



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:29 AM UTC

PDB ID : 8OV5 / pdb_00008ov5
Title : PERIDININ-CHLOROPHYLL-PROTEIN OF AMPHIDIUM
CARTERAE, 100K
Authors : Hofmann, E.; Johanning, S.
Deposited on : 2023-04-25
Resolution : 1.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

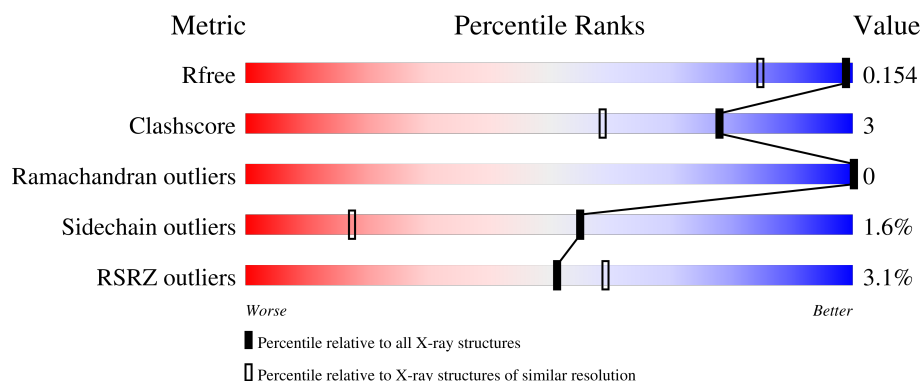
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	312	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
2	CLA	M	602	X	-	-	-
2	CLA	N	601	X	-	-	-
2	CLA	N	602	X	-	-	-
2	CLA	O	602	X	-	-	-
3	PID	M	613[A]	X	-	-	-
3	PID	M	613[B]	X	-	-	-
3	PID	O	623[B]	X	-	-	-

2 Entry composition

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.

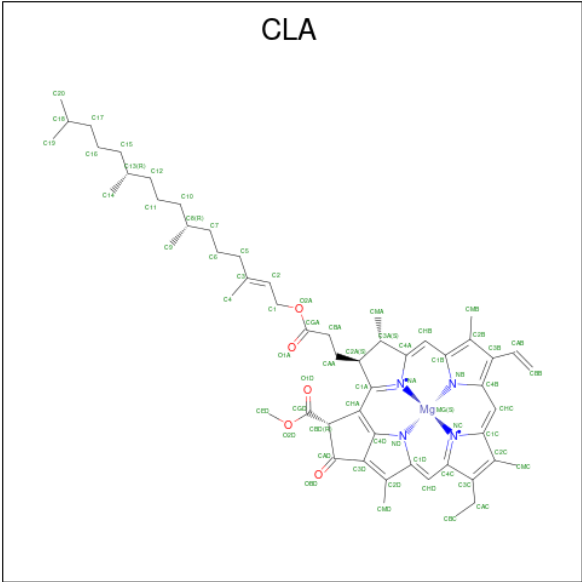
- Molecule 1 is a protein called Peridinin-chlorophyll a-binding protein 1, chloroplastic.

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

There are 6 discrepancies between the modelled and reference sequences:

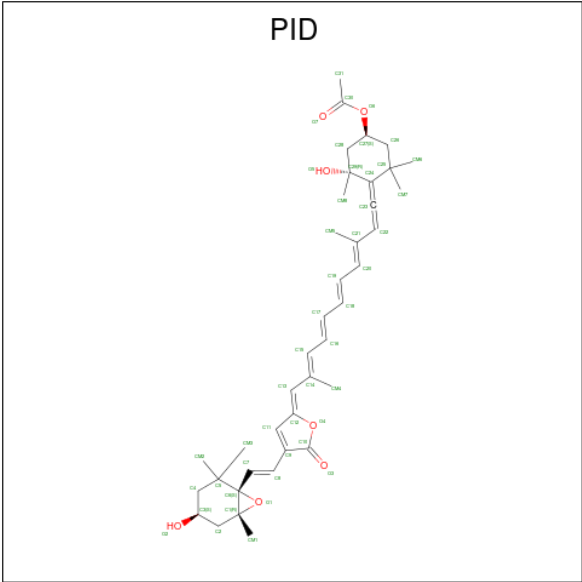
Chain	Residue	Modelled	Actual	Comment	Reference
M	128	ASN	SER	conflict	UNP P80484
M	276	VAL	ALA	conflict	UNP P80484
N	128	ASN	SER	conflict	UNP P80484
N	276	VAL	ALA	conflict	UNP P80484
O	128	ASN	SER	conflict	UNP P80484
O	276	VAL	ALA	conflict	UNP P80484

- 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
2	M	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
2	M	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
2	N	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
2	N	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
2	O	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
2	O	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 3 is PERIDININ (CCD ID: PID) (formula: C₃₉H₅₀O₇) (labeled as "Ligand of Interest" by depositor).



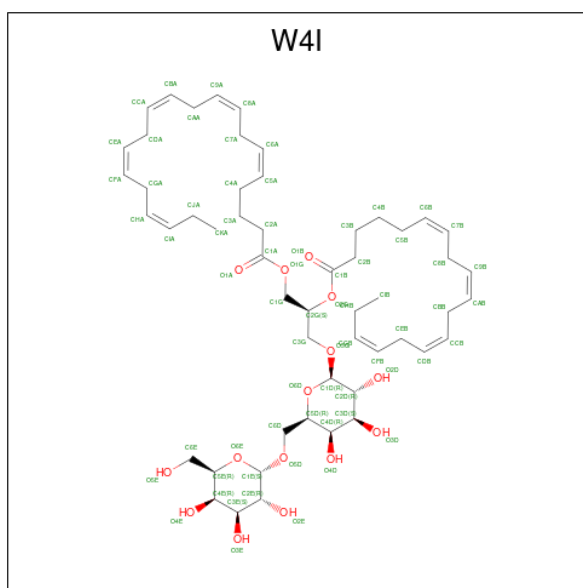
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	1	Total	C	H	O	0	0
			96	39	50	7		
3	M	1	Total	C	H	O	0	0
			96	39	50	7		
3	M	1	Total	C	H	O	0	1
			102	41	53	8		
3	M	1	Total	C	H	O	0	0
			96	39	50	7		
3	M	1	Total	C	H	O	0	0
			96	39	50	7		
3	M	1	Total	C	H	O	0	0
			96	39	50	7		
3	M	1	Total	C	H	O	0	1
			192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

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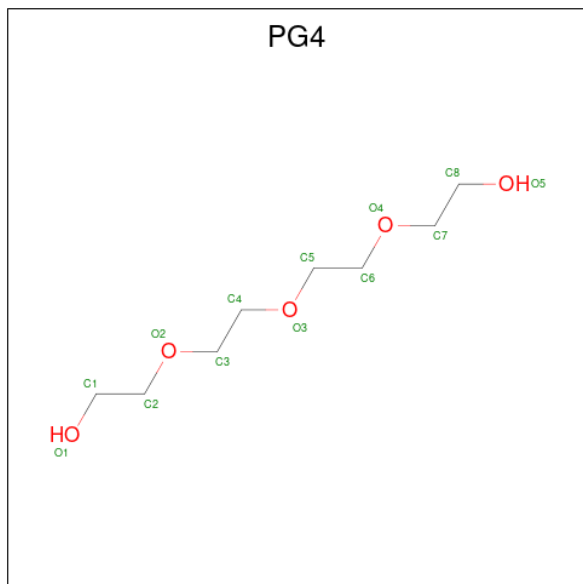
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	N	1	Total 192	C 78	H 100	O 14	0	1
3	N	1	Total 96	C 39	H 50	O 7	0	0
3	O	1	Total 96	C 39	H 50	O 7	0	0
3	O	1	Total 96	C 39	H 50	O 7	0	0
3	O	1	Total 102	C 41	H 53	O 8	0	1
3	O	1	Total 96	C 39	H 50	O 7	0	0
3	O	1	Total 96	C 39	H 50	O 7	0	0
3	O	1	Total 96	C 39	H 50	O 7	0	0
3	O	1	Total 192	C 78	H 100	O 14	0	1
3	O	1	Total 96	C 39	H 50	O 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-tetraenyl]oxy-propyl] (5 {Z},8 {Z},11 {Z},14 {Z},17 {Z})-icosa-5,8,11,14,17-pentaenoate (CCD ID: W4I) (formula: C₅₃H₈₂O₁₅) (labeled as "Ligand of Interest" by depositor).



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

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



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

- Molecule 6 is water.

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

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

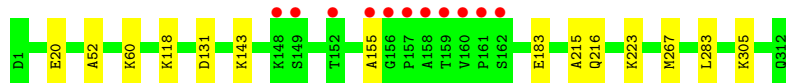
3 Residue-property plots [i](#)

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.

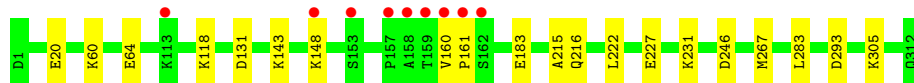
- Molecule 1: Peridinin-chlorophyll a-binding protein 1, chloroplastic



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PG4, PID, 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

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.

All (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
1:O:222[B]:LEU:HD21	3:O:613[B]:PID:O7	1.96	0.66
1:O:118:LYS:NZ	6:O:705:HOH:O	2.21	0.62
1:N:118:LYS:NZ	6:N:703:HOH:O	2.27	0.60
3:N:623[A]:PID:C9	3:N:624:PID:HM12	2.32	0.60
1:M:183[A]:GLU:OE2	1:M:293:ASP:OD2	2.20	0.59
1:N:216[B]:GLN:HG3	6:N:903:HOH:O	2.02	0.58
1:N:60[B]:LYS:HD2	1:N:215:ALA:HA	1.86	0.58
1:M:183[A]:GLU:OE2	6:M:820:HOH:O	2.17	0.56
1:N:20[B]:GLU:OE2	1:N:131:ASP:OD2	2.25	0.55
1:M:155:ALA:HB3	6:M:916:HOH:O	2.06	0.55
1:O:222[B]:LEU:HG	3:O:613[B]:PID:H311	1.88	0.54
1:M:222[B]:LEU:HD21	3:M:613[B]:PID:O7	2.06	0.54
1:M:60[B]:LYS:HD2	1:M:215:ALA:HA	1.90	0.52
1:N:60[A]:LYS:HE3	6:N:708:HOH:O	2.10	0.52
1:O:216[A]:GLN:HG3	6:O:901:HOH:O	2.09	0.52
1:O:20[B]:GLU:OE2	1:O:131:ASP:OD2	2.28	0.51
1:O:60[B]:LYS:HD2	1:O:215:ALA:HA	1.91	0.51
3:M:623[A]:PID:C9	3:M:624:PID:HM12	2.40	0.50
1:M:216[A]:GLN:HG3	6:M:952:HOH:O	2.09	0.50
1:M:52:ALA:O	1:M:223[A]:LYS:NZ	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:52:ALA:O	1:N:223[A]:LYS:NZ	2.38	0.50
1:O:183[A]:GLU:OE2	1:O:293:ASP:OD2	2.30	0.50
1:N:267:MET:SD	3:N:623[B]:PID:H11	2.52	0.49
1:M:20[B]:GLU:OE2	1:M:131:ASP:OD2	2.31	0.49
1:N:155:ALA:HB3	6:N:1006:HOH:O	2.13	0.48
1:O:222[B]:LEU:CD2	3:O:613[B]:PID:O7	2.61	0.48
1:O:160:VAL:HG12	1:O:161:PRO:O	2.12	0.47
1:O:267:MET:SD	3:O:623[B]:PID:H11	2.55	0.47
3:M:623[A]:PID:C10	3:M:624:PID:HM12	2.45	0.46
3:N:623[A]:PID:C10	3:N:624:PID:HM12	2.47	0.45
2:N:602:CLA:HBB1	2:N:602:CLA:HHC	1.99	0.44
1:M:222[B]:LEU:CD2	3:M:613[B]:PID:O7	2.67	0.42
1:M:56:PRO:O	1:M:60[B]:LYS:HG2	2.20	0.41
3:O:623[B]:PID:C9	3:O:624:PID:HM12	2.50	0.41
3:O:623[B]:PID:C10	3:O:624:PID:HM12	2.49	0.41
1:M:8:LYS:HE2	6:M:893:HOH:O	2.21	0.40
3:O:611:PID:H16	3:O:611:PID:HM41	1.91	0.40

All (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
6:M:1325:HOH:O	6:O:1092:HOH:O[4_546]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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 ⓘ

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

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	143	LYS
1	M	149	SER
1	M	283	LEU
1	M	305[A]	LYS
1	M	305[B]	LYS
1	N	143	LYS
1	N	283	LEU
1	N	305[A]	LYS
1	N	305[B]	LYS
1	O	143	LYS
1	O	148	LYS
1	O	283	LEU
1	O	305[A]	LYS
1	O	305[B]	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	N	621	-	43,49,49	0.88	3 (6%)	52,76,76	0.80	1 (1%)
2	CLA	M	602	6	69,73,73	1.12	4 (5%)	82,113,113	1.27	2 (2%)
2	CLA	M	601	6	69,73,73	1.12	5 (7%)	82,113,113	1.22	4 (4%)
3	PID	N	613[B]	-	43,49,49	1.17	4 (9%)	52,76,76	0.87	1 (1%)
3	PID	M	611	-	43,49,49	1.24	2 (4%)	52,76,76	0.92	0
4	W4I	M	615[A]	-	57,57,69	1.34	7 (12%)	65,65,83	1.17	7 (10%)
3	PID	N	624	-	43,49,49	0.97	2 (4%)	52,76,76	0.83	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PID	O	623[A]	-	43,49,49	1.18	2 (4%)	52,76,76	1.04	6 (11%)
5	PG4	M	651	-	12,12,12	0.15	0	11,11,11	0.45	0
3	PID	O	611	-	43,49,49	1.16	2 (4%)	52,76,76	0.89	1 (1%)
3	PID	N	613[A]	-	43,49,49	1.21	5 (11%)	52,76,76	0.92	2 (3%)
2	CLA	O	602	6	69,73,73	1.09	5 (7%)	82,113,113	1.16	6 (7%)
3	PID	M	621	-	43,49,49	0.89	1 (2%)	52,76,76	0.91	2 (3%)
5	PG4	O	651	-	12,12,12	0.12	0	11,11,11	0.52	0
3	PID	N	623[B]	-	43,49,49	0.96	2 (4%)	52,76,76	0.75	1 (1%)
3	PID	M	624	-	43,49,49	0.87	0	52,76,76	0.88	2 (3%)
3	PID	N	623[A]	-	43,49,49	0.90	1 (2%)	52,76,76	0.77	1 (1%)
2	CLA	N	602	6	69,73,73	1.16	7 (10%)	82,113,113	1.33	5 (6%)
2	CLA	N	601	6	69,73,73	1.03	4 (5%)	82,113,113	1.39	5 (6%)
3	PID	M	623[B]	-	43,49,49	0.99	3 (6%)	52,76,76	0.97	3 (5%)
3	PID	N	614	-	43,49,49	0.88	1 (2%)	52,76,76	0.81	1 (1%)
3	PID	O	622	-	43,49,49	1.10	3 (6%)	52,76,76	1.07	2 (3%)
3	PID	O	624	-	43,49,49	0.80	0	52,76,76	0.76	0
4	W4I	M	625[B]	-	69,69,69	0.74	1 (1%)	83,83,83	0.72	0
4	W4I	O	615[B]	-	57,57,69	1.39	7 (12%)	65,65,83	1.13	5 (7%)
5	PG4	N	651	-	12,12,12	0.12	0	11,11,11	0.50	0
4	W4I	O	625[B]	-	69,69,69	0.86	2 (2%)	83,83,83	0.78	1 (1%)
3	PID	M	613[B]	-	43,49,49	0.96	2 (4%)	52,76,76	0.91	1 (1%)
2	CLA	O	601	6	69,73,73	1.13	4 (5%)	82,113,113	1.17	2 (2%)
3	PID	M	623[A]	-	43,49,49	1.18	3 (6%)	52,76,76	0.93	1 (1%)
4	W4I	M	625[A]	-	69,69,69	0.74	1 (1%)	83,83,83	0.74	0
3	PID	M	613[A]	-	43,49,49	1.05	3 (6%)	52,76,76	0.93	1 (1%)
4	W4I	O	615[A]	-	57,57,69	1.38	7 (12%)	65,65,83	1.12	5 (7%)
4	W4I	M	615[B]	-	57,57,69	1.34	7 (12%)	65,65,83	1.21	7 (10%)
4	W4I	O	625[A]	-	69,69,69	0.85	2 (2%)	83,83,83	0.79	1 (1%)
3	PID	O	621	-	43,49,49	0.99	3 (6%)	52,76,76	0.83	1 (1%)
3	PID	O	612	-	43,49,49	1.44	2 (4%)	52,76,76	0.93	3 (5%)
3	PID	M	614	-	43,49,49	0.89	2 (4%)	52,76,76	0.82	2 (3%)
4	W4I	N	615[B]	-	57,57,69	1.43	9 (15%)	65,65,83	1.18	7 (10%)
3	PID	M	622	-	43,49,49	0.97	2 (4%)	52,76,76	1.04	4 (7%)
3	PID	O	614	-	43,49,49	0.83	2 (4%)	52,76,76	0.91	3 (5%)
3	PID	O	623[B]	-	43,49,49	1.22	5 (11%)	52,76,76	0.95	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PID	N	611	-	43,49,49	1.23	1 (2%)	52,76,76	0.89	1 (1%)
4	W4I	N	615[A]	-	57,57,69	1.42	9 (15%)	65,65,83	1.21	7 (10%)
3	PID	O	613[B]	-	43,49,49	1.11	2 (4%)	52,76,76	0.81	0
3	PID	N	612	-	43,49,49	1.26	2 (4%)	52,76,76	0.95	2 (3%)
4	W4I	N	625[B]	-	69,69,69	0.89	2 (2%)	83,83,83	0.81	4 (4%)
4	W4I	N	625[A]	-	69,69,69	0.89	2 (2%)	83,83,83	0.82	4 (4%)
3	PID	N	622	-	43,49,49	1.00	2 (4%)	52,76,76	1.07	4 (7%)
3	PID	M	612	-	43,49,49	1.45	4 (9%)	52,76,76	0.88	1 (1%)
3	PID	O	613[A]	-	43,49,49	1.21	3 (6%)	52,76,76	0.89	1 (1%)

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	N	621	-	-	0/24/93/93	0/4/4/4
2	CLA	M	602	6	1/1/20/20	1/39/115/115	-
2	CLA	M	601	6	-	0/39/115/115	-
3	PID	N	613[B]	-	-	0/24/93/93	0/4/4/4
3	PID	M	611	-	-	0/24/93/93	0/4/4/4
4	W4I	M	615[A]	-	-	11/52/72/97	0/1/1/2
3	PID	N	624	-	-	0/24/93/93	0/4/4/4
3	PID	O	623[A]	-	-	0/24/93/93	0/4/4/4
5	PG4	M	651	-	-	3/10/10/10	-
3	PID	O	611	-	-	0/24/93/93	0/4/4/4
3	PID	N	613[A]	-	-	0/24/93/93	0/4/4/4
2	CLA	O	602	6	1/1/20/20	0/39/115/115	-
3	PID	M	621	-	-	0/24/93/93	0/4/4/4
5	PG4	O	651	-	-	4/10/10/10	-
3	PID	N	623[B]	-	-	0/24/93/93	0/4/4/4
3	PID	M	624	-	-	0/24/93/93	0/4/4/4
3	PID	N	623[A]	-	-	0/24/93/93	0/4/4/4
2	CLA	N	602	6	1/1/20/20	0/39/115/115	-
2	CLA	N	601	6	1/1/20/20	0/39/115/115	-
3	PID	M	623[B]	-	-	0/24/93/93	0/4/4/4
3	PID	N	614	-	-	0/24/93/93	0/4/4/4
3	PID	O	613[A]	-	-	0/24/93/93	0/4/4/4
3	PID	O	622	-	-	0/24/93/93	0/4/4/4
3	PID	O	624	-	-	0/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	W4I	M	625[B]	-	-	4/57/97/97	0/2/2/2
4	W4I	O	615[B]	-	-	9/52/72/97	0/1/1/2
4	W4I	O	625[B]	-	-	4/57/97/97	0/2/2/2
5	PG4	N	651	-	-	2/10/10/10	-
3	PID	M	613[B]	-	1/1/25/25	0/24/93/93	0/4/4/4
2	CLA	O	601	6	-	0/39/115/115	-
3	PID	M	623[A]	-	-	0/24/93/93	0/4/4/4
4	W4I	M	625[A]	-	-	6/57/97/97	0/2/2/2
3	PID	M	613[A]	-	1/1/25/25	0/24/93/93	0/4/4/4
4	W4I	O	615[A]	-	-	8/52/72/97	0/1/1/2
4	W4I	M	615[B]	-	-	14/52/72/97	0/1/1/2
4	W4I	O	625[A]	-	-	6/57/97/97	0/2/2/2
3	PID	O	621	-	-	0/24/93/93	0/4/4/4
3	PID	O	612	-	-	0/24/93/93	0/4/4/4
3	PID	M	614	-	-	0/24/93/93	0/4/4/4
4	W4I	N	615[B]	-	-	17/52/72/97	0/1/1/2
3	PID	M	622	-	-	0/24/93/93	0/4/4/4
3	PID	O	614	-	-	0/24/93/93	0/4/4/4
3	PID	N	611	-	-	0/24/93/93	0/4/4/4
4	W4I	N	615[A]	-	-	16/52/72/97	0/1/1/2
3	PID	O	613[B]	-	-	0/24/93/93	0/4/4/4
3	PID	N	612	-	-	0/24/93/93	0/4/4/4
4	W4I	N	625[B]	-	-	3/57/97/97	0/2/2/2
4	W4I	N	625[A]	-	-	5/57/97/97	0/2/2/2
3	PID	N	622	-	-	0/24/93/93	0/4/4/4
3	PID	M	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

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	612	PID	C2-C3	-6.96	1.42	1.52
3	M	612	PID	C2-C3	-6.62	1.42	1.52
3	N	612	PID	C2-C3	-5.64	1.44	1.52
2	M	602	CLA	MG-NA	5.21	2.18	2.06
3	M	611	PID	C4-C3	-5.04	1.45	1.52
2	O	602	CLA	MG-NA	4.91	2.17	2.06
2	N	602	CLA	MG-NA	4.88	2.17	2.06
3	N	611	PID	C4-C3	-4.87	1.45	1.52
4	N	615[A]	W4I	C3G-C2G	4.39	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	615[B]	W4I	C3G-C2G	4.39	1.64	1.50
4	O	615[A]	W4I	C6D-C5D	4.36	1.66	1.51
4	O	615[B]	W4I	C6D-C5D	4.36	1.66	1.51
2	O	601	CLA	MG-NA	4.32	2.16	2.06
4	M	615[A]	W4I	C6D-C5D	4.29	1.66	1.51
4	M	615[B]	W4I	C6D-C5D	4.29	1.66	1.51
4	N	615[A]	W4I	C6D-C5D	4.14	1.65	1.51
4	N	615[B]	W4I	C6D-C5D	4.14	1.65	1.51
3	O	611	PID	C4-C3	-3.97	1.46	1.52
2	M	601	CLA	MG-NA	3.96	2.15	2.06
4	M	615[A]	W4I	C3G-C2G	3.95	1.63	1.50
4	M	615[B]	W4I	C3G-C2G	3.95	1.63	1.50
2	N	601	CLA	MG-NA	3.74	2.15	2.06
3	O	623[A]	PID	C2-C3	-3.70	1.47	1.52
4	M	615[A]	W4I	C4D-C5D	3.51	1.60	1.53
4	M	615[B]	W4I	C4D-C5D	3.51	1.60	1.53
3	N	623[B]	PID	C2-C3	-3.50	1.47	1.52
4	N	615[A]	W4I	C1G-C2G	3.26	1.61	1.50
4	N	615[B]	W4I	C1G-C2G	3.26	1.61	1.50
3	O	613[A]	PID	O6-C30	-3.26	1.27	1.35
3	O	613[A]	PID	C4-C3	-3.23	1.47	1.52
3	O	613[B]	PID	C4-C3	-3.23	1.47	1.52
3	O	623[B]	PID	C6-C7	-3.20	1.45	1.50
3	O	623[B]	PID	C4-C3	-3.14	1.47	1.52
4	N	615[A]	W4I	O3G-C1D	3.07	1.45	1.40
4	N	615[B]	W4I	O3G-C1D	3.07	1.45	1.40
4	O	615[A]	W4I	C4D-C5D	3.04	1.59	1.53
4	O	615[B]	W4I	C4D-C5D	3.04	1.59	1.53
4	O	615[A]	W4I	C3G-C2G	3.00	1.60	1.50
4	O	615[B]	W4I	C3G-C2G	3.00	1.60	1.50
2	O	601	CLA	C1D-ND	2.96	1.41	1.37
3	M	613[A]	PID	O6-C30	-2.96	1.28	1.35
3	N	613[A]	PID	C13-C14	-2.93	1.40	1.45
3	N	613[B]	PID	C13-C14	-2.93	1.40	1.45
3	M	623[A]	PID	C2-C3	-2.86	1.48	1.52
3	O	612	PID	CM1-C1	-2.78	1.47	1.51
4	N	615[A]	W4I	C4D-C5D	2.76	1.58	1.53
4	N	615[B]	W4I	C4D-C5D	2.76	1.58	1.53
3	M	623[A]	PID	CM1-C1	-2.73	1.47	1.51
3	N	613[A]	PID	O1-C1	-2.73	1.42	1.46
3	N	613[B]	PID	O1-C1	-2.73	1.42	1.46
2	M	601	CLA	C1D-ND	2.71	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	613[A]	PID	C4-C3	-2.70	1.48	1.52
3	N	613[B]	PID	C4-C3	-2.70	1.48	1.52
4	N	615[A]	W4I	C1D-C2D	2.69	1.60	1.52
4	N	615[B]	W4I	C1D-C2D	2.69	1.60	1.52
4	O	615[A]	W4I	C1D-C2D	2.69	1.60	1.52
4	O	615[B]	W4I	C1D-C2D	2.69	1.60	1.52
3	O	622	PID	C13-C14	-2.68	1.40	1.45
2	N	602	CLA	C1D-ND	2.68	1.41	1.37
3	M	623[B]	PID	C4-C3	-2.64	1.48	1.52
3	O	623[B]	PID	C11-C12	-2.62	1.39	1.44
3	O	613[A]	PID	CM1-C1	-2.61	1.47	1.51
3	O	613[B]	PID	CM1-C1	-2.61	1.47	1.51
4	O	615[A]	W4I	O3G-C1D	2.61	1.44	1.40
4	O	615[B]	W4I	O3G-C1D	2.61	1.44	1.40
4	O	625[A]	W4I	O5D-C6D	-2.59	1.39	1.43
4	O	625[B]	W4I	O5D-C6D	-2.59	1.39	1.43
2	M	602	CLA	C4B-NB	2.54	1.41	1.37
4	O	615[A]	W4I	C1G-C2G	2.54	1.58	1.50
4	O	615[B]	W4I	C1G-C2G	2.54	1.58	1.50
2	N	602	CLA	C1B-C2B	2.53	1.49	1.43
4	N	625[A]	W4I	O3G-C3G	-2.50	1.39	1.43
4	N	625[B]	W4I	O3G-C3G	-2.50	1.39	1.43
3	O	621	PID	C2-C3	-2.50	1.48	1.52
3	N	612	PID	C4-C5	-2.49	1.50	1.54
3	M	611	PID	O2-C3	2.49	1.50	1.43
3	M	613[A]	PID	C4-C3	-2.49	1.48	1.52
3	M	613[B]	PID	C4-C3	-2.49	1.48	1.52
3	O	623[B]	PID	C9-C10	-2.48	1.43	1.48
3	N	614	PID	CM8-C29	-2.48	1.49	1.52
3	N	624	PID	C4-C3	-2.48	1.48	1.52
3	M	612	PID	CM1-C1	-2.45	1.48	1.51
2	M	602	CLA	C1B-C2B	2.44	1.48	1.43
3	M	622	PID	C4-C3	-2.44	1.48	1.52
3	O	622	PID	C4-C3	-2.44	1.48	1.52
4	M	615[A]	W4I	C1G-C2G	2.43	1.58	1.50
4	M	615[B]	W4I	C1G-C2G	2.43	1.58	1.50
4	O	615[A]	W4I	C3D-C2D	2.42	1.58	1.52
4	O	615[B]	W4I	C3D-C2D	2.42	1.58	1.52
3	M	623[B]	PID	C2-C3	-2.42	1.48	1.52
3	N	613[A]	PID	O6-C30	-2.42	1.29	1.35
3	M	612	PID	CM2-C5	2.40	1.58	1.53
3	M	614	PID	C9-C10	-2.39	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	601	CLA	C1D-ND	2.39	1.41	1.37
2	M	601	CLA	C4B-NB	2.38	1.41	1.37
4	N	615[A]	W4I	O2G-C1B	2.34	1.40	1.34
4	N	615[B]	W4I	O2G-C1B	2.34	1.40	1.34
3	O	623[B]	PID	C4-C5	-2.33	1.51	1.54
2	O	602	CLA	C3B-C4B	2.32	1.49	1.42
3	M	623[A]	PID	C4-C5	-2.32	1.51	1.54
2	N	602	CLA	C4B-NB	2.32	1.40	1.37
2	O	602	CLA	C1B-C2B	2.30	1.48	1.43
3	O	621	PID	C11-C12	-2.30	1.39	1.44
3	N	622	PID	C4-C3	-2.27	1.49	1.52
2	N	601	CLA	C1B-C2B	2.25	1.48	1.43
2	O	602	CLA	C4B-NB	2.25	1.40	1.37
3	O	621	PID	C9-C10	-2.24	1.43	1.48
2	M	601	CLA	C3B-C4B	2.23	1.49	1.42
2	M	601	CLA	C1B-C2B	2.22	1.48	1.43
4	O	625[A]	W4I	O1A-C1A	-2.21	1.15	1.22
4	O	625[B]	W4I	O1A-C1A	-2.21	1.15	1.22
3	N	621	PID	C11-C12	-2.21	1.39	1.44
2	N	602	CLA	MG-NC	2.21	2.11	2.06
3	N	613[A]	PID	CM1-C1	-2.20	1.48	1.51
3	N	613[B]	PID	CM1-C1	-2.20	1.48	1.51
3	N	623[B]	PID	C13-C14	-2.20	1.41	1.45
3	M	613[A]	PID	C2-C3	-2.18	1.49	1.52
3	M	613[B]	PID	C2-C3	-2.18	1.49	1.52
3	M	621	PID	CM1-C1	-2.18	1.48	1.51
2	O	601	CLA	C3B-C4B	2.16	1.49	1.42
4	N	615[A]	W4I	O1G-C1A	2.15	1.39	1.33
4	N	615[B]	W4I	O1G-C1A	2.15	1.39	1.33
4	M	615[A]	W4I	O2G-C1B	2.15	1.40	1.34
4	M	615[B]	W4I	O2G-C1B	2.15	1.40	1.34
4	N	625[A]	W4I	O4D-C4D	-2.14	1.37	1.43
4	N	625[B]	W4I	O4D-C4D	-2.14	1.37	1.43
2	O	601	CLA	C1B-C2B	2.14	1.48	1.43
2	N	602	CLA	C3B-C4B	2.14	1.49	1.42
2	O	602	CLA	C1D-ND	2.14	1.40	1.37
3	N	623[A]	PID	C9-C10	-2.13	1.44	1.48
3	O	614	PID	CM8-C29	-2.12	1.49	1.52
3	N	622	PID	C11-C12	-2.12	1.40	1.44
3	O	622	PID	O5-C29	2.12	1.47	1.43
3	M	612	PID	O2-C3	2.12	1.49	1.43
2	M	602	CLA	C3B-C4B	2.12	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	625[A]	W4I	O5D-C6D	-2.11	1.40	1.43
4	M	625[B]	W4I	O5D-C6D	-2.11	1.40	1.43
3	M	623[B]	PID	O1-C1	-2.10	1.43	1.46
3	O	623[A]	PID	C9-C10	-2.08	1.44	1.48
2	N	602	CLA	CHC-C1C	2.08	1.42	1.38
3	O	614	PID	C13-C14	-2.07	1.41	1.45
3	M	614	PID	C13-C14	-2.06	1.42	1.45
4	M	615[A]	W4I	C1D-C2D	2.05	1.58	1.52
4	M	615[B]	W4I	C1D-C2D	2.05	1.58	1.52
3	O	611	PID	C13-C14	-2.04	1.42	1.45
4	N	615[A]	W4I	C3D-C2D	2.04	1.57	1.52
4	N	615[B]	W4I	C3D-C2D	2.04	1.57	1.52
4	M	615[A]	W4I	O3G-C1D	2.03	1.43	1.40
4	M	615[B]	W4I	O3G-C1D	2.03	1.43	1.40
3	N	621	PID	C9-C10	-2.03	1.44	1.48
3	N	621	PID	C13-C14	-2.01	1.42	1.45
3	N	624	PID	C6-C7	-2.01	1.47	1.50
2	N	601	CLA	C3B-C4B	2.01	1.48	1.42
3	M	622	PID	C6-C7	-2.00	1.47	1.50

