



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 08:52 pm BST

PDB ID : 8OW6 / pdb_00008ow6
Title : PERIDININ-CHLOROPHYLL-PROTEIN OF HETEROCAPSA PYG-
MAEA, 100K
Authors : Hofmann, E.; Schulte, T.
Deposited on : 2023-04-27
Resolution : 1.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

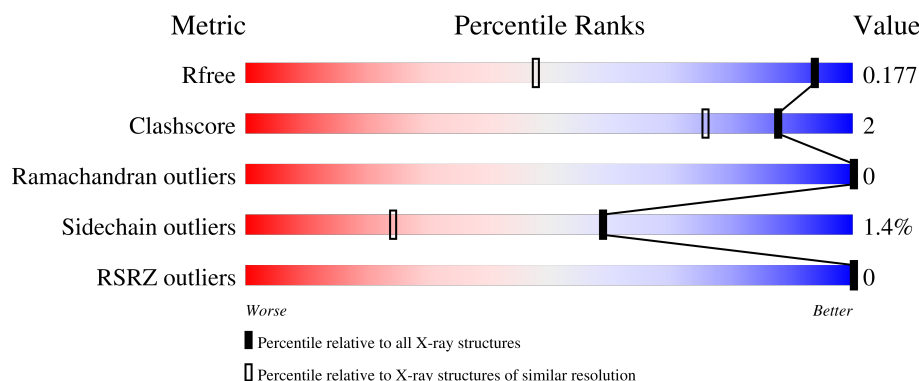
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

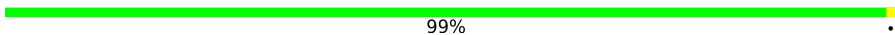
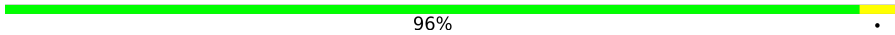
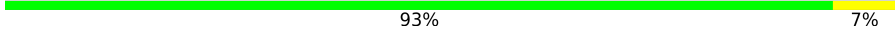
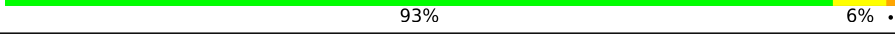
The reported resolution of this entry is 1.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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

Mol	Chain	Length	Quality of chain
1	A	149	 99%
1	C	149	 96%
2	B	149	 93% 7%
2	D	149	 93% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PID	D	613	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12518 atoms, of which 5917 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-chl a protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	149	Total	C	H	N	O	S	0	3	0
			2205	701	1098	180	219	7			
1	C	149	Total	C	H	N	O	S	0	5	0
			2228	707	1112	182	220	7			

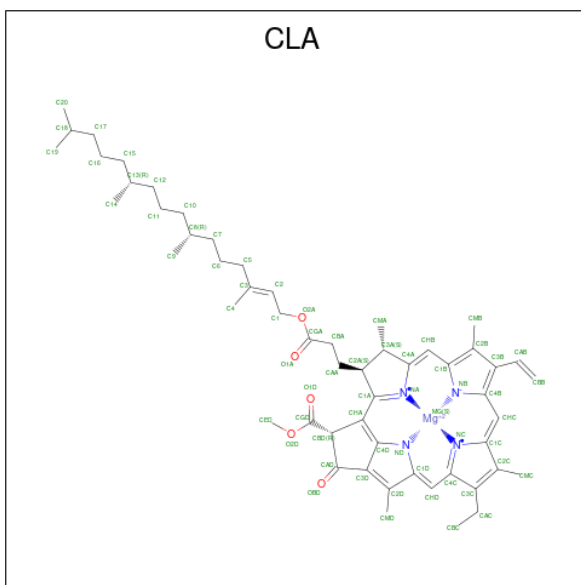
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	ALA	VAL	conflict	UNP Q9FEY4
C	108	ALA	VAL	conflict	UNP Q9FEY4

- Molecule 2 is a protein called Peridinin-chl a protein.

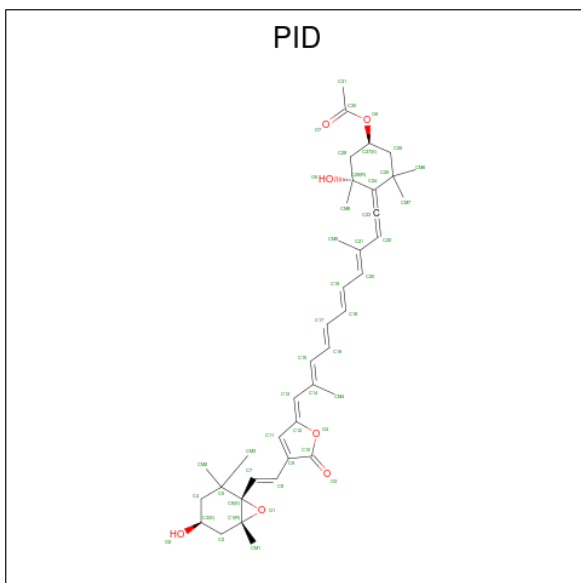
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	149	Total	C	H	N	O	S	0	15	0
			2322	732	1165	187	231	7			
2	D	149	Total	C	H	N	O	S	0	7	0
			2276	720	1142	184	223	7			

