wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2026 – 04:50 am BST

PDB ID	:	8OV5 / pdb_00008ov5
Title	:	PERIDININ-CHLOROPHYLL-PROTEIN OF AMPHIDINIUM CARTERAE, 100K
Authors	:	Hofmann, E.; Johanning, S.
Deposited on	:	2023-04-25
Resolution	:	1.15 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

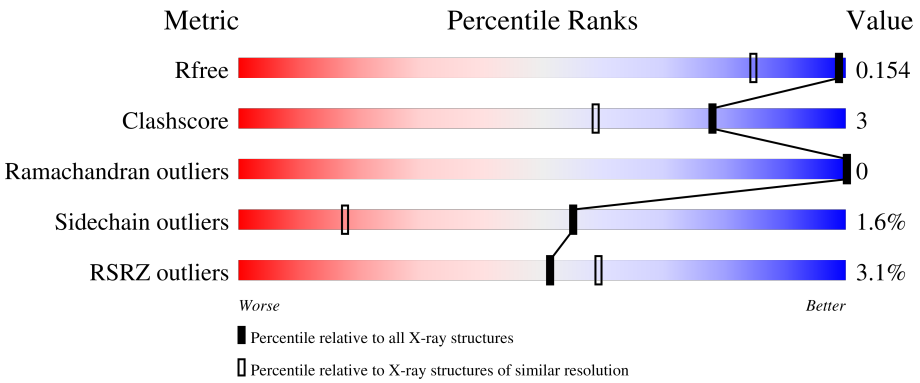
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.15 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}	180053	1380 (1.16-1.12)
Clashscore	190562	1393 (1.16-1.12)
Ramachandran outliers	187476	1369 (1.16-1.12)
Sidechain outliers	187428	1369 (1.16-1.12)
RSRZ outliers	180081	1379 (1.16-1.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	3% 94% 6%
1	N	312	4% 96% .
1	O	312	3% 94% 6%

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
3	PID	M	613[A]	X	-	-	-
3	PID	M	613[B]	X	-	-	-
3	PID	O	623[B]	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20859 atoms, of which 9740 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.

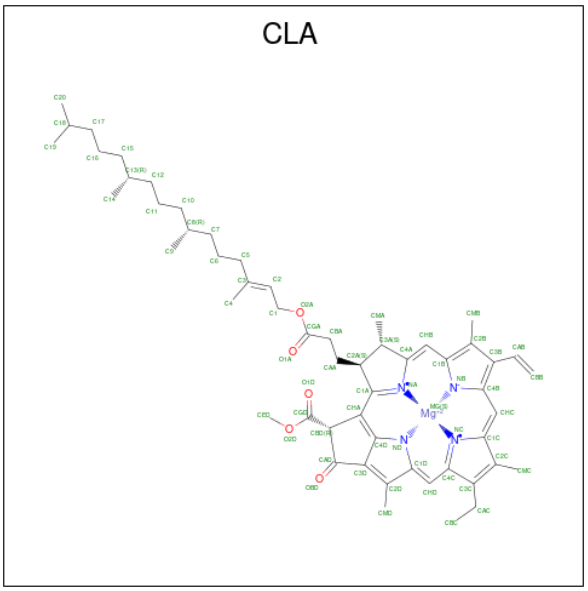
- Molecule 1 is a protein called Peridinin-chlorophyll a-binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	M	312	4870	1525	2460	402	471	12	0	27	0
1	N	312	4870	1525	2460	402	471	12	0	27	0
1	O	312	4869	1525	2459	402	471	12	0	27	0

There are 6 discrepancies between the modelled and reference sequences:

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

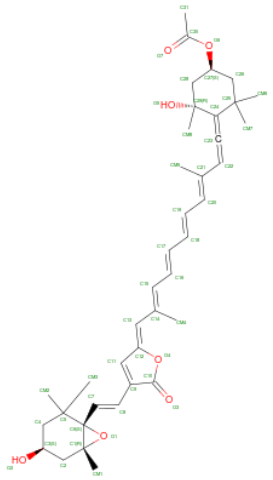
- Molecule 2 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
2	M	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
2	M	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
2	N	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
2	N	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
2	O	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
2	O	1	137	55	72	1	4	5	0	0

- Molecule 3 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).

PID



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	M	1	96	39	50	7	0	0
			Total	C	H	O		
3	M	1	96	39	50	7	0	0
			Total	C	H	O		
3	M	1	102	41	53	8	0	1
			Total	C	H	O		
3	M	1	96	39	50	7	0	0
			Total	C	H	O		
3	M	1	96	39	50	7	0	0
			Total	C	H	O		
3	M	1	96	39	50	7	0	0
			Total	C	H	O		
3	M	1	192	78	100	14	0	1
			Total	C	H	O		
3	M	1	96	39	50	7	0	0
			Total	C	H	O		
3	N	1	96	39	50	7	0	0
			Total	C	H	O		
3	N	1	96	39	50	7	0	0
			Total	C	H	O		
3	N	1	102	41	53	8	0	1
			Total	C	H	O		
3	N	1	96	39	50	7	0	0
			Total	C	H	O		
3	N	1	96	39	50	7	0	0
			Total	C	H	O		
3	N	1	96	39	50	7	0	0

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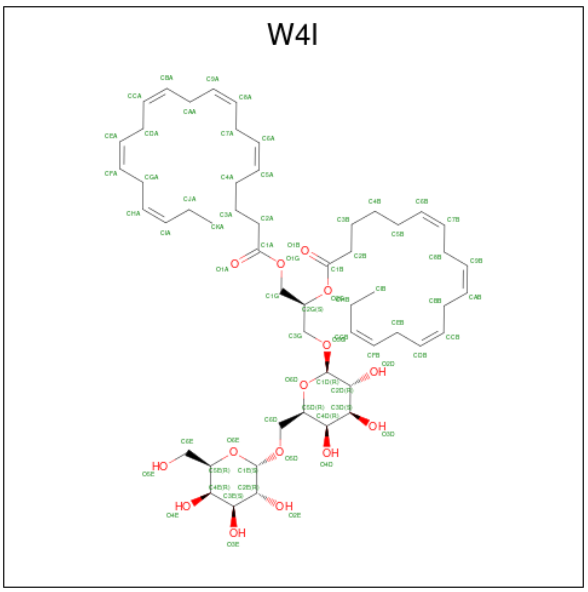
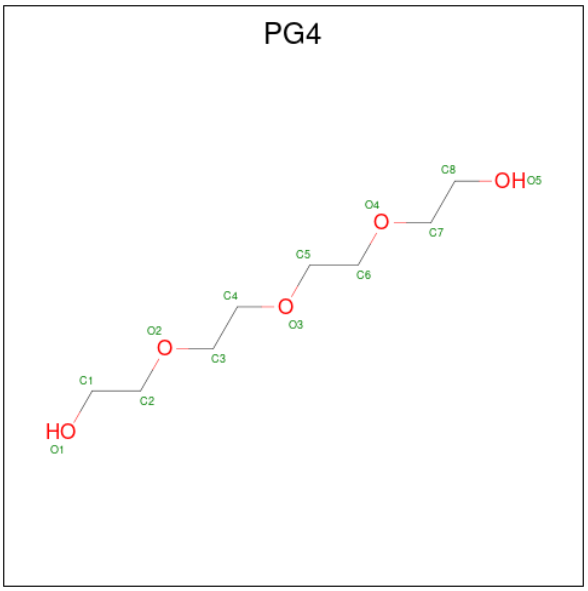
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	N	1	192	78	100	14	0	1
			Total	C	H	O		
3	N	1	96	39	50	7	0	0
			Total	C	H	O		
3	O	1	96	39	50	7	0	0
			Total	C	H	O		
3	O	1	96	39	50	7	0	0
			Total	C	H	O		
3	O	1	102	41	53	8	0	1
			Total	C	H	O		
3	O	1	96	39	50	7	0	0
			Total	C	H	O		
3	O	1	96	39	50	7	0	0
			Total	C	H	O		
3	O	1	96	39	50	7	0	0
			Total	C	H	O		
3	O	1	192	78	100	14	0	1
			Total	C	H	O		
3	O	1	96	39	50	7	0	0

- Molecule 4 is [(2 {S})-3-[(2 {R},3 {R},4 {S},5 {R},6 {R})-6-[[(2 {S},3 {R},4 {S},5 {R},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-2-[(6 {Z},9 {Z},12 {Z},15 {Z})-octadeca-6,9,12,15-tetraenoyl]oxy-propyl] (5 {Z},8 {Z},11 {Z},14 {Z},17 {Z})-icosa-5,8,11,14,17-pentaenoate (CCD ID: W4I) (formula: $C_{53}H_{82}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	M	1	147	55	82	10	0	1
			Total	C	H	O		
4	M	1	164	59	90	15	0	1
			Total	C	H	O		
4	N	1	147	55	82	10	0	1
			Total	C	H	O		
4	N	1	164	59	90	15	0	1
			Total	C	H	O		
4	O	1	147	55	82	10	0	1
			Total	C	H	O		
4	O	1	164	59	90	15	0	1

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	M	1	31	8	18	5	0	0
			Total	C	H	O		
5	N	1	31	8	18	5	0	0
			Total	C	H	O		
5	O	1	31	8	18	5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	M	621	621	621	0	1

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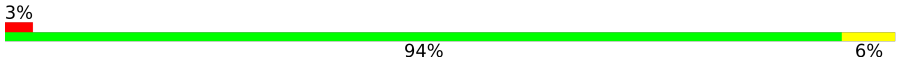
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	N	562	562	562	0	1
			Total	O		
6	O	609	609	609	0	1

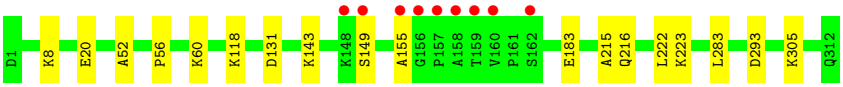
3 Residue-property plots (i)

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

• Molecule 1: Peridinin-chlorophyll a-binding protein 1, chloroplastic

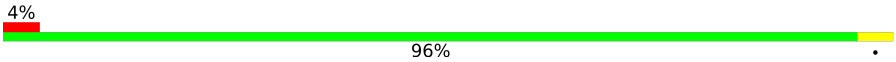
Chain M:

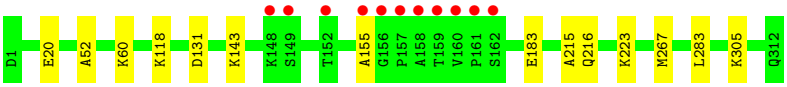




• Molecule 1: Peridinin-chlorophyll a-binding protein 1, chloroplastic

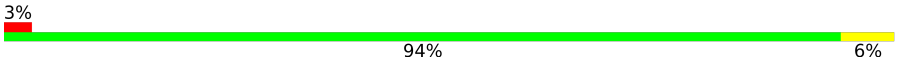
Chain N:

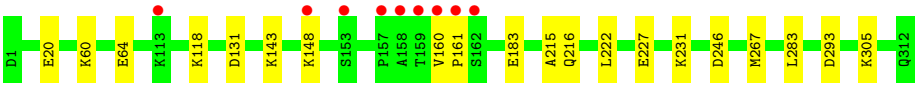




• Molecule 1: Peridinin-chlorophyll a-binding protein 1, chloroplastic

Chain O:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	197.14Å 115.61Å 65.88Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	43.38 – 1.15 43.38 – 1.15	Depositor EDS
% Data completeness (in resolution range)	85.6 (43.38-1.15) 79.6 (43.38-1.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.90 (at 1.15Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.141 , 0.155 0.141 , 0.154	Depositor DCC
R_{free} test set	22204 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	20859	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, PG4, CLA, W4I

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	0.38	0/2545	0.55	0/3449
1	N	0.34	0/2545	0.51	0/3449
1	O	0.38	0/2540	0.54	0/3442
All	All	0.37	0/7630	0.53	0/10340

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	2410	2460	2364	14	0
1	N	2410	2460	2364	11	0
1	O	2410	2459	2363	15	2
2	M	130	144	144	0	0
2	N	130	144	144	1	0
2	O	130	144	144	0	0
3	M	417	453	406	5	0
3	N	417	453	406	4	0
3	O	417	453	406	9	0
4	M	139	172	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	139	172	0	0	0
4	O	139	172	0	0	0
5	M	13	18	18	0	0
5	N	13	18	18	0	0
5	O	13	18	18	0	0
6	M	621	0	0	5	6
6	N	562	0	0	5	0
6	O	609	0	0	5	4
All	All	11119	9740	8795	52	6

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 3.

The worst 5 of 52 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:N:183[A]:GLU:OE2	6:N:747:HOH:O	2.07	0.72
1:O:64:GLU:OE2	6:O:763:HOH:O	2.08	0.69
1:O:227:GLU:OE1	6:O:776:HOH:O	2.11	0.69
1:M:118:LYS:NZ	6:M:703:HOH:O	2.27	0.69
1:O:183[A]:GLU:OE2	6:O:703:HOH:O	2.12	0.66

The worst 5 of 6 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)
1:O:231:LYS:NZ	6:M:1184:HOH:O[4_555]	2.00	0.20
6:M:1184:HOH:O	6:O:951:HOH:O[4_545]	2.03	0.17
1:O:246:ASP:OD1	6:M:1184:HOH:O[4_555]	2.05	0.15
6:M:744:HOH:O	6:O:1061:HOH:O[4_545]	2.12	0.08
6:M:1184:HOH:O	6:O:970:HOH:O[4_545]	2.13	0.07

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	339/312 (109%)	339 (100%)	0	0	100	100
1	N	339/312 (109%)	339 (100%)	0	0	100	100
1	O	338/312 (108%)	338 (100%)	0	0	100	100
All	All	1016/936 (108%)	1016 (100%)	0	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	259/233 (111%)	254 (98%)	5 (2%)	50	11
1	N	259/233 (111%)	255 (98%)	4 (2%)	57	19
1	O	259/233 (111%)	254 (98%)	5 (2%)	50	11
All	All	777/699 (111%)	763 (98%)	14 (2%)	55	13

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	305[A]	LYS
1	N	305[B]	LYS
1	O	305[B]	LYS
1	O	283	LEU
1	O	305[A]	LYS

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

Mol	Chain	Res	Type
1	N	36	GLN
1	O	30	GLN
1	O	36	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

51 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	612	-	41,49,49	1.47	4 (9%)	49,76,76	0.82	1 (2%)
2	CLA	N	601	6	69,73,73	1.15	6 (8%)	83,113,113	1.40	5 (6%)
3	PID	N	612	-	41,49,49	1.29	3 (7%)	49,76,76	0.98	2 (4%)
4	W4I	M	615[B]	-	57,57,69	1.36	6 (10%)	63,65,83	1.24	7 (11%)
3	PID	M	613[A]	-	41,49,49	1.11	4 (9%)	49,76,76	0.89	1 (2%)
3	PID	O	611	-	41,49,49	1.21	2 (4%)	49,76,76	0.87	1 (2%)
4	W4I	O	615[B]	-	57,57,69	1.40	7 (12%)	63,65,83	1.16	5 (7%)
3	PID	O	622	-	41,49,49	1.11	3 (7%)	49,76,76	1.02	1 (2%)
4	W4I	M	625[A]	-	69,69,69	0.75	1 (1%)	81,83,83	0.75	0
3	PID	O	613[A]	-	41,49,49	1.28	4 (9%)	49,76,76	0.83	1 (2%)
3	PID	O	614	-	41,49,49	0.86	0	49,76,76	0.84	2 (4%)
3	PID	M	621	-	41,49,49	0.95	2 (4%)	49,76,76	0.83	1 (2%)
5	PG4	N	651	-	12,12,12	0.12	0	11,11,11	0.51	0
3	PID	M	623[A]	-	41,49,49	1.24	5 (12%)	49,76,76	0.90	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	W4I	N	625[A]	-	69,69,69	0.89	2 (2%)	81,83,83	0.83	3 (3%)
4	W4I	O	625[A]	-	69,69,69	0.85	3 (4%)	81,83,83	0.81	1 (1%)
3	PID	N	623[A]	-	41,49,49	0.94	1 (2%)	49,76,76	0.69	0
3	PID	N	613[B]	-	41,49,49	1.20	5 (12%)	49,76,76	0.85	1 (2%)
4	W4I	N	615[B]	-	57,57,69	1.44	9 (15%)	63,65,83	1.20	7 (11%)
3	PID	N	621	-	41,49,49	0.92	1 (2%)	49,76,76	0.71	0
3	PID	N	624	-	41,49,49	1.00	2 (4%)	49,76,76	0.82	2 (4%)
3	PID	O	612	-	41,49,49	1.46	4 (9%)	49,76,76	0.91	2 (4%)
3	PID	O	623[B]	-	41,49,49	1.14	5 (12%)	49,76,76	0.94	3 (6%)
5	PG4	M	651	-	12,12,12	0.15	0	11,11,11	0.46	0
3	PID	M	613[B]	-	41,49,49	1.02	3 (7%)	49,76,76	0.87	1 (2%)
2	CLA	M	602	6	69,73,73	1.22	5 (7%)	83,113,113	1.28	3 (3%)
4	W4I	M	625[B]	-	69,69,69	0.74	1 (1%)	81,83,83	0.73	0
2	CLA	N	602	6	69,73,73	1.24	8 (11%)	83,113,113	1.34	5 (6%)
3	PID	M	622	-	41,49,49	0.93	1 (2%)	49,76,76	1.02	3 (6%)
3	PID	M	623[B]	-	41,49,49	1.09	3 (7%)	49,76,76	0.96	2 (4%)
3	PID	O	613[B]	-	41,49,49	1.18	3 (7%)	49,76,76	0.75	0
4	W4I	M	615[A]	-	57,57,69	1.36	6 (10%)	63,65,83	1.20	7 (11%)
3	PID	O	621	-	41,49,49	1.03	3 (7%)	49,76,76	0.80	1 (2%)
4	W4I	N	625[B]	-	69,69,69	0.89	2 (2%)	81,83,83	0.82	3 (3%)
4	W4I	O	625[B]	-	69,69,69	0.86	3 (4%)	81,83,83	0.79	1 (1%)
3	PID	M	624	-	41,49,49	0.92	1 (2%)	49,76,76	0.89	2 (4%)
3	PID	N	623[B]	-	41,49,49	1.00	3 (7%)	49,76,76	0.74	1 (2%)
3	PID	O	624	-	41,49,49	0.81	0	49,76,76	0.69	0
4	W4I	O	615[A]	-	57,57,69	1.40	7 (12%)	63,65,83	1.14	5 (7%)
3	PID	M	614	-	41,49,49	0.86	1 (2%)	49,76,76	0.76	1 (2%)
3	PID	N	622	-	41,49,49	1.05	3 (7%)	49,76,76	1.05	3 (6%)
2	CLA	M	601	6	69,73,73	1.24	6 (8%)	83,113,113	1.25	5 (6%)
3	PID	N	613[A]	-	41,49,49	1.24	6 (14%)	49,76,76	0.89	2 (4%)
4	W4I	N	615[A]	-	57,57,69	1.44	9 (15%)	63,65,83	1.23	7 (11%)
3	PID	N	614	-	41,49,49	0.89	1 (2%)	49,76,76	0.74	0
5	PG4	O	651	-	12,12,12	0.13	0	11,11,11	0.53	0
2	CLA	O	602	6	69,73,73	1.21	6 (8%)	83,113,113	1.18	6 (7%)
2	CLA	O	601	6	69,73,73	1.24	5 (7%)	83,113,113	1.18	4 (4%)
3	PID	M	611	-	41,49,49	1.24	2 (4%)	49,76,76	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PID	N	611	-	41,49,49	1.25	2 (4%)	49,76,76	0.85	0
3	PID	O	623[A]	-	41,49,49	1.22	2 (4%)	49,76,76	0.94	4 (8%)

