Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 05:38 AM EST

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

This is a 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 (i) symbol.

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

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

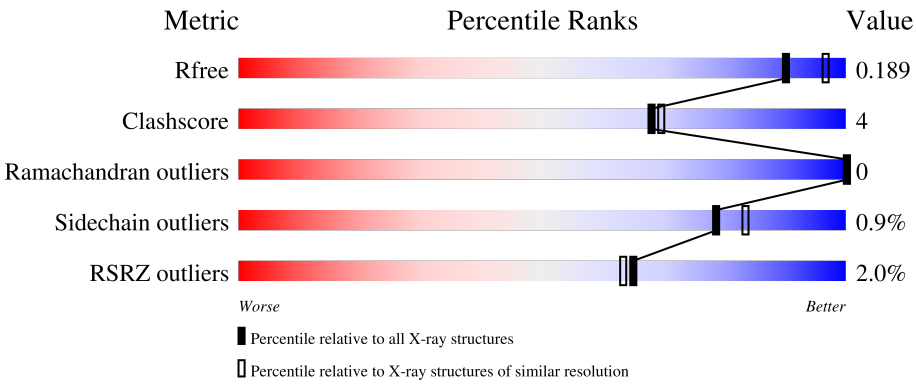
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	M	312	.% 96% .
1	N	312	3% 96% .
1	O	312	2% 95% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	M	601	X	-	-	-
2	CLA	M	602	X	-	-	-
2	CLA	N	601	X	-	-	-
2	CLA	N	602	X	-	-	-
2	CLA	O	601	X	-	-	-
2	CLA	O	602	X	-	-	-
3	PID	M	613	X	-	-	-
3	PID	N	613	X	-	-	-
3	PID	O	613	X	-	-	-
4	DGD	M	615	X	-	-	-
4	DGD	N	615	X	-	-	-
4	DGD	O	615	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9152 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

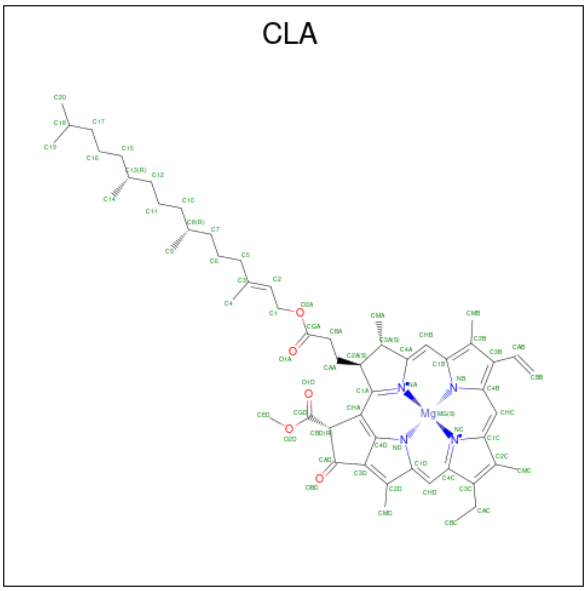
- Molecule 1 is a protein called PERIDININ-CHLOROPHYLL PROTEIN.

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

There are 9 discrepancies between the modelled and reference sequences:

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

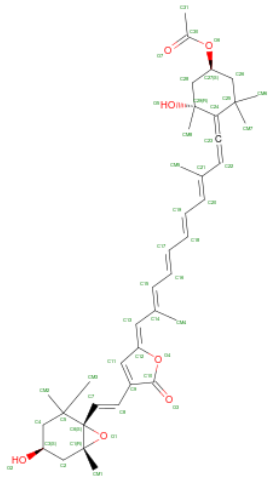
- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

PID



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

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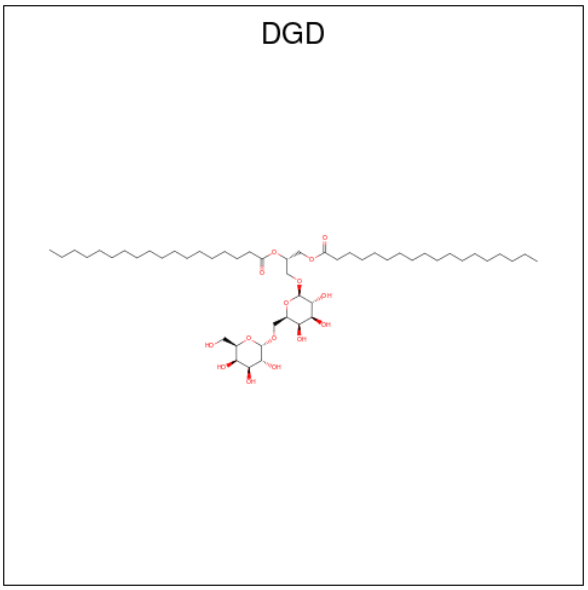
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	N	1	46	39	7	0	0
			Total	C	O		
3	N	1	46	39	7	0	0
			Total	C	O		
3	O	1	46	39	7	0	0
			Total	C	O		
3	O	1	46	39	7	0	0
			Total	C	O		
3	O	1	46	39	7	0	0
			Total	C	O		
3	O	1	46	39	7	0	0
			Total	C	O		
3	O	1	46	39	7	0	0
			Total	C	O		
3	O	1	46	39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

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



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

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

- Molecule 5 is water.

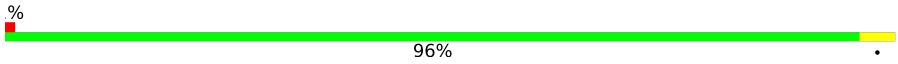
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	M	139	139	139	0	0
			Total	O		
5	N	137	137	137	0	0
			Total	O		
5	O	140	140	140	0	0

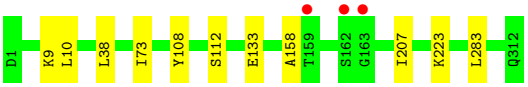
3 Residue-property plots (i)

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 PROTEIN

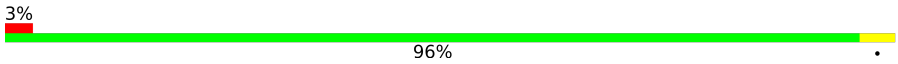
Chain M:

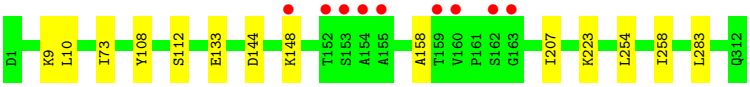




• Molecule 1: PERIDININ-CHLOROPHYLL PROTEIN

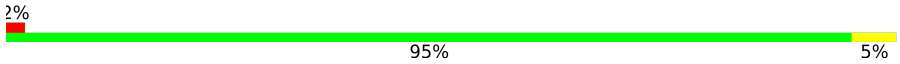
Chain N:

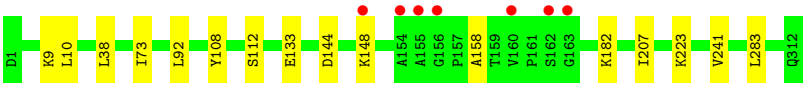




• Molecule 1: PERIDININ-CHLOROPHYLL PROTEIN

Chain O:





4 Data and refinement statistics (i)

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	M	0.58	0/2323	0.60	0/3154
1	N	0.56	0/2323	0.58	0/3154
1	O	0.59	0/2323	0.60	0/3154
All	All	0.58	0/6969	0.59	0/9462

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:73:ILE:HD11	3:O:614:PID:HM72	1.27	1.15
1:M:73:ILE:HD11	3:M:614:PID:HM72	1.30	1.07
1:N:73:ILE:HD11	3:N:614:PID:HM72	1.31	1.06
1:O:73:ILE:HD11	3:O:614:PID:CM7	2.12	0.75
2:M:602:CLA:HBB1	2:M:602:CLA:HHC	1.71	0.72
2:O:602:CLA:HHC	2:O:602:CLA:HBB1	1.74	0.69
2:N:602:CLA:HBB1	2:N:602:CLA:HHC	1.76	0.68
2:N:601:CLA:HBB1	2:N:601:CLA:HHC	1.78	0.66
2:O:601:CLA:HBB1	2:O:601:CLA:HHC	1.78	0.66
1:M:73:ILE:HD11	3:M:614:PID:CM7	2.17	0.65
2:M:601:CLA:HBB1	2:M:601:CLA:HHC	1.78	0.65
1:O:112:SER:HA	4:O:615:DGD:HB51	1.80	0.63
1:N:73:ILE:HD11	3:N:614:PID:CM7	2.19	0.63
1:N:112:SER:HA	4:N:615:DGD:HB51	1.81	0.62
1:M:112:SER:HA	4:M:615:DGD:HB51	1.82	0.62
3:N:611:PID:H3	4:N:615:DGD:HD61	1.85	0.59
3:M:611:PID:H3	4:M:615:DGD:HD61	1.85	0.59
3:O:611:PID:H3	4:O:615:DGD:HD61	1.85	0.59
4:N:615:DGD:HA22	4:N:615:DGD:HB62	1.88	0.55
4:M:615:DGD:HA22	4:M:615:DGD:HB62	1.88	0.54
1:O:9:LYS:N	1:O:9:LYS:HD2	2.24	0.52
1:M:9:LYS:HD2	1:M:9:LYS:N	2.25	0.52
1:N:9:LYS:N	1:N:9:LYS:HD2	2.25	0.51
1:M:108:TYR:CD1	4:M:615:DGD:HB82	2.47	0.50
1:O:108:TYR:CD1	4:O:615:DGD:HB82	2.47	0.49
1:N:207:ILE:HD12	3:N:611:PID:H261	1.94	0.49
1:N:108:TYR:CD1	4:N:615:DGD:HB82	2.48	0.49
1:O:207:ILE:HD12	3:O:611:PID:H261	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:158:ALA:HB2	1:O:223:LYS:HD3	1.94	0.47
4:O:615:DGD:HA22	4:O:615:DGD:HB62	1.96	0.47
4:O:615:DGD:HBN2	4:O:615:DGD:HBG3	1.73	0.47
1:M:207:ILE:HD12	3:M:611:PID:H261	1.97	0.46
4:M:615:DGD:HBG3	4:M:615:DGD:HBN2	1.72	0.45
1:M:158:ALA:HB2	1:M:223:LYS:HD3	2.00	0.44
3:O:622:PID:H312	4:O:615:DGD:HBG2	2.00	0.44
4:M:625:DGD:O1A	3:N:621:PID:H11	2.17	0.44
3:M:622:PID:H312	4:M:615:DGD:HBG2	2.00	0.43
4:O:615:DGD:HD2	4:O:615:DGD:HG31	1.73	0.43
4:M:615:DGD:HD2	4:M:615:DGD:HG31	1.75	0.43
4:M:615:DGD:HA21	4:M:615:DGD:HB91	2.01	0.43
1:O:144:ASP:O	1:O:148:LYS:HG2	2.19	0.42
3:M:623:PID:H16	4:O:625:DGD:HBT1	2.01	0.42
1:N:133:GLU:HG2	4:N:615:DGD:O5E	2.19	0.42
3:M:611:PID:H11	4:M:615:DGD:O1A	2.20	0.42
1:O:133:GLU:HG2	4:O:615:DGD:O5E	2.19	0.42
1:O:38:LEU:HD23	1:O:38:LEU:HA	1.84	0.42
4:N:615:DGD:HBG3	4:N:615:DGD:HBN2	1.73	0.42
1:O:92:LEU:HD22	2:O:601:CLA:HMD3	2.01	0.42
1:O:182:LYS:HG2	1:O:241:VAL:HG11	2.01	0.42
1:N:158:ALA:HB2	1:N:223:LYS:HD3	2.00	0.42
4:N:625:DGD:O1A	3:O:621:PID:H11	2.20	0.42
1:M:133:GLU:HG2	4:M:615:DGD:O5E	2.19	0.41
2:M:602:CLA:H203	2:M:602:CLA:H161	1.83	0.41
3:O:611:PID:H11	4:O:615:DGD:O1A	2.21	0.41
3:N:612:PID:HM52	4:N:615:DGD:HAH1	2.02	0.41
3:N:622:PID:H312	4:N:615:DGD:HBG2	2.02	0.41
3:O:621:PID:H16	3:O:621:PID:HM41	1.93	0.41
3:M:612:PID:HM52	4:M:615:DGD:HAH1	2.00	0.41
3:O:613:PID:H16	3:O:613:PID:HM41	1.93	0.41
4:N:615:DGD:HA21	4:N:615:DGD:HB91	2.03	0.41
3:N:624:PID:H16	3:N:624:PID:HM41	1.86	0.41
1:M:38:LEU:HA	1:M:38:LEU:HD23	1.84	0.40
3:M:621:PID:H11	4:O:625:DGD:O1A	2.20	0.40
1:N:144:ASP:O	1:N:148:LYS:HG2	2.22	0.40
3:N:612:PID:H16	3:N:612:PID:HM41	1.91	0.40
2:O:602:CLA:H203	2:O:602:CLA:H161	1.85	0.40
1:N:254:LEU:O	1:N:258:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
1	N	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
1	O	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
All	All	930/936 (99%)	921 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	233/233 (100%)	231 (99%)	2 (1%)	78	83
1	N	233/233 (100%)	231 (99%)	2 (1%)	78	83
1	O	233/233 (100%)	231 (99%)	2 (1%)	78	83
All	All	699/699 (100%)	693 (99%)	6 (1%)	78	83

All (6) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	O	283	LEU

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

Mol	Chain	Res	Type
1	M	216	GLN
1	N	216	GLN
1	O	216	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DGD	O	625	-	67,67,67	0.76	1 (1%)	81,81,81	0.96	5 (6%)
2	CLA	N	602	5	65,73,73	1.59	11 (16%)	76,113,113	1.75	11 (14%)
3	PID	N	612	-	41,49,49	1.84	11 (26%)	49,76,76	2.17	19 (38%)
2	CLA	M	601	5	65,73,73	1.53	11 (16%)	76,113,113	1.61	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PID	M	621	-	41,49,49	1.86	11 (26%)	49,76,76	2.08	13 (26%)
3	PID	M	624	-	41,49,49	1.76	9 (21%)	49,76,76	1.92	12 (24%)
3	PID	N	623	-	41,49,49	1.81	8 (19%)	49,76,76	2.13	15 (30%)
3	PID	M	614	-	41,49,49	1.90	11 (26%)	49,76,76	2.22	13 (26%)
3	PID	N	611	-	41,49,49	1.85	10 (24%)	49,76,76	2.17	18 (36%)
3	PID	O	612	-	41,49,49	1.76	12 (29%)	49,76,76	2.17	17 (34%)
3	PID	N	621	-	41,49,49	1.77	9 (21%)	49,76,76	2.12	15 (30%)
3	PID	O	611	-	41,49,49	1.79	10 (24%)	49,76,76	2.12	17 (34%)
2	CLA	O	602	5	65,73,73	1.52	8 (12%)	76,113,113	1.62	12 (15%)
3	PID	N	624	-	41,49,49	1.87	11 (26%)	49,76,76	2.16	17 (34%)
3	PID	M	611	-	41,49,49	1.90	13 (31%)	49,76,76	2.17	15 (30%)
3	PID	N	614	-	41,49,49	1.89	12 (29%)	49,76,76	2.31	16 (32%)
3	PID	O	614	-	41,49,49	1.83	11 (26%)	49,76,76	2.21	15 (30%)
3	PID	N	622	-	41,49,49	1.95	11 (26%)	49,76,76	2.20	14 (28%)
3	PID	O	624	-	41,49,49	1.75	10 (24%)	49,76,76	1.99	16 (32%)
4	DGD	M	615	-	67,67,67	0.85	2 (2%)	81,81,81	1.39	7 (8%)
2	CLA	M	602	5	65,73,73	1.55	8 (12%)	76,113,113	1.73	9 (11%)
4	DGD	N	625	-	67,67,67	0.78	1 (1%)	81,81,81	0.97	5 (6%)
3	PID	M	612	-	41,49,49	1.91	10 (24%)	49,76,76	2.15	19 (38%)
2	CLA	O	601	5	65,73,73	1.56	11 (16%)	76,113,113	1.59	8 (10%)
3	PID	N	613	-	41,49,49	1.84	10 (24%)	49,76,76	2.18	16 (32%)
3	PID	M	623	-	41,49,49	1.76	10 (24%)	49,76,76	2.13	15 (30%)
3	PID	O	613	-	41,49,49	1.67	9 (21%)	49,76,76	2.25	16 (32%)
3	PID	O	623	-	41,49,49	1.68	7 (17%)	49,76,76	1.97	15 (30%)
3	PID	M	622	-	41,49,49	1.83	10 (24%)	49,76,76	2.18	15 (30%)
3	PID	O	622	-	41,49,49	1.90	10 (24%)	49,76,76	2.17	14 (28%)
2	CLA	N	601	5	65,73,73	1.51	12 (18%)	76,113,113	1.54	10 (13%)
4	DGD	M	625	-	67,67,67	0.73	0	81,81,81	0.89	4 (4%)
3	PID	O	621	-	41,49,49	1.62	7 (17%)	49,76,76	1.88	15 (30%)
4	DGD	O	615	-	67,67,67	0.85	1 (1%)	81,81,81	1.39	8 (9%)
4	DGD	N	615	-	67,67,67	0.77	1 (1%)	81,81,81	1.39	7 (8%)
3	PID	M	613	-	41,49,49	1.77	10 (24%)	49,76,76	2.19	14 (28%)

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
4	DGD	O	625	-	-	24/55/95/95	0/2/2/2
2	CLA	N	602	5	1/1/15/20	2/37/115/115	-
3	PID	N	612	-	-	1/24/93/93	0/4/4/4
2	CLA	M	601	5	2/2/15/20	3/37/115/115	-
3	PID	M	621	-	-	1/24/93/93	0/4/4/4
3	PID	M	624	-	-	0/24/93/93	0/4/4/4
3	PID	N	623	-	-	1/24/93/93	0/4/4/4
3	PID	M	614	-	-	0/24/93/93	0/4/4/4
3	PID	N	611	-	-	1/24/93/93	0/4/4/4
3	PID	O	612	-	-	1/24/93/93	0/4/4/4
3	PID	N	621	-	-	1/24/93/93	0/4/4/4
3	PID	O	611	-	-	1/24/93/93	0/4/4/4
2	CLA	O	602	5	1/1/15/20	2/37/115/115	-
3	PID	N	624	-	-	1/24/93/93	0/4/4/4
3	PID	M	611	-	-	1/24/93/93	0/4/4/4
3	PID	N	614	-	-	0/24/93/93	0/4/4/4
3	PID	O	614	-	-	0/24/93/93	0/4/4/4
3	PID	N	622	-	-	1/24/93/93	0/4/4/4
3	PID	O	624	-	-	0/24/93/93	0/4/4/4
4	DGD	M	615	-	3/3/13/13	33/55/95/95	0/2/2/2
2	CLA	M	602	5	1/1/15/20	1/37/115/115	-
4	DGD	N	625	-	-	25/55/95/95	0/2/2/2
3	PID	M	612	-	-	1/24/93/93	0/4/4/4
2	CLA	O	601	5	2/2/15/20	4/37/115/115	-
3	PID	O	613	-	1/1/14/25	1/24/93/93	0/4/4/4
3	PID	M	623	-	-	0/24/93/93	0/4/4/4
3	PID	N	613	-	1/1/14/25	1/24/93/93	0/4/4/4
3	PID	O	623	-	-	0/24/93/93	0/4/4/4
3	PID	M	622	-	-	1/24/93/93	0/4/4/4
3	PID	O	622	-	-	1/24/93/93	0/4/4/4
2	CLA	N	601	5	2/2/15/20	3/37/115/115	-
4	DGD	M	625	-	-	25/55/95/95	0/2/2/2
3	PID	O	621	-	-	1/24/93/93	0/4/4/4
4	DGD	O	615	-	3/3/13/13	33/55/95/95	0/2/2/2
4	DGD	N	615	-	3/3/13/13	33/55/95/95	0/2/2/2
3	PID	M	613	-	1/1/14/25	1/24/93/93	0/4/4/4