- Molecule 3 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



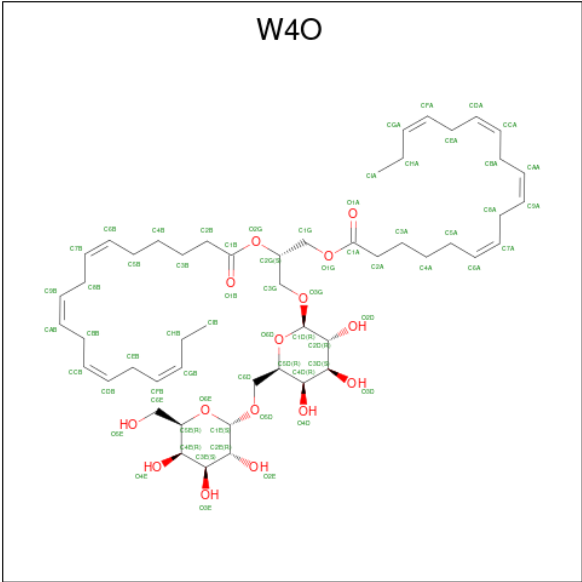
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
3	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
3	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
3	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

- Molecule 4 is PERIDININ (CCD ID: PID) (formula: $\text{C}_{39}\text{H}_{50}\text{O}_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			96	39	50	7		
4	A	1	Total	C	H	O	0	0
			96	39	50	7		
4	A	1	Total	C	H	O	0	0
			96	39	50	7		
4	A	1	Total	C	H	O	0	0
			96	39	50	7		
4	B	1	Total	C	H	O	0	0
			96	39	50	7		
4	B	1	Total	C	H	O	0	0
			96	39	50	7		
4	B	1	Total	C	H	O	0	0
			96	39	50	7		
4	B	1	Total	C	H	O	0	0
			96	39	50	7		
4	C	1	Total	C	H	O	0	0
			96	39	50	7		
4	C	1	Total	C	H	O	0	0
			96	39	50	7		
4	C	1	Total	C	H	O	0	0
			96	39	50	7		
4	C	1	Total	C	H	O	0	0
			96	39	50	7		
4	D	1	Total	C	H	O	0	0
			96	39	50	7		
4	D	1	Total	C	H	O	0	0
			96	39	50	7		
4	D	1	Total	C	H	O	0	0
			96	39	50	7		
4	D	1	Total	C	H	O	0	0
			96	39	50	7		

- Molecule 5 is [(2 {S})-3-[(2 {R},3 {R},4 {S},5 {R},6 {R})-6-[(2 {S},3 {R},4 {S},5 {R},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-2-[(6 {Z},9 {Z},12 {Z},15 {Z})-octadeca-6,9,12,15-tetraenoyl]oxy-propyl (6 {Z},9 {Z},12 {Z},15 {Z})-octadeca-6,9,12,15-tetraenoate (CCD ID: W4O) (formula: C₅₁H₈₀O₁₅) (labeled as "Ligand of Interest" by depositor).

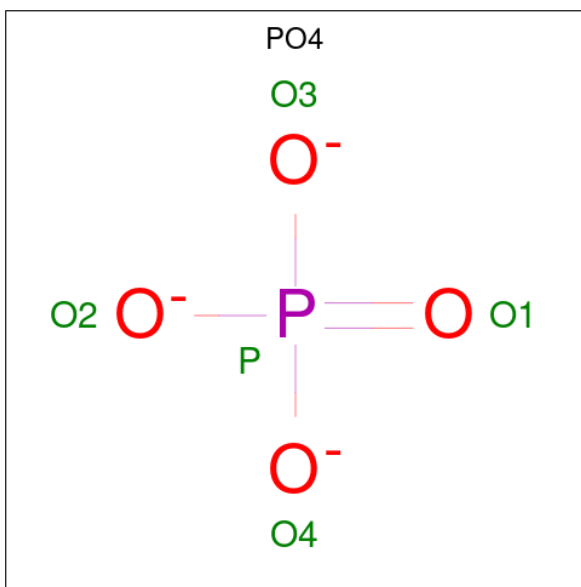


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			144	51	78	15		
5	B	1	Total	C	H	O	0	0
			144	51	78	15		
5	C	1	Total	C	H	O	0	0
			144	51	78	15		
5	D	1	Total	C	H	O	0	0
			144	51	78	15		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K	0	0
			1 1		
6	B	1	Total K	0	0
			1 1		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		

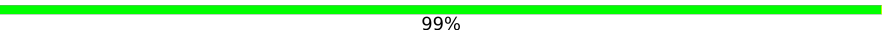
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	240	Total	O	0	0
			240	240		
9	B	233	Total	O	0	0
			233	233		
9	C	181	Total	O	0	0
			181	181		
9	D	165	Total	O	0	0
			165	165		

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-chl a protein

Chain A:  99% .

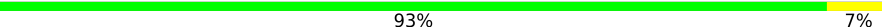


- Molecule 1: Peridinin-chl a protein

Chain C:  96% .

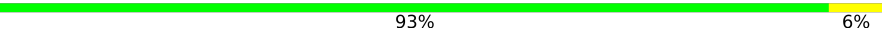


- Molecule 2: Peridinin-chl a protein

Chain B:  93% 7% .