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	612	-	-	0/24/93/93	0/4/4/4
2	CLA	N	601	6	-	1/39/115/115	-
3	PID	N	612	-	-	0/24/93/93	0/4/4/4
4	W4I	M	615[B]	-	-	14/52/72/97	0/1/1/2
3	PID	M	613[A]	-	1/1/25/25	0/24/93/93	0/4/4/4
3	PID	O	611	-	-	0/24/93/93	0/4/4/4
4	W4I	O	615[B]	-	-	9/52/72/97	0/1/1/2
3	PID	O	622	-	-	0/24/93/93	0/4/4/4
4	W4I	M	625[A]	-	-	6/57/97/97	0/2/2/2
3	PID	O	613[A]	-	-	0/24/93/93	0/4/4/4
3	PID	O	614	-	-	0/24/93/93	0/4/4/4
3	PID	M	621	-	-	0/24/93/93	0/4/4/4
5	PG4	N	651	-	-	2/10/10/10	-
3	PID	M	623[A]	-	-	0/24/93/93	0/4/4/4
4	W4I	N	625[A]	-	-	5/57/97/97	0/2/2/2
4	W4I	O	625[A]	-	-	6/57/97/97	0/2/2/2
3	PID	N	623[A]	-	-	0/24/93/93	0/4/4/4
3	PID	N	613[B]	-	-	0/24/93/93	0/4/4/4
4	W4I	N	615[B]	-	-	17/52/72/97	0/1/1/2
3	PID	N	621	-	-	0/24/93/93	0/4/4/4
3	PID	N	624	-	-	0/24/93/93	0/4/4/4
3	PID	O	612	-	-	0/24/93/93	0/4/4/4
3	PID	O	623[B]	-	1/1/25/25	0/24/93/93	0/4/4/4
5	PG4	M	651	-	-	2/10/10/10	-
3	PID	M	613[B]	-	1/1/25/25	0/24/93/93	0/4/4/4
2	CLA	M	602	6	-	0/39/115/115	-
4	W4I	M	625[B]	-	-	4/57/97/97	0/2/2/2
2	CLA	N	602	6	-	0/39/115/115	-
3	PID	M	622	-	-	0/24/93/93	0/4/4/4
3	PID	M	623[B]	-	-	0/24/93/93	0/4/4/4
3	PID	O	613[B]	-	-	0/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	W4I	M	615[A]	-	-	11/52/72/97	0/1/1/2
3	PID	O	621	-	-	0/24/93/93	0/4/4/4
4	W4I	N	625[B]	-	-	3/57/97/97	0/2/2/2
4	W4I	O	625[B]	-	-	4/57/97/97	0/2/2/2
3	PID	M	624	-	-	0/24/93/93	0/4/4/4
3	PID	N	623[B]	-	-	0/24/93/93	0/4/4/4
3	PID	O	624	-	-	0/24/93/93	0/4/4/4
4	W4I	O	615[A]	-	-	8/52/72/97	0/1/1/2
3	PID	M	614	-	-	0/24/93/93	0/4/4/4
3	PID	N	622	-	-	0/24/93/93	0/4/4/4
2	CLA	M	601	6	-	1/39/115/115	-
3	PID	N	613[A]	-	-	0/24/93/93	0/4/4/4
4	W4I	N	615[A]	-	-	16/52/72/97	0/1/1/2
3	PID	N	614	-	-	0/24/93/93	0/4/4/4
5	PG4	O	651	-	-	4/10/10/10	-
2	CLA	O	602	6	-	0/39/115/115	-
2	CLA	O	601	6	-	1/39/115/115	-
3	PID	M	611	-	-	0/24/93/93	0/4/4/4
3	PID	N	611	-	-	0/24/93/93	0/4/4/4
3	PID	O	623[A]	-	-	0/24/93/93	0/4/4/4

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	612	PID	C2-C3	-6.86	1.42	1.52
3	M	612	PID	C2-C3	-6.53	1.42	1.52
3	N	612	PID	C2-C3	-5.56	1.44	1.52
2	M	602	CLA	MG-NA	5.21	2.18	2.06
3	M	611	PID	C4-C3	-4.97	1.45	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	601	CLA	C4A-NA-C1A	8.15	110.37	106.71
2	N	602	CLA	C4A-NA-C1A	7.81	110.22	106.71
2	O	601	CLA	C4A-NA-C1A	7.31	109.99	106.71
2	M	602	CLA	C4A-NA-C1A	7.10	109.90	106.71
2	O	602	CLA	C4A-NA-C1A	5.82	109.32	106.71

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	613[A]	PID	C6
3	M	613[B]	PID	C6
3	O	623[B]	PID	C6

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	615[A]	W4I	CHA-CIA-CJA-CKA
4	M	615[B]	W4I	CHA-CIA-CJA-CKA
4	N	615[A]	W4I	CHA-CIA-CJA-CKA
4	N	615[B]	W4I	CHA-CIA-CJA-CKA
4	O	625[A]	W4I	CFA-CGA-CHA-CIA

There are no ring outliers.

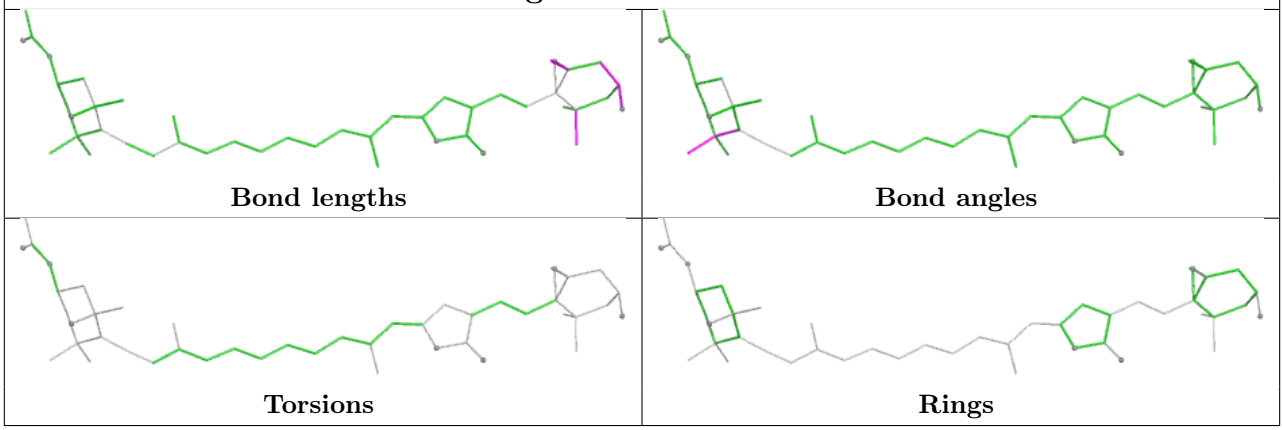
15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	611	PID	1	0
3	O	614	PID	1	0
3	M	623[A]	PID	2	0
3	N	623[A]	PID	2	0
3	N	624	PID	2	0
3	O	623[B]	PID	3	0
3	M	613[B]	PID	2	0
2	N	602	CLA	1	0
3	O	613[B]	PID	3	0
3	O	621	PID	1	0
3	M	624	PID	2	0
3	N	623[B]	PID	1	0
3	O	624	PID	2	0
3	M	614	PID	1	0
3	N	614	PID	1	0

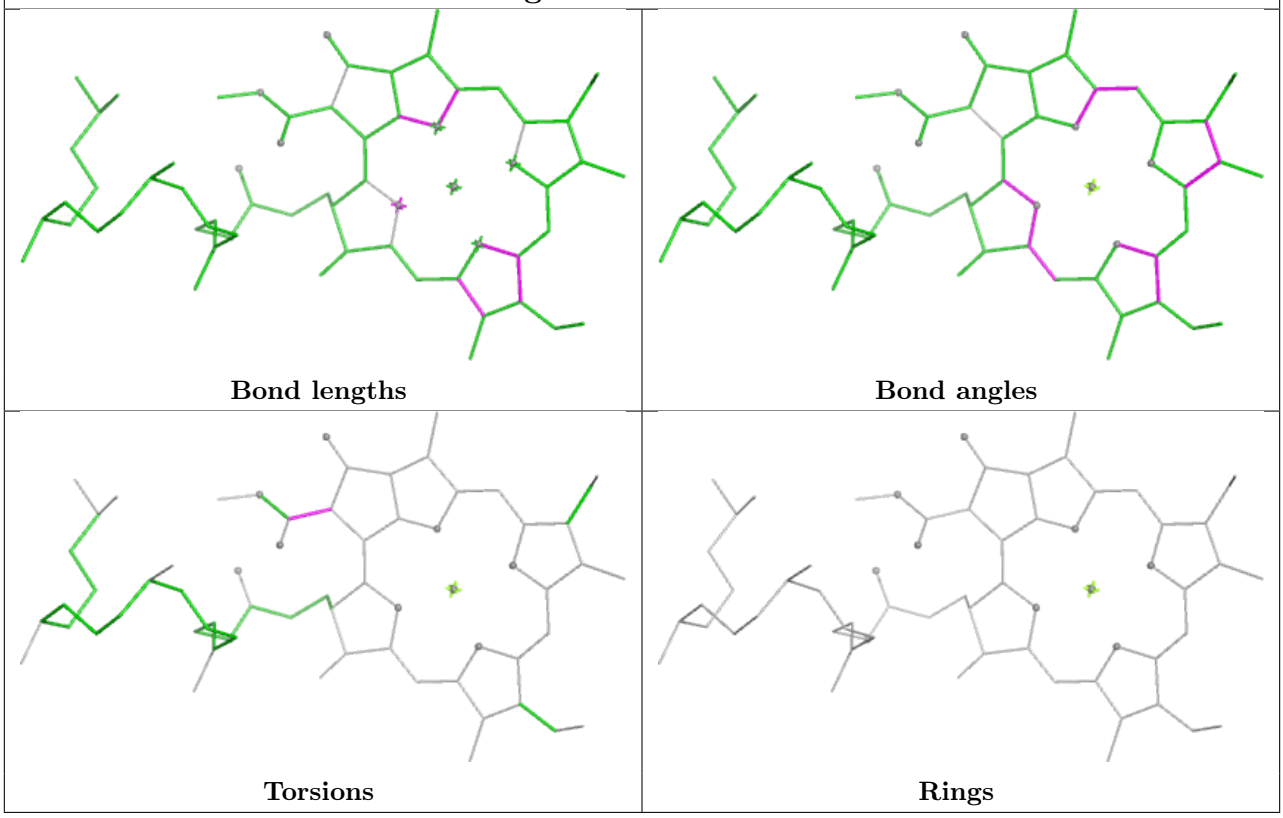
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 M 612



Ligand CLA N 601



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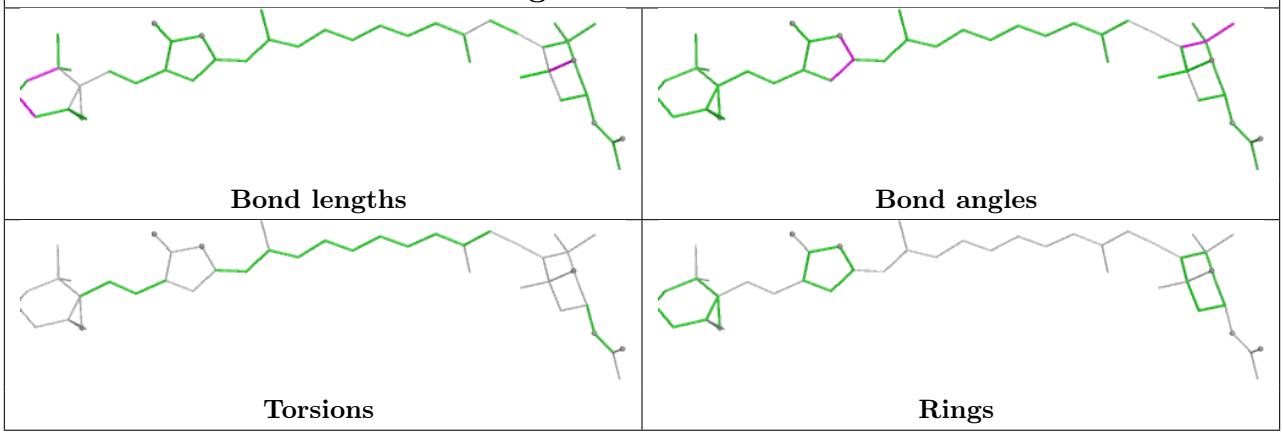
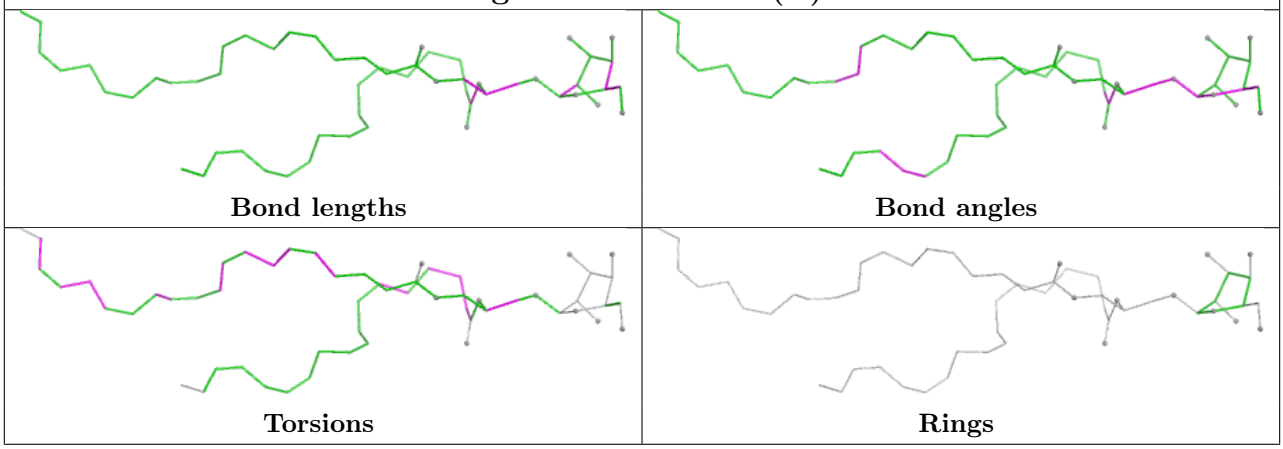


Ligand W4I M 615 (B)



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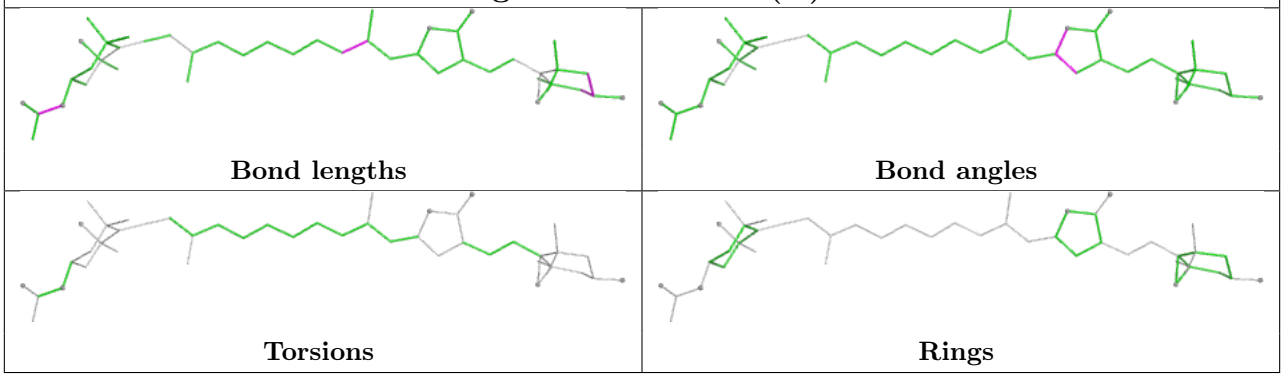

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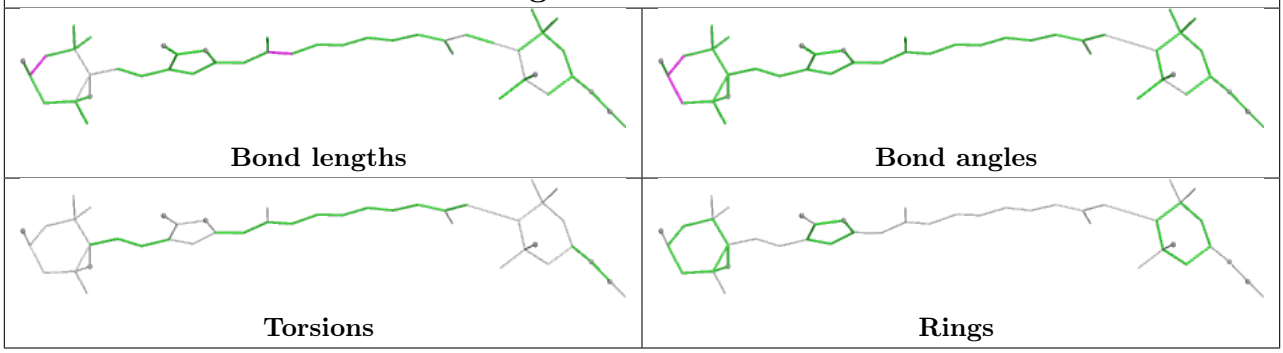
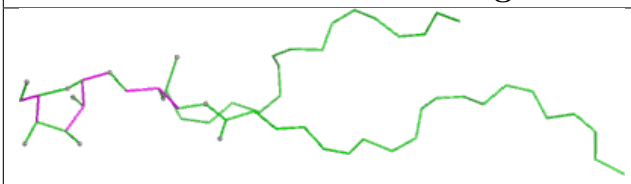
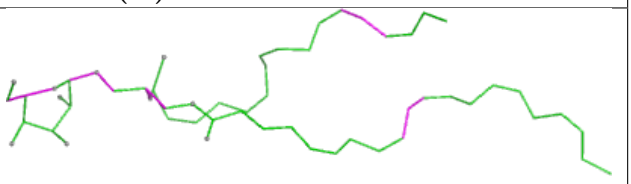
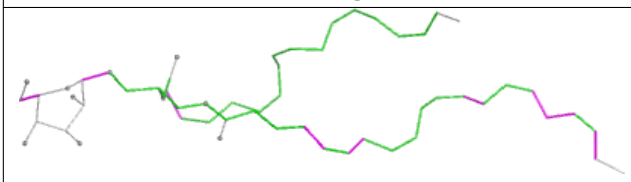
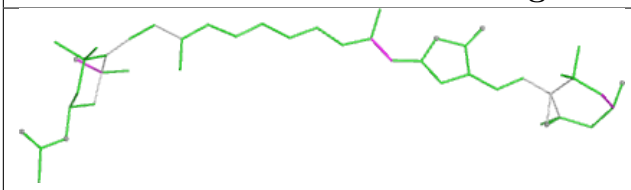
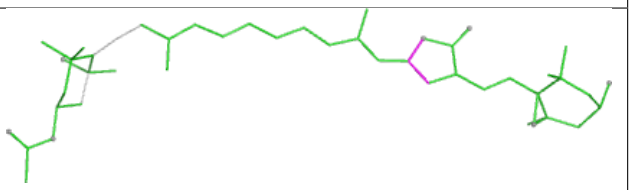
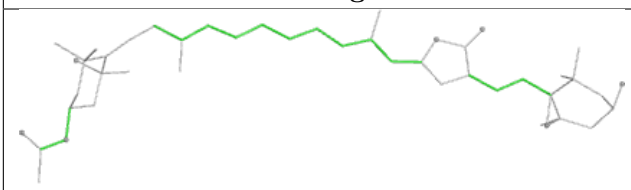
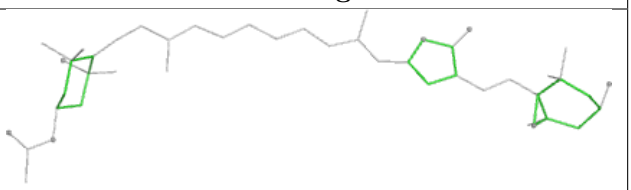
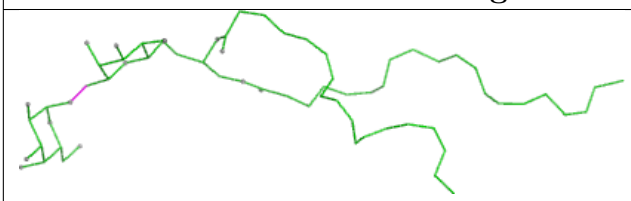
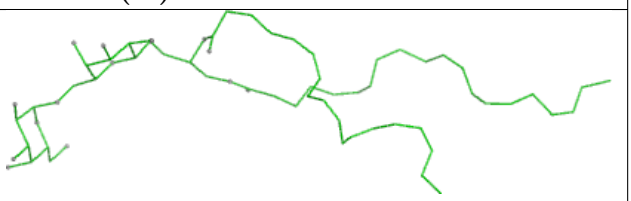
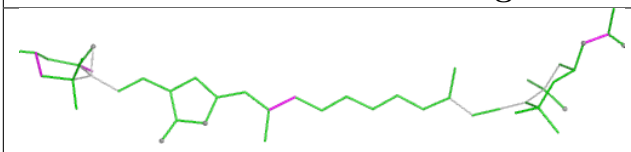