All (309) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	602	CLA	MG-NA	7.58	2.24	2.06
2	N	602	CLA	MG-NA	7.11	2.23	2.06
2	O	602	CLA	MG-NA	6.92	2.22	2.06
2	O	601	CLA	MG-NA	6.23	2.21	2.06
2	M	601	CLA	MG-NA	5.54	2.19	2.06
2	N	601	CLA	MG-NA	5.51	2.19	2.06
3	N	613	PID	C23-C22	5.29	1.40	1.32
3	N	612	PID	C8-C7	5.23	1.44	1.32
3	M	611	PID	C23-C22	4.98	1.40	1.32
3	M	612	PID	C8-C7	4.98	1.43	1.32
2	O	602	CLA	C4B-NB	4.92	1.39	1.35
3	N	624	PID	C23-C22	4.91	1.40	1.32
3	N	624	PID	C8-C7	4.85	1.43	1.32
3	N	622	PID	C23-C22	4.84	1.40	1.32
3	M	614	PID	C15-C14	4.79	1.42	1.35
3	N	622	PID	C8-C7	4.79	1.43	1.32
3	M	614	PID	C23-C22	4.79	1.39	1.32
3	N	611	PID	C8-C7	4.75	1.43	1.32
3	O	622	PID	C8-C7	4.71	1.42	1.32
3	M	624	PID	C23-C22	4.66	1.39	1.32
3	M	611	PID	C8-C7	4.65	1.42	1.32
3	M	614	PID	C8-C7	4.64	1.42	1.32
2	O	601	CLA	O2D-CGD	4.59	1.44	1.33
3	N	614	PID	C8-C7	4.58	1.42	1.32
3	N	611	PID	C15-C14	4.58	1.41	1.35
3	N	621	PID	C23-C22	4.56	1.39	1.32
3	N	614	PID	C15-C14	4.54	1.41	1.35
2	N	602	CLA	C4B-NB	4.54	1.39	1.35
3	O	614	PID	C8-C7	4.52	1.42	1.32
3	O	622	PID	C23-C22	4.48	1.39	1.32
3	N	621	PID	C8-C7	4.47	1.42	1.32
3	M	622	PID	C8-C7	4.46	1.42	1.32
3	N	623	PID	C8-C7	4.44	1.42	1.32
2	M	601	CLA	O2D-CGD	4.43	1.44	1.33
3	O	612	PID	C8-C7	4.42	1.42	1.32
3	N	622	PID	C20-C21	4.42	1.41	1.35
3	O	621	PID	C23-C22	4.32	1.39	1.32
3	O	621	PID	C8-C7	4.30	1.42	1.32
2	N	602	CLA	C1B-NB	4.30	1.39	1.35
3	M	611	PID	C15-C14	4.30	1.41	1.35
3	O	611	PID	C15-C14	4.28	1.41	1.35
2	O	601	CLA	C1B-NB	4.28	1.39	1.35
3	M	624	PID	C8-C7	4.27	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	614	PID	C15-C14	4.25	1.41	1.35
3	O	623	PID	C8-C7	4.21	1.41	1.32
3	M	622	PID	C20-C21	4.21	1.41	1.35
3	O	623	PID	C15-C14	4.17	1.41	1.35
3	N	623	PID	C15-C14	4.09	1.41	1.35
3	M	622	PID	C15-C14	4.07	1.41	1.35
3	M	623	PID	C8-C7	4.05	1.41	1.32
3	M	624	PID	O1-C1	4.03	1.52	1.46
3	M	621	PID	C23-C22	4.03	1.38	1.32
3	N	613	PID	C15-C14	4.02	1.41	1.35
3	N	611	PID	C23-C22	4.02	1.38	1.32
3	M	613	PID	C23-C22	4.00	1.38	1.32
3	M	621	PID	C8-C7	3.99	1.41	1.32
2	M	601	CLA	C4B-NB	3.99	1.38	1.35
3	M	623	PID	C15-C14	3.93	1.41	1.35
3	N	613	PID	C8-C7	3.92	1.41	1.32
3	M	612	PID	C15-C14	3.88	1.40	1.35
3	O	622	PID	C20-C21	3.87	1.40	1.35
3	O	624	PID	C23-C22	3.84	1.38	1.32
3	N	612	PID	C20-C21	3.81	1.40	1.35
3	O	613	PID	C23-C22	3.81	1.38	1.32
2	M	602	CLA	C4B-NB	3.80	1.38	1.35
3	N	614	PID	C23-C22	3.80	1.38	1.32
3	N	621	PID	C15-C14	3.78	1.40	1.35
3	M	613	PID	C15-C14	3.74	1.40	1.35
3	M	623	PID	C23-C22	3.71	1.38	1.32
3	N	623	PID	C20-C21	3.71	1.40	1.35
3	O	611	PID	C23-C22	3.71	1.38	1.32
3	M	613	PID	C20-C21	3.70	1.40	1.35
3	O	622	PID	C15-C14	3.70	1.40	1.35
3	M	612	PID	C23-C22	3.68	1.38	1.32
3	M	612	PID	C20-C21	3.64	1.40	1.35
3	O	614	PID	C23-C22	3.64	1.38	1.32
3	O	611	PID	C8-C7	3.63	1.40	1.32
3	M	622	PID	C23-C22	3.62	1.38	1.32
3	M	621	PID	C20-C21	3.62	1.40	1.35
3	M	613	PID	C8-C7	3.60	1.40	1.32
3	O	623	PID	C23-C22	3.56	1.37	1.32
3	O	611	PID	C20-C21	3.54	1.40	1.35
3	N	623	PID	C23-C22	3.53	1.37	1.32
3	O	624	PID	C20-C21	3.52	1.40	1.35
3	M	612	PID	O4-C10	-3.50	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	624	PID	C8-C7	3.48	1.40	1.32
3	O	612	PID	C15-C14	3.48	1.40	1.35
3	N	611	PID	C20-C21	3.47	1.40	1.35
3	N	614	PID	C20-C21	3.46	1.40	1.35
3	O	613	PID	C15-C14	3.45	1.40	1.35
2	N	601	CLA	C4B-NB	3.42	1.38	1.35
2	O	602	CLA	C1B-NB	3.39	1.38	1.35
3	O	622	PID	O4-C10	-3.38	1.32	1.39
3	N	612	PID	C15-C14	3.38	1.40	1.35
3	O	613	PID	C8-C7	3.37	1.39	1.32
3	N	624	PID	O1-C1	3.36	1.51	1.46
3	N	613	PID	C20-C21	3.35	1.40	1.35
3	M	621	PID	C25-C24	3.35	1.60	1.54
3	M	621	PID	C15-C14	3.30	1.40	1.35
2	O	602	CLA	C3B-C2B	-3.29	1.35	1.40
2	N	601	CLA	O2D-CGD	3.28	1.41	1.33
3	N	612	PID	C23-C22	3.27	1.37	1.32
2	M	602	CLA	C1B-NB	3.26	1.38	1.35
2	N	601	CLA	C1B-NB	3.24	1.38	1.35
3	O	612	PID	C20-C21	3.24	1.40	1.35
3	O	612	PID	C23-C22	3.21	1.37	1.32
2	N	601	CLA	C3B-C2B	-3.18	1.36	1.40
3	N	622	PID	C15-C14	3.16	1.40	1.35
3	M	623	PID	C20-C21	3.14	1.40	1.35
3	M	621	PID	CM8-C29	3.14	1.57	1.52
2	M	601	CLA	C3B-C2B	-3.13	1.36	1.40
2	M	602	CLA	CHC-C1C	3.13	1.43	1.35
3	N	621	PID	C20-C21	3.13	1.39	1.35
3	M	624	PID	C20-C21	3.12	1.39	1.35
3	M	623	PID	O4-C10	-3.10	1.33	1.39
3	M	613	PID	O4-C10	-3.07	1.33	1.39
3	M	621	PID	CM4-C14	3.06	1.57	1.50
3	N	624	PID	C15-C14	3.04	1.39	1.35
2	O	601	CLA	C4B-NB	3.04	1.37	1.35
3	O	614	PID	CM5-C21	3.03	1.57	1.50
3	O	624	PID	O4-C10	-3.03	1.33	1.39
3	N	623	PID	O4-C10	-3.01	1.33	1.39
3	M	613	PID	O1-C1	2.99	1.50	1.46
2	O	602	CLA	C2-C3	2.98	1.40	1.33
3	M	623	PID	CM4-C14	2.97	1.57	1.50
3	O	614	PID	O4-C12	2.96	1.43	1.38
3	N	612	PID	O4-C10	-2.94	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	624	PID	CM1-C1	2.94	1.56	1.51
2	M	602	CLA	C2-C3	2.92	1.40	1.33
3	O	611	PID	O4-C12	2.91	1.43	1.38
3	M	611	PID	C20-C21	2.91	1.39	1.35
2	N	601	CLA	O2D-CED	-2.89	1.38	1.45
3	N	623	PID	C17-C16	2.89	1.43	1.36
3	M	614	PID	C20-C21	2.88	1.39	1.35
3	M	622	PID	CM5-C21	2.87	1.56	1.50
3	O	613	PID	C20-C21	2.86	1.39	1.35
3	N	624	PID	C20-C21	2.83	1.39	1.35
3	M	614	PID	CM5-C21	2.81	1.56	1.50
3	N	624	PID	O4-C10	-2.81	1.33	1.39
3	O	611	PID	CM4-C14	2.81	1.56	1.50
3	O	621	PID	C15-C14	2.80	1.39	1.35
3	M	612	PID	O1-C1	2.78	1.50	1.46
2	M	601	CLA	CMC-C2C	2.78	1.56	1.50
2	N	601	CLA	O2A-CGA	2.77	1.41	1.33
3	M	624	PID	CM5-C21	2.75	1.56	1.50
2	M	601	CLA	O1D-CGD	2.75	1.28	1.21
3	M	611	PID	C19-C18	2.75	1.43	1.36
3	M	621	PID	O4-C12	2.74	1.43	1.38
2	M	601	CLA	CHC-C1C	2.73	1.42	1.35
3	O	623	PID	O4-C10	-2.73	1.33	1.39
3	M	614	PID	O4-C12	2.73	1.43	1.38
2	N	601	CLA	MG-ND	-2.72	2.00	2.05
3	O	623	PID	C20-C21	2.72	1.39	1.35
3	N	622	PID	C25-C24	2.72	1.59	1.54
3	O	612	PID	O6-C30	-2.71	1.29	1.35
3	O	621	PID	C20-C21	2.70	1.39	1.35
3	O	614	PID	O4-C10	-2.70	1.33	1.39
3	M	624	PID	CM4-C14	2.69	1.56	1.50
3	N	623	PID	O4-C12	2.68	1.43	1.38
3	O	614	PID	C20-C21	2.67	1.39	1.35
3	O	623	PID	C17-C16	2.67	1.42	1.36
3	M	611	PID	O1-C1	2.66	1.50	1.46
3	N	621	PID	CM8-C29	2.66	1.57	1.52
2	M	602	CLA	CMD-C2D	2.65	1.56	1.50
3	O	613	PID	O4-C12	2.65	1.42	1.38
2	O	601	CLA	CHC-C1C	2.65	1.41	1.35
2	N	602	CLA	C2-C3	2.62	1.39	1.33
3	N	623	PID	O1-C1	2.61	1.50	1.46
3	O	612	PID	O4-C10	-2.61	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	613	PID	O4-C12	2.60	1.42	1.38
2	O	601	CLA	CMC-C2C	2.59	1.56	1.50
3	M	623	PID	C17-C16	2.59	1.42	1.36
3	O	613	PID	O4-C10	-2.59	1.34	1.39
3	N	621	PID	C19-C18	2.59	1.42	1.36
2	O	601	CLA	C3B-C2B	-2.58	1.36	1.40
3	N	614	PID	O4-C10	-2.58	1.34	1.39
3	M	622	PID	C2-C1	2.58	1.55	1.52
3	O	622	PID	CM5-C21	2.57	1.56	1.50
3	O	624	PID	CM5-C21	2.57	1.56	1.50
3	O	624	PID	C15-C14	2.56	1.39	1.35
3	M	612	PID	O6-C30	-2.56	1.29	1.35
2	O	601	CLA	CAC-C3C	2.55	1.57	1.51
3	N	612	PID	O6-C30	-2.54	1.29	1.35
3	M	621	PID	C19-C18	2.54	1.42	1.36
2	O	602	CLA	CMA-C3A	2.54	1.58	1.53
3	N	614	PID	O4-C12	2.53	1.42	1.38
2	N	601	CLA	C3B-CAB	-2.53	1.42	1.47
4	M	615	DGD	O5D-C1E	2.52	1.44	1.40
3	M	624	PID	O4-C10	-2.52	1.34	1.39
3	O	624	PID	CM4-C14	2.51	1.56	1.50
3	M	614	PID	O4-C10	-2.51	1.34	1.39
3	N	613	PID	O4-C10	-2.50	1.34	1.39
2	N	602	CLA	C4-C3	2.49	1.57	1.50
3	M	611	PID	C13-C14	-2.49	1.41	1.45
3	M	622	PID	O4-C10	-2.48	1.34	1.39
4	O	615	DGD	O5D-C1E	2.47	1.44	1.40
3	N	612	PID	O1-C1	2.47	1.49	1.46
3	M	621	PID	O1-C1	2.47	1.49	1.46
3	M	612	PID	C25-C24	2.45	1.58	1.54
3	N	614	PID	CM5-C21	2.45	1.55	1.50
3	N	622	PID	C19-C18	2.44	1.42	1.36
3	N	613	PID	O1-C1	2.44	1.49	1.46
3	M	614	PID	O1-C1	2.43	1.49	1.46
2	N	601	CLA	CHC-C1C	2.43	1.41	1.35
3	N	614	PID	C19-C18	2.42	1.42	1.36
3	O	624	PID	O1-C1	2.42	1.49	1.46
3	O	614	PID	C17-C16	2.42	1.42	1.36
3	N	614	PID	O1-C1	2.42	1.49	1.46
3	N	611	PID	C13-C14	-2.41	1.41	1.45
2	O	601	CLA	O1D-CGD	2.41	1.27	1.21
4	N	615	DGD	O5D-C1E	2.41	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	602	CLA	CMC-C2C	2.41	1.55	1.50
3	O	612	PID	C19-C18	2.40	1.42	1.36
3	N	611	PID	O4-C12	2.39	1.42	1.38
3	M	614	PID	C17-C16	2.39	1.42	1.36
4	N	625	DGD	O5D-C1E	2.39	1.44	1.40
2	N	602	CLA	CMD-C2D	2.39	1.55	1.50
3	M	612	PID	C17-C16	2.38	1.42	1.36
3	M	621	PID	O4-C10	-2.38	1.34	1.39
3	N	611	PID	O4-C10	-2.38	1.34	1.39
3	N	622	PID	C2-C1	2.38	1.55	1.52
3	M	622	PID	O6-C30	-2.37	1.29	1.35
2	N	602	CLA	C3B-CAB	-2.37	1.43	1.47
3	O	612	PID	C25-C24	2.37	1.58	1.54
3	O	611	PID	C17-C16	2.37	1.42	1.36
3	N	622	PID	CM4-C14	2.37	1.55	1.50
3	O	613	PID	C8-C9	-2.37	1.40	1.46
3	O	624	PID	CM1-C1	2.36	1.55	1.51
3	N	624	PID	C19-C18	2.35	1.42	1.36
3	O	612	PID	CM4-C14	2.35	1.55	1.50
3	N	622	PID	O1-C1	2.35	1.49	1.46
3	N	612	PID	C19-C18	2.35	1.42	1.36
2	O	601	CLA	C2-C3	2.35	1.38	1.33
3	N	621	PID	O4-C10	-2.34	1.34	1.39
3	N	611	PID	C17-C16	2.34	1.42	1.36
3	N	621	PID	CM4-C14	2.31	1.55	1.50
3	O	611	PID	C28-C27	2.31	1.55	1.51
3	O	621	PID	C25-C24	2.31	1.58	1.54
3	N	622	PID	CM5-C21	2.30	1.55	1.50
3	N	611	PID	CM4-C14	2.30	1.55	1.50
3	N	624	PID	CM4-C14	2.30	1.55	1.50
2	N	602	CLA	CHC-C1C	2.30	1.40	1.35
2	M	601	CLA	C1B-NB	2.30	1.37	1.35
2	O	602	CLA	CHC-C1C	2.29	1.40	1.35
2	N	602	CLA	C3B-C2B	-2.27	1.37	1.40
3	M	622	PID	O4-C12	2.27	1.42	1.38
3	M	613	PID	C17-C16	2.27	1.41	1.36
3	N	624	PID	CM5-C21	2.26	1.55	1.50
3	O	622	PID	CM4-C14	2.26	1.55	1.50
3	N	611	PID	C19-C18	2.26	1.41	1.36
3	O	621	PID	O4-C10	-2.25	1.34	1.39
2	N	602	CLA	O2D-CGD	2.25	1.38	1.33
3	O	621	PID	C17-C16	2.25	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	612	PID	O4-C12	2.24	1.42	1.38
3	M	611	PID	O4-C12	2.23	1.42	1.38
3	N	613	PID	C8-C9	-2.23	1.40	1.46
2	N	602	CLA	MG-ND	-2.23	2.01	2.05
3	M	613	PID	O6-C30	-2.23	1.30	1.35
3	O	624	PID	C19-C18	2.22	1.41	1.36
2	N	601	CLA	O1D-CGD	2.22	1.26	1.21
3	N	622	PID	O4-C10	-2.21	1.35	1.39
3	N	612	PID	O4-C12	2.20	1.42	1.38
3	M	611	PID	CM5-C21	2.20	1.55	1.50
2	M	601	CLA	MG-NC	2.20	2.11	2.06
3	M	612	PID	O4-C12	2.19	1.42	1.38
3	M	611	PID	O4-C10	-2.19	1.35	1.39
3	M	623	PID	CM5-C21	2.19	1.55	1.50
3	O	613	PID	O1-C1	2.19	1.49	1.46
3	M	624	PID	C15-C14	2.18	1.38	1.35
2	O	601	CLA	O2D-CED	-2.18	1.40	1.45
3	M	613	PID	O4-C12	2.17	1.42	1.38
3	N	624	PID	C8-C9	-2.16	1.40	1.46
3	N	612	PID	CM4-C14	2.16	1.55	1.50
3	N	614	PID	C17-C16	2.16	1.41	1.36
3	N	613	PID	C13-C14	-2.15	1.41	1.45
3	N	614	PID	CM4-C14	2.15	1.55	1.50
3	M	613	PID	C8-C9	-2.15	1.40	1.46
2	N	601	CLA	CMC-C2C	2.14	1.55	1.50
3	M	614	PID	C19-C18	2.14	1.41	1.36
3	M	611	PID	C2-C1	2.14	1.55	1.52
3	N	621	PID	O4-C12	2.14	1.42	1.38
3	M	622	PID	C13-C14	-2.12	1.41	1.45
3	O	614	PID	C26-C27	2.11	1.55	1.51
3	O	612	PID	C17-C16	2.11	1.41	1.36
3	O	622	PID	C13-C14	-2.11	1.41	1.45
2	O	602	CLA	C4-C3	2.10	1.56	1.50
3	M	624	PID	C19-C18	2.10	1.41	1.36
2	M	601	CLA	C2-C3	2.10	1.38	1.33
3	O	613	PID	C13-C14	-2.09	1.41	1.45
2	M	601	CLA	O2A-CGA	2.09	1.39	1.33
3	M	623	PID	O4-C12	2.09	1.41	1.38
3	O	622	PID	C25-C24	2.09	1.58	1.54
3	O	611	PID	O4-C10	-2.09	1.35	1.39
3	M	623	PID	C19-C18	2.09	1.41	1.36
4	O	625	DGD	C4D-C5D	2.08	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	611	PID	CM4-C14	2.07	1.55	1.50
3	O	623	PID	O1-C1	2.07	1.49	1.46
2	M	602	CLA	C3B-C2B	-2.07	1.37	1.40
3	O	614	PID	C8-C9	-2.07	1.41	1.46
3	N	612	PID	C25-C24	2.05	1.58	1.54
3	N	614	PID	C8-C9	-2.04	1.41	1.46
3	M	614	PID	C13-C14	-2.04	1.41	1.45
3	N	613	PID	C17-C16	2.04	1.41	1.36
3	O	612	PID	O1-C1	2.03	1.49	1.46
3	O	611	PID	C2-C1	2.03	1.55	1.52
4	M	615	DGD	O3G-C1D	2.03	1.43	1.40
3	O	614	PID	O1-C1	2.02	1.49	1.46
3	M	611	PID	C28-C27	2.00	1.55	1.51
3	O	622	PID	C26-C27	2.00	1.55	1.51

All (465) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	602	CLA	C4A-NA-C1A	9.74	111.09	106.71
2	N	602	CLA	C4A-NA-C1A	9.72	111.08	106.71
2	M	601	CLA	C4A-NA-C1A	9.41	110.94	106.71
3	N	613	PID	O3-C10-C9	-8.65	120.89	130.74
2	O	602	CLA	C4A-NA-C1A	8.36	110.46	106.71
2	O	601	CLA	C4A-NA-C1A	8.30	110.44	106.71
3	O	613	PID	O3-C10-C9	-8.08	121.54	130.74
3	O	614	PID	O3-C10-C9	-7.93	121.71	130.74
3	M	613	PID	O3-C10-C9	-7.91	121.73	130.74
2	N	601	CLA	C4A-NA-C1A	7.81	110.22	106.71
4	M	615	DGD	O6E-C5E-C4E	7.57	123.44	109.69
4	O	615	DGD	O6E-C5E-C4E	7.56	123.43	109.69
4	N	615	DGD	O6E-C5E-C4E	7.48	123.28	109.69
3	M	614	PID	O3-C10-C9	-7.31	122.42	130.74
3	N	614	PID	O3-C10-C9	-7.25	122.49	130.74
3	M	614	PID	O4-C12-C11	6.82	111.50	107.36
3	N	614	PID	O4-C12-C11	6.80	111.48	107.36
3	N	622	PID	O3-C10-C9	-6.56	123.27	130.74
3	N	623	PID	O4-C12-C11	6.53	111.32	107.36
3	M	611	PID	O3-C10-C9	-6.42	123.43	130.74
3	O	611	PID	O3-C10-C9	-6.35	123.51	130.74
3	N	611	PID	O3-C10-C9	-6.29	123.58	130.74
3	O	624	PID	O4-C12-C11	6.23	111.14	107.36
3	M	623	PID	O3-C10-C9	-6.18	123.70	130.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	624	PID	O4-C12-C11	6.17	111.10	107.36
3	N	624	PID	O4-C12-C11	6.16	111.09	107.36
3	O	612	PID	O3-C10-C9	-6.14	123.75	130.74
3	O	614	PID	O4-C12-C11	6.04	111.02	107.36
3	N	624	PID	O3-C10-C9	-6.02	123.88	130.74
3	M	611	PID	O4-C12-C11	6.02	111.01	107.36
3	N	612	PID	O4-C12-C11	6.01	111.01	107.36
3	O	622	PID	O3-C10-C9	-5.98	123.93	130.74
3	N	611	PID	O4-C12-C11	5.98	110.98	107.36
3	O	622	PID	O4-C12-C11	5.93	110.95	107.36
3	M	623	PID	O4-C12-C11	5.92	110.95	107.36
3	M	622	PID	O4-C12-C11	5.91	110.94	107.36
3	M	613	PID	O4-C12-C11	5.88	110.92	107.36
3	M	622	PID	O3-C10-C9	-5.86	124.07	130.74
3	M	621	PID	O3-C10-C9	-5.81	124.13	130.74
3	M	612	PID	O4-C12-C11	5.78	110.86	107.36
3	O	623	PID	O3-C10-C9	-5.69	124.26	130.74
3	N	623	PID	O3-C10-C9	-5.69	124.27	130.74
3	N	622	PID	O4-C12-C11	5.67	110.80	107.36
3	O	613	PID	O4-C12-C11	5.58	110.74	107.36
3	M	612	PID	O3-C10-C9	-5.56	124.41	130.74
3	N	612	PID	O3-C10-C9	-5.52	124.45	130.74
3	O	612	PID	O4-C12-C11	5.44	110.66	107.36
3	N	621	PID	O4-C12-C11	5.43	110.65	107.36
3	M	614	PID	C12-O4-C10	-5.39	104.84	107.65
3	N	614	PID	C12-O4-C10	-5.38	104.85	107.65
3	N	623	PID	C12-O4-C10	-5.28	104.91	107.65
3	O	623	PID	O4-C12-C11	5.25	110.54	107.36
3	N	621	PID	O3-C10-C9	-5.22	124.80	130.74
3	O	611	PID	O4-C12-C11	5.19	110.51	107.36
3	N	611	PID	C12-O4-C10	-5.09	105.00	107.65
2	M	602	CLA	O2D-CGD-CBD	5.06	120.25	111.27
3	N	613	PID	O4-C12-C11	4.99	110.38	107.36
2	O	602	CLA	O2D-CGD-CBD	4.96	120.08	111.27
3	O	621	PID	O3-C10-C9	-4.96	125.10	130.74
2	N	602	CLA	O2D-CGD-CBD	4.95	120.06	111.27
3	M	623	PID	C12-O4-C10	-4.94	105.08	107.65
3	O	624	PID	O3-C10-C9	-4.93	125.12	130.74
3	N	621	PID	C12-O4-C10	-4.81	105.15	107.65
3	N	624	PID	C12-O4-C10	-4.78	105.16	107.65
3	M	621	PID	O4-C12-C11	4.76	110.25	107.36
3	M	624	PID	O3-C10-C9	-4.65	125.45	130.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	614	PID	C12-O4-C10	-4.64	105.23	107.65
4	O	615	DGD	O6D-C5D-C6D	4.61	115.97	106.67
4	N	615	DGD	O6D-C5D-C6D	4.58	115.92	106.67
3	O	613	PID	C1-C2-C3	4.55	121.76	112.75
3	O	611	PID	C12-O4-C10	-4.53	105.29	107.65
3	N	622	PID	C12-O4-C10	-4.53	105.30	107.65
3	M	611	PID	C12-O4-C10	-4.52	105.30	107.65
4	M	615	DGD	O6D-C5D-C6D	4.50	115.74	106.67
3	M	613	PID	C1-C2-C3	4.44	121.54	112.75
3	O	621	PID	O4-C12-C11	4.37	110.01	107.36
3	M	621	PID	O1-C1-C2	4.37	116.67	113.38
3	N	613	PID	C1-C2-C3	4.36	121.36	112.75
2	N	601	CLA	O2D-CGD-CBD	4.34	118.97	111.27
3	O	622	PID	C12-O4-C10	-4.26	105.43	107.65
3	M	622	PID	C12-O4-C10	-4.22	105.45	107.65
3	O	612	PID	C12-O4-C10	-4.22	105.46	107.65
3	M	621	PID	C12-O4-C10	-4.18	105.48	107.65
3	M	621	PID	O6-C30-C31	4.16	118.74	111.09
3	O	613	PID	C12-O4-C10	-4.14	105.50	107.65
3	N	621	PID	O6-C30-C31	4.10	118.63	111.09
3	N	612	PID	C19-C20-C21	-4.02	121.57	127.31
3	M	622	PID	C1-C2-C3	3.99	120.65	112.75
2	O	602	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
3	O	623	PID	O6-C30-C31	3.97	118.39	111.09
3	N	614	PID	O6-C30-C31	3.95	118.36	111.09
3	M	622	PID	C19-C20-C21	-3.93	121.70	127.31
3	M	612	PID	C12-O4-C10	-3.91	105.62	107.65
3	O	612	PID	C19-C20-C21	-3.90	121.74	127.31
3	O	622	PID	C19-C20-C21	-3.90	121.74	127.31
3	M	612	PID	C19-C20-C21	-3.90	121.74	127.31
3	O	622	PID	C1-C2-C3	3.88	120.43	112.75
3	N	623	PID	O6-C30-C31	3.87	118.21	111.09
3	M	613	PID	O6-C30-C31	3.85	118.18	111.09
3	N	621	PID	O1-C1-C2	3.84	116.27	113.38
3	O	614	PID	O6-C30-C31	3.81	118.09	111.09
3	N	622	PID	C1-C2-C3	3.78	120.23	112.75
3	N	622	PID	C19-C20-C21	-3.78	121.91	127.31
3	M	614	PID	O6-C30-C31	3.78	118.04	111.09
3	N	622	PID	C17-C16-C15	-3.74	115.81	123.47
2	N	602	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
2	O	601	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
3	N	612	PID	C12-O4-C10	-3.69	105.73	107.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	622	PID	C17-C16-C15	-3.66	115.98	123.47
2	M	602	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
3	N	624	PID	O6-C30-C31	3.64	117.78	111.09
3	O	621	PID	O6-C30-C31	3.63	117.76	111.09
3	N	621	PID	O4-C10-C9	3.62	111.07	108.04
3	N	613	PID	O6-C30-C31	3.62	117.74	111.09
3	M	623	PID	O6-C30-C31	3.59	117.69	111.09
2	O	601	CLA	O2D-CGD-CBD	3.58	117.64	111.27
3	M	621	PID	O4-C10-C9	3.58	111.03	108.04
3	N	611	PID	O6-C30-C31	3.57	117.65	111.09
3	O	613	PID	O6-C30-C31	3.56	117.64	111.09
3	O	622	PID	O6-C30-C31	3.52	117.56	111.09
2	M	601	CLA	O2D-CGD-CBD	3.51	117.51	111.27
3	O	611	PID	O6-C30-C31	3.51	117.56	111.09
3	O	622	PID	C17-C16-C15	-3.51	116.28	123.47
3	N	614	PID	C16-C15-C14	-3.50	122.31	127.31
3	N	624	PID	O4-C10-C9	3.48	110.95	108.04
3	M	624	PID	O6-C30-C31	3.44	117.42	111.09
3	O	624	PID	O6-C30-C31	3.44	117.42	111.09
3	O	621	PID	C18-C19-C20	-3.43	116.44	123.47
2	N	601	CLA	O2A-CGA-CBA	3.43	122.67	111.91
4	N	625	DGD	C1D-O6D-C5D	-3.43	106.96	113.69
3	N	623	PID	O4-C10-C9	3.42	110.90	108.04
3	N	622	PID	O6-C30-C31	3.39	117.32	111.09
4	N	615	DGD	C3G-O3G-C1D	-3.38	107.13	113.74
3	N	614	PID	CM1-C1-C6	-3.38	116.59	122.26
3	M	622	PID	C17-C18-C19	-3.38	117.30	124.81
3	O	624	PID	C16-C15-C14	-3.37	122.50	127.31
3	M	621	PID	C18-C19-C20	-3.36	116.59	123.47
3	M	622	PID	O6-C30-C31	3.35	117.26	111.09
2	M	601	CLA	O2A-CGA-CBA	3.35	122.42	111.91
3	N	624	PID	C16-C15-C14	-3.35	122.53	127.31
3	M	611	PID	C1-C2-C3	3.34	119.36	112.75
2	O	601	CLA	O2A-CGA-CBA	3.31	122.29	111.91
3	M	624	PID	C12-O4-C10	-3.31	105.93	107.65
3	O	611	PID	C18-C19-C20	-3.31	116.70	123.47
3	O	621	PID	O4-C10-C9	3.30	110.80	108.04
3	N	612	PID	CM3-C5-C4	-3.30	103.25	108.98
2	N	602	CLA	O2A-CGA-CBA	3.29	122.23	111.91
3	M	611	PID	O6-C30-C31	3.28	117.11	111.09
3	N	613	PID	C19-C20-C21	-3.27	122.64	127.31
3	O	622	PID	C17-C18-C19	-3.26	117.56	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	612	PID	CM3-C5-C4	-3.24	103.35	108.98
3	M	611	PID	C16-C15-C14	-3.24	122.69	127.31
3	M	613	PID	C11-C12-C13	-3.23	121.18	128.34
3	M	624	PID	C16-C15-C14	-3.23	122.70	127.31
3	O	614	PID	CM1-C1-C6	-3.22	116.86	122.26
3	O	611	PID	C1-C2-C3	3.22	119.13	112.75
3	M	614	PID	CM1-C1-C6	-3.21	116.88	122.26
3	M	622	PID	C27-O6-C30	-3.20	111.92	117.90
3	N	612	PID	C1-C2-C3	3.20	119.07	112.75
3	N	613	PID	C11-C12-C13	-3.19	121.29	128.34
3	N	611	PID	C11-C12-C13	-3.18	121.29	128.34
3	N	612	PID	CM1-C1-C6	-3.18	116.94	122.26
3	M	623	PID	O4-C10-C9	3.18	110.70	108.04
3	O	613	PID	C11-C12-C13	-3.17	121.31	128.34
4	M	615	DGD	C3G-O3G-C1D	-3.17	107.55	113.74
4	M	615	DGD	O2G-C1B-C2B	3.16	118.32	111.50
3	N	614	PID	C27-O6-C30	-3.16	112.01	117.90
4	O	615	DGD	O2G-C1B-C2B	3.13	118.25	111.50
3	O	624	PID	C12-O4-C10	-3.13	106.02	107.65
3	O	623	PID	CM1-C1-C6	-3.12	117.03	122.26
3	O	613	PID	C19-C20-C21	-3.12	122.85	127.31
3	O	612	PID	CM3-C5-C4	-3.12	103.56	108.98
2	M	602	CLA	O2A-CGA-CBA	3.10	121.62	111.91
3	M	612	PID	C1-C2-C3	3.09	118.87	112.75
4	O	615	DGD	C3G-O3G-C1D	-3.09	107.70	113.74
3	M	611	PID	C11-C12-C13	-3.09	121.51	128.34
3	O	621	PID	C12-O4-C10	-3.08	106.05	107.65
2	O	602	CLA	O2A-CGA-CBA	3.08	121.58	111.91
3	O	621	PID	C17-C16-C15	-3.08	117.17	123.47
3	N	614	PID	C11-C12-C13	-3.07	121.55	128.34
3	N	621	PID	C11-C12-C13	-3.07	121.55	128.34
3	M	614	PID	C16-C15-C14	-3.06	122.94	127.31
4	N	615	DGD	O2G-C1B-C2B	3.06	118.09	111.50
3	O	611	PID	C11-C12-C13	-3.05	121.58	128.34
3	M	613	PID	C19-C20-C21	-3.05	122.95	127.31
3	N	611	PID	C1-C2-C3	3.04	118.76	112.75
3	M	611	PID	C6-C7-C8	-3.03	119.58	125.99
3	M	611	PID	C18-C19-C20	-3.02	117.28	123.47
3	N	622	PID	CM1-C1-C6	-3.01	117.21	122.26
3	O	622	PID	O4-C10-C9	2.99	110.54	108.04
3	M	613	PID	C12-O4-C10	-2.99	106.10	107.65
3	N	611	PID	C18-C19-C20	-2.98	117.37	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	613	PID	C12-O4-C10	-2.97	106.10	107.65
3	N	623	PID	C19-C20-C21	-2.97	123.07	127.31
3	O	611	PID	C6-C7-C8	-2.97	119.72	125.99
3	O	612	PID	O4-C10-C9	2.96	110.51	108.04
3	M	612	PID	C17-C16-C15	-2.95	117.44	123.47
3	N	622	PID	C17-C18-C19	-2.95	118.25	124.81
3	M	614	PID	C11-C12-C13	-2.94	121.83	128.34
2	O	601	CLA	CED-O2D-CGD	2.94	122.58	115.94
3	N	622	PID	C27-O6-C30	-2.93	112.44	117.90
3	M	612	PID	CM1-C1-C6	-2.93	117.36	122.26
3	O	622	PID	C27-O6-C30	-2.92	112.45	117.90
3	N	621	PID	C18-C19-C20	-2.91	117.50	123.47
3	N	611	PID	C6-C7-C8	-2.91	119.85	125.99
3	O	612	PID	C1-C2-C3	2.91	118.50	112.75
3	M	621	PID	C11-C12-C13	-2.90	121.92	128.34
3	O	623	PID	C17-C16-C15	-2.90	117.53	123.47
3	M	622	PID	CM1-C1-C2	2.90	117.54	114.28
3	O	623	PID	C19-C20-C21	-2.90	123.17	127.31
3	O	612	PID	CM1-C1-C6	-2.90	117.40	122.26
3	M	623	PID	C19-C20-C21	-2.90	123.18	127.31
3	N	624	PID	CM1-C1-C6	-2.86	117.47	122.26
3	O	623	PID	C12-O4-C10	-2.86	106.17	107.65
3	O	614	PID	C16-C15-C14	-2.85	123.24	127.31
3	N	611	PID	C16-C15-C14	-2.85	123.25	127.31
3	O	623	PID	C18-C19-C20	-2.84	117.65	123.47
3	O	614	PID	C18-C19-C20	-2.84	117.65	123.47
3	O	624	PID	CM1-C1-C6	-2.84	117.50	122.26
4	O	625	DGD	C1D-O6D-C5D	-2.82	108.15	113.69
4	O	625	DGD	O3G-C1D-C2D	-2.82	103.90	108.30
3	O	614	PID	C11-C12-C13	-2.81	122.13	128.34
3	M	624	PID	O4-C10-C9	2.80	110.38	108.04
3	N	614	PID	C19-C20-C21	-2.80	123.32	127.31
3	M	622	PID	CM1-C1-C6	-2.79	117.58	122.26
3	N	621	PID	C16-C15-C14	-2.79	123.33	127.31
3	M	613	PID	O1-C1-C2	2.77	115.47	113.38
4	O	625	DGD	O2G-C2G-C1G	-2.76	98.39	108.40
4	O	615	DGD	O6D-C1D-C2D	2.76	116.19	110.35
3	O	614	PID	CM1-C1-C2	2.76	117.39	114.28
3	O	622	PID	CM1-C1-C6	-2.75	117.65	122.26
3	N	611	PID	C8-C9-C11	-2.75	122.08	127.37
3	N	622	PID	O4-C10-C9	2.74	110.33	108.04
3	N	612	PID	O6-C30-C31	2.74	116.13	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	623	PID	C27-O6-C30	-2.74	112.80	117.90
2	M	601	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
3	N	623	PID	C27-O6-C30	-2.72	112.82	117.90
3	O	621	PID	C11-C12-C13	-2.72	122.31	128.34
3	N	624	PID	C19-C20-C21	-2.72	123.43	127.31
3	O	611	PID	C8-C9-C11	-2.72	122.15	127.37
3	O	624	PID	C18-C19-C20	-2.70	117.94	123.47
3	M	614	PID	CM1-C1-C2	2.70	117.31	114.28
3	M	614	PID	C19-C20-C21	-2.69	123.47	127.31
2	N	601	CLA	CMB-C2B-C1B	-2.69	124.34	128.46
3	M	613	PID	C16-C15-C14	-2.68	123.48	127.31
3	N	623	PID	C11-C12-C13	-2.68	122.41	128.34
3	M	611	PID	C8-C9-C11	-2.68	122.23	127.37
3	M	612	PID	C16-C15-C14	-2.68	123.49	127.31
3	O	624	PID	C19-C20-C21	-2.67	123.50	127.31
3	N	623	PID	C17-C16-C15	-2.67	118.01	123.47
3	N	612	PID	C16-C15-C14	-2.66	123.51	127.31
3	M	612	PID	C6-C7-C8	-2.65	120.38	125.99
3	O	613	PID	C16-C15-C14	-2.65	123.52	127.31
3	O	612	PID	C17-C16-C15	-2.65	118.04	123.47
3	M	624	PID	C18-C19-C20	-2.64	118.06	123.47
2	O	602	CLA	CMB-C2B-C3B	2.64	129.62	124.68
3	N	613	PID	C16-C15-C14	-2.64	123.55	127.31
3	M	623	PID	C11-C12-C13	-2.64	122.51	128.34
3	O	621	PID	C16-C15-C14	-2.64	123.55	127.31
3	M	621	PID	C17-C16-C15	-2.63	118.08	123.47
3	M	612	PID	O6-C30-C31	2.63	115.93	111.09
3	N	612	PID	C6-C7-C8	-2.63	120.44	125.99
4	N	625	DGD	O6D-C1D-O3G	-2.62	103.78	109.97
4	O	625	DGD	O6D-C1D-O3G	-2.61	103.78	109.97
3	N	614	PID	C18-C19-C20	-2.61	118.12	123.47
3	M	612	PID	O4-C10-C9	2.61	110.22	108.04
3	N	623	PID	CM1-C1-C6	-2.61	117.89	122.26
3	M	613	PID	C8-C9-C11	-2.61	122.36	127.37
3	N	624	PID	C11-C12-C13	-2.61	122.57	128.34
3	N	612	PID	C17-C16-C15	-2.60	118.15	123.47
3	M	614	PID	C18-C19-C20	-2.60	118.15	123.47
4	N	615	DGD	C1E-O6E-C5E	2.60	118.79	113.69
3	O	624	PID	C17-C16-C15	-2.59	118.16	123.47
3	O	613	PID	C8-C9-C11	-2.59	122.40	127.37
3	M	623	PID	C17-C16-C15	-2.58	118.18	123.47
4	N	625	DGD	O2G-C1B-C2B	2.58	117.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	623	PID	C11-C12-C13	-2.57	122.66	128.34
3	O	614	PID	C27-O6-C30	-2.56	113.13	117.90
3	M	624	PID	C11-C12-C13	-2.55	122.69	128.34
3	M	623	PID	CM1-C1-C6	-2.55	117.99	122.26
3	O	613	PID	CM1-C1-C6	-2.55	117.99	122.26
4	O	625	DGD	O2G-C1B-C2B	2.55	116.99	111.50
3	O	624	PID	O4-C10-C9	2.54	110.16	108.04
3	N	622	PID	CM1-C1-C2	2.54	117.14	114.28
3	N	613	PID	C8-C9-C11	-2.54	122.49	127.37
3	M	623	PID	C27-O6-C30	-2.53	113.17	117.90
3	O	611	PID	C16-C15-C14	-2.53	123.70	127.31
3	M	622	PID	C11-C12-C13	-2.53	122.75	128.34
3	M	624	PID	C17-C16-C15	-2.52	118.31	123.47
3	N	612	PID	CM1-C1-C2	2.52	117.12	114.28
2	O	602	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
2	O	601	CLA	CMB-C2B-C3B	2.52	129.39	124.68
3	M	611	PID	CM1-C1-C2	2.52	117.11	114.28
4	N	615	DGD	O6D-C1D-C2D	2.51	115.67	110.35
3	O	624	PID	C11-C12-C13	-2.50	122.80	128.34
3	O	622	PID	C11-C12-C13	-2.50	122.80	128.34
3	M	612	PID	C27-O6-C30	-2.50	113.24	117.90
2	N	602	CLA	CMB-C2B-C3B	2.50	129.35	124.68
4	M	615	DGD	O6D-C1D-C2D	2.49	115.61	110.35
2	M	602	CLA	CMB-C2B-C3B	2.48	129.32	124.68
3	N	624	PID	C27-O6-C30	-2.48	113.27	117.90
4	M	625	DGD	C1D-O6D-C5D	-2.47	108.83	113.69
3	O	612	PID	C16-C15-C14	-2.47	123.78	127.31
2	O	601	CLA	CHD-C1D-ND	-2.47	122.19	124.45
3	O	611	PID	C19-C20-C21	-2.47	123.79	127.31
3	O	612	PID	O6-C30-C31	2.46	115.62	111.09
3	N	622	PID	C11-C12-C13	-2.46	122.90	128.34
3	M	612	PID	C11-C12-C13	-2.46	122.91	128.34
3	N	614	PID	CM1-C1-C2	2.45	117.04	114.28
3	O	613	PID	C17-C16-C15	-2.45	118.45	123.47
3	N	613	PID	CM1-C1-C6	-2.45	118.16	122.26
2	N	601	CLA	CED-O2D-CGD	2.44	121.46	115.94
4	M	625	DGD	O2G-C1B-C2B	2.44	116.76	111.50
3	M	623	PID	C18-C19-C20	-2.44	118.48	123.47
4	M	625	DGD	O6D-C1D-O3G	-2.44	104.20	109.97
3	O	611	PID	CM1-C1-C2	2.44	117.02	114.28
2	N	602	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
3	N	621	PID	C27-O6-C30	-2.44	113.36	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	623	PID	C16-C15-C14	-2.43	123.84	127.31
4	M	615	DGD	C1E-O6E-C5E	2.43	118.45	113.69
3	M	622	PID	O4-C10-C9	2.42	110.07	108.04
2	N	602	CLA	C1-C2-C3	2.42	130.23	126.04
3	O	612	PID	CM1-C1-C2	2.41	117.00	114.28
3	N	623	PID	C18-C19-C20	-2.41	118.53	123.47
3	O	614	PID	C19-C20-C21	-2.41	123.87	127.31
3	O	622	PID	CM1-C1-C2	2.41	116.99	114.28
3	O	623	PID	CM1-C1-C2	2.40	116.98	114.28
4	O	615	DGD	C1E-O6E-C5E	2.40	118.40	113.69
2	O	602	CLA	CED-O2D-CGD	2.40	121.37	115.94
3	N	621	PID	C17-C16-C15	-2.39	118.58	123.47
3	N	611	PID	C26-C25-C24	-2.39	106.89	109.21
3	N	612	PID	C27-O6-C30	-2.38	113.46	117.90
3	N	612	PID	C17-C18-C19	-2.38	119.52	124.81
2	M	602	CLA	CHD-C1D-ND	-2.38	122.27	124.45
3	N	612	PID	CM4-C14-C15	-2.38	119.60	122.92
3	O	613	PID	O1-C1-C2	2.37	115.17	113.38
2	O	602	CLA	C3A-C2A-C1A	2.37	104.89	101.34
3	M	612	PID	O6-C30-O7	-2.36	118.27	122.96
3	O	611	PID	C18-C17-C16	-2.36	119.56	124.81
3	M	613	PID	CM1-C1-C6	-2.36	118.31	122.26
3	O	623	PID	O4-C10-C9	2.36	110.01	108.04
3	O	612	PID	C11-C12-C13	-2.35	123.13	128.34
2	M	602	CLA	C1-C2-C3	2.35	130.11	126.04
3	N	611	PID	C19-C20-C21	-2.35	123.96	127.31
3	O	611	PID	C17-C16-C15	-2.33	118.69	123.47
3	N	624	PID	CM4-C14-C15	-2.33	119.67	122.92
3	M	612	PID	CM1-C1-C2	2.32	116.89	114.28
3	M	614	PID	C27-O6-C30	-2.31	113.58	117.90
3	N	612	PID	C11-C12-C13	-2.31	123.22	128.34
3	N	621	PID	C8-C9-C11	-2.31	122.93	127.37
3	N	613	PID	O4-C12-C13	2.31	127.81	122.89
3	O	612	PID	C17-C18-C19	-2.30	119.68	124.81
4	M	615	DGD	O5D-C6D-C5D	2.30	113.31	109.05
2	M	602	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
3	N	623	PID	C8-C9-C11	-2.30	122.95	127.37
3	N	611	PID	C18-C17-C16	-2.30	119.70	124.81
3	N	621	PID	O4-C12-C13	2.29	127.78	122.89
3	O	612	PID	C8-C9-C11	-2.29	122.96	127.37
3	O	621	PID	C27-O6-C30	-2.29	113.62	117.90
3	N	612	PID	CM2-C5-C4	2.28	112.95	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	621	PID	O4-C12-C13	2.28	127.76	122.89
2	M	601	CLA	CHD-C1D-ND	-2.28	122.36	124.45
2	N	602	CLA	CHD-C1D-ND	-2.28	122.36	124.45
3	N	624	PID	C17-C16-C15	-2.28	118.81	123.47
3	M	624	PID	C8-C9-C11	-2.27	123.00	127.37
3	M	613	PID	C17-C16-C15	-2.27	118.83	123.47
3	M	612	PID	C17-C18-C19	-2.26	119.77	124.81
3	O	614	PID	C17-C16-C15	-2.25	118.86	123.47
3	N	612	PID	C8-C9-C11	-2.25	123.04	127.37
3	N	613	PID	C17-C16-C15	-2.25	118.87	123.47
3	M	624	PID	CM1-C1-C6	-2.25	118.50	122.26
3	O	613	PID	CM1-C1-C2	2.24	116.80	114.28
3	N	624	PID	C18-C19-C20	-2.23	118.90	123.47
3	M	614	PID	C8-C9-C11	-2.23	123.09	127.37
3	M	611	PID	C18-C17-C16	-2.23	119.85	124.81
3	N	621	PID	C4-C3-C2	-2.23	106.47	110.77
3	N	614	PID	C8-C9-C11	-2.22	123.10	127.37
3	M	611	PID	CM1-C1-C6	-2.22	118.54	122.26
3	M	621	PID	C8-C9-C11	-2.22	123.11	127.37
3	O	614	PID	C6-C7-C8	-2.20	121.34	125.99
3	M	622	PID	C16-C15-C14	-2.20	124.18	127.31
3	N	612	PID	O4-C10-C9	2.19	109.87	108.04
3	O	621	PID	O4-C12-C13	2.19	127.57	122.89
2	N	601	CLA	C1-C2-C3	2.19	129.83	126.04
3	O	613	PID	O4-C12-C13	2.19	127.56	122.89
3	O	621	PID	C8-C9-C11	-2.19	123.17	127.37
3	N	623	PID	CM1-C1-C2	2.19	116.74	114.28
3	N	611	PID	C27-O6-C30	-2.19	113.82	117.90
2	N	601	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
2	O	601	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
4	N	625	DGD	O2G-C2G-C1G	-2.18	100.51	108.40
2	N	602	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
3	N	624	PID	CM1-C1-C2	2.17	116.72	114.28
3	O	623	PID	C8-C9-C11	-2.17	123.20	127.37
3	M	621	PID	C16-C15-C14	-2.17	124.21	127.31
2	N	601	CLA	CHD-C1D-ND	-2.17	122.46	124.45
4	O	615	DGD	O5D-C6D-C5D	2.17	113.06	109.05
3	M	612	PID	CM4-C14-C15	-2.16	119.89	122.92
3	N	614	PID	CM7-C25-C24	-2.16	108.54	110.47
4	M	625	DGD	O2G-C2G-C1G	-2.16	100.59	108.40
4	N	615	DGD	O5D-C6D-C5D	2.16	113.03	109.05
3	O	614	PID	C8-C9-C11	-2.15	123.23	127.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	601	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
3	O	614	PID	CM7-C25-C24	-2.15	108.54	110.47
3	O	621	PID	C6-C7-C8	-2.15	121.45	125.99
3	N	614	PID	CM4-C14-C15	-2.15	119.91	122.92
3	O	624	PID	C8-C9-C11	-2.14	123.25	127.37
3	M	623	PID	CM1-C1-C2	2.14	116.69	114.28
3	N	624	PID	O4-C10-O3	2.14	124.25	120.12
3	M	613	PID	C17-C18-C19	-2.14	120.05	124.81
3	O	613	PID	C6-C7-C8	-2.14	121.48	125.99
2	M	601	CLA	CED-O2D-CGD	2.13	120.76	115.94
3	O	612	PID	C6-C7-C8	-2.13	121.49	125.99
3	N	611	PID	CM1-C1-C2	2.13	116.67	114.28
3	O	621	PID	C18-C17-C16	-2.12	120.08	124.81
3	M	623	PID	C8-C9-C11	-2.12	123.29	127.37
3	O	611	PID	O4-C12-C13	2.12	127.42	122.89
3	M	612	PID	C8-C9-C11	-2.12	123.30	127.37
3	M	613	PID	O4-C12-C13	2.12	127.41	122.89
2	N	601	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
2	O	602	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
3	M	622	PID	C8-C9-C11	-2.10	123.33	127.37
4	N	625	DGD	O3G-C3G-C2G	-2.09	105.84	110.90
3	N	613	PID	CM1-C1-C2	2.09	116.64	114.28
3	N	613	PID	C17-C18-C19	-2.09	120.15	124.81
2	N	602	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
3	N	613	PID	C27-O6-C30	-2.09	114.01	117.90
2	N	602	CLA	C3C-C4C-NC	-2.08	108.23	110.57
3	M	621	PID	O4-C10-O3	2.08	124.14	120.12
2	O	602	CLA	C2C-C1C-NC	-2.08	108.02	109.97
2	M	601	CLA	C1-C2-C3	2.08	129.63	126.04
3	N	621	PID	C6-C7-C8	-2.07	121.61	125.99
3	M	624	PID	CM1-C1-C2	2.07	116.61	114.28
3	N	611	PID	CM1-C1-C6	-2.07	118.79	122.26
3	N	611	PID	O4-C12-C13	2.07	127.30	122.89
2	O	602	CLA	CHD-C1D-ND	-2.07	122.55	124.45
3	N	614	PID	O4-C10-C9	2.07	109.77	108.04
2	N	601	CLA	C3A-C2A-C1A	2.07	104.43	101.34
3	O	611	PID	O4-C10-C9	2.06	109.76	108.04
3	O	622	PID	C16-C15-C14	-2.05	124.38	127.31
2	O	602	CLA	C1-C2-C3	2.05	129.59	126.04
3	N	614	PID	C17-C16-C15	-2.05	119.28	123.47
3	N	623	PID	C4-C3-C2	-2.05	106.82	110.77
3	N	613	PID	O1-C1-C2	2.05	114.92	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	622	PID	C8-C9-C11	-2.04	123.44	127.37
3	N	623	PID	C16-C15-C14	-2.04	124.39	127.31
3	O	611	PID	C26-C25-C24	-2.04	107.23	109.21
2	M	602	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
3	N	624	PID	C6-C7-C8	-2.03	121.69	125.99
3	O	624	PID	CM1-C1-C2	2.03	116.57	114.28
3	O	623	PID	C6-C7-C8	-2.03	121.70	125.99
4	O	615	DGD	O6D-C5D-C4D	2.03	113.38	109.69
3	M	611	PID	O4-C12-C13	2.03	127.21	122.89
3	M	611	PID	C19-C20-C21	-2.02	124.42	127.31
3	N	611	PID	C17-C16-C15	-2.02	119.33	123.47
3	O	624	PID	C26-C25-C24	-2.02	107.25	109.21
3	O	624	PID	O1-C1-C2	2.02	114.90	113.38
3	O	623	PID	C16-C15-C14	-2.01	124.44	127.31
3	M	614	PID	C17-C16-C15	-2.01	119.36	123.47
3	O	612	PID	C26-C25-C24	-2.01	107.26	109.21
3	O	621	PID	O4-C10-O3	2.00	123.99	120.12
3	O	624	PID	CM4-C14-C15	-2.00	120.11	122.92
3	O	613	PID	C18-C19-C20	-2.00	119.37	123.47
3	N	624	PID	C4-C3-C2	-2.00	106.90	110.77
3	M	623	PID	CM4-C14-C15	-2.00	120.12	122.92