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	601	CLA	C4A-NA-C1A	8.09	110.37	106.68
2	N	602	CLA	C4A-NA-C1A	7.75	110.22	106.68
2	O	601	CLA	C4A-NA-C1A	7.26	109.99	106.68
2	M	602	CLA	C4A-NA-C1A	7.06	109.90	106.68
2	O	602	CLA	C4A-NA-C1A	5.79	109.32	106.68
2	M	601	CLA	C4A-NA-C1A	5.64	109.25	106.68
2	N	601	CLA	C3B-C4B-NB	-4.33	106.67	110.53
2	M	601	CLA	C3B-C4B-NB	-4.23	106.75	110.53
2	M	602	CLA	C3B-C4B-NB	-4.17	106.81	110.53
4	O	615[A]	W4I	O6D-C5D-C6D	3.72	115.67	106.44
4	O	615[B]	W4I	O6D-C5D-C6D	3.72	115.67	106.44
4	M	615[A]	W4I	C1D-O6D-C5D	3.66	120.86	113.72
4	M	615[B]	W4I	C1D-O6D-C5D	3.66	120.86	113.72
4	N	615[A]	W4I	O6D-C5D-C6D	3.59	115.35	106.44
4	N	615[B]	W4I	O6D-C5D-C6D	3.59	115.35	106.44
4	O	615[A]	W4I	CFB-CEB-CDB	3.53	129.40	112.02
4	O	615[B]	W4I	CFB-CEB-CDB	3.53	129.40	112.02
4	N	615[A]	W4I	CFB-CEB-CDB	3.44	128.96	112.02
4	N	615[B]	W4I	CFB-CEB-CDB	3.44	128.96	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	615[A]	W4I	CFB-CEB-CDB	3.36	128.57	112.02
4	M	615[B]	W4I	CFB-CEB-CDB	3.36	128.57	112.02
3	O	614	PID	O4-C12-C11	3.29	109.25	107.39
2	O	602	CLA	C3B-C4B-NB	-3.27	107.61	110.53
2	N	602	CLA	C3B-C4B-NB	-3.19	107.68	110.53
3	O	622	PID	C22-C23-C24	-3.07	174.03	177.66
4	M	615[A]	W4I	O6D-C5D-C6D	3.04	113.97	106.44
4	M	615[B]	W4I	O6D-C5D-C6D	3.04	113.97	106.44
3	O	623[B]	PID	C26-C25-C24	-3.04	106.26	109.21
4	N	615[A]	W4I	CBA-CAA-C9A	3.02	126.90	112.02
3	M	622	PID	O4-C12-C11	3.01	109.10	107.39
2	O	601	CLA	C3B-C4B-NB	-2.99	107.86	110.53
4	O	615[A]	W4I	C3G-O3G-C1D	2.82	119.84	113.80
4	O	615[B]	W4I	C3G-O3G-C1D	2.82	119.84	113.80
3	M	624	PID	O4-C12-C11	2.80	108.97	107.39
3	O	613[A]	PID	C27-O6-C30	2.80	122.78	117.85
3	O	623[A]	PID	O3-C10-C9	2.77	133.92	131.04
3	M	614	PID	C22-C23-C24	-2.74	174.43	177.66
3	O	614	PID	C22-C23-C24	-2.74	174.43	177.66
4	N	615[A]	W4I	O3G-C3G-C2G	2.73	117.47	110.82
4	N	615[B]	W4I	O3G-C3G-C2G	2.73	117.47	110.82
3	O	621	PID	O4-C12-C11	2.73	108.94	107.39
3	M	612	PID	CM7-C25-C24	2.71	112.90	110.47
3	O	623[A]	PID	C12-O4-C10	2.70	108.99	107.68
3	N	622	PID	O4-C12-C11	2.59	108.86	107.39
4	N	615[A]	W4I	O2G-C1B-C2B	2.58	117.07	111.48
4	N	615[B]	W4I	O2G-C1B-C2B	2.58	117.07	111.48
3	O	623[A]	PID	CM2-C5-C4	-2.57	104.45	108.97
3	O	623[B]	PID	CM7-C25-C24	2.52	112.73	110.47
3	N	622	PID	CM7-C25-C24	2.49	112.70	110.47
3	M	624	PID	C12-O4-C10	-2.48	106.47	107.68
2	M	601	CLA	CHD-C1D-ND	-2.47	121.33	124.80
3	N	613[A]	PID	C27-O6-C30	2.44	122.16	117.85
4	N	615[A]	W4I	C1D-O6D-C5D	2.44	118.48	113.72
4	N	615[B]	W4I	C1D-O6D-C5D	2.44	118.48	113.72
4	M	615[A]	W4I	C3G-O3G-C1D	2.43	119.01	113.80
4	M	615[B]	W4I	C3G-O3G-C1D	2.43	119.01	113.80
3	M	613[A]	PID	O4-C12-C11	2.43	108.77	107.39
3	M	613[B]	PID	O4-C12-C11	2.43	108.77	107.39
3	M	614	PID	C26-C25-C24	-2.41	106.87	109.21
3	O	612	PID	O4-C12-C11	2.41	108.75	107.39
3	N	621	PID	C22-C23-C24	-2.40	174.83	177.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	623[B]	PID	O4-C12-C11	2.40	108.75	107.39
3	M	622	PID	C26-C25-C24	-2.39	106.89	109.21
3	O	623[A]	PID	C22-C23-C24	-2.38	174.86	177.66
3	O	611	PID	C4-C3-C2	2.37	115.22	110.79
4	O	615[A]	W4I	O2G-C2G-C1G	-2.37	99.86	108.34
4	O	615[B]	W4I	O2G-C2G-C1G	-2.37	99.86	108.34
4	M	615[B]	W4I	CBA-CAA-C9A	2.34	123.57	112.02
3	N	612	PID	O4-C12-C11	2.34	108.72	107.39
3	N	612	PID	CM7-C25-C24	2.34	112.57	110.47
3	O	622	PID	O4-C12-C11	2.34	108.71	107.39
3	N	623[A]	PID	C22-C23-C24	-2.32	174.92	177.66
3	M	621	PID	CM7-C25-C24	2.32	112.55	110.47
3	M	621	PID	C22-C23-C24	-2.32	174.93	177.66
3	M	623[B]	PID	CM7-C25-C24	2.31	112.54	110.47
2	O	602	CLA	CHA-C1A-NA	-2.29	121.20	126.39
4	O	615[A]	W4I	CBA-CAA-C9A	2.26	123.17	112.02
3	O	612	PID	C29-C24-C25	-2.26	117.45	119.70
4	O	625[A]	W4I	O1G-C1A-O1A	-2.26	117.98	123.63
4	O	625[B]	W4I	O1G-C1A-O1A	-2.26	117.98	123.63
4	N	625[A]	W4I	O1G-C1A-O1A	-2.26	117.98	123.63
4	N	625[B]	W4I	O1G-C1A-O1A	-2.26	117.98	123.63
2	N	602	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
3	M	622	PID	C22-C23-C24	-2.25	175.01	177.66
4	M	615[A]	W4I	O3G-C3G-C2G	2.25	116.28	110.82
4	M	615[B]	W4I	O3G-C3G-C2G	2.25	116.28	110.82
2	N	602	CLA	CHD-C1D-ND	-2.24	121.65	124.80
4	N	615[A]	W4I	C3G-O3G-C1D	2.23	118.58	113.80
4	N	615[B]	W4I	C3G-O3G-C1D	2.23	118.58	113.80
2	N	601	CLA	CHB-C4A-NA	2.23	127.62	124.40
3	N	622	PID	C4-C3-C2	2.22	114.94	110.79
3	N	611	PID	C8-C9-C10	2.21	127.94	123.60
4	M	615[A]	W4I	O2G-C1B-C2B	2.20	116.23	111.48
4	M	615[B]	W4I	O2G-C1B-C2B	2.20	116.23	111.48
4	N	615[B]	W4I	CBA-CAA-C9A	2.17	122.73	112.02
3	N	622	PID	C22-C23-C24	-2.16	175.11	177.66
3	O	612	PID	C22-C23-C24	-2.14	175.13	177.66
2	N	602	CLA	CHB-C4A-NA	2.14	127.49	124.40
4	M	615[A]	W4I	CBA-CAA-C9A	2.14	122.57	112.02
3	O	623[A]	PID	C7-C8-C9	2.14	128.75	126.06
3	N	614	PID	C22-C23-C24	-2.13	175.15	177.66
2	M	601	CLA	CAC-C3C-C4C	2.13	127.56	124.79
3	O	623[A]	PID	C29-C24-C25	-2.12	117.59	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	625[A]	W4I	C4E-C3E-C2E	-2.12	107.11	110.83
4	N	625[B]	W4I	C4E-C3E-C2E	-2.12	107.11	110.83
2	O	602	CLA	C4-C3-C5	2.11	118.89	115.23
3	M	622	PID	C4-C3-C2	2.11	114.73	110.79
3	N	623[B]	PID	O4-C12-C11	2.10	108.58	107.39
3	N	613[A]	PID	C12-O4-C10	2.10	108.70	107.68
3	N	613[B]	PID	C12-O4-C10	2.10	108.70	107.68
2	O	602	CLA	C4D-CHA-C1A	2.09	123.74	121.24
3	O	614	PID	C28-C27-C26	2.09	113.64	109.89
3	M	623[B]	PID	CM6-C25-C24	-2.07	108.61	110.47
3	M	623[B]	PID	C22-C23-C24	-2.06	175.23	177.66
2	N	601	CLA	CHD-C1D-ND	-2.06	121.91	124.80
3	M	623[A]	PID	O3-C10-C9	2.05	133.18	131.04
2	O	602	CLA	CHD-C1D-ND	-2.04	121.93	124.80
2	N	601	CLA	C1C-C2C-C3C	-2.03	104.84	106.98
4	N	625[A]	W4I	O6D-C1D-O3G	-2.03	105.24	110.04
4	N	625[B]	W4I	O6D-C1D-O3G	-2.03	105.24	110.04
3	N	624	PID	C29-C24-C25	-2.01	117.70	119.70
4	N	625[A]	W4I	C3D-C4D-C5D	-2.01	106.59	110.23
4	N	625[B]	W4I	C3D-C4D-C5D	-2.01	106.59	110.23
4	O	615[B]	W4I	CBA-CAA-C9A	2.00	121.87	112.02

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	M	602	CLA	ND
2	N	601	CLA	ND
2	N	602	CLA	ND
2	O	602	CLA	ND
3	M	613[A]	PID	C6
3	M	613[B]	PID	C6
3	O	623[B]	PID	C6

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	625[A]	W4I	CFA-CGA-CHA-CIA
5	N	651	PG4	O3-C5-C6-O4
4	M	615[A]	W4I	C2B-C3B-C4B-C5B
4	M	615[B]	W4I	C2B-C3B-C4B-C5B
5	N	651	PG4	O2-C3-C4-O3
4	N	615[A]	W4I	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
4	N	615[B]	W4I	C4D-C5D-C6D-O5D
5	M	651	PG4	O3-C5-C6-O4
5	O	651	PG4	O3-C5-C6-O4
5	M	651	PG4	O2-C3-C4-O3
5	O	651	PG4	O2-C3-C4-O3
4	N	615[A]	W4I	O6D-C5D-C6D-O5D
4	N	615[B]	W4I	O6D-C5D-C6D-O5D
4	O	615[A]	W4I	C1B-C2B-C3B-C4B
4	O	615[B]	W4I	C1B-C2B-C3B-C4B
5	O	651	PG4	O4-C7-C8-O5
4	N	615[A]	W4I	C1G-C2G-C3G-O3G
4	N	615[B]	W4I	C1G-C2G-C3G-O3G
4	N	615[A]	W4I	CHA-CIA-CJA-CKA
4	N	615[B]	W4I	CHA-CIA-CJA-CKA
4	N	615[A]	W4I	C2A-C3A-C4A-C5A
4	N	615[B]	W4I	C2A-C3A-C4A-C5A
4	O	615[A]	W4I	O6D-C5D-C6D-O5D
4	O	615[B]	W4I	O6D-C5D-C6D-O5D
4	M	615[A]	W4I	O2G-C2G-C3G-O3G
4	M	615[B]	W4I	O2G-C2G-C3G-O3G
4	N	615[A]	W4I	O2G-C2G-C3G-O3G
4	N	615[B]	W4I	O2G-C2G-C3G-O3G
4	M	615[A]	W4I	C1G-C2G-C3G-O3G
4	M	615[B]	W4I	C1G-C2G-C3G-O3G
4	M	615[A]	W4I	CEA-CFA-CGA-CHA
4	M	615[A]	W4I	CFA-CGA-CHA-CIA
4	M	615[B]	W4I	C5A-C6A-C7A-C8A
4	M	615[B]	W4I	C6A-C7A-C8A-C9A
4	M	615[B]	W4I	C8A-C9A-CAA-CBA
4	M	615[B]	W4I	CBA-CCA-CDA-CEA
4	M	615[B]	W4I	CEA-CFA-CGA-CHA
4	M	615[B]	W4I	CFA-CGA-CHA-CIA
4	M	625[A]	W4I	CFA-CGA-CHA-CIA
4	N	615[A]	W4I	CBA-CCA-CDA-CEA
4	N	615[A]	W4I	CFA-CGA-CHA-CIA
4	N	615[B]	W4I	C6A-C7A-C8A-C9A
4	N	615[B]	W4I	CFA-CGA-CHA-CIA
4	N	625[A]	W4I	C9A-CAA-CBA-CCA
4	N	625[A]	W4I	CFA-CGA-CHA-CIA
4	N	625[B]	W4I	C9A-CAA-CBA-CCA
4	O	615[A]	W4I	CBA-CCA-CDA-CEA
4	O	615[A]	W4I	CFA-CGA-CHA-CIA

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Mol	Chain	Res	Type	Atoms
4	O	615[B]	W4I	C5A-C6A-C7A-C8A
4	O	615[B]	W4I	CBA-CCA-CDA-CEA
4	O	615[B]	W4I	CFA-CGA-CHA-CIA
4	O	625[A]	W4I	C9A-CAA-CBA-CCA
4	O	625[A]	W4I	CBA-CCA-CDA-CEA
4	O	625[A]	W4I	CCB-CDB-CEB-CFB
4	O	625[B]	W4I	C9A-CAA-CBA-CCA
4	O	625[B]	W4I	CCB-CDB-CEB-CFB
4	O	615[A]	W4I	C2D-C1D-O3G-C3G
4	O	615[B]	W4I	C2D-C1D-O3G-C3G
4	M	615[A]	W4I	CHA-CIA-CJA-CKA
4	M	615[B]	W4I	CHA-CIA-CJA-CKA
4	M	625[A]	W4I	C2G-C3G-O3G-C1D
4	M	625[B]	W4I	C2G-C3G-O3G-C1D
4	N	625[A]	W4I	C2G-C3G-O3G-C1D
4	N	625[B]	W4I	C2G-C3G-O3G-C1D
4	O	625[A]	W4I	C2G-C3G-O3G-C1D
4	O	625[B]	W4I	C2G-C3G-O3G-C1D
4	N	615[A]	W4I	C1A-C2A-C3A-C4A
4	N	615[B]	W4I	C1A-C2A-C3A-C4A
4	M	615[A]	W4I	C1B-C2B-C3B-C4B
4	M	615[B]	W4I	C1B-C2B-C3B-C4B
4	M	615[A]	W4I	C4B-C5B-C6B-C7B
4	M	615[B]	W4I	C4B-C5B-C6B-C7B
2	M	602	CLA	CHA-CBD-CGD-O1D
5	O	651	PG4	C5-C6-O4-C7
4	O	615[A]	W4I	CHA-CIA-CJA-CKA
4	O	615[B]	W4I	CHA-CIA-CJA-CKA
4	N	615[A]	W4I	C2A-C1A-O1G-C1G
4	N	615[B]	W4I	C2A-C1A-O1G-C1G
4	N	615[B]	W4I	C3A-C4A-C5A-C6A
4	O	615[B]	W4I	C3A-C4A-C5A-C6A
4	M	615[A]	W4I	CBA-CCA-CDA-CEA
4	M	625[A]	W4I	C9A-CAA-CBA-CCA
4	M	625[A]	W4I	CBA-CCA-CDA-CEA
4	M	625[A]	W4I	C9B-CAB-CBB-CCB
4	M	625[A]	W4I	CCB-CDB-CEB-CFB
4	M	625[B]	W4I	C9A-CAA-CBA-CCA
4	M	625[B]	W4I	C9B-CAB-CBB-CCB
4	M	625[B]	W4I	CCB-CDB-CEB-CFB
4	N	615[A]	W4I	CEA-CFA-CGA-CHA
4	N	615[A]	W4I	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
4	N	615[B]	W4I	C5A-C6A-C7A-C8A
4	N	615[B]	W4I	CEA-CFA-CGA-CHA
4	N	615[B]	W4I	CAB-CBB-CCB-CDB
4	N	625[A]	W4I	CBA-CCA-CDA-CEA
4	N	625[A]	W4I	CCB-CDB-CEB-CFB
4	N	625[B]	W4I	CCB-CDB-CEB-CFB
4	O	615[A]	W4I	CEA-CFA-CGA-CHA
4	O	615[B]	W4I	CEA-CFA-CGA-CHA
4	O	625[A]	W4I	C9B-CAB-CBB-CCB
4	O	625[B]	W4I	C9B-CAB-CBB-CCB
4	N	615[A]	W4I	O1A-C1A-O1G-C1G
4	N	615[B]	W4I	O1A-C1A-O1G-C1G
4	M	615[B]	W4I	C3A-C4A-C5A-C6A
4	N	615[A]	W4I	C3A-C4A-C5A-C6A
4	M	615[A]	W4I	O2G-C1B-C2B-C3B
4	M	615[B]	W4I	O2G-C1B-C2B-C3B
4	O	615[A]	W4I	C3A-C4A-C5A-C6A
4	N	615[A]	W4I	O1G-C1G-C2G-O2G
4	N	615[B]	W4I	O1G-C1G-C2G-O2G
4	N	615[A]	W4I	CFB-CGB-CHB-CIB
4	N	615[B]	W4I	CFB-CGB-CHB-CIB
4	M	615[A]	W4I	C3A-C4A-C5A-C6A
5	M	651	PG4	C5-C6-O4-C7

There are no ring outliers.