Ligand W4I O 615 (B)	
 Bond lengths	 Bond angles
 Torsions	Rings

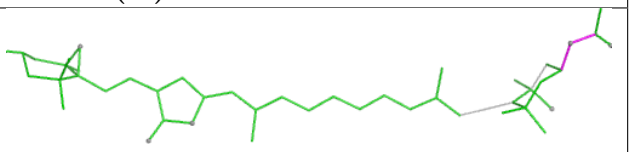
Ligand PID O 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand W4I M 625 (A)	
 Bond lengths	 Bond angles
Torsions	Rings

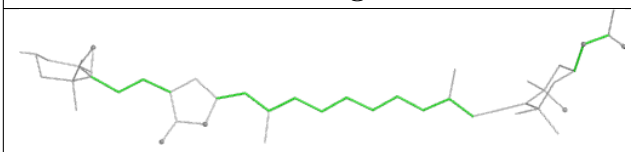
Ligand PID O 613 (A)



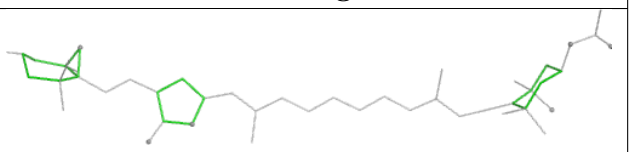
Bond lengths



Bond angles

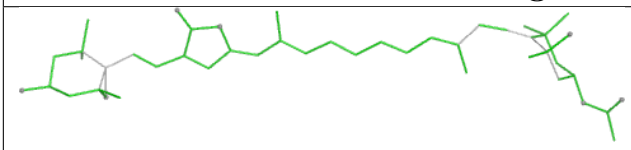


Torsions

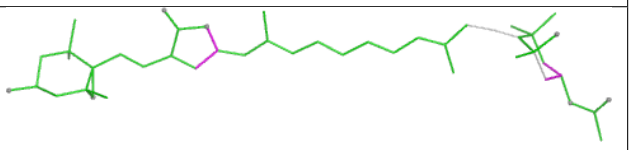


Rings

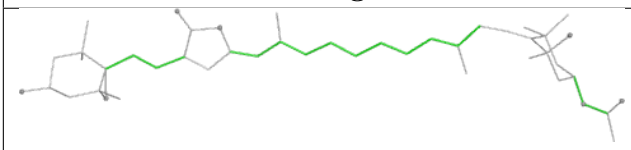
Ligand PID O 614



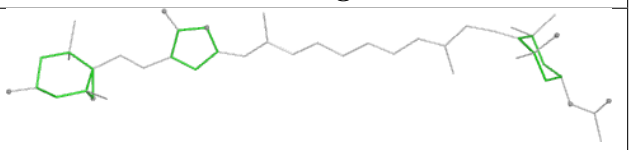
Bond lengths



Bond angles

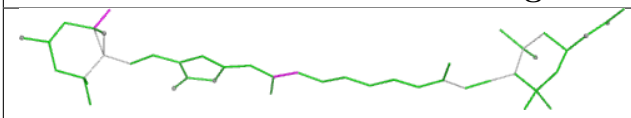


Torsions

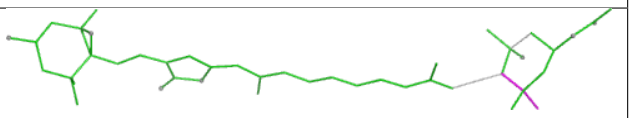


Rings

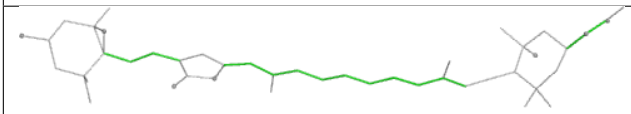
Ligand PID M 621



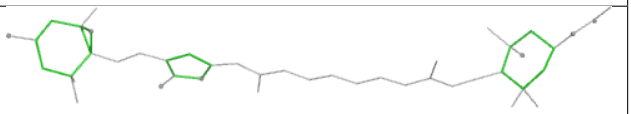
Bond lengths



Bond angles

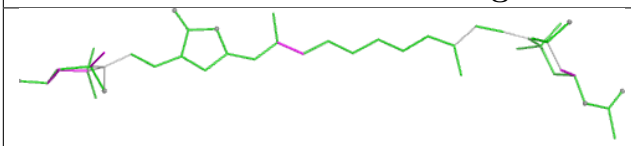


Torsions

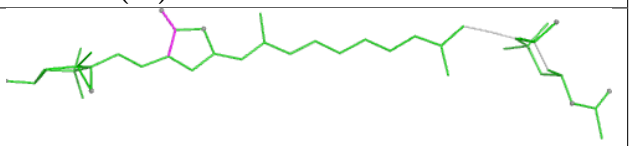


Rings

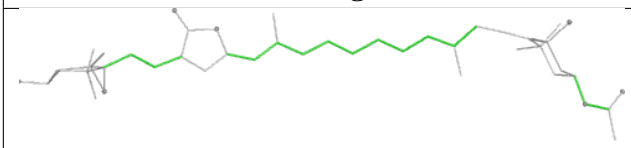
Ligand PID M 623 (A)



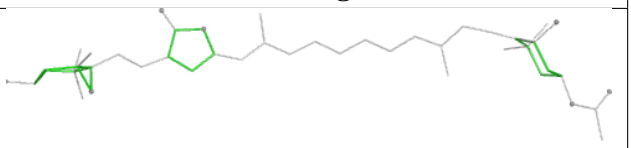
Bond lengths



Bond angles



Torsions



Rings

Ligand W4I N 625 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand W4I O 625 (A)

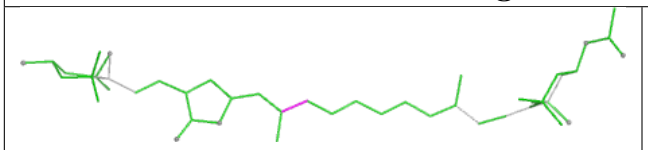
Bond lengths

Bond angles

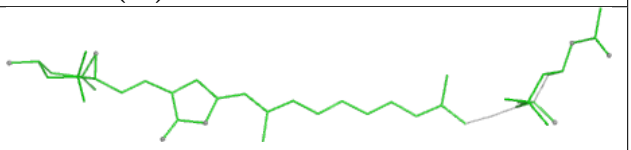
Torsions

Rings

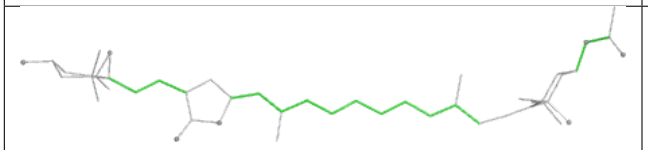
Ligand PID N 623 (A)



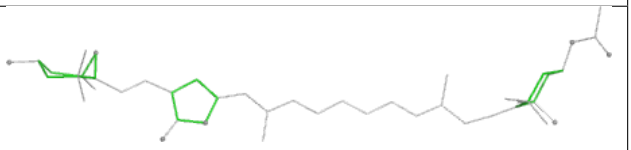
Bond lengths



Bond angles

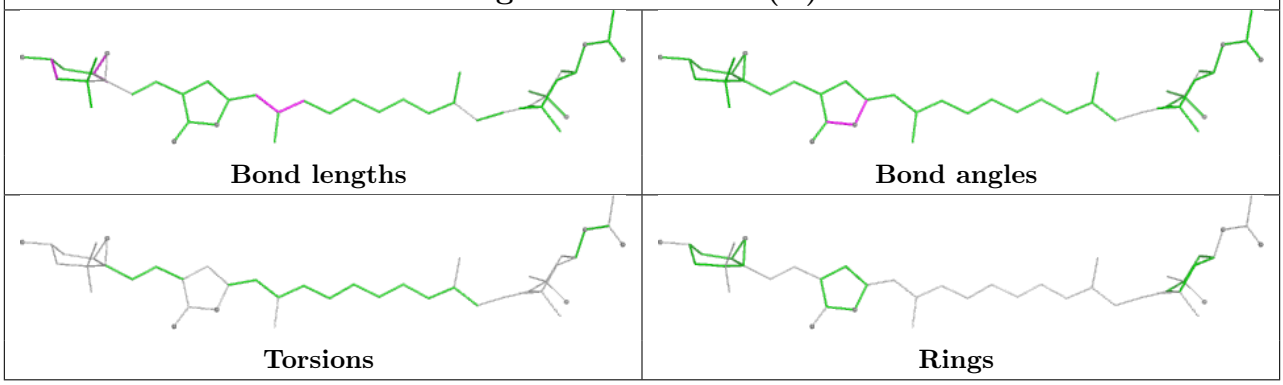


Torsions

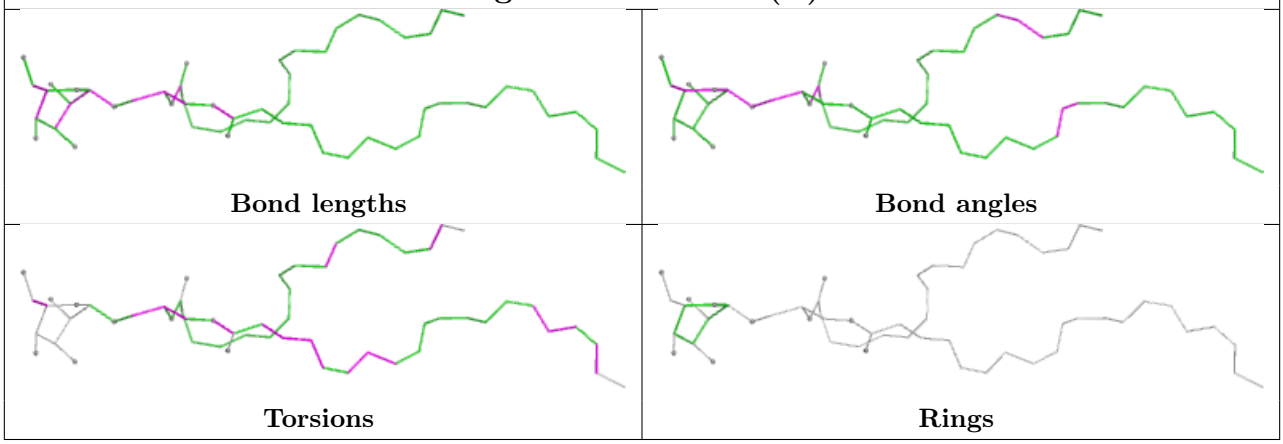


Rings

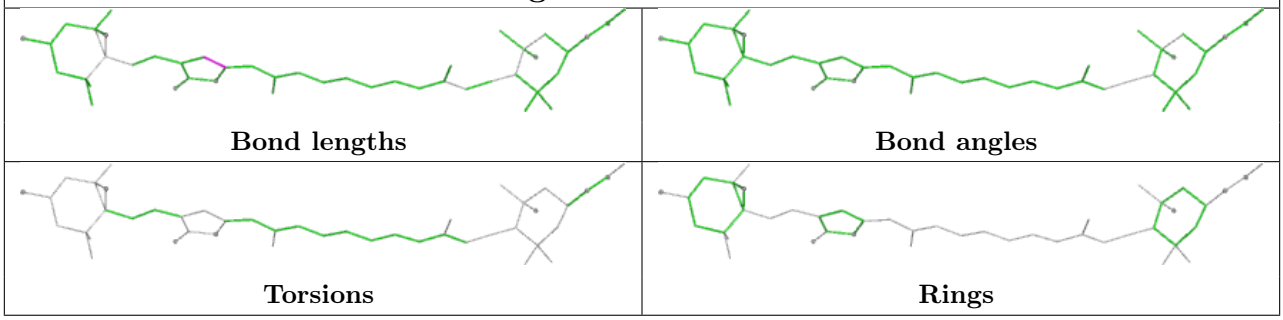
Ligand PID N 613 (B)



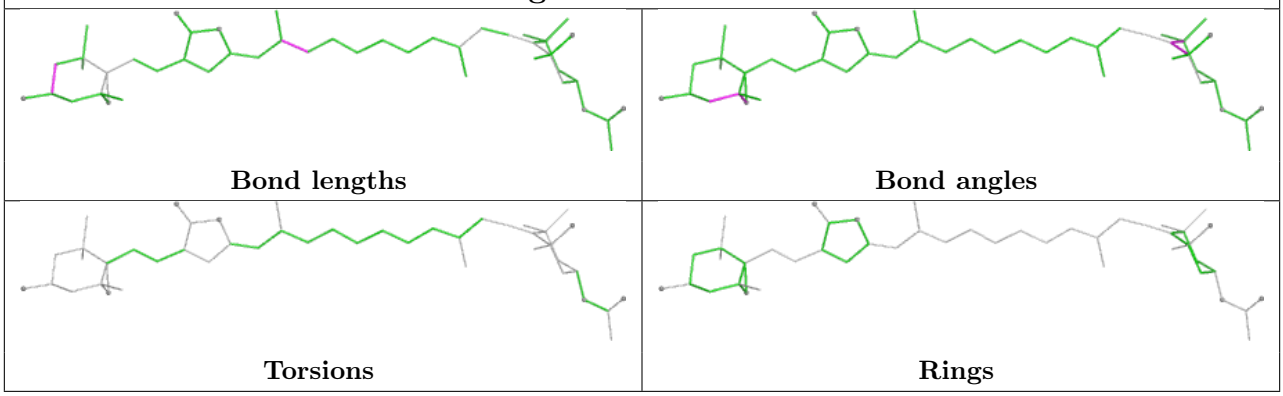
Ligand W4I N 615 (B)

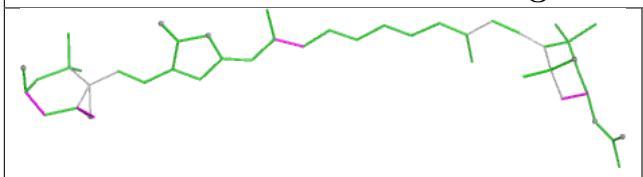
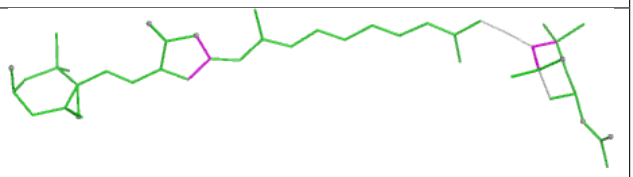
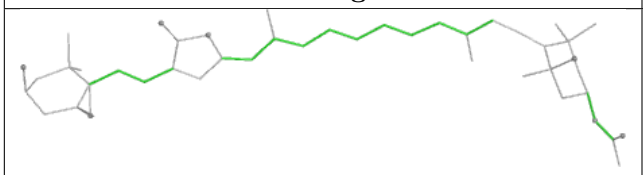
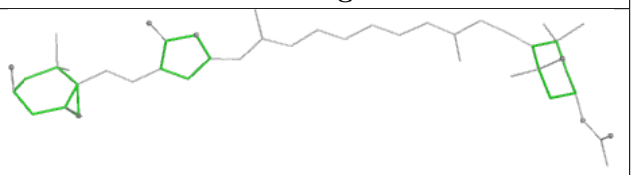


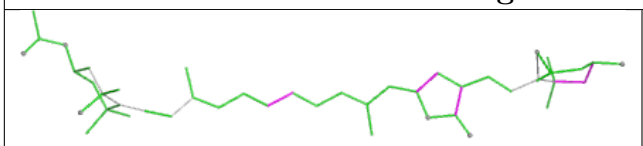
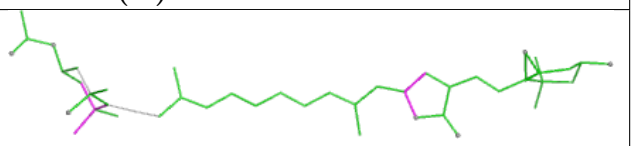
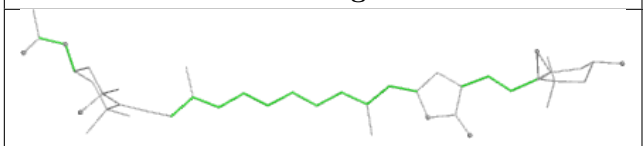
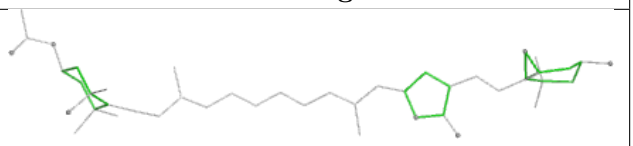
Ligand PID N 621

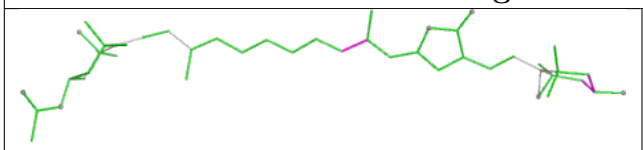
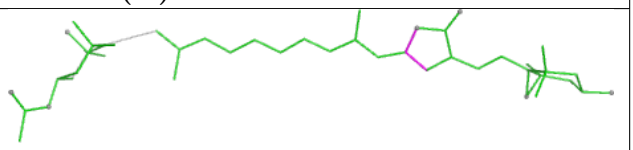
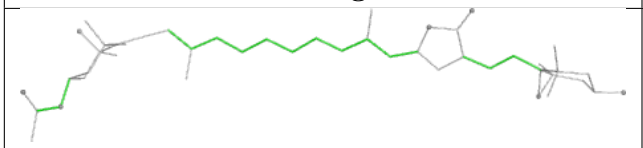
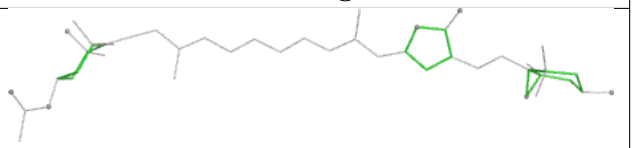


Ligand PID N 624

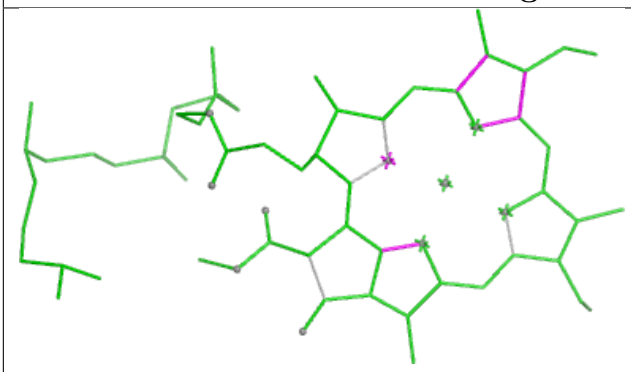


Ligand PID O 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

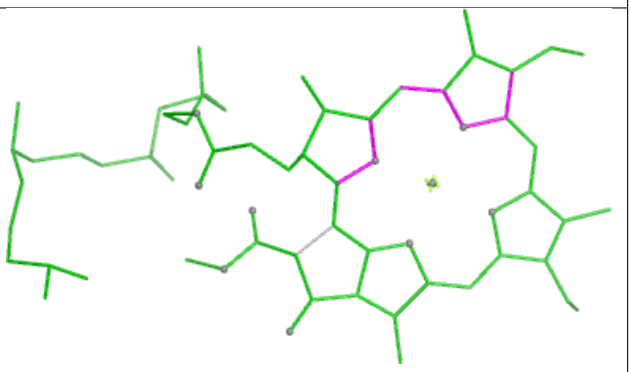
Ligand PID O 623 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PID M 613 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