All (21) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	M	601	CLA	C8
2	M	601	CLA	ND
2	M	602	CLA	ND
2	N	601	CLA	C8
2	N	601	CLA	ND
2	N	602	CLA	ND
2	O	601	CLA	C8
2	O	601	CLA	ND
2	O	602	CLA	ND
3	M	613	PID	C3
3	N	613	PID	C3
3	O	613	PID	C3
4	M	615	DGD	C2D
4	M	615	DGD	C5D
4	M	615	DGD	C5E
4	N	615	DGD	C2D
4	N	615	DGD	C5D

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Mol	Chain	Res	Type	Atom
4	N	615	DGD	C5E
4	O	615	DGD	C2D
4	O	615	DGD	C5D
4	O	615	DGD	C5E

All (205) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	615	DGD	O2G-C2G-C3G-O3G
4	M	615	DGD	O6D-C1D-O3G-C3G
4	M	615	DGD	C4D-C5D-C6D-O5D
4	N	615	DGD	O2G-C2G-C3G-O3G
4	N	615	DGD	O6D-C1D-O3G-C3G
4	N	615	DGD	C4D-C5D-C6D-O5D
4	O	615	DGD	O2G-C2G-C3G-O3G
4	O	615	DGD	O6D-C1D-O3G-C3G
4	O	615	DGD	C4D-C5D-C6D-O5D
4	M	615	DGD	O6D-C5D-C6D-O5D
4	N	615	DGD	O6D-C5D-C6D-O5D
4	O	615	DGD	O6D-C5D-C6D-O5D
4	M	625	DGD	C5B-C6B-C7B-C8B
4	N	625	DGD	C5B-C6B-C7B-C8B
4	O	625	DGD	C5B-C6B-C7B-C8B
4	O	625	DGD	C8B-C9B-CAB-CBB
4	O	615	DGD	C7B-C8B-C9B-CAB
4	M	625	DGD	C8B-C9B-CAB-CBB
4	N	615	DGD	C7B-C8B-C9B-CAB
4	N	625	DGD	C8B-C9B-CAB-CBB
4	M	615	DGD	C7B-C8B-C9B-CAB
4	M	615	DGD	O6E-C5E-C6E-O5E
4	N	615	DGD	O6E-C5E-C6E-O5E
4	O	615	DGD	O6E-C5E-C6E-O5E
4	M	615	DGD	C1A-C2A-C3A-C4A
4	N	615	DGD	C1A-C2A-C3A-C4A
4	O	615	DGD	C1A-C2A-C3A-C4A
4	M	625	DGD	CAB-CBB-CCB-CDB
3	M	612	PID	O7-C30-O6-C27
3	N	622	PID	O7-C30-O6-C27
4	O	625	DGD	CAB-CBB-CCB-CDB
3	O	612	PID	O7-C30-O6-C27
4	N	625	DGD	CAB-CBB-CCB-CDB
3	M	622	PID	O7-C30-O6-C27

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Mol	Chain	Res	Type	Atoms
3	M	613	PID	C19-C20-C21-CM5
3	M	621	PID	C19-C20-C21-CM5
3	N	613	PID	C19-C20-C21-CM5
3	N	621	PID	C19-C20-C21-CM5
3	O	613	PID	C19-C20-C21-CM5
4	M	615	DGD	C5B-C6B-C7B-C8B
4	M	625	DGD	CAA-CBA-CCA-CDA
4	M	625	DGD	C6B-C7B-C8B-C9B
4	N	615	DGD	C5B-C6B-C7B-C8B
4	N	625	DGD	C6A-C7A-C8A-C9A
4	N	625	DGD	C6B-C7B-C8B-C9B
4	O	625	DGD	CAA-CBA-CCA-CDA
4	O	625	DGD	C6B-C7B-C8B-C9B
4	M	625	DGD	C4B-C5B-C6B-C7B
4	N	615	DGD	CEB-CFB-CGB-CHB
4	N	625	DGD	C9A-CAA-CBA-CCA
4	N	625	DGD	CAA-CBA-CCA-CDA
4	N	625	DGD	CEB-CFB-CGB-CHB
4	O	625	DGD	C4B-C5B-C6B-C7B
3	O	622	PID	O7-C30-O6-C27
4	M	615	DGD	CEB-CFB-CGB-CHB
4	O	615	DGD	C5B-C6B-C7B-C8B
4	O	615	DGD	CEB-CFB-CGB-CHB
4	M	615	DGD	C9B-CAB-CBB-CCB
4	O	625	DGD	C9A-CAA-CBA-CCA
3	N	612	PID	O7-C30-O6-C27
4	M	625	DGD	C6A-C7A-C8A-C9A
4	M	625	DGD	C9A-CAA-CBA-CCA
4	M	625	DGD	CEB-CFB-CGB-CHB
4	O	625	DGD	CEB-CFB-CGB-CHB
4	O	625	DGD	C6A-C7A-C8A-C9A
4	O	615	DGD	C9B-CAB-CBB-CCB
4	M	615	DGD	C3B-C4B-C5B-C6B
4	M	625	DGD	CBA-CCA-CDA-CEA
4	N	615	DGD	C3B-C4B-C5B-C6B
4	N	615	DGD	CBA-CCA-CDA-CEA
4	N	615	DGD	C9B-CAB-CBB-CCB
4	N	625	DGD	CBA-CCA-CDA-CEA
4	O	625	DGD	CCB-CDB-CEB-CFB
4	O	615	DGD	C3B-C4B-C5B-C6B
4	N	625	DGD	C4B-C5B-C6B-C7B
4	M	615	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
4	M	625	DGD	CCB-CDB-CEB-CFB
4	N	615	DGD	C4A-C5A-C6A-C7A
4	N	625	DGD	CCB-CDB-CEB-CFB
4	O	625	DGD	CBA-CCA-CDA-CEA
4	O	615	DGD	C4A-C5A-C6A-C7A
4	O	615	DGD	CBA-CCA-CDA-CEA
4	M	615	DGD	C4A-C5A-C6A-C7A
2	O	601	CLA	C3-C5-C6-C7
4	M	615	DGD	CEA-CFA-CGA-CHA
4	M	615	DGD	CBB-CCB-CDB-CEB
4	O	615	DGD	CAB-CBB-CCB-CDB
2	N	601	CLA	C3-C5-C6-C7
4	N	615	DGD	CAB-CBB-CCB-CDB
4	M	615	DGD	CAB-CBB-CCB-CDB
4	N	615	DGD	CBB-CCB-CDB-CEB
4	O	615	DGD	CBB-CCB-CDB-CEB
4	N	615	DGD	CEA-CFA-CGA-CHA
4	O	615	DGD	CEA-CFA-CGA-CHA
4	O	615	DGD	C2D-C1D-O3G-C3G
4	M	615	DGD	CDA-CEA-CFA-CGA
4	N	625	DGD	CEA-CFA-CGA-CHA
4	O	615	DGD	CDA-CEA-CFA-CGA
4	O	625	DGD	C1A-C2A-C3A-C4A
4	N	615	DGD	CDA-CEA-CFA-CGA
2	M	601	CLA	C3-C5-C6-C7
4	O	625	DGD	CEA-CFA-CGA-CHA
4	M	615	DGD	C1G-C2G-C3G-O3G
4	M	625	DGD	CEA-CFA-CGA-CHA
4	N	615	DGD	C1G-C2G-C3G-O3G
4	N	625	DGD	C7B-C8B-C9B-CAB
4	O	615	DGD	CFA-CGA-CHA-CIA
4	O	615	DGD	C1G-C2G-C3G-O3G
4	M	625	DGD	C2G-C3G-O3G-C1D
4	N	625	DGD	C2G-C3G-O3G-C1D
4	O	625	DGD	C2G-C3G-O3G-C1D
4	O	625	DGD	CFB-CGB-CHB-CIB
4	M	625	DGD	CFB-CGB-CHB-CIB
4	N	625	DGD	CFB-CGB-CHB-CIB
4	O	625	DGD	CFA-CGA-CHA-CIA
4	M	615	DGD	CFA-CGA-CHA-CIA
4	M	625	DGD	CFA-CGA-CHA-CIA
4	N	615	DGD	CFA-CGA-CHA-CIA

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Mol	Chain	Res	Type	Atoms
4	N	625	DGD	CFA-CGA-CHA-CIA
4	O	625	DGD	C8A-C9A-CAA-CBA
3	N	624	PID	C19-C20-C21-CM5
4	N	625	DGD	C1A-C2A-C3A-C4A
4	M	625	DGD	C8A-C9A-CAA-CBA
4	M	615	DGD	C2D-C1D-O3G-C3G
4	N	615	DGD	C2D-C1D-O3G-C3G
4	O	625	DGD	C9B-CAB-CBB-CCB
4	M	625	DGD	C7B-C8B-C9B-CAB
4	O	615	DGD	C9A-CAA-CBA-CCA
4	M	625	DGD	C1A-C2A-C3A-C4A
4	O	615	DGD	O1A-C1A-O1G-C1G
4	M	625	DGD	C9B-CAB-CBB-CCB
4	M	615	DGD	C7A-C8A-C9A-CAA
4	N	625	DGD	CDA-CEA-CFA-CGA
4	N	625	DGD	C8A-C9A-CAA-CBA
4	N	615	DGD	O1A-C1A-O1G-C1G
4	O	615	DGD	C7A-C8A-C9A-CAA
4	M	615	DGD	C5A-C6A-C7A-C8A
4	N	625	DGD	C3A-C4A-C5A-C6A
4	M	615	DGD	C9A-CAA-CBA-CCA
4	M	615	DGD	O1A-C1A-O1G-C1G
4	O	615	DGD	C6B-C7B-C8B-C9B
4	N	615	DGD	C9A-CAA-CBA-CCA
4	M	625	DGD	CDA-CEA-CFA-CGA
4	O	625	DGD	CCA-CDA-CEA-CFA
4	O	625	DGD	C7B-C8B-C9B-CAB
4	N	615	DGD	C6B-C7B-C8B-C9B
4	O	625	DGD	C3A-C4A-C5A-C6A
4	O	625	DGD	CDA-CEA-CFA-CGA
4	M	615	DGD	C6B-C7B-C8B-C9B
4	O	615	DGD	CFB-CGB-CHB-CIB
4	N	615	DGD	C7A-C8A-C9A-CAA
4	O	615	DGD	C5A-C6A-C7A-C8A
3	N	611	PID	C19-C20-C21-CM5
3	O	611	PID	C19-C20-C21-CM5
3	O	621	PID	C19-C20-C21-CM5
4	M	615	DGD	C2A-C3A-C4A-C5A
4	N	615	DGD	C5A-C6A-C7A-C8A
2	N	601	CLA	CAD-CBD-CGD-O2D
2	O	601	CLA	CAD-CBD-CGD-O2D
4	N	615	DGD	CFB-CGB-CHB-CIB

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Mol	Chain	Res	Type	Atoms
4	M	625	DGD	C3A-C4A-C5A-C6A
4	N	625	DGD	C9B-CAB-CBB-CCB
4	M	615	DGD	CFB-CGB-CHB-CIB
4	O	615	DGD	C2A-C3A-C4A-C5A
4	N	615	DGD	C2A-C3A-C4A-C5A
4	M	615	DGD	C2E-C1E-O5D-C6D
4	N	625	DGD	CCA-CDA-CEA-CFA
4	M	615	DGD	C3A-C4A-C5A-C6A
3	N	623	PID	C19-C20-C21-CM5
4	N	615	DGD	O6E-C1E-O5D-C6D
4	N	615	DGD	C2E-C1E-O5D-C6D
4	O	615	DGD	C2E-C1E-O5D-C6D
4	M	615	DGD	O6E-C1E-O5D-C6D
4	N	615	DGD	C3A-C4A-C5A-C6A
4	M	625	DGD	CCA-CDA-CEA-CFA
4	O	615	DGD	C3A-C4A-C5A-C6A
4	O	625	DGD	C5A-C6A-C7A-C8A
4	O	615	DGD	O6E-C1E-O5D-C6D
4	N	625	DGD	C5A-C6A-C7A-C8A
4	N	625	DGD	C7A-C8A-C9A-CAA
2	M	601	CLA	C12-C13-C15-C16
2	N	601	CLA	C12-C13-C15-C16
2	O	601	CLA	C12-C13-C15-C16
4	N	615	DGD	C8B-C9B-CAB-CBB
2	M	602	CLA	CAD-CBD-CGD-O2D
2	N	602	CLA	CAD-CBD-CGD-O2D
2	O	602	CLA	CAD-CBD-CGD-O2D
2	O	602	CLA	O2A-C1-C2-C3
4	M	625	DGD	C5A-C6A-C7A-C8A
4	O	615	DGD	O2G-C1B-C2B-C3B
4	M	625	DGD	C4A-C5A-C6A-C7A
2	O	601	CLA	C4-C3-C5-C6
4	O	615	DGD	C8B-C9B-CAB-CBB
4	O	625	DGD	C7A-C8A-C9A-CAA
4	M	625	DGD	C7A-C8A-C9A-CAA
4	N	615	DGD	O2G-C1B-C2B-C3B
3	M	611	PID	C19-C20-C21-CM5
4	M	615	DGD	O2G-C1B-C2B-C3B
2	M	601	CLA	C4-C3-C5-C6
4	M	615	DGD	C8B-C9B-CAB-CBB
2	N	602	CLA	CAA-CBA-CGA-O2A
4	N	625	DGD	C4A-C5A-C6A-C7A

Continued on next page...

