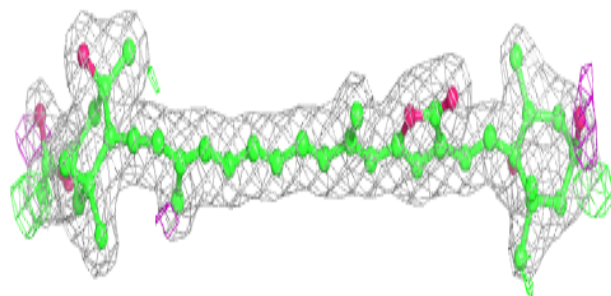
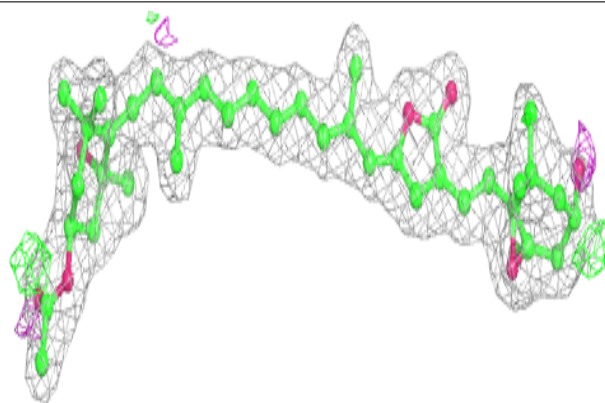


**Electron density around PID N 612:**

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

**Electron density around PID M 612:**

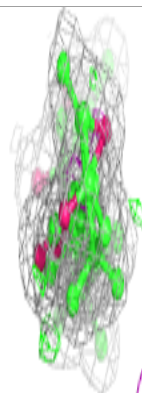
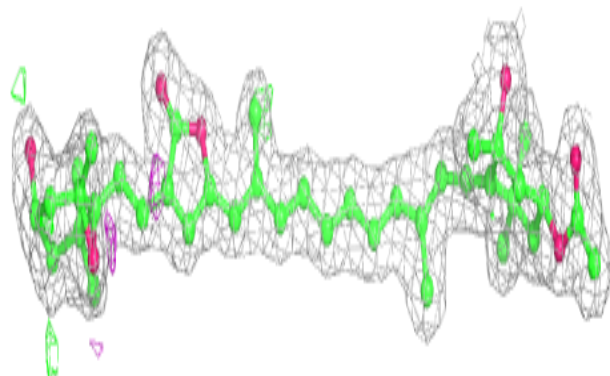
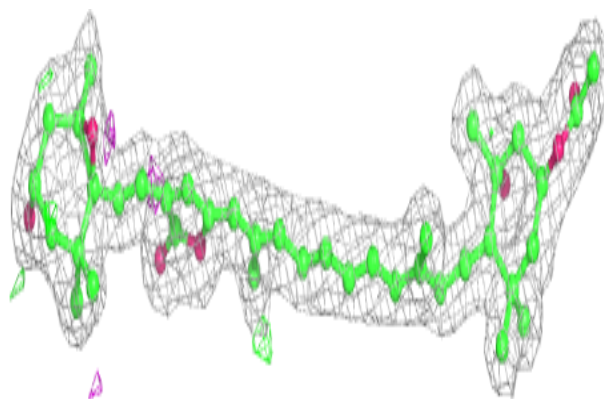
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



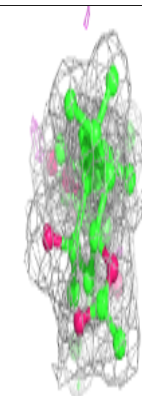
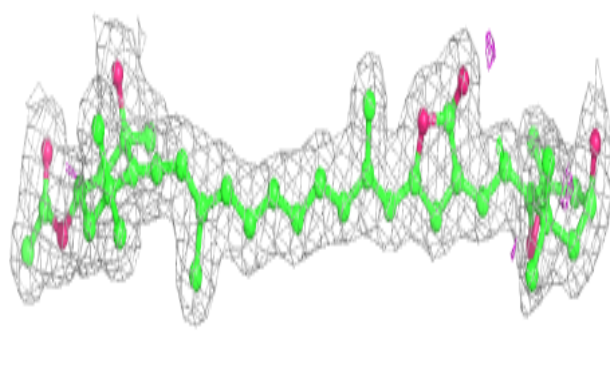
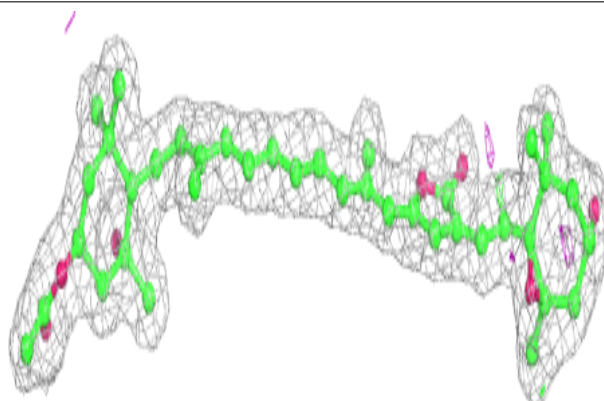


**Electron density around PID N 611:**

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

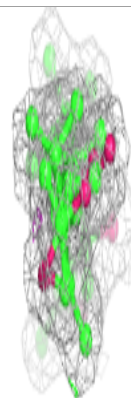
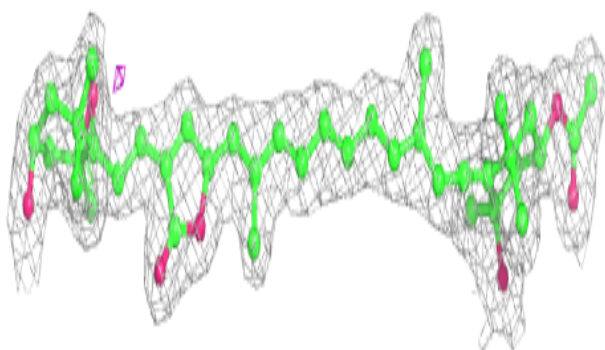
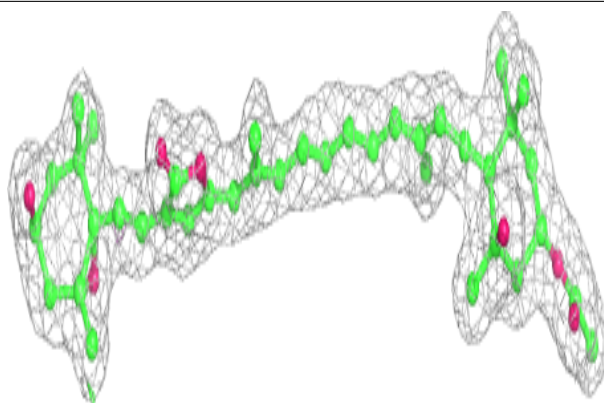
**Electron density around PID O 611:**