15 monomers are involved in 19 short contacts:

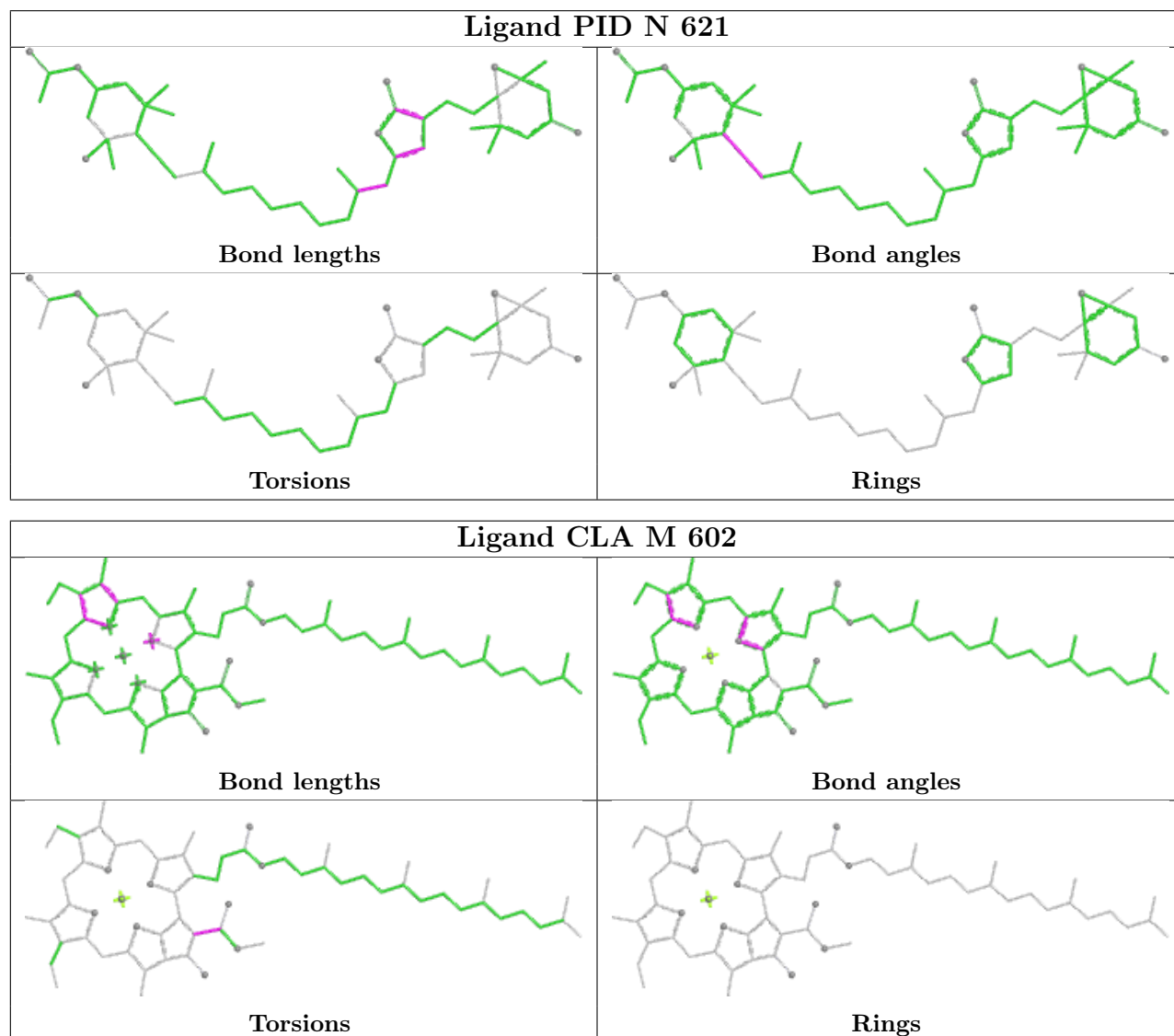
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	624	PID	2	0
3	O	611	PID	1	0
3	N	623[B]	PID	1	0
3	M	624	PID	2	0
3	N	623[A]	PID	2	0
2	N	602	CLA	1	0
3	N	614	PID	1	0
3	O	624	PID	2	0
3	M	613[B]	PID	2	0
3	M	623[A]	PID	2	0
3	O	621	PID	1	0
3	M	614	PID	1	0
3	O	614	PID	1	0
3	O	623[B]	PID	3	0

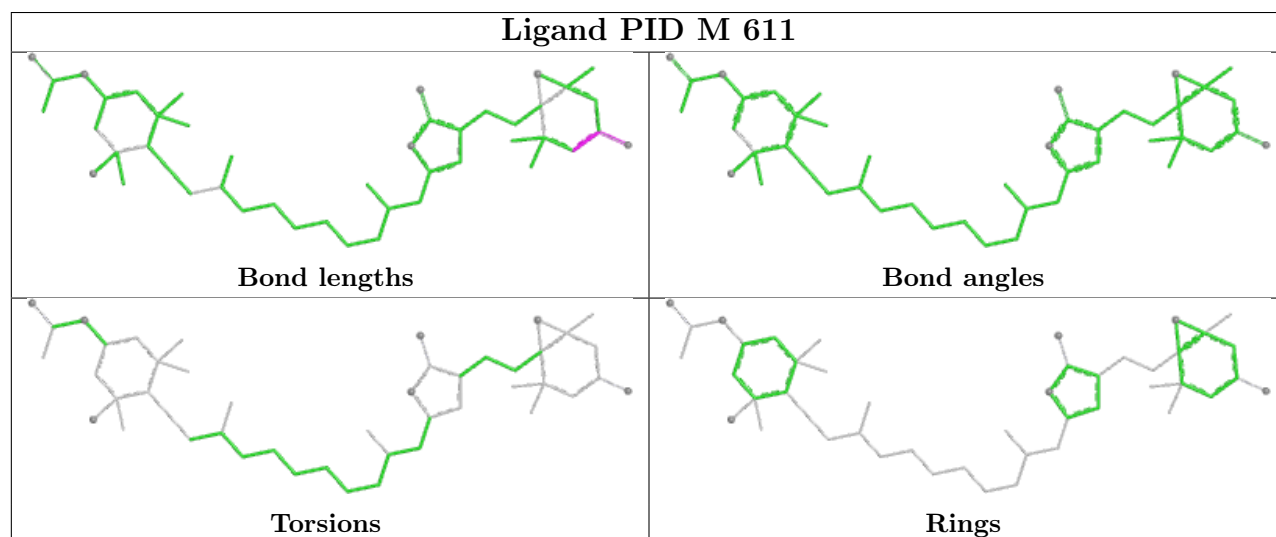
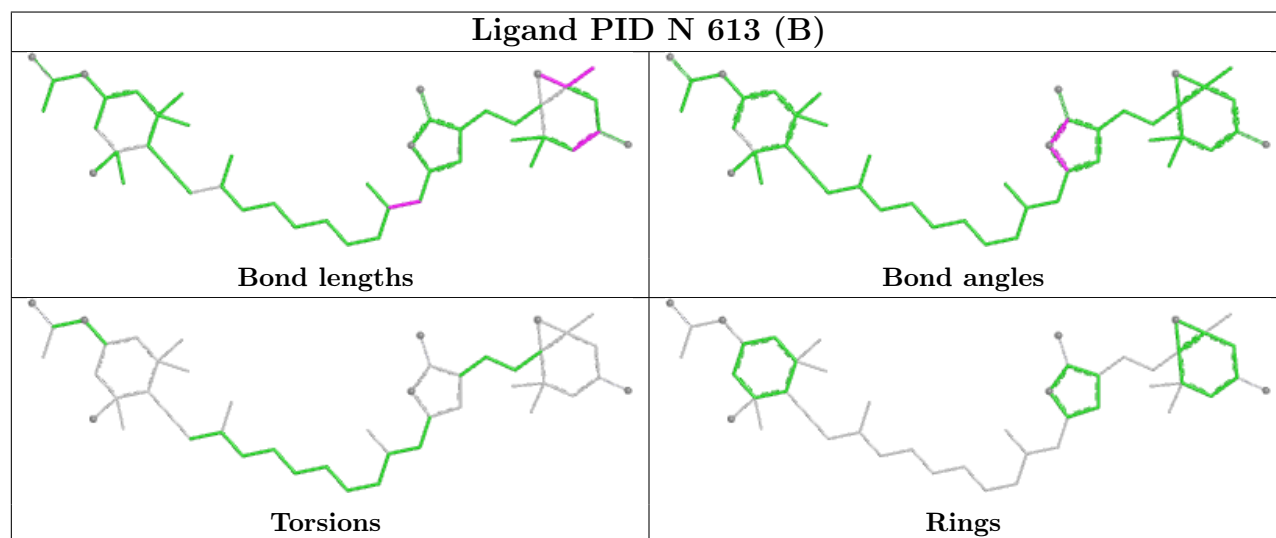
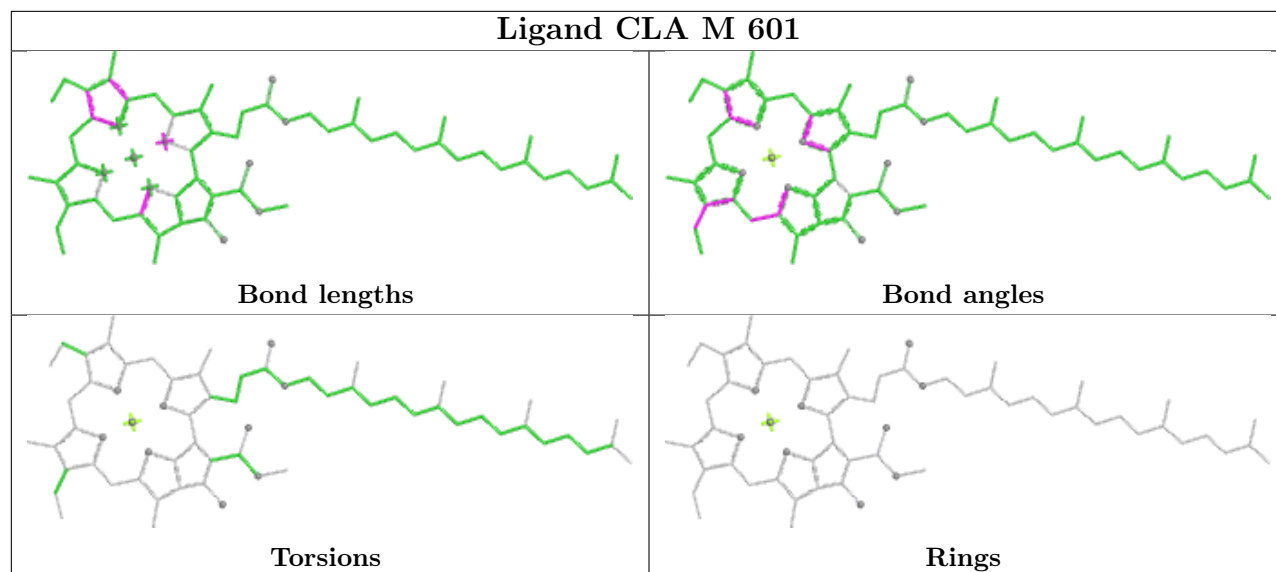
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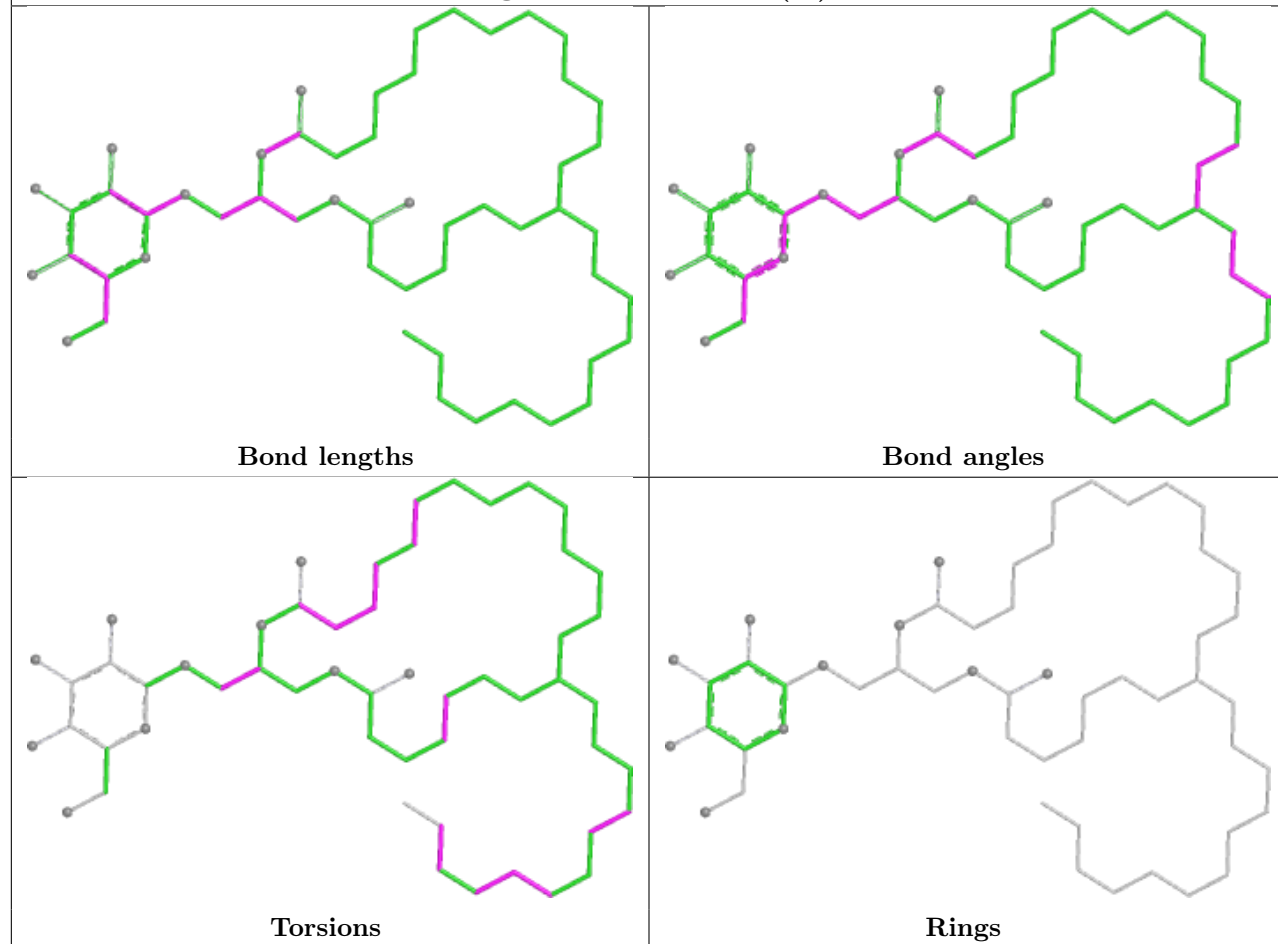
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	613[B]	PID	3	0

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

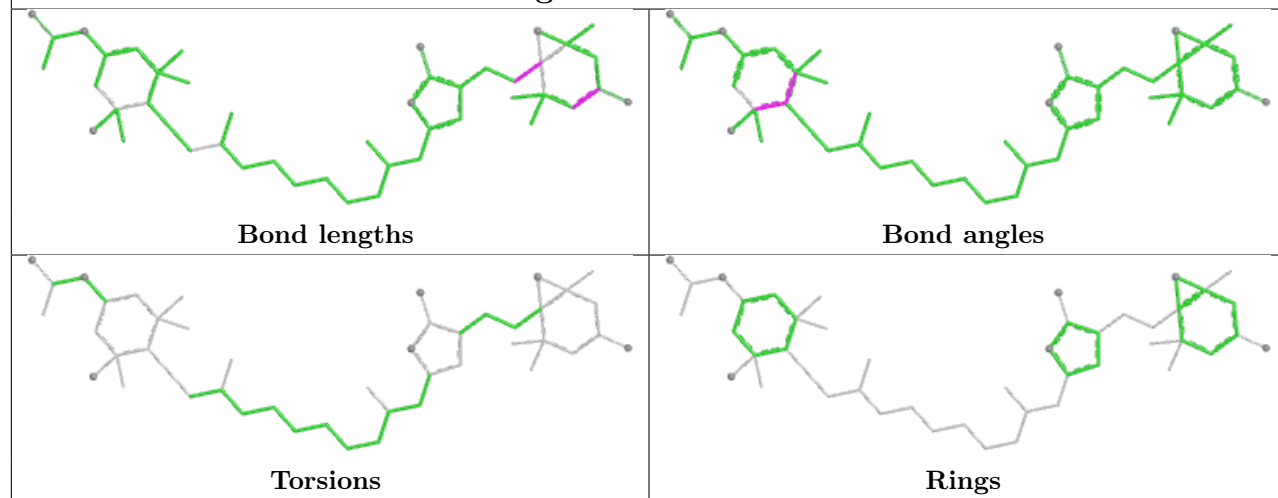




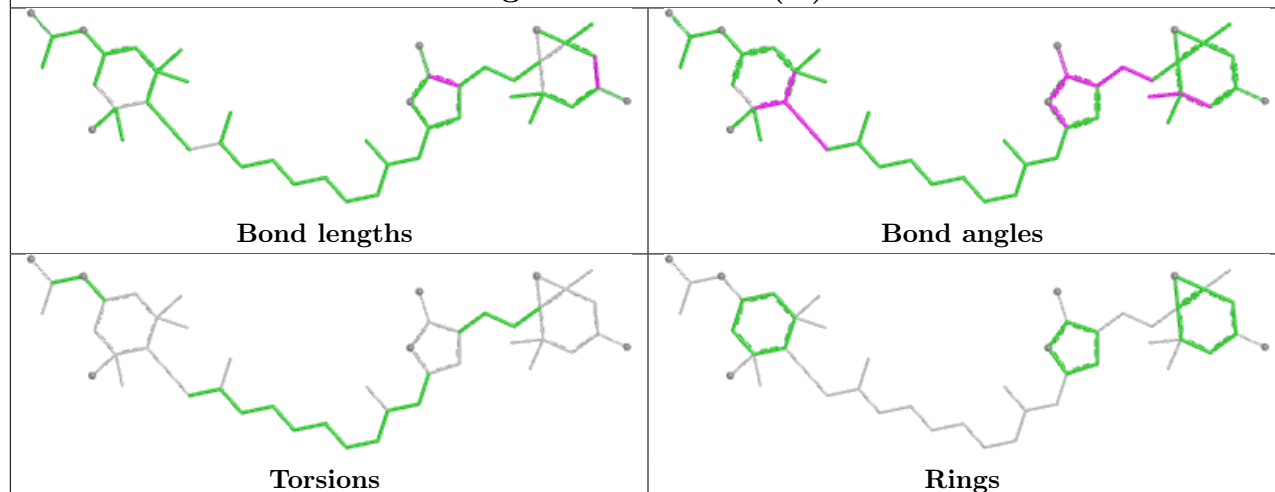
Ligand W4I M 615 (A)



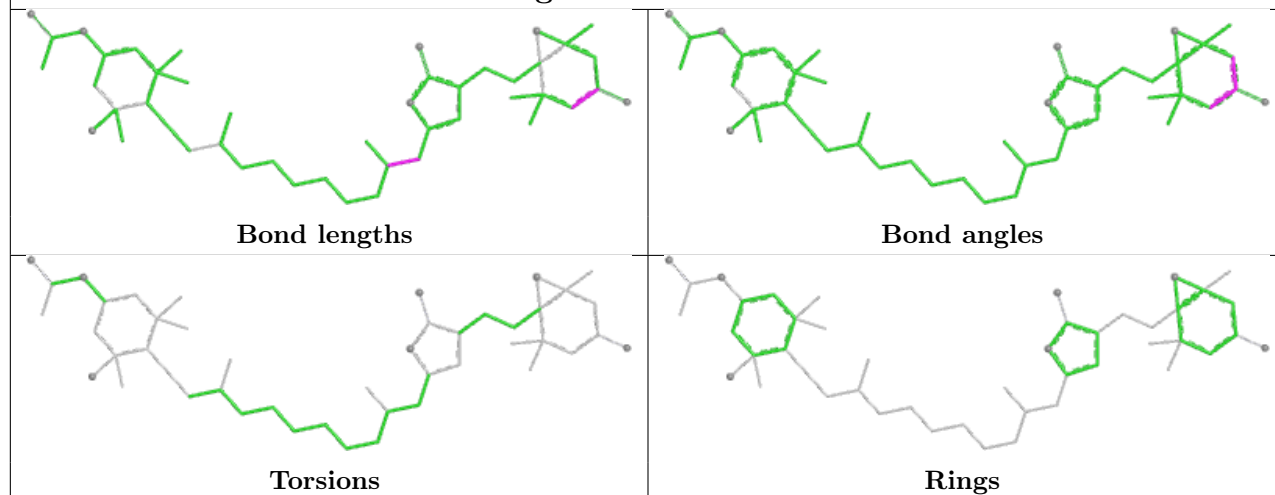
Ligand PID N 624



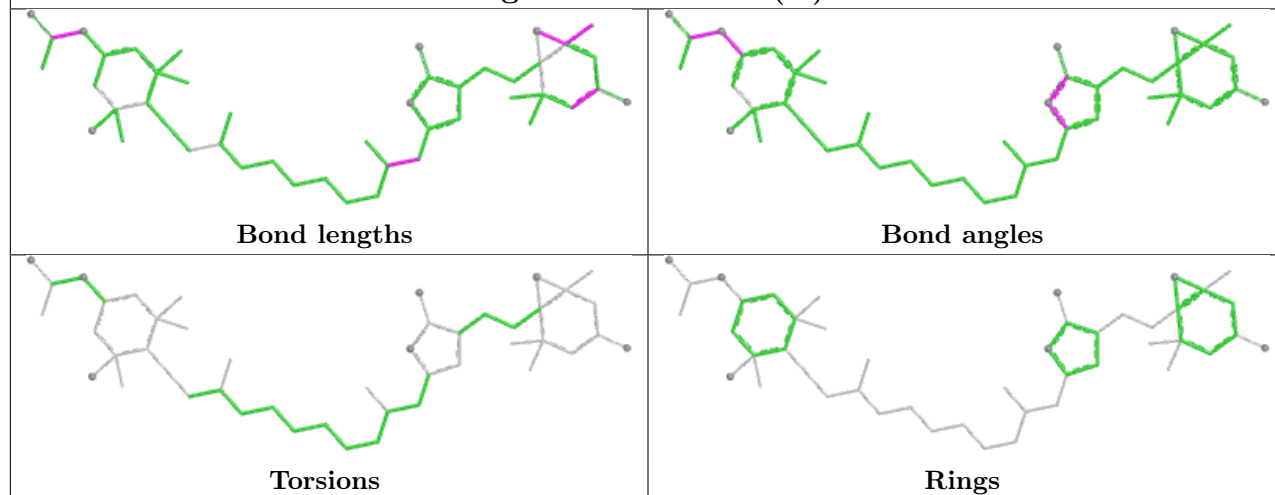
Ligand PID O 623 (A)

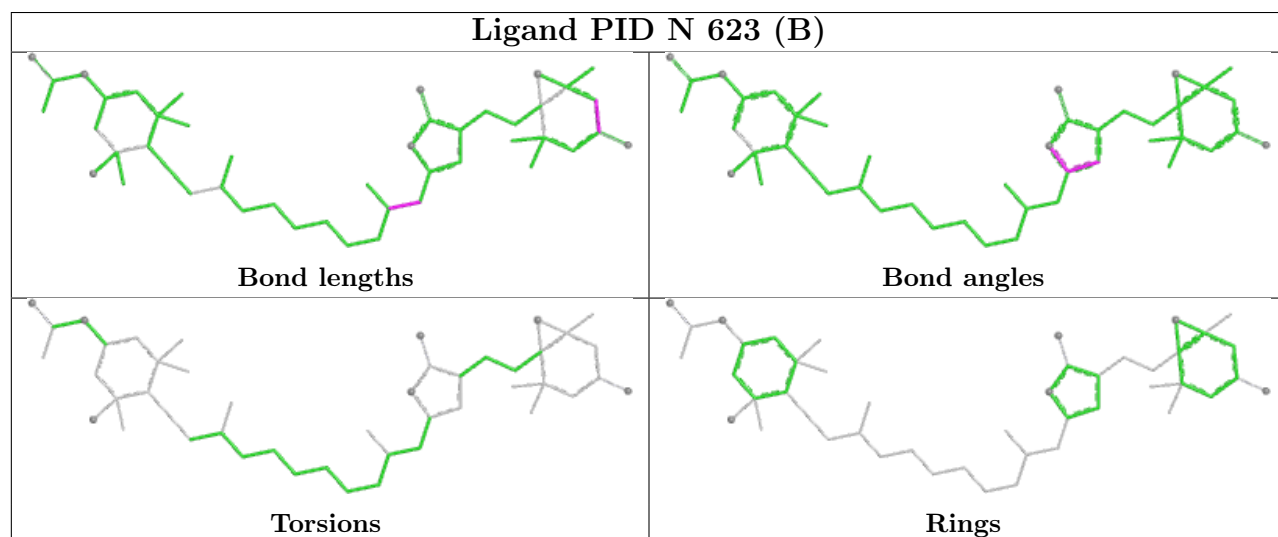
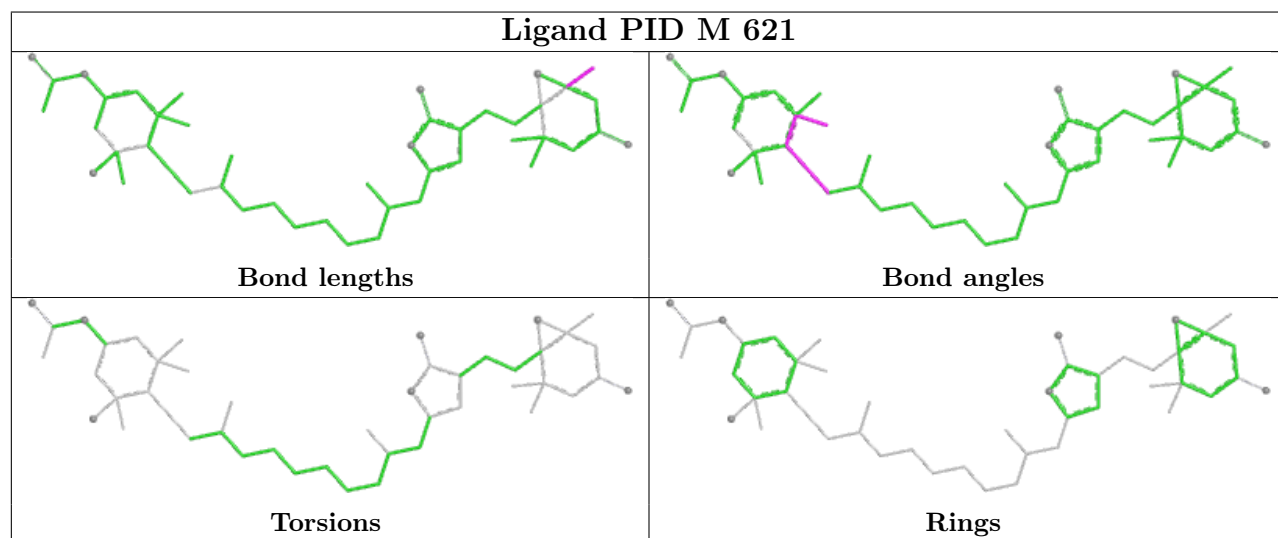
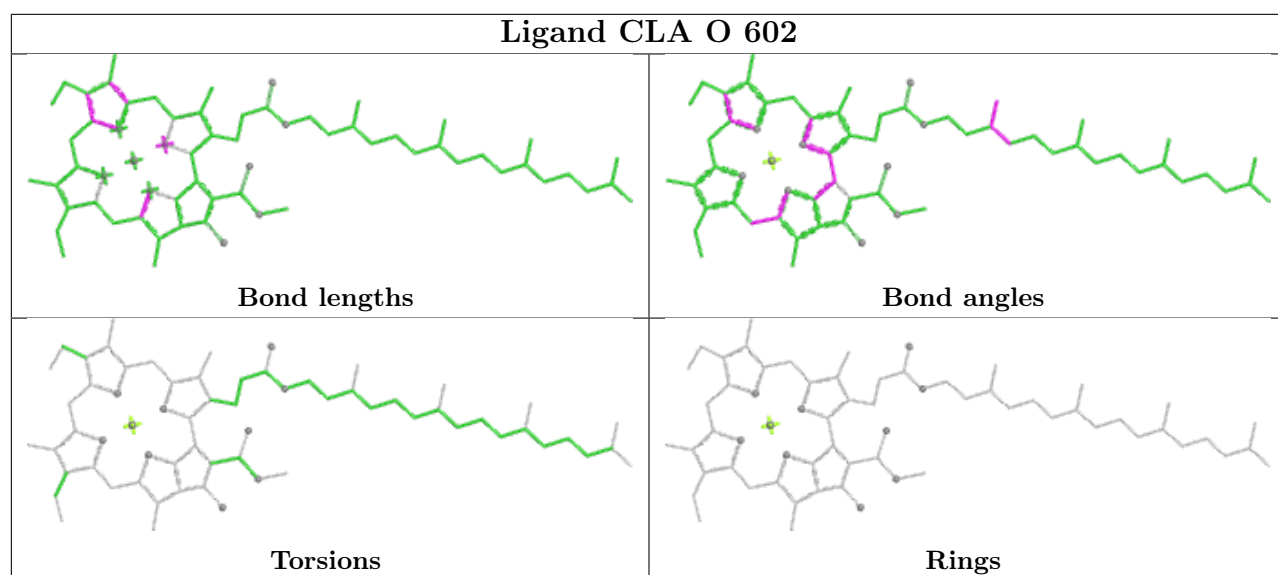


Ligand PID O 611

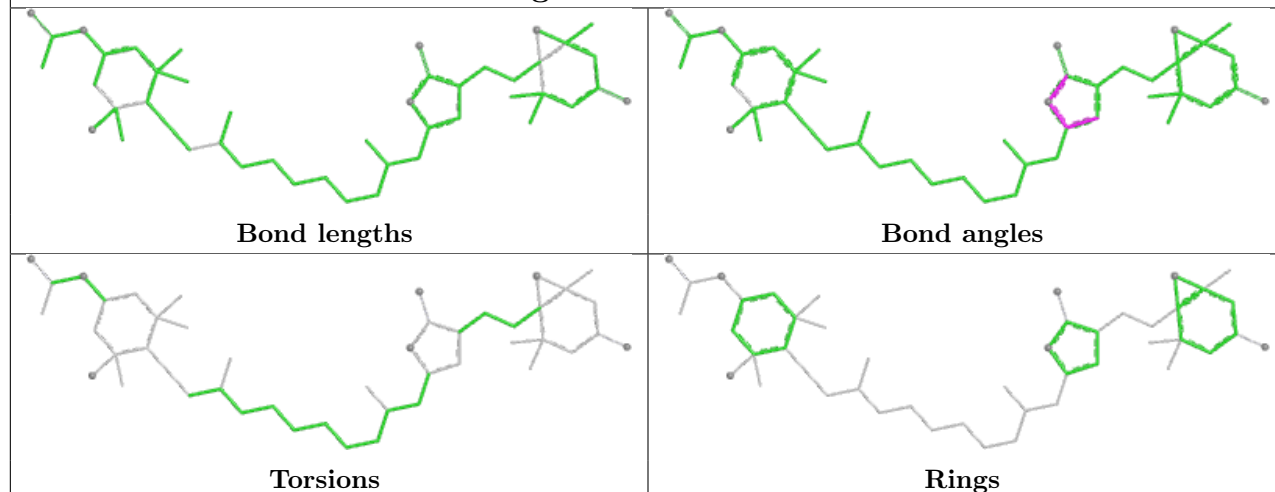


Ligand PID N 613 (A)