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Mol	Chain	Res	Type	Atoms
4	M	615	DGD	O1B-C1B-C2B-C3B
4	N	615	DGD	O1B-C1B-C2B-C3B
4	O	615	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

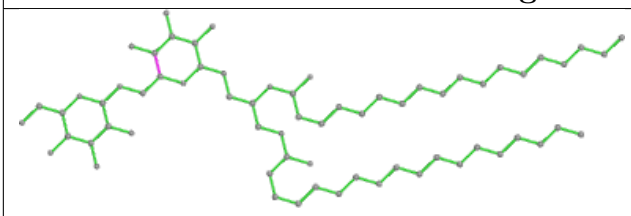
29 monomers are involved in 55 short contacts:

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

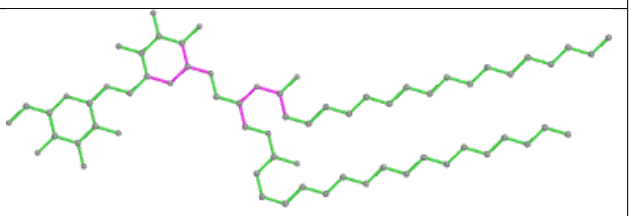
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

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

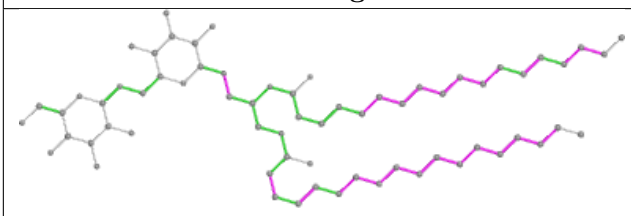
Ligand DGD O 625



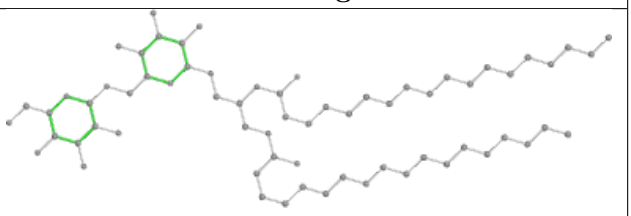
Bond lengths



Bond angles

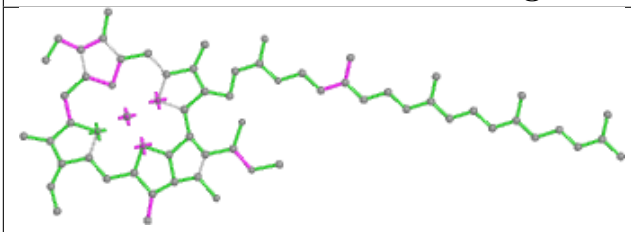


Torsions

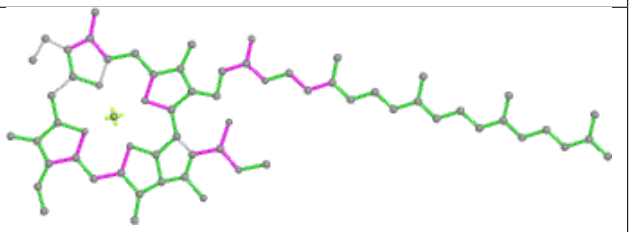


Rings

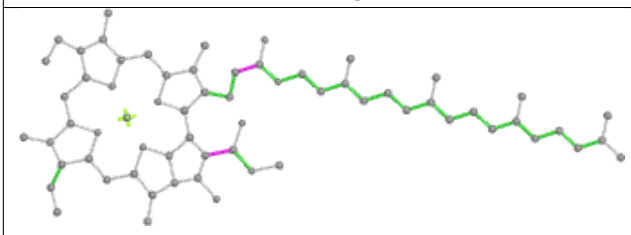
Ligand CLA N 602



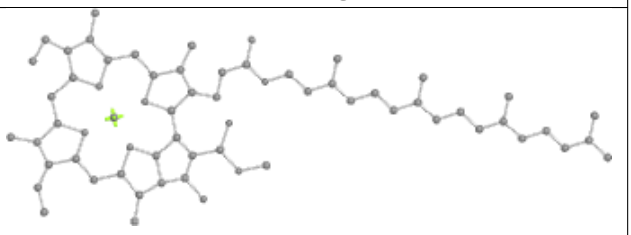
Bond lengths



Bond angles

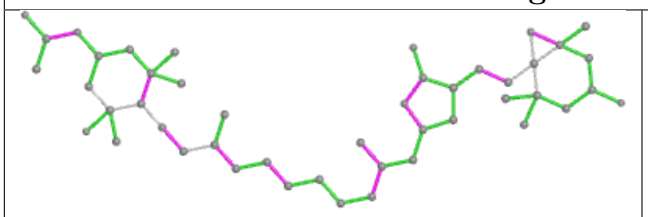


Torsions

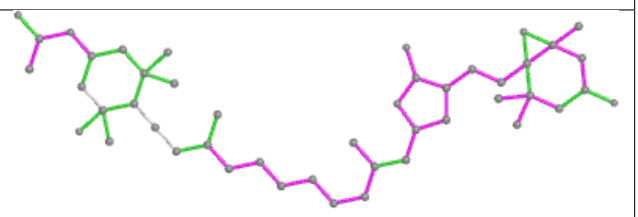


Rings

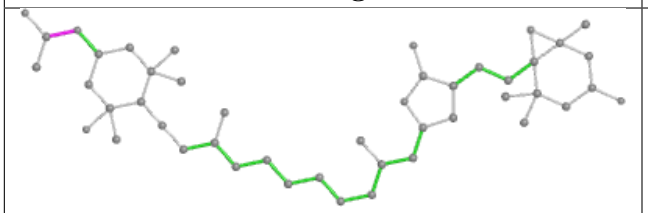
Ligand PID N 612



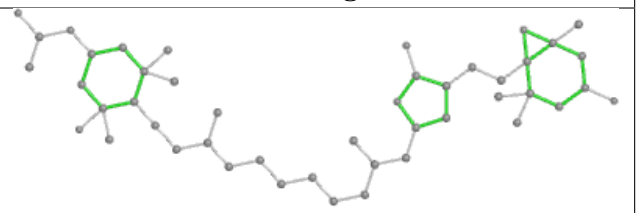
Bond lengths



Bond angles

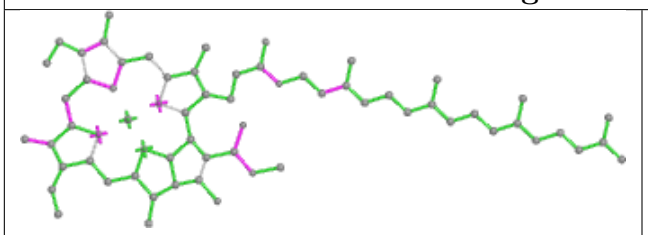


Torsions



Rings

Ligand CLA M 601



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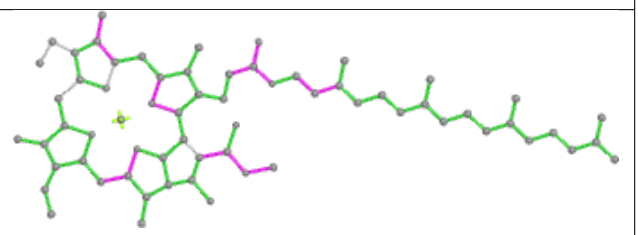
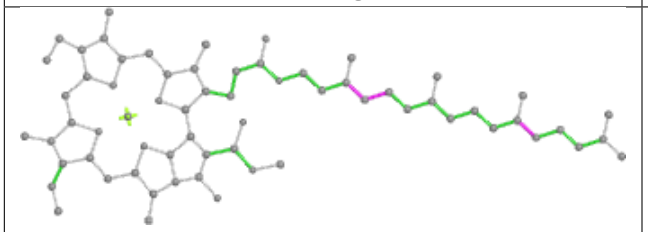


Bond angles



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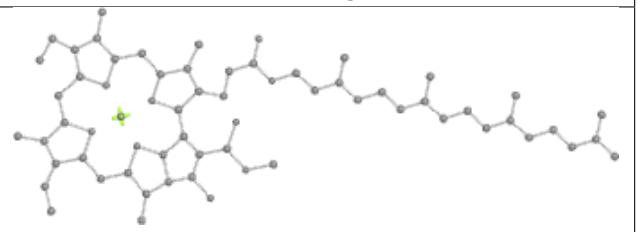
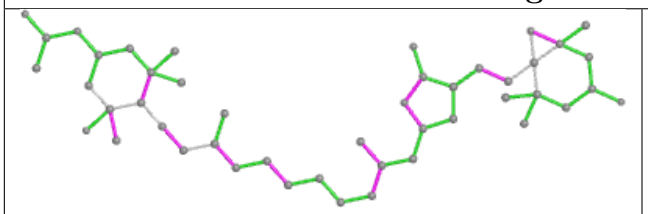


Rings

Ligand PID M 621



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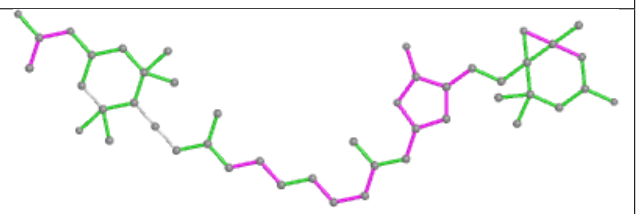
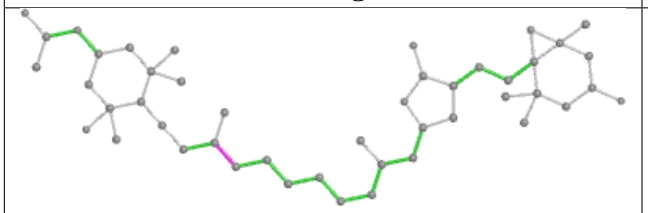


Bond angles



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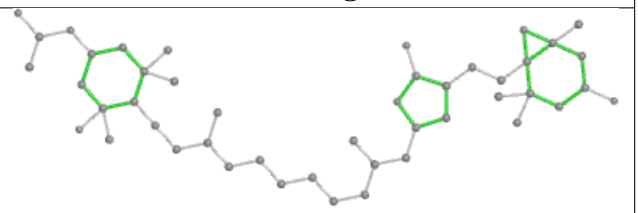

Rings

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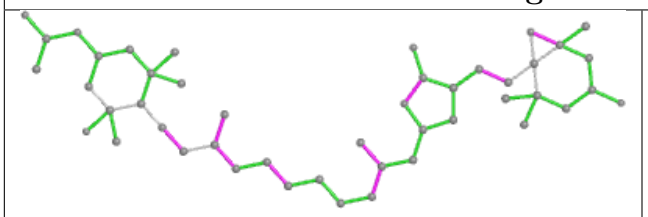

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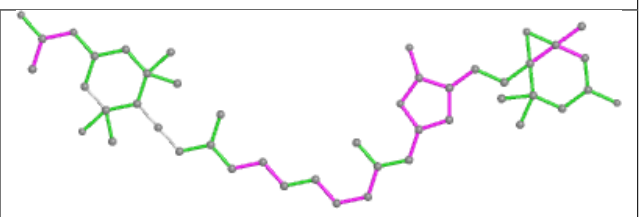

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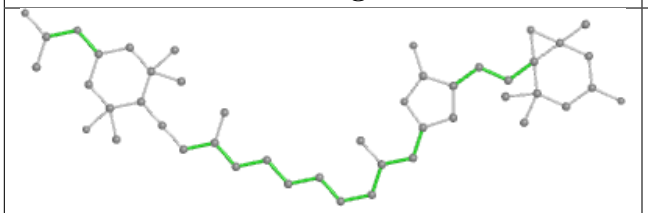

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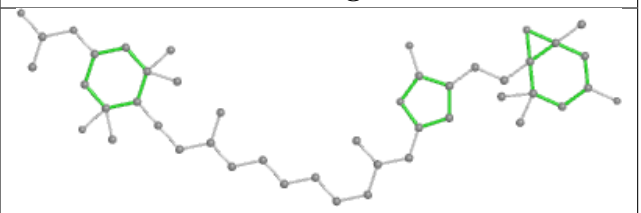
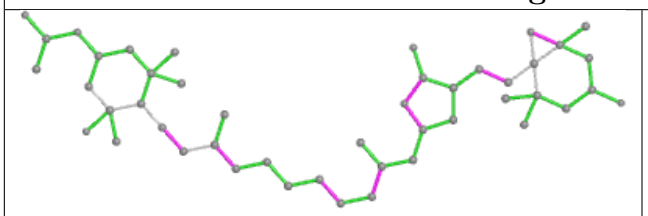


Rings

Ligand PID N 623



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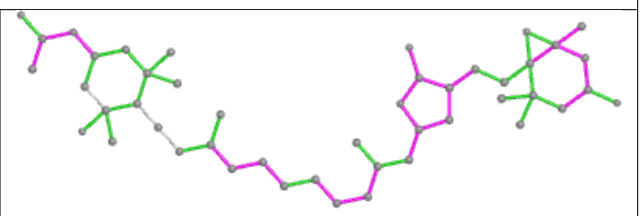

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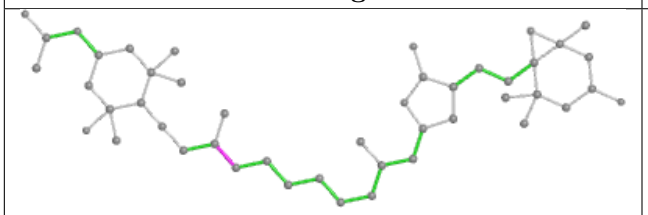

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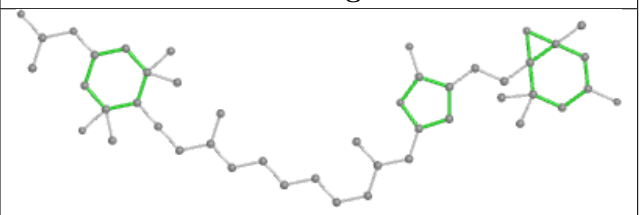

Rings

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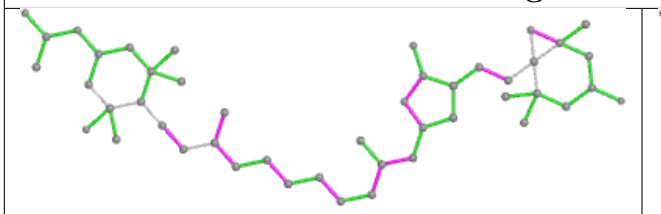

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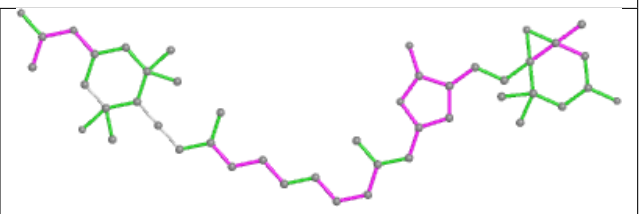
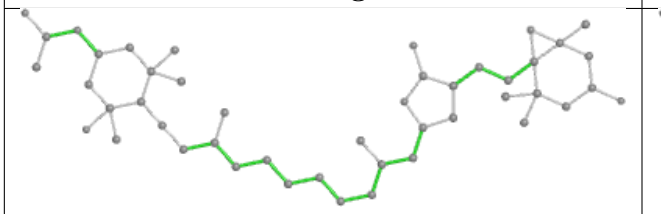


Bond angles



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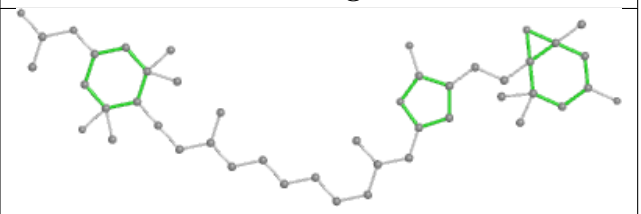
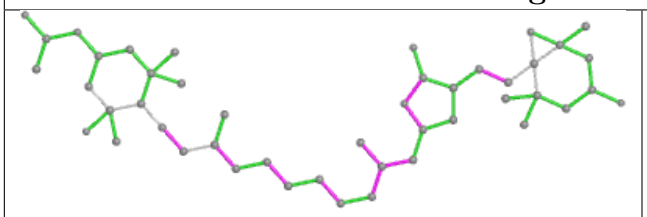


Rings

Ligand PID N 611



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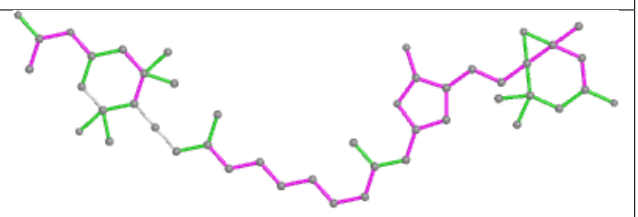
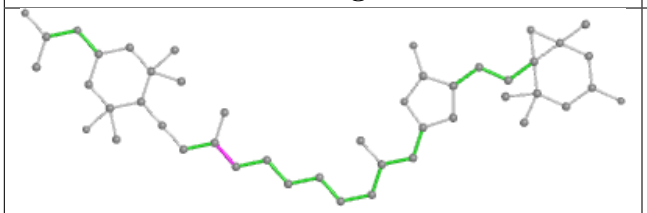


Bond angles



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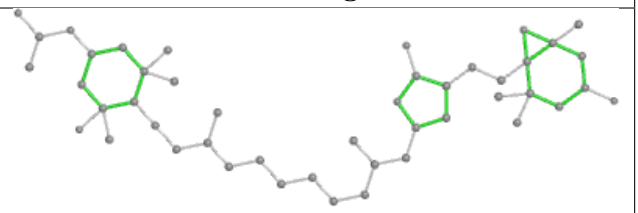
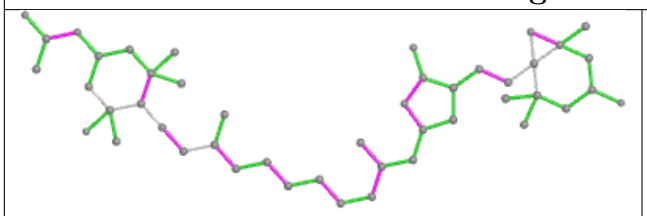


Rings

Ligand PID O 612



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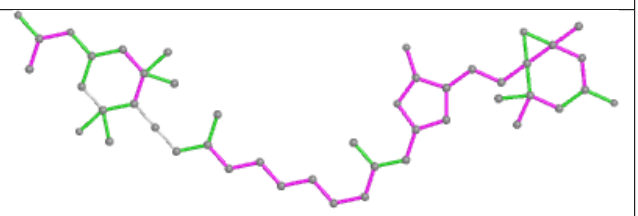
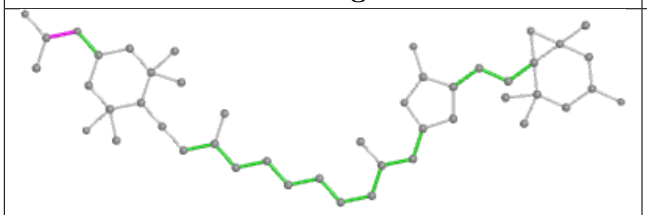


Bond angles



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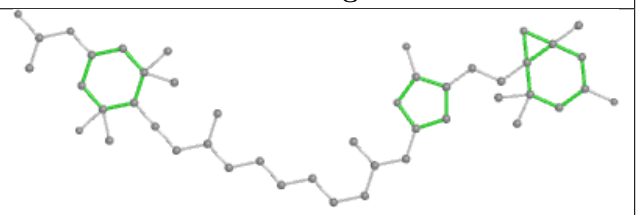
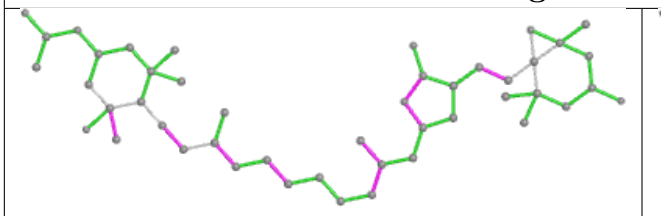
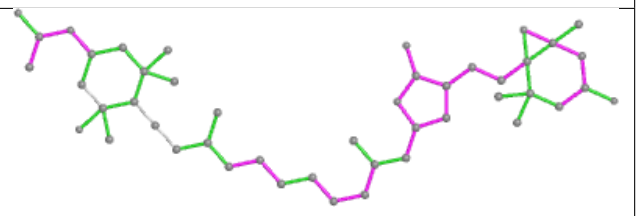


Rings

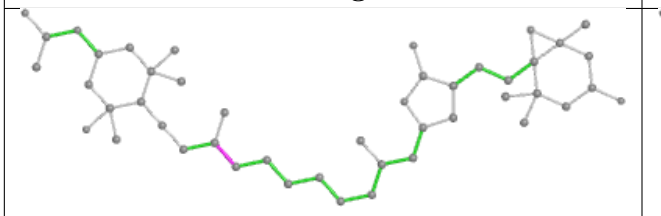
Ligand PID N 621



Bond lengths



Bond angles



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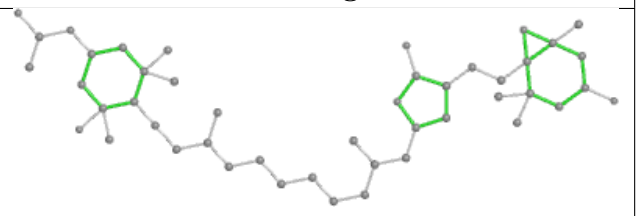
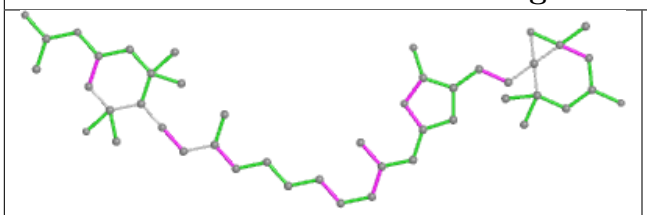
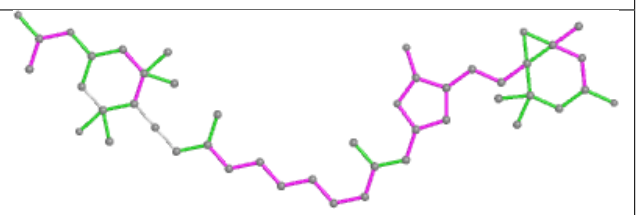


Rings

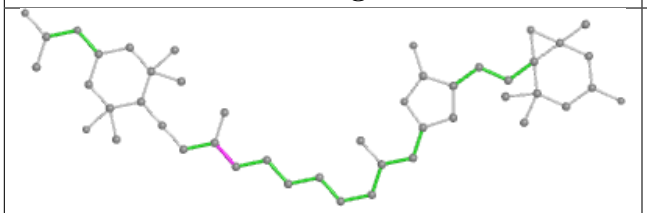
Ligand PID O 611



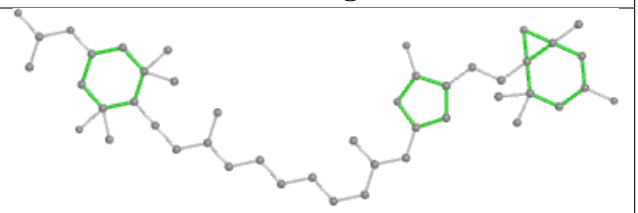
Bond lengths



Bond angles

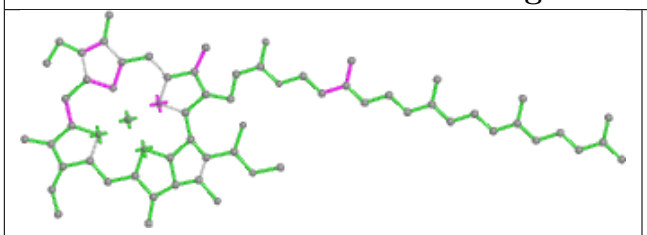


Torsions



Rings

Ligand CLA O 602



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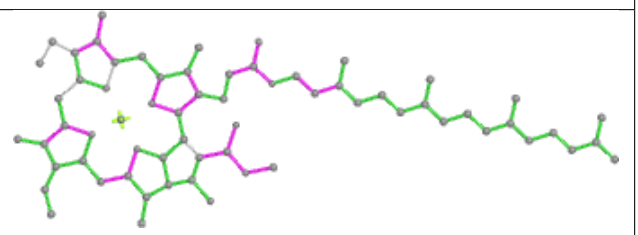
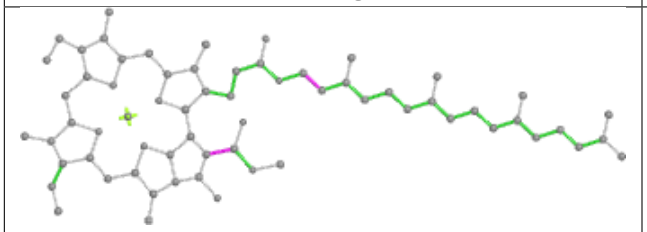


Bond angles



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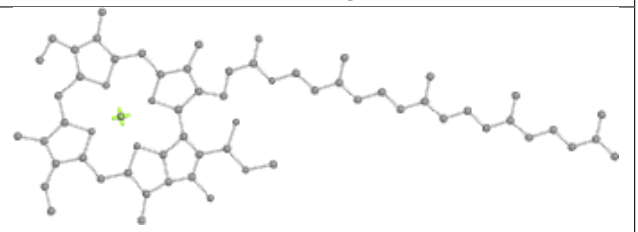
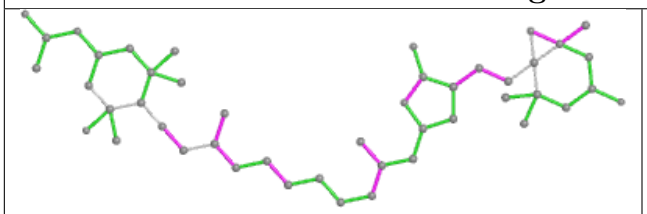


Rings

Ligand PID N 624



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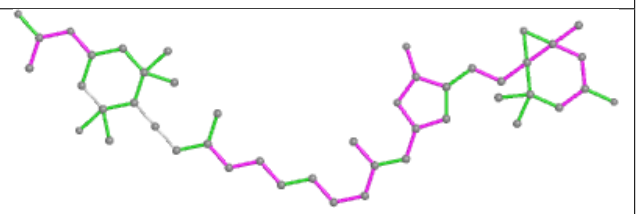
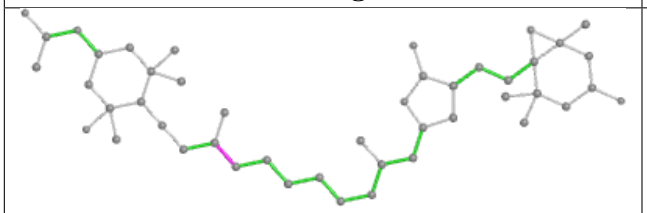


Bond angles



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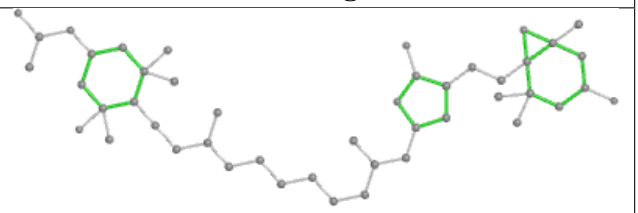
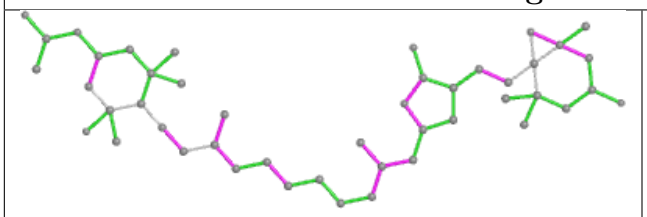


Rings

Ligand PID M 611



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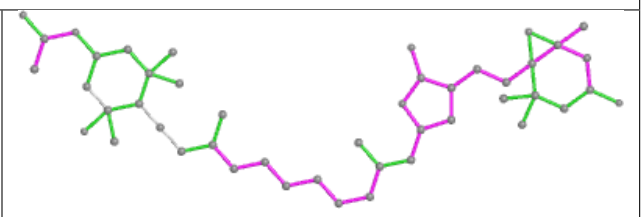
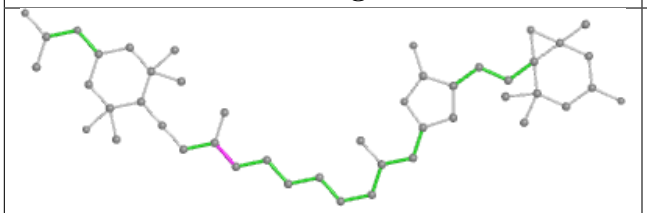


Bond angles



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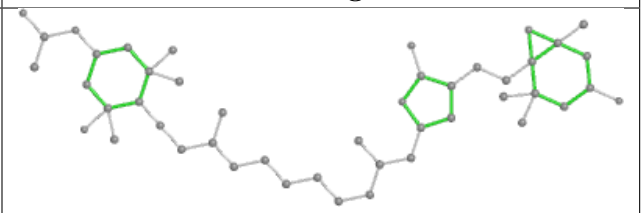

Rings

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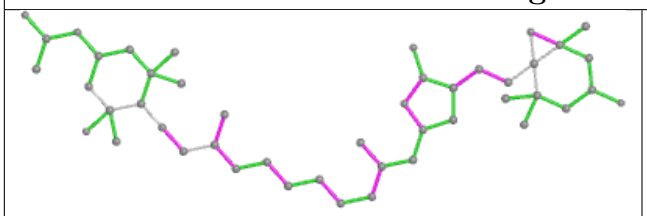

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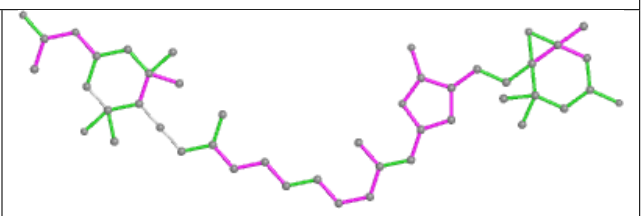
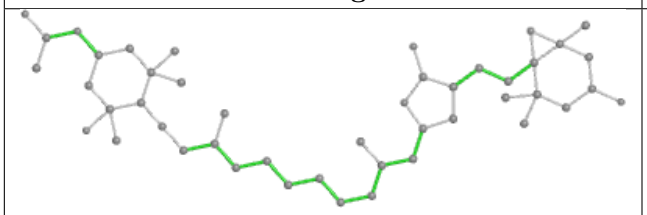


Bond angles



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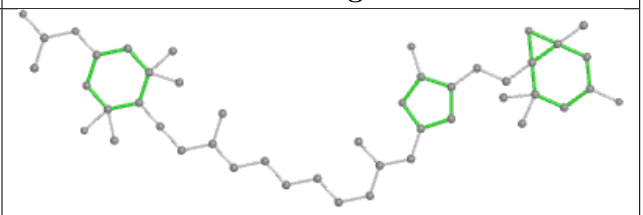

Rings

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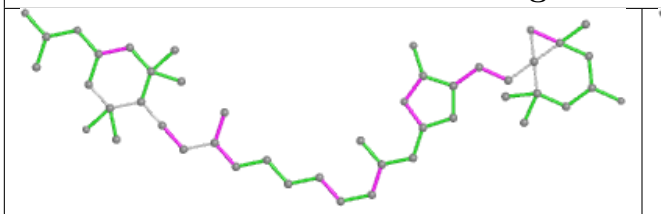

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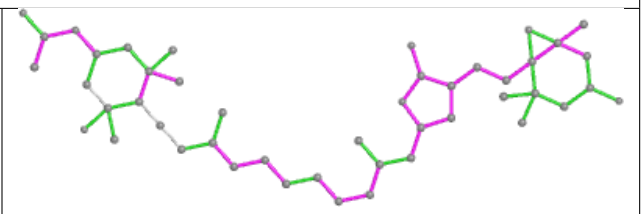
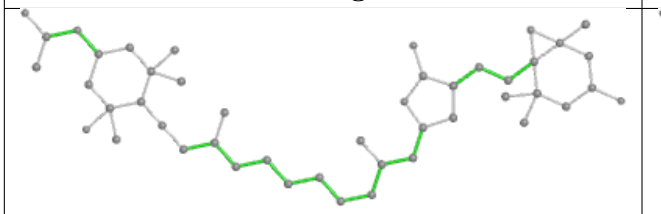