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

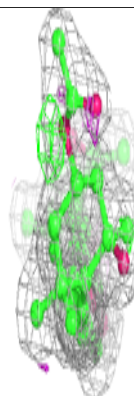
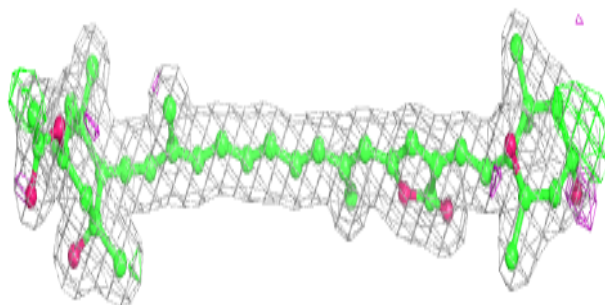
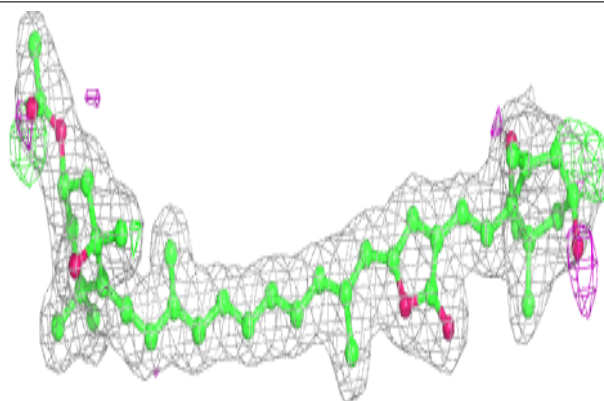


**Electron density around PID M 611:**

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

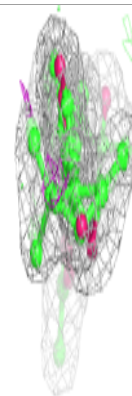
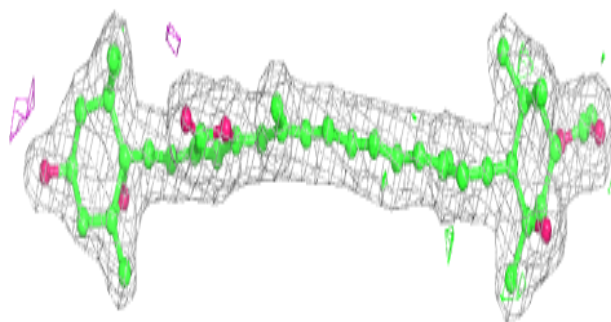
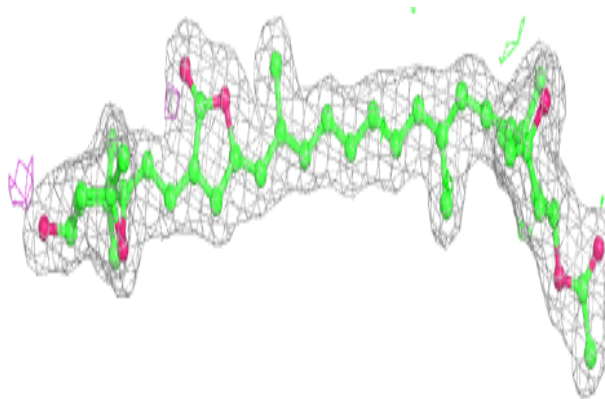
**Electron density around PID O 612:**

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

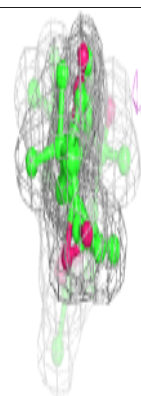
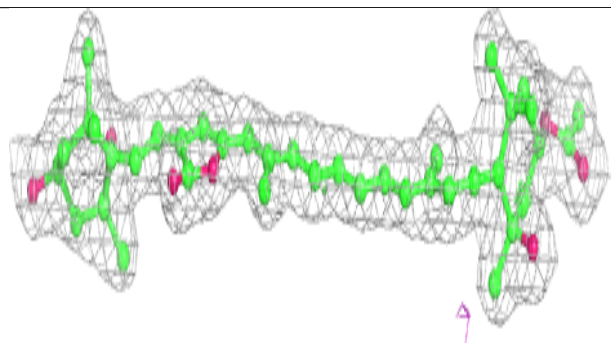
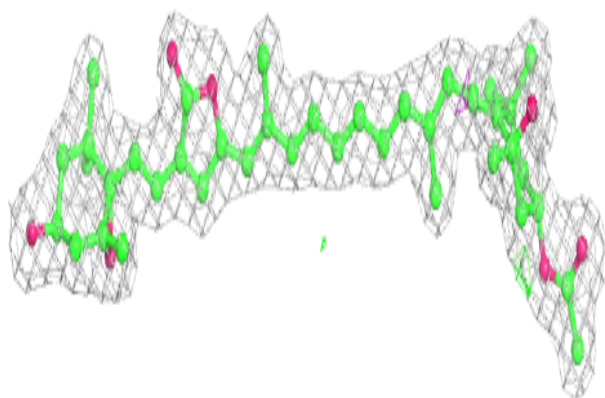


**Electron density around PID N 623:**

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

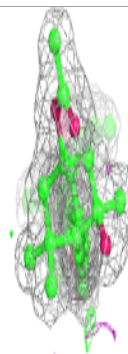
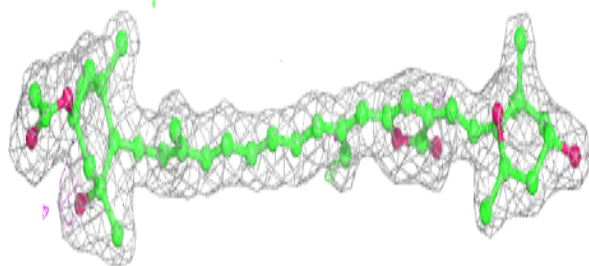
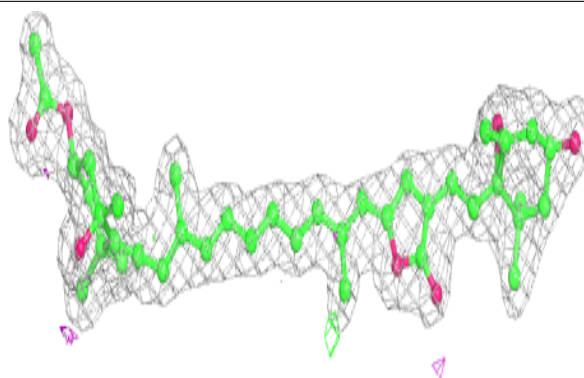
**Electron density around PID M 614:**