- Molecule 2: Peridinin-chl a protein

Chain D:  93% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants a, b, c, α , β , γ	90.61Å 90.61Å 155.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.50 – 1.20 43.50 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.50-1.20) 96.3 (43.50-1.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.149 , 0.171 0.151 , 0.177	Depositor DCC
R_{free} test set	2139 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å ²)	9.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.368 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12518	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, K, PID, CLA, CL, W4O, PO4

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	A	0.64	0/1135	0.50	0/1522
1	C	0.59	0/1145	0.50	0/1536
2	B	0.62	0/1228	0.48	0/1644
2	D	0.57	0/1165	0.49	0/1560
All	All	0.61	0/4673	0.49	0/6262

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	A	1107	1098	1073	0	0
1	C	1116	1112	1089	4	0
2	B	1157	1165	1103	7	0
2	D	1134	1142	1115	6	0
3	A	65	72	72	0	0
3	B	65	72	72	0	0
3	C	65	72	72	0	0
3	D	65	72	72	0	0
4	A	184	200	200	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	184	200	200	2	0
4	C	184	200	200	4	0
4	D	184	200	200	2	0
5	A	66	78	0	0	0
5	B	66	78	0	0	0
5	C	66	78	0	0	0
5	D	66	78	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	1
7	A	5	0	0	0	0
8	B	1	0	0	0	0
9	A	240	0	0	0	10
9	B	233	0	0	3	6
9	C	181	0	0	2	2
9	D	165	0	0	2	1
All	All	6601	5917	5468	23	12

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 2.

All (23) 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)
2:B:125:LYS:NZ	9:B:722:HOH:O	1.96	0.99
4:C:613:PID:H311	2:D:62:ALA:HB2	1.60	0.84
4:C:613:PID:C31	2:D:62:ALA:HB2	2.19	0.73
2:D:106:TYR:OH	9:D:738:HOH:O	2.00	0.69
4:A:613:PID:H311	2:B:62:ALA:HB2	1.74	0.69
2:B:54:ASP:OD2	9:B:729:HOH:O	2.10	0.69
1:C:142:LYS:HD3	4:C:614:PID:HM13	1.74	0.69
4:A:613:PID:C31	2:B:62:ALA:HB2	2.23	0.68
1:C:5:ASP:OD1	9:C:702:HOH:O	2.13	0.65
1:C:84:GLU:OE1	9:C:703:HOH:O	2.16	0.62
4:A:613:PID:C9	4:A:614:PID:HM12	2.32	0.59
1:C:62:ALA:HB2	4:D:613:PID:H313	1.94	0.49
4:C:613:PID:C9	4:C:614:PID:HM12	2.44	0.48
2:B:9:LYS:NZ	2:B:140:GLU:OE2	2.39	0.47
4:B:613:PID:C9	4:B:614:PID:HM12	2.47	0.44
2:D:19[B]:LYS:HG2	2:D:77:VAL:HG11	1.98	0.44
2:D:10:LEU:HD22	2:D:141:PHE:CG	2.53	0.43
2:B:19[A]:LYS:HG2	2:B:77:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:ASP:OD2	9:D:706:HOH:O	2.21	0.43
4:D:613:PID:C9	4:D:614:PID:HM12	2.50	0.42
4:B:612:PID:C8	4:B:612:PID:HM11	2.50	0.41
2:B:41:LYS:HG2	9:B:711:HOH:O	2.20	0.41
4:A:613:PID:C11	4:A:614:PID:HM12	2.51	0.41

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:607:K:K	6:B:607:K:K[4_555]	1.31	0.89
9:A:856:HOH:O	9:C:775:HOH:O[3_555]	1.81	0.39
9:A:838:HOH:O	9:B:847:HOH:O[2_445]	1.89	0.31
9:A:828:HOH:O	9:B:910:HOH:O[3_555]	1.94	0.26
9:A:777:HOH:O	9:B:836:HOH:O[3_555]	1.95	0.25
9:A:928:HOH:O	9:B:920:HOH:O[5_555]	1.95	0.25
9:C:844:HOH:O	9:D:761:HOH:O[2_555]	1.97	0.23
9:A:820:HOH:O	9:A:907:HOH:O[2_445]	2.12	0.08
9:A:888:HOH:O	9:B:881:HOH:O[3_555]	2.12	0.08
9:A:742:HOH:O	9:A:869:HOH:O[2_445]	2.16	0.04
9:A:786:HOH:O	9:A:786:HOH:O[5_555]	2.16	0.04
9:A:864:HOH:O	9:B:848:HOH:O[2_445]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/149 (99%)	146 (99%)	2 (1%)	0	100	100
1	C	150/149 (101%)	148 (99%)	2 (1%)	0	100	100
2	B	160/149 (107%)	158 (99%)	2 (1%)	0	100	100
2	D	153/149 (103%)	151 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	611/596 (102%)	603 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	111/108 (103%)	110 (99%)	1 (1%)	70	40
1	C	111/108 (103%)	110 (99%)	1 (1%)	70	40
2	B	123/109 (113%)	122 (99%)	1 (1%)	73	44
2	D	115/109 (106%)	110 (96%)	5 (4%)	26	2
All	All	460/434 (106%)	452 (98%)	8 (2%)	59	18