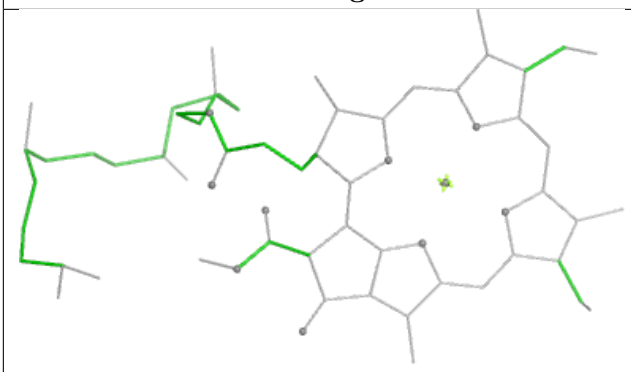
Ligand CLA M 602



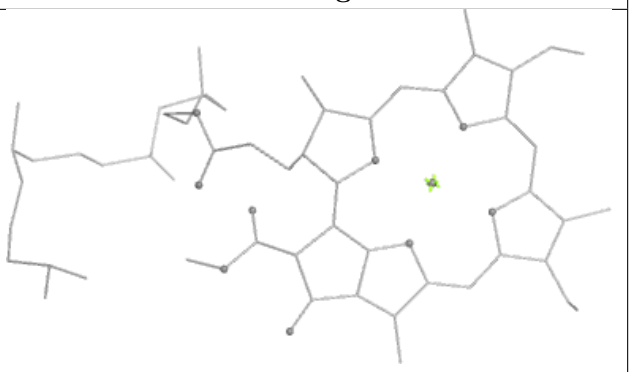
Bond lengths



Bond angles



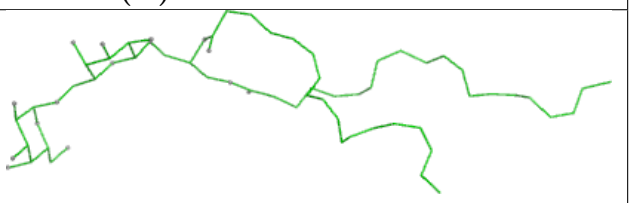
Torsions



Rings

Ligand W4I M 625 (B)

Bond lengths

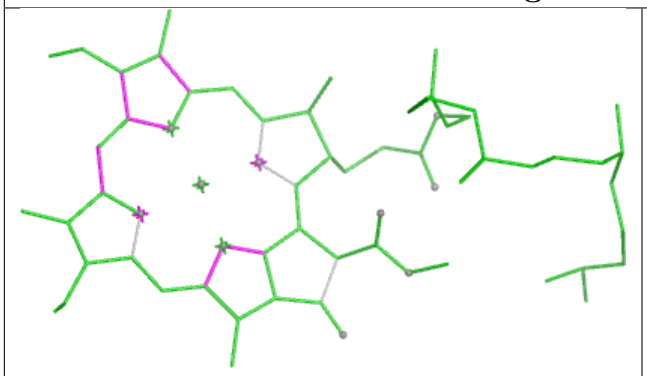


Bond angles

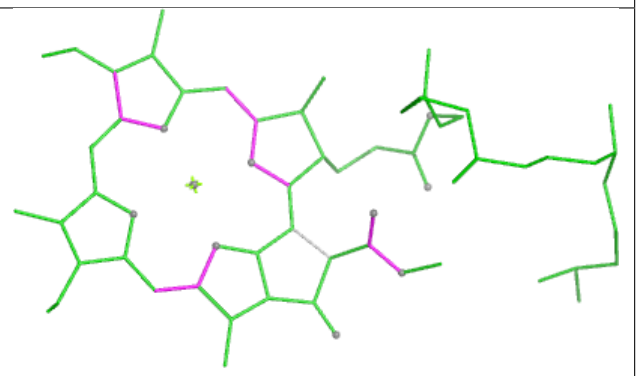
Torsions

Rings

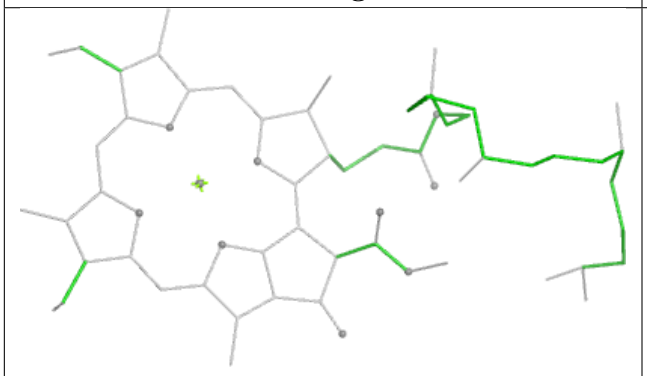
Ligand CLA N 602



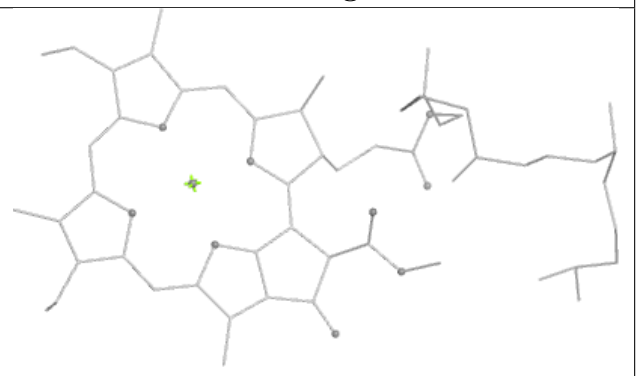
Bond lengths



Bond angles

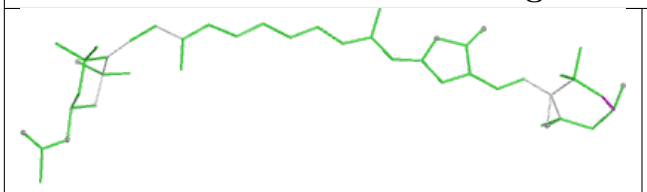


Torsions

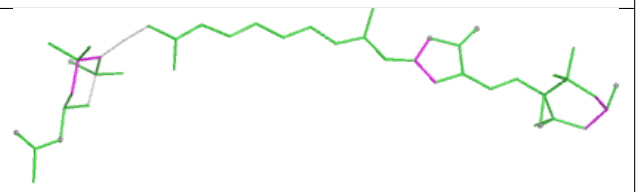


Rings

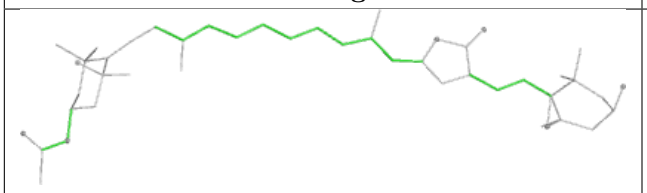
Ligand PID M 622



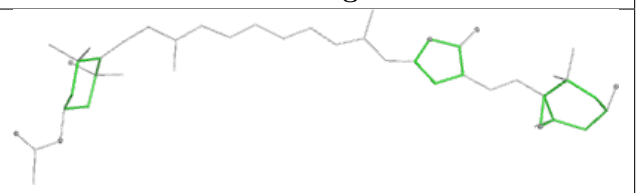
Bond lengths



Bond angles

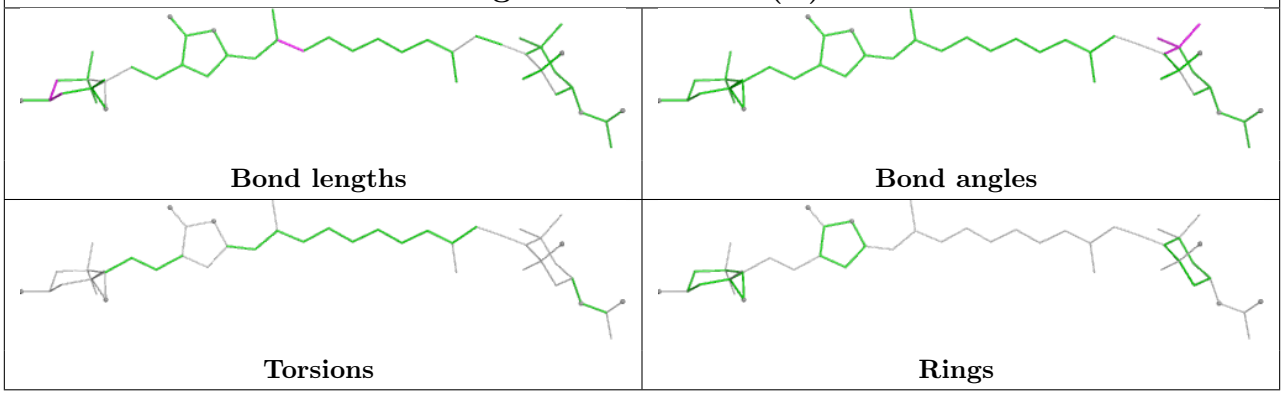


Torsions

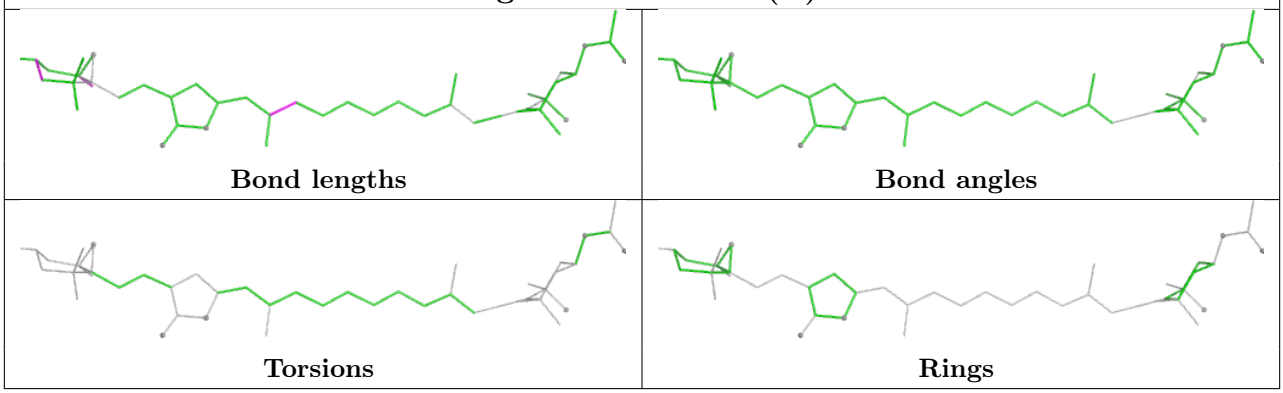


Rings

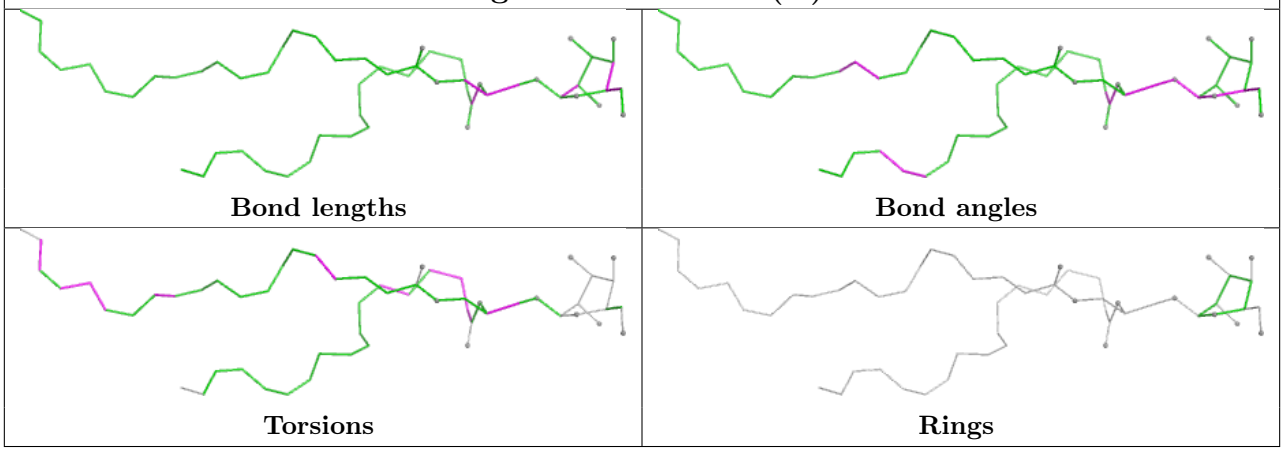
Ligand PID M 623 (B)



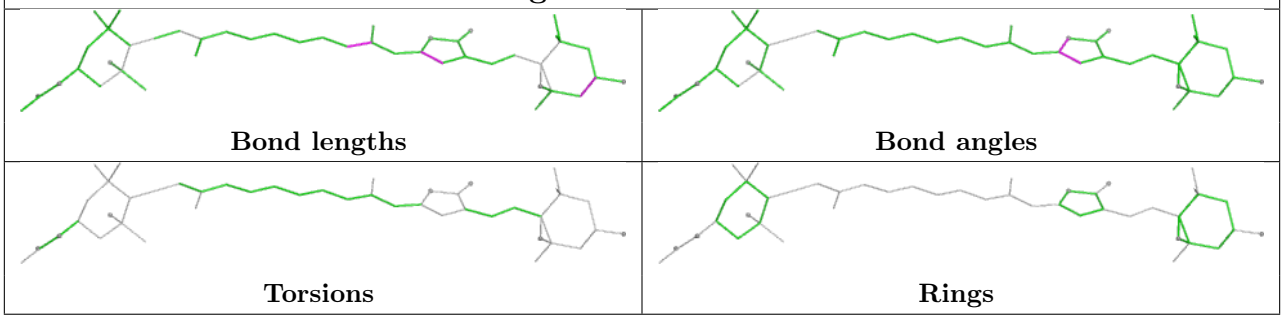
Ligand PID O 613 (B)



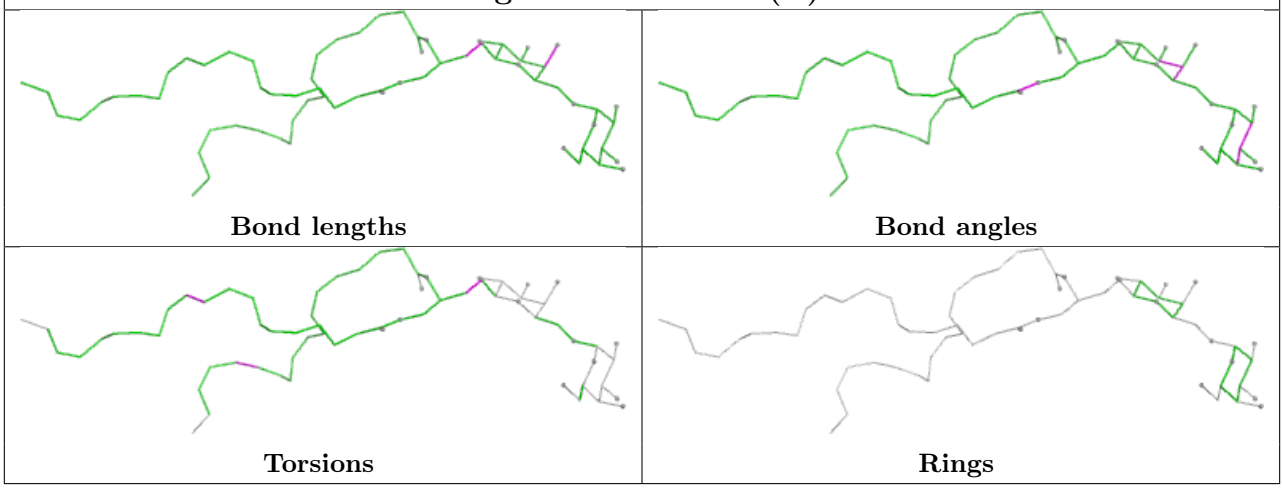
Ligand W4I M 615 (A)



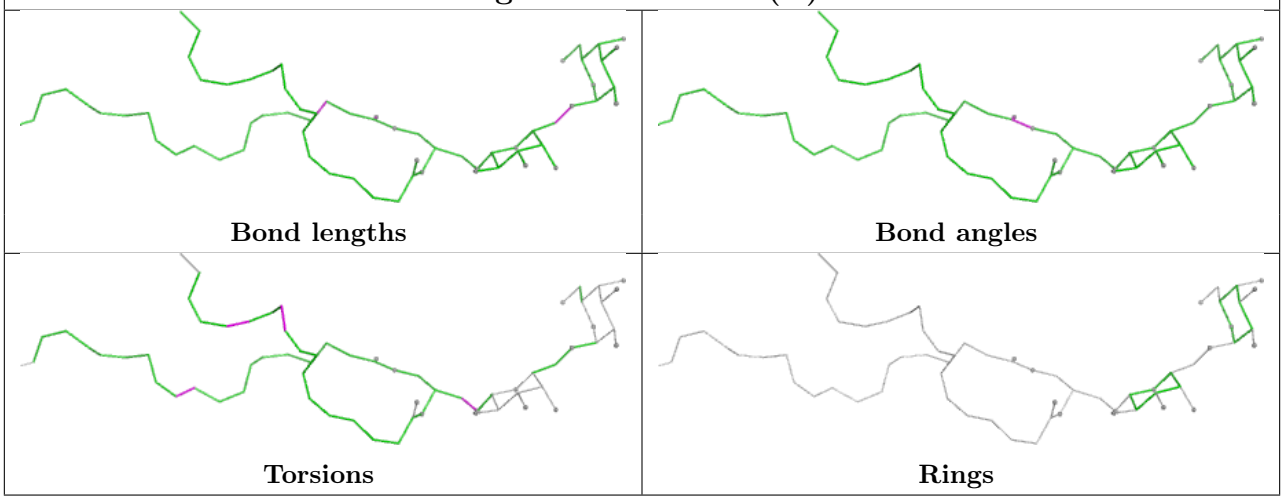
Ligand PID O 621



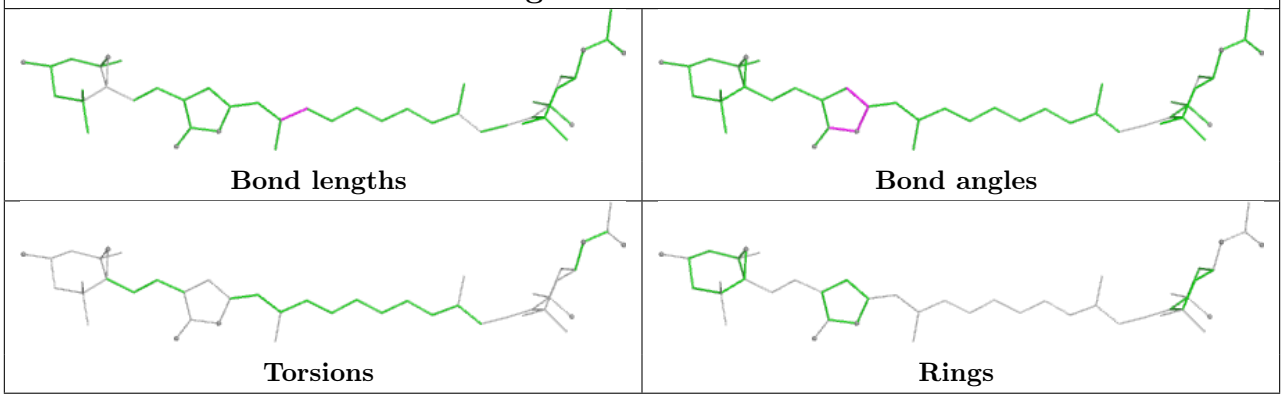
Ligand W4I N 625 (B)



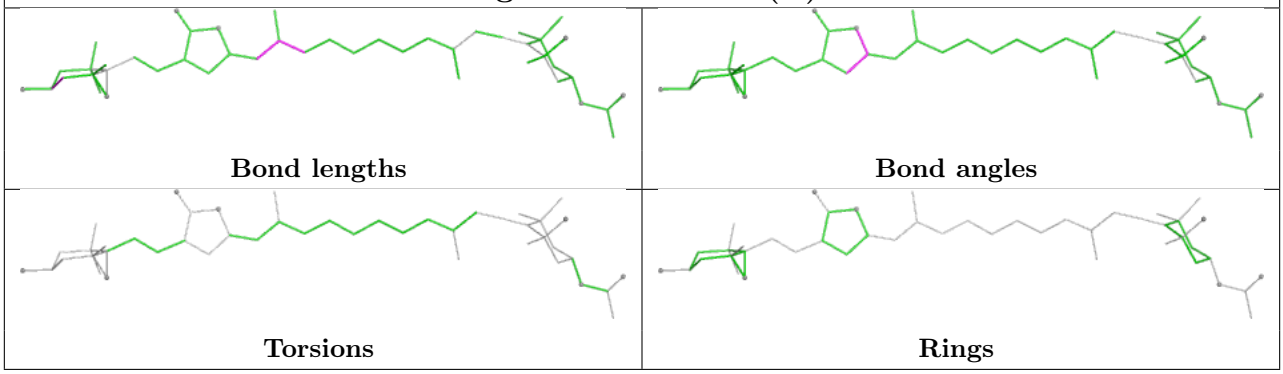
Ligand W4I O 625 (B)