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

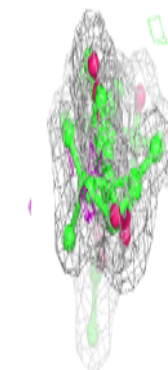
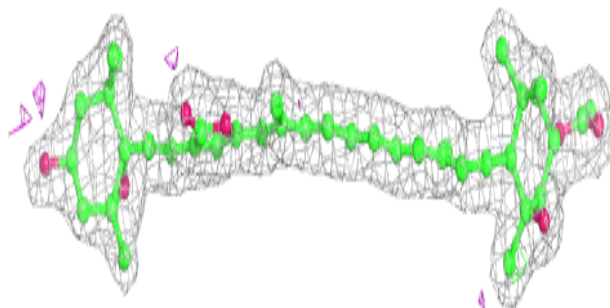
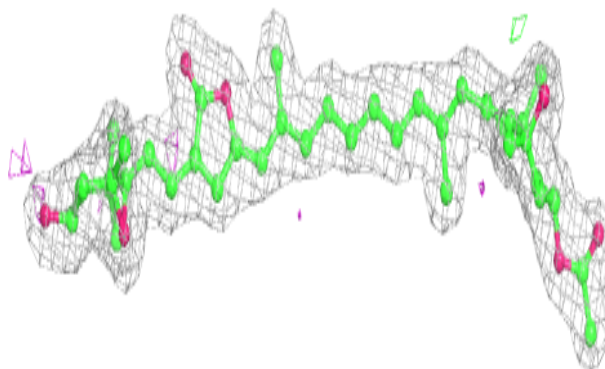


**Electron density around PID N 614:**

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

**Electron density around PID O 623:**

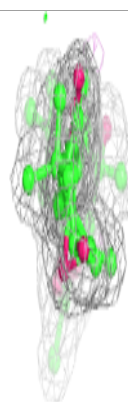
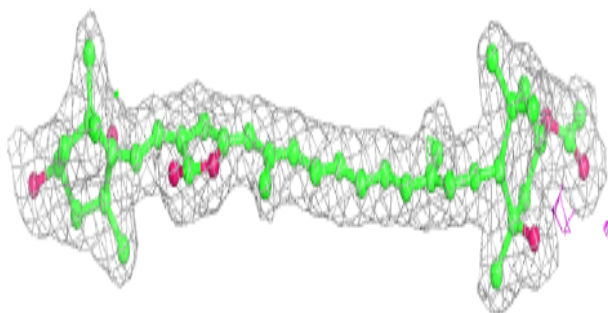
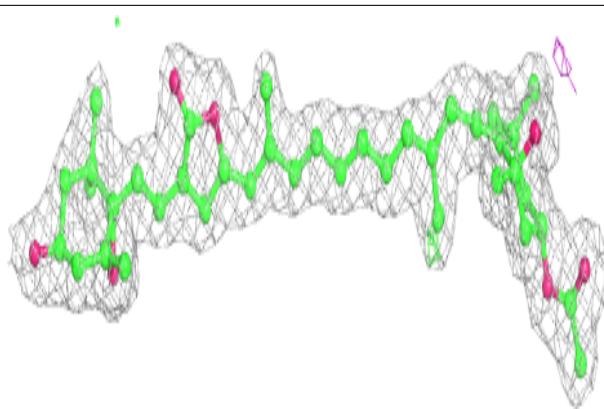
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



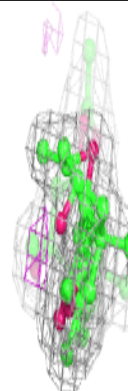
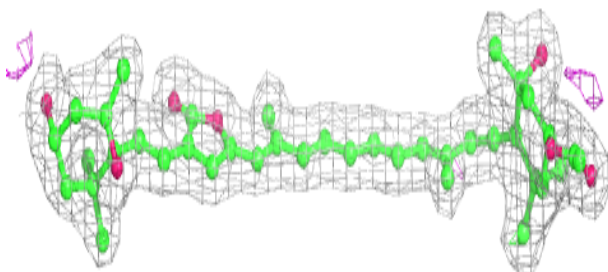
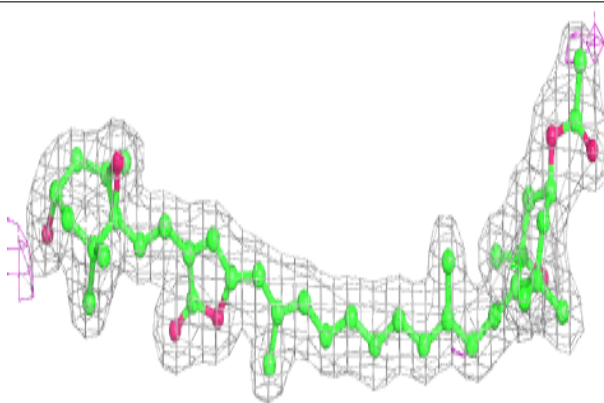


