



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:11 pm BST

PDB ID : 3IIS  
Title : Structure of the reconstituted Peridinin-Chlorophyll a-Protein (RFPCP)  
Authors : Schulte, T.; Hofmann, E.  
Deposited on : 2009-08-03  
Resolution : 1.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

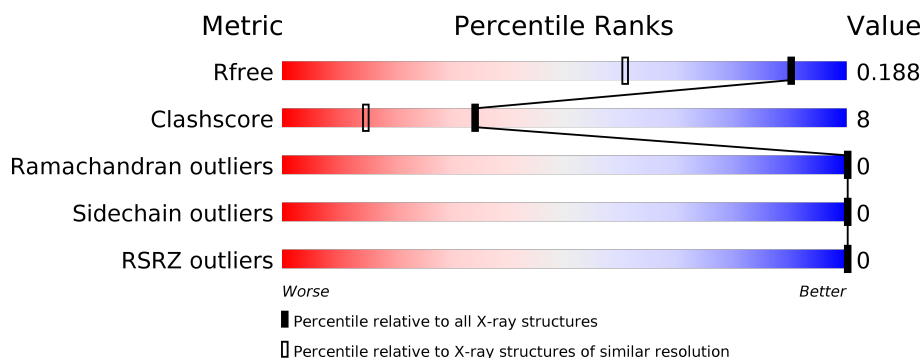
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	151	

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
7	CL	M	161[A]	-	-	X	-
7	CL	M	161[B]	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 1910 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

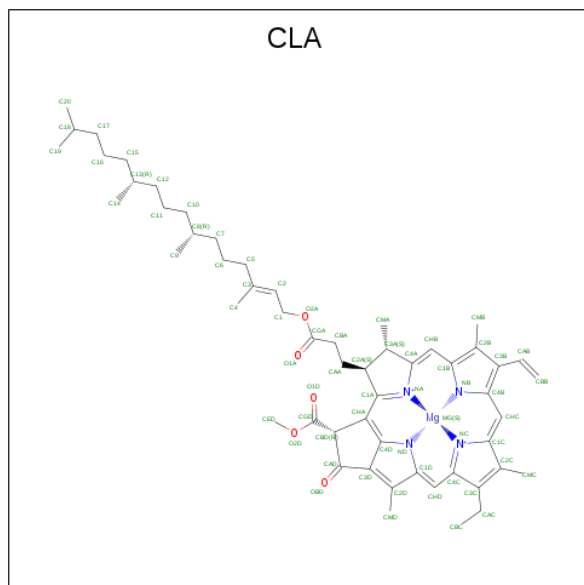
- Molecule 1 is a protein called Peridinin-chlorophyll a-binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	151	1249	795	208	240	6	0	18	0

There are 2 discrepancies between the modelled and reference sequences:

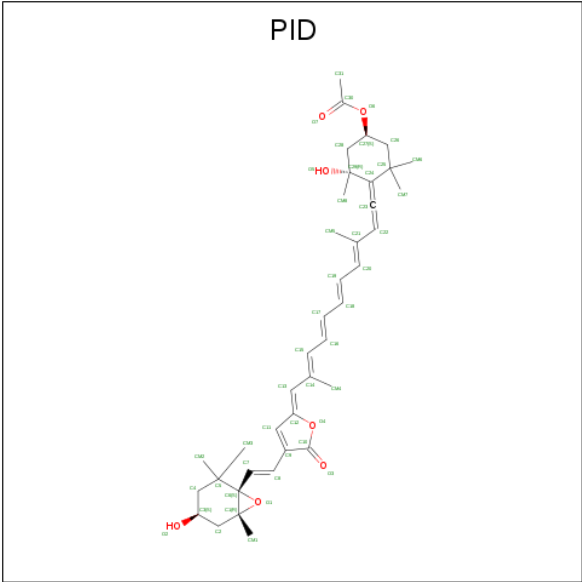
Chain	Residue	Modelled	Actual	Comment	Reference
M	87	SER	ASN	SEE REMARK 999	UNP P80484
M	128	ASN	SER	SEE REMARK 999	UNP P80484

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



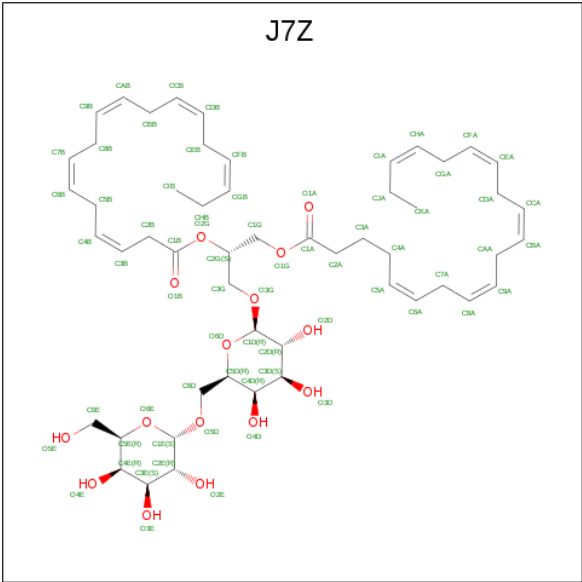
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
2	M	1	68	58	1	4	5	0	1

- Molecule 3 is PERIDININ (three-letter code: PID) (formula:  $C_{39}H_{50}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	1
			57	48	9		
3	M	1	Total	C	O	0	1
			51	42	9		
3	M	1	Total	C	O	0	1
			62	51	11		
3	M	1	Total	C	O	0	0
			46	39	7		

- Molecule 4 is (2S)-3-[(6-O-alpha-D-galactopyranosyl-beta-D-galactopyranosyl)oxy]-2-[(3Z,6Z,9Z,12Z,15Z)-octadeca-3,6,9,12,15-pentaenoxy]propyl (5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoate (three-letter code: J7Z) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	1
			75	59	16		

- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	4	Total	Cd	0	1
			5	5		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	3	Total	K	0	1
			4	4		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	5	Total	Cl	0	2
			7	7		


- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	286	Total	O	0	0
			286	286		

### 3 Residue-property plots

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

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

Chain M:  89% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.69Å 81.62Å 75.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.85 – 1.40 35.86 – 1.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.85-1.40) 95.7 (35.86-1.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.152 , 0.187 0.153 , 0.188	Depositor DCC
$R_{free}$ test set	2002 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	1910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: J7Z, CL, K, PID, CLA, CD

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	0.73	0/1291	0.77	2/1736 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	M	5	ASP	CB-CG-OD1	6.71	124.34	118.30
1	M	5	ASP	CB-CG-OD2	-5.54	113.31	118.30

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	1249	0	1284	21	0
2	M	68	0	6	1	0
3	M	216	0	146	2	0
4	M	75	0	24	0	0
5	M	5	0	0	2	0
6	M	4	0	0	1	0
7	M	7	0	0	8	0
8	M	286	0	0	11	0
All	All	1910	0	1460	27	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (27) 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)
6:M:155:K:K	7:M:162[B]:CL:CL	1.86	1.20
5:M:152[B]:CD:CD	7:M:159:CL:CL	1.60	1.07
1:M:30[B]:GLN:NE2	8:M:355:HOH:O	1.86	1.07
5:M:153:CD:CD	7:M:161[B]:CL:CL	1.52	0.95
1:M:116:ASP:OD2	7:M:161[B]:CL:CL	2.33	0.84
1:M:134[B]:LYS:HE3	8:M:320:HOH:O	1.90	0.71
1:M:39[B]:GLU:OE2	8:M:283:HOH:O	2.07	0.71
1:M:64[A]:GLU:OE1	8:M:411:HOH:O	2.09	0.70
1:M:105:MET:CA	8:M:247:HOH:O	2.25	0.66
1:M:102[B]:ASN:ND2	8:M:207:HOH:O	2.29	0.64
1:M:134[B]:LYS:HD3	8:M:324:HOH:O	1.97	0.63
1:M:64[B]:GLU:OE2	8:M:258:HOH:O	2.18	0.56
1:M:116:ASP:OD1	7:M:161[B]:CL:CL	2.61	0.56
1:M:116:ASP:OD1	7:M:161[A]:CL:CL	2.61	0.55
1:M:116:ASP:CG	7:M:161[B]:CL:CL	2.81	0.55
1:M:105:MET:C	8:M:247:HOH:O	2.44	0.54
1:M:105:MET:HA	8:M:247:HOH:O	1.99	0.52
3:M:613[A]:PID:O2	8:M:190:HOH:O	1.85	0.52
1:M:118:LYS:HG3	7:M:161[A]:CL:CL	2.47	0.51
1:M:44:ILE:HD13	1:M:47[B]:MET:HE3	1.92	0.51
1:M:44:ILE:HD13	1:M:47[B]:MET:CE	2.44	0.48
3:M:613[A]:PID:HM22	3:M:613[A]:PID:O2	2.13	0.48
1:M:57[A]:LYS:HE3	1:M:57[A]:LYS:HB3	1.55	0.47
1:M:8[A]:LYS:HD3	1:M:8[A]:LYS:O	2.19	0.43
1:M:19[A]:LYS:HG2	1:M:79:VAL:HG11	2.01	0.42

There are no symmetry-related clashes.