Bond angles



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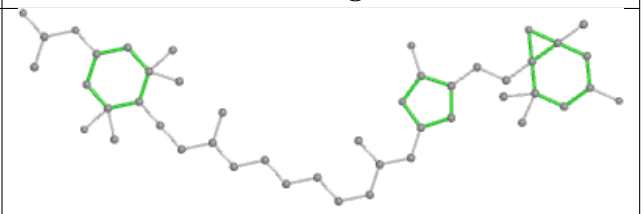
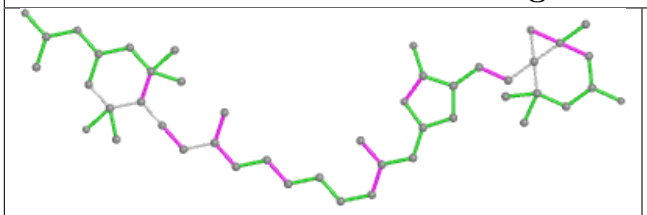


Rings

Ligand PID N 622



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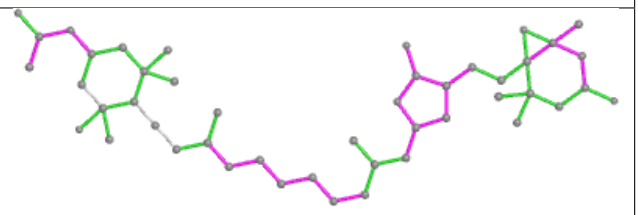
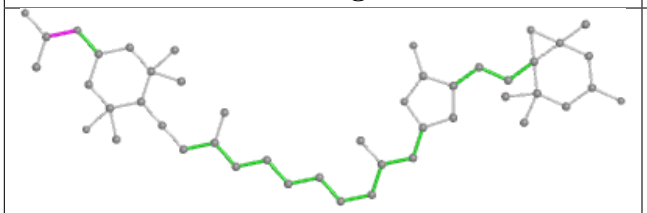


Bond angles



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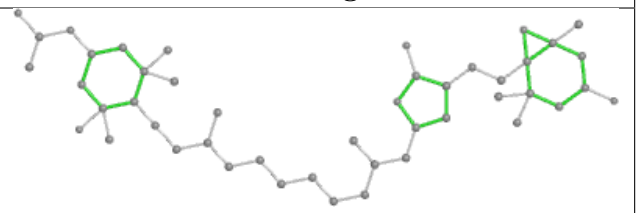

Rings

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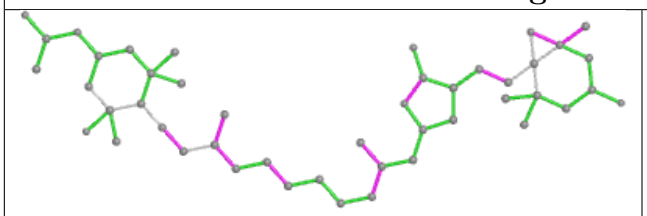

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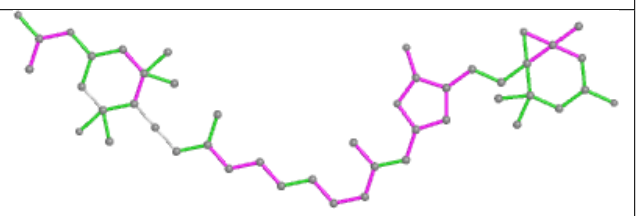
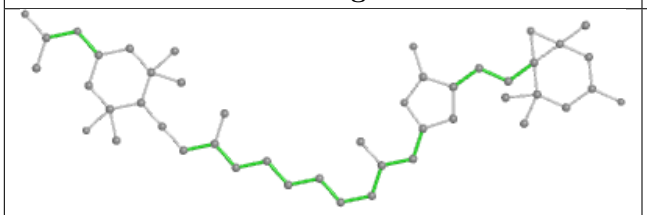


Bond angles



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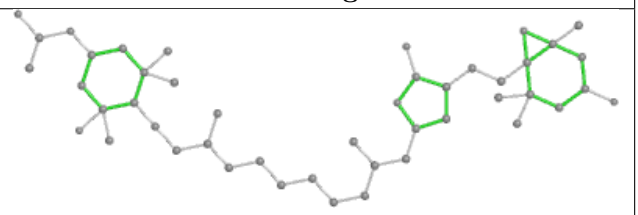
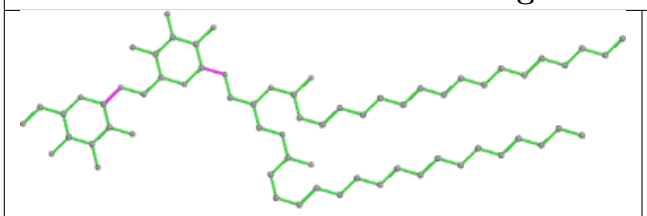


Rings

Ligand DGD M 615



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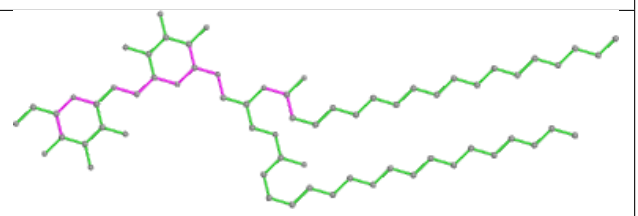
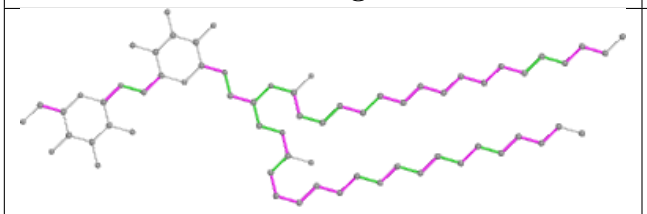
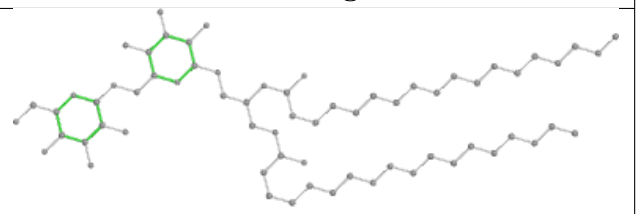


Bond angles

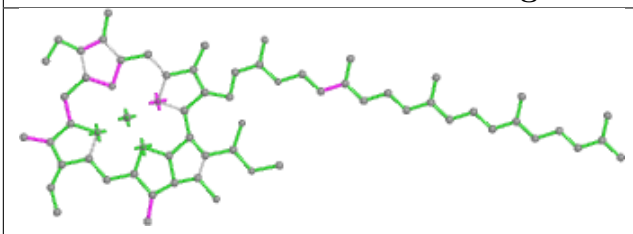


Torsions



Rings

Ligand CLA M 602



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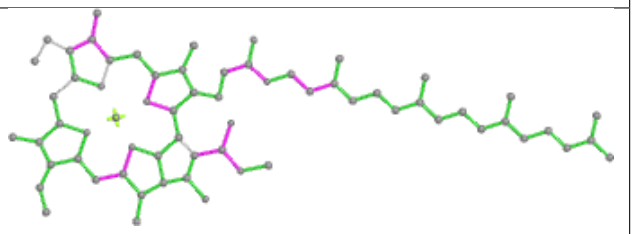
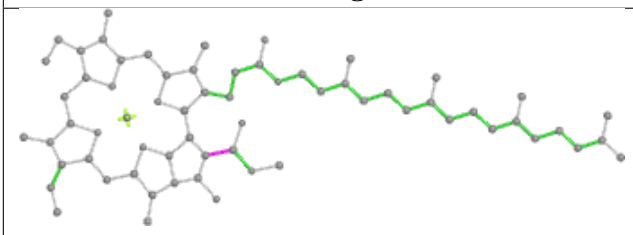


Bond angles



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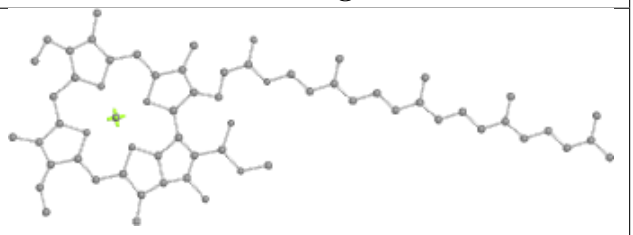
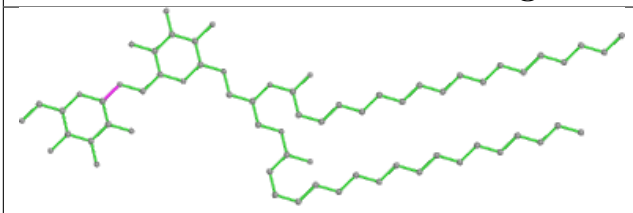


Rings

Ligand DGD N 625



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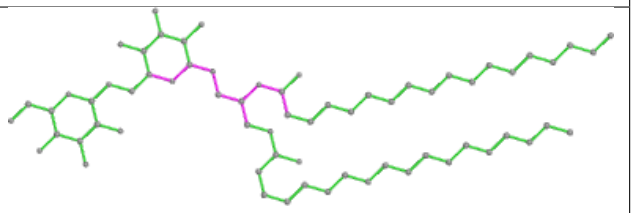
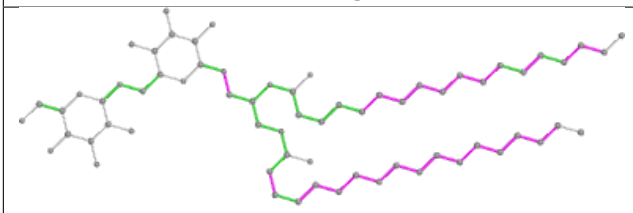


Bond angles



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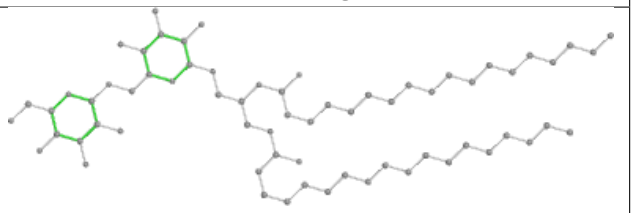
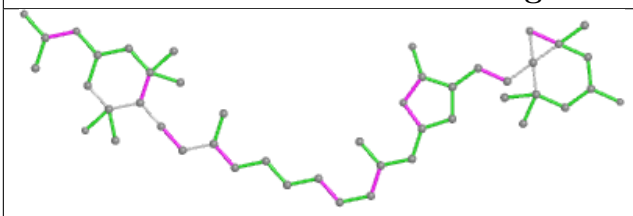


Rings

Ligand PID M 612



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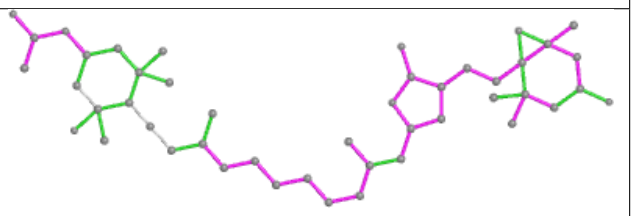
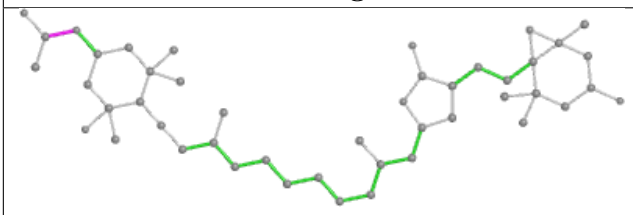


Bond angles



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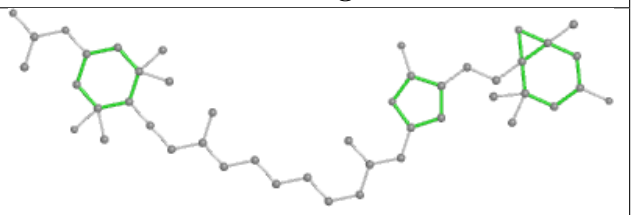
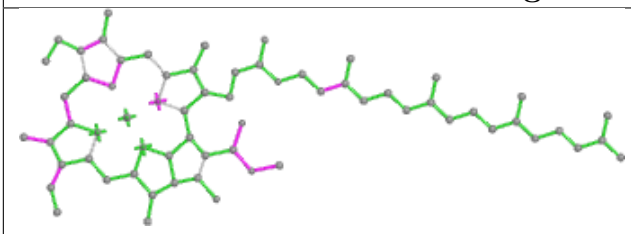
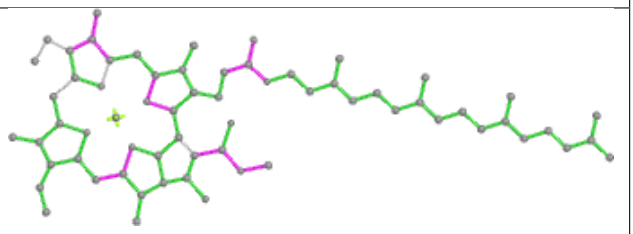


Rings

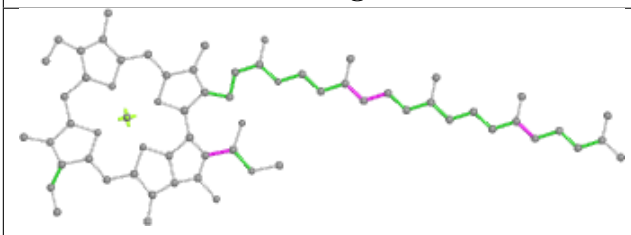
Ligand CLA O 601



Bond lengths



Bond angles



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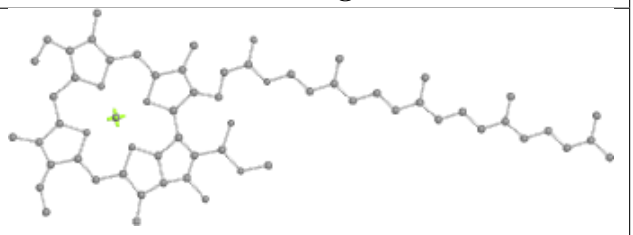
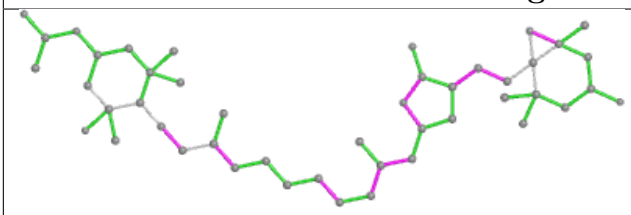


Rings

Ligand PID N 613



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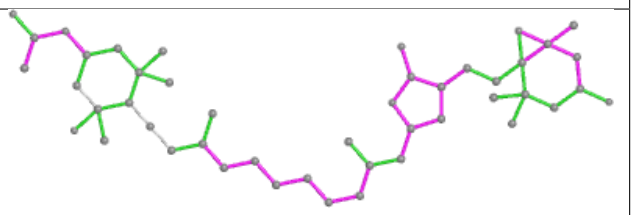
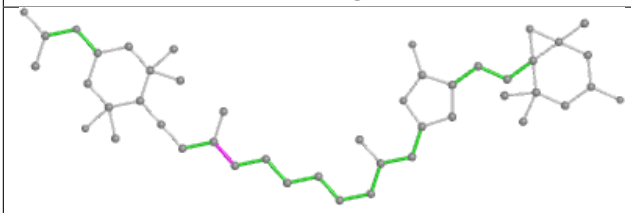
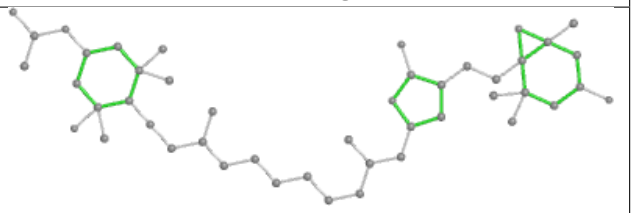


Bond angles

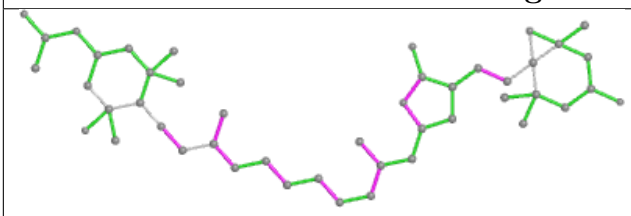


Torsions



Rings

Ligand PID M 623



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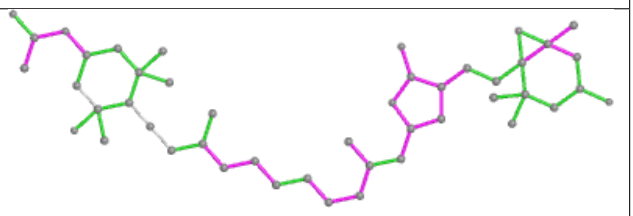
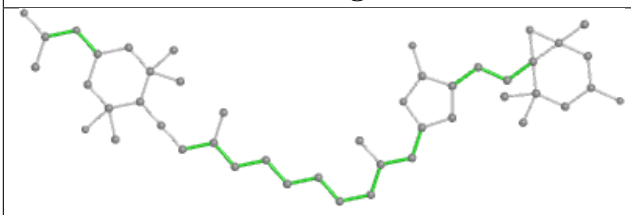


Bond angles



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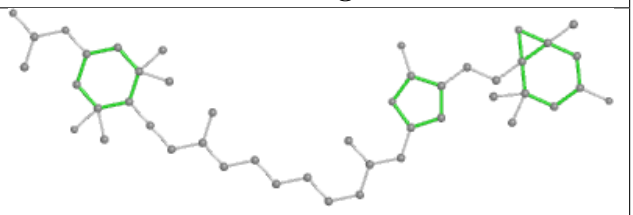
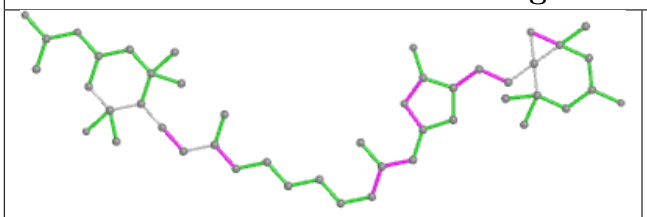


Rings

Ligand PID O 613



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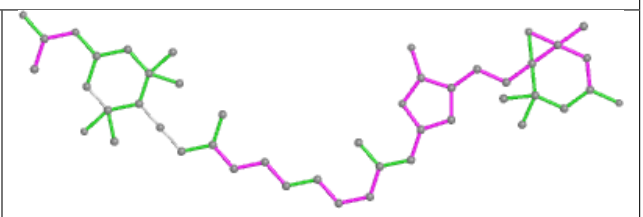

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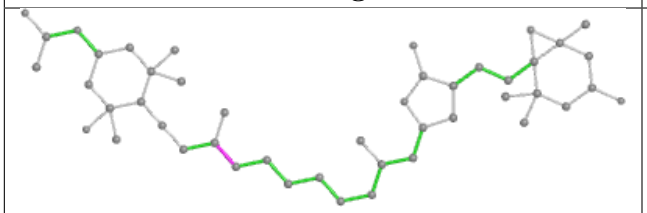

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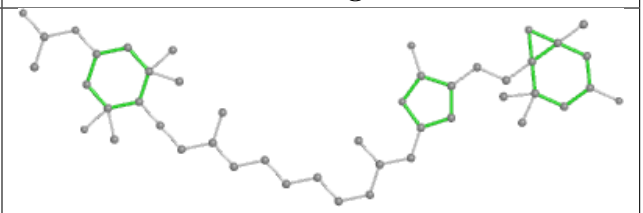

Rings

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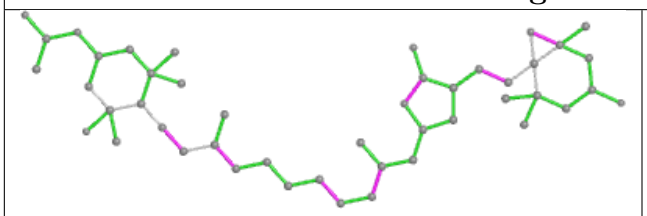

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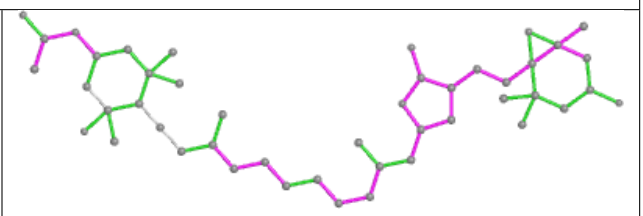
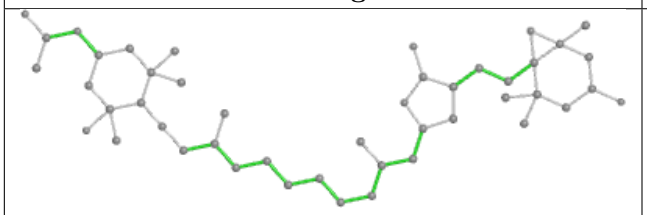


Bond angles



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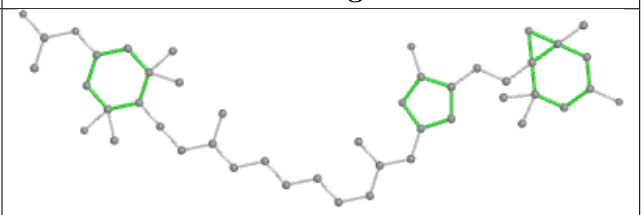
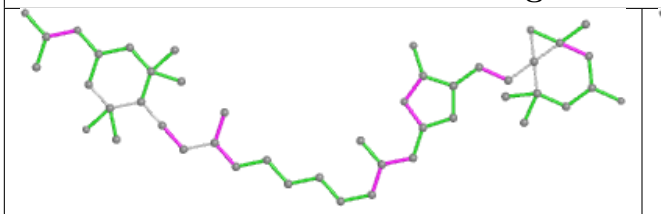


Rings

Ligand PID M 622



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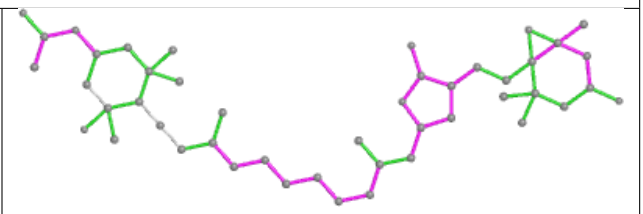
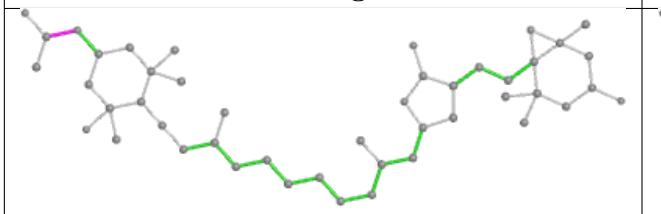
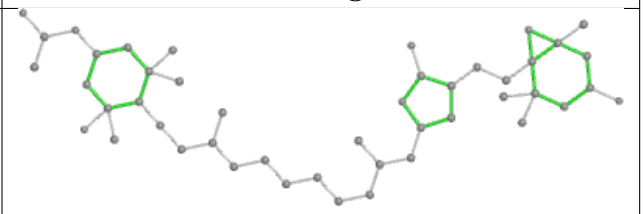


Bond angles

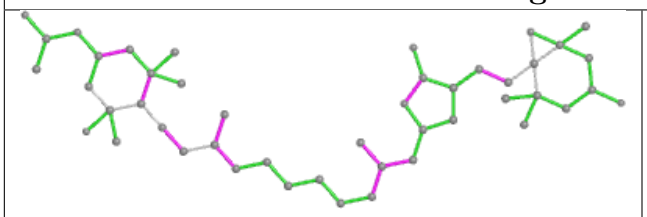


Torsions



Rings

Ligand PID O 622



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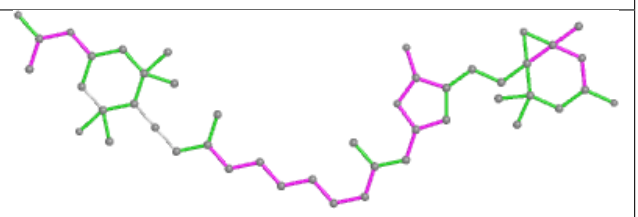
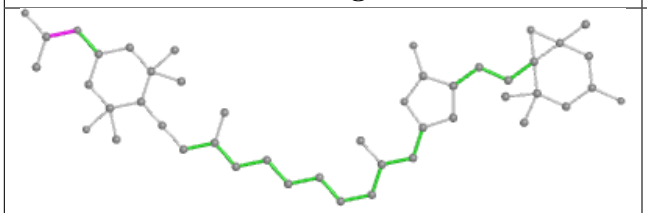
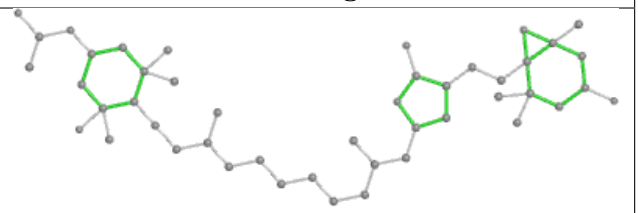


Bond angles

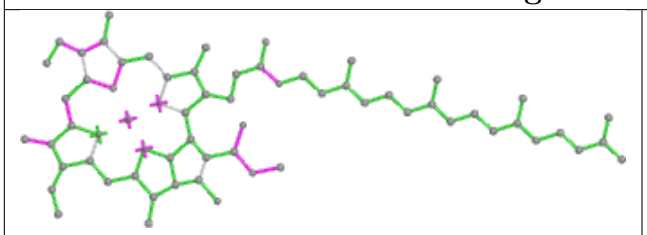


Torsions



Rings

Ligand CLA N 601



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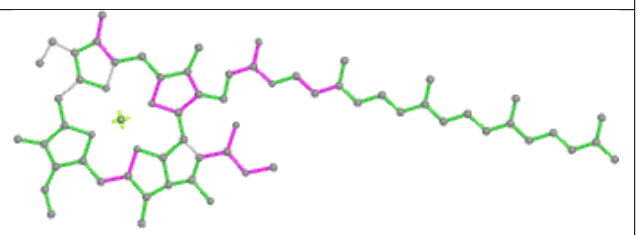

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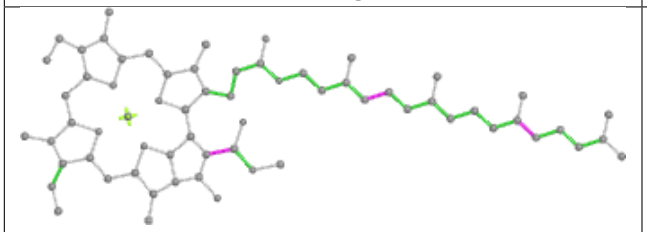

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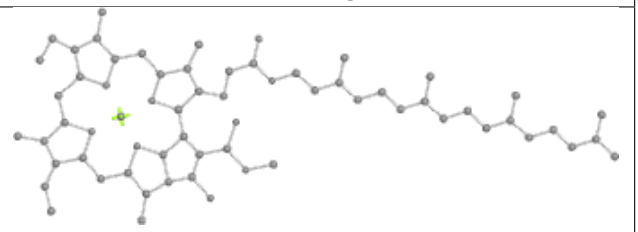
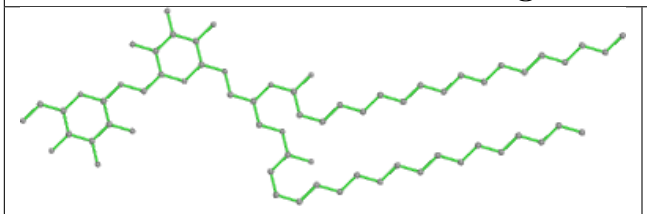


Rings

Ligand DGD M 625



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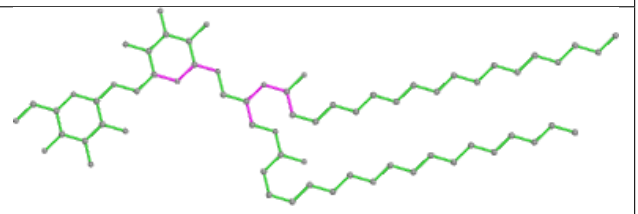
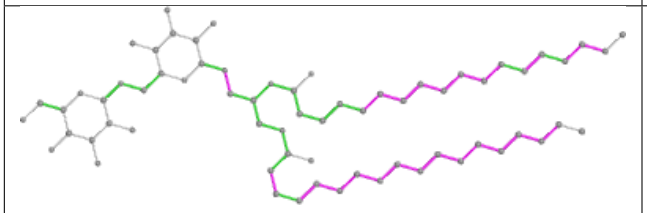


Bond angles



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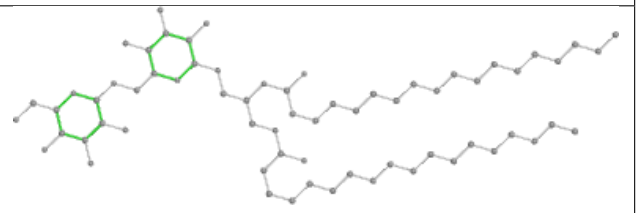
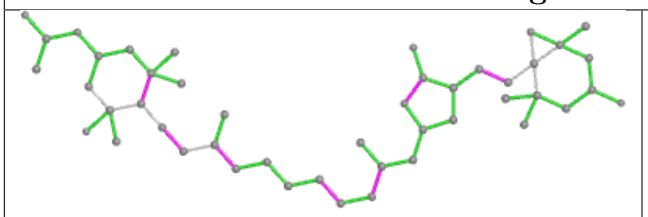
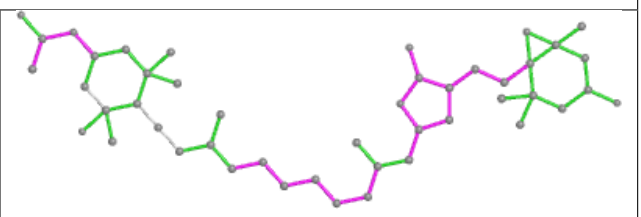