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ASP
2	B	117	ASP
1	C	117	ASP
2	D	19[A]	LYS
2	D	19[B]	LYS
2	D	117	ASP
2	D	136[A]	LYS
2	D	136[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	HYP	C	32	1	6,8,9	1.18	1 (16%)	5,10,12	2.21	2 (40%)
1	HYP	A	32	1	6,8,9	1.41	1 (16%)	5,10,12	2.51	2 (40%)
2	HYP	D	32	2	6,8,9	1.00	0	5,10,12	2.72	3 (60%)
2	HYP	B	32	2	6,8,9	1.19	1 (16%)	5,10,12	2.99	4 (80%)

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
1	HYP	C	32	1	-	0/0/11/13	0/1/1/1
1	HYP	A	32	1	-	0/0/11/13	0/1/1/1
2	HYP	D	32	2	-	0/0/11/13	0/1/1/1
2	HYP	B	32	2	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	HYP	OD1-CG	-2.77	1.35	1.43
1	C	32	HYP	OD1-CG	-2.41	1.36	1.43
2	B	32	HYP	OD1-CG	-2.34	1.36	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	HYP	CB-CG-CD	-5.39	96.66	103.27
2	D	32	HYP	CB-CG-CD	-4.66	97.55	103.27
1	A	32	HYP	CB-CG-CD	-4.36	97.92	103.27
1	C	32	HYP	CB-CG-CD	-3.59	98.86	103.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	32	HYP	OD1-CG-CB	2.64	116.56	110.03
2	B	32	HYP	OD1-CG-CB	2.48	116.17	110.03
1	A	32	HYP	OD1-CG-CB	2.44	116.07	110.03
1	C	32	HYP	OD1-CG-CB	2.36	115.88	110.03
2	B	32	HYP	OD1-CG-CD	2.26	115.29	110.35
2	D	32	HYP	OD1-CG-CD	2.19	115.14	110.35
2	B	32	HYP	O-C-CA	-2.00	119.53	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	B	601	9	69,73,73	1.28	12 (17%)	83,113,113	1.04	5 (6%)
3	CLA	D	601	9	69,73,73	1.28	10 (14%)	83,113,113	1.11	6 (7%)
3	CLA	C	601	9	69,73,73	1.28	10 (14%)	83,113,113	1.25	5 (6%)
4	PID	D	611	-	41,49,49	1.27	6 (14%)	49,76,76	0.84	2 (4%)
3	CLA	A	601	9	69,73,73	1.28	8 (11%)	83,113,113	1.36	8 (9%)
5	W4O	A	615	-	67,67,67	1.28	9 (13%)	79,81,81	1.25	9 (11%)
4	PID	C	612	-	41,49,49	1.68	11 (26%)	49,76,76	1.12	5 (10%)
7	PO4	A	608	6	4,4,4	0.97	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PID	B	614	-	41,49,49	1.39	4 (9%)	49,76,76	0.86	1 (2%)
4	PID	B	612	-	41,49,49	1.43	8 (19%)	49,76,76	1.06	4 (8%)
4	PID	C	614	-	41,49,49	1.42	10 (24%)	49,76,76	1.13	4 (8%)
4	PID	C	613	-	41,49,49	1.69	11 (26%)	49,76,76	0.91	1 (2%)
4	PID	B	613	-	41,49,49	1.28	4 (9%)	49,76,76	1.08	5 (10%)
4	PID	D	613	-	41,49,49	1.66	7 (17%)	49,76,76	0.88	2 (4%)
5	W4O	B	615	-	67,67,67	1.37	8 (11%)	79,81,81	1.25	9 (11%)
4	PID	C	611	-	41,49,49	1.46	8 (19%)	49,76,76	0.81	1 (2%)
4	PID	B	611	-	41,49,49	1.47	4 (9%)	49,76,76	0.83	1 (2%)
5	W4O	D	615	-	67,67,67	1.29	7 (10%)	79,81,81	1.23	8 (10%)
4	PID	A	613	-	41,49,49	1.65	7 (17%)	49,76,76	0.93	2 (4%)
4	PID	A	614	-	41,49,49	1.15	4 (9%)	49,76,76	0.77	1 (2%)
5	W4O	C	615	-	67,67,67	1.33	8 (11%)	79,81,81	1.27	10 (12%)
4	PID	A	611	-	41,49,49	1.60	5 (12%)	49,76,76	0.92	2 (4%)
4	PID	A	612	-	41,49,49	1.53	6 (14%)	49,76,76	1.02	5 (10%)
4	PID	D	614	-	41,49,49	1.19	3 (7%)	49,76,76	0.93	2 (4%)
4	PID	D	612	-	41,49,49	1.37	9 (21%)	49,76,76	1.01	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	B	601	9	-	1/39/115/115	-
3	CLA	D	601	9	-	1/39/115/115	-
3	CLA	C	601	9	-	2/39/115/115	-
4	PID	D	611	-	-	0/24/93/93	0/4/4/4
3	CLA	A	601	9	-	5/39/115/115	-
5	W4O	A	615	-	-	11/55/95/95	0/2/2/2
4	PID	C	612	-	-	0/24/93/93	0/4/4/4
4	PID	B	614	-	-	0/24/93/93	0/4/4/4
4	PID	B	612	-	-	0/24/93/93	0/4/4/4
4	PID	C	614	-	-	0/24/93/93	0/4/4/4
4	PID	C	613	-	-	0/24/93/93	0/4/4/4
4	PID	B	613	-	-	0/24/93/93	0/4/4/4
4	PID	D	613	-	1/1/25/25	0/24/93/93	0/4/4/4
5	W4O	B	615	-	-	9/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PID	C	611	-	-	0/24/93/93	0/4/4/4
4	PID	B	611	-	-	0/24/93/93	0/4/4/4
5	W4O	D	615	-	-	8/55/95/95	0/2/2/2
4	PID	A	613	-	-	0/24/93/93	0/4/4/4
4	PID	A	614	-	-	0/24/93/93	0/4/4/4
5	W4O	C	615	-	-	11/55/95/95	0/2/2/2
4	PID	A	611	-	-	0/24/93/93	0/4/4/4
4	PID	A	612	-	-	0/24/93/93	0/4/4/4
4	PID	D	614	-	-	0/24/93/93	0/4/4/4
4	PID	D	612	-	-	0/24/93/93	0/4/4/4