## 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	167/151 (111%)	166 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	132/114 (116%)	132 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	24	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 16 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	PID	M	612[B]	-	41,49,49	1.30	5 (12%)	49,76,76	3.94	17 (34%)
3	PID	M	614	-	41,49,49	1.15	4 (9%)	49,76,76	2.96	15 (30%)
3	PID	M	613[A]	-	41,49,49	1.23	3 (7%)	49,76,76	2.50	18 (36%)
2	CLA	M	601[B]	-	59,73,73	1.44	9 (15%)	67,113,113	1.45	10 (14%)
4	J7Z	M	615[A]	-	69,69,69	0.72	2 (2%)	80,83,83	1.02	5 (6%)
3	PID	M	612[A]	-	41,49,49	1.36	5 (12%)	49,76,76	3.92	17 (34%)
2	CLA	M	601[A]	-	59,73,73	1.42	9 (15%)	67,113,113	1.47	10 (14%)
3	PID	M	611[B]	-	41,49,49	1.28	5 (12%)	49,76,76	2.79	12 (24%)
3	PID	M	611[A]	-	41,49,49	1.28	4 (9%)	49,76,76	2.72	14 (28%)
4	J7Z	M	615[B]	-	69,69,69	0.72	2 (2%)	80,83,83	1.11	7 (8%)
3	PID	M	613[B]	-	41,49,49	1.14	2 (4%)	49,76,76	2.46	15 (30%)

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[B]	-	-	0/24/93/93	0/4/4/4
3	PID	M	614	-	-	0/24/93/93	0/4/4/4
3	PID	M	613[A]	-	-	2/24/93/93	0/4/4/4
2	CLA	M	601[B]	-	-	2/37/135/135	-
4	J7Z	M	615[A]	-	-	7/57/97/97	0/2/2/2
3	PID	M	612[A]	-	-	0/24/93/93	0/4/4/4
2	CLA	M	601[A]	-	-	2/37/135/135	-
3	PID	M	611[B]	-	-	0/24/93/93	0/4/4/4
3	PID	M	611[A]	-	-	0/24/93/93	0/4/4/4
4	J7Z	M	615[B]	-	-	8/57/97/97	0/2/2/2
3	PID	M	613[B]	-	-	0/24/93/93	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	601[B]	CLA	CHC-C1C	4.42	1.46	1.35
2	M	601[A]	CLA	CHC-C1C	4.42	1.46	1.35
2	M	601[B]	CLA	C4B-NB	4.05	1.38	1.35
2	M	601[A]	CLA	C4B-NB	4.05	1.38	1.35
3	M	612[A]	PID	O6-C30	3.98	1.44	1.35
3	M	614	PID	C13-C12	3.89	1.47	1.36
3	M	612[A]	PID	C13-C12	3.88	1.47	1.36
3	M	612[B]	PID	C13-C12	3.88	1.47	1.36
3	M	613[A]	PID	C13-C12	3.70	1.46	1.36
3	M	613[B]	PID	C13-C12	3.70	1.46	1.36
3	M	611[B]	PID	C13-C12	3.70	1.46	1.36
3	M	611[A]	PID	C13-C12	3.70	1.46	1.36
2	M	601[B]	CLA	OBD-CAD	3.68	1.27	1.22
2	M	601[A]	CLA	OBD-CAD	3.68	1.27	1.22
3	M	613[A]	PID	O6-C30	3.64	1.43	1.35
2	M	601[B]	CLA	C1B-CHB	3.23	1.50	1.41
2	M	601[A]	CLA	C1B-CHB	3.23	1.50	1.41
3	M	613[B]	PID	O6-C30	3.21	1.42	1.35
3	M	612[A]	PID	O3-C10	3.15	1.28	1.21
3	M	612[B]	PID	O3-C10	3.15	1.28	1.21
4	M	615[B]	J7Z	O2G-C1B	3.02	1.42	1.34
4	M	615[A]	J7Z	O2G-C1B	3.02	1.42	1.34
3	M	613[A]	PID	C26-C27	2.86	1.56	1.51
3	M	612[B]	PID	O6-C30	2.85	1.41	1.35
2	M	601[B]	CLA	O2D-CGD	2.83	1.40	1.33
2	M	601[A]	CLA	O2D-CGD	2.83	1.40	1.33
3	M	614	PID	C2-C1	2.78	1.56	1.52
3	M	611[B]	PID	O3-C10	2.65	1.27	1.21
3	M	611[A]	PID	O3-C10	2.65	1.27	1.21
2	M	601[B]	CLA	CHD-C4C	2.60	1.48	1.41
2	M	601[A]	CLA	CHD-C4C	2.60	1.48	1.41
3	M	611[B]	PID	O6-C30	2.57	1.41	1.35
3	M	611[A]	PID	O6-C30	2.57	1.41	1.35
4	M	615[B]	J7Z	O5D-C1E	2.52	1.44	1.40
4	M	615[A]	J7Z	O5D-C1E	2.52	1.44	1.40
3	M	614	PID	O3-C10	2.51	1.26	1.21
2	M	601[B]	CLA	C4C-C3C	-2.22	1.41	1.45
2	M	601[A]	CLA	C4C-C3C	-2.22	1.41	1.45
3	M	611[B]	PID	C11-C12	-2.18	1.40	1.44
3	M	611[A]	PID	C11-C12	-2.18	1.40	1.44
2	M	601[B]	CLA	MG-NA	2.14	2.11	2.06
2	M	601[A]	CLA	MG-NA	2.14	2.11	2.06
3	M	614	PID	O6-C30	2.13	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	612[A]	PID	O1-C1	-2.07	1.43	1.46
3	M	612[B]	PID	O1-C1	-2.07	1.43	1.46
3	M	611[B]	PID	O1-C1	-2.02	1.43	1.46
3	M	612[A]	PID	C2-C1	2.02	1.54	1.52
3	M	612[B]	PID	C2-C1	2.02	1.54	1.52
2	M	601[B]	CLA	CAA-C2A	2.00	1.57	1.54
2	M	601[A]	CLA	CAA-C2A	2.00	1.57	1.54