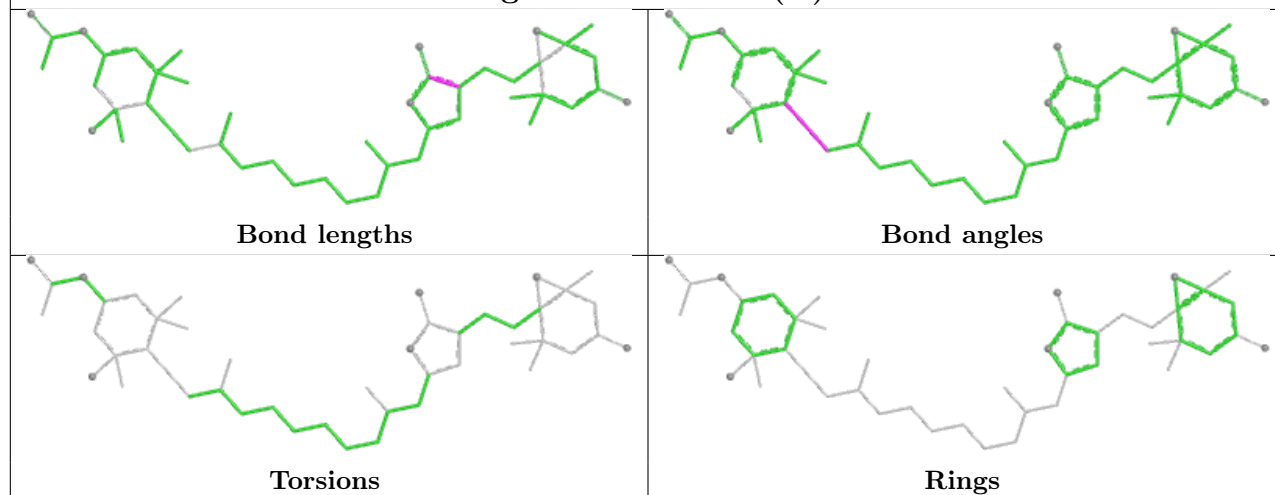




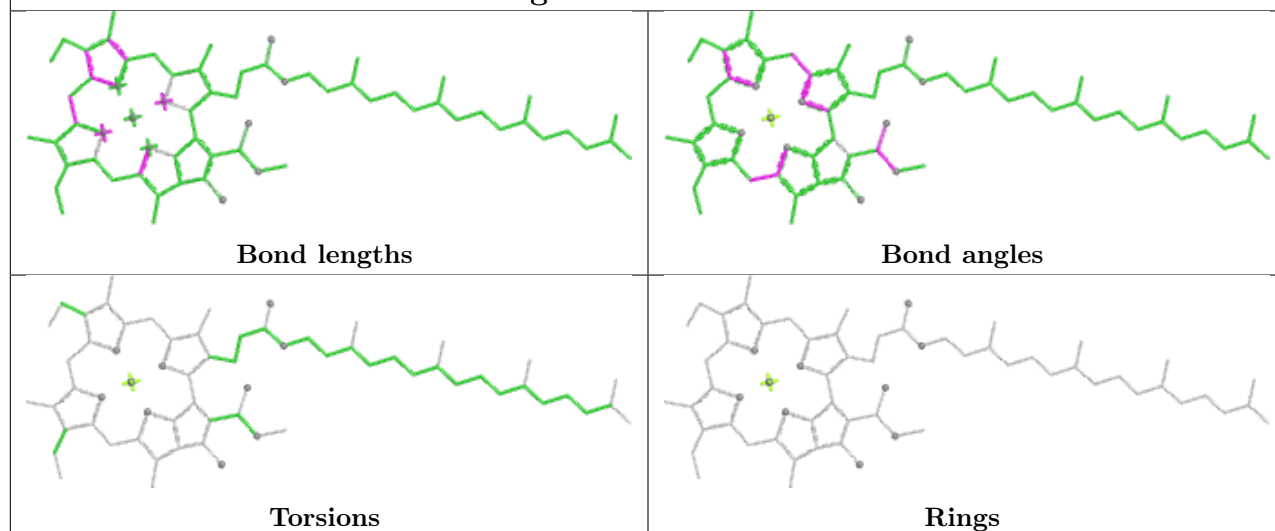
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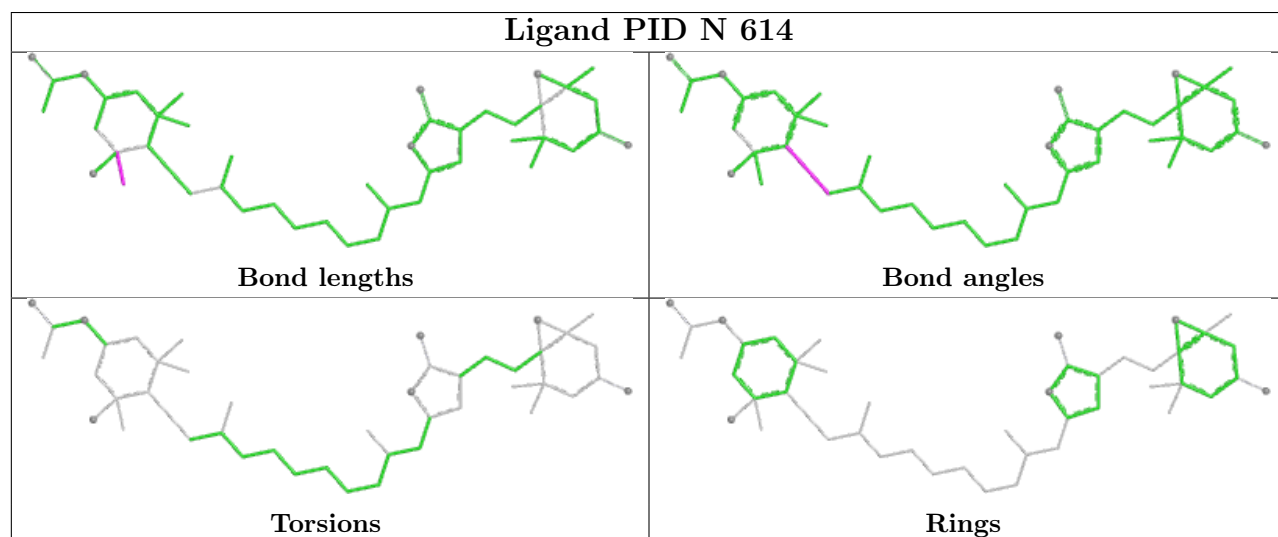
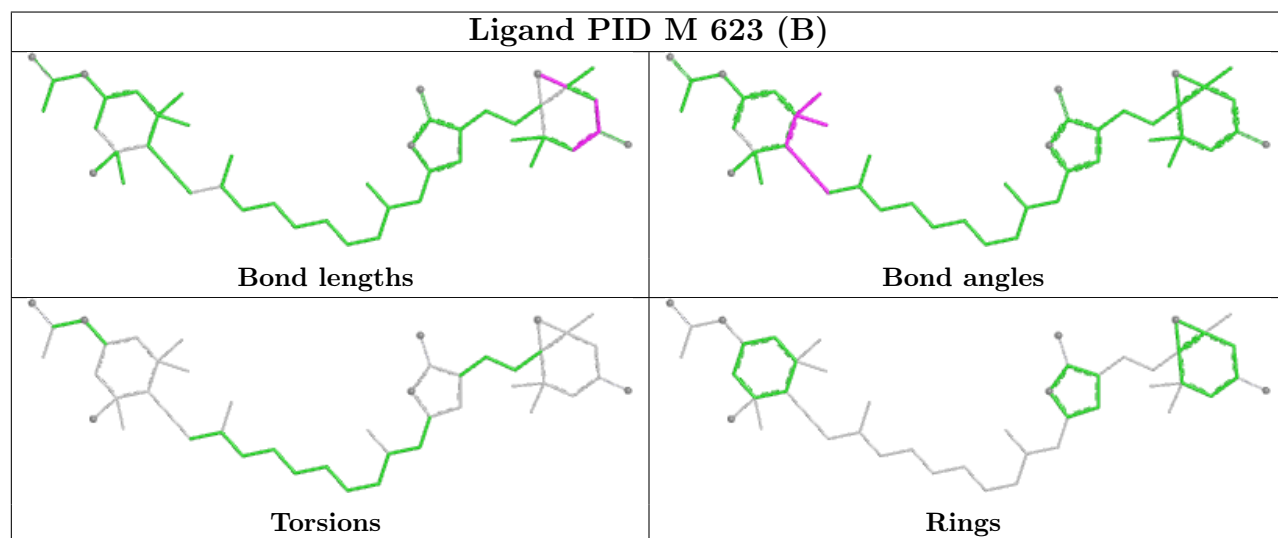
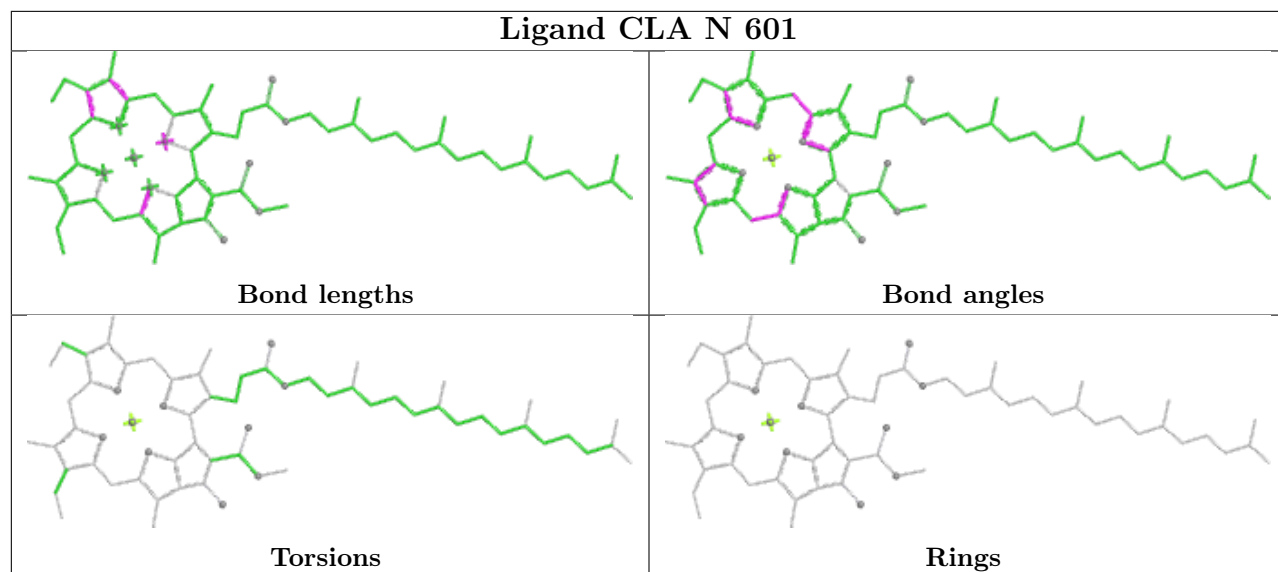


Ligand PID N 623 (A)

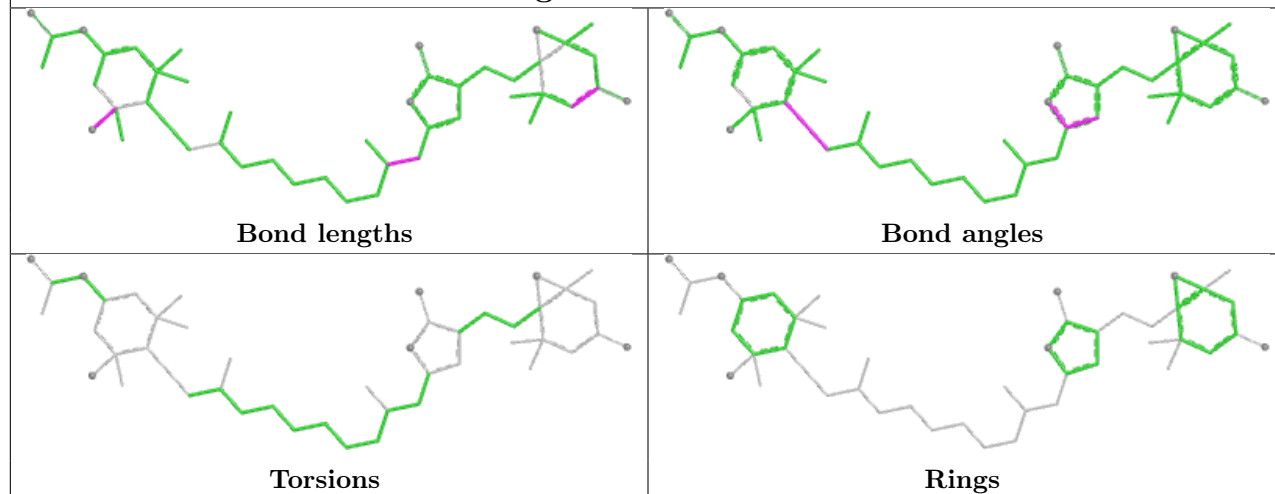


Ligand CLA N 602

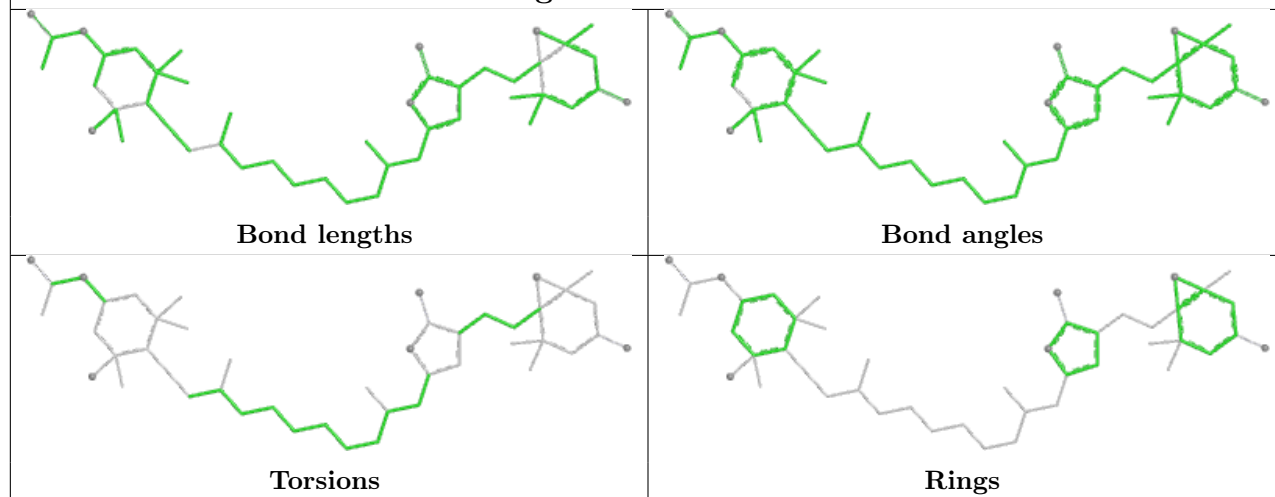


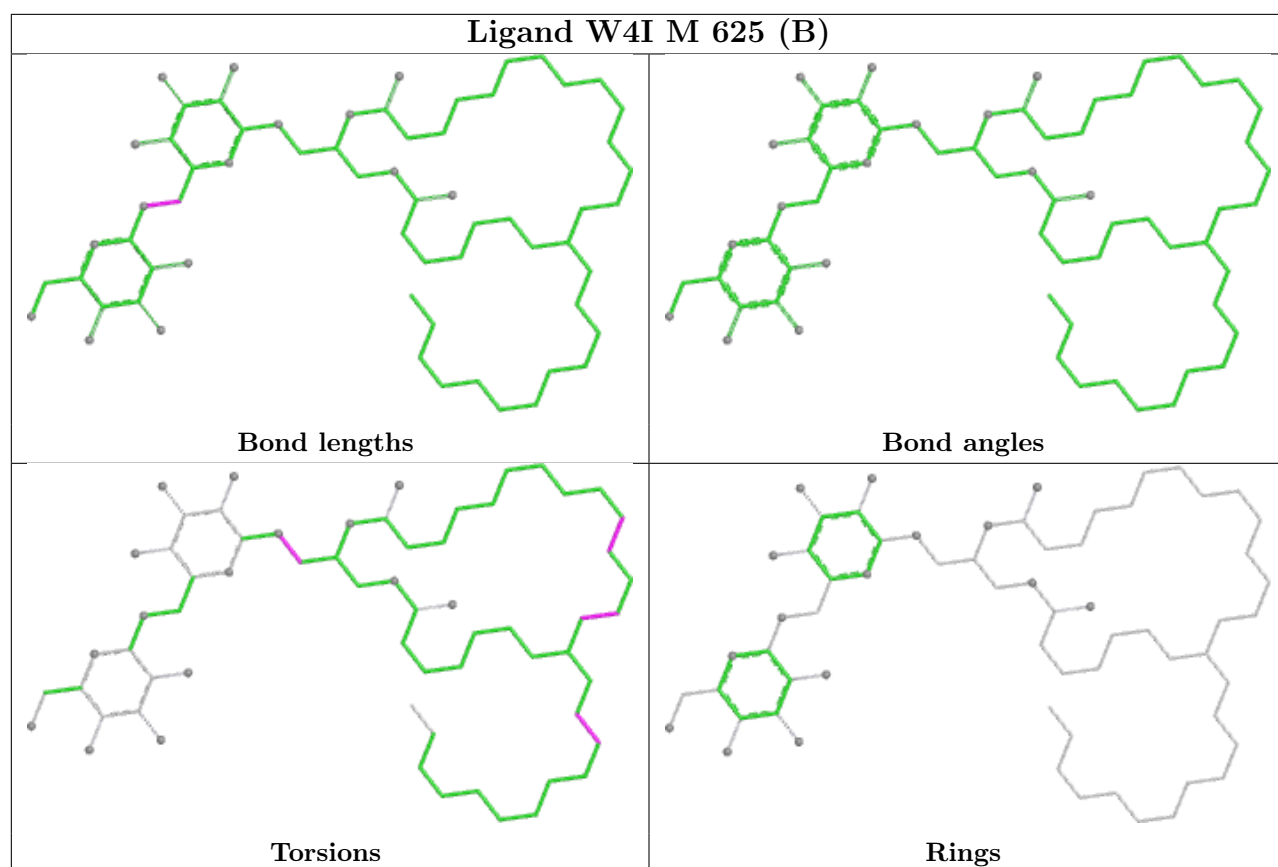


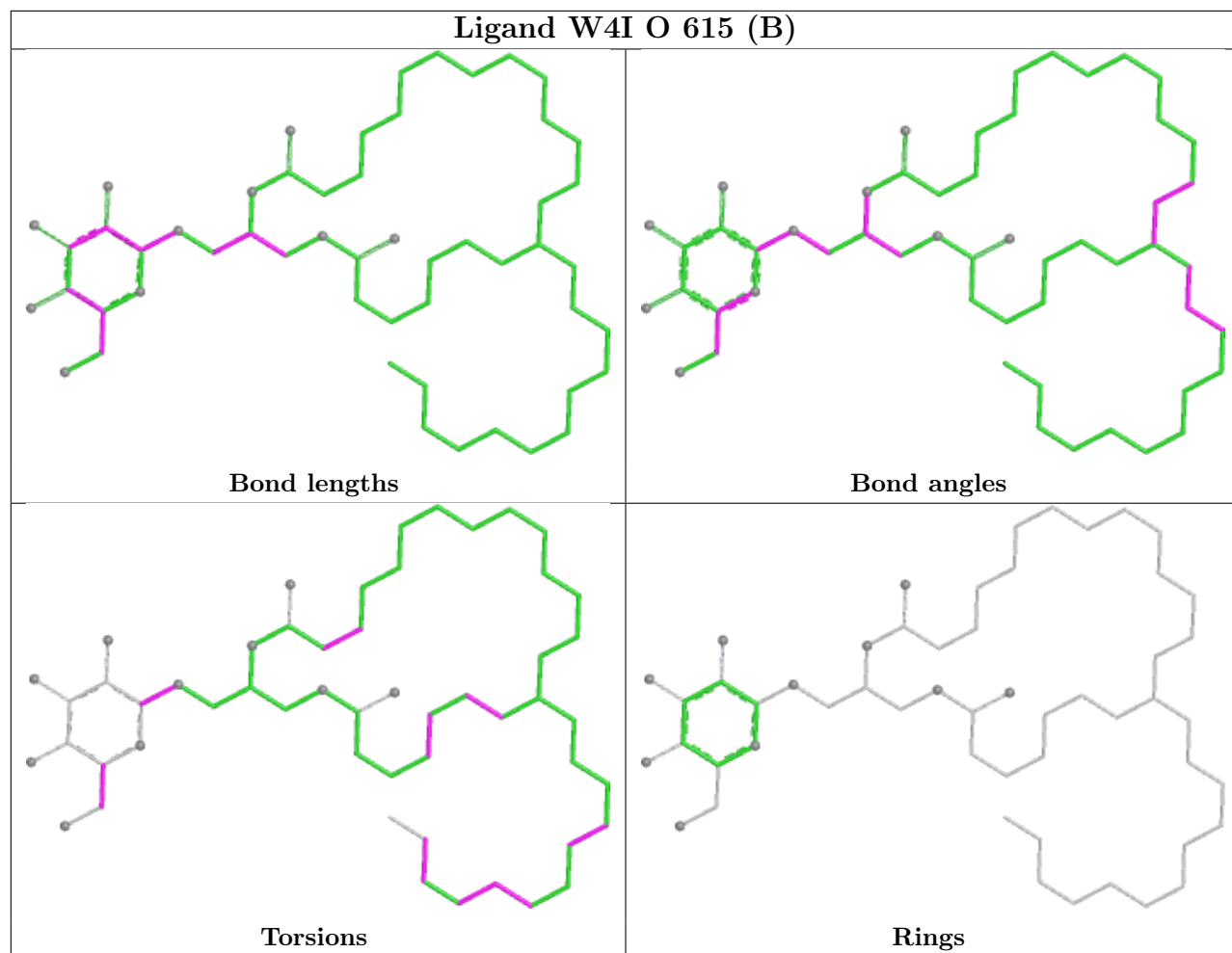
Ligand PID O 622



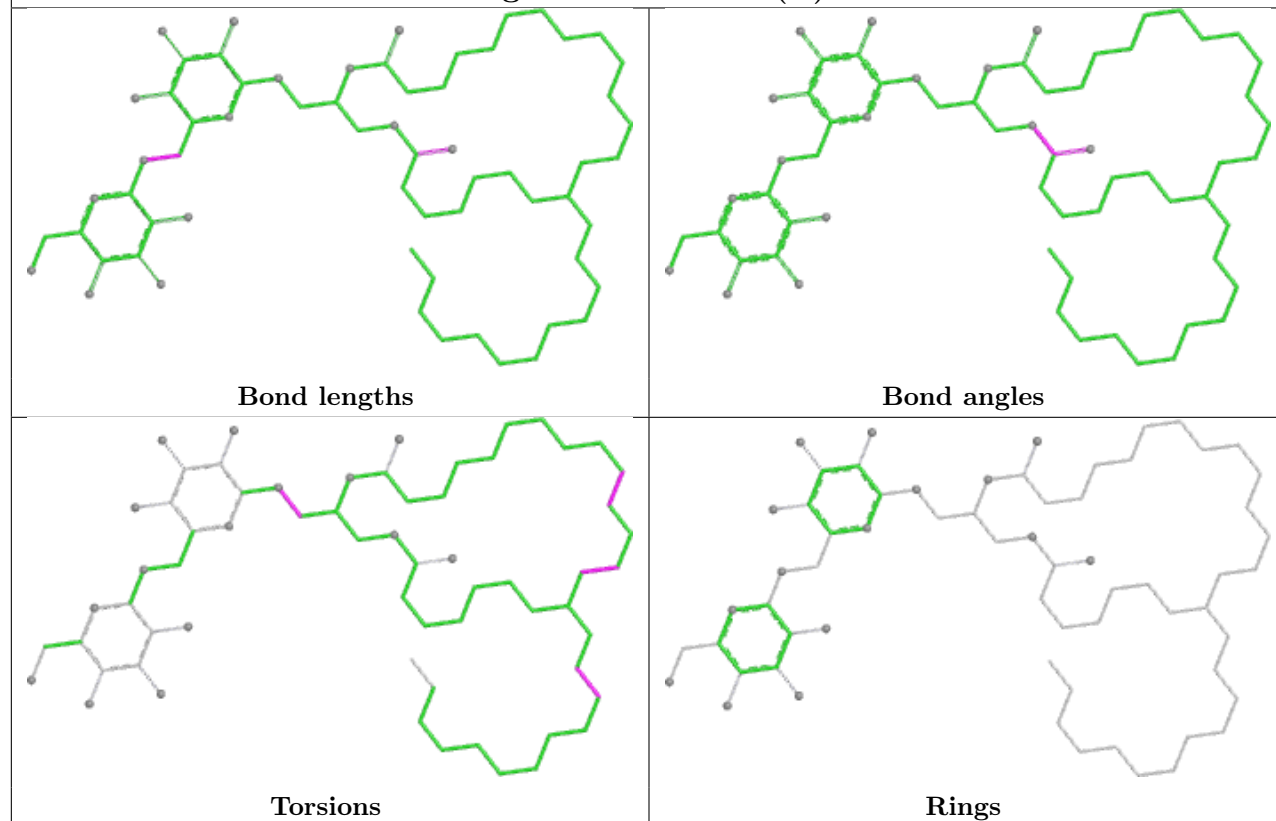
Ligand PID O 624



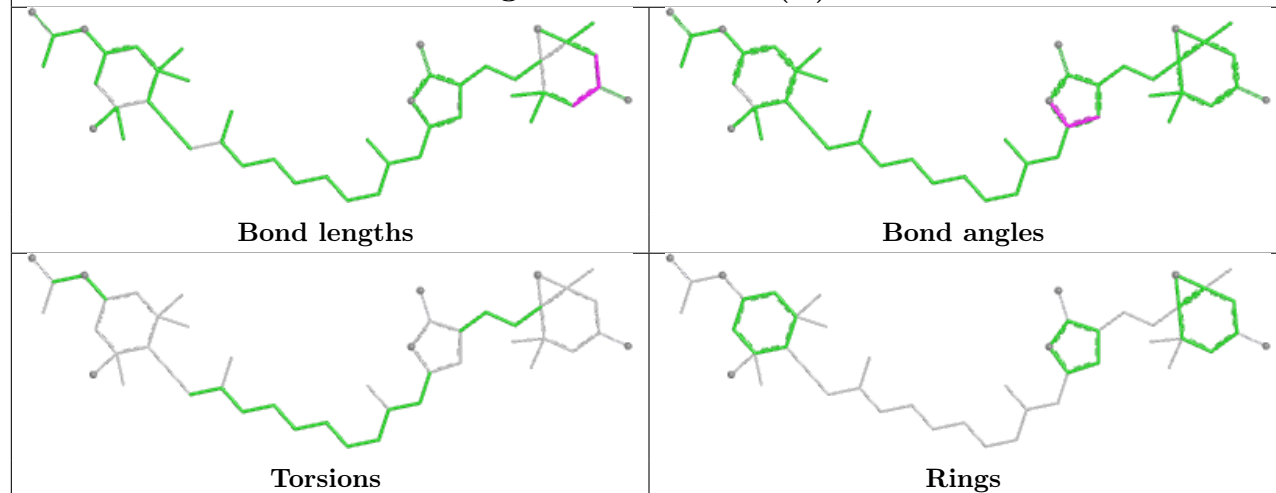




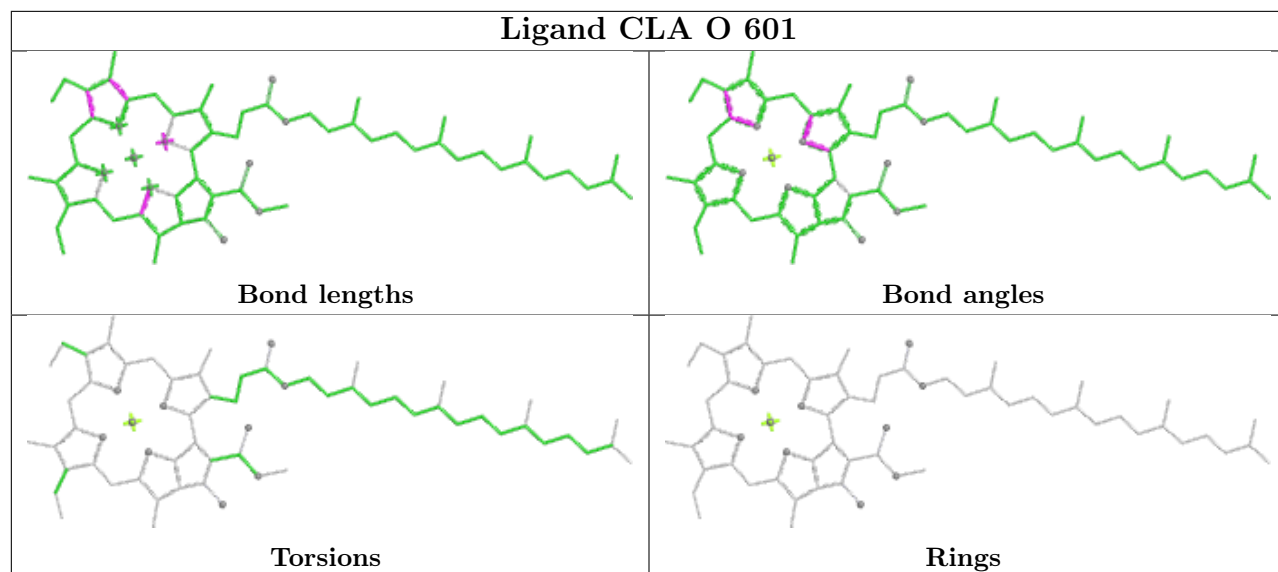
Ligand W4I O 625 (B)