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	612	PID	C4-C3	-5.40	1.44	1.52
4	A	611	PID	C2-C3	-4.56	1.45	1.52
4	B	611	PID	O1-C1	-4.49	1.39	1.46
3	A	601	CLA	MG-NA	4.44	2.16	2.06
4	D	613	PID	C2-C3	-4.40	1.46	1.52
5	C	615	W4O	O3G-C3G	-4.38	1.35	1.43
4	A	613	PID	CM1-C1	-4.36	1.45	1.51
5	D	615	W4O	O3G-C3G	-4.28	1.35	1.43
3	C	601	CLA	MG-NA	4.26	2.16	2.06
5	B	615	W4O	O3G-C3G	-4.20	1.36	1.43
4	C	612	PID	C4-C3	-4.11	1.46	1.52
4	B	614	PID	C2-C3	-4.06	1.46	1.52
4	D	613	PID	C4-C3	-4.05	1.46	1.52
5	B	615	W4O	O1G-C1G	-3.98	1.36	1.45
3	D	601	CLA	C1D-ND	3.94	1.42	1.37
4	A	613	PID	C4-C5	-3.93	1.48	1.54
4	B	611	PID	CM1-C1	-3.91	1.45	1.51
4	C	613	PID	C4-C5	-3.81	1.48	1.54
4	A	613	PID	C2-C3	-3.78	1.46	1.52
4	C	612	PID	O1-C1	-3.75	1.40	1.46
4	C	613	PID	C4-C3	-3.71	1.47	1.52
4	B	613	PID	CM1-C1	-3.71	1.46	1.51
3	D	601	CLA	C4D-ND	-3.69	1.32	1.37
4	A	611	PID	O1-C1	-3.68	1.40	1.46
4	A	612	PID	O1-C1	-3.66	1.41	1.46
4	D	613	PID	C4-C5	-3.65	1.48	1.54
4	D	614	PID	CM1-C1	-3.65	1.46	1.51
4	A	613	PID	CM3-C5	-3.64	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	611	PID	C4-C3	-3.57	1.47	1.52
4	A	611	PID	C4-C3	-3.56	1.47	1.52
5	B	615	W4O	C4A-C3A	-3.51	1.31	1.51
4	B	614	PID	O1-C1	-3.50	1.41	1.46
3	B	601	CLA	MG-NA	3.49	2.14	2.06
4	C	613	PID	O1-C1	-3.44	1.41	1.46
5	A	615	W4O	C4A-C3A	-3.43	1.32	1.51
4	D	612	PID	O1-C1	-3.42	1.41	1.46
4	B	614	PID	CM1-C1	-3.39	1.46	1.51
3	B	601	CLA	C4D-ND	-3.38	1.33	1.37
4	B	612	PID	C4-C3	-3.38	1.47	1.52
5	C	615	W4O	C4E-C3E	3.32	1.60	1.52
5	D	615	W4O	O6D-C5D	-3.29	1.36	1.44
3	C	601	CLA	C1D-ND	3.25	1.41	1.37
3	C	601	CLA	C4D-ND	-3.24	1.33	1.37
3	C	601	CLA	C3B-C4B	3.21	1.50	1.42
5	C	615	W4O	C4A-C3A	-3.19	1.33	1.51
3	A	601	CLA	C4B-NB	3.14	1.41	1.37
4	C	612	PID	C2-C3	-3.14	1.47	1.52
3	A	601	CLA	C1D-ND	3.12	1.41	1.37
5	B	615	W4O	C4E-C5E	3.12	1.59	1.53
5	D	615	W4O	C4A-C3A	-3.11	1.34	1.51
4	B	614	PID	CM8-C29	-3.08	1.47	1.52
4	C	613	PID	C2-C3	-3.07	1.47	1.52
4	A	613	PID	O1-C1	-3.07	1.41	1.46
5	D	615	W4O	O4D-C4D	-3.05	1.35	1.43
3	D	601	CLA	C3B-C4B	3.04	1.49	1.42
3	A	601	CLA	MG-NC	3.00	2.13	2.06
4	C	612	PID	C11-C12	-3.00	1.38	1.44
4	B	612	PID	C11-C12	-2.97	1.38	1.44
3	B	601	CLA	C1D-ND	2.96	1.41	1.37
4	A	612	PID	CM1-C1	-2.93	1.47	1.51
4	B	612	PID	O1-C1	-2.92	1.42	1.46
4	C	614	PID	C2-C3	-2.90	1.48	1.52
3	B	601	CLA	C3B-C4B	2.90	1.49	1.42
4	C	613	PID	C2-C1	-2.88	1.48	1.52
5	A	615	W4O	O1G-C1G	-2.86	1.38	1.45
4	C	613	PID	CM8-C29	-2.85	1.48	1.52
4	D	614	PID	CM8-C29	-2.83	1.48	1.52
5	A	615	W4O	O2G-C2G	-2.82	1.39	1.46
4	C	611	PID	C2-C3	-2.78	1.48	1.52
4	B	613	PID	O1-C1	-2.77	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	611	PID	O1-C1	-2.76	1.42	1.46
3	A	601	CLA	C3B-C4B	2.74	1.49	1.42
4	D	613	PID	CM8-C29	-2.74	1.48	1.52
4	D	613	PID	O1-C1	-2.74	1.42	1.46
3	D	601	CLA	C1B-NB	-2.74	1.34	1.37
4	B	611	PID	CM3-C5	-2.68	1.48	1.53
4	D	612	PID	C11-C12	-2.67	1.39	1.44
4	A	614	PID	C2-C3	-2.67	1.48	1.52
4	C	614	PID	O4-C10	-2.64	1.34	1.39
4	C	612	PID	O4-C12	-2.63	1.33	1.38
4	D	612	PID	C2-C1	-2.62	1.48	1.52
5	A	615	W4O	C4E-C3E	2.62	1.59	1.52
3	A	601	CLA	C4D-ND	-2.62	1.34	1.37
4	C	613	PID	O6-C30	-2.61	1.29	1.35
4	D	611	PID	CM8-C29	-2.60	1.48	1.52
5	C	615	W4O	O6D-C5D	-2.60	1.38	1.44
5	C	615	W4O	C4E-C5E	2.59	1.58	1.53
4	C	612	PID	O4-C10	-2.57	1.34	1.39
4	C	614	PID	O1-C1	-2.57	1.42	1.46