**Electron density around PID O 614:**

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

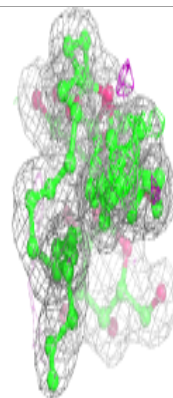
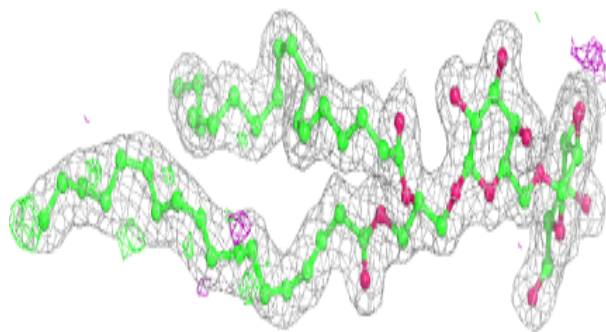
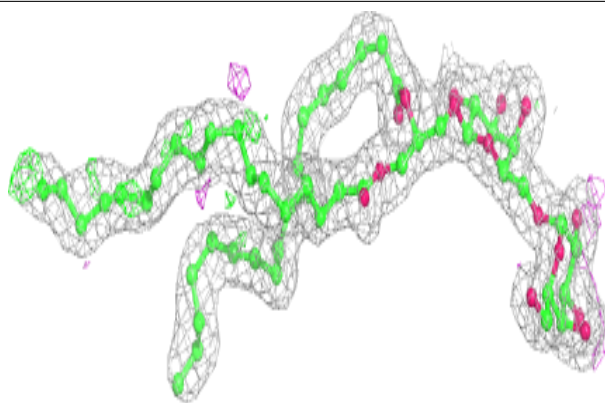
**Electron density around PID M 622:**

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

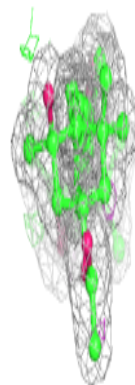
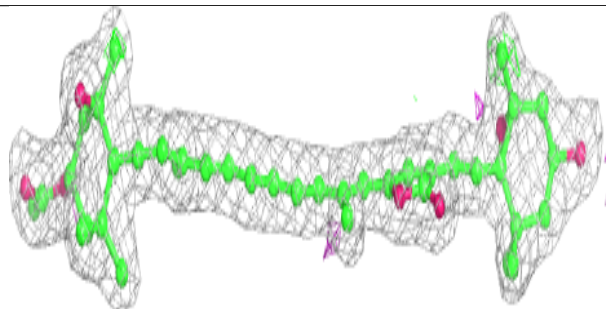
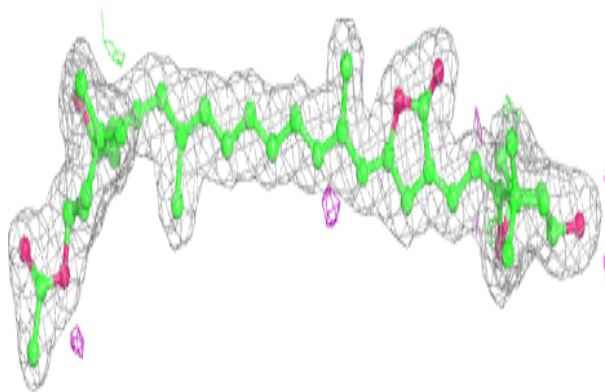


**Electron density around DGD N 625:**

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

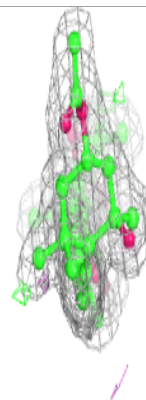
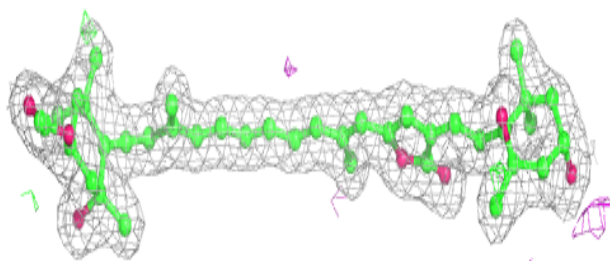
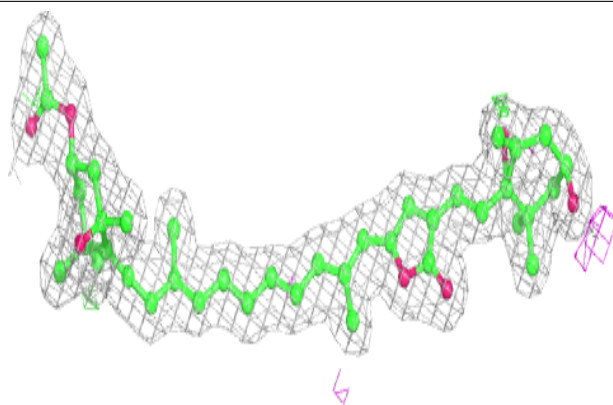
**Electron density around PID M 623:**

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

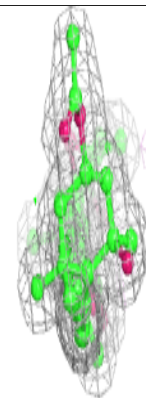
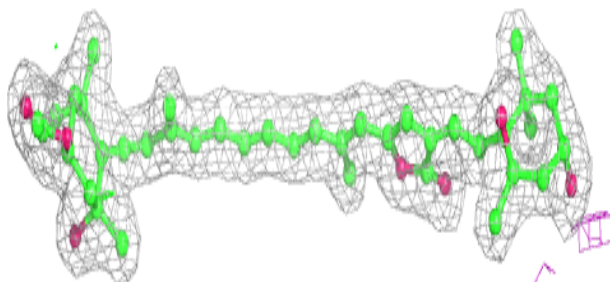
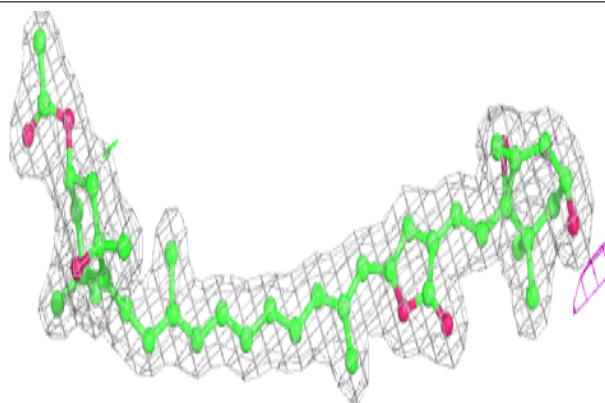