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	612[A]	PID	O4-C12-C11	19.00	118.88	107.36
3	M	612[B]	PID	O4-C12-C11	19.00	118.88	107.36
3	M	612[A]	PID	C12-O4-C10	-13.90	100.42	107.65
3	M	612[B]	PID	C12-O4-C10	-13.90	100.42	107.65
3	M	611[B]	PID	O4-C12-C11	12.93	115.20	107.36
3	M	611[A]	PID	O4-C12-C11	12.93	115.20	107.36
3	M	614	PID	O4-C12-C11	12.76	115.10	107.36
3	M	613[A]	PID	O4-C12-C11	10.01	113.43	107.36
3	M	613[B]	PID	O4-C12-C11	10.01	113.43	107.36
3	M	614	PID	C12-O4-C10	-9.98	102.46	107.65
3	M	611[B]	PID	O1-C1-C2	8.85	120.03	113.38
3	M	613[A]	PID	O1-C1-CM1	6.74	123.13	115.06
3	M	613[B]	PID	O1-C1-C2	6.66	118.38	113.38
3	M	611[A]	PID	O1-C1-C2	6.55	118.31	113.38
2	M	601[B]	CLA	C4D-C3D-CAD	-5.72	105.28	108.47
2	M	601[A]	CLA	C4D-C3D-CAD	-5.72	105.28	108.47
3	M	614	PID	O1-C1-C2	5.54	117.54	113.38
3	M	612[A]	PID	O1-C1-CM1	5.28	121.38	115.06
3	M	612[B]	PID	O1-C1-CM1	5.28	121.38	115.06
3	M	614	PID	O4-C10-C9	5.11	112.31	108.04
3	M	611[B]	PID	C12-O4-C10	-5.10	105.00	107.65
3	M	611[A]	PID	C12-O4-C10	-5.10	105.00	107.65
3	M	613[A]	PID	C12-O4-C10	-4.70	105.21	107.65
3	M	613[B]	PID	C12-O4-C10	-4.70	105.21	107.65
3	M	613[A]	PID	C6-C7-C8	-4.49	116.49	125.99
3	M	611[A]	PID	O1-C1-CM1	4.44	120.37	115.06
3	M	612[B]	PID	O6-C27-C28	-4.35	96.76	107.59
3	M	612[A]	PID	O4-C10-C9	4.28	111.62	108.04
3	M	612[B]	PID	O4-C10-C9	4.28	111.62	108.04
3	M	612[A]	PID	C11-C12-C13	-4.18	119.10	128.34
3	M	612[B]	PID	C11-C12-C13	-4.18	119.10	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	611[B]	PID	C8-C9-C11	-4.04	119.60	127.37
3	M	611[A]	PID	C8-C9-C11	-4.04	119.60	127.37
3	M	612[A]	PID	C6-C7-C8	-3.93	117.69	125.99
3	M	612[B]	PID	C6-C7-C8	-3.93	117.69	125.99
3	M	614	PID	O3-C10-C9	-3.91	126.29	130.74
2	M	601[B]	CLA	C2C-C1C-NC	3.89	113.61	109.97
2	M	601[A]	CLA	C2C-C1C-NC	3.89	113.61	109.97
2	M	601[B]	CLA	C4A-NA-C1A	-3.88	104.96	106.71
2	M	601[A]	CLA	C4A-NA-C1A	-3.88	104.96	106.71
4	M	615[B]	J7Z	O6E-C5E-C6E	3.85	116.02	106.44
3	M	611[B]	PID	C6-C7-C8	-3.80	117.96	125.99
3	M	613[B]	PID	O1-C1-CM1	3.73	119.53	115.06
3	M	613[B]	PID	O6-C27-C26	-3.65	98.51	107.59
3	M	613[A]	PID	O6-C27-C26	3.60	116.55	107.59
3	M	614	PID	C18-C19-C20	-3.51	116.28	123.47
3	M	613[B]	PID	C6-C7-C8	-3.25	119.11	125.99
3	M	611[A]	PID	C6-C7-C8	-3.22	119.18	125.99
4	M	615[B]	J7Z	O2E-C2E-C3E	-3.20	102.95	110.35
4	M	615[A]	J7Z	O2E-C2E-C3E	-3.20	102.95	110.35
3	M	612[A]	PID	O1-C1-C2	3.19	115.78	113.38
3	M	612[B]	PID	O1-C1-C2	3.19	115.78	113.38
3	M	613[A]	PID	O6-C30-C31	3.14	116.88	111.09
3	M	612[A]	PID	C26-C25-C24	-3.11	106.19	109.21
3	M	612[B]	PID	C26-C25-C24	-3.11	106.19	109.21
3	M	611[B]	PID	C11-C12-C13	-3.07	121.56	128.34
3	M	611[A]	PID	C11-C12-C13	-3.07	121.56	128.34
3	M	614	PID	CM1-C1-C6	-3.00	117.24	122.26
3	M	612[A]	PID	CM1-C1-C6	-2.97	117.28	122.26
3	M	612[B]	PID	CM1-C1-C6	-2.97	117.28	122.26
3	M	612[A]	PID	O6-C30-C31	2.96	116.54	111.09
3	M	613[A]	PID	C11-C12-C13	-2.93	121.85	128.34
3	M	613[B]	PID	C11-C12-C13	-2.93	121.85	128.34
3	M	614	PID	C29-C24-C25	-2.93	116.78	119.70
3	M	612[A]	PID	CM7-C25-C24	2.93	113.09	110.47
3	M	612[B]	PID	CM7-C25-C24	2.93	113.09	110.47
3	M	614	PID	C6-C7-C8	-2.92	119.81	125.99
3	M	613[B]	PID	CM1-C1-C6	-2.89	117.41	122.26
3	M	612[A]	PID	O6-C27-C28	2.84	114.65	107.59
2	M	601[B]	CLA	C4-C3-C5	2.77	119.93	115.27
2	M	601[A]	CLA	C4-C3-C5	2.77	119.93	115.27
2	M	601[B]	CLA	C3C-C4C-NC	2.76	113.67	110.57
2	M	601[A]	CLA	C3C-C4C-NC	2.76	113.67	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	601[B]	CLA	OBD-CAD-CBD	-2.74	121.98	125.89
2	M	601[A]	CLA	OBD-CAD-CBD	-2.74	121.98	125.89
3	M	614	PID	O6-C30-C31	2.69	116.03	111.09
3	M	613[A]	PID	CM1-C1-C6	-2.67	117.78	122.26
3	M	613[A]	PID	O1-C1-C2	2.65	115.37	113.38
3	M	611[B]	PID	C18-C19-C20	-2.63	118.09	123.47
3	M	611[A]	PID	C18-C19-C20	-2.63	118.09	123.47
3	M	611[A]	PID	CM1-C1-C2	-2.62	111.34	114.28
3	M	612[B]	PID	O6-C27-C26	2.60	114.07	107.59
3	M	611[A]	PID	O1-C1-C6	-2.60	56.81	58.96
2	M	601[A]	CLA	CMB-C2B-C3B	2.57	129.50	124.68
3	M	612[A]	PID	O1-C1-C6	-2.55	56.85	58.96
3	M	612[B]	PID	O1-C1-C6	-2.55	56.85	58.96
3	M	613[A]	PID	O6-C27-C28	-2.53	101.29	107.59
3	M	614	PID	O6-C30-O7	-2.53	117.94	122.96
3	M	613[A]	PID	CM6-C25-C24	2.49	112.70	110.47
3	M	613[B]	PID	CM6-C25-C24	2.49	112.70	110.47
3	M	611[B]	PID	O1-C1-C6	-2.45	56.93	58.96
4	M	615[B]	J7Z	C2B-C3B-C4B	-2.43	119.35	125.03
3	M	613[A]	PID	O5-C29-CM8	-2.38	105.16	109.39
3	M	613[B]	PID	O5-C29-CM8	-2.38	105.16	109.39
3	M	613[A]	PID	CM4-C14-C13	2.37	124.52	119.05
3	M	613[B]	PID	CM4-C14-C13	2.37	124.52	119.05
3	M	612[A]	PID	C17-C18-C19	-2.35	119.58	124.81
3	M	612[B]	PID	C17-C18-C19	-2.35	119.58	124.81
3	M	611[B]	PID	O6-C30-O7	-2.33	118.34	122.96
3	M	611[A]	PID	O6-C30-O7	-2.33	118.34	122.96
4	M	615[B]	J7Z	O1G-C1A-O1A	-2.30	117.78	123.59
4	M	615[A]	J7Z	O1G-C1A-O1A	-2.30	117.78	123.59
3	M	613[A]	PID	O1-C1-C6	-2.24	57.10	58.96
4	M	615[B]	J7Z	C4E-C3E-C2E	2.24	114.73	110.82
4	M	615[A]	J7Z	C4E-C3E-C2E	2.24	114.73	110.82
3	M	611[B]	PID	O5-C29-CM8	-2.22	105.45	109.39
3	M	611[A]	PID	O5-C29-CM8	-2.22	105.45	109.39
4	M	615[B]	J7Z	C3D-C4D-C5D	-2.21	106.30	110.24
4	M	615[A]	J7Z	C3D-C4D-C5D	-2.21	106.30	110.24
2	M	601[B]	CLA	CHA-C1A-NA	-2.19	121.39	126.40
2	M	601[A]	CLA	CHA-C1A-NA	-2.19	121.39	126.40
3	M	614	PID	C11-C12-C13	-2.17	123.54	128.34
3	M	613[A]	PID	C8-C9-C11	-2.16	123.21	127.37
3	M	613[B]	PID	C8-C9-C11	-2.16	123.21	127.37
4	M	615[B]	J7Z	C1D-O6D-C5D	-2.16	109.45	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	615[A]	J7Z	C1D-O6D-C5D	-2.16	109.45	113.69
2	M	601[B]	CLA	CMB-C2B-C3B	2.16	128.71	124.68
3	M	613[A]	PID	C18-C19-C20	-2.15	119.07	123.47
3	M	613[B]	PID	C18-C19-C20	-2.15	119.07	123.47
2	M	601[B]	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
2	M	601[A]	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
3	M	612[A]	PID	C8-C9-C11	-2.11	123.31	127.37
3	M	612[B]	PID	C8-C9-C11	-2.11	123.31	127.37
3	M	613[A]	PID	O3-C10-C9	-2.11	128.34	130.74
3	M	613[B]	PID	O3-C10-C9	-2.11	128.34	130.74
3	M	614	PID	O2-C3-C2	-2.09	105.65	109.80
3	M	612[A]	PID	C17-C16-C15	-2.06	119.26	123.47
3	M	612[B]	PID	C17-C16-C15	-2.06	119.26	123.47
3	M	612[A]	PID	C18-C19-C20	-2.06	119.26	123.47
3	M	612[B]	PID	C18-C19-C20	-2.06	119.26	123.47
3	M	611[B]	PID	C18-C17-C16	-2.05	120.24	124.81
3	M	611[A]	PID	C18-C17-C16	-2.05	120.24	124.81
3	M	611[B]	PID	O3-C10-C9	-2.05	128.41	130.74
3	M	611[A]	PID	O3-C10-C9	-2.05	128.41	130.74
3	M	614	PID	C1-C2-C3	-2.05	108.69	112.75
2	M	601[B]	CLA	CHD-C4C-C3C	-2.04	121.84	124.84
2	M	601[A]	CLA	CHD-C4C-C3C	-2.04	121.84	124.84
3	M	613[A]	PID	O4-C10-C9	2.02	109.73	108.04
3	M	613[B]	PID	O4-C10-C9	2.02	109.73	108.04
3	M	614	PID	C8-C9-C11	-2.02	123.49	127.37

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	615[B]	J7Z	CCB-CDB-CEB-CFB
4	M	615[A]	J7Z	CCB-CDB-CEB-CFB
4	M	615[B]	J7Z	O6E-C5E-C6E-O5E
4	M	615[B]	J7Z	C1B-C2B-C3B-C4B
3	M	613[A]	PID	C31-C30-O6-C27
3	M	613[A]	PID	O7-C30-O6-C27
4	M	615[B]	J7Z	C3B-C4B-C5B-C6B
4	M	615[A]	J7Z	C3B-C4B-C5B-C6B
4	M	615[A]	J7Z	O6E-C5E-C6E-O5E
4	M	615[B]	J7Z	C9B-CAB-CBB-CCB
4	M	615[B]	J7Z	CBA-CCA-CDA-CEA
4	M	615[A]	J7Z	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
4	M	615[A]	J7Z	CBA-CCA-CDA-CEA
4	M	615[B]	J7Z	CHA-CIA-CJA-CKA
4	M	615[A]	J7Z	CHA-CIA-CJA-CKA
2	M	601[B]	CLA	CAD-CBD-CGD-O2D
2	M	601[A]	CLA	CAD-CBD-CGD-O2D
4	M	615[B]	J7Z	O6D-C5D-C6D-O5D
4	M	615[A]	J7Z	O6D-C5D-C6D-O5D
2	M	601[B]	CLA	CAA-CBA-CGA-O2A
2	M	601[A]	CLA	CAA-CBA-CGA-O2A

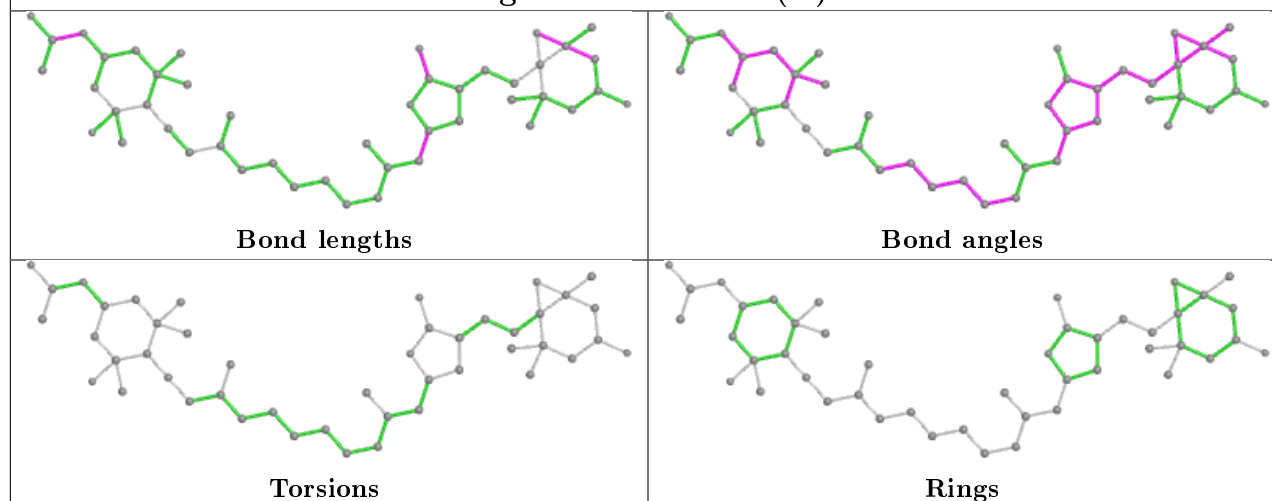
There are no ring outliers.