3	A	601	CLA	CMB-C2B	-2.57	1.45	1.50
5	B	615	W4O	O4D-C4D	-2.57	1.36	1.43
4	B	612	PID	C15-C14	2.55	1.39	1.35
4	C	611	PID	CM6-C25	-2.54	1.48	1.53
4	D	611	PID	O6-C30	-2.53	1.29	1.35
3	C	601	CLA	CMC-C2C	-2.53	1.45	1.50
3	B	601	CLA	MG-NB	-2.52	2.00	2.05
4	B	612	PID	CM1-C1	-2.52	1.47	1.51
4	C	614	PID	C28-C27	-2.51	1.47	1.51
3	A	601	CLA	C1B-C2B	2.50	1.49	1.43
3	C	601	CLA	O2D-CED	-2.49	1.39	1.45
4	C	613	PID	CM7-C25	-2.49	1.48	1.53
4	C	611	PID	CM3-C5	-2.48	1.49	1.53
4	D	611	PID	CM1-C1	-2.47	1.48	1.51
4	D	612	PID	O4-C10	-2.46	1.34	1.39
4	B	612	PID	C9-C10	-2.45	1.42	1.48
5	D	615	W4O	O2E-C2E	-2.44	1.37	1.43
5	B	615	W4O	O2G-C2G	-2.43	1.40	1.46
3	B	601	CLA	CMD-C2D	-2.43	1.45	1.50
5	A	615	W4O	C4E-C5E	2.43	1.58	1.53
4	A	613	PID	C28-C27	-2.42	1.47	1.51
4	C	613	PID	C28-C27	-2.41	1.47	1.51
3	C	601	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	614	PID	C4-C3	-2.40	1.48	1.52
5	C	615	W4O	O4D-C4D	-2.40	1.37	1.43
4	B	611	PID	C4-C5	-2.39	1.50	1.54
5	B	615	W4O	O6D-C5D	-2.37	1.38	1.44
4	A	612	PID	C2-C3	-2.35	1.48	1.52
4	D	611	PID	CM4-C14	-2.34	1.46	1.50
4	D	614	PID	C2-C3	-2.32	1.49	1.52
5	A	615	W4O	C3G-C2G	2.32	1.57	1.50
5	B	615	W4O	C3E-C2E	2.29	1.58	1.52
4	A	612	PID	C11-C12	-2.29	1.39	1.44
3	D	601	CLA	CMC-C2C	-2.27	1.46	1.50
4	C	614	PID	O4-C12	-2.27	1.34	1.38
4	B	613	PID	C4-C3	-2.25	1.49	1.52
4	B	612	PID	O4-C10	-2.24	1.34	1.39
3	D	601	CLA	MG-NA	2.23	2.11	2.06
5	D	615	W4O	O1G-C1G	-2.23	1.40	1.45
4	D	612	PID	CM7-C25	-2.21	1.49	1.53
4	C	612	PID	C2-C1	-2.21	1.48	1.52
4	A	613	PID	CM5-C21	-2.20	1.46	1.50
4	D	611	PID	C28-C27	-2.20	1.47	1.51
3	D	601	CLA	MG-NC	2.20	2.11	2.06
4	D	611	PID	C13-C14	-2.20	1.41	1.45
5	C	615	W4O	C6E-C5E	2.19	1.59	1.51
4	A	614	PID	O1-C1	-2.18	1.43	1.46
3	B	601	CLA	CMB-C2B	-2.18	1.46	1.50
4	C	612	PID	O6-C27	-2.18	1.41	1.46
5	D	615	W4O	C4E-C3E	2.15	1.57	1.52
4	C	612	PID	C15-C14	2.13	1.38	1.35
3	B	601	CLA	C1B-NB	-2.13	1.35	1.37
4	D	612	PID	C4-C3	-2.13	1.49	1.52
3	B	601	CLA	MG-NC	2.12	2.11	2.06
4	C	614	PID	C2-C1	-2.11	1.49	1.52
3	D	601	CLA	O2D-CED	-2.11	1.40	1.45
5	A	615	W4O	O4D-C4D	-2.11	1.38	1.43
3	D	601	CLA	CMD-C2D	-2.11	1.46	1.50
3	B	601	CLA	C1B-C2B	2.10	1.48	1.43
4	C	614	PID	O5-C29	-2.10	1.39	1.43
4	C	611	PID	C13-C14	-2.09	1.41	1.45
4	D	613	PID	CM5-C21	-2.08	1.46	1.50
3	B	601	CLA	C1C-NC	-2.08	1.34	1.37
4	B	613	PID	C15-C14	2.08	1.38	1.35
3	C	601	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	612	PID	C9-C10	-2.07	1.43	1.48
4	B	612	PID	O4-C12	-2.07	1.34	1.38
3	C	601	CLA	MG-NC	2.06	2.11	2.06
4	A	614	PID	C15-C14	2.06	1.38	1.35
4	C	613	PID	CM1-C1	-2.05	1.48	1.51
4	A	612	PID	CM8-C29	-2.05	1.49	1.52
4	D	612	PID	C11-C9	-2.05	1.34	1.39
5	A	615	W4O	C4A-C5A	-2.05	1.44	1.52
4	C	611	PID	O6-C30	-2.05	1.30	1.35
3	D	601	CLA	CMB-C2B	-2.04	1.46	1.50
4	C	614	PID	CM1-C1	-2.04	1.48	1.51
3	C	601	CLA	C4B-NB	2.04	1.40	1.37
4	C	611	PID	C4-C5	-2.03	1.51	1.54
3	B	601	CLA	O2D-CED	-2.03	1.40	1.45
4	A	611	PID	C28-C27	-2.03	1.47	1.51
4	A	611	PID	CM1-C1	-2.02	1.48	1.51
4	A	614	PID	C9-C10	-2.02	1.43	1.48
4	D	612	PID	CM1-C1	-2.01	1.48	1.51
5	A	615	W4O	C1E-C2E	2.01	1.58	1.52
4	C	613	PID	CM3-C5	-2.01	1.49	1.53
4	C	614	PID	C4-C5	-2.01	1.51	1.54
4	C	612	PID	C11-C9	-2.01	1.34	1.39
4	C	612	PID	CM5-C21	-2.00	1.46	1.50
5	C	615	W4O	C1G-C2G	2.00	1.56	1.50
4	D	613	PID	C15-C14	2.00	1.38	1.35