**Electron density around PID O 622:**

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

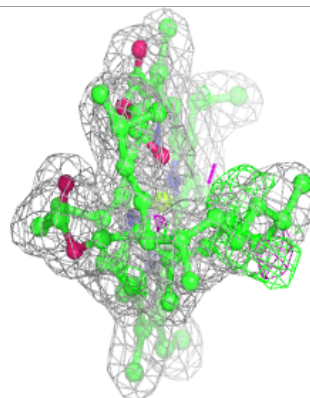
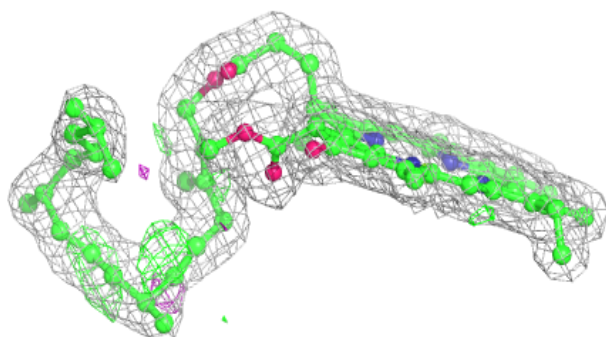
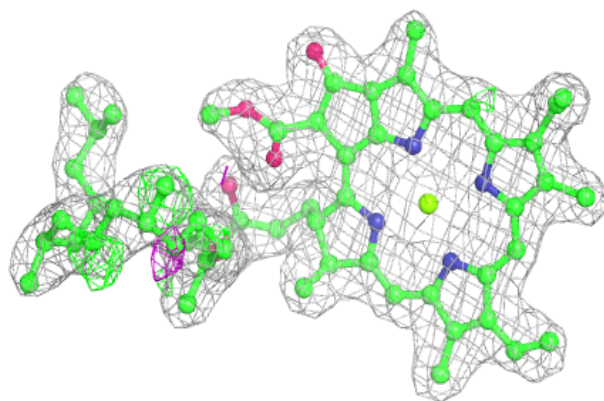
**Electron density around PID N 622:**

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

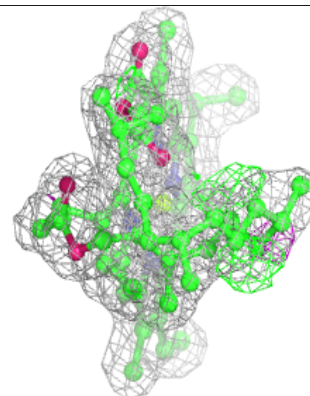
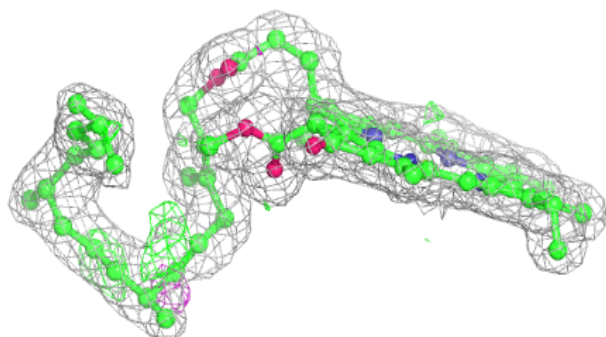
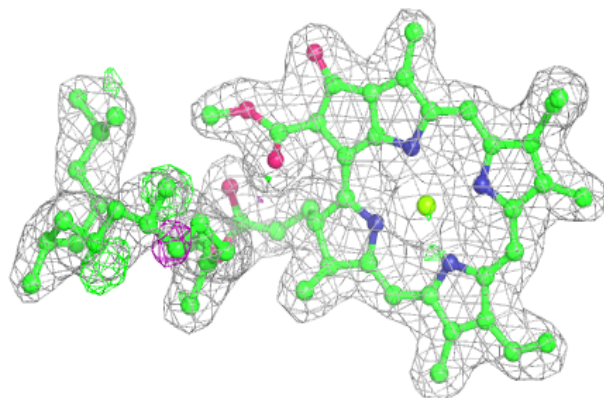


**Electron density around CLA N 601:**

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

**Electron density around CLA M 601:**

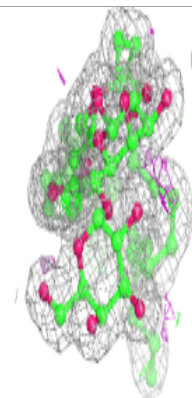
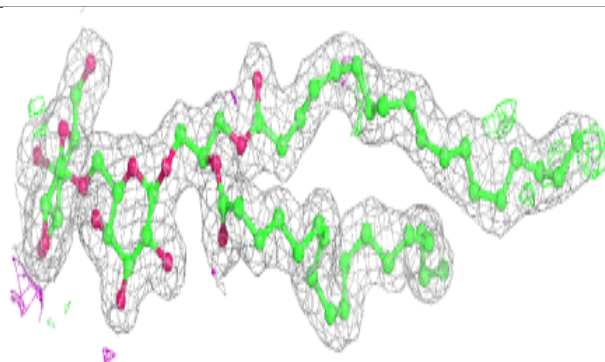
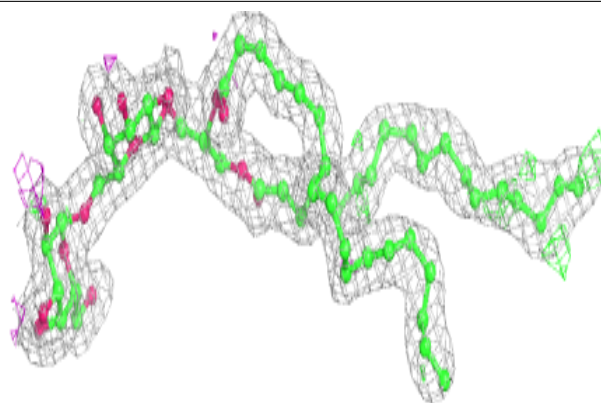
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



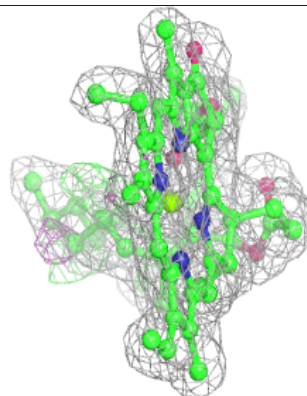
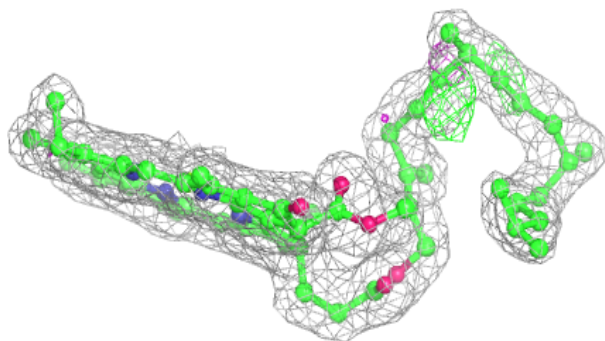
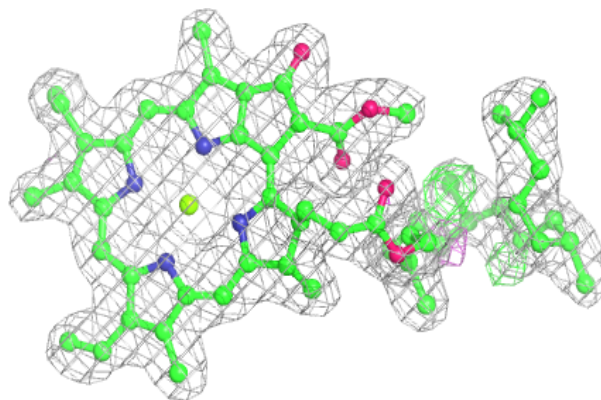