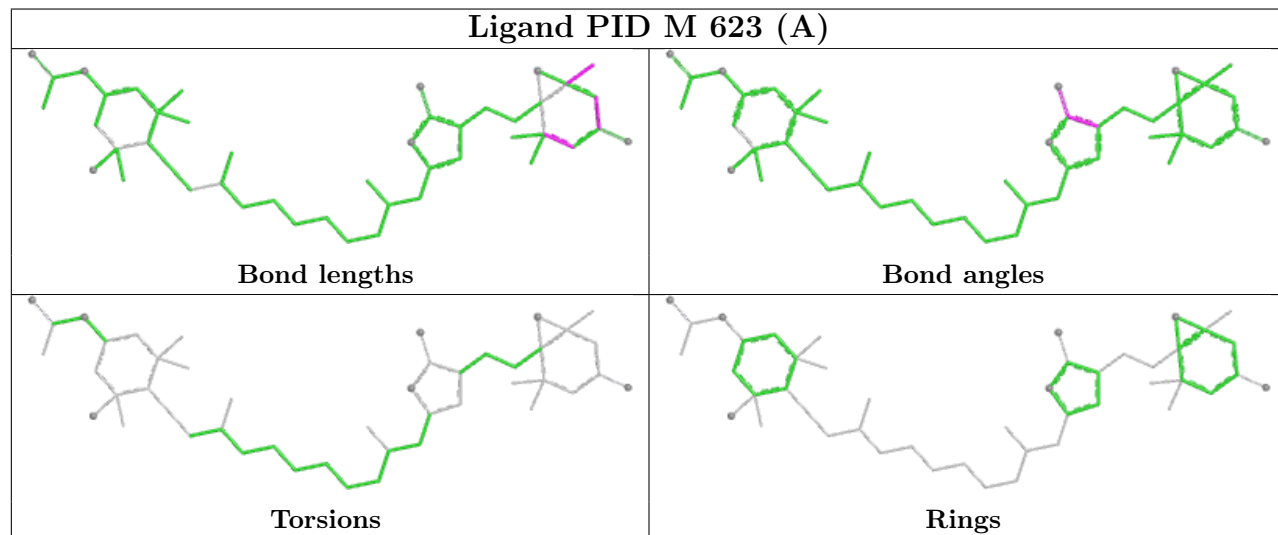
Ligand PID M 613 (B)

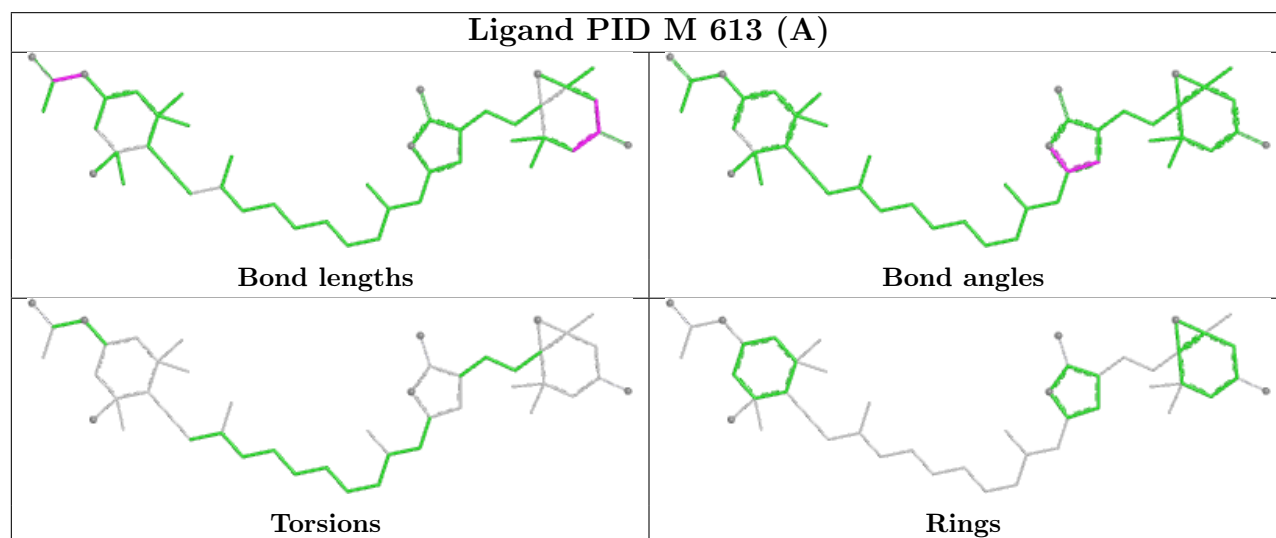
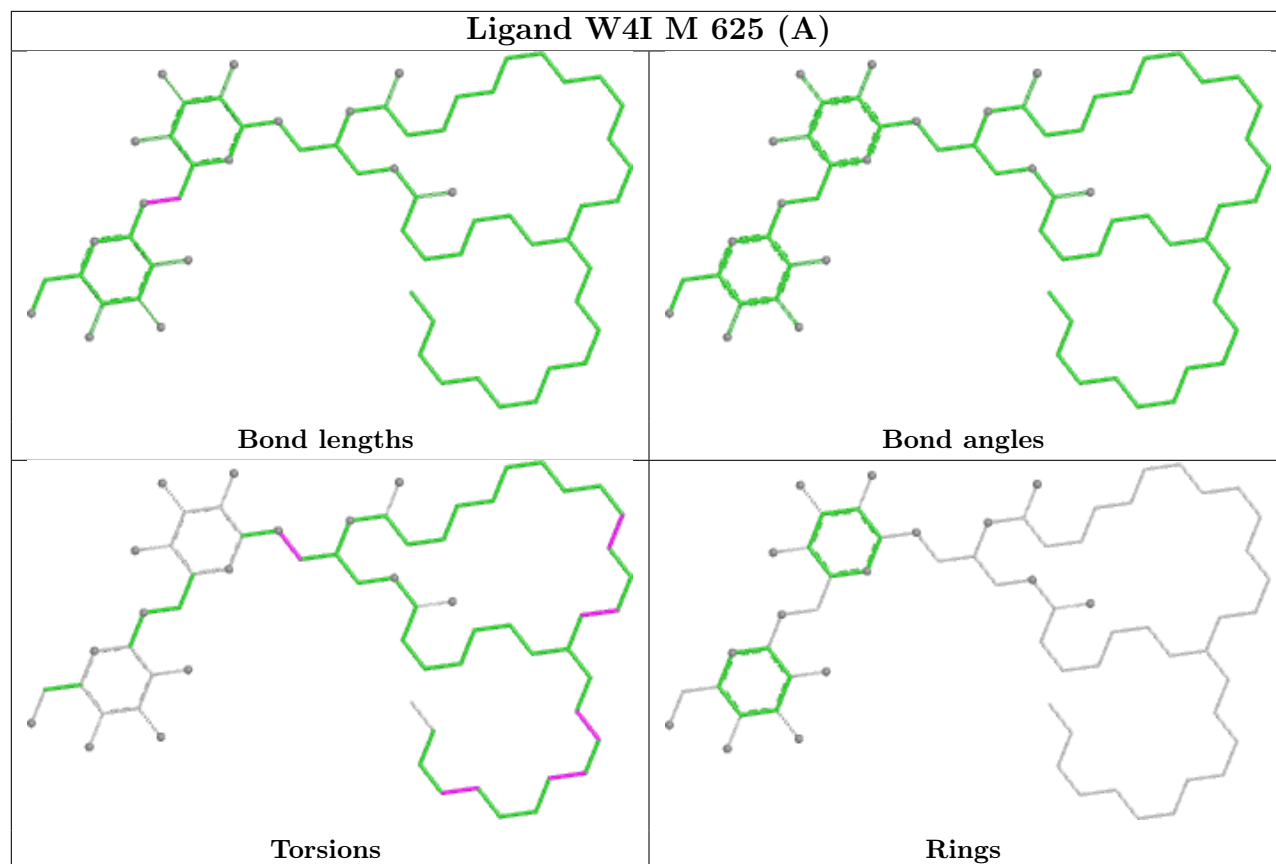


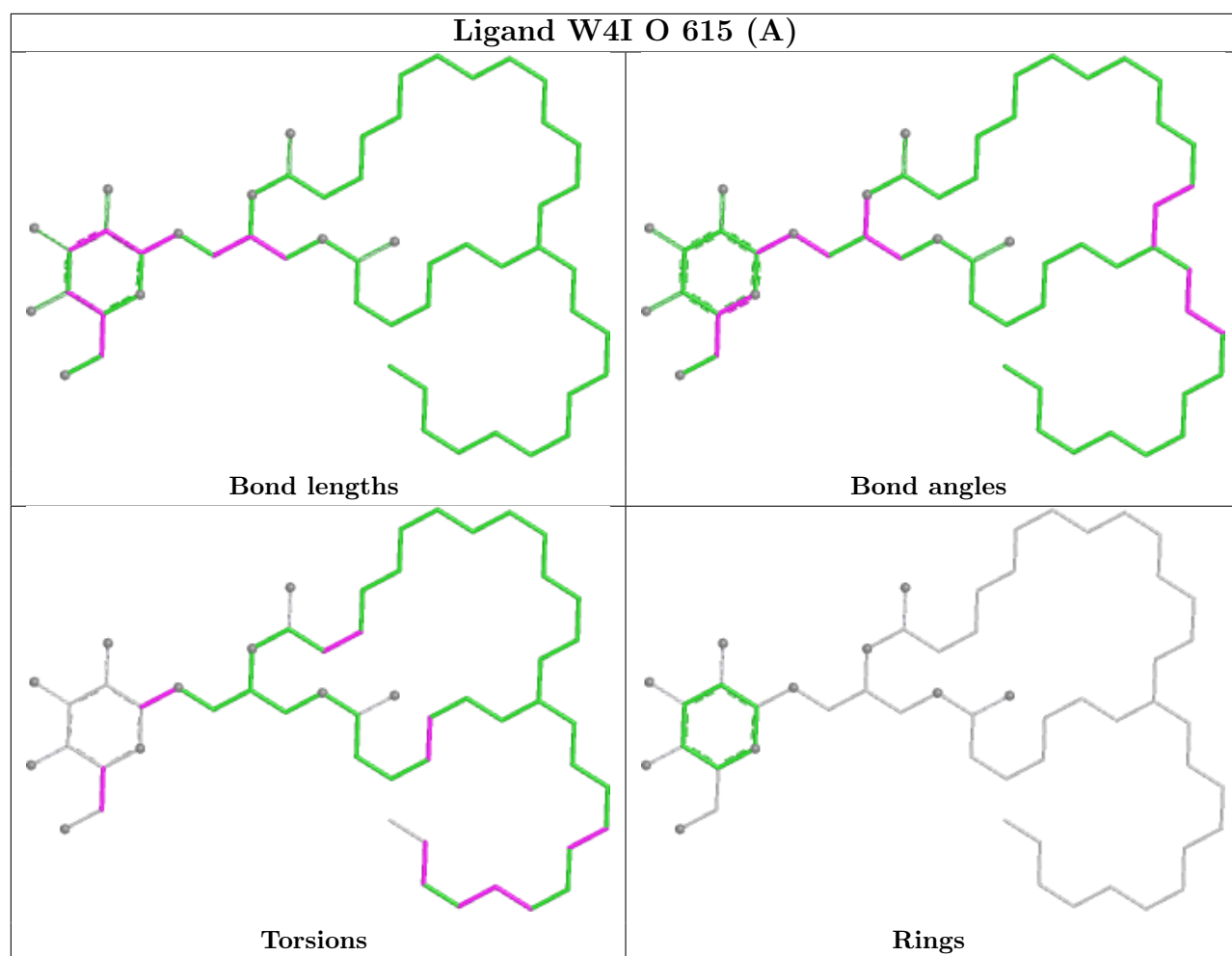
Ligand CLA O 601

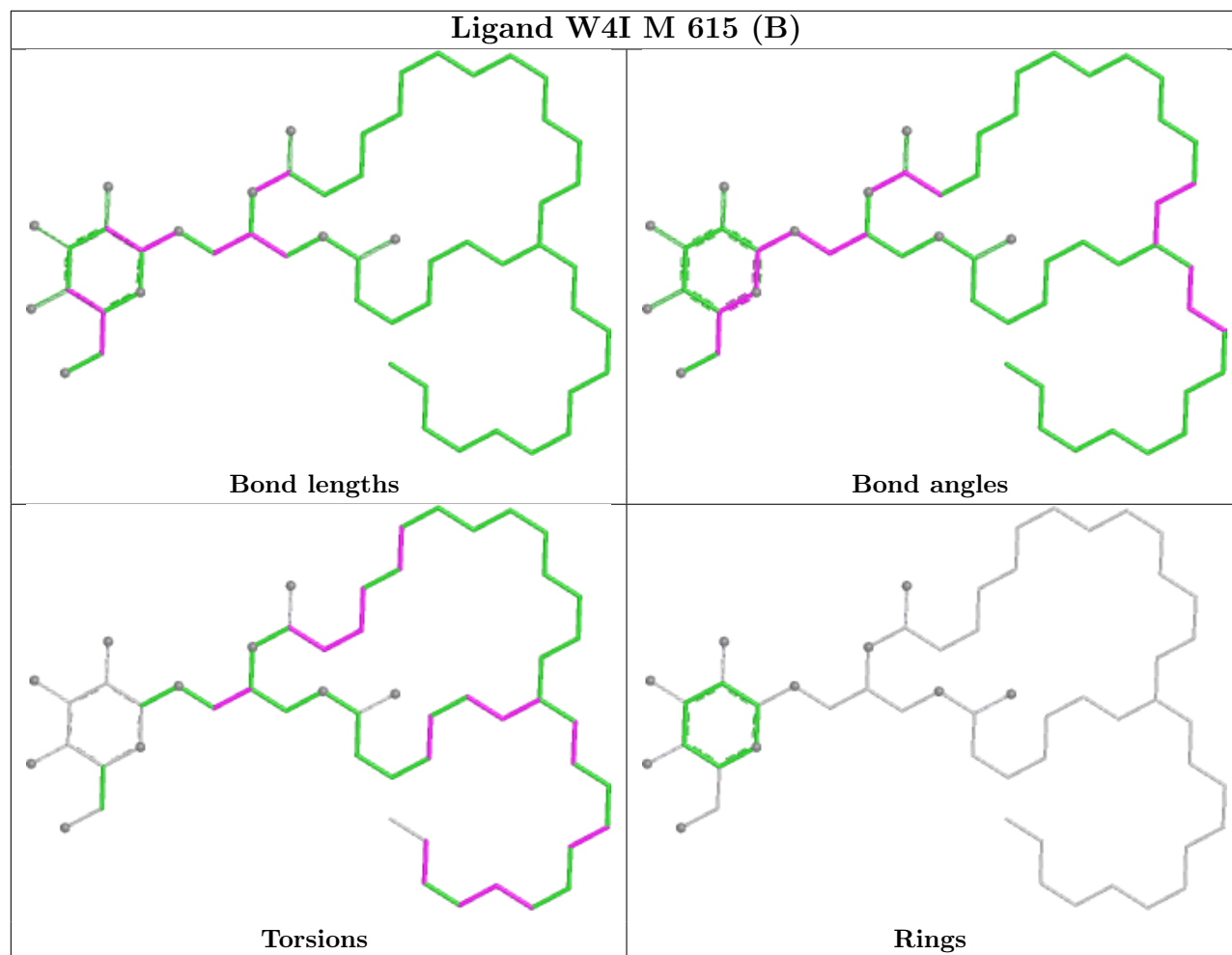


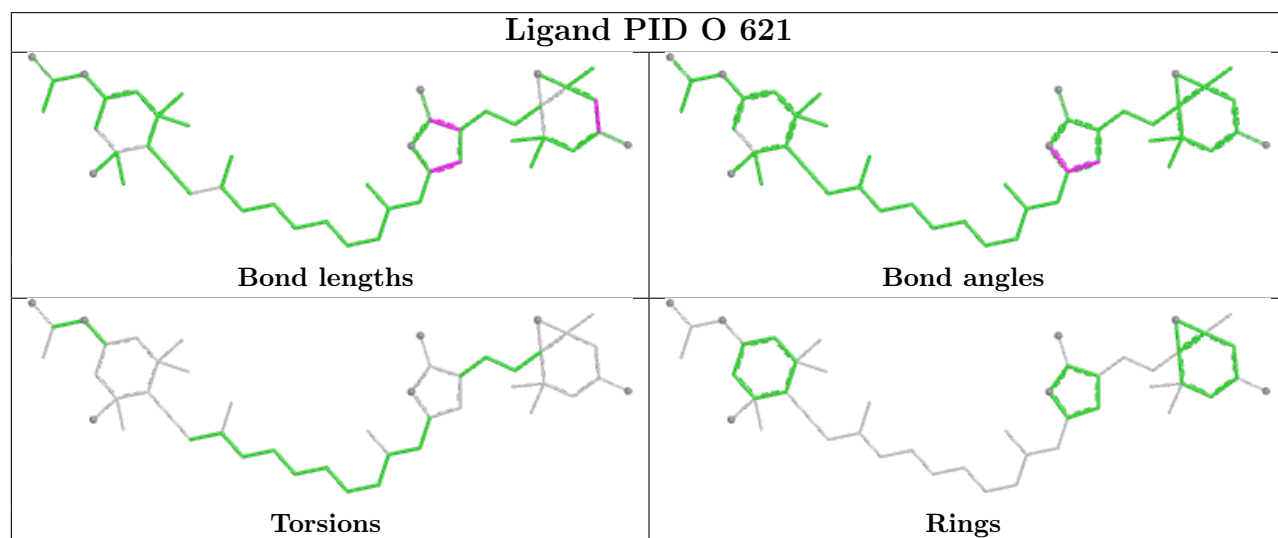
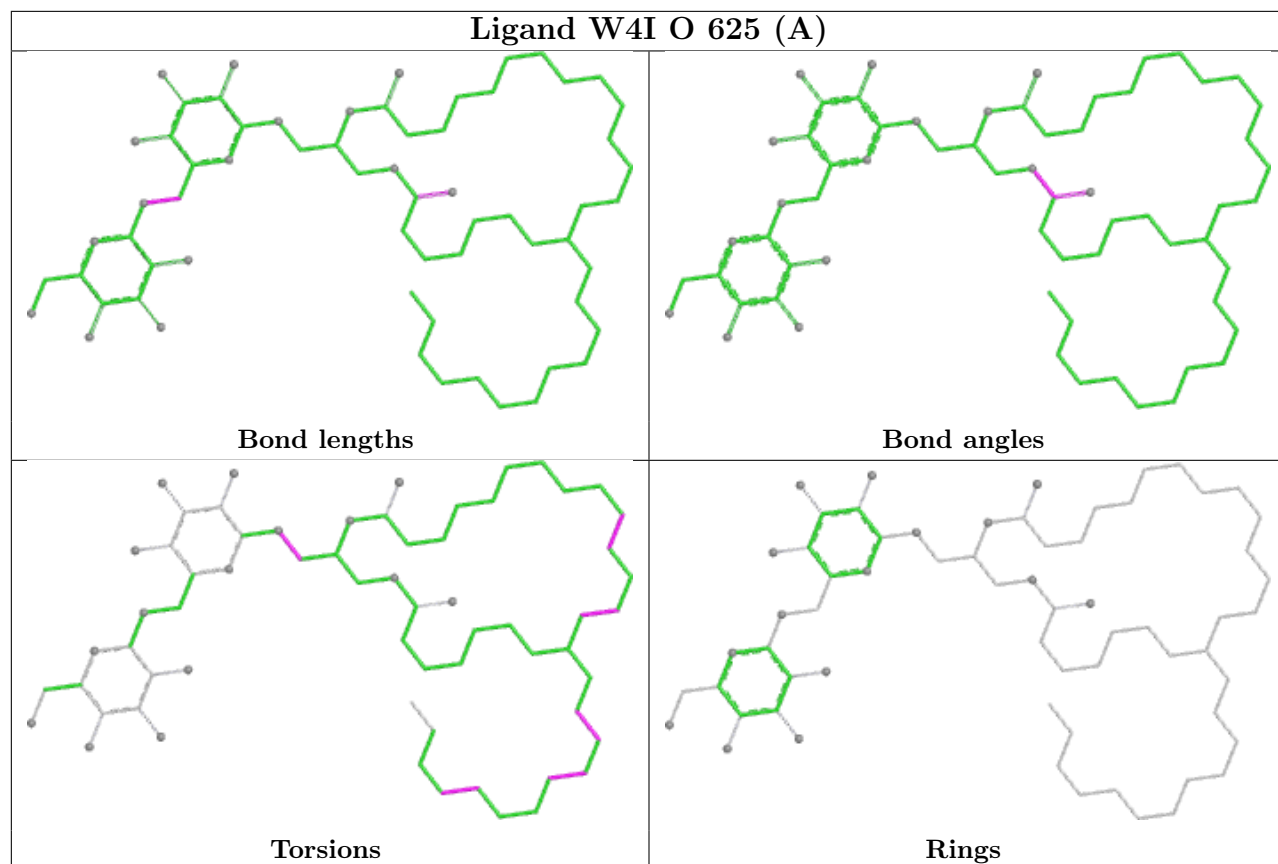
Ligand PID M 623 (A)