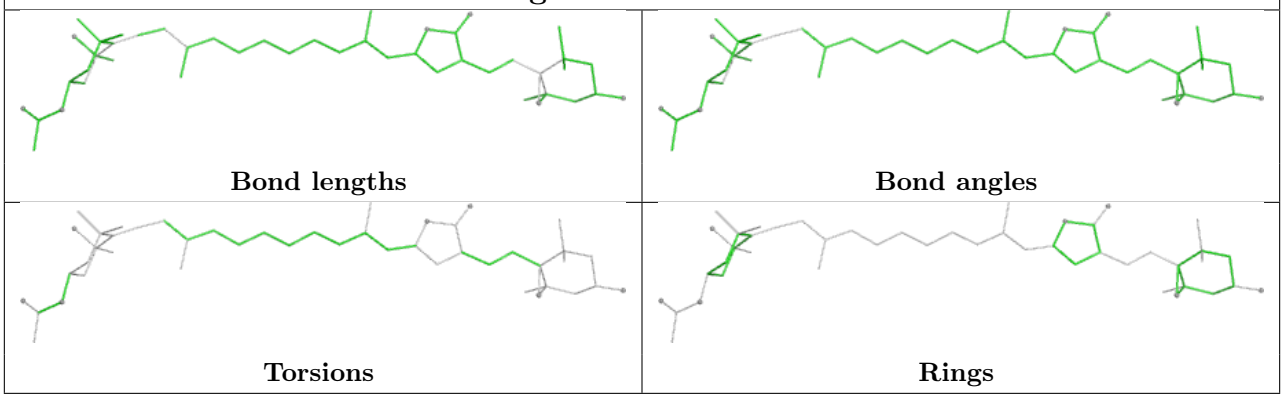
Ligand PID M 624



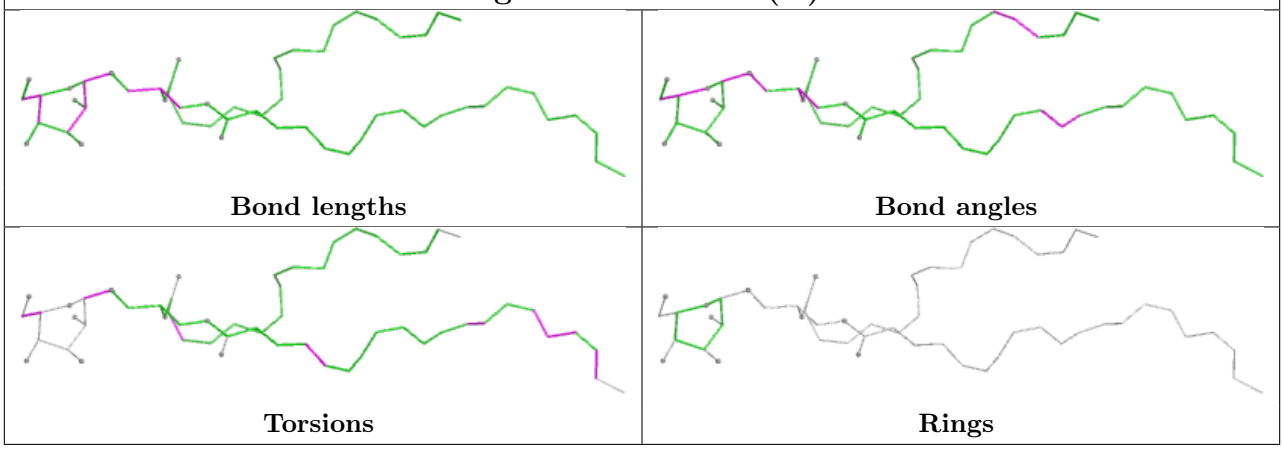
Ligand PID N 623 (B)



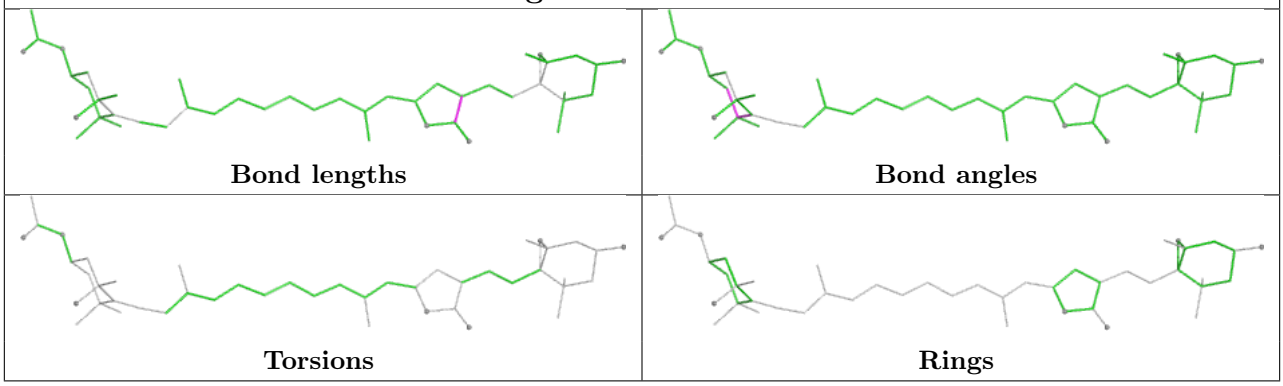
Ligand PID O 624



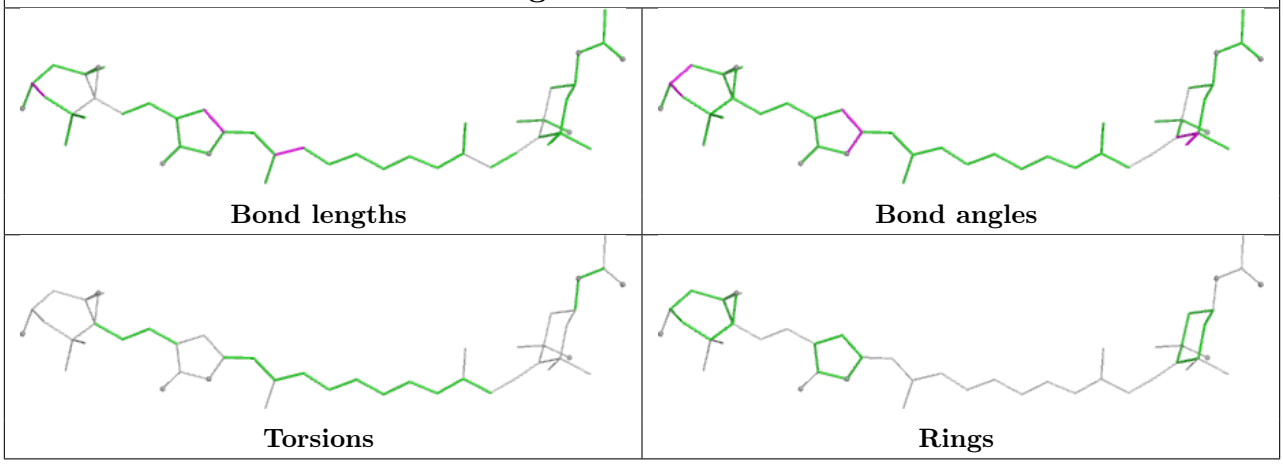
Ligand W4I O 615 (A)



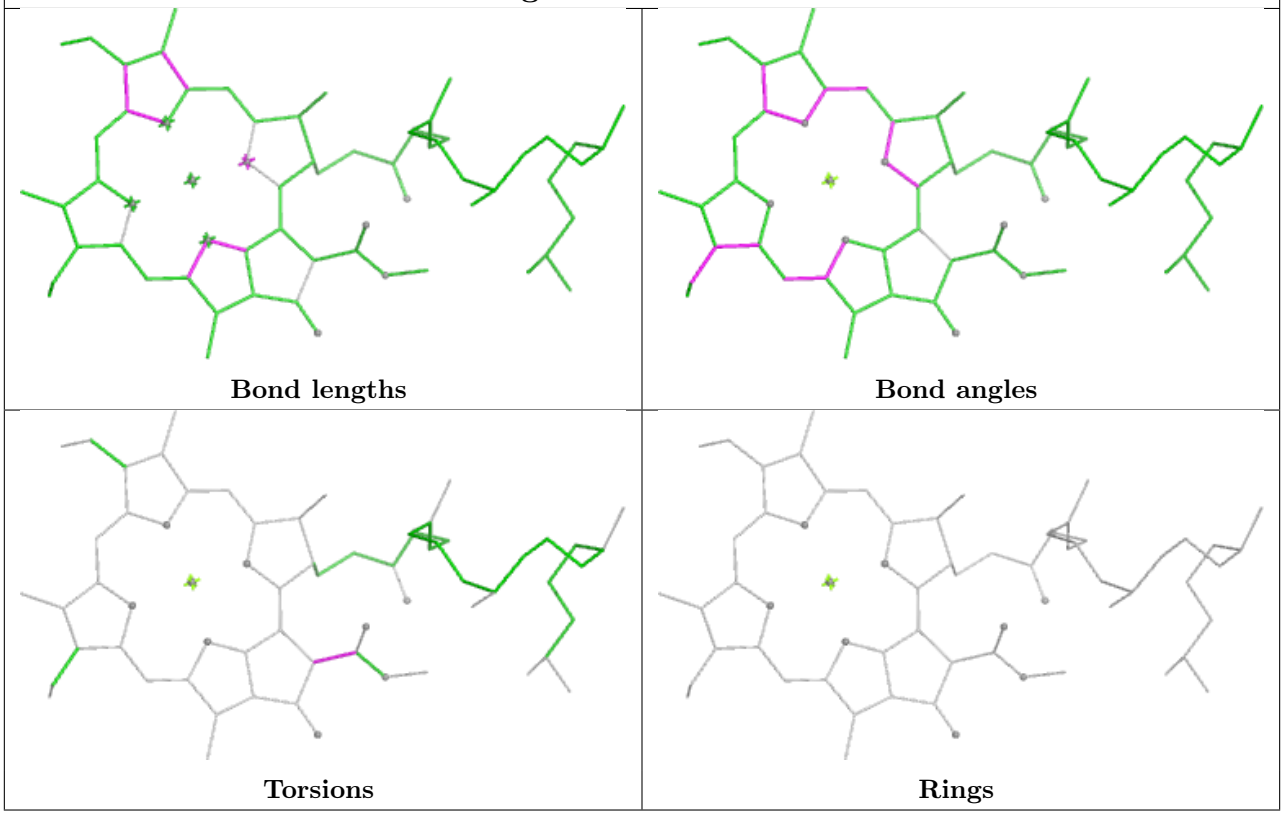
Ligand PID M 614



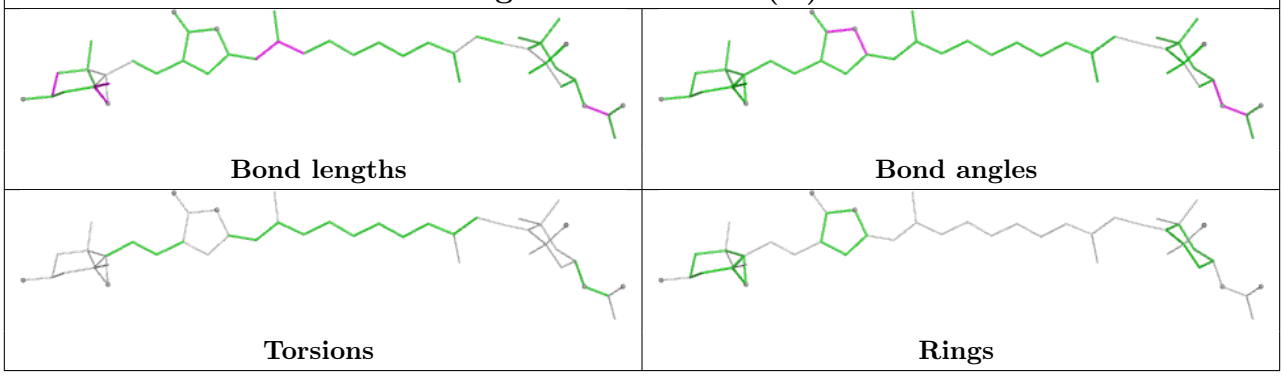
Ligand PID N 622



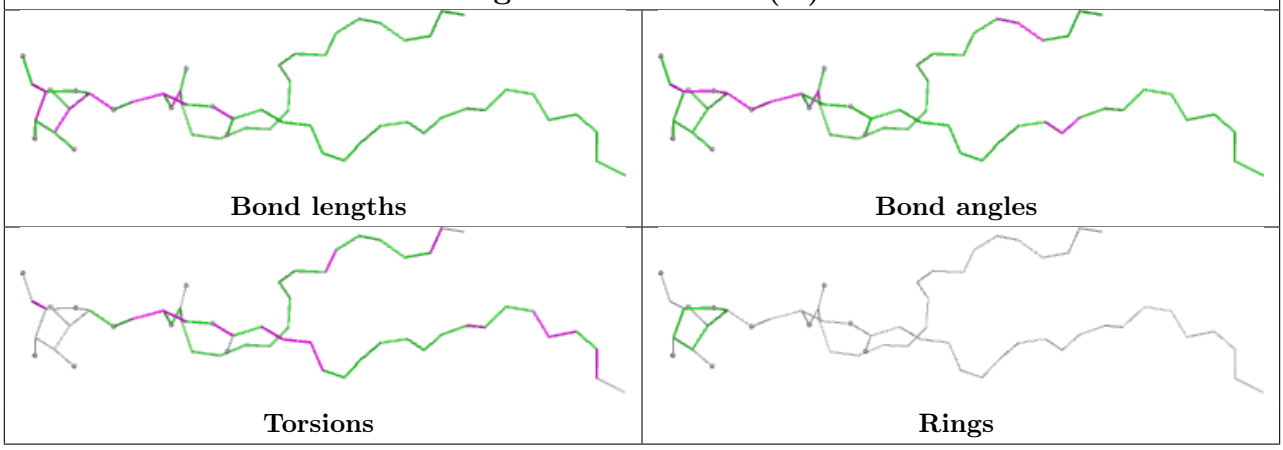
Ligand CLA M 601



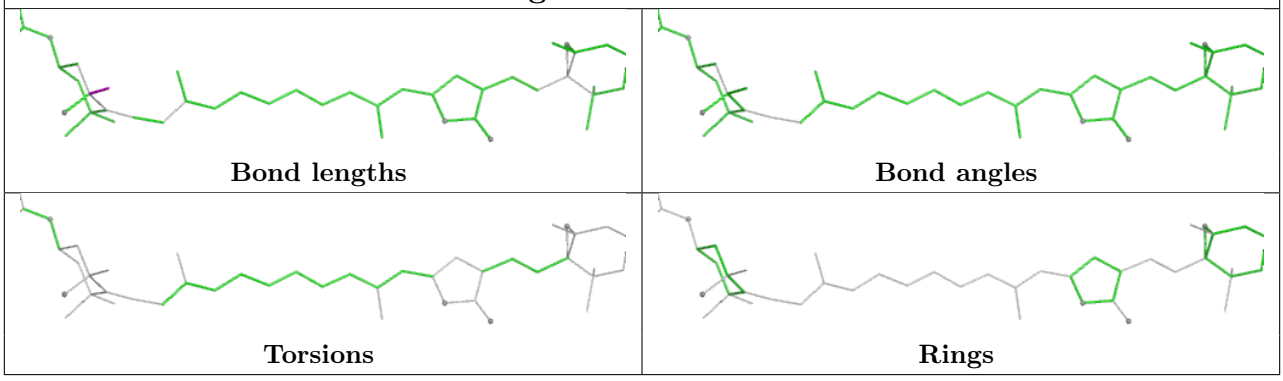
Ligand PID N 613 (A)



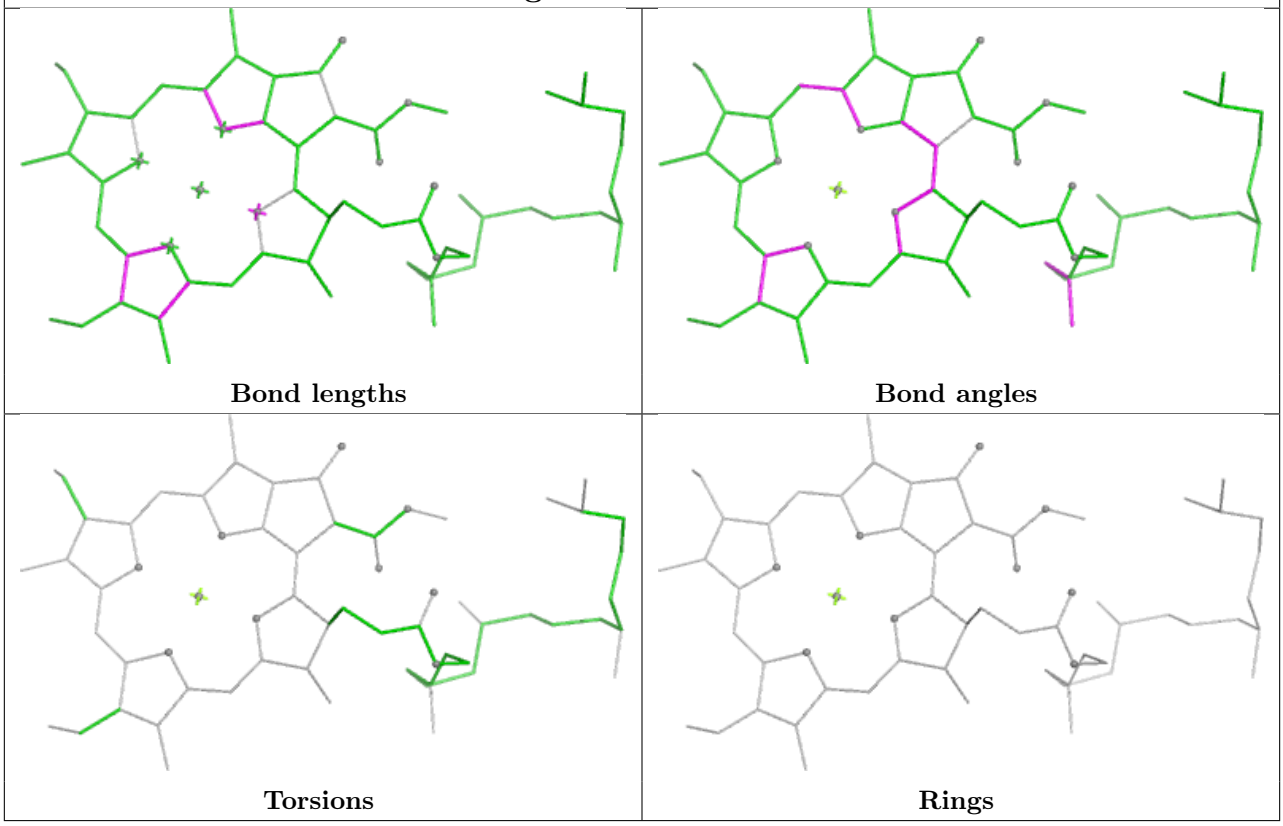
Ligand W4I N 615 (A)