**Electron density around DGD O 625:**

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

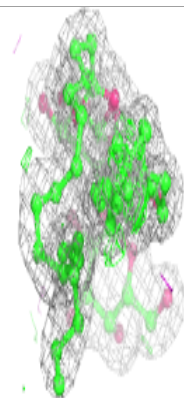
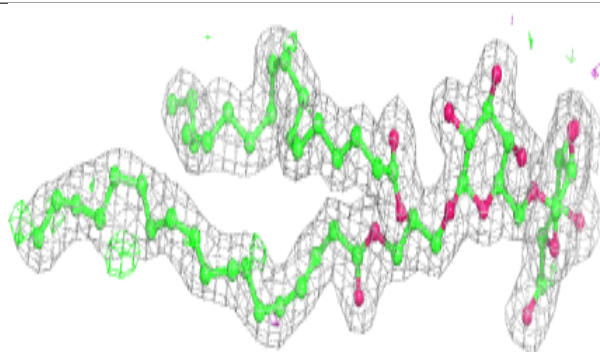
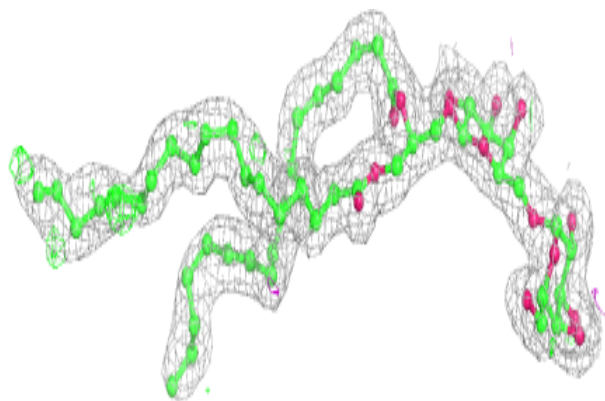
**Electron density around CLA O 601:**

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

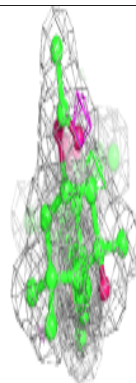
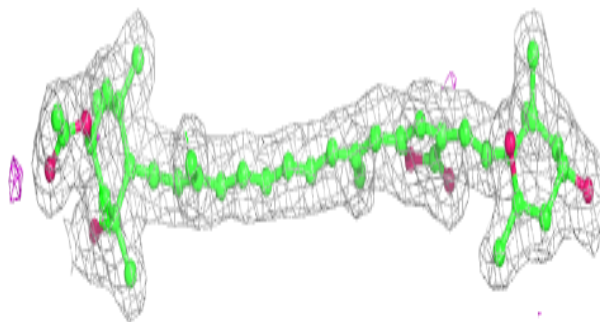
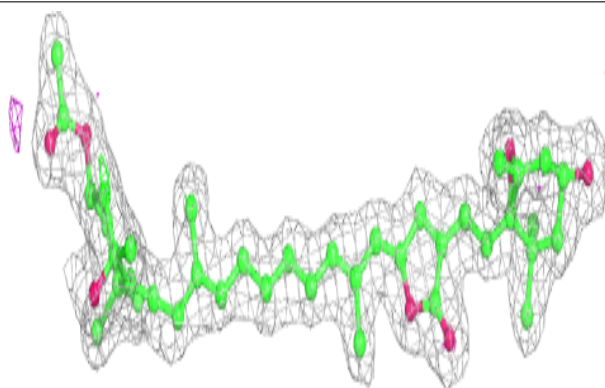


**Electron density around DGD M 625:**

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

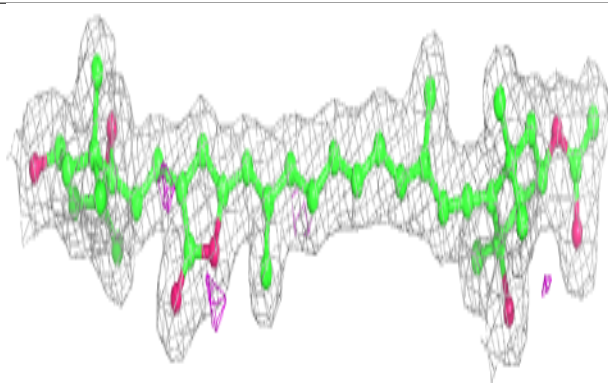
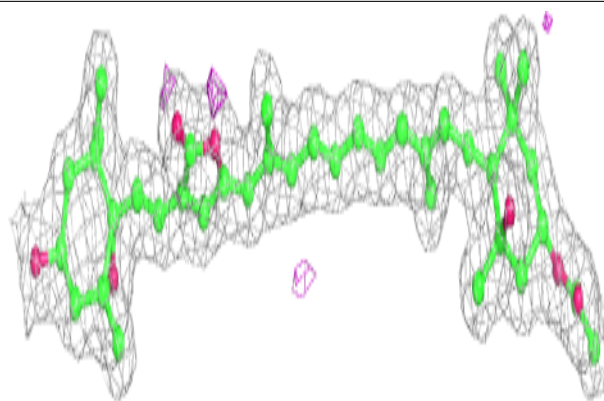
**Electron density around PID M 624:**