Rings

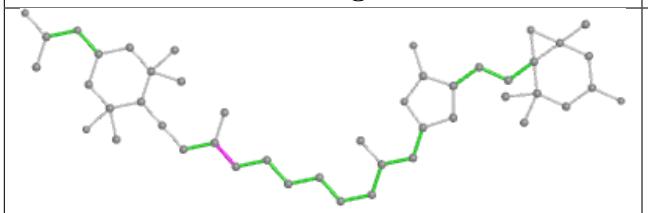
Ligand PID O 621



Bond lengths



Bond angles



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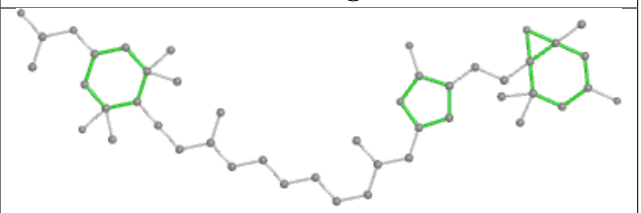
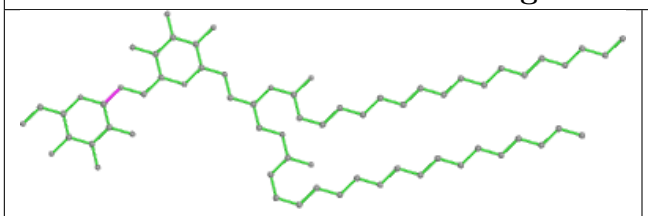
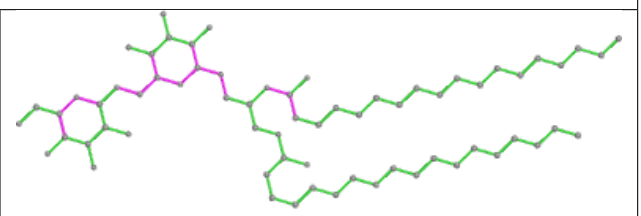


Rings

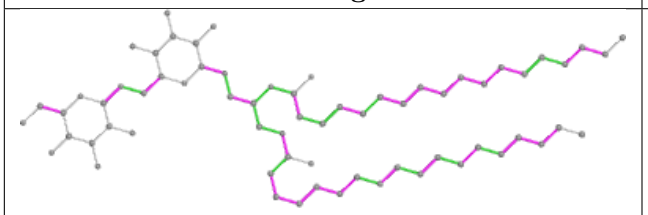
Ligand DGD O 615



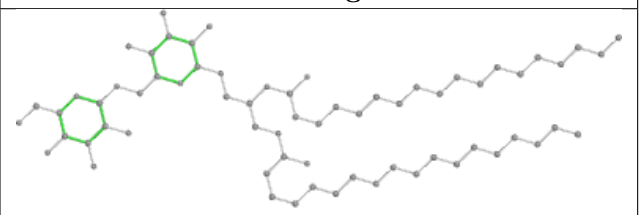
Bond lengths



Bond angles

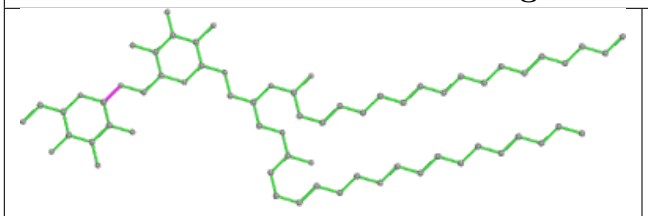


Torsions

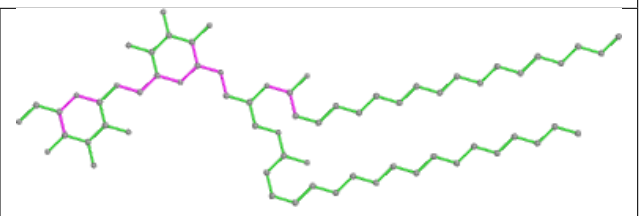


Rings

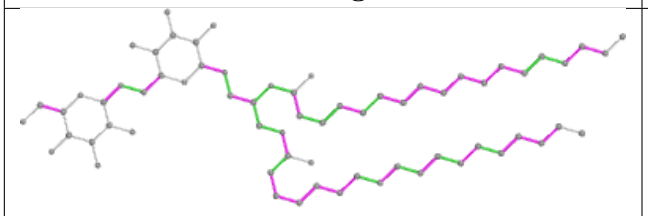
Ligand DGD N 615



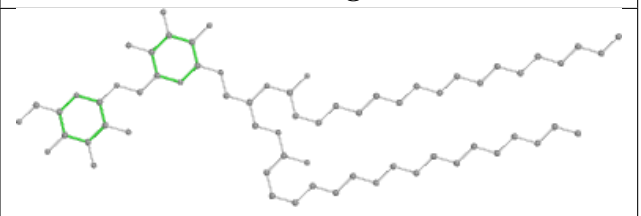
Bond lengths



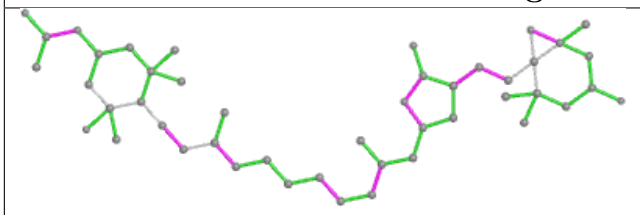
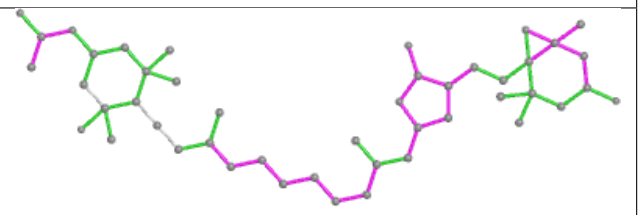
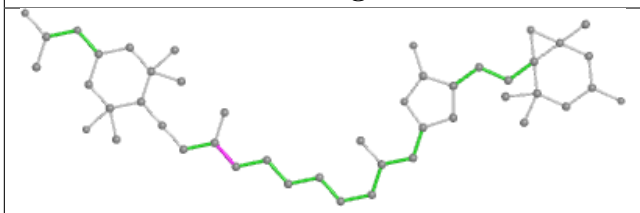
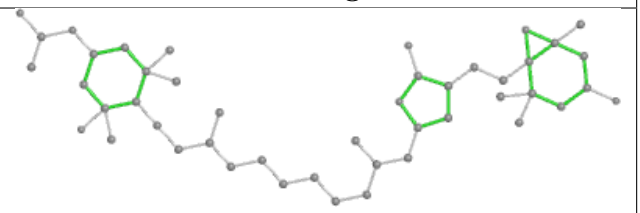
Bond angles



Torsions



Rings

Ligand PID M 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	M	312/312 (100%)	-0.66	3 (0%)	82	81	20, 31, 53, 63	0
1	N	312/312 (100%)	-0.51	9 (2%)	51	50	22, 34, 57, 66	0
1	O	312/312 (100%)	-0.68	7 (2%)	62	60	21, 29, 51, 64	0
All	All	936/936 (100%)	-0.62	19 (2%)	65	63	20, 31, 53, 66	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	159	THR	3.7
1	M	162	SER	3.5
1	N	163	GLY	3.2
1	O	163	GLY	3.2
1	N	153	SER	3.1
1	M	163	GLY	2.9
1	N	162	SER	2.8
1	N	154	ALA	2.8
1	O	156	GLY	2.7
1	N	155	ALA	2.7
1	O	162	SER	2.6
1	M	159	THR	2.6
1	N	148	LYS	2.6
1	N	152	THR	2.5
1	O	154	ALA	2.5
1	O	148	LYS	2.3
1	O	160	VAL	2.2
1	O	155	ALA	2.1
1	N	160	VAL	2.0

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 monosaccharides 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
4	DGD	N	615	66/66	0.61	0.25	42,51,105,106	0
4	DGD	O	615	66/66	0.64	0.25	37,49,104,104	0
4	DGD	M	615	66/66	0.66	0.24	38,50,105,105	0
3	PID	N	613	46/46	0.86	0.15	30,40,57,61	0
3	PID	O	613	46/46	0.89	0.13	23,34,54,60	0
3	PID	M	613	46/46	0.89	0.15	25,36,56,61	0
3	PID	N	612	46/46	0.91	0.14	26,29,40,51	0
3	PID	N	611	46/46	0.92	0.11	21,30,41,45	0
3	PID	O	611	46/46	0.92	0.12	19,26,36,43	0
3	PID	M	612	46/46	0.92	0.13	24,27,37,47	0
3	PID	M	611	46/46	0.93	0.12	20,28,39,41	0
3	PID	O	612	46/46	0.93	0.14	20,25,35,48	0
3	PID	N	623	46/46	0.93	0.13	22,30,38,42	0
3	PID	M	614	46/46	0.94	0.10	24,34,41,44	0
3	PID	N	614	46/46	0.94	0.10	25,38,44,49	0
3	PID	O	623	46/46	0.94	0.12	18,24,34,42	0
3	PID	M	623	46/46	0.95	0.11	18,26,33,38	0
3	PID	O	614	46/46	0.95	0.10	20,30,38,41	0
4	DGD	N	625	66/66	0.95	0.11	19,24,38,41	0
3	PID	M	622	46/46	0.95	0.12	18,25,29,33	0
2	CLA	O	601	65/65	0.96	0.14	21,26,43,45	0
2	CLA	M	601	65/65	0.96	0.14	22,29,43,46	0
4	DGD	M	625	66/66	0.96	0.11	22,25,41,43	0
3	PID	N	622	46/46	0.96	0.11	21,26,33,37	0
2	CLA	N	601	65/65	0.96	0.15	26,32,46,47	0
4	DGD	O	625	66/66	0.96	0.10	19,24,39,41	0
3	PID	O	622	46/46	0.96	0.11	18,24,29,32	0

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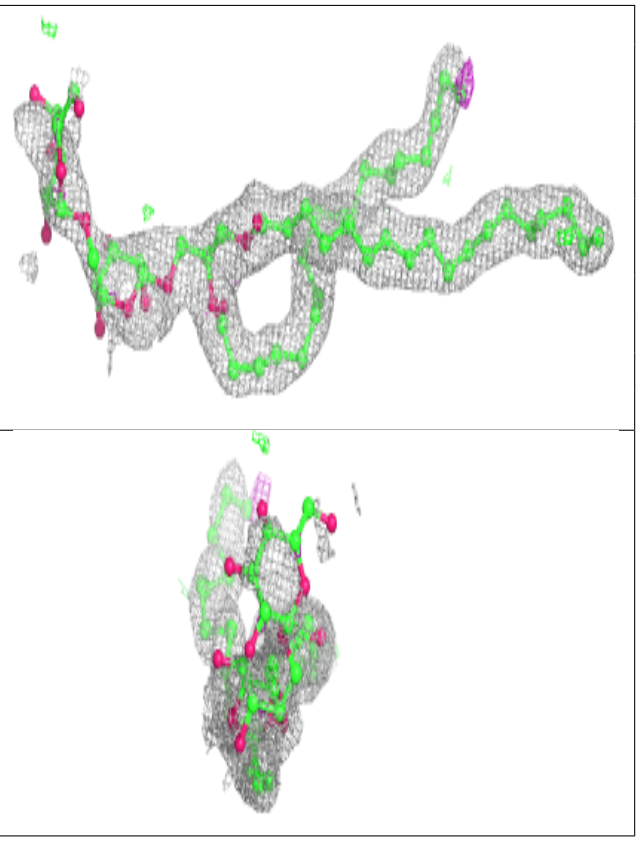
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PID	M	624	46/46	0.97	0.08	19,22,26,34	0
3	PID	N	624	46/46	0.97	0.08	22,26,31,35	0
3	PID	O	621	46/46	0.97	0.09	17,21,25,26	0
2	CLA	N	602	65/65	0.97	0.11	19,26,34,37	0
2	CLA	M	602	65/65	0.97	0.11	19,23,33,35	0
3	PID	O	624	46/46	0.97	0.08	19,23,28,32	0
3	PID	N	621	46/46	0.98	0.08	20,22,28,29	0
3	PID	M	621	46/46	0.98	0.09	17,21,26,28	0
2	CLA	O	602	65/65	0.98	0.11	18,22,31,34	0

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

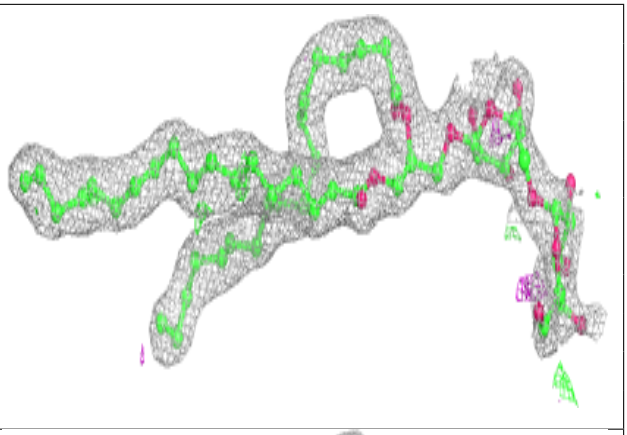
Electron density around DGD N 615:

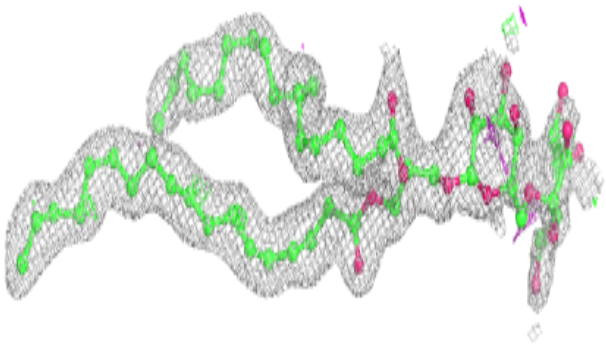
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

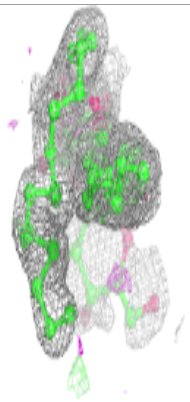


Electron density around DGD O 615:

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

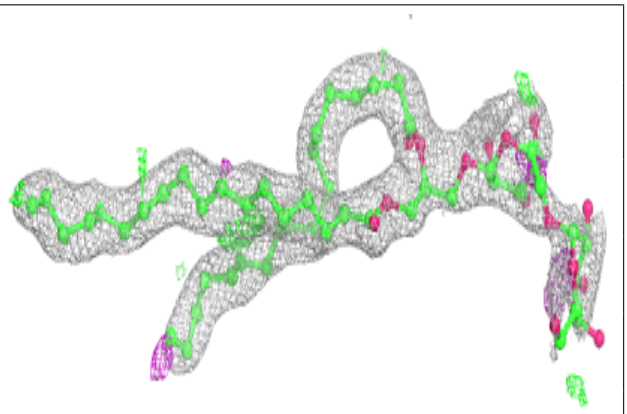


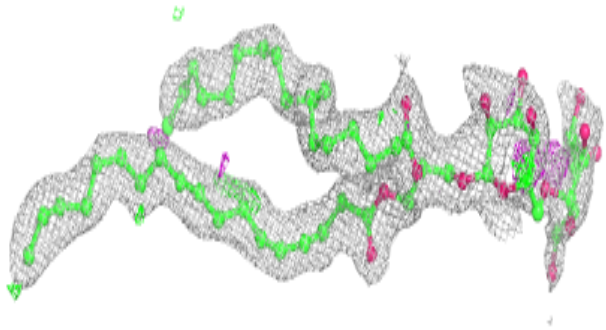


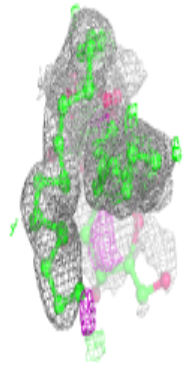


Electron density around DGD M 615:

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

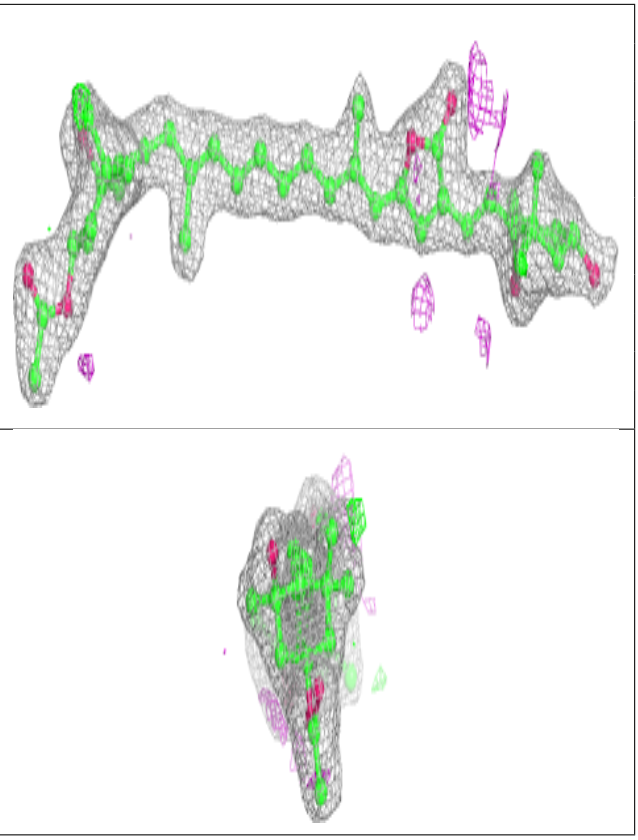






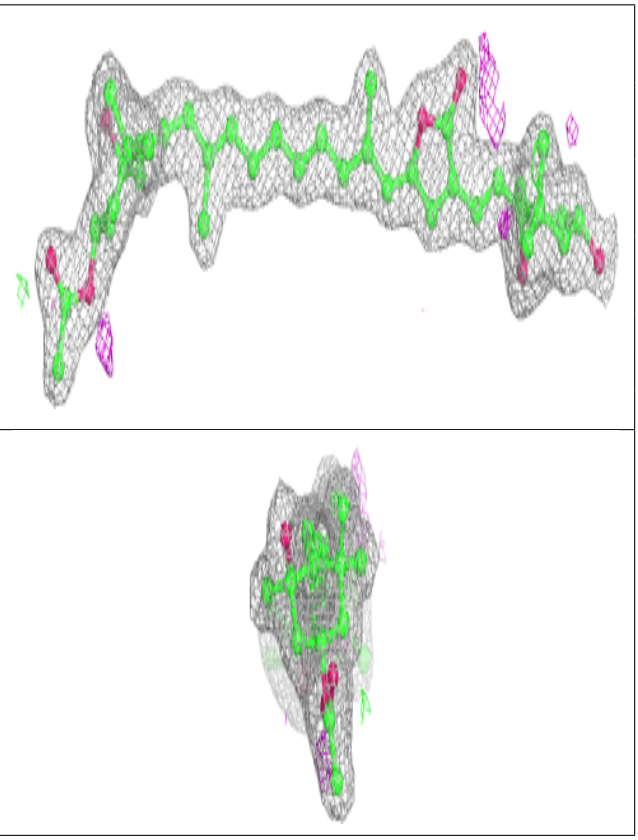
Electron density around PID N 613:

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



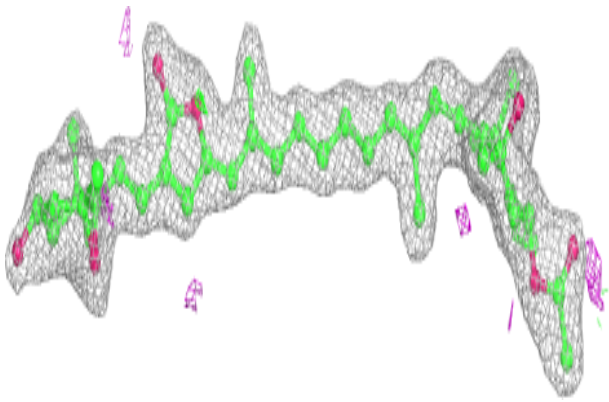
Electron density around PID O 613:

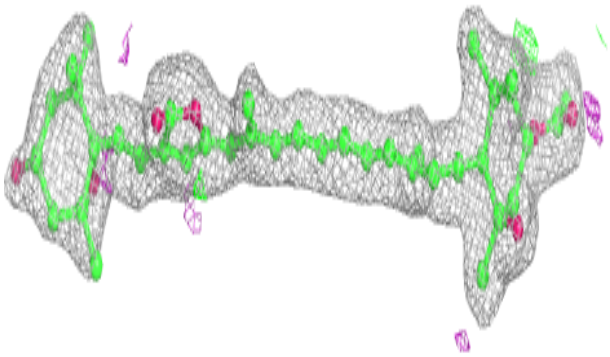
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

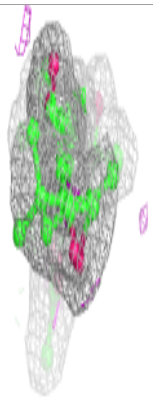


Electron density around PID M 613:

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

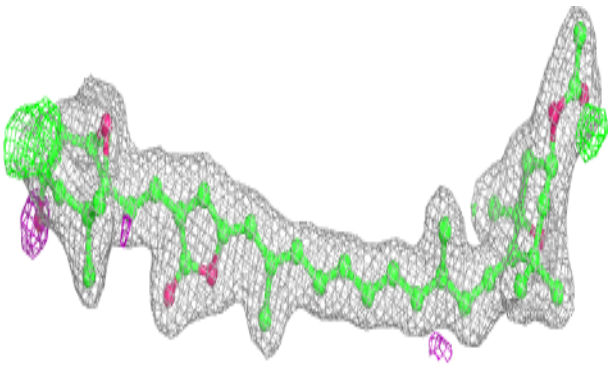


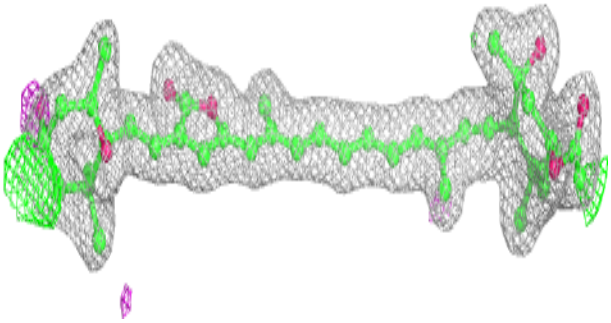


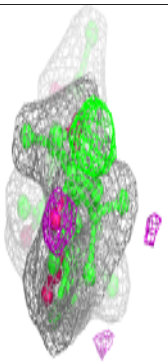


Electron density around PID N 612:

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

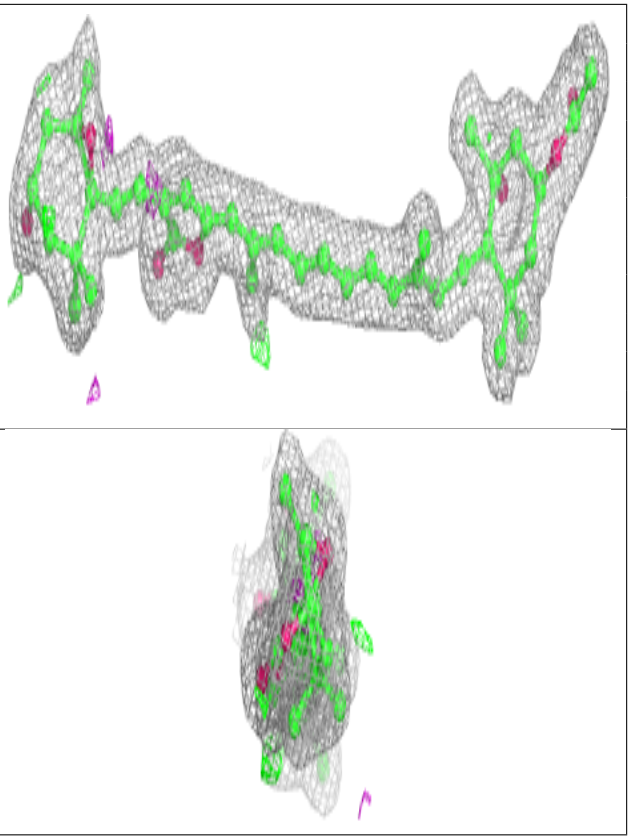






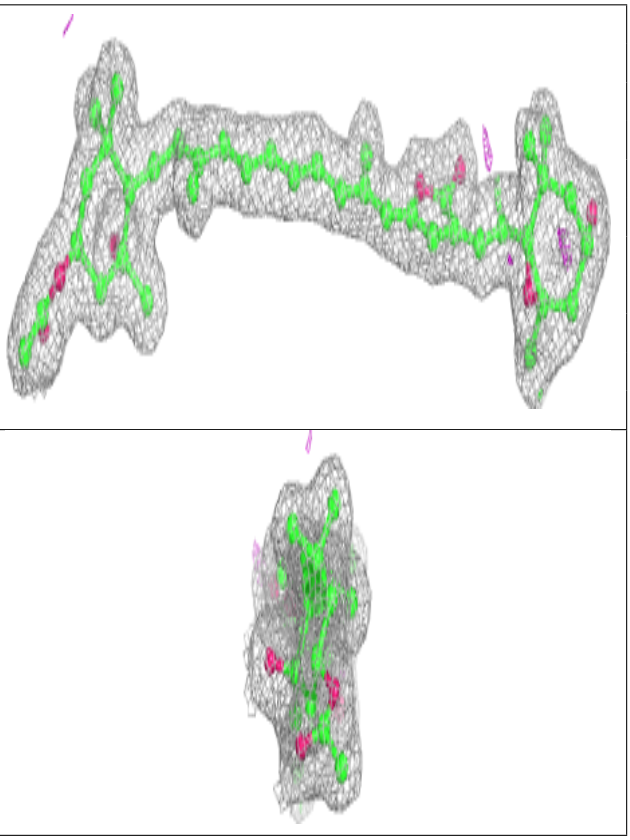
Electron density around PID N 611:

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



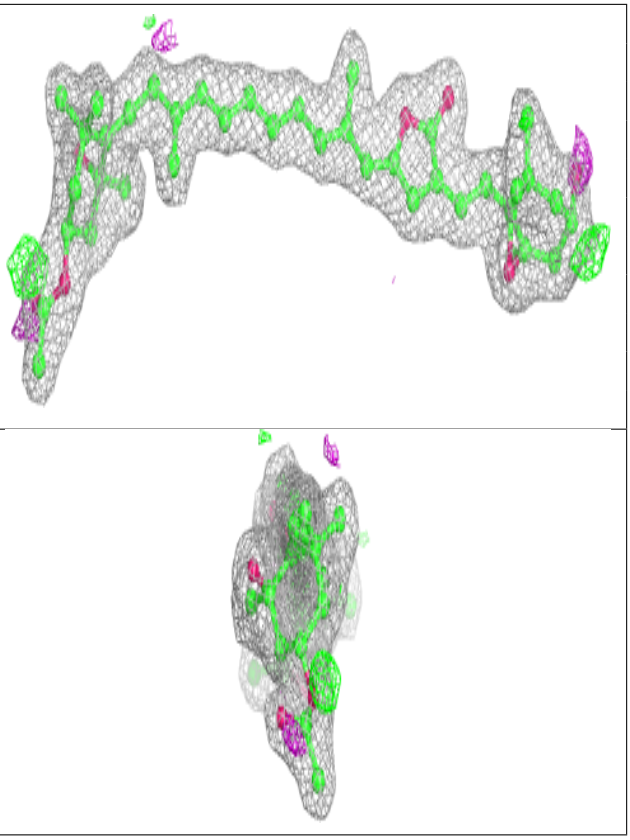
Electron density around PID O 611:

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



Electron density around PID M 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 611:

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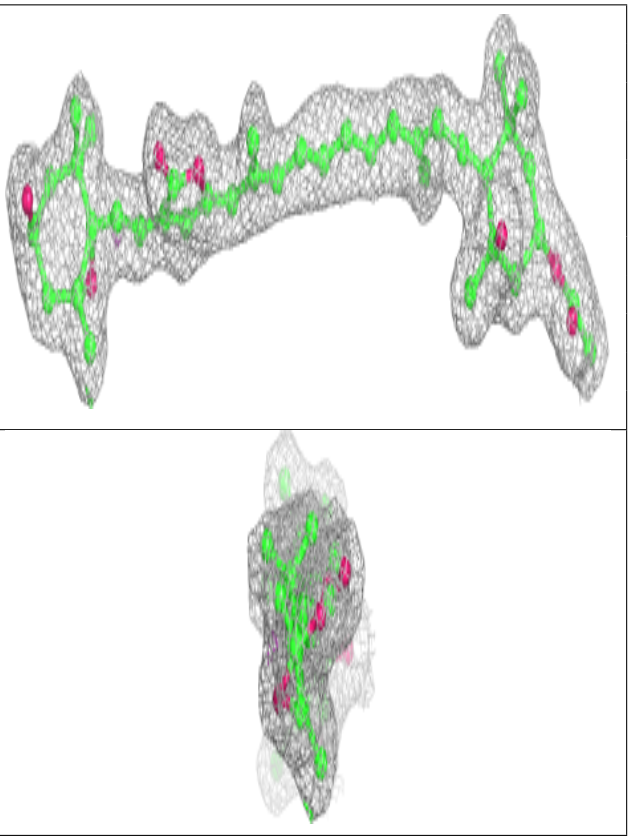
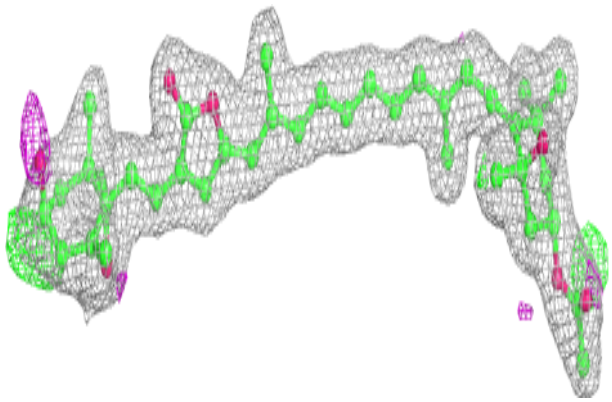
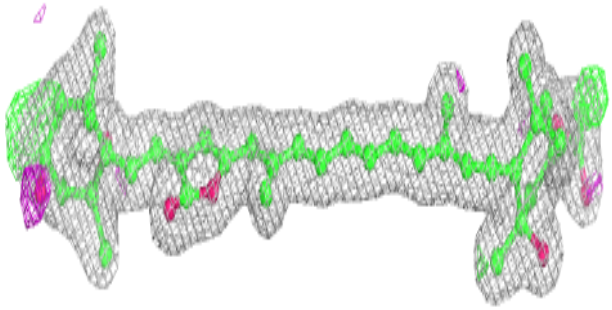
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