2 monomers are involved in 3 short contacts:

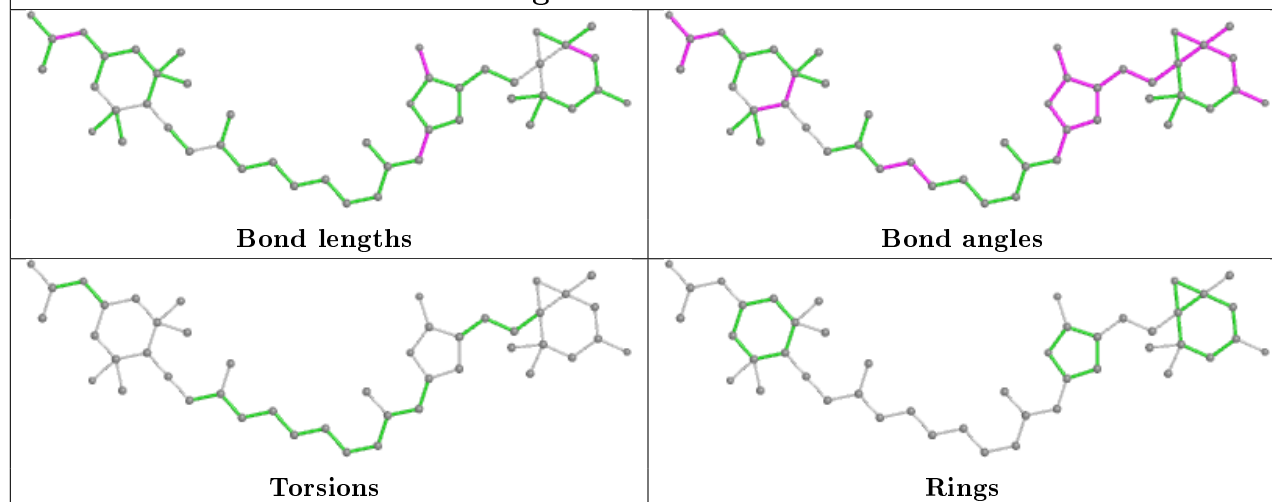
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	613[A]	PID	2	0
2	M	601[A]	CLA	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

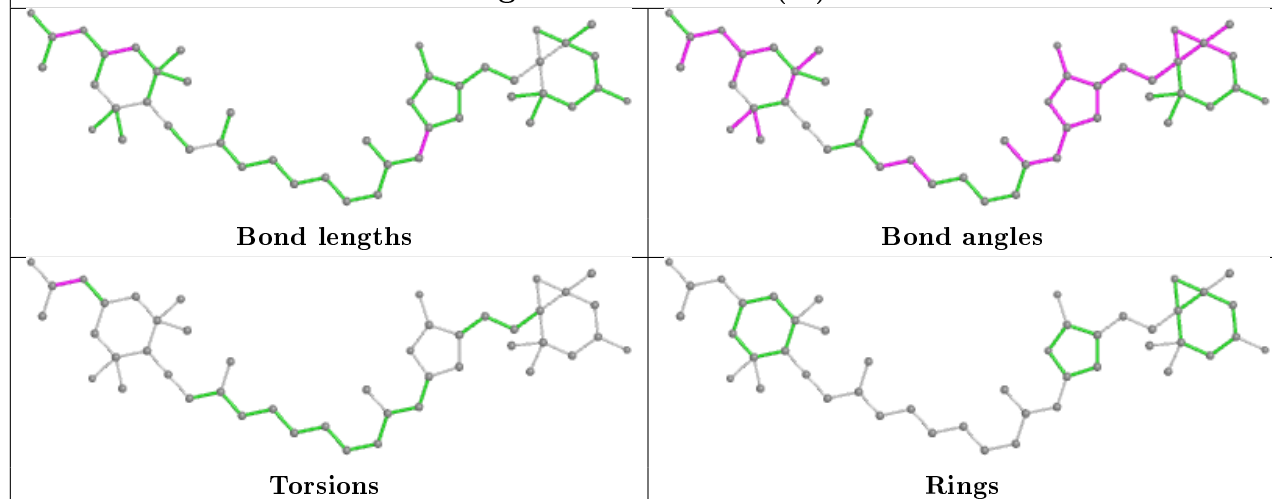
## Ligand PID M 612 (B)

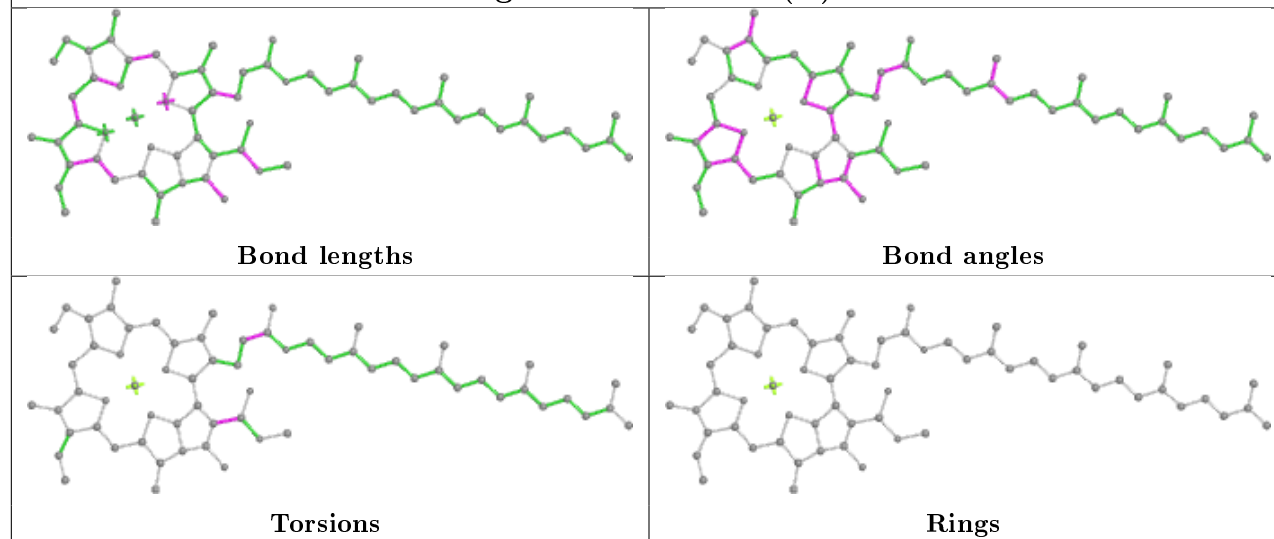
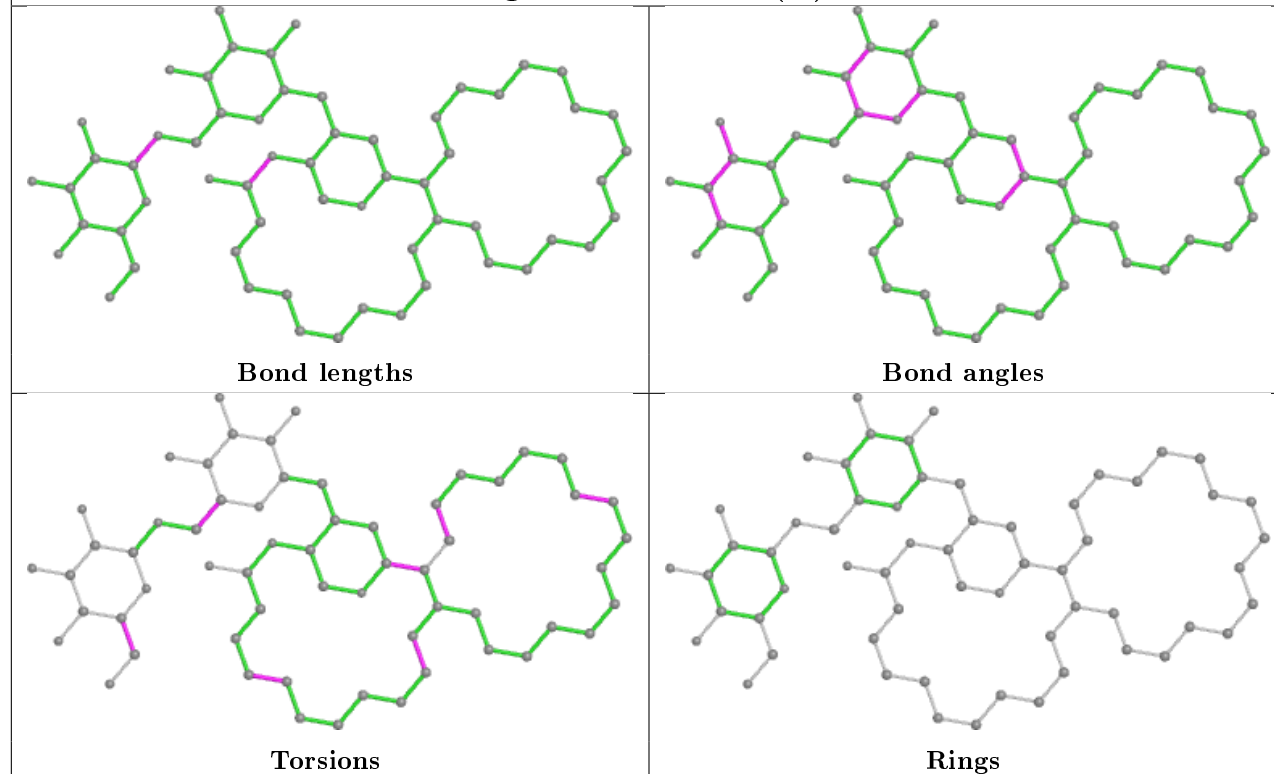