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

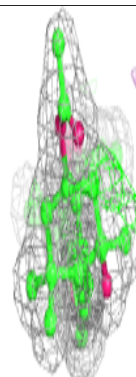
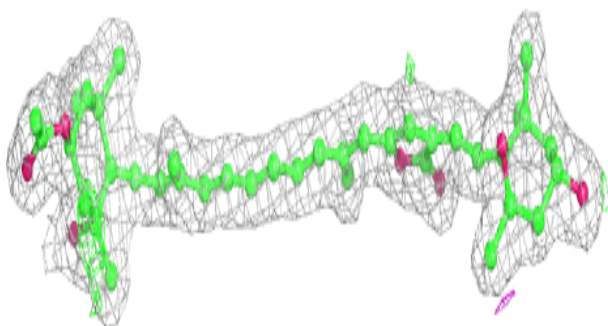
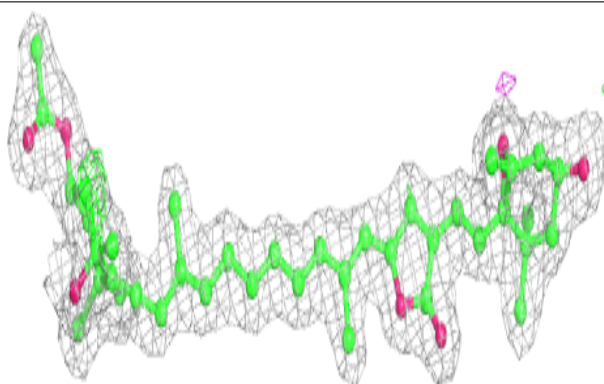


**Electron density around PID O 621:**

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

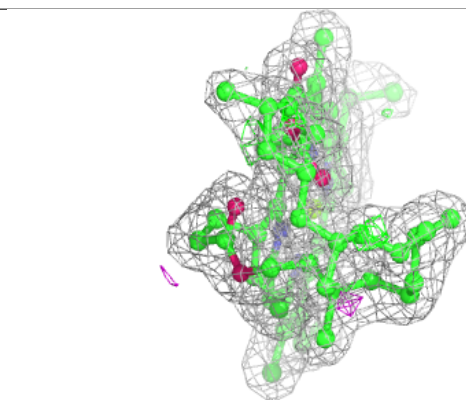
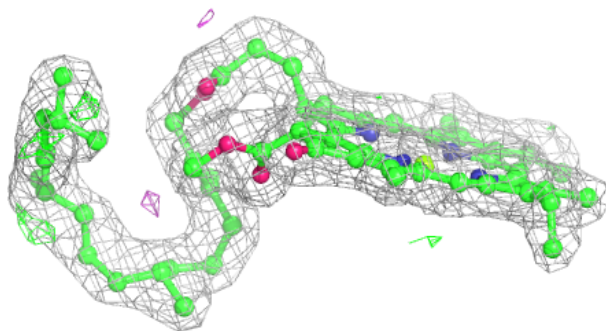
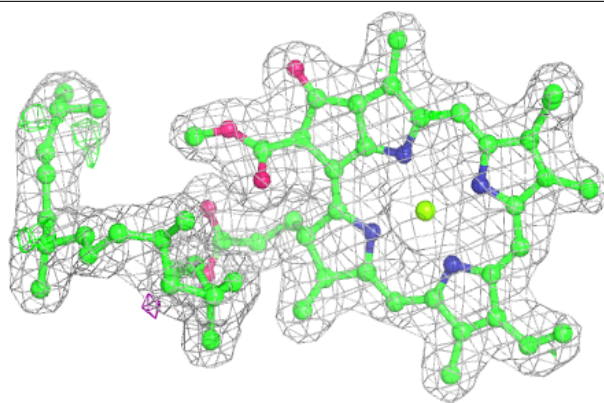
**Electron density around PID O 624:**

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

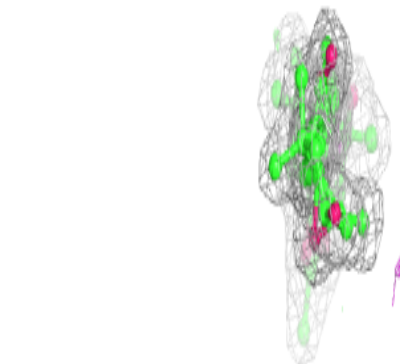
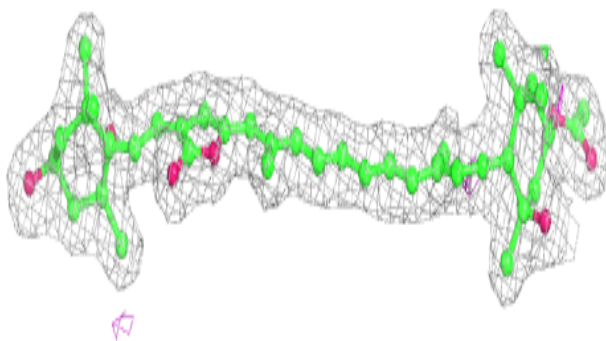
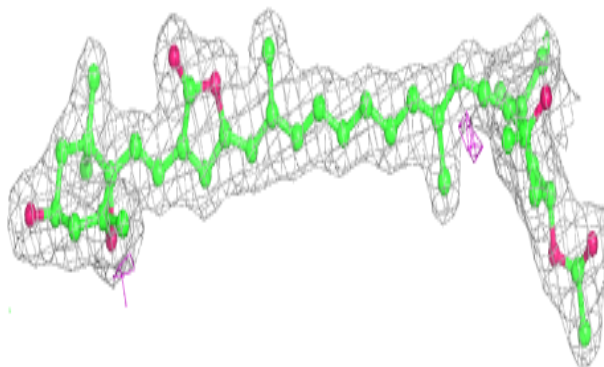


**Electron density around CLA N 602:**

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

**Electron density around PID N 624:**

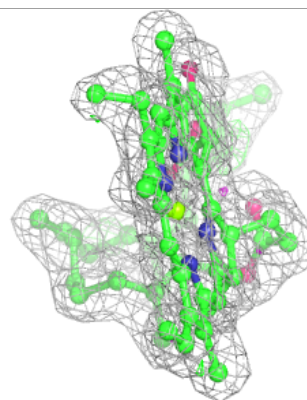
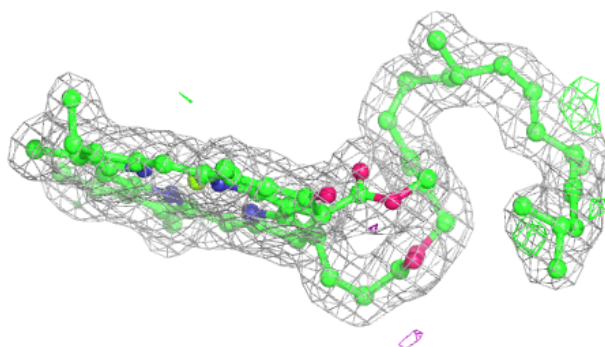
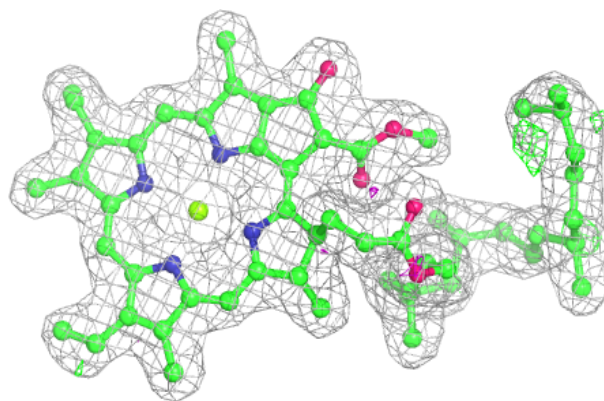
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