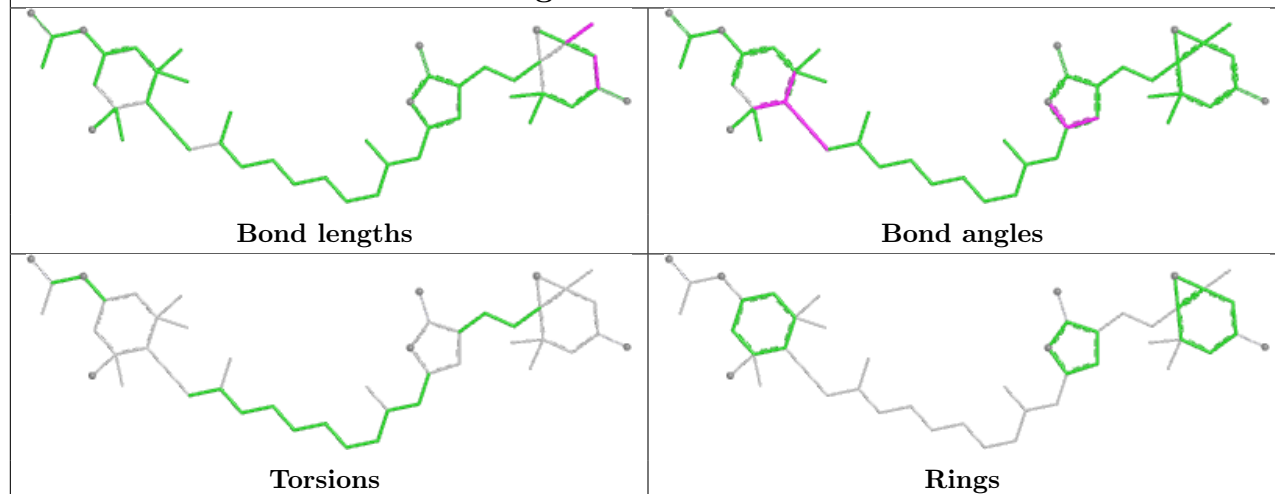




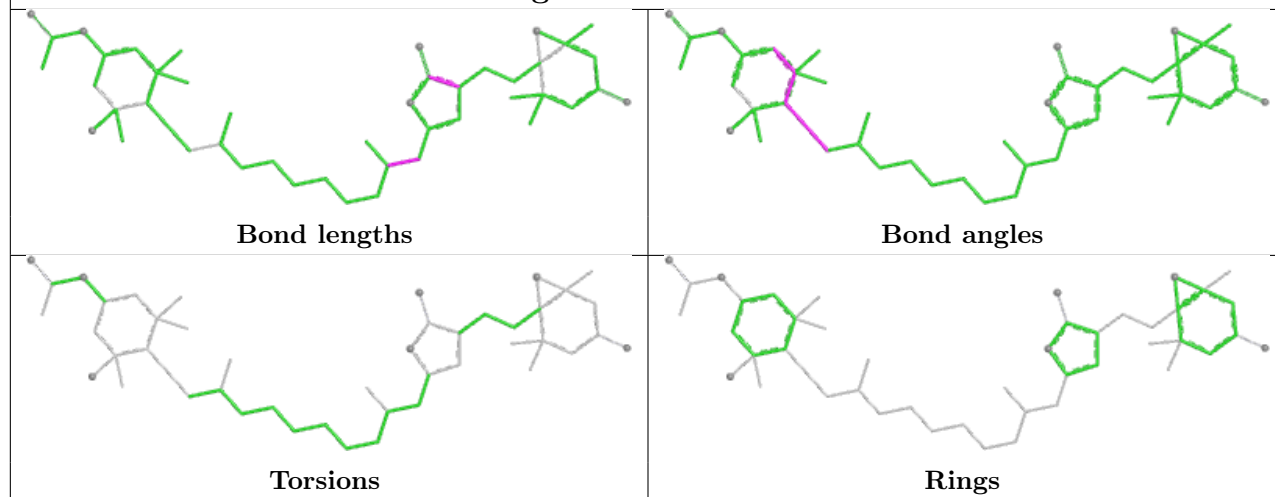




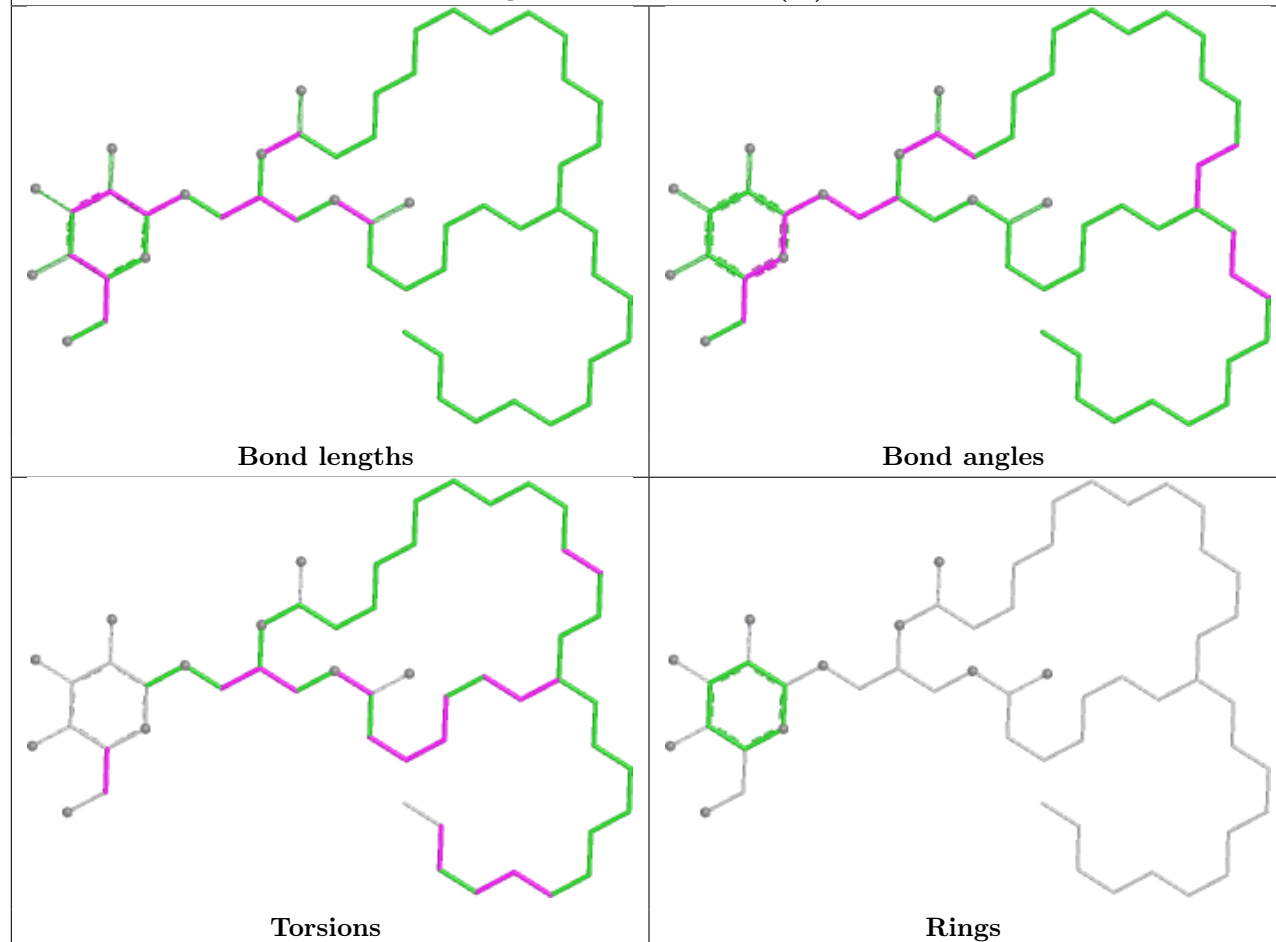
Ligand PID O 612



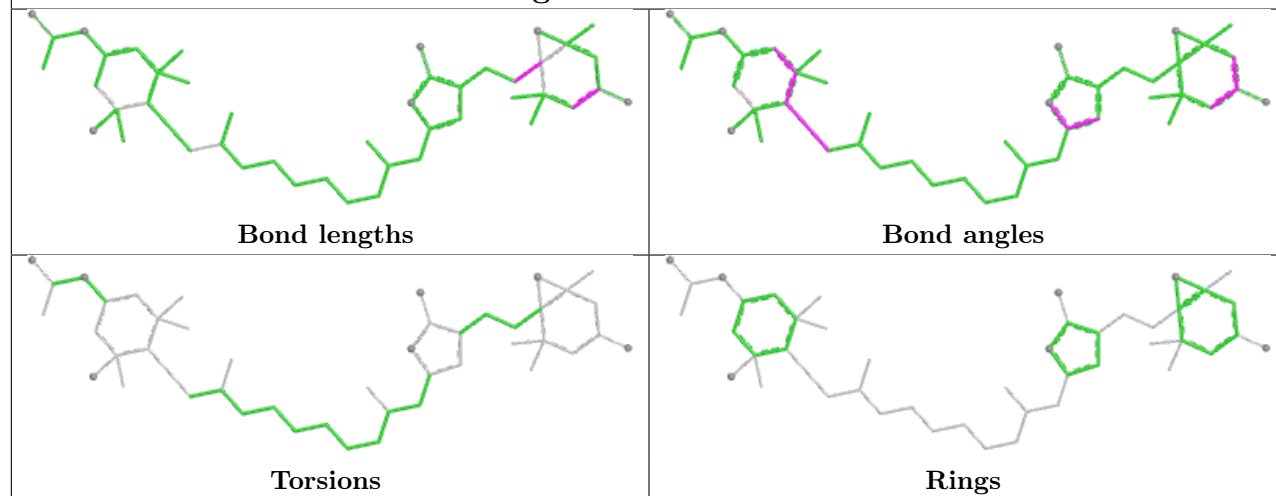
Ligand PID M 614



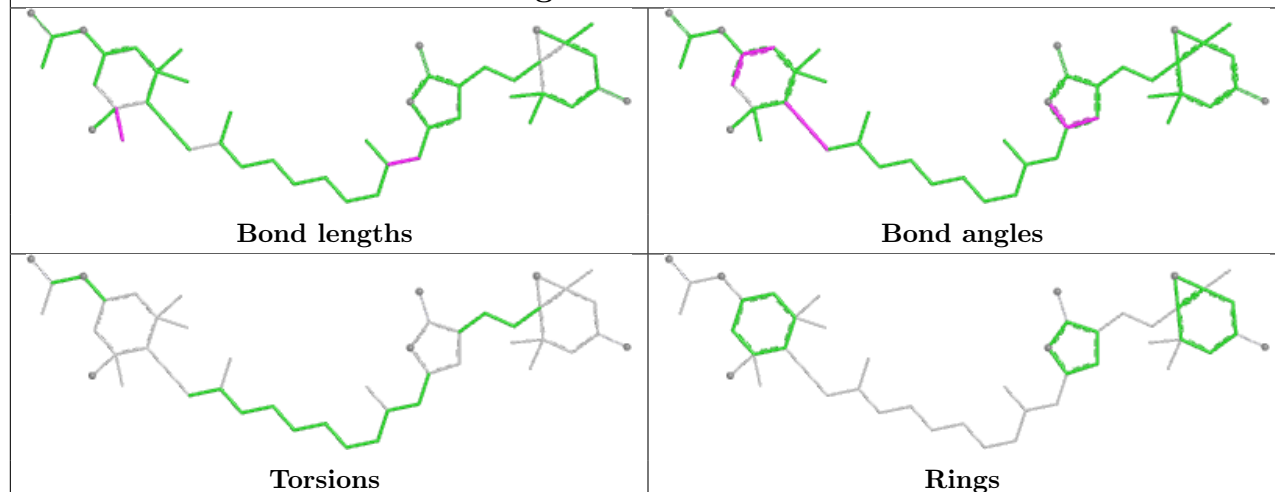
Ligand W4I N 615 (B)



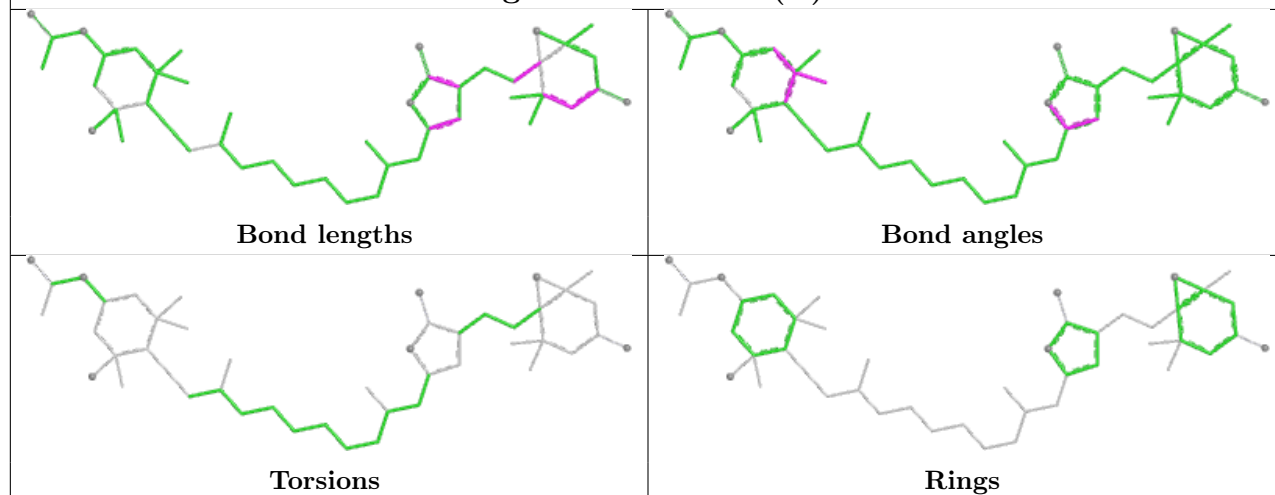
Ligand PID M 622



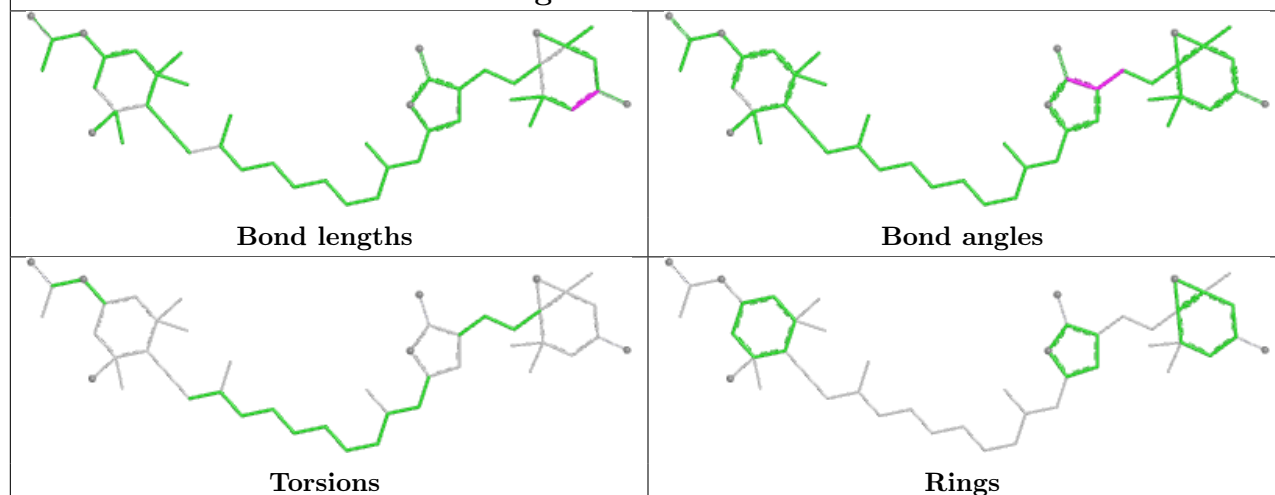
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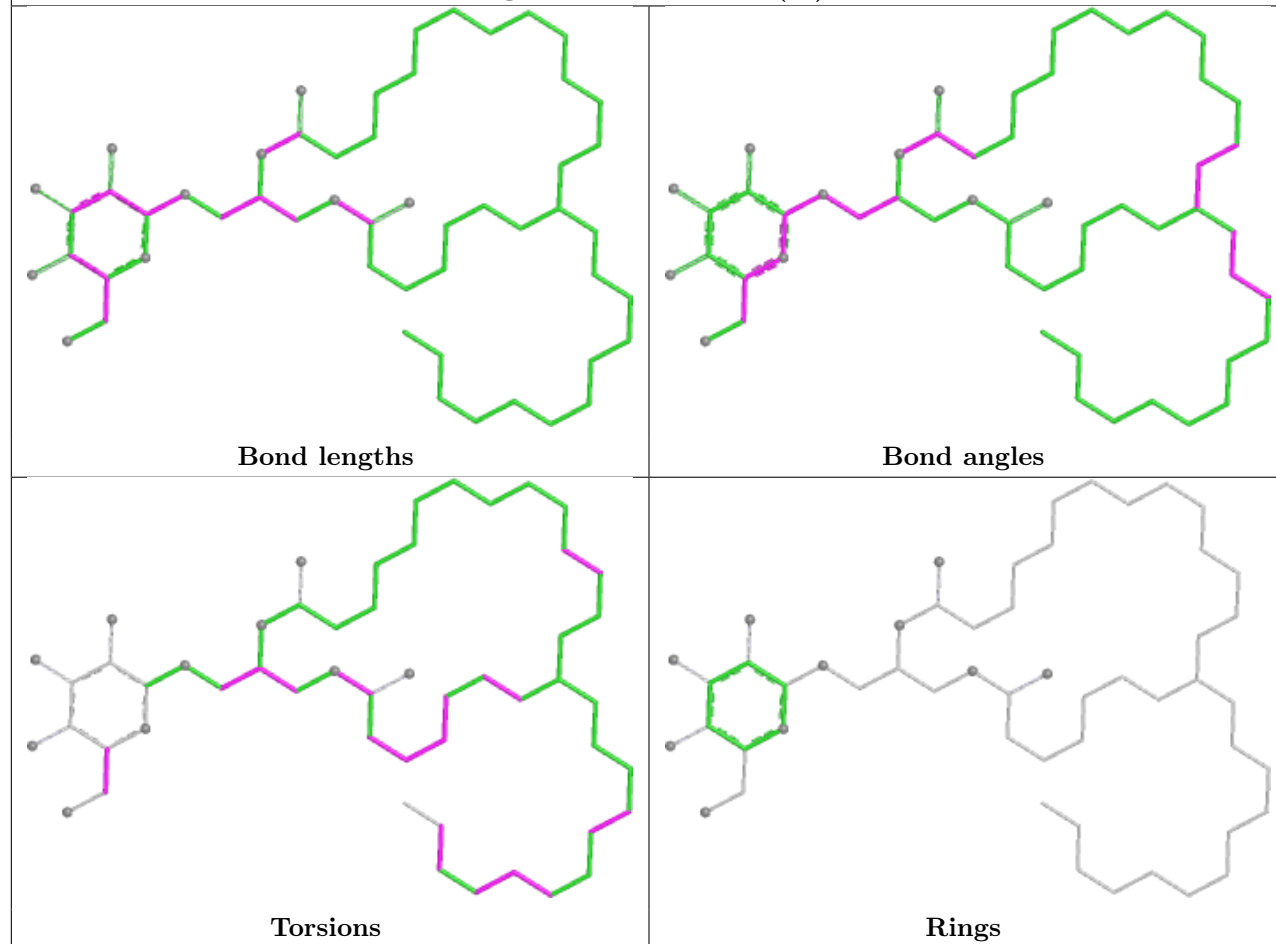
Ligand PID O 623 (B)



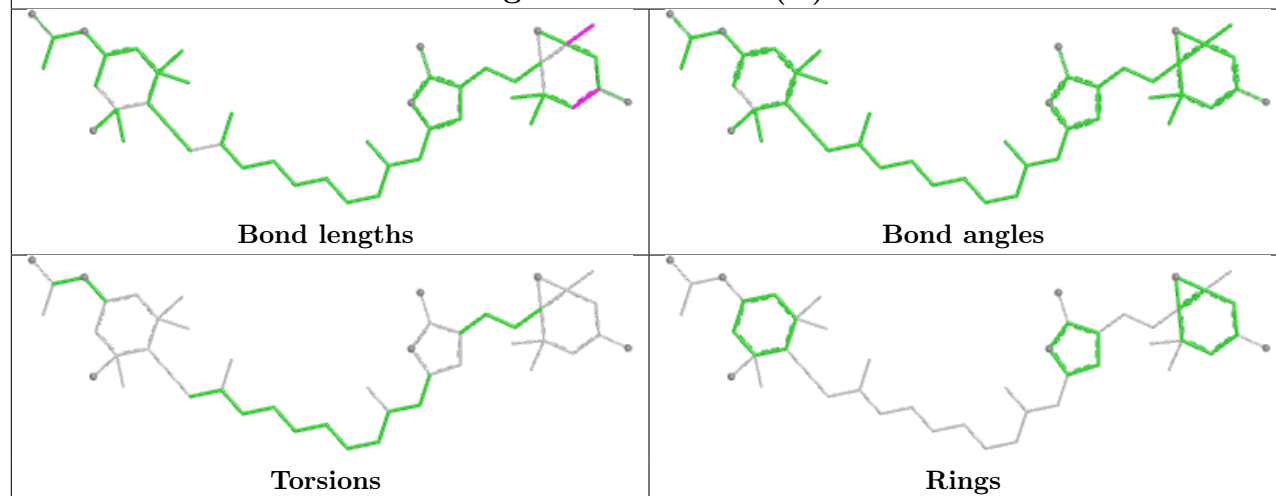
Ligand PID N 611

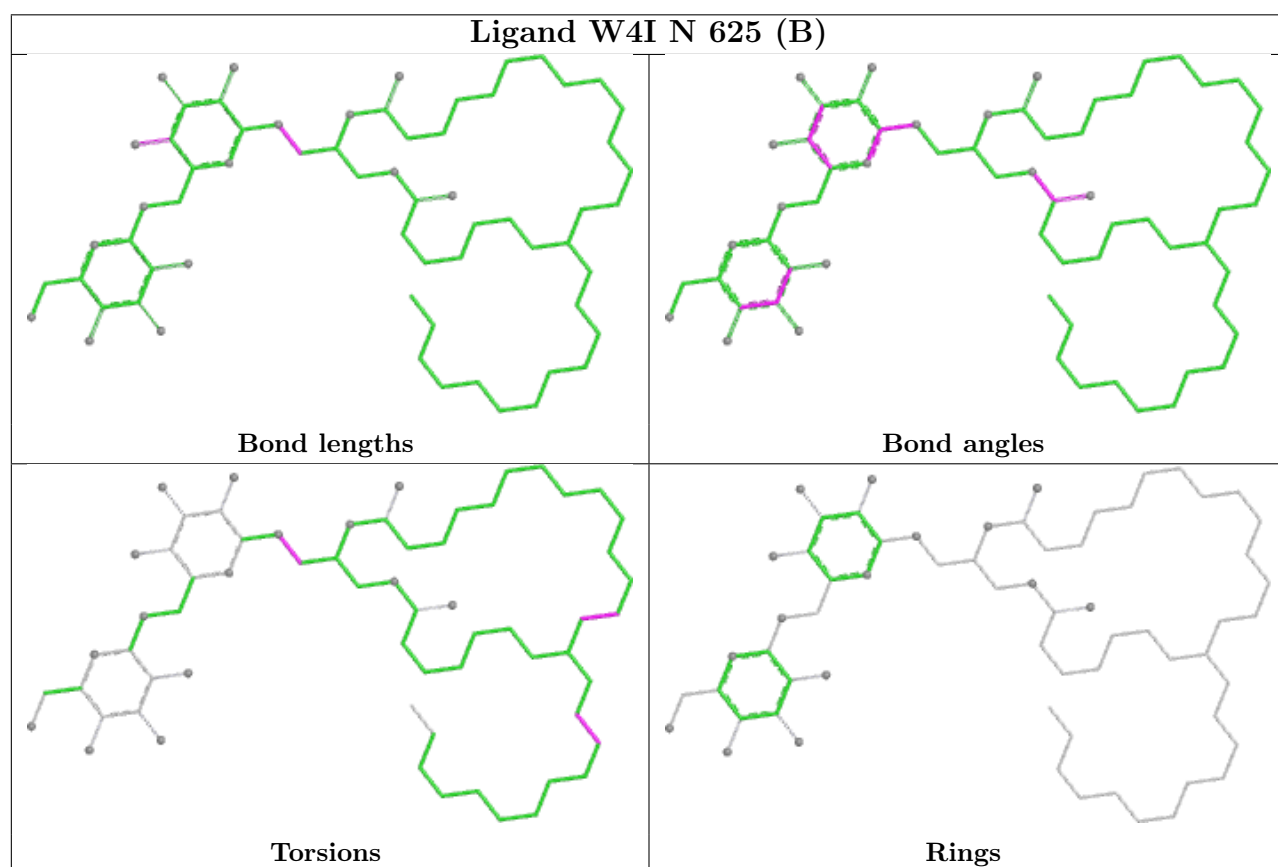
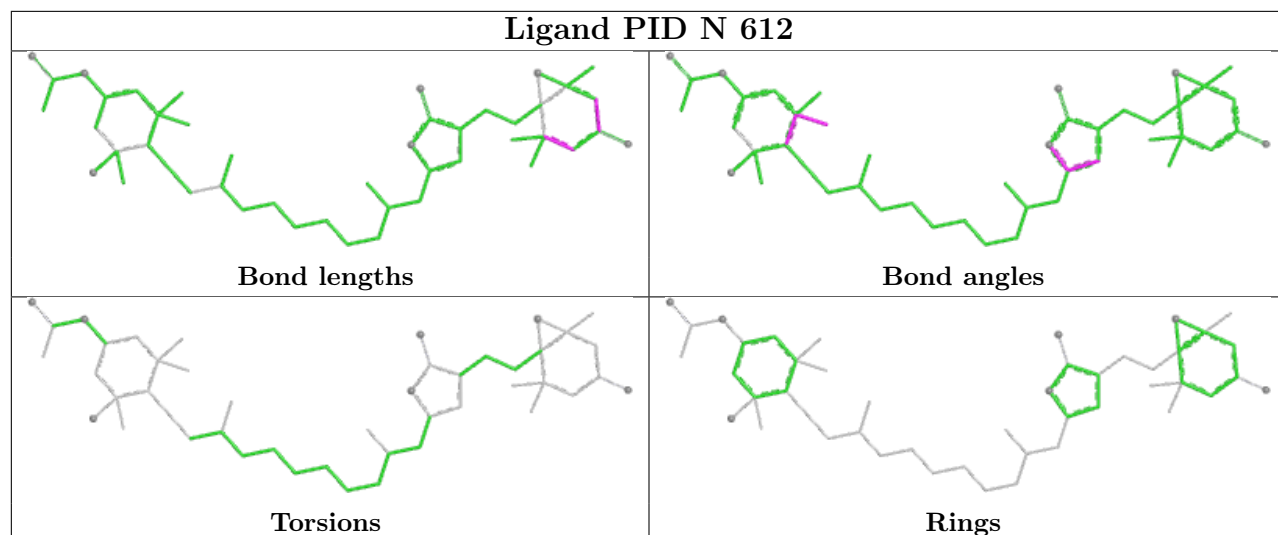


Ligand W4I N 615 (A)

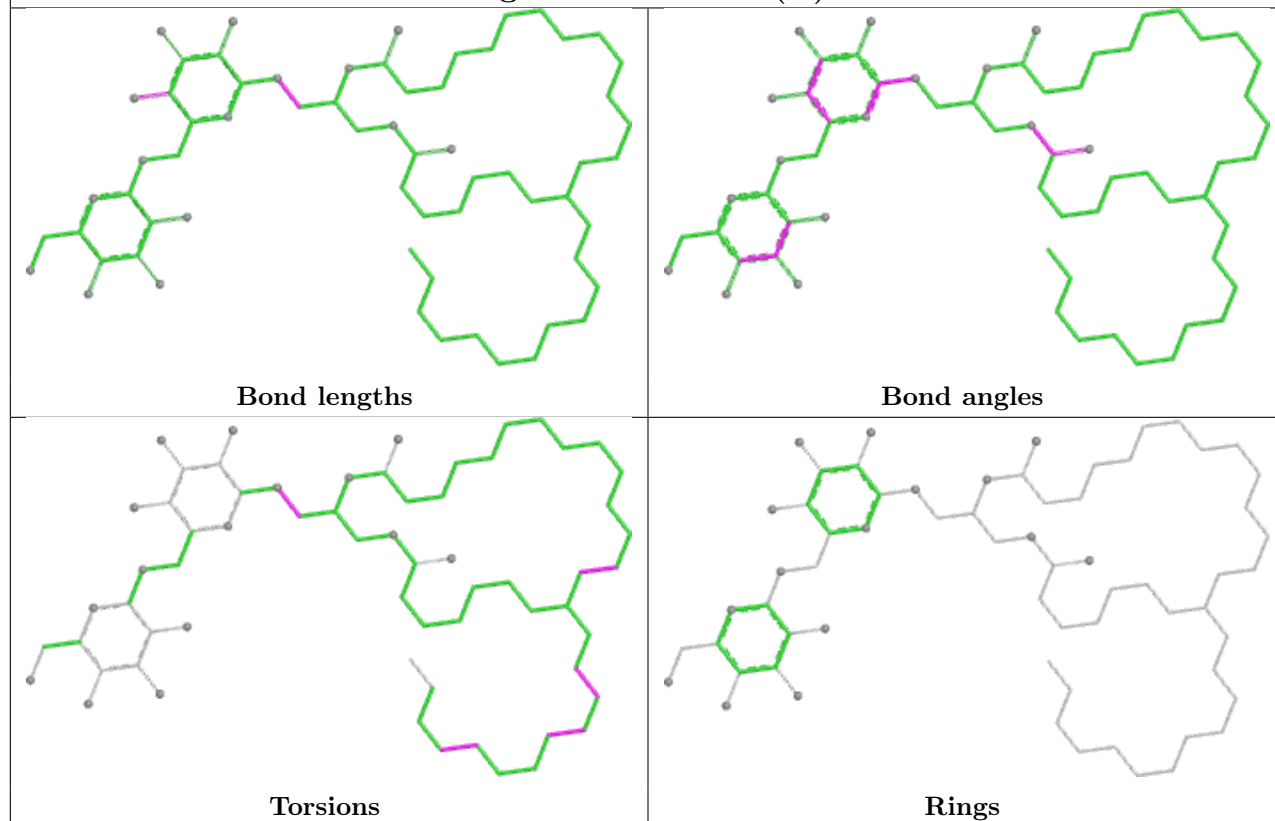


Ligand PID O 613 (B)