## Ligand PID M 614

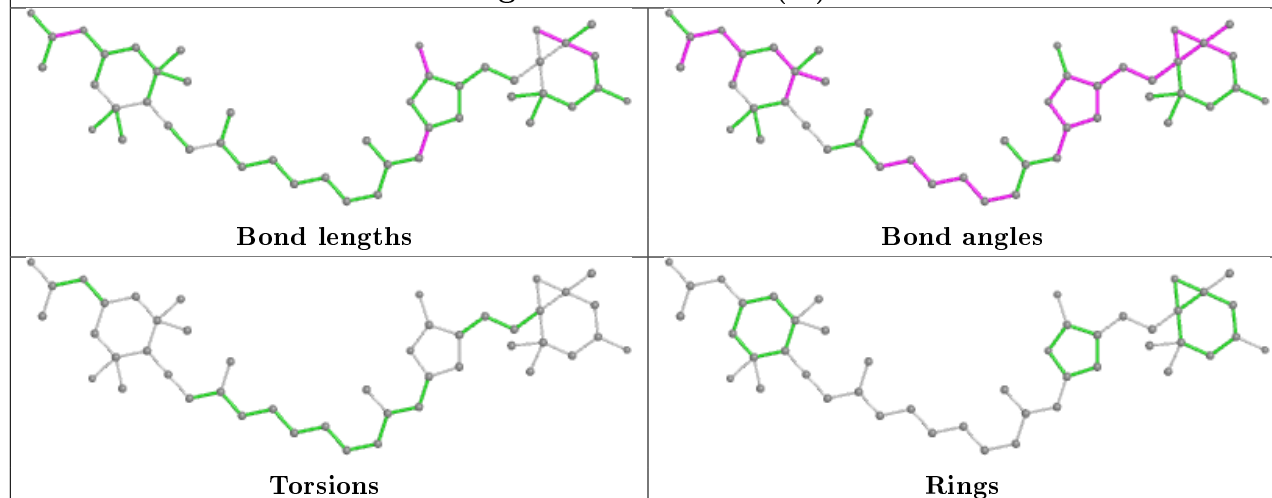


## Ligand PID M 613 (A)

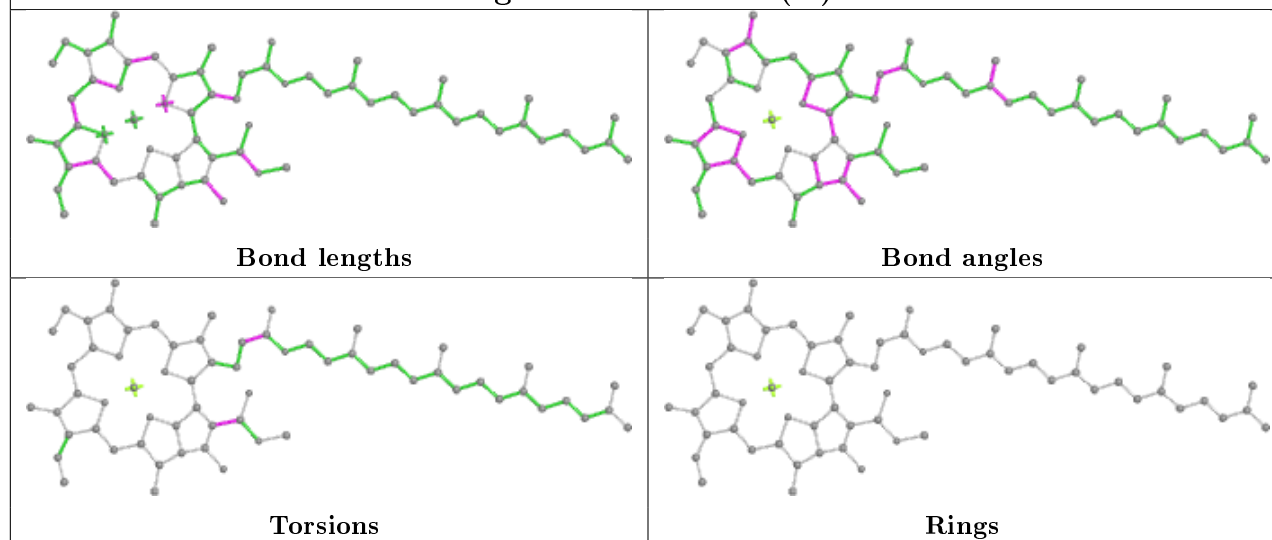


**Ligand CLA M 601 (B)****Ligand J7Z M 615 (A)**

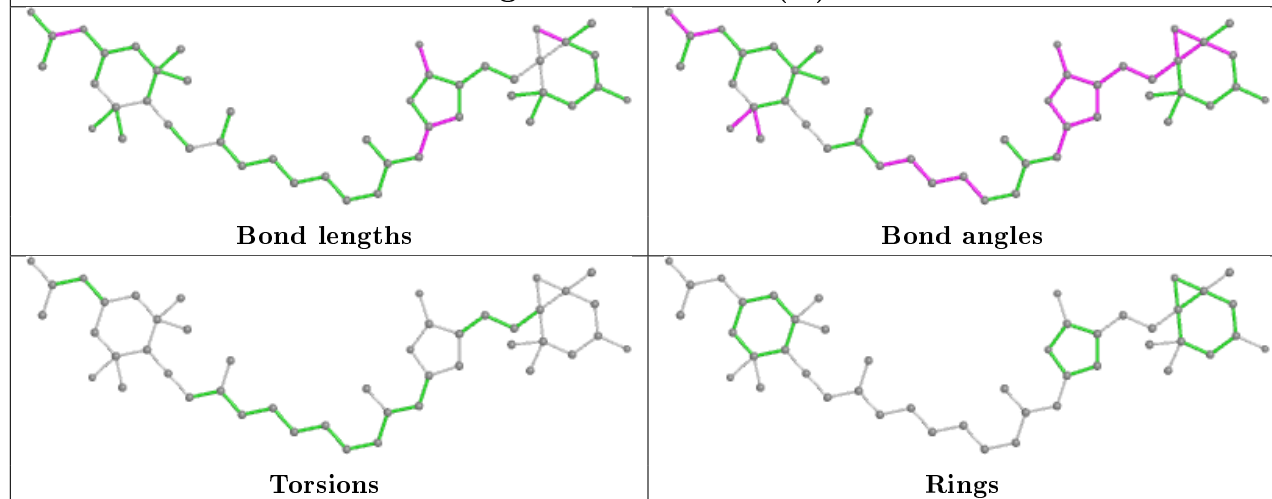
## Ligand PID M 612 (A)



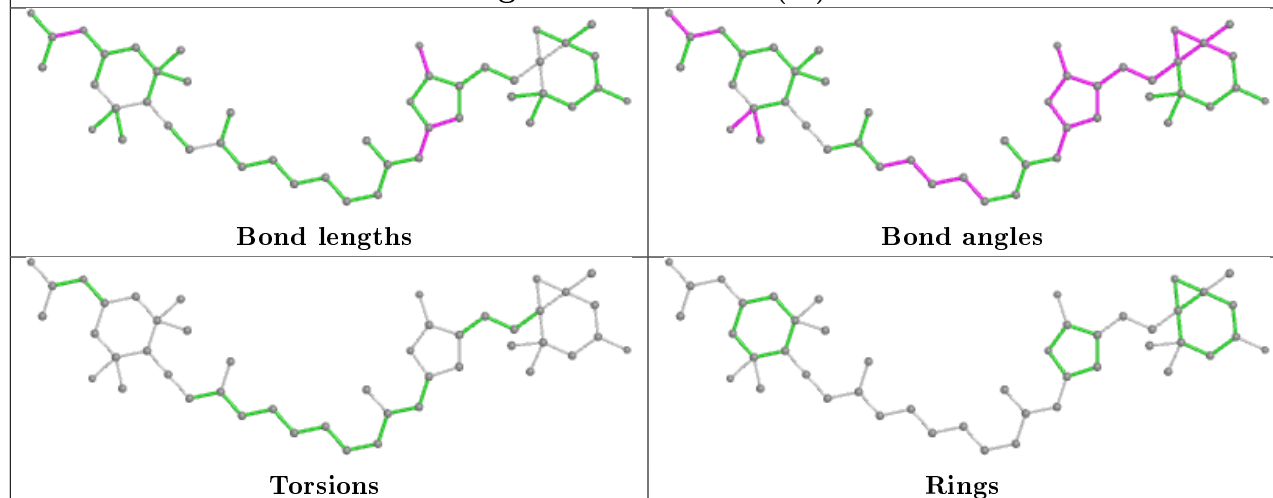
## Ligand CLA M 601 (A)