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	CLA	C4A-NA-C1A	7.86	110.24	106.71
3	C	601	CLA	C4A-NA-C1A	6.76	109.75	106.71
3	D	601	CLA	C4A-NA-C1A	4.95	108.93	106.71
5	A	615	W4O	O5D-C1E-C2E	4.61	115.50	108.30
5	D	615	W4O	C4A-C3A-C2A	4.37	128.89	113.19
4	C	614	PID	C12-O4-C10	4.16	109.82	107.65
5	A	615	W4O	C4A-C3A-C2A	4.01	127.62	113.19
5	D	615	W4O	O5D-C1E-C2E	3.91	114.41	108.30
5	C	615	W4O	C4A-C3A-C2A	3.85	127.01	113.19
5	B	615	W4O	C4A-C3A-C2A	3.83	126.96	113.19
5	B	615	W4O	C3A-C4A-C5A	3.59	129.43	113.79
5	D	615	W4O	C3A-C4A-C5A	3.50	129.04	113.79
5	C	615	W4O	O5D-C6D-C5D	-3.50	102.58	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	615	W4O	O5D-C1E-C2E	3.41	113.62	108.30
5	A	615	W4O	C3A-C4A-C5A	3.38	128.50	113.79
5	C	615	W4O	O6D-C5D-C6D	3.27	113.26	106.67
5	B	615	W4O	O5D-C1E-C2E	3.22	113.33	108.30
4	C	614	PID	CM7-C25-C24	3.20	113.33	110.47
4	A	612	PID	O4-C12-C11	3.18	109.29	107.36
3	B	601	CLA	C4A-NA-C1A	3.17	108.13	106.71
5	A	615	W4O	C1D-O6D-C5D	3.17	119.90	113.69
4	B	612	PID	C12-O4-C10	3.09	109.26	107.65
5	C	615	W4O	C3A-C4A-C5A	3.07	127.16	113.79
3	C	601	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
5	B	615	W4O	C1D-O6D-C5D	3.04	119.66	113.69
4	D	613	PID	C12-O4-C10	2.88	109.15	107.65
5	B	615	W4O	O6D-C5D-C6D	2.87	112.46	106.67
3	D	601	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
3	A	601	CLA	O1D-CGD-CBD	2.84	130.31	124.48
4	B	613	PID	C12-O4-C10	2.81	109.11	107.65
4	C	612	PID	C12-O4-C10	2.81	109.11	107.65
3	D	601	CLA	C3B-C4B-NB	-2.81	107.91	110.52
3	B	601	CLA	C3B-C4B-NB	-2.74	107.98	110.52
4	A	612	PID	CM1-C1-C2	2.70	117.32	114.28
5	D	615	W4O	O6D-C1D-O3G	-2.70	103.58	109.97
4	B	613	PID	O3-C10-C9	2.68	133.79	130.74
5	B	615	W4O	C6D-O5D-C1E	2.67	118.96	113.74
3	C	601	CLA	C3B-C4B-NB	-2.63	108.08	110.52
3	A	601	CLA	C3B-C4B-NB	-2.57	108.13	110.52
4	B	612	PID	CM1-C1-C6	-2.52	118.03	122.26
4	D	612	PID	C12-O4-C10	2.52	108.96	107.65
3	A	601	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
3	A	601	CLA	CHB-C4A-NA	2.50	127.97	124.51
5	D	615	W4O	O6D-C5D-C6D	2.46	111.64	106.67
4	C	612	PID	O4-C12-C11	2.46	108.85	107.36
4	A	611	PID	C12-O4-C10	2.41	108.90	107.65
5	A	615	W4O	O6D-C5D-C6D	2.40	111.50	106.67
3	A	601	CLA	C3A-C2A-C1A	2.39	104.91	101.34