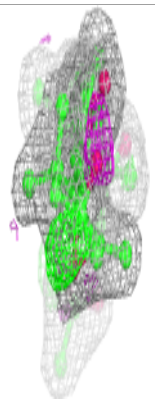


Electron density around PID O 612:

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

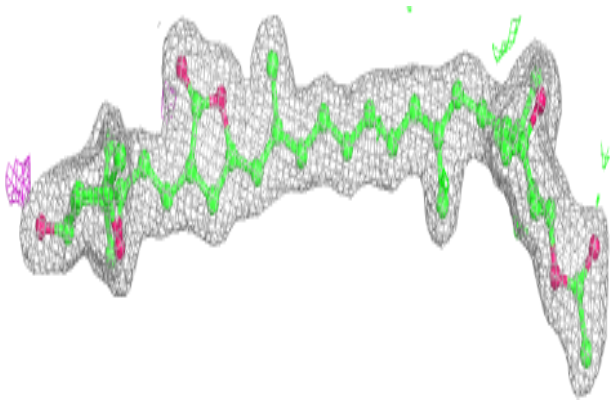


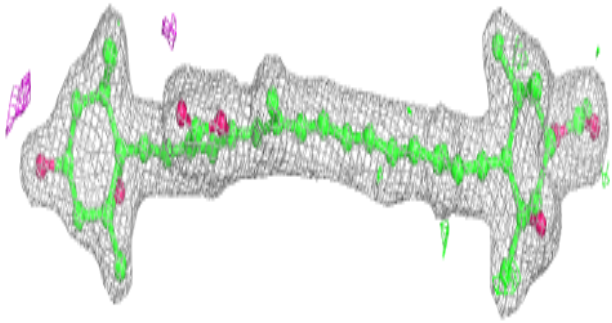


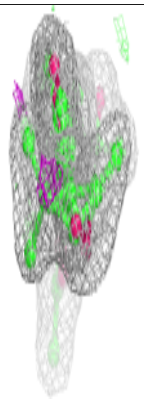


Electron density around PID N 623:

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

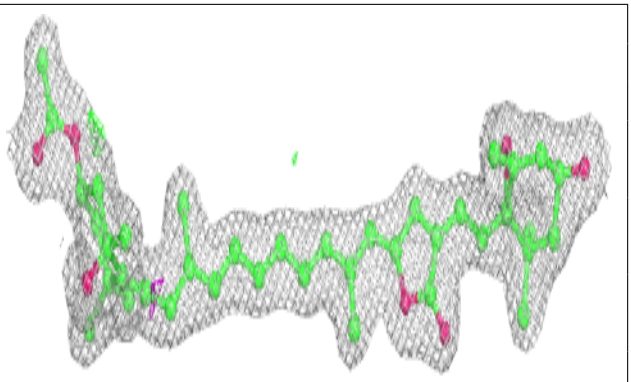


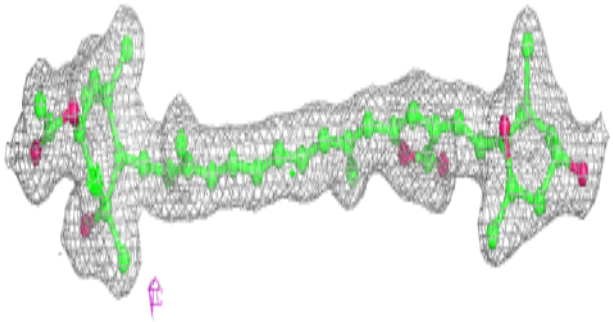


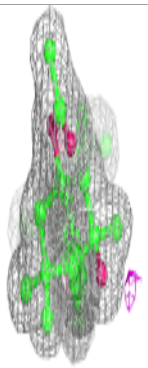


Electron density around PID M 614:

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

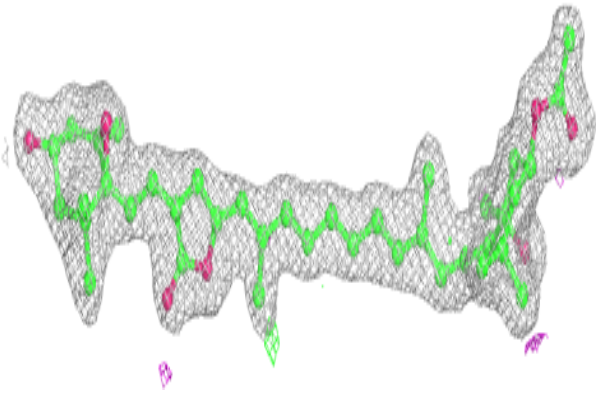


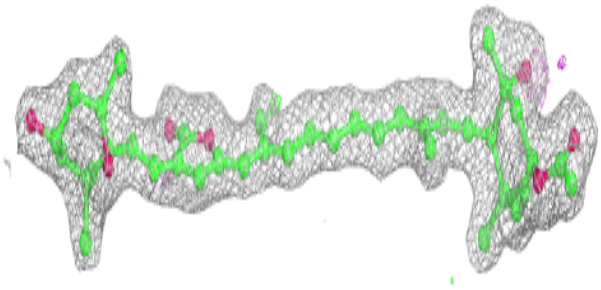


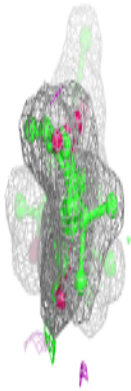


Electron density around PID N 614:

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

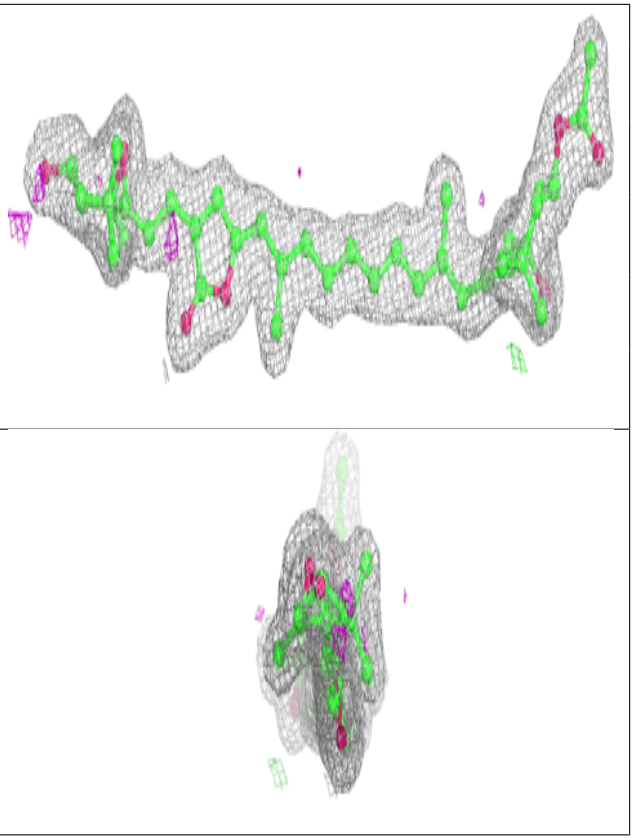






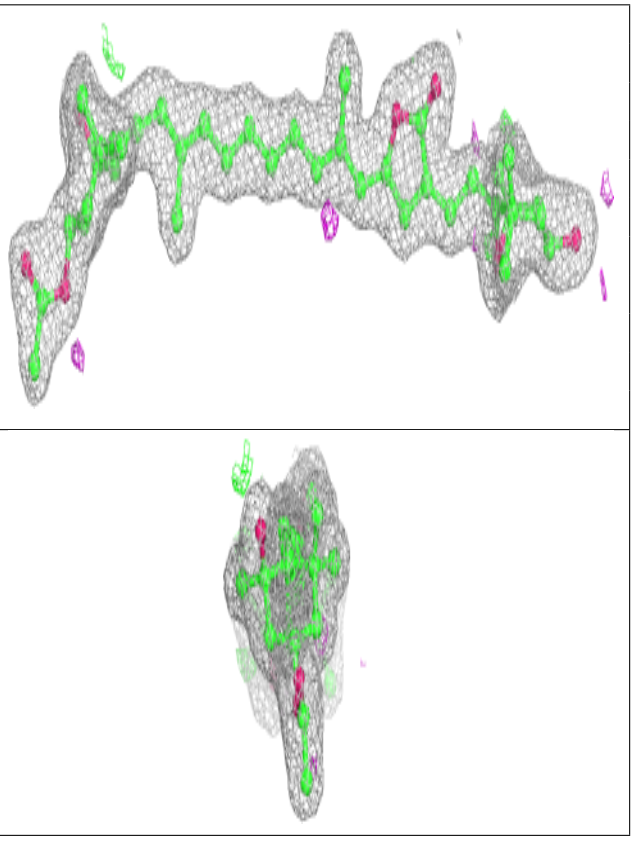
Electron density around PID O 623:

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



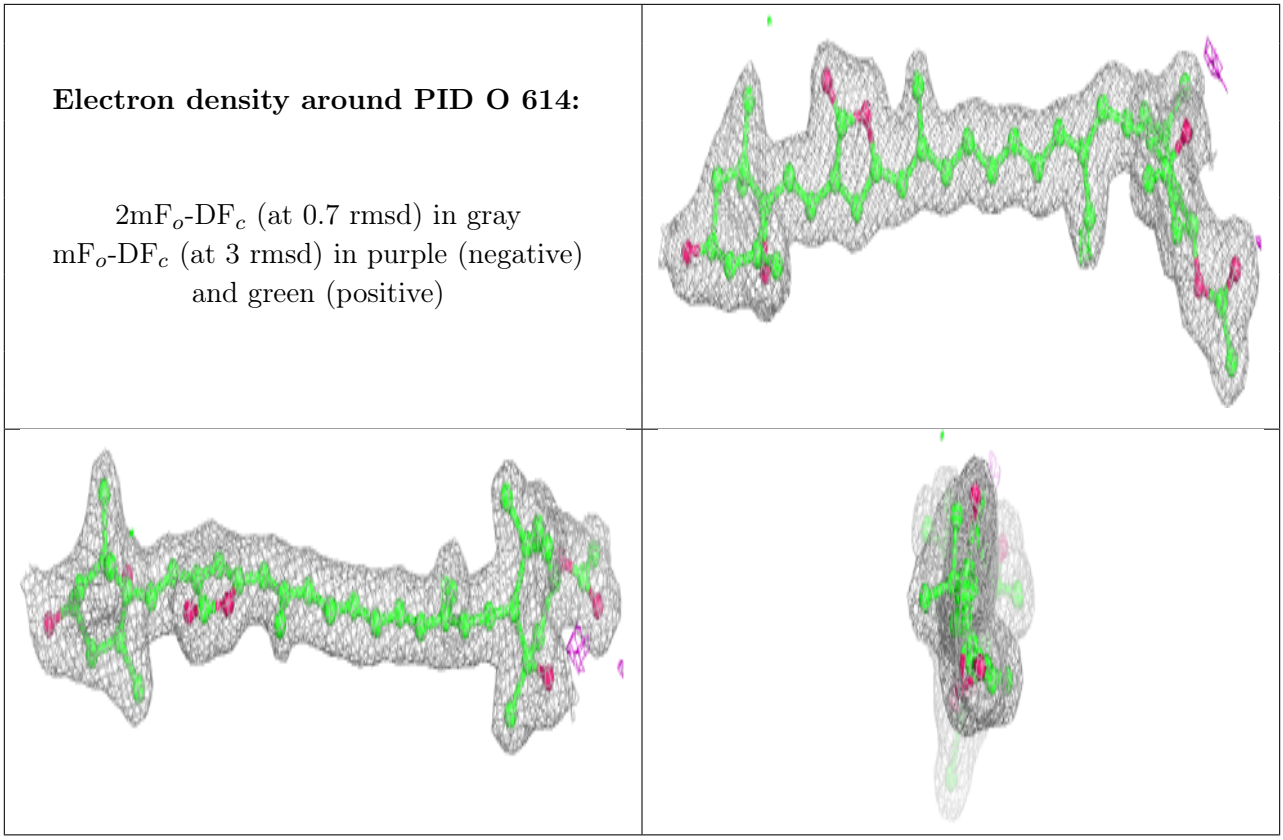
Electron density around PID M 623:

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



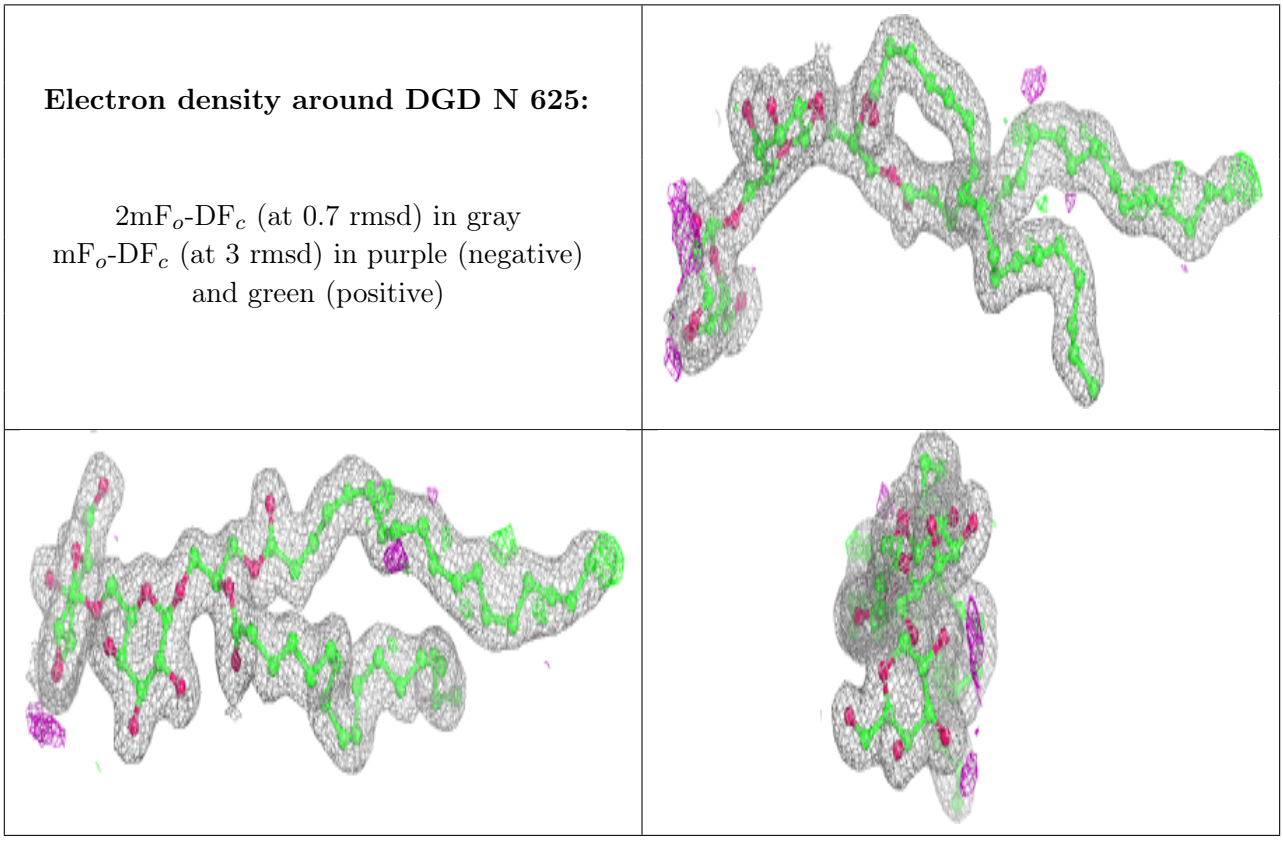
Electron density around PID O 614:

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



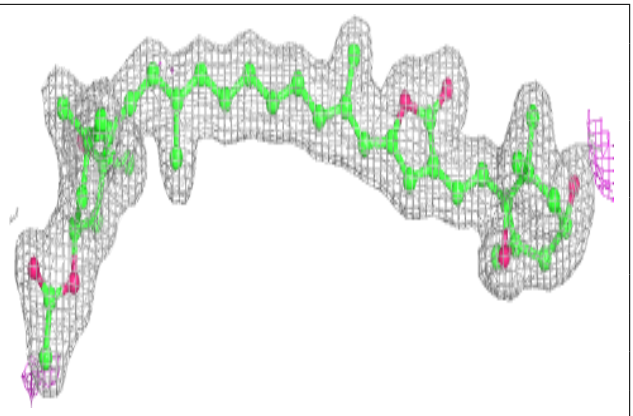
Electron density around DGD N 625:

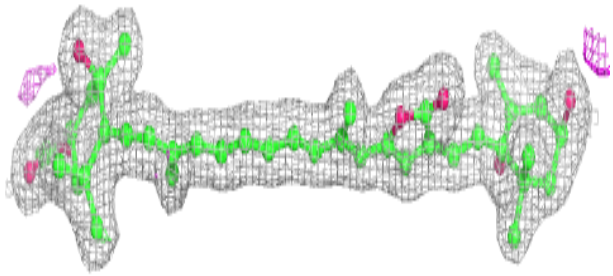
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

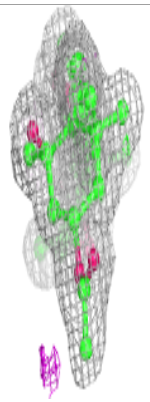


Electron density around PID M 622:

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

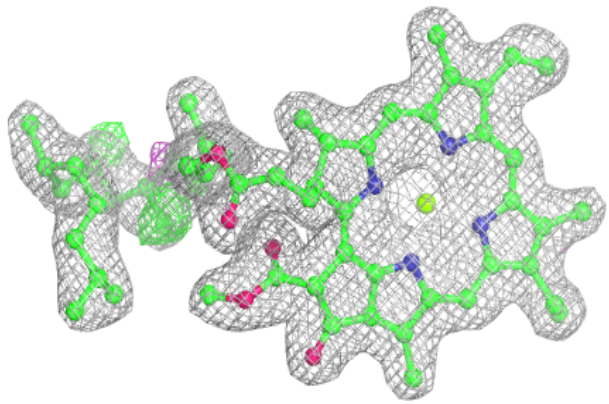


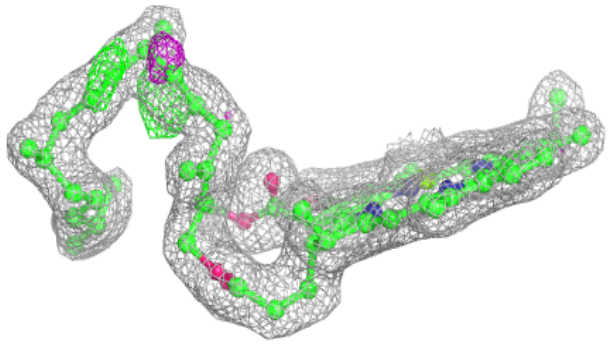


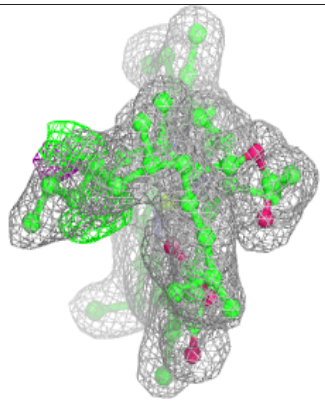


Electron density around CLA O 601:

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

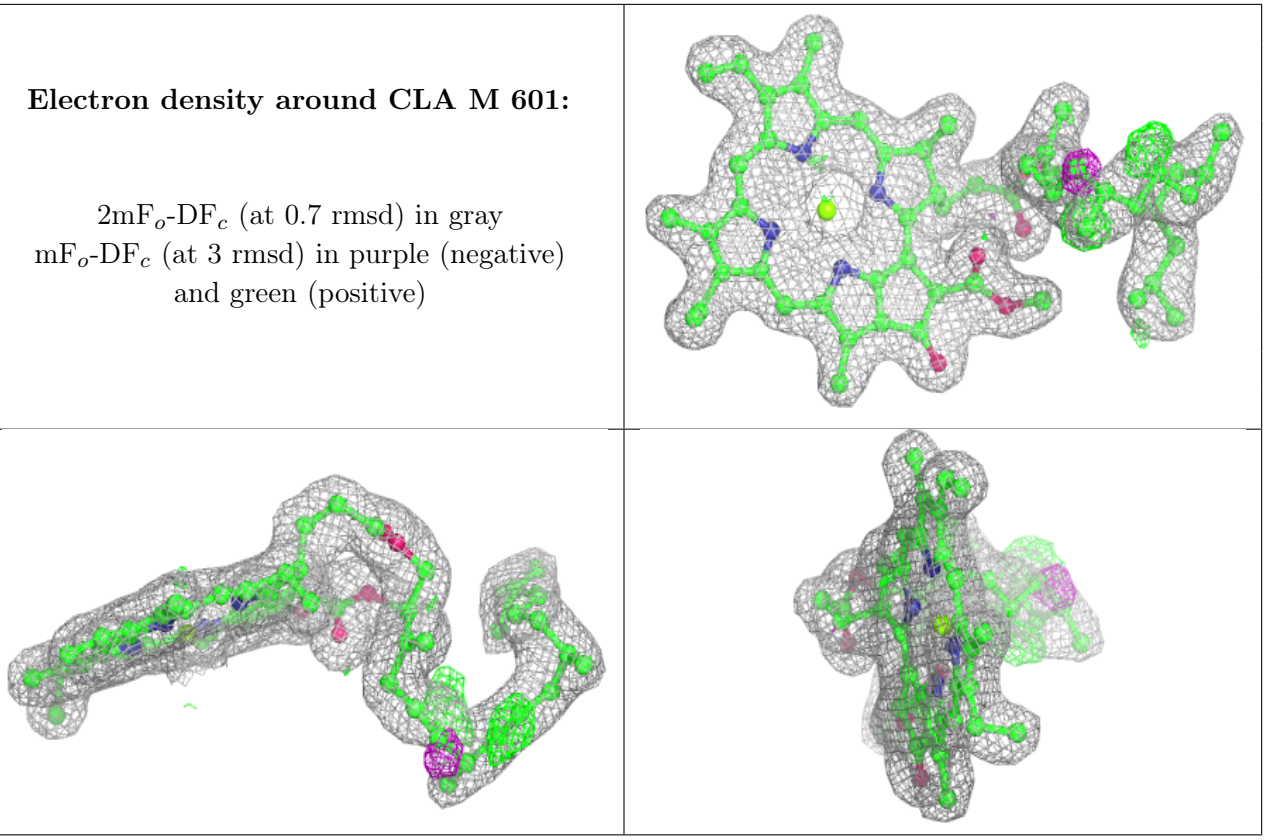






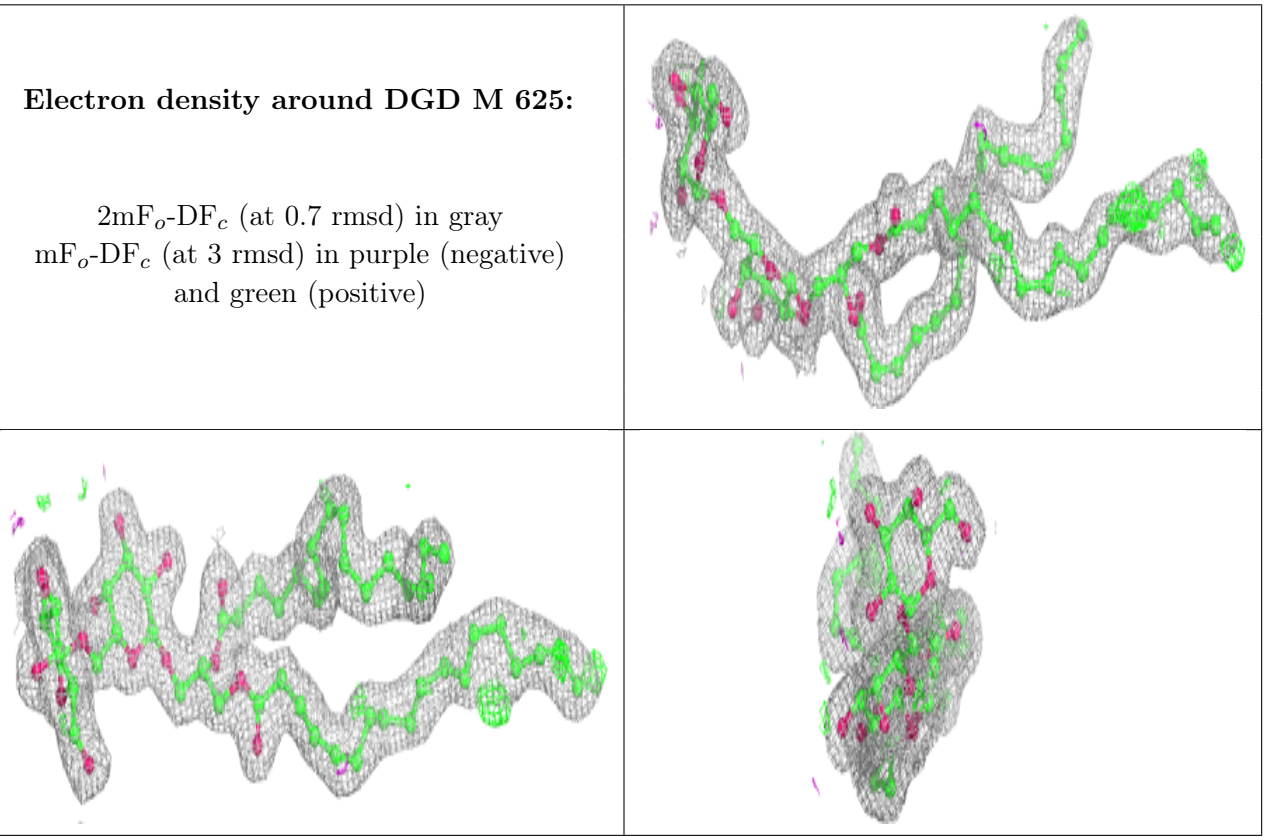
Electron density around CLA M 601:

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



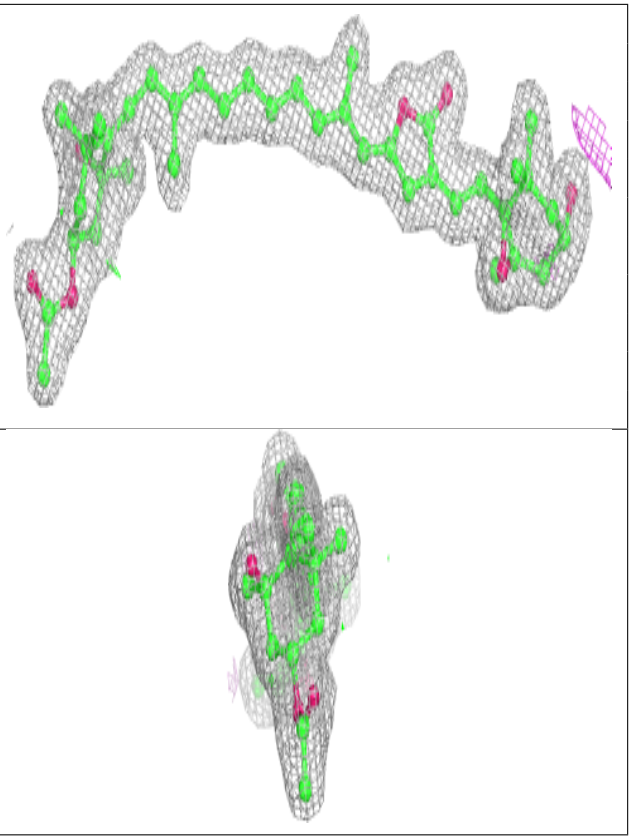
Electron density around DGD M 625:

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



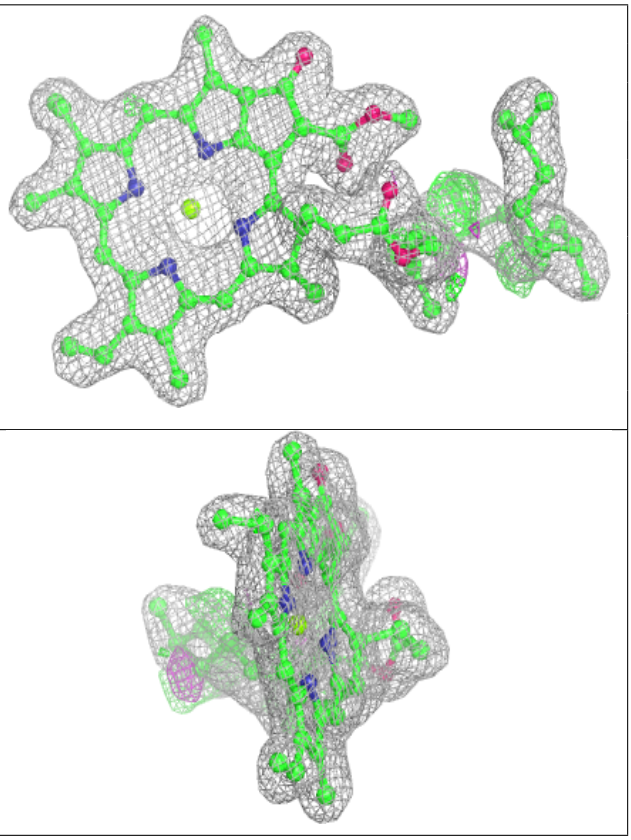
Electron density around PID N 622:

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



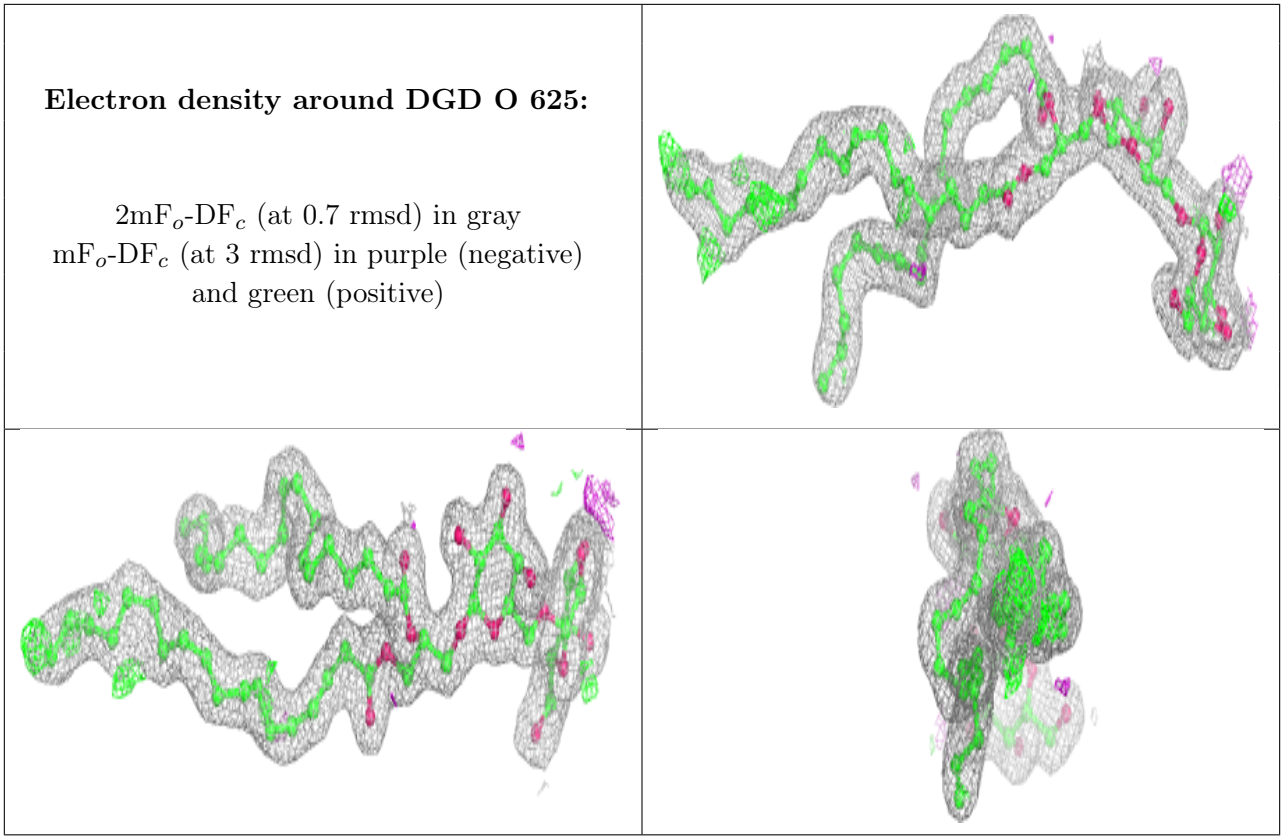
Electron density around CLA N 601:

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



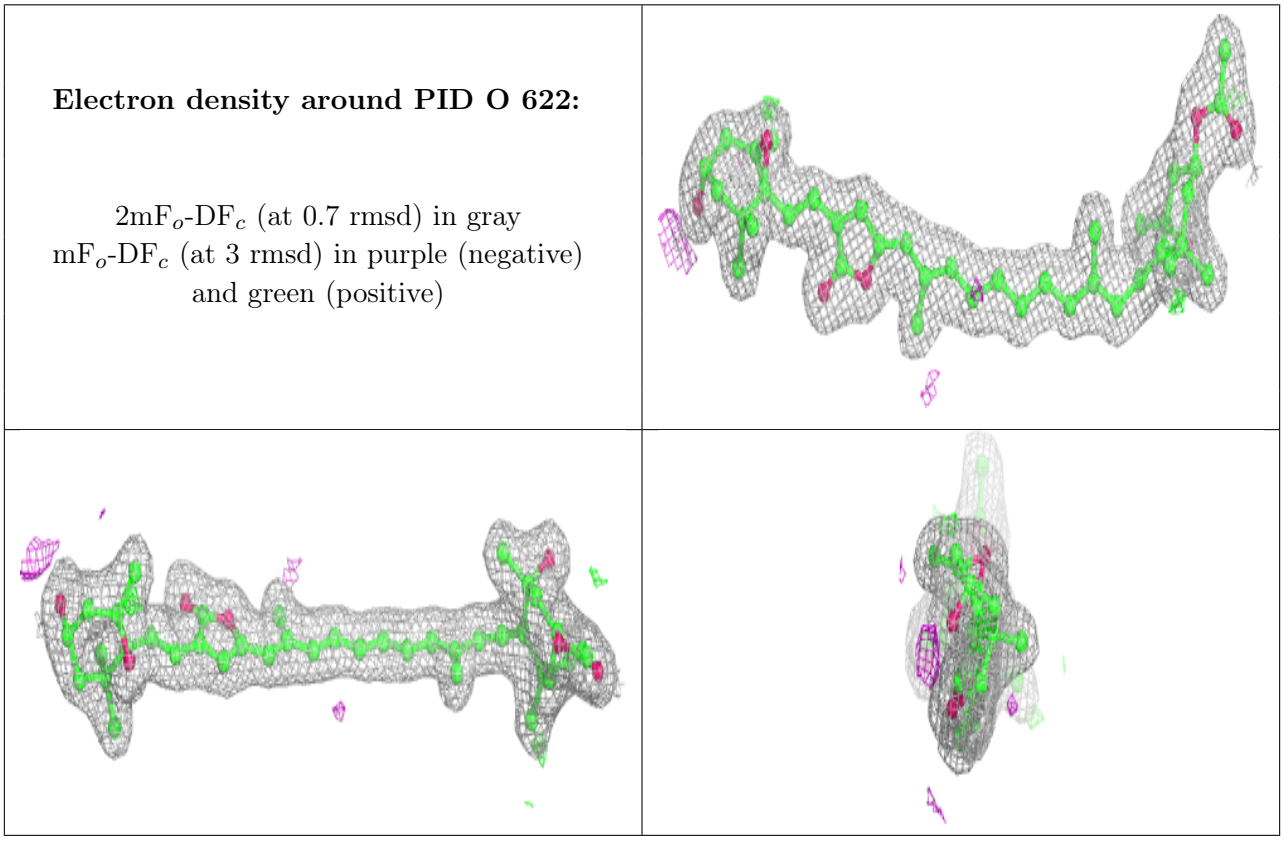
Electron density around DGD O 625:

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



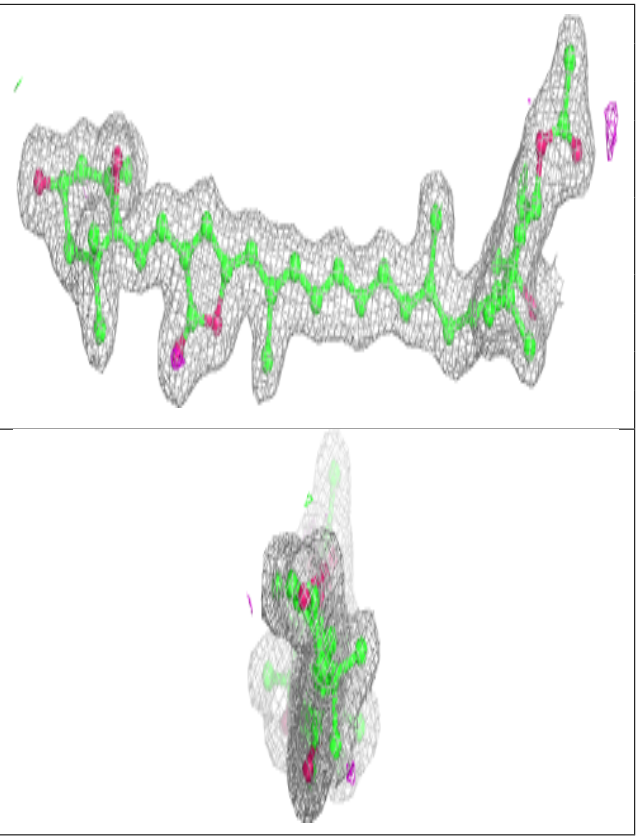
Electron density around PID O 622:

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



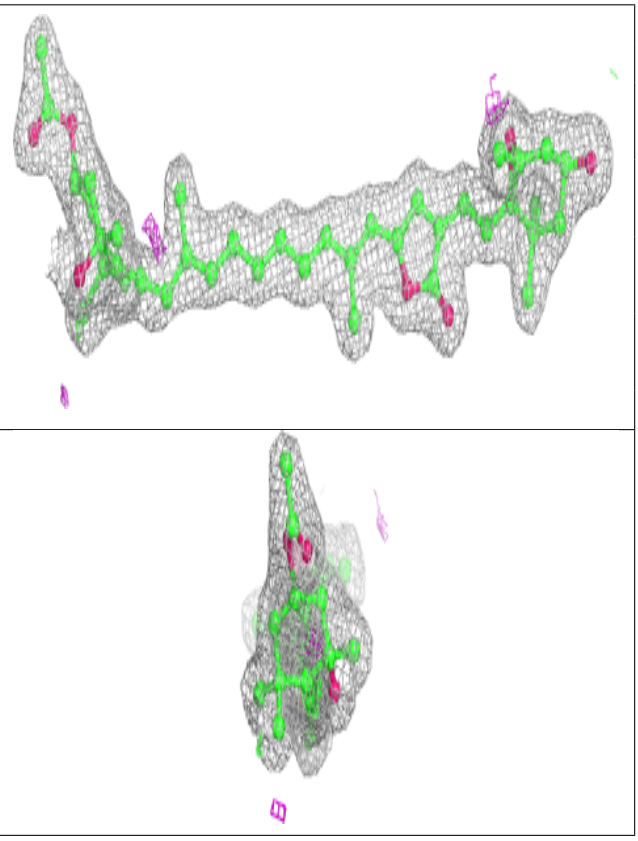
Electron density around PID M 624:

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



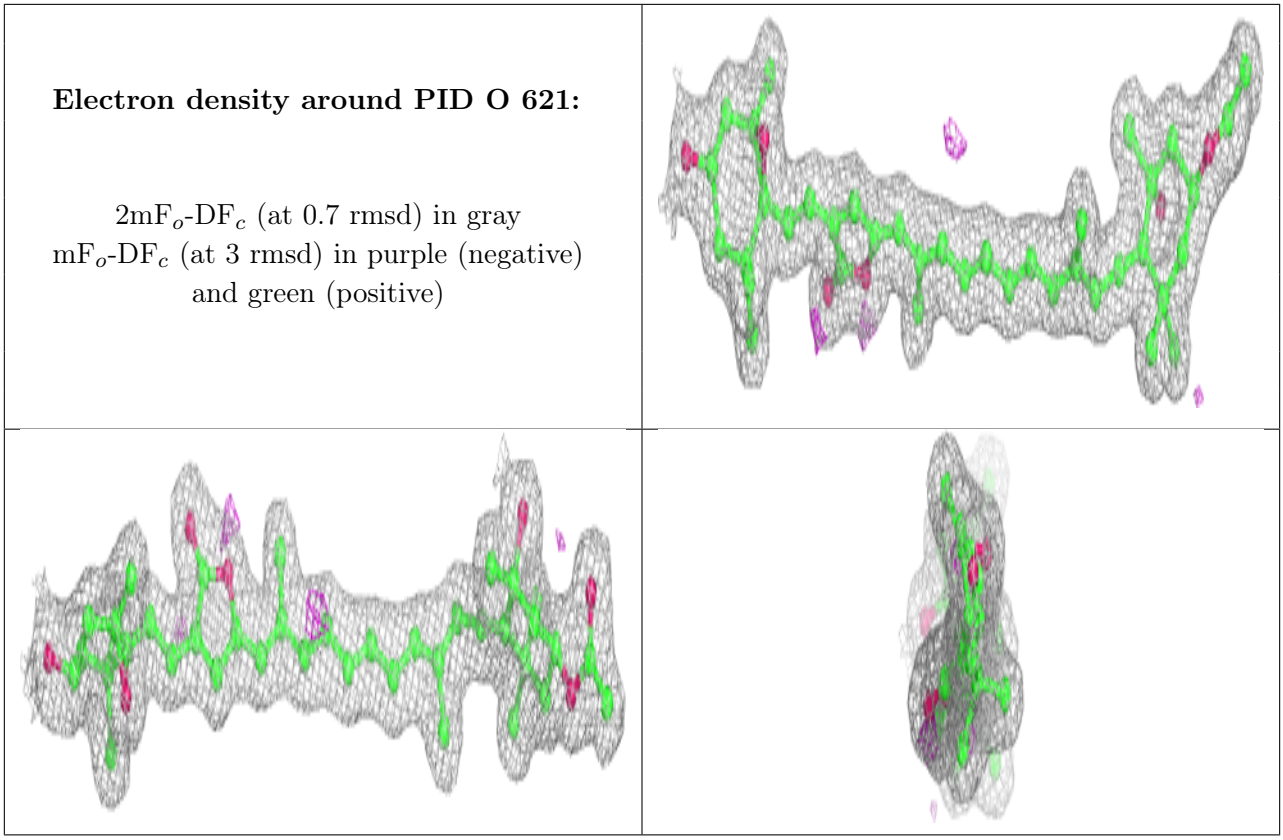
Electron density around PID N 624:

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



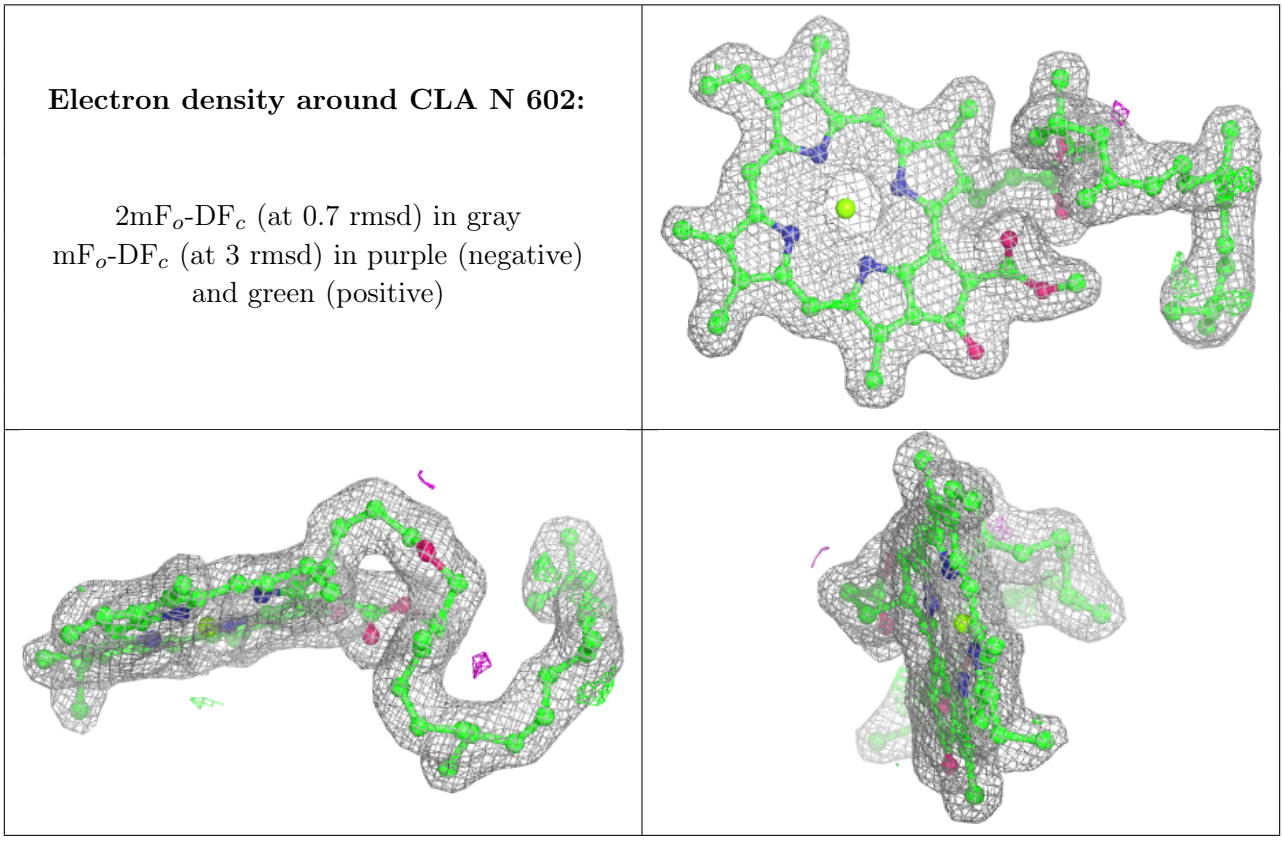
Electron density around PID O 621:

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



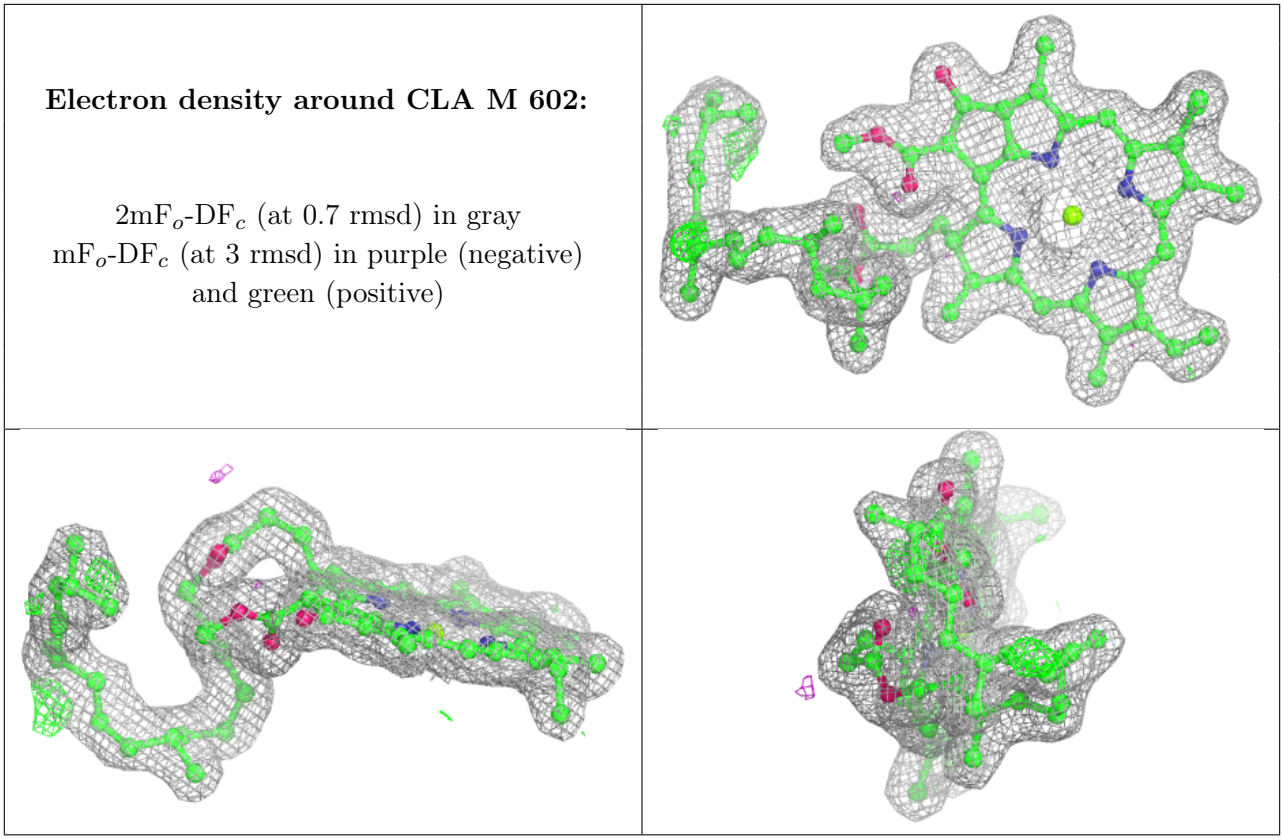
Electron density around CLA N 602:

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



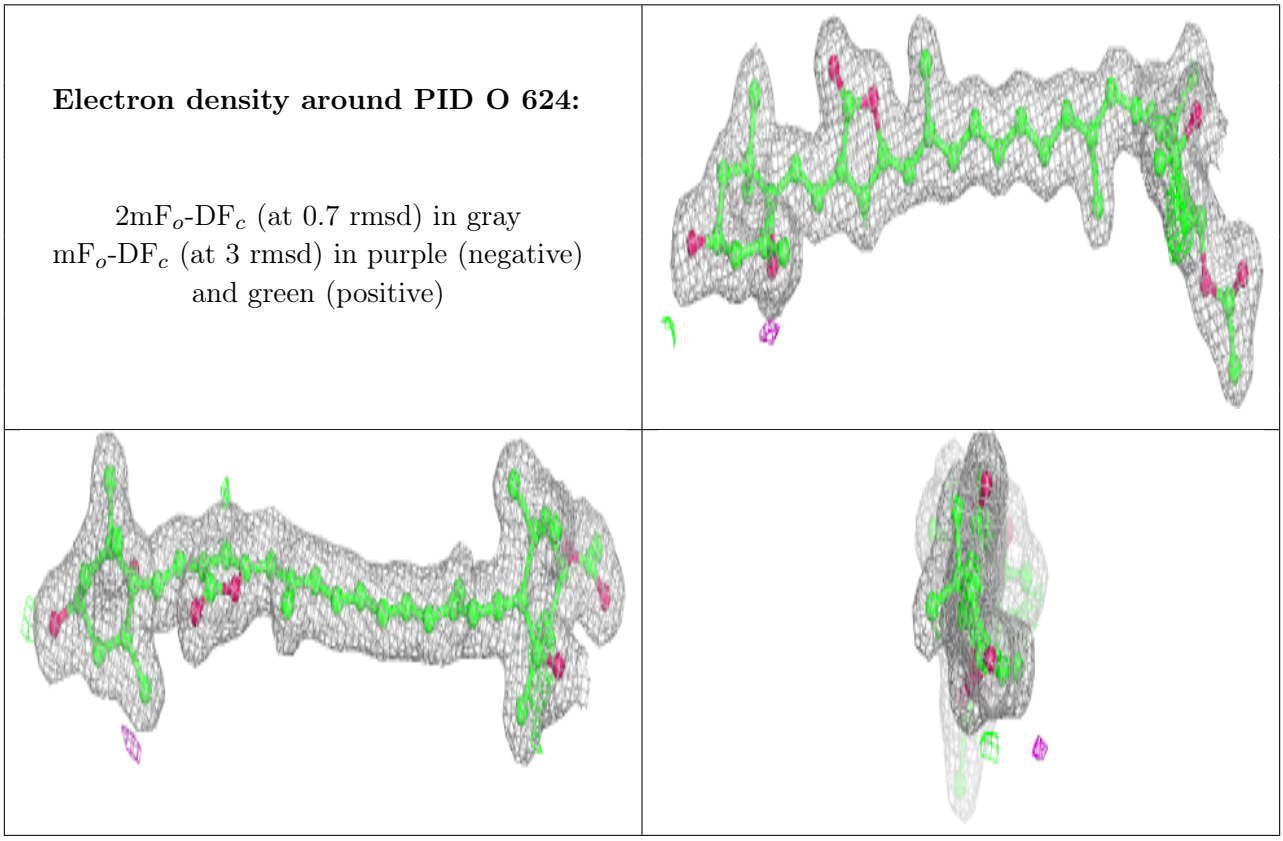
Electron density around CLA M 602:

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



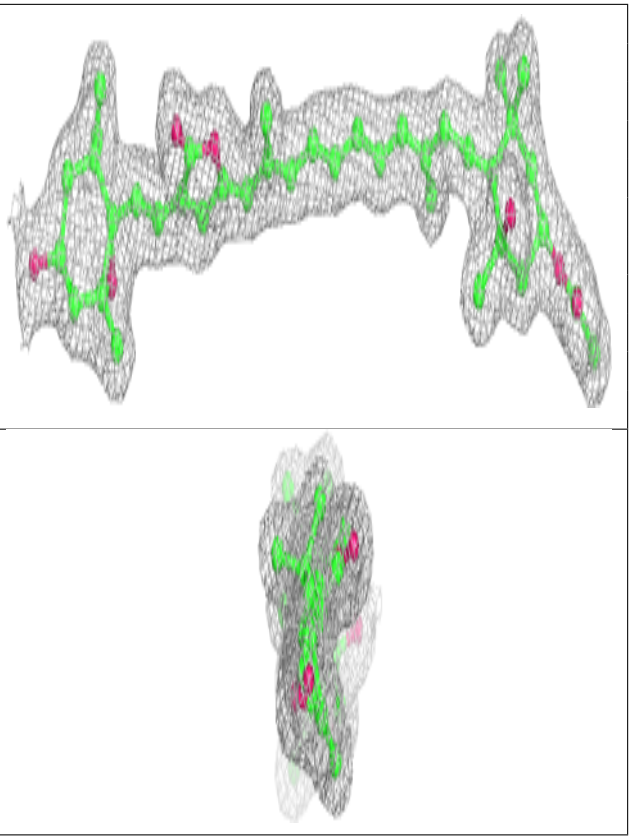
Electron density around PID O 624:

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



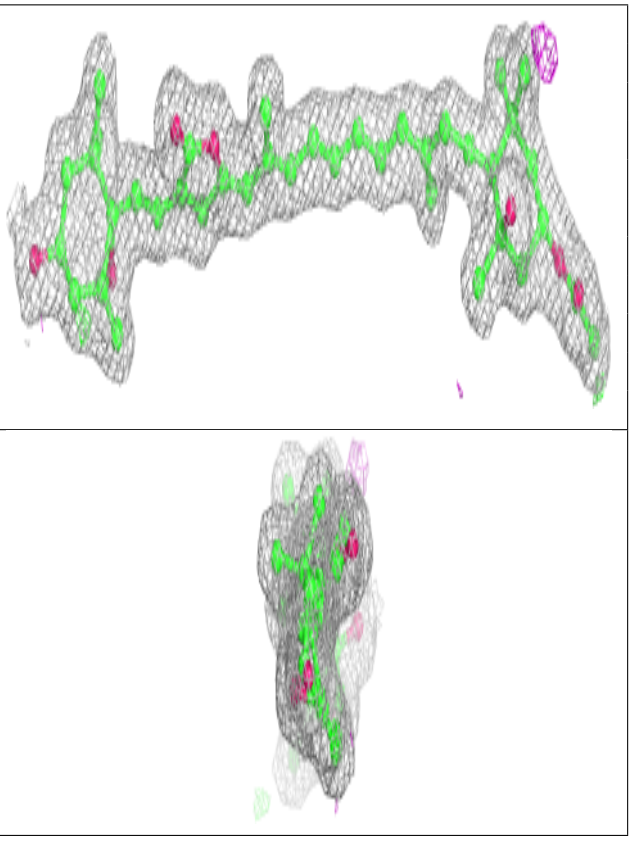
Electron density around PID N 621:

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



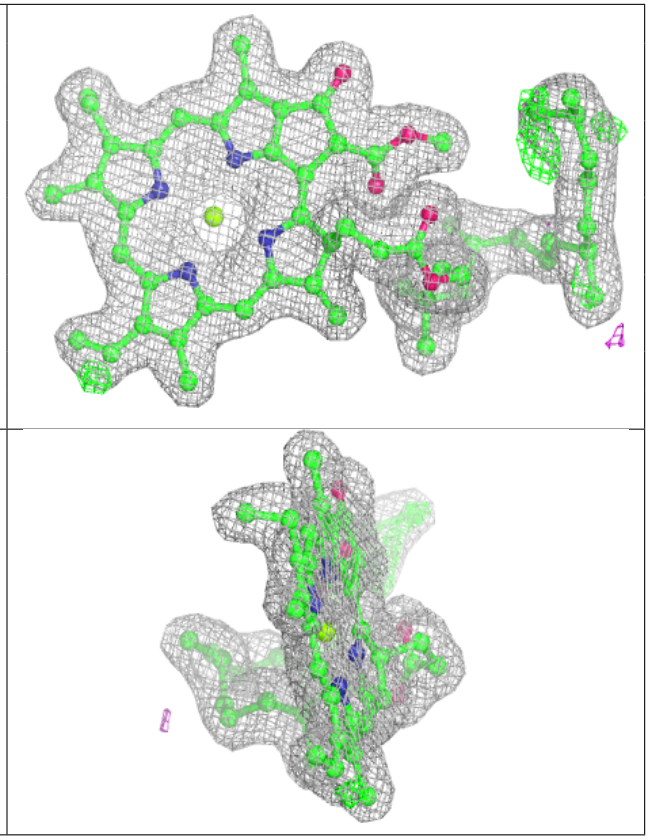
Electron density around PID M 621:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.