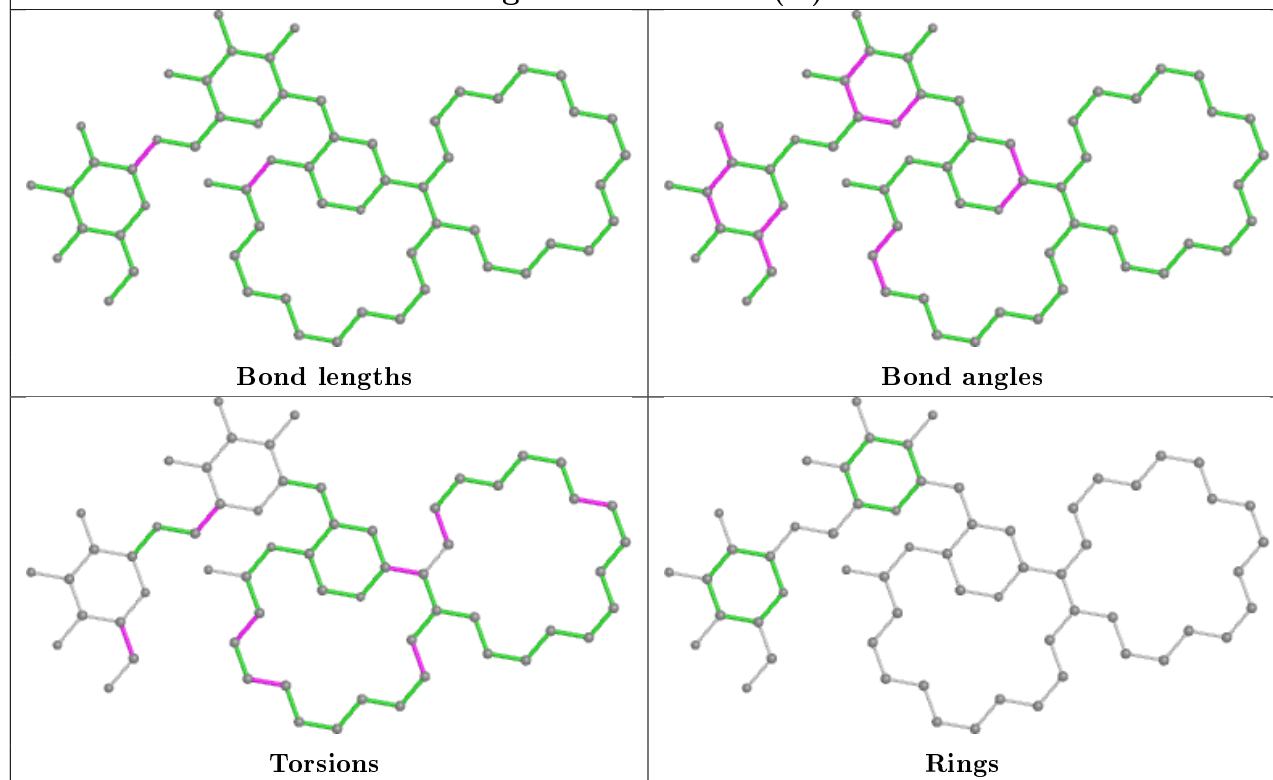
## Ligand PID M 611 (B)

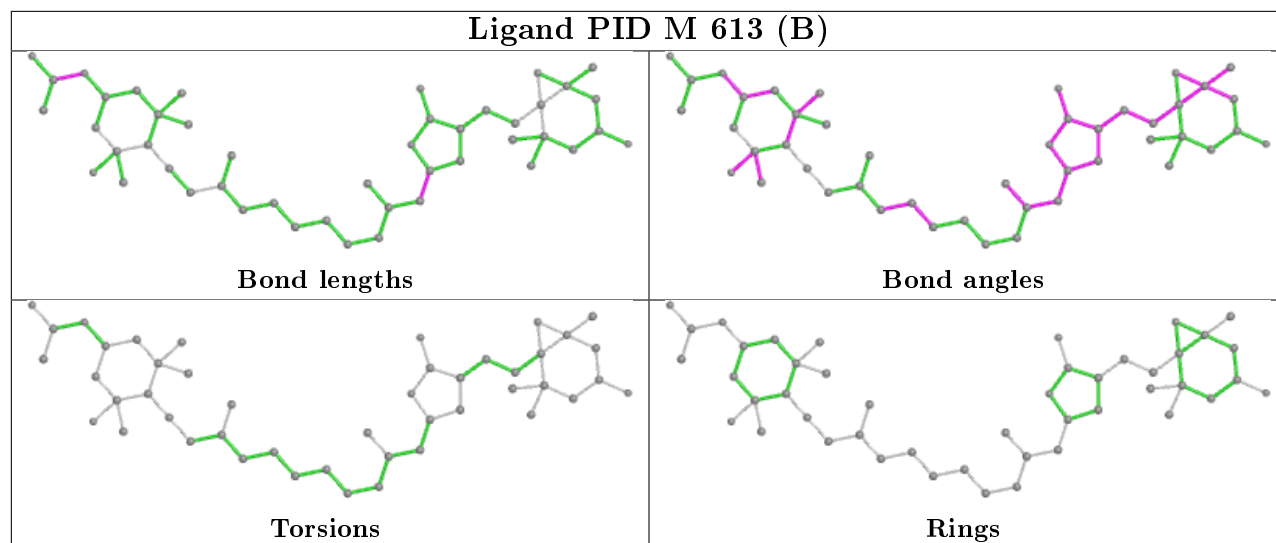


## Ligand PID M 611 (A)



## Ligand J7Z M 615 (B)





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	M	151/151 (100%)	-0.47	0 100 100	5, 8, 14, 20	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	CL	M	159	1/1	0.87	0.09	25,25,25,25	1
7	CL	M	162[B]	1/1	0.93	0.10	15,15,15,15	1
7	CL	M	162[A]	1/1	0.93	0.10	4,4,4,4	1
3	PID	M	612[A]	46/46	0.94	0.10	4,7,22,25	5
3	PID	M	612[B]	46/46	0.94	0.10	2,6,22,25	5
4	J7Z	M	615[A]	68/68	0.95	0.09	7,11,24,26	7
4	J7Z	M	615[B]	68/68	0.95	0.09	7,11,24,26	7
6	K	M	155	1/1	0.97	0.06	11,11,11,11	1
7	CL	M	161[B]	1/1	0.97	0.09	9,9,9,9	1

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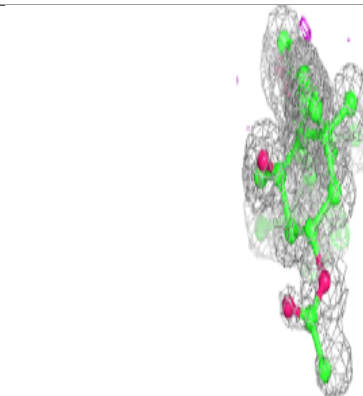
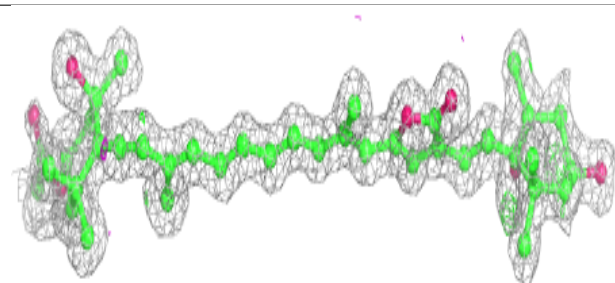
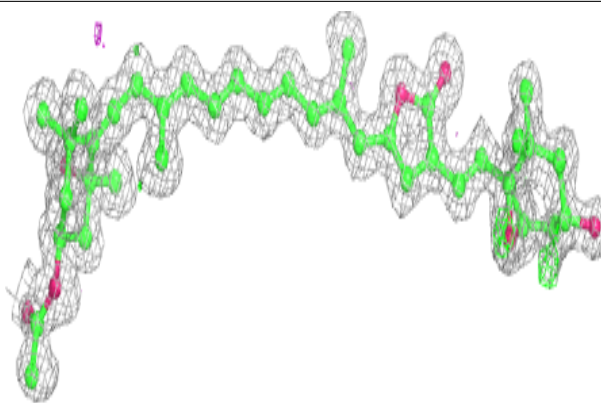
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PID	M	614	46/46	0.97	0.07	3,6,8,11	0
7	CL	M	161[A]	1/1	0.97	0.09	2,2,2,2	1
2	CLA	M	601[B]	65/65	0.97	0.08	3,6,8,11	3
2	CLA	M	601[A]	65/65	0.97	0.08	3,6,8,10	3
3	PID	M	611[B]	46/46	0.97	0.07	2,5,7,9	11
3	PID	M	611[A]	46/46	0.97	0.07	4,5,8,10	11
6	K	M	156[A]	1/1	0.98	0.07	9,9,9,9	1
3	PID	M	613[B]	46/46	0.98	0.08	3,6,8,12	16
5	CD	M	154	1/1	0.98	0.04	13,13,13,13	1
3	PID	M	613[A]	46/46	0.98	0.08	3,6,10,15	16
6	K	M	156[B]	1/1	0.98	0.07	20,20,20,20	1
7	CL	M	160	1/1	0.99	0.04	20,20,20,20	1
6	K	M	157	1/1	0.99	0.04	8,8,8,8	1
5	CD	M	152[B]	1/1	0.99	0.05	11,11,11,11	1
5	CD	M	152[A]	1/1	0.99	0.05	9,9,9,9	1
7	CL	M	158	1/1	0.99	0.06	7,7,7,7	0
5	CD	M	153	1/1	1.00	0.03	7,7,7,7	1
5	CD	M	151	1/1	1.00	0.04	6,6,6,6	0