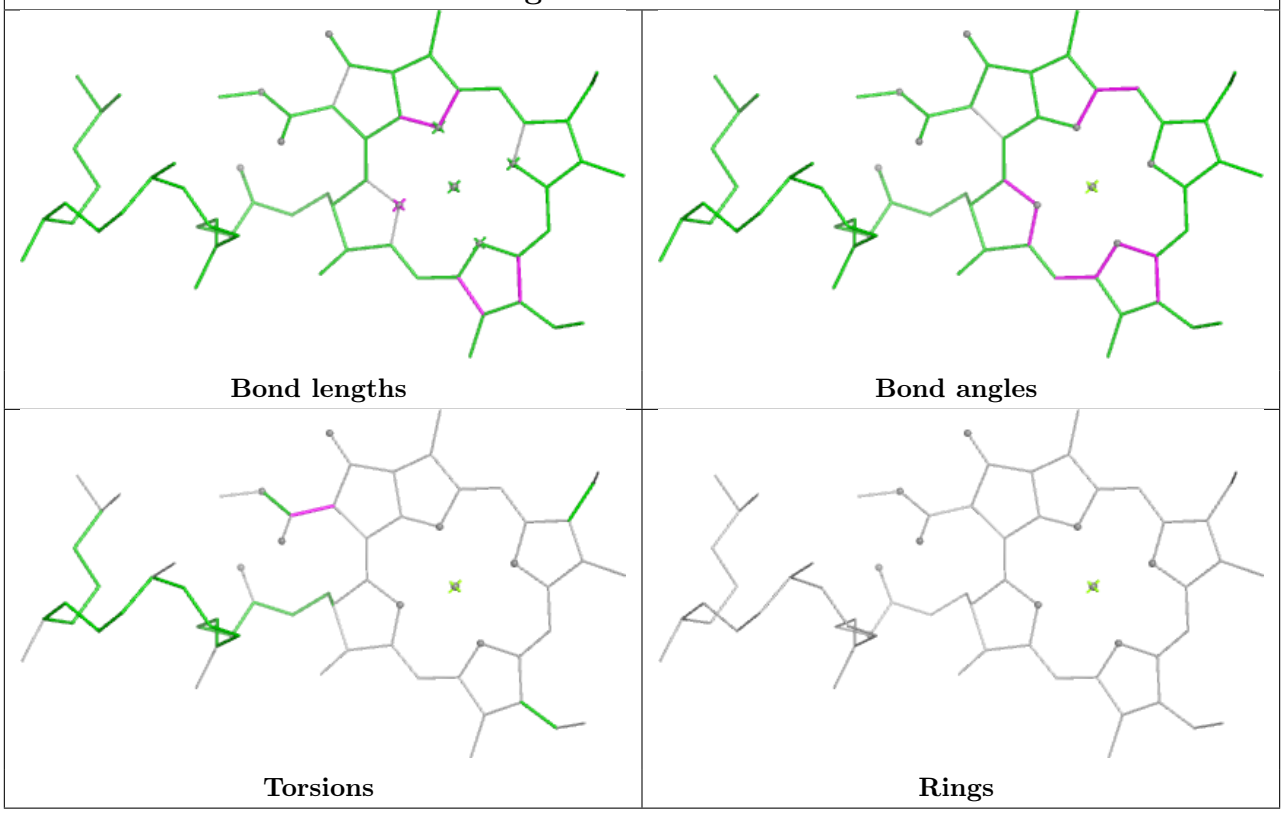
Ligand PID N 614



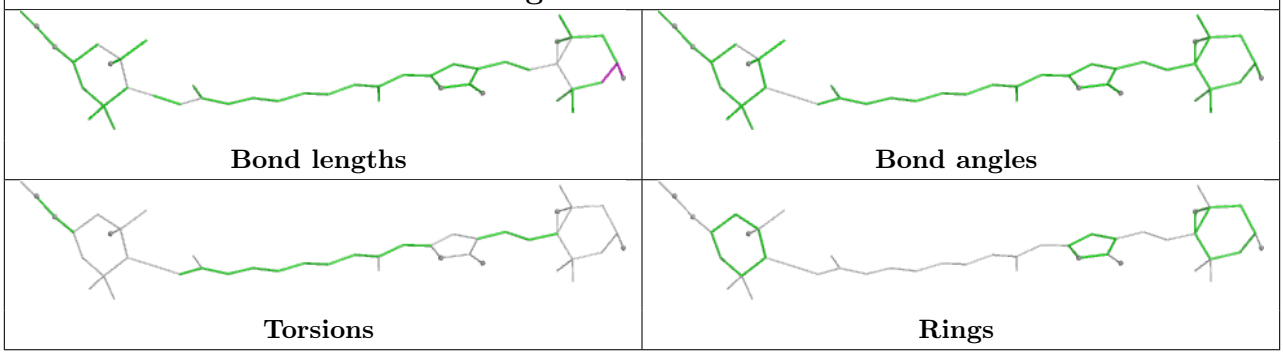
Ligand CLA O 602



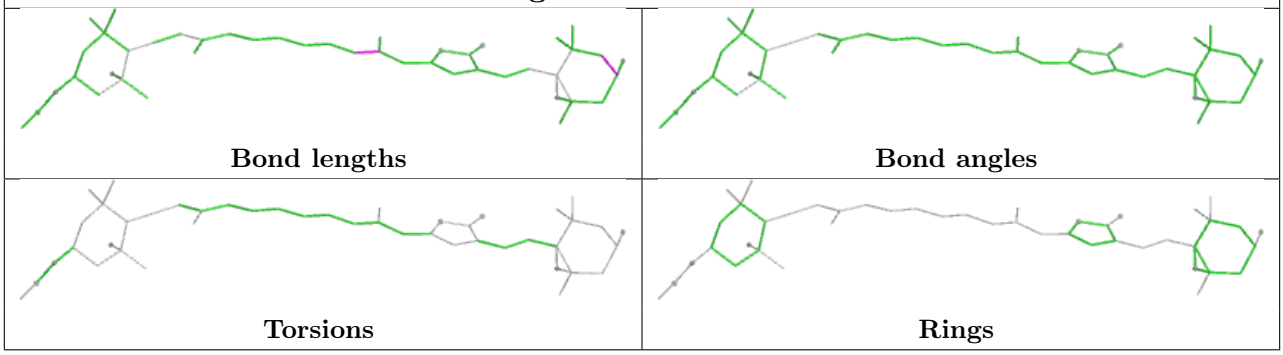
Ligand CLA O 601

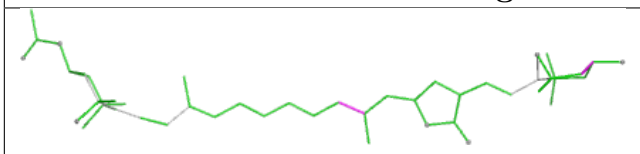
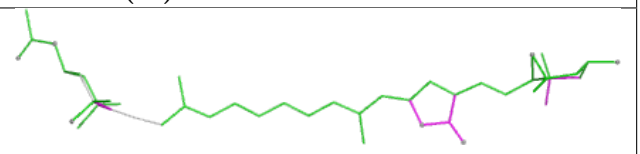
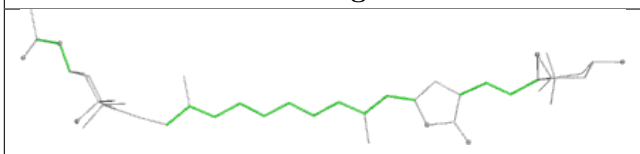
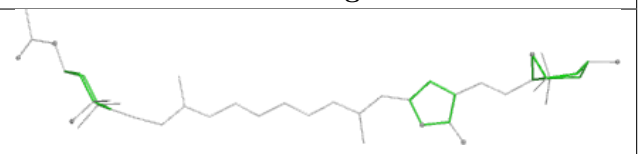


Ligand PID M 611



Ligand PID N 611



Ligand PID O 623 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95th 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^2)	Q<0.9
1	M	312/312 (100%)	-0.29	9 (2%)	53	62	5, 15, 27, 40	17 (5%)
1	N	312/312 (100%)	-0.09	11 (3%)	47	55	6, 18, 32, 49	17 (5%)
1	O	312/312 (100%)	-0.31	9 (2%)	53	62	5, 14, 27, 38	17 (5%)
All	All	936/936 (100%)	-0.23	29 (3%)	51	59	5, 16, 29, 49	51 (5%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	160	VAL	9.7
1	O	160	VAL	7.4
1	N	159	THR	5.6
1	M	155	ALA	4.6
1	M	160	VAL	4.5

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PG4	N	651	13/13	0.79	0.22	59,71,73,73	0
4	W4I	N	615[B]	57/68	0.81	0.16	26,41,58,59	19
5	PG4	M	651	13/13	0.81	0.22	56,67,69,70	0
4	W4I	N	615[A]	57/68	0.81	0.16	26,41,58,59	19
4	W4I	O	615[A]	57/68	0.85	0.15	21,33,55,56	19
4	W4I	O	615[B]	57/68	0.85	0.15	21,33,55,56	19
4	W4I	M	615[A]	57/68	0.85	0.14	21,34,54,55	19
4	W4I	M	615[B]	57/68	0.85	0.14	21,34,54,55	19
5	PG4	O	651	13/13	0.85	0.16	42,51,58,58	0
3	PID	N	613[B]	46/46	0.97	0.06	14,19,34,36	6
3	PID	N	613[A]	46/46	0.97	0.06	14,19,34,36	6
3	PID	N	623[B]	46/46	0.98	0.04	8,12,15,18	96
3	PID	O	611	46/46	0.98	0.04	9,13,22,26	0
3	PID	O	612	46/46	0.98	0.05	10,13,21,26	0
3	PID	O	613[A]	46/46	0.98	0.05	10,15,30,33	6
3	PID	O	613[B]	46/46	0.98	0.05	10,15,30,33	6
3	PID	M	611	46/46	0.98	0.04	9,14,23,28	0
3	PID	M	612	46/46	0.98	0.04	11,14,23,28	0
3	PID	M	613[A]	46/46	0.98	0.05	11,15,31,34	6
3	PID	M	613[B]	46/46	0.98	0.05	11,15,31,34	6
4	W4I	N	625[A]	68/68	0.98	0.05	10,16,23,25	14
4	W4I	N	625[B]	68/68	0.98	0.05	10,16,23,25	14
3	PID	N	612	46/46	0.98	0.05	12,16,22,27	0
2	CLA	N	601	65/65	0.98	0.04	11,17,26,29	0
4	W4I	O	625[A]	68/68	0.98	0.05	10,15,20,24	14
4	W4I	O	625[B]	68/68	0.98	0.05	10,15,20,24	14
2	CLA	N	602	65/65	0.98	0.04	10,15,19,20	0
3	PID	N	614	46/46	0.98	0.04	13,17,26,28	0
3	PID	N	623[A]	46/46	0.98	0.04	8,13,16,19	96
3	PID	M	624	46/46	0.99	0.03	8,11,13,15	0
3	PID	O	614	46/46	0.99	0.04	10,14,20,23	0
3	PID	O	621	46/46	0.99	0.04	9,11,14,16	0
3	PID	O	622	46/46	0.99	0.04	9,13,18,19	0
3	PID	O	623[A]	46/46	0.99	0.03	5,11,14,15	96
3	PID	O	623[B]	46/46	0.99	0.03	7,11,14,16	96
3	PID	O	624	46/46	0.99	0.03	8,11,13,14	0
3	PID	N	611	46/46	0.99	0.04	11,15,25,30	0
2	CLA	M	601	65/65	0.99	0.04	10,14,24,26	0
4	W4I	M	625[A]	68/68	0.99	0.05	10,14,21,23	14
4	W4I	M	625[B]	68/68	0.99	0.05	10,14,21,23	14
2	CLA	M	602	65/65	0.99	0.04	8,11,16,18	0
2	CLA	O	601	65/65	0.99	0.04	9,14,22,25	0
2	CLA	O	602	65/65	0.99	0.04	8,11,17,20	0

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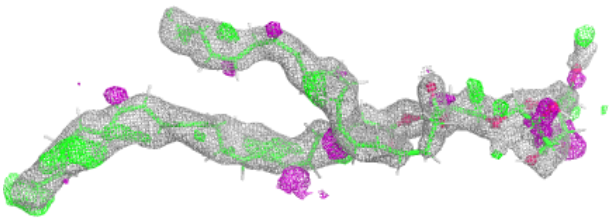
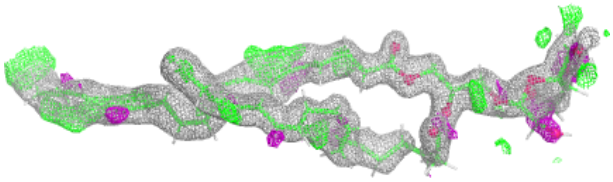
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PID	N	621	46/46	0.99	0.03	10,13,17,18	0
3	PID	N	622	46/46	0.99	0.04	11,15,19,19	0
3	PID	M	614	46/46	0.99	0.04	11,14,20,23	0
3	PID	M	621	46/46	0.99	0.03	9,11,15,16	0
3	PID	N	624	46/46	0.99	0.04	11,14,16,18	0
3	PID	M	622	46/46	0.99	0.04	10,13,19,20	0
3	PID	M	623[A]	46/46	0.99	0.03	7,10,13,14	96
3	PID	M	623[B]	46/46	0.99	0.03	6,11,13,15	96

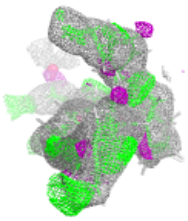
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W4I N 615 (B):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

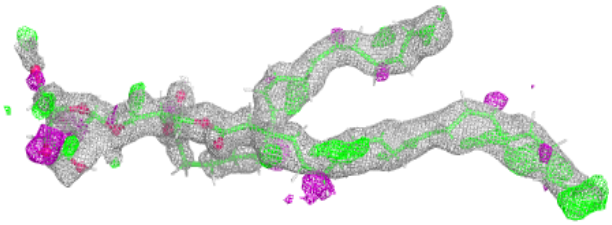


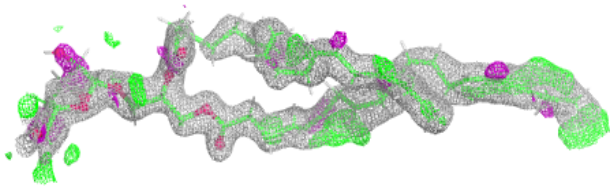


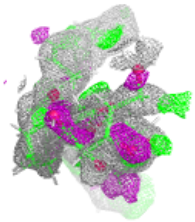


Electron density around W4I N 615 (A):

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







Electron density around W4I O 615 (A):

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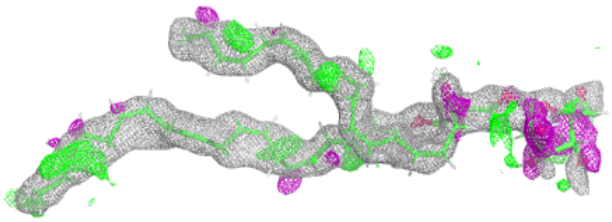
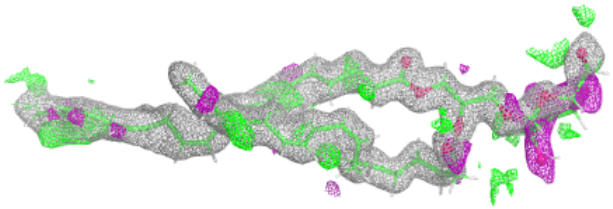
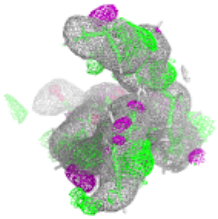
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around W4I O 615 (B):

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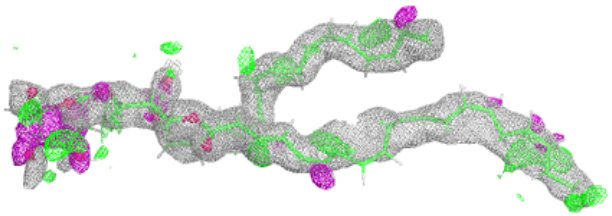
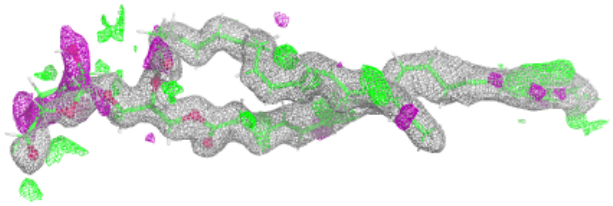
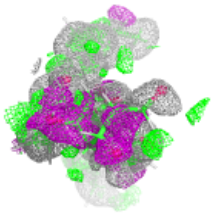
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

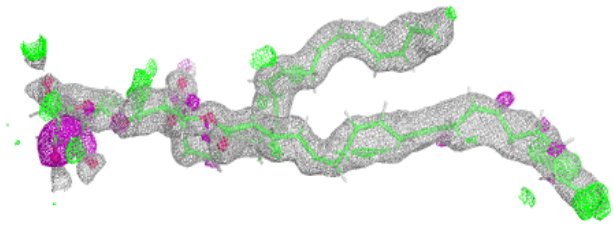


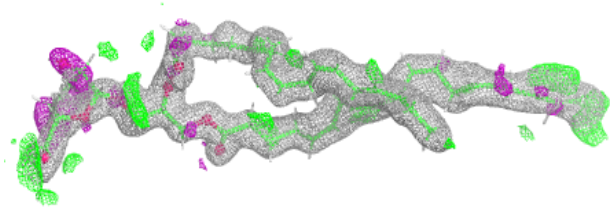


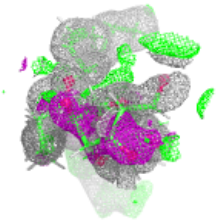


Electron density around W4I M 615 (A):

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

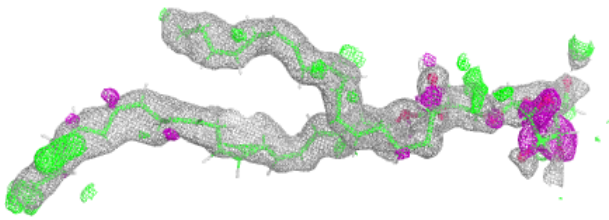


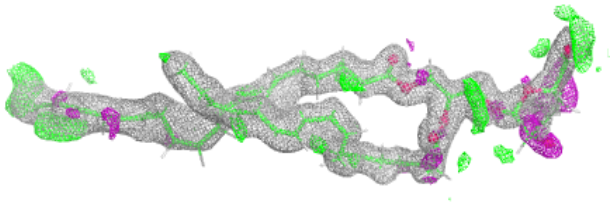


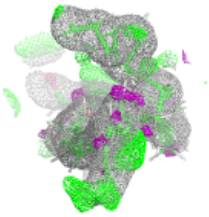


Electron density around W4I M 615 (B):

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

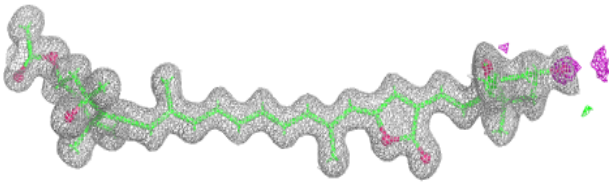


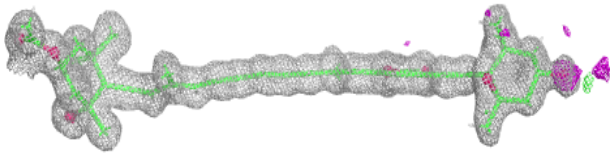


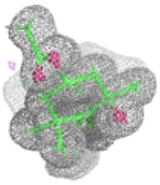


Electron density around PID N 613 (B):

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

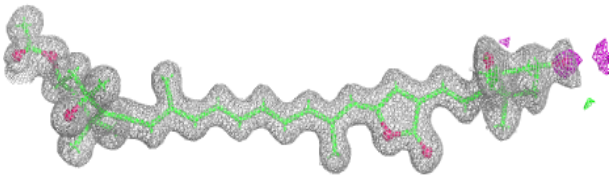


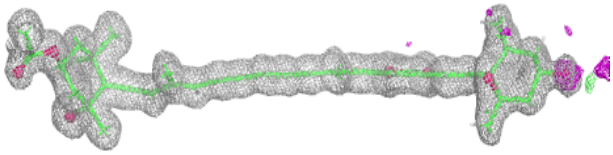


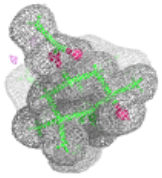


Electron density around PID N 613 (A):

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

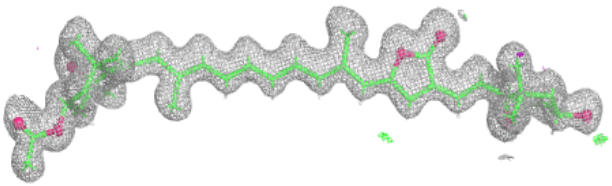


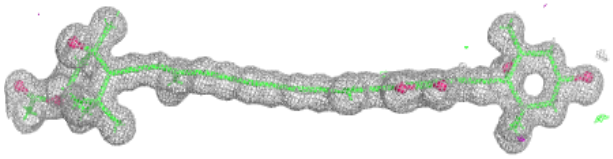


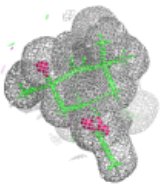


Electron density around PID N 623 (B):

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

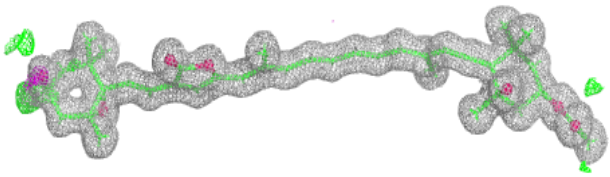


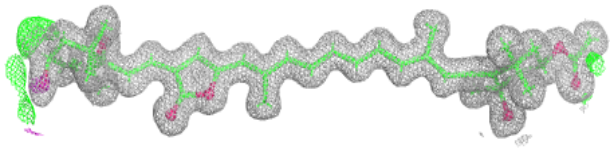


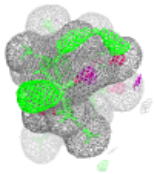


Electron density around PID O 611:

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

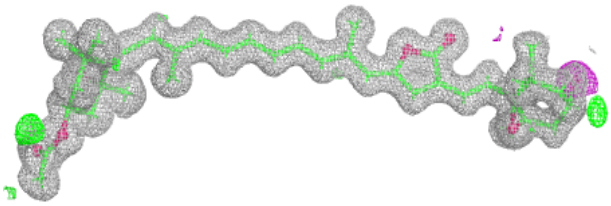


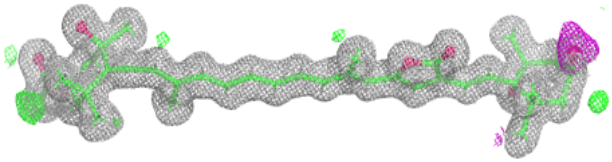


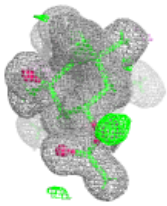


Electron density around PID O 612:

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

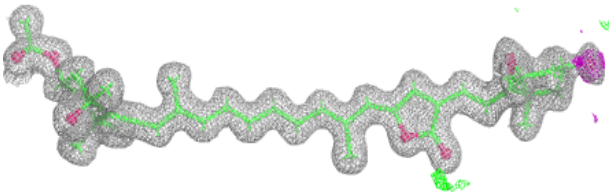


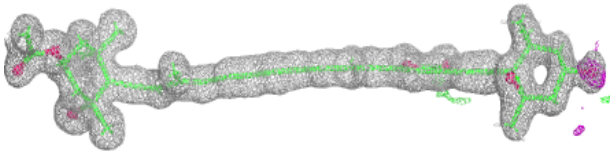


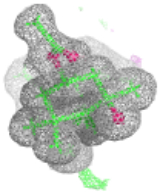


Electron density around PID O 613 (A):

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

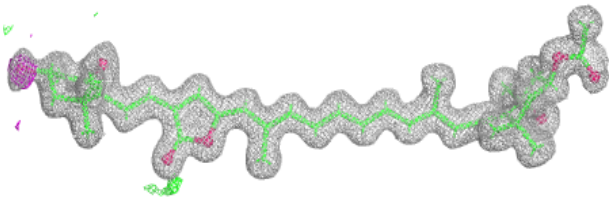


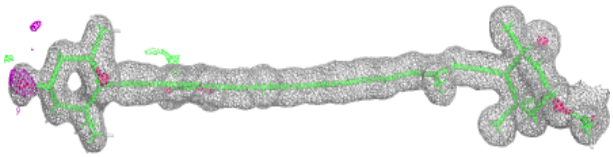


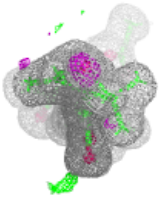


Electron density around PID O 613 (B):

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

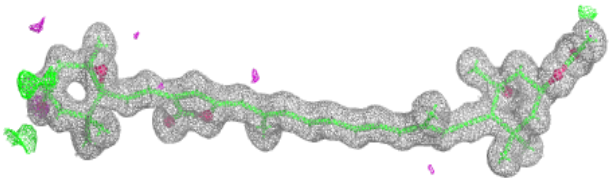


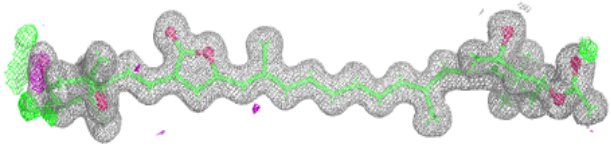


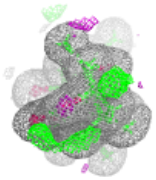


Electron density around PID M 611:

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

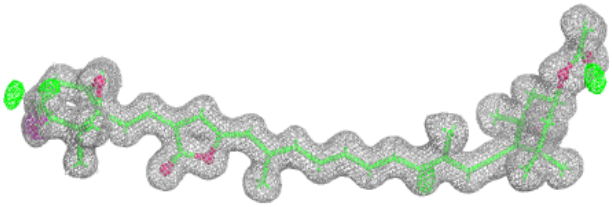


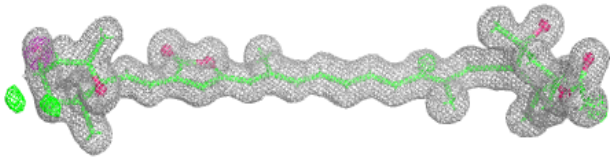


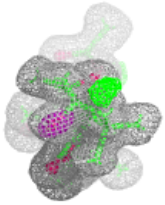


Electron density around PID M 612:

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

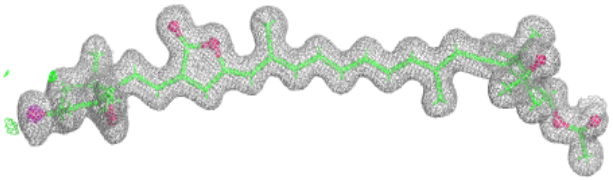


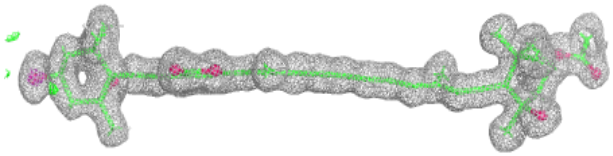


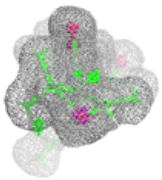


Electron density around PID M 613 (A):

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

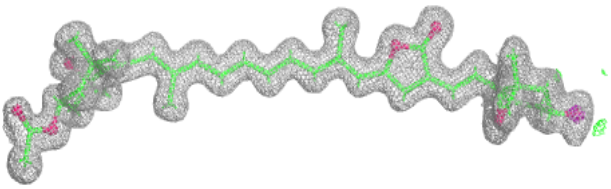


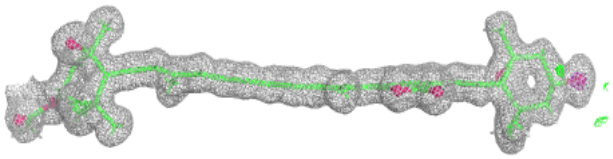


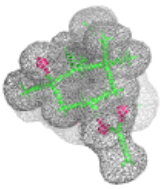


Electron density around PID M 613 (B):

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

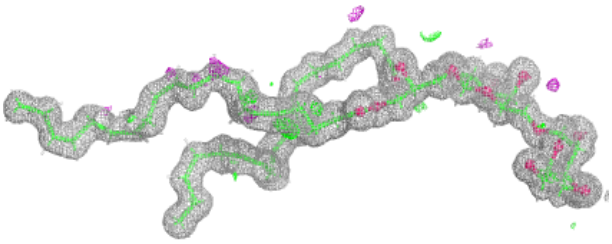


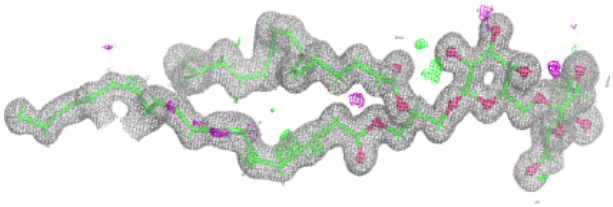


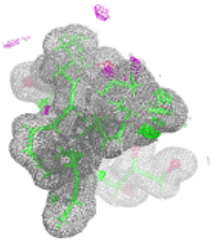


Electron density around W4I N 625 (A):

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

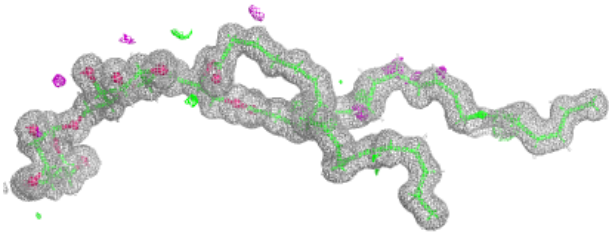


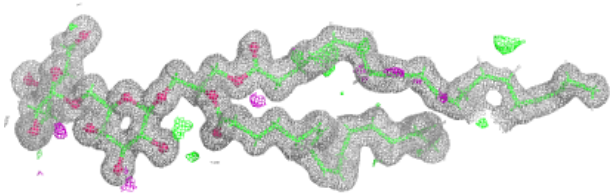


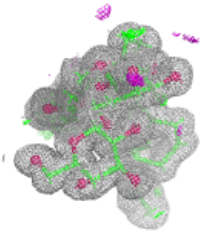


Electron density around W4I N 625 (B):

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

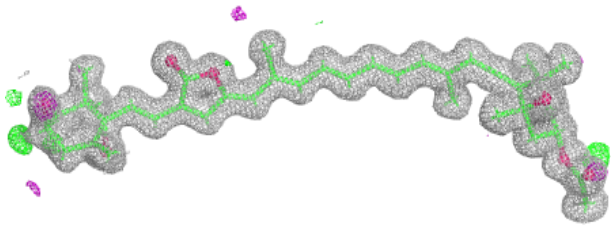


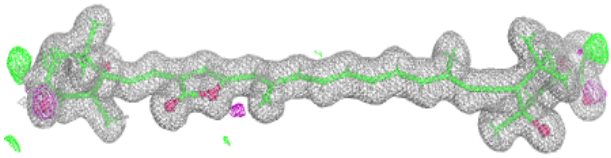


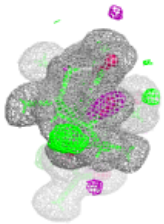


Electron density around PID N 612:

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

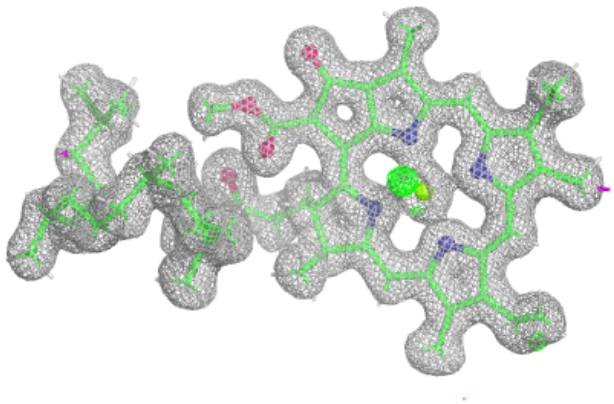


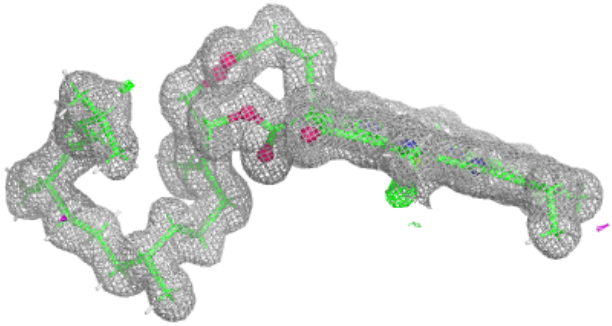


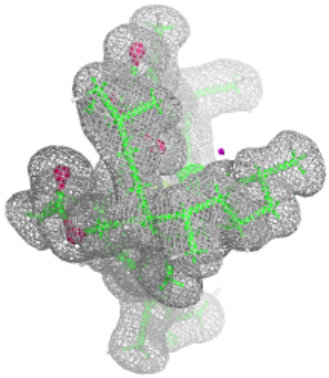


Electron density around CLA N 601:

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

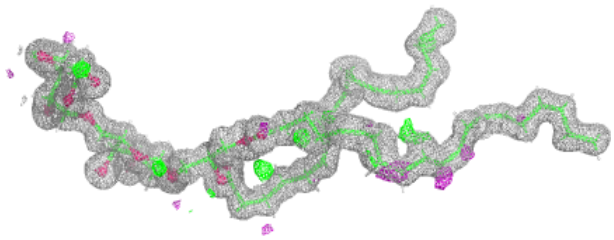


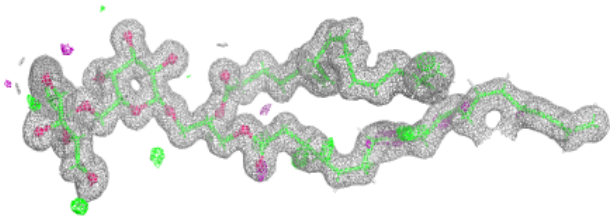


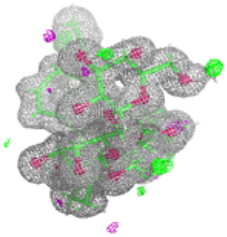


Electron density around W4I O 625 (A):

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

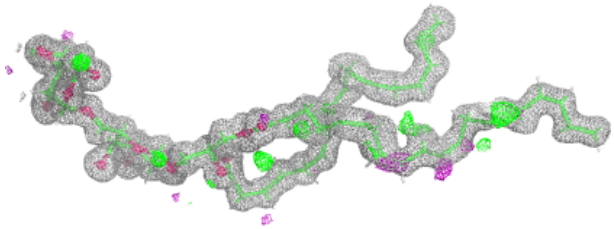


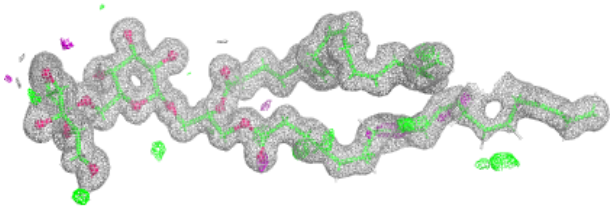


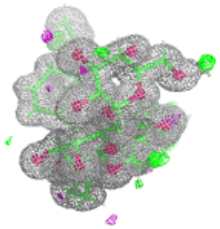


Electron density around W4I O 625 (B):

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

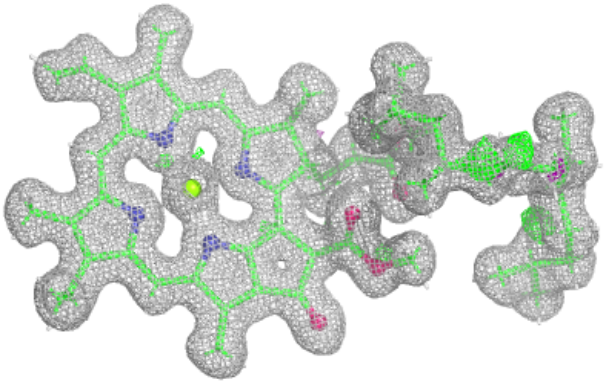


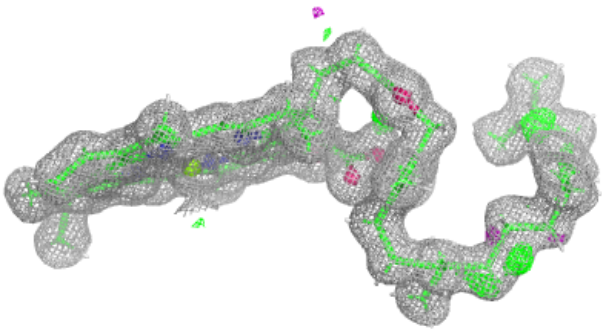


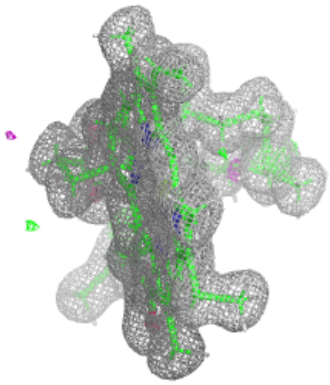


Electron density around CLA N 602:

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

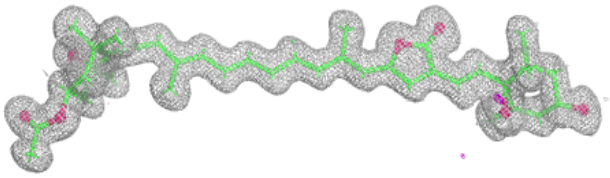


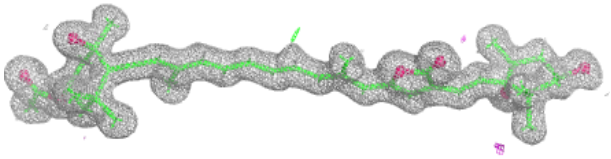


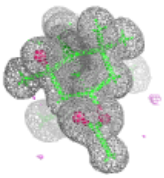


Electron density around PID N 614:

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

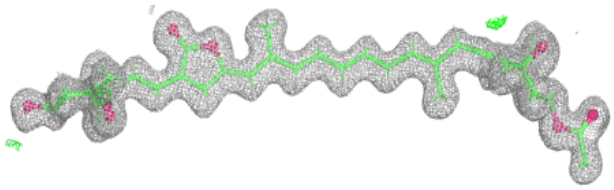


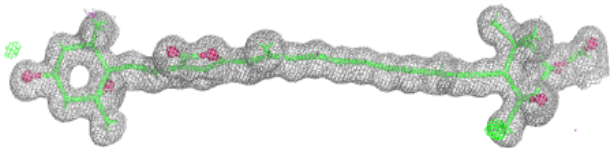


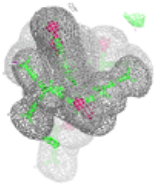


Electron density around PID N 623 (A):

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

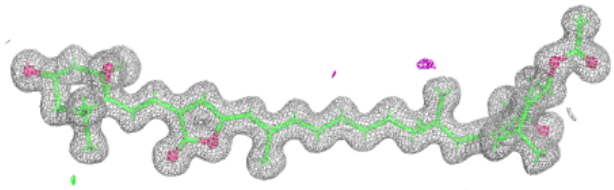


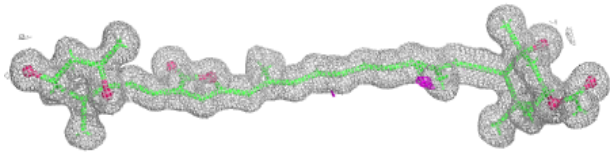


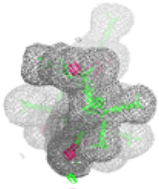


Electron density around PID M 624:

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

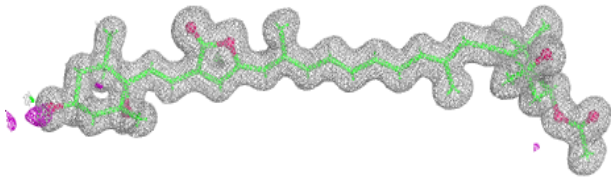


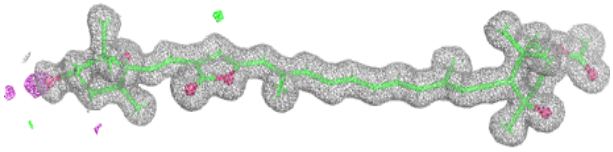


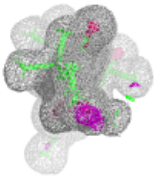


Electron density around PID O 614:

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

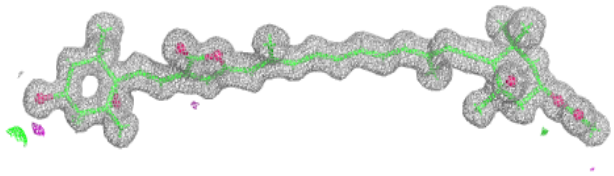


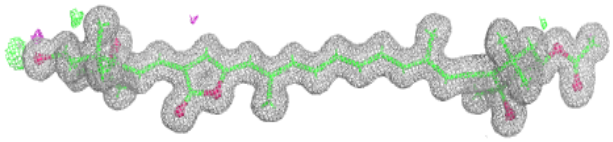


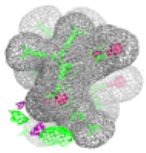


Electron density around PID O 621:

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

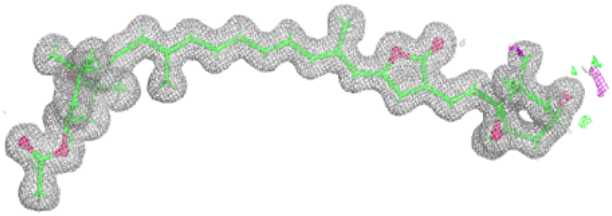


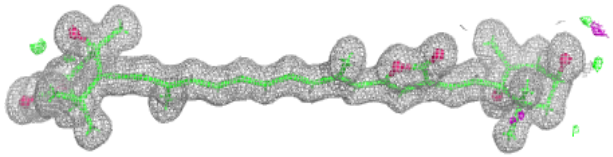


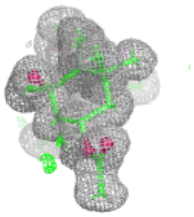


Electron density around PID O 622:

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

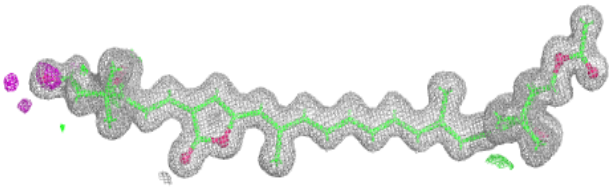


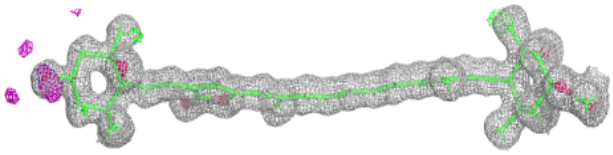


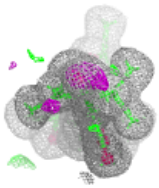


Electron density around PID O 623 (A):

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

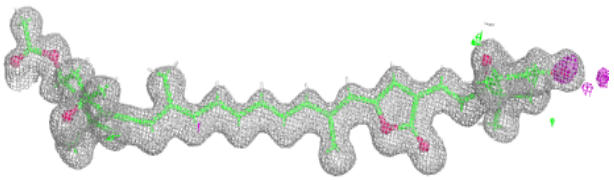


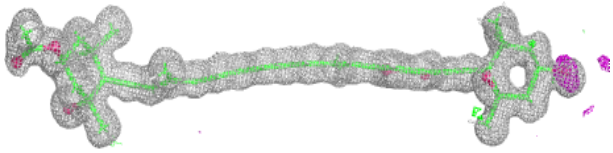


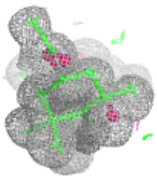


Electron density around PID O 623 (B):

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

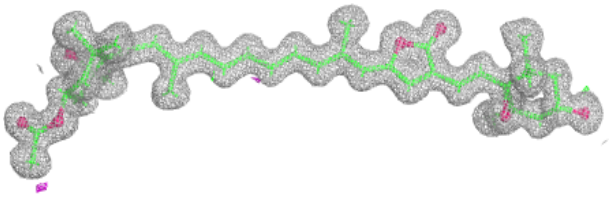


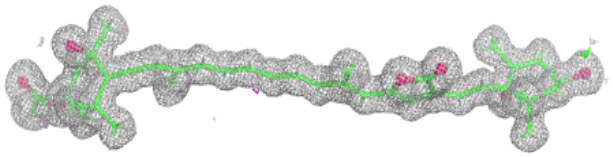


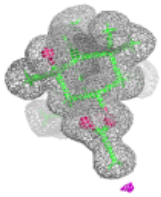


Electron density around PID O 624:

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

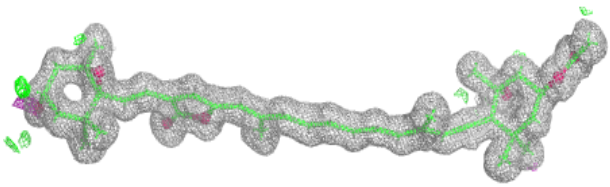


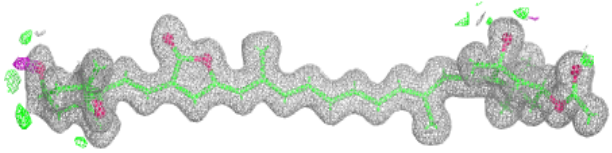


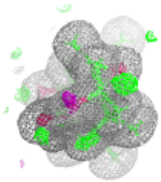


Electron density around PID N 611:

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

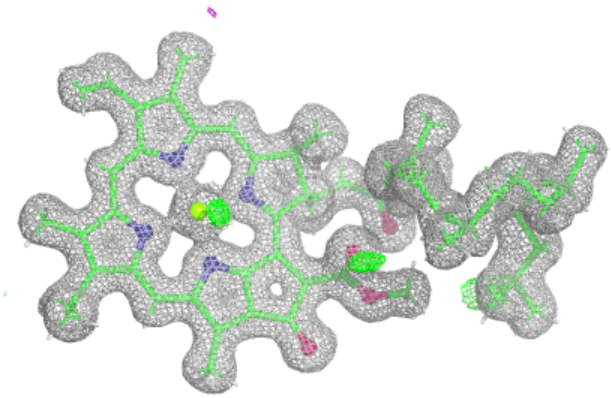


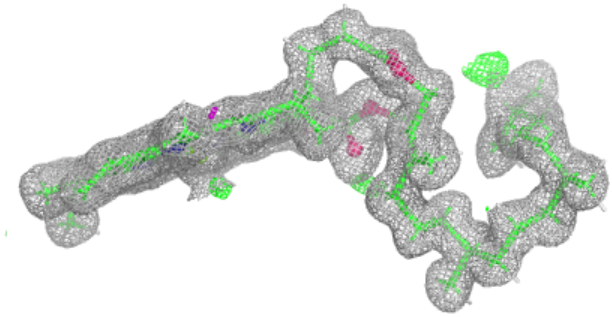


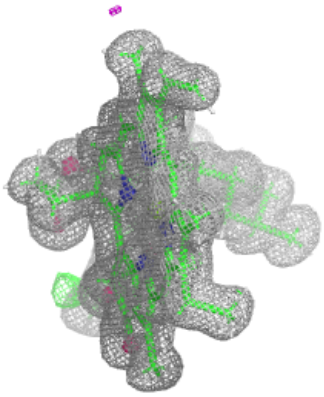


Electron density around CLA M 601:

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

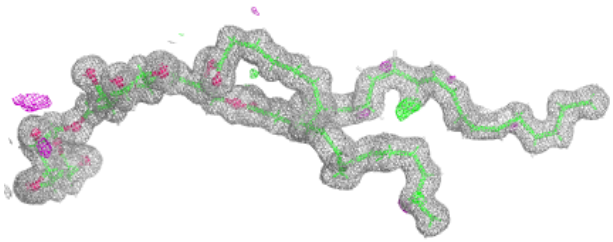


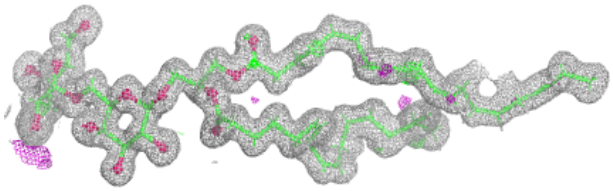


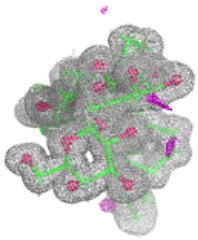


Electron density around W4I M 625 (A):

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

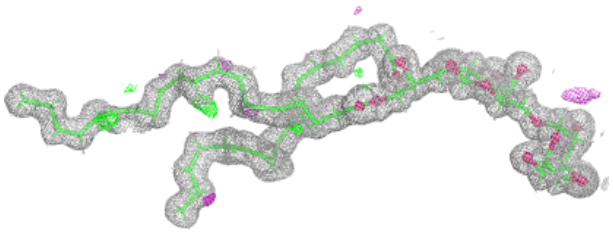


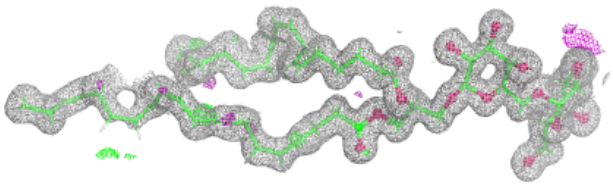


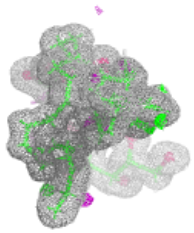


Electron density around W4I M 625 (B):

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

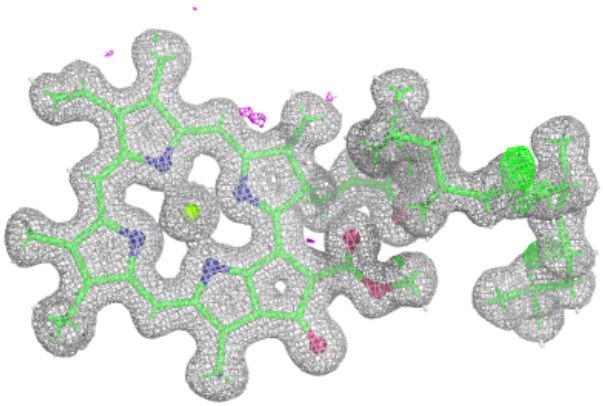


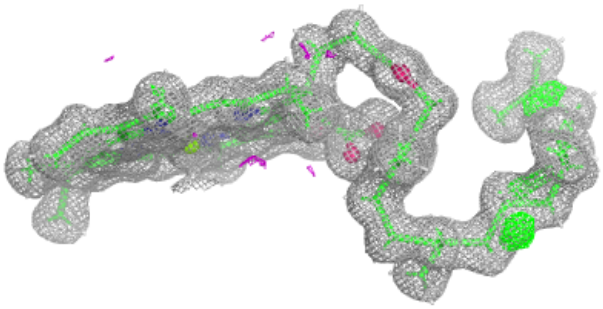


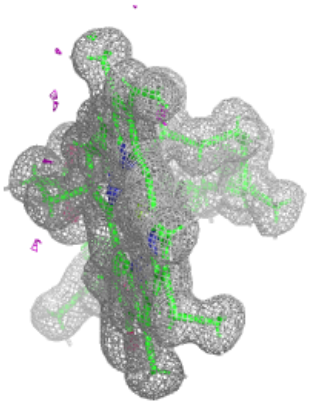


Electron density around CLA M 602:

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

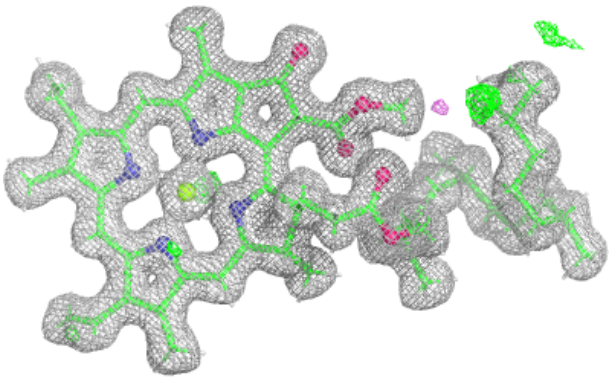


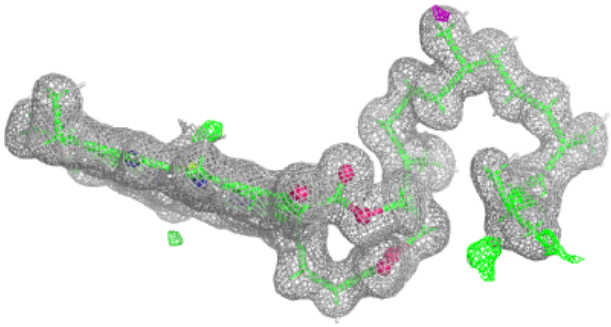


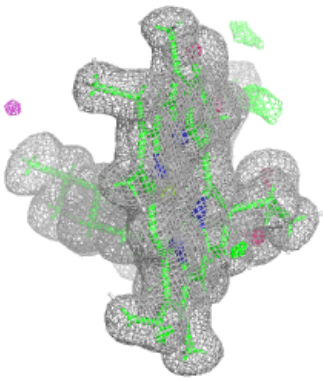


Electron density around CLA O 601:

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

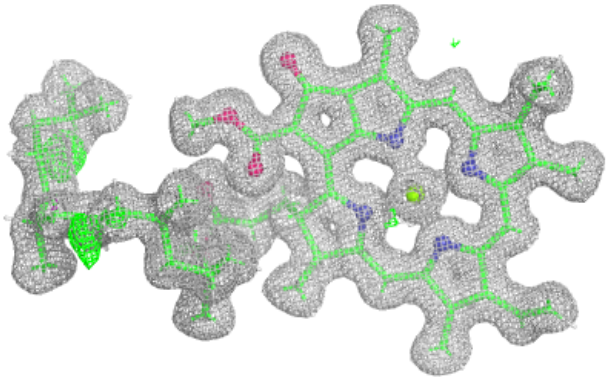


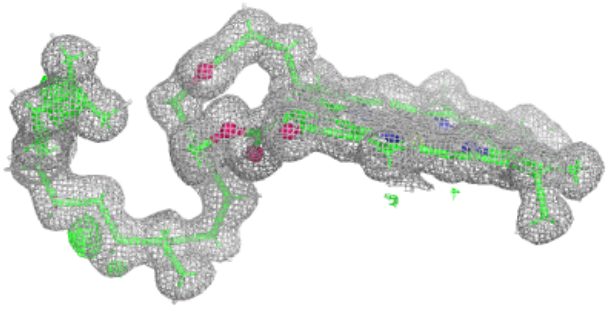


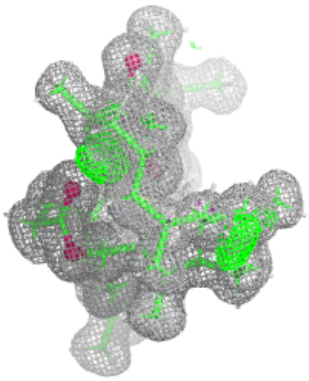


Electron density around CLA O 602:

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

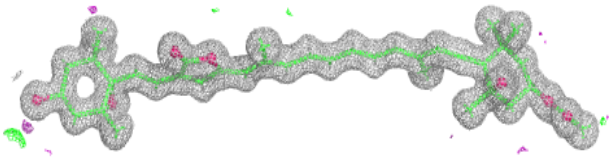


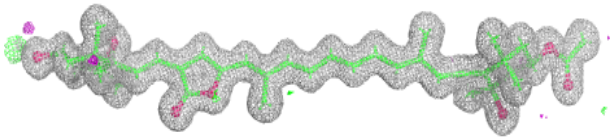


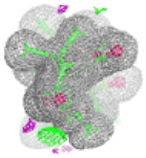


Electron density around PID N 621:

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

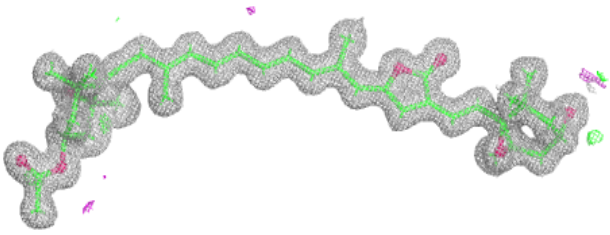


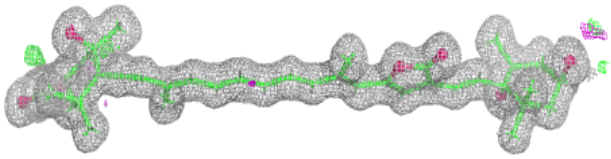


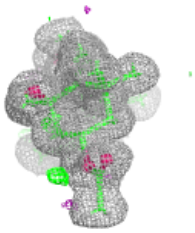


Electron density around PID N 622:

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

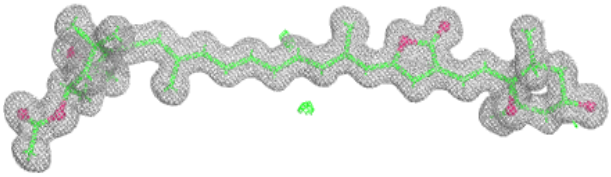


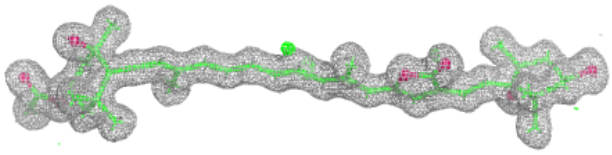


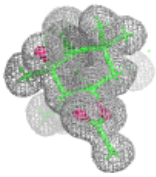


Electron density around PID M 614:

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

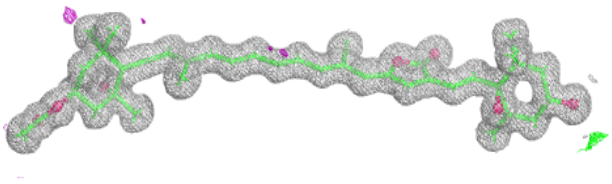


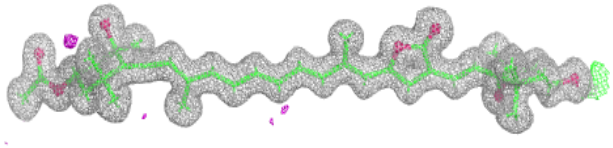


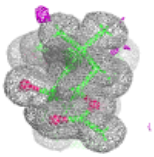


Electron density around PID M 621:

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

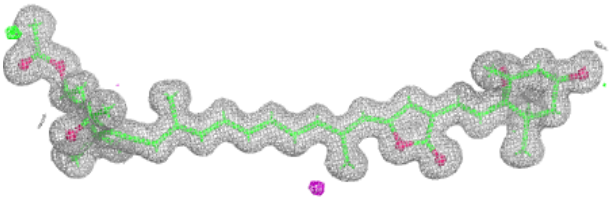


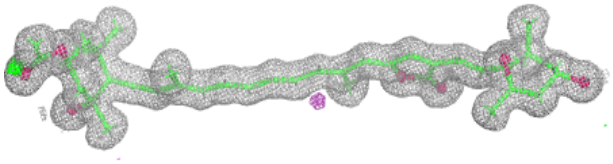


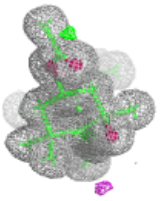


Electron density around PID N 624:

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

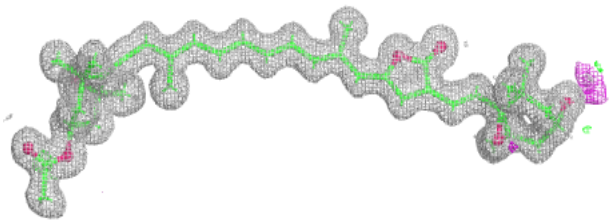


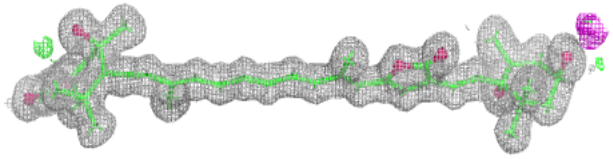


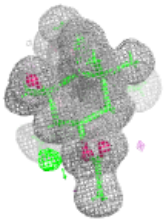


Electron density around PID M 622:

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

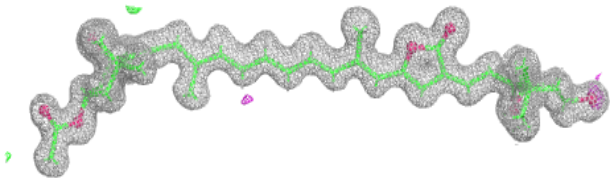


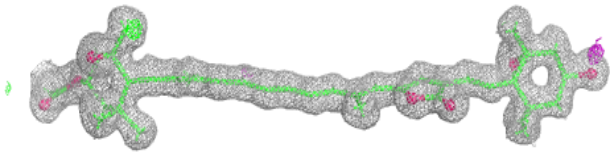


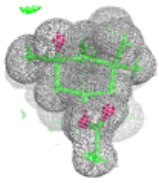


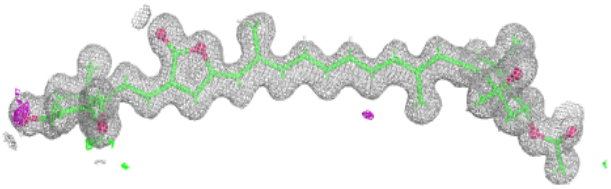
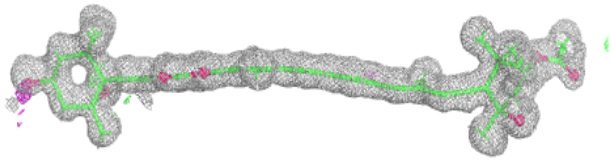
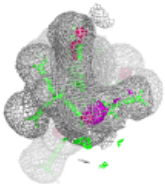
Electron density around PID M 623 (A):

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







Electron density around PID M 623 (B): $2mF_o$-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.