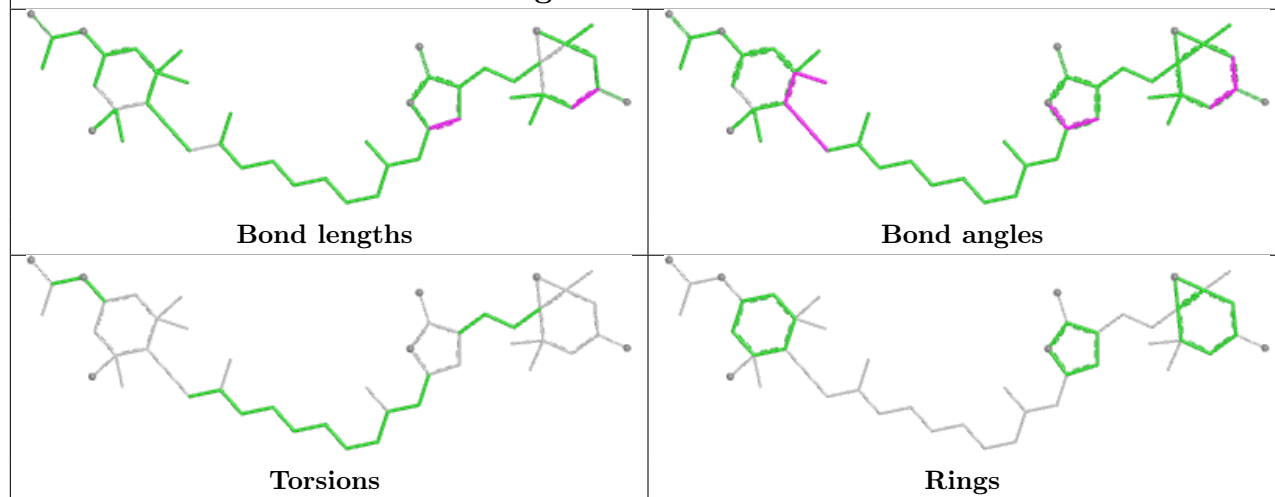


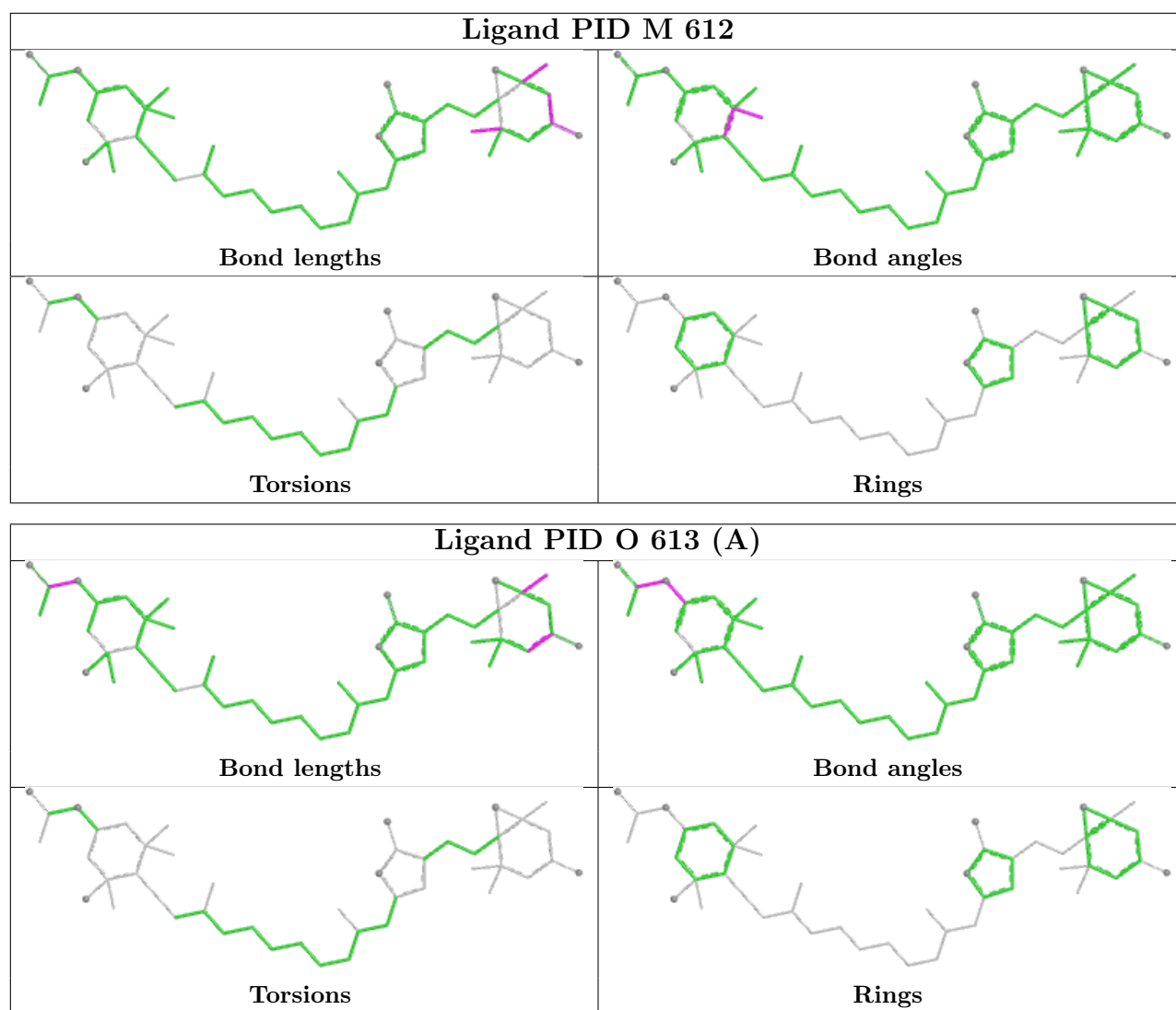


Ligand W4I N 625 (A)



Ligand PID N 622





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)

All (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
1	M	159	THR	4.0
1	N	155	ALA	3.8
1	O	161	PRO	3.7
1	N	161	PRO	3.5
1	N	158	ALA	3.3
1	N	157	PRO	3.2
1	O	157	PRO	3.2
1	O	162	SER	3.1
1	M	157	PRO	3.1
1	M	158	ALA	3.1
1	O	159	THR	3.0
1	N	156	GLY	3.0
1	M	162	SER	2.6
1	M	156	GLY	2.5
1	N	149	SER	2.5
1	N	152	THR	2.5
1	N	162	SER	2.5
1	O	158	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	153	SER	2.3
1	M	149	SER	2.2
1	O	148	LYS	2.2
1	M	148	LYS	2.2
1	N	148	LYS	2.2
1	O	113[A]	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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

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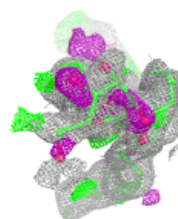
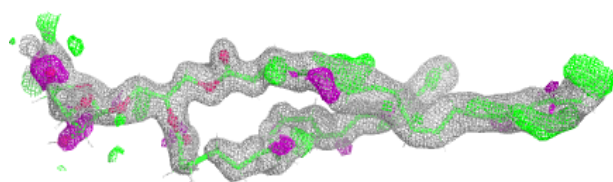
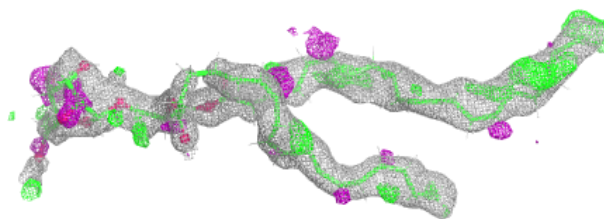
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PID	M	612	46/46	0.98	0.04	11,14,23,28	0
3	PID	M	613[A]	46/46	0.98	0.05	11,15,31,34	6
3	PID	M	613[B]	46/46	0.98	0.05	11,15,31,34	6
4	W4I	N	625[A]	68/68	0.98	0.05	10,16,23,25	14
4	W4I	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
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

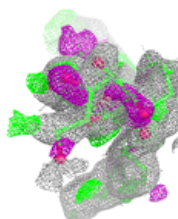
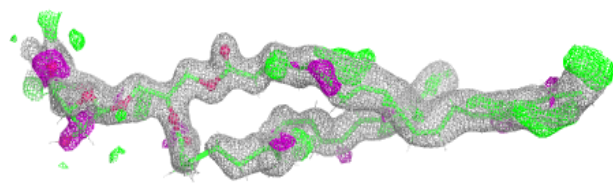
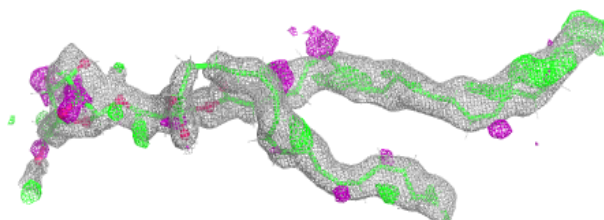
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

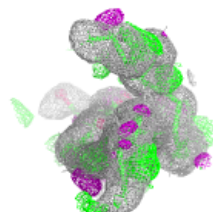
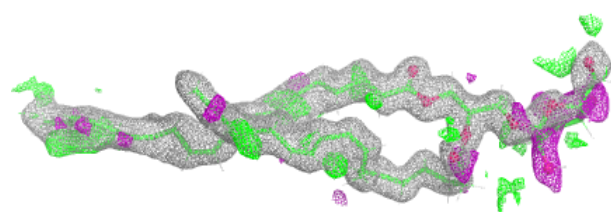
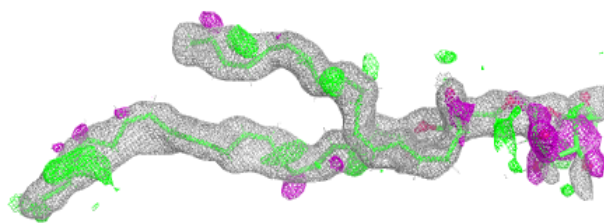
**Electron density around W4I N 615 (A):**

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

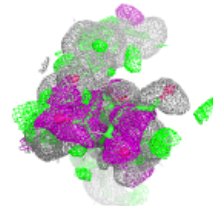
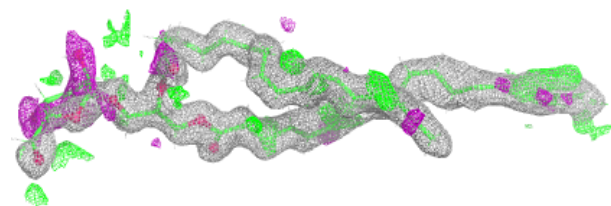
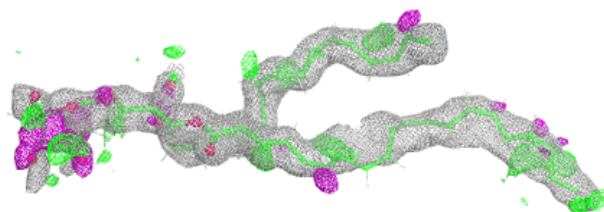


Electron density around W4I O 615 (A):

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

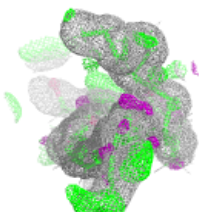
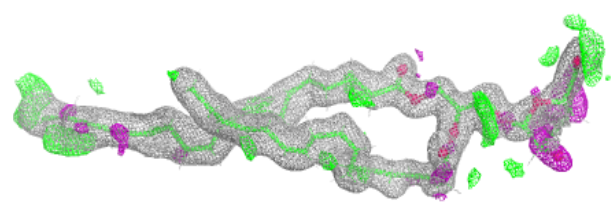
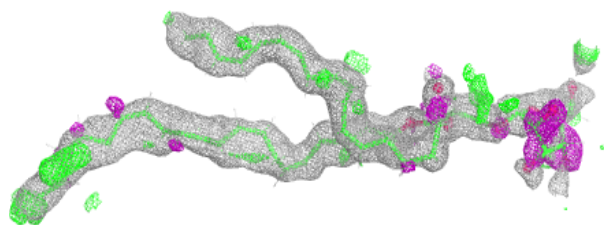
**Electron density around W4I O 615 (B):**

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

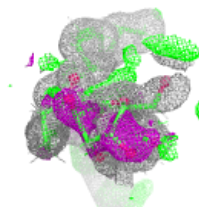
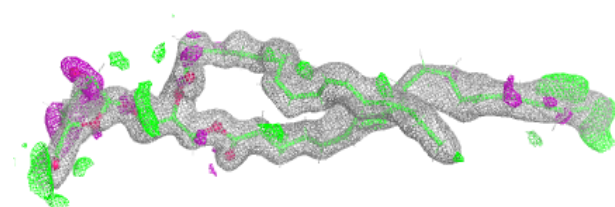
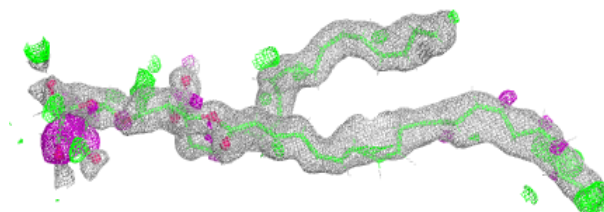


Electron density around W4I M 615 (A):

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

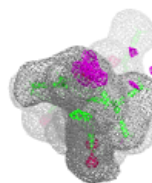
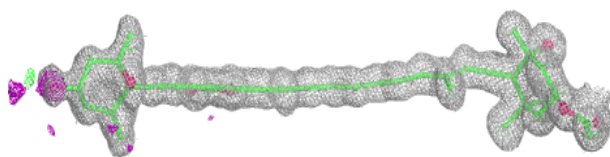
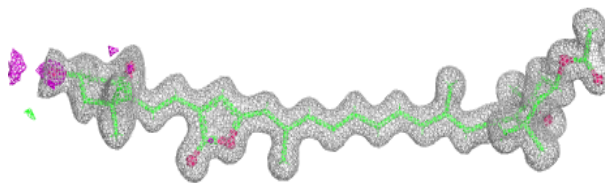
**Electron density around W4I M 615 (B):**

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

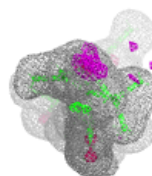
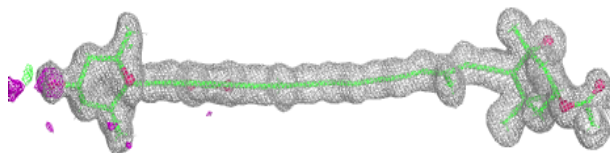
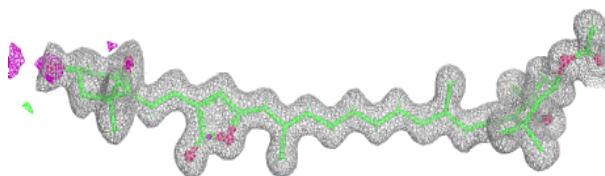


Electron density around PID N 613 (B):

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

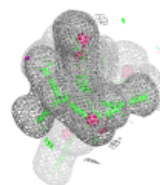
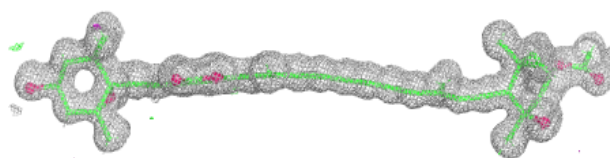
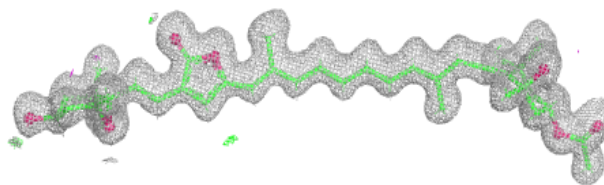
**Electron density around PID N 613 (A):**

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

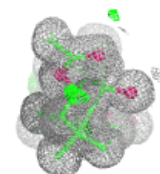
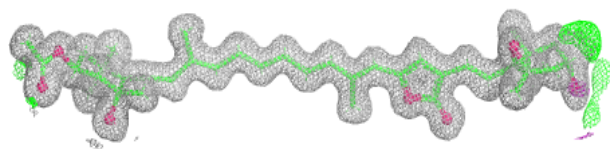
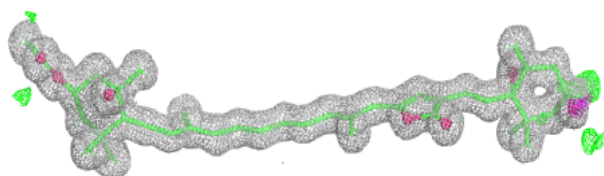


Electron density around PID N 623 (B):

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

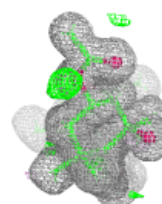
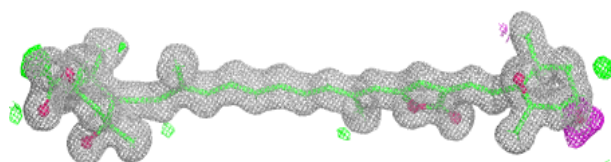
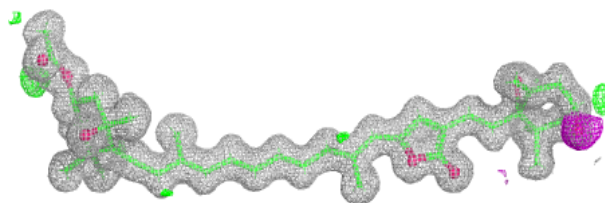
**Electron density around PID O 611:**

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

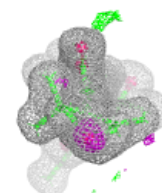
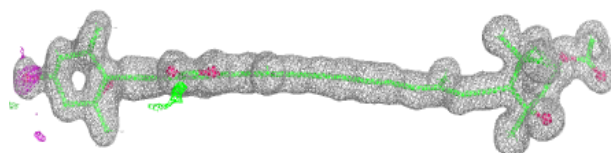
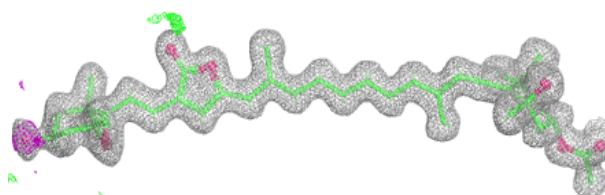


Electron density around PID O 612:

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

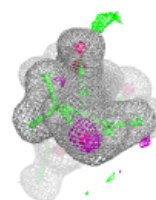
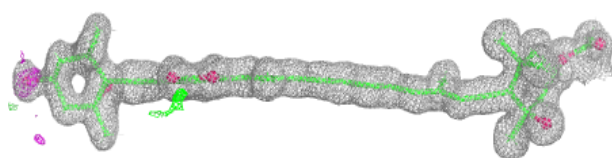
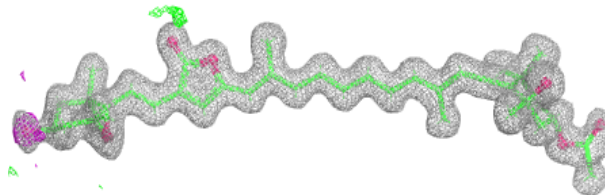
**Electron density around PID O 613 (A):**

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

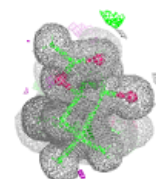
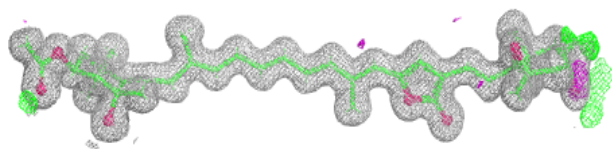
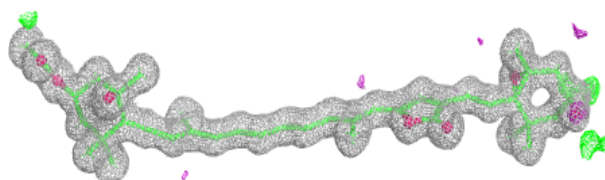


Electron density around PID O 613 (B):

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

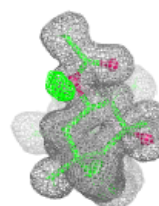
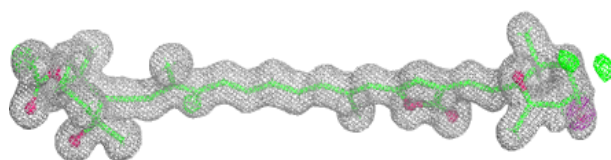
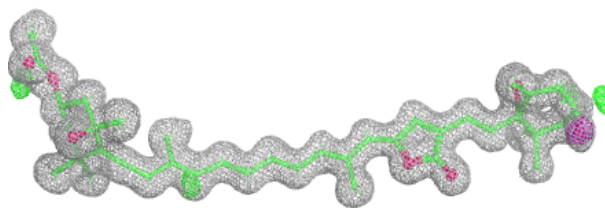
**Electron density around PID M 611:**

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

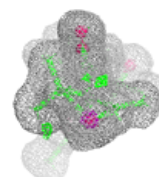
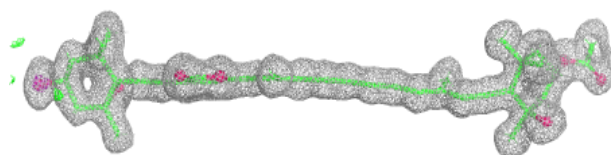
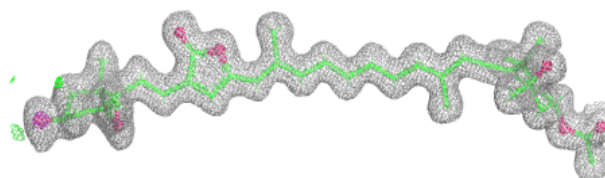


Electron density around PID M 612:

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

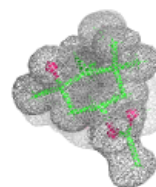
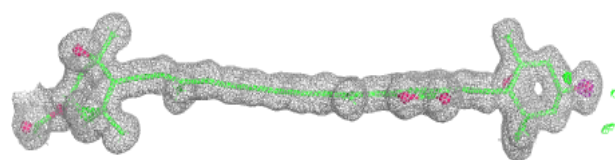
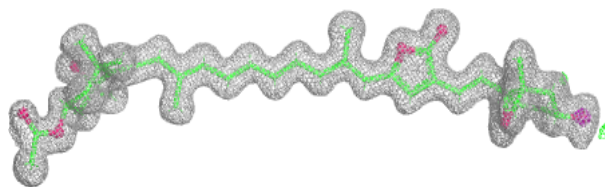
**Electron density around PID M 613 (A):**

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

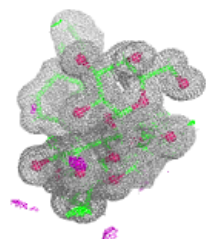
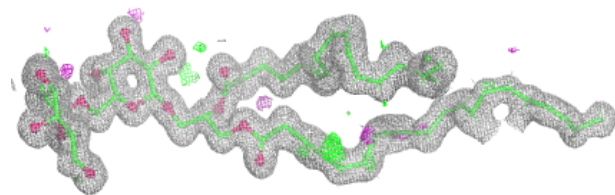
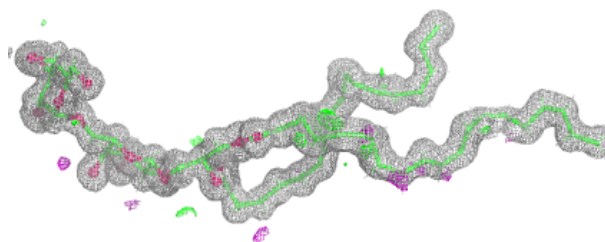


Electron density around PID M 613 (B):

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

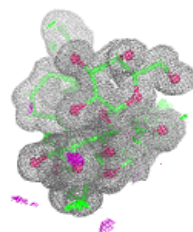
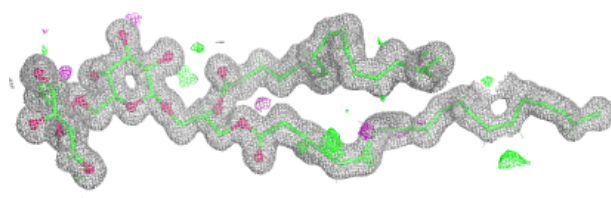
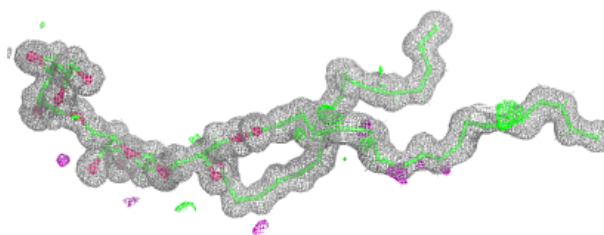
**Electron density around W4I N 625 (A):**

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

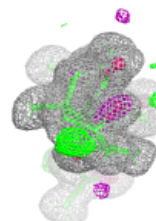
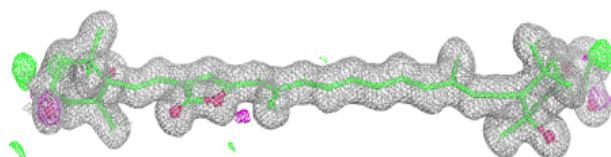
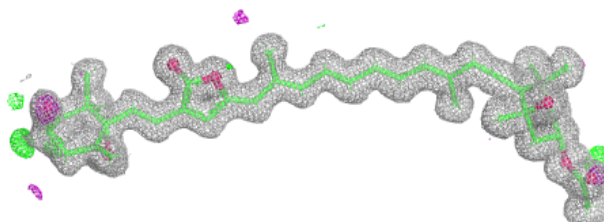


Electron density around W4I N 625 (B):

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

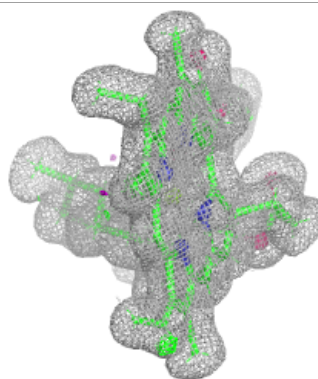
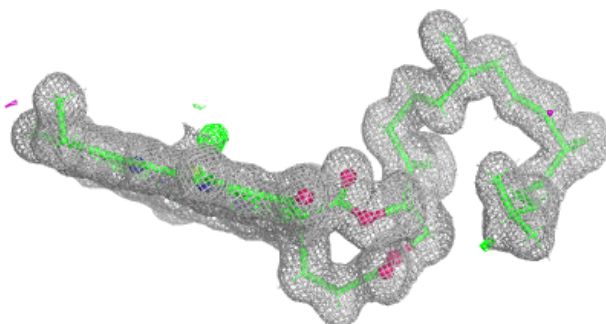
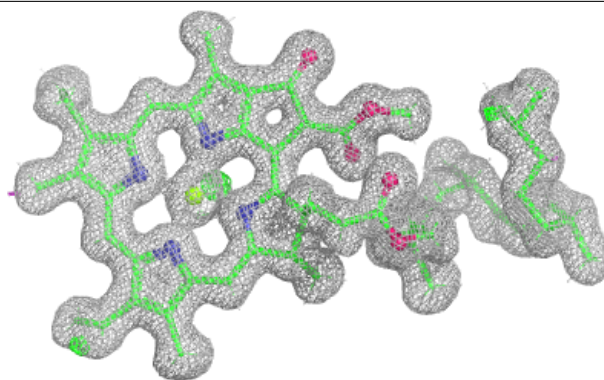
**Electron density around PID N 612:**

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

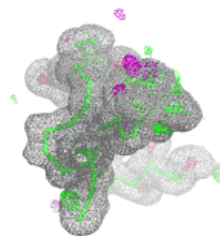
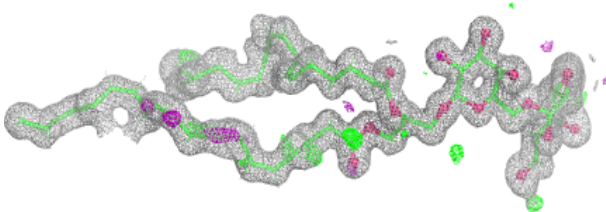
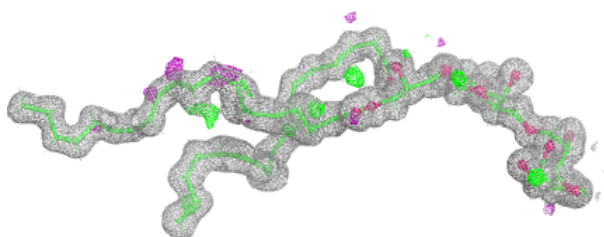


Electron density around CLA N 601:

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

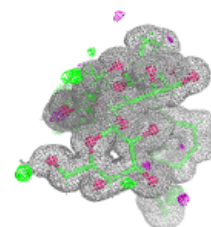
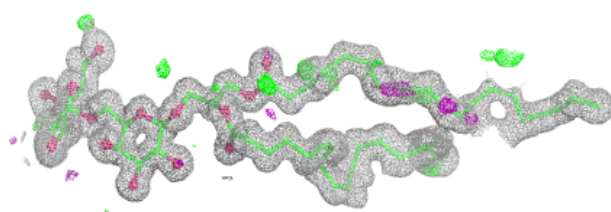
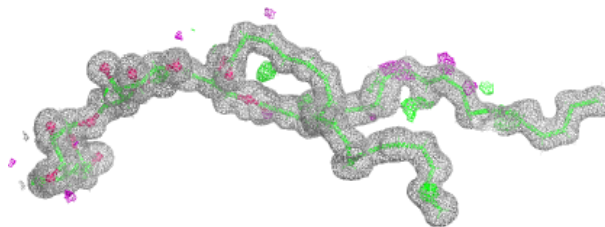
**Electron density around W4I O 625 (A):**

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

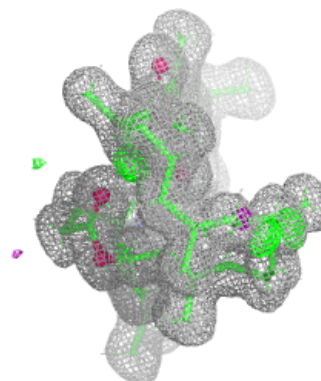
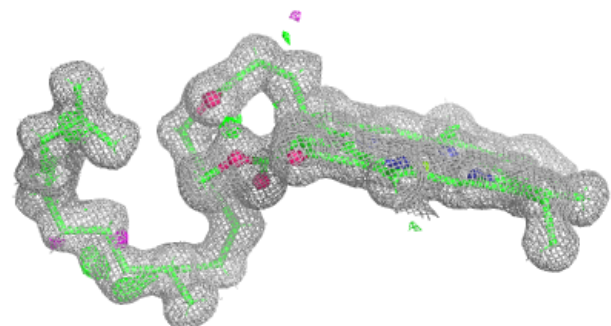
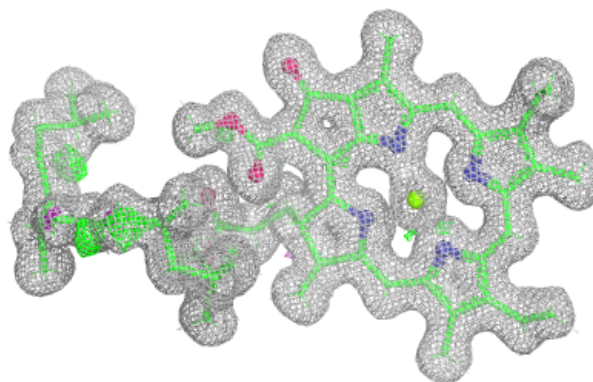


Electron density around W4I O 625 (B):

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

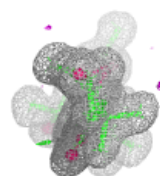
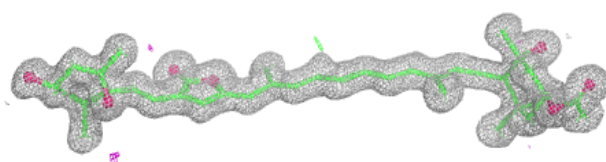
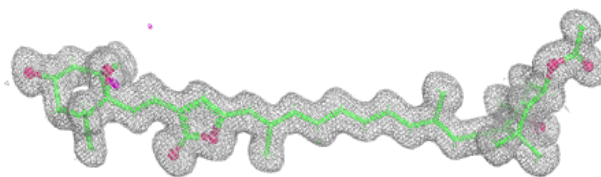
**Electron density around CLA N 602:**

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

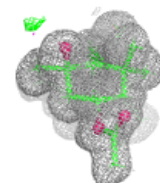
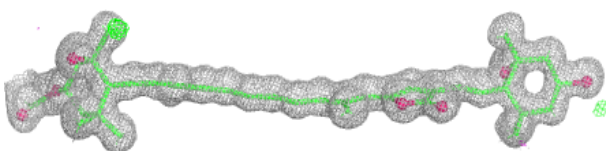
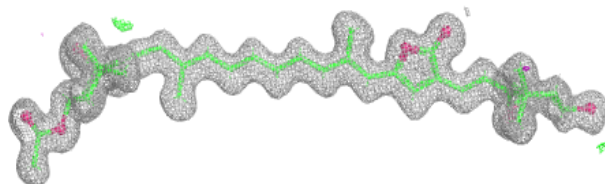


Electron density around PID N 614:

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

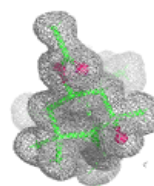
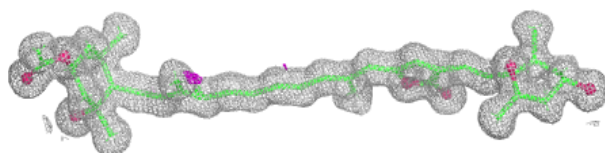
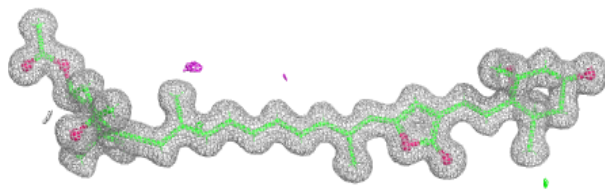
**Electron density around PID N 623 (A):**

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

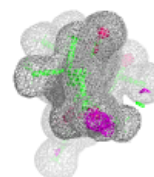
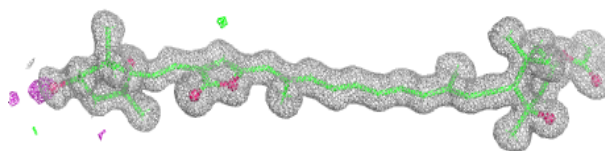
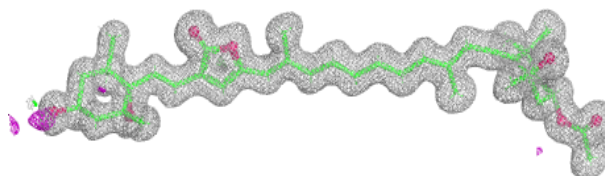


Electron density around PID M 624:

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

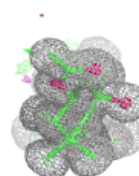
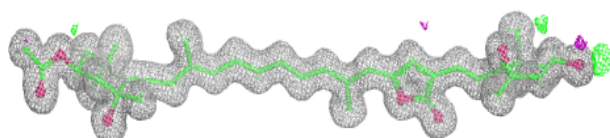
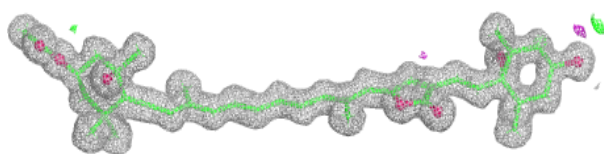
**Electron density around PID O 614:**

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

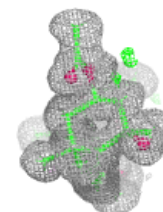
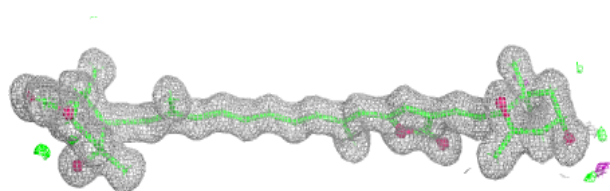
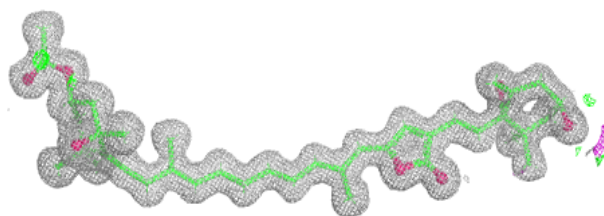


Electron density around PID O 621:

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

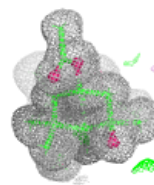
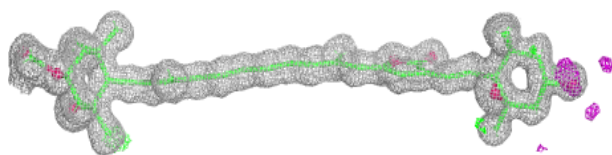
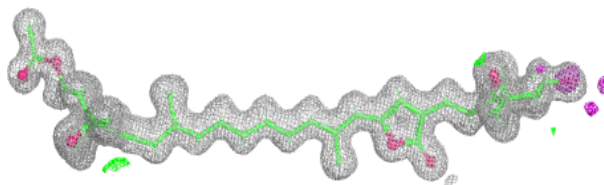
**Electron density around PID O 622:**

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

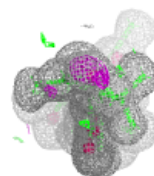
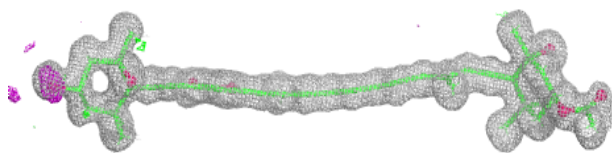
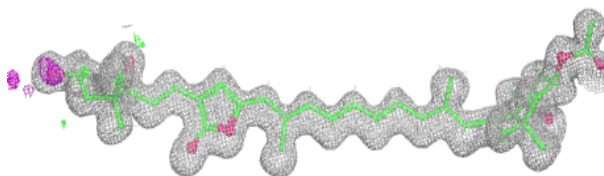


Electron density around PID O 623 (A):

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

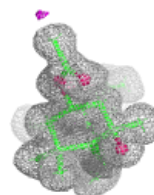
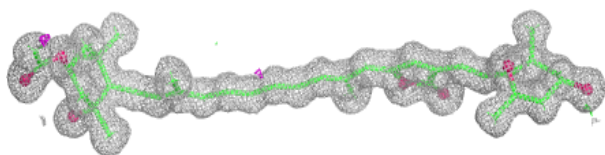
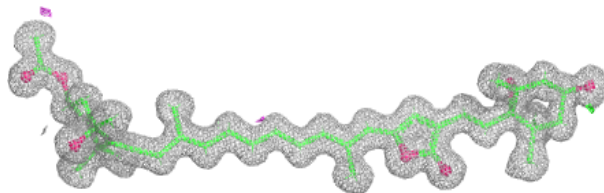
**Electron density around PID O 623 (B):**

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

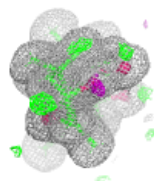
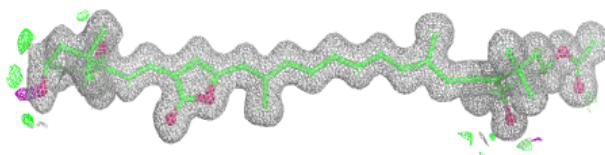
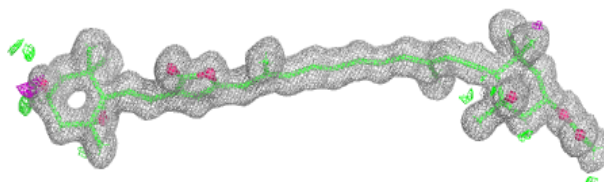


Electron density around PID O 624:

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

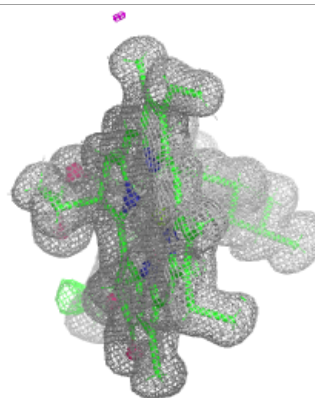
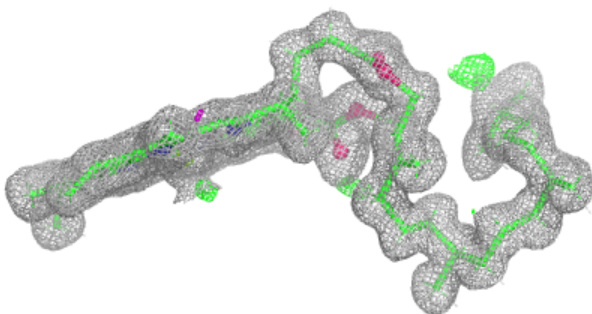
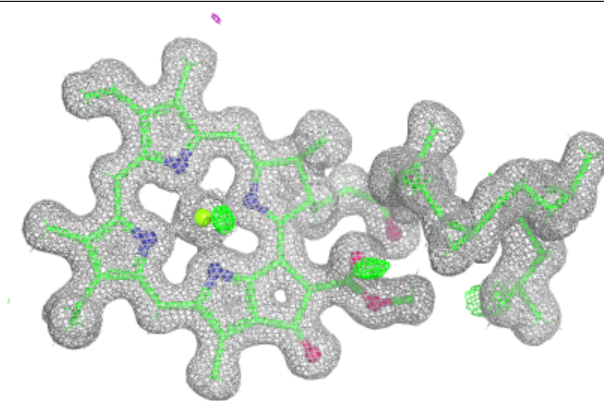
**Electron density around PID N 611:**

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

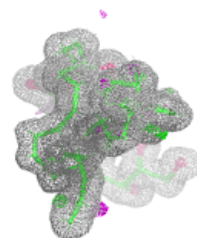
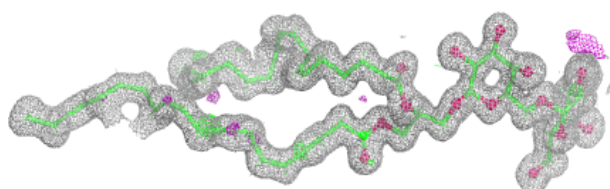
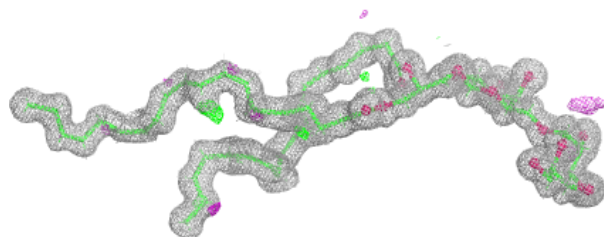


Electron density around CLA M 601:

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

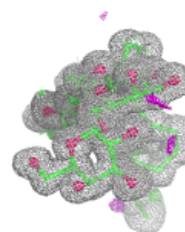
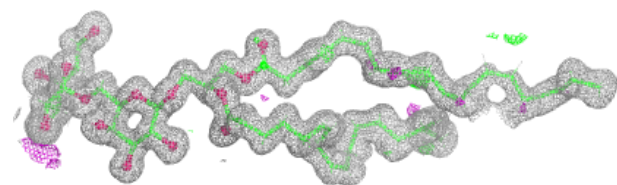
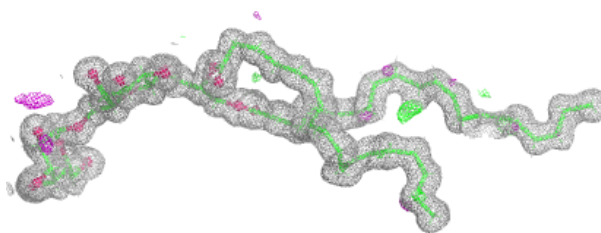
**Electron density around W4I M 625 (A):**

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

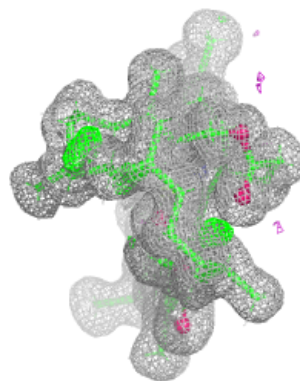
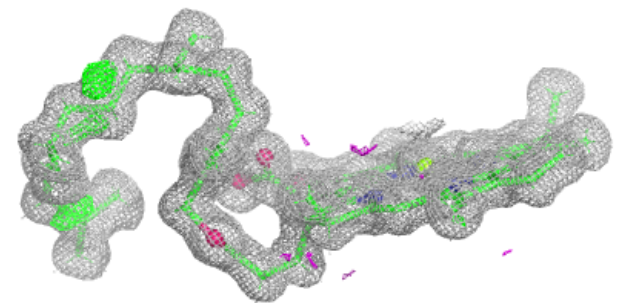
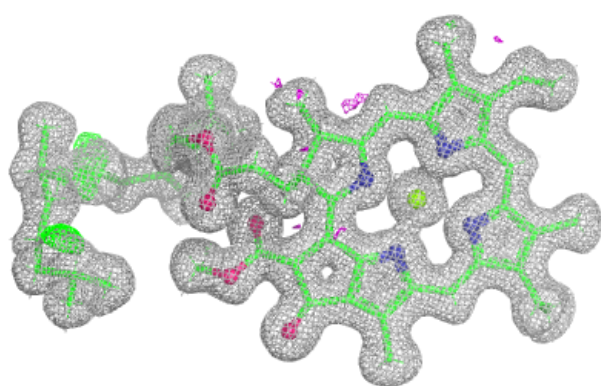


Electron density around W4I M 625 (B):

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

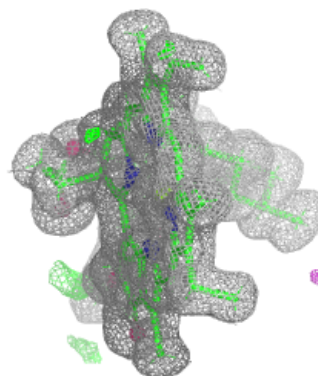
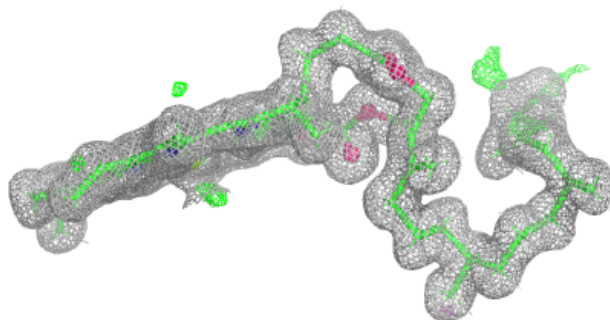
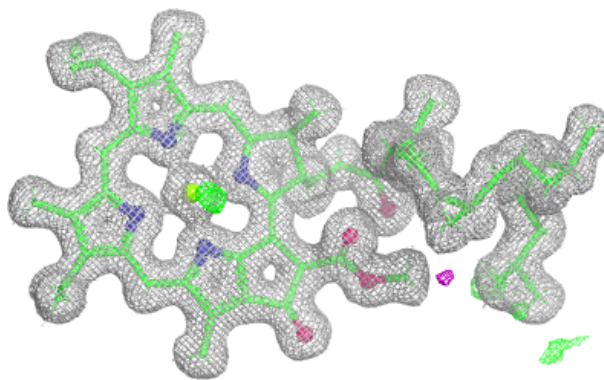
**Electron density around CLA M 602:**

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

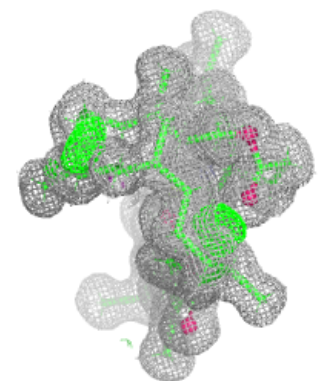
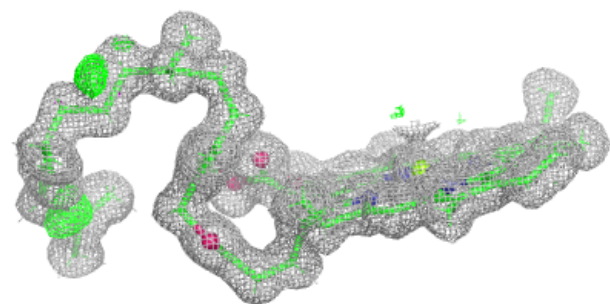
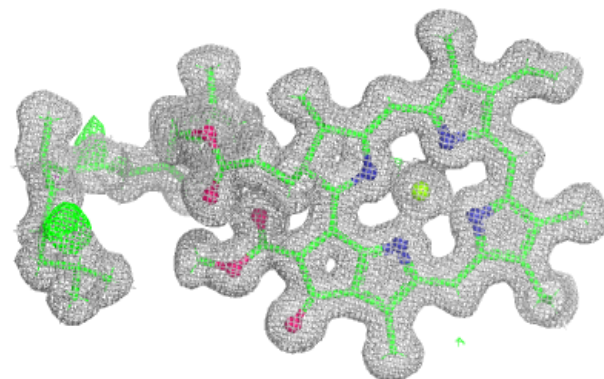


Electron density around CLA O 601:

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

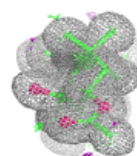
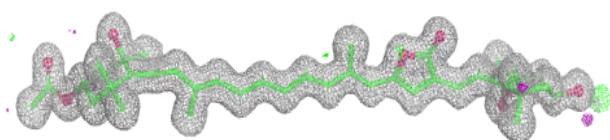
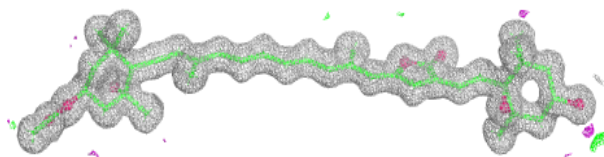
**Electron density around CLA O 602:**

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

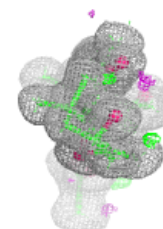
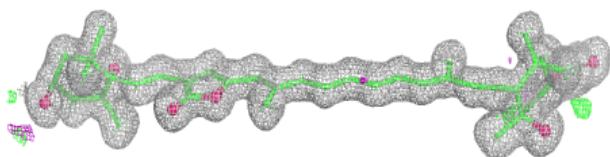
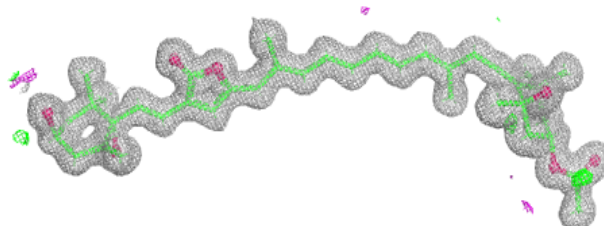


Electron density around PID N 621:

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

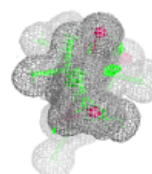
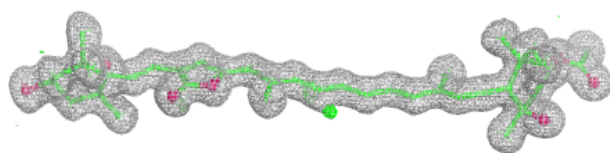
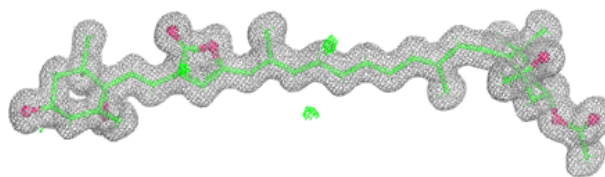
**Electron density around PID N 622:**

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

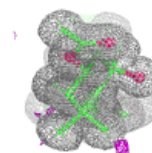
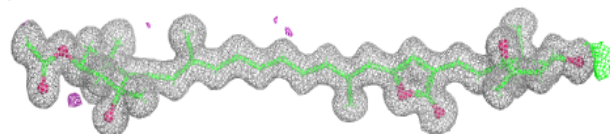
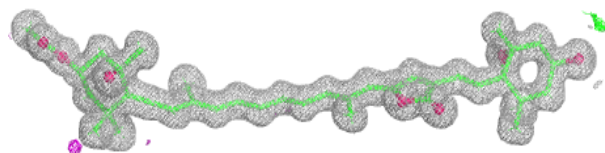


Electron density around PID M 614:

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

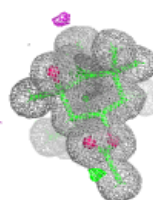
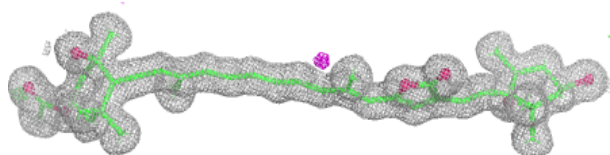
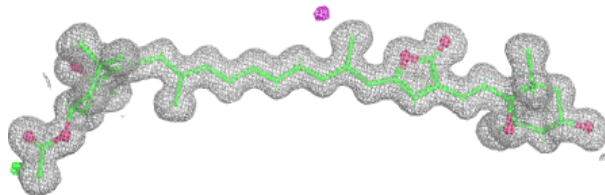
**Electron density around PID M 621:**

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

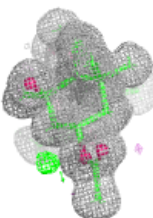
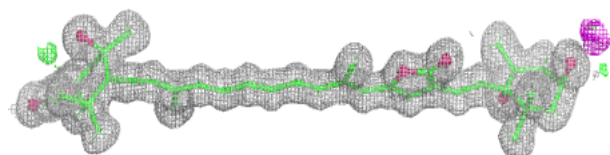
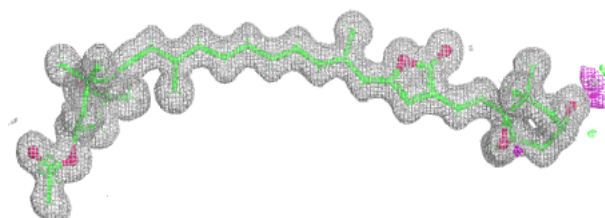


Electron density around PID N 624:

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

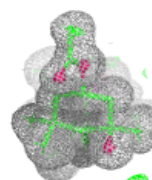
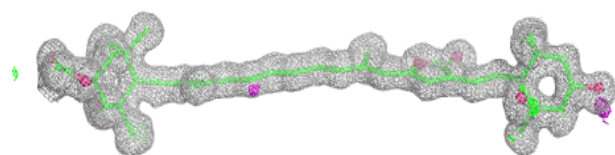
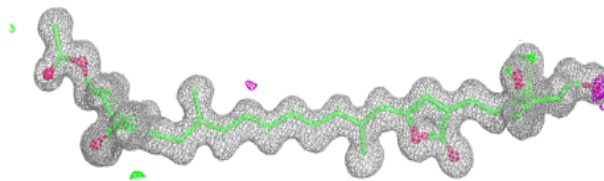
**Electron density around PID M 622:**

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

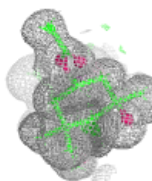
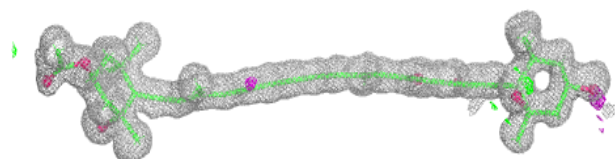
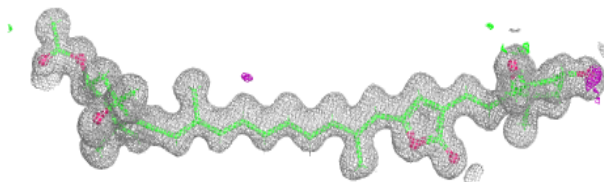


Electron density around PID M 623 (A):

$2mF_o-DF_c$ (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.