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

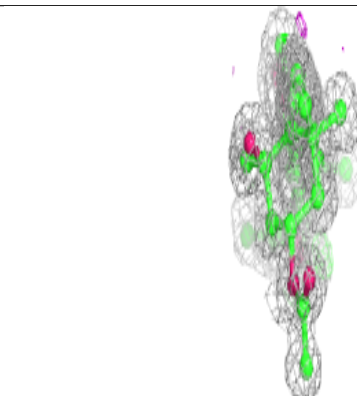
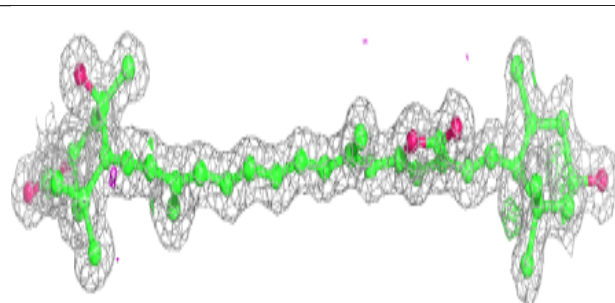
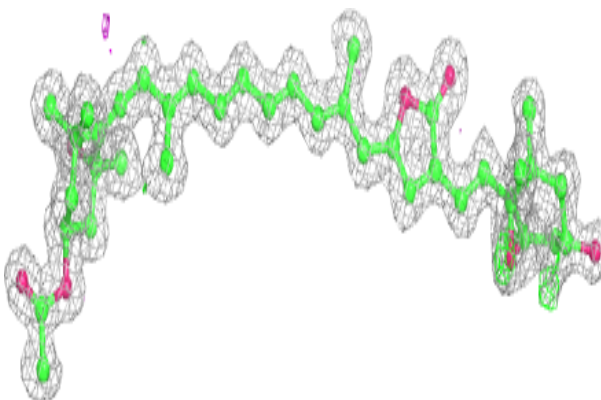


**Electron density around PID M 612 (A):**

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

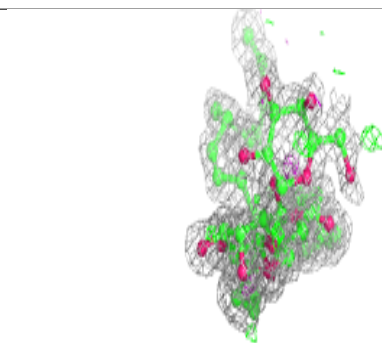
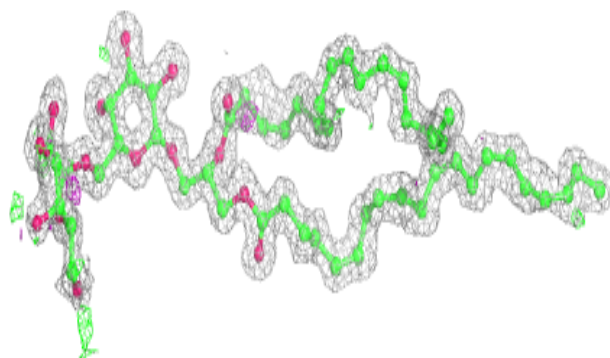
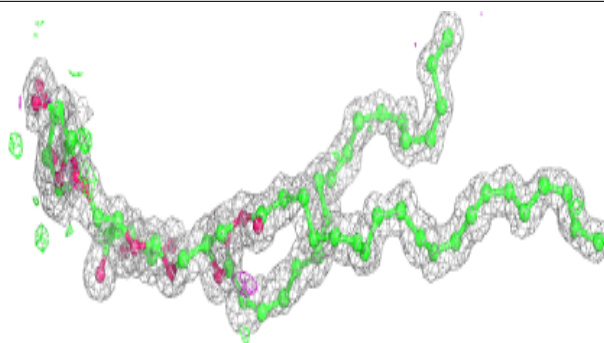
**Electron density around PID M 612 (B):**

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

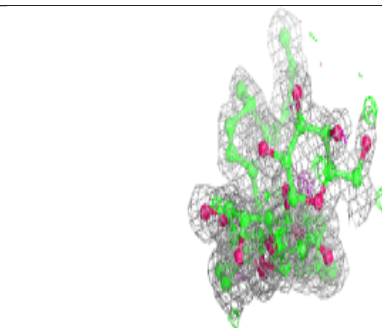
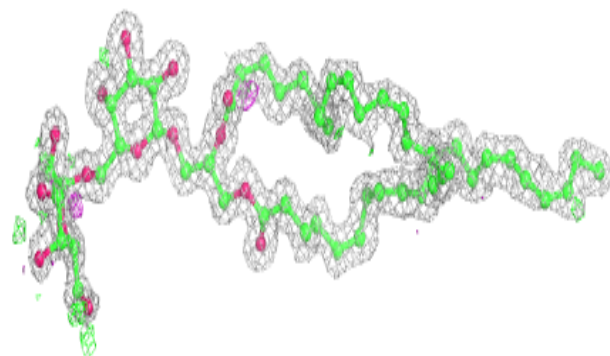
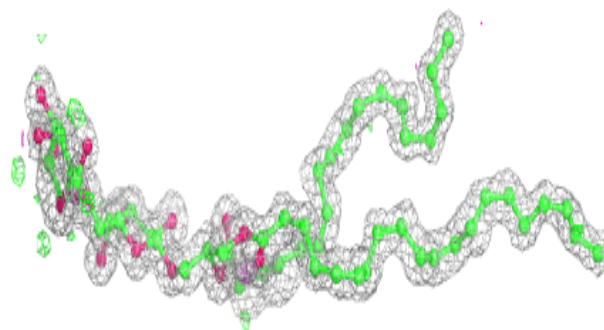


**Electron density around J7Z M 615 (A):**

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

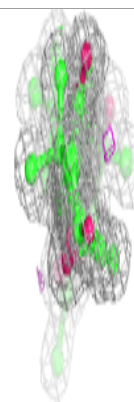
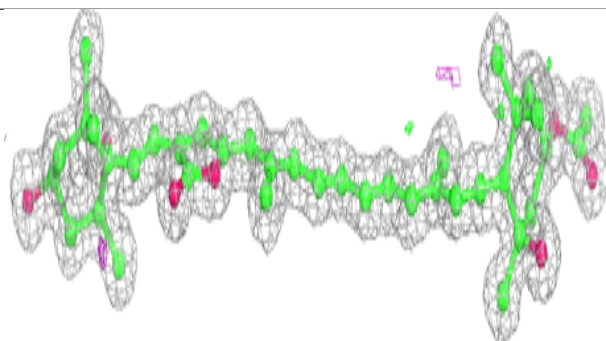
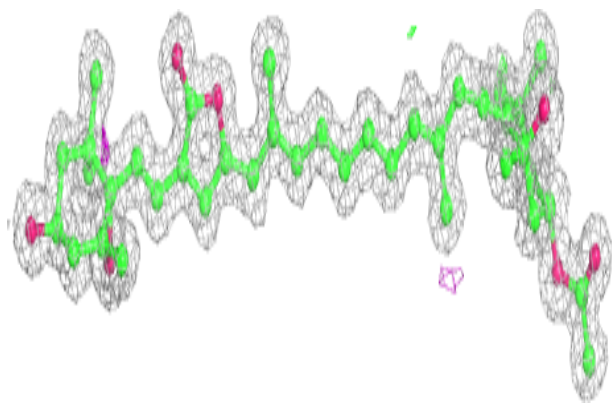
**Electron density around J7Z M 615 (B):**

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

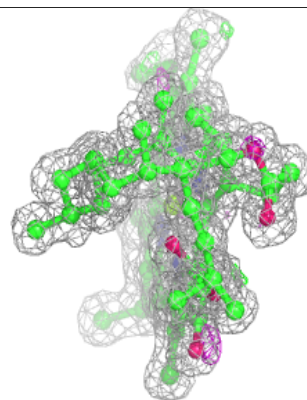
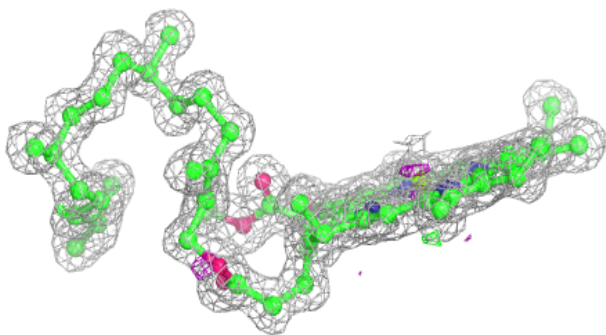
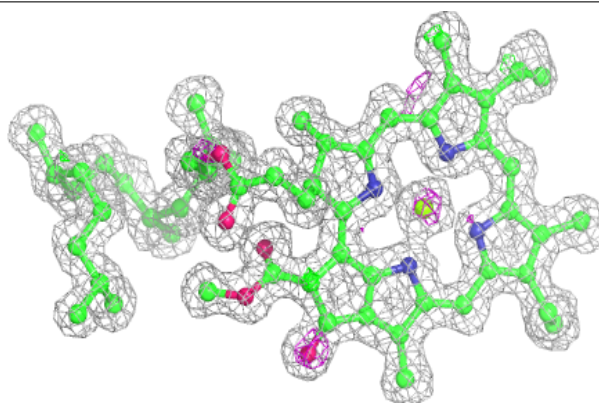