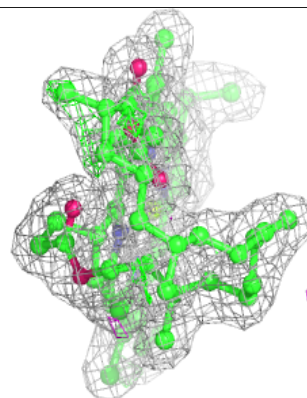
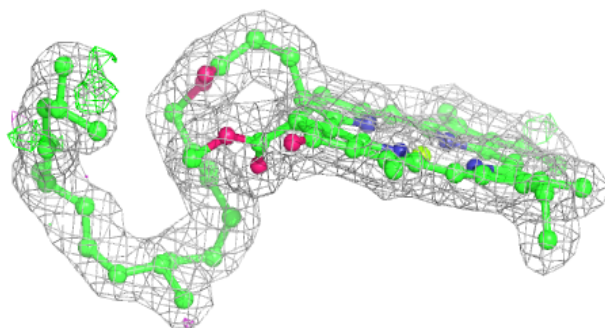
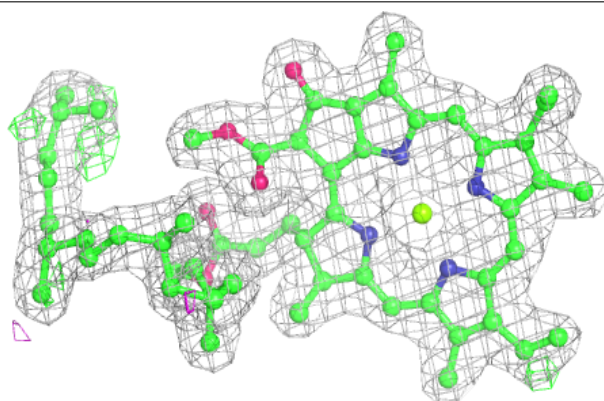


**Electron density around CLA M 602:**

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

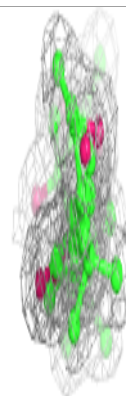
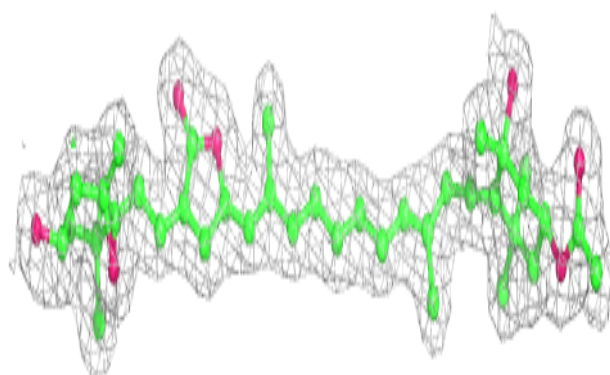
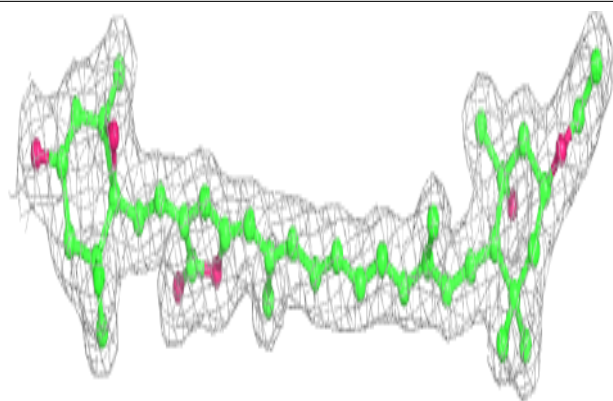
**Electron density around CLA O 602:**

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

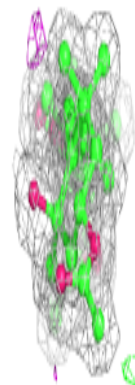
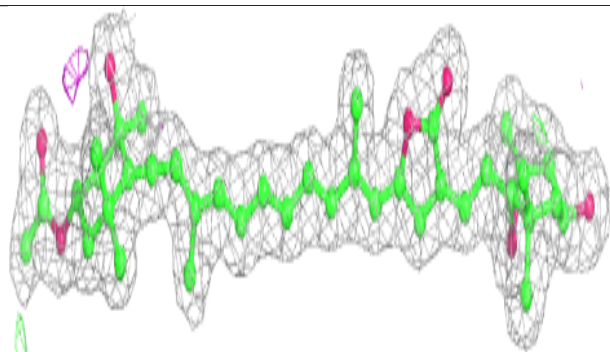
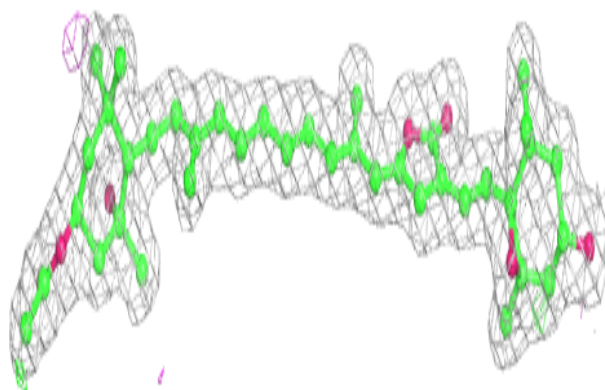


**Electron density around PID N 621:**

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

**Electron density around PID M 621:**

$2mF_o-DF_c$  (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.