**Electron density around PID M 614:**

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

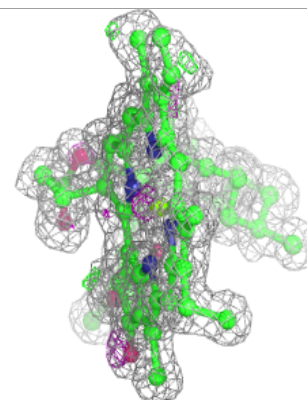
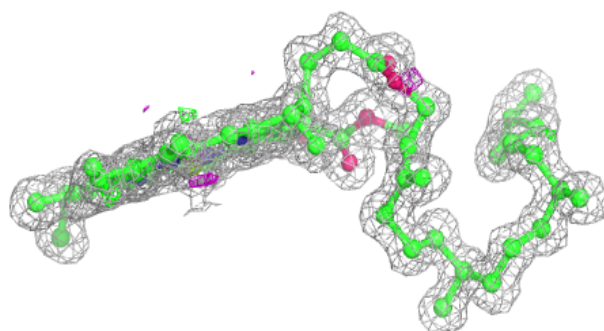
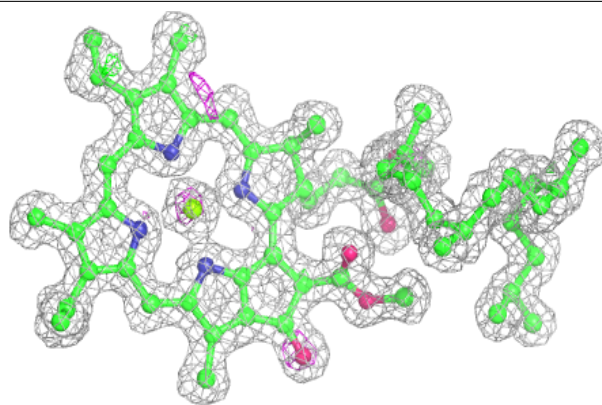
**Electron density around CLA M 601 (B):**

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

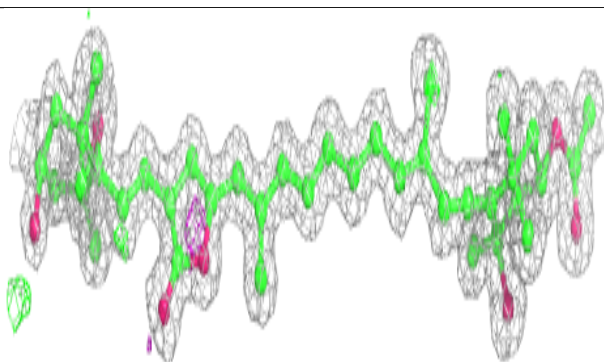
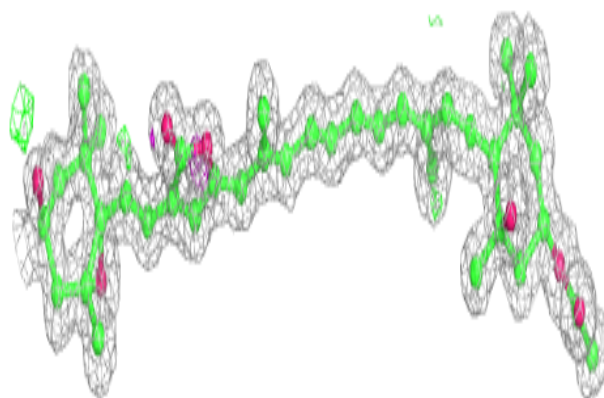


**Electron density around CLA M 601 (A):**

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

**Electron density around PID M 611 (B):**

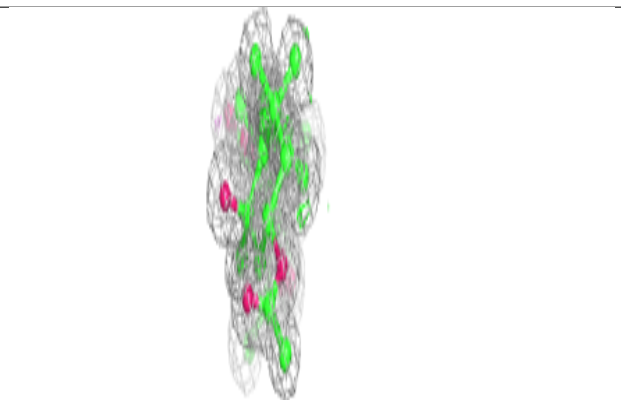
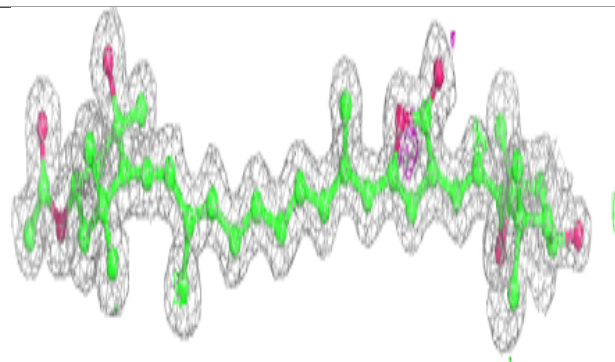
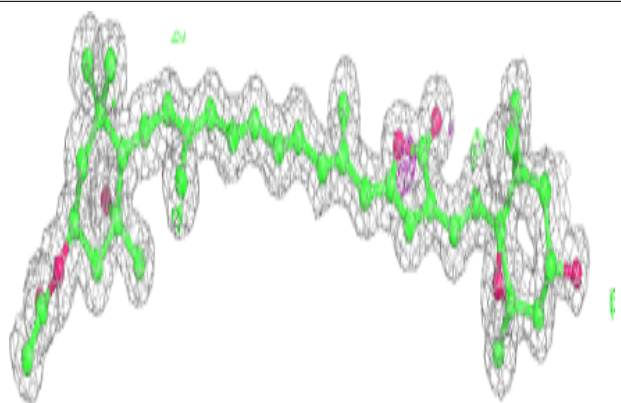
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



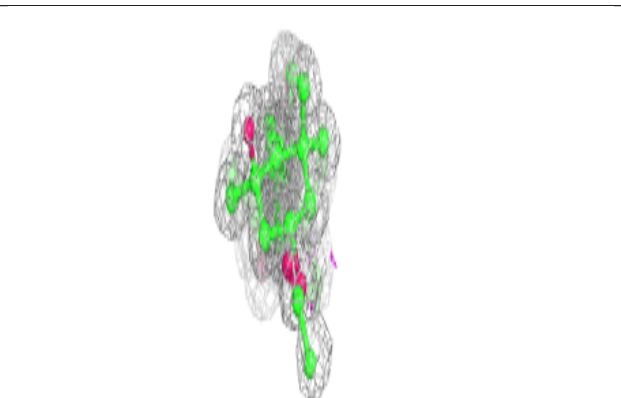
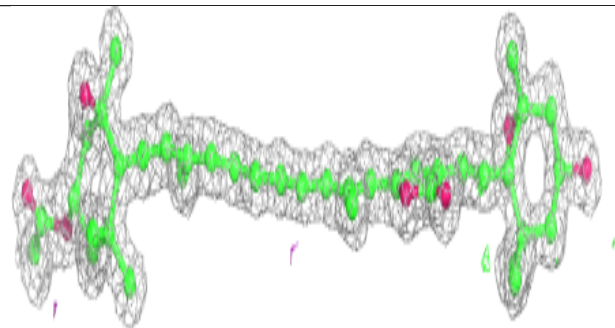
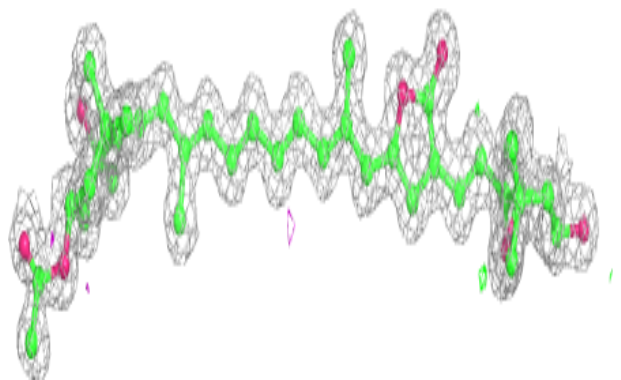


**Electron density around PID M 611 (A):**

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

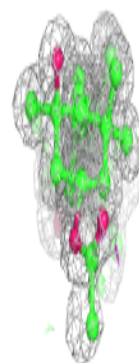
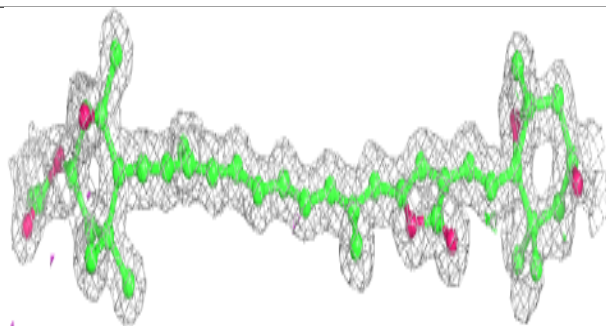
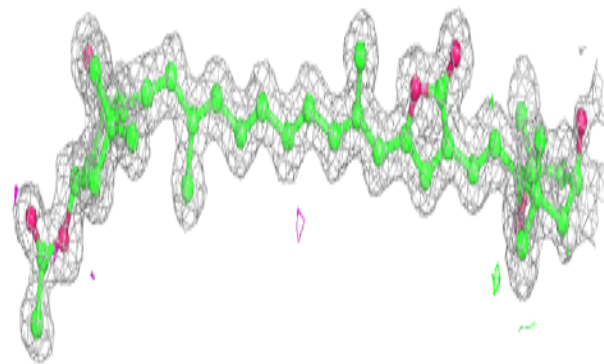
**Electron density around PID M 613 (B):**

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



**Electron density around 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.