3	D	601	CLA	CHD-C1D-ND	-2.38	122.26	124.45
4	B	613	PID	C27-O6-C30	2.38	122.33	117.90
5	C	615	W4O	O6D-C1D-O3G	-2.38	104.34	109.97
4	B	611	PID	O4-C12-C11	2.37	108.80	107.36
4	D	611	PID	C19-C20-C21	2.35	130.66	127.31
4	C	612	PID	O1-C1-C2	-2.35	111.62	113.38
5	D	615	W4O	O5D-C6D-C5D	-2.33	104.74	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	615	W4O	C3G-O3G-C1D	2.31	118.25	113.74
4	C	612	PID	C29-C24-C25	-2.31	117.41	119.70
3	A	601	CLA	C2D-C1D-ND	-2.30	108.41	110.10
3	B	601	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
5	A	615	W4O	O6D-C1D-O3G	-2.29	104.55	109.97
4	A	613	PID	C12-O4-C10	2.28	108.84	107.65
4	C	614	PID	C28-C27-C26	2.28	113.86	109.88
4	B	612	PID	C16-C15-C14	2.28	130.56	127.31
5	C	615	W4O	O6E-C1E-O5D	-2.25	104.63	109.97
4	B	612	PID	C1-C2-C3	2.25	117.20	112.75
4	B	613	PID	O1-C1-CM1	2.25	117.75	115.06
3	C	601	CLA	CHB-C4A-NA	2.24	127.61	124.51
5	A	615	W4O	O5E-C6E-C5E	-2.24	103.61	111.29
4	C	612	PID	CM7-C25-C24	2.23	112.46	110.47
4	D	614	PID	C29-C24-C25	-2.20	117.51	119.70
4	C	613	PID	CM1-C1-C2	2.19	116.75	114.28
5	C	615	W4O	C1D-O6D-C5D	2.19	117.99	113.69
3	A	601	CLA	C2A-C1A-CHA	2.19	127.69	123.86
5	B	615	W4O	O6E-C5E-C4E	2.19	113.67	109.69
3	B	601	CLA	CHB-C1B-NB	2.19	126.57	124.26
4	B	614	PID	O1-C1-CM1	2.18	117.67	115.06
5	D	615	W4O	O5E-C6E-C5E	-2.17	103.86	111.29
4	D	614	PID	CM7-C25-C24	2.16	112.40	110.47
4	B	613	PID	C29-C24-C25	-2.13	117.58	119.70
3	D	601	CLA	CHB-C4A-NA	2.13	127.46	124.51
4	A	613	PID	CM7-C25-C24	2.13	112.38	110.47
5	A	615	W4O	C9A-C8A-C7A	-2.13	101.55	112.02
5	D	615	W4O	O6E-C1E-O5D	-2.13	104.94	109.97
3	D	601	CLA	O1D-CGD-CBD	2.13	128.83	124.48
5	C	615	W4O	O1G-C1G-C2G	2.11	114.59	108.43
5	B	615	W4O	O5E-C6E-C5E	-2.11	104.04	111.29
4	C	611	PID	C19-C20-C21	2.11	130.32	127.31
5	C	615	W4O	C6D-O5D-C1E	2.11	117.86	113.74
4	A	614	PID	C28-C27-C26	2.10	113.54	109.88
3	C	601	CLA	CHB-C1B-NB	2.09	126.47	124.26
4	D	612	PID	O1-C1-C2	-2.09	111.81	113.38
4	C	614	PID	C29-C24-C25	-2.08	117.63	119.70
4	A	611	PID	O2-C3-C2	-2.08	105.66	109.80
5	A	615	W4O	O6E-C1E-O5D	-2.06	105.10	109.97
4	D	612	PID	C18-C19-C20	2.05	127.67	123.47
4	A	612	PID	C29-C24-C25	-2.04	117.67	119.70
3	B	601	CLA	O2A-CGA-O1A	-2.04	118.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	612	PID	C18-C19-C20	2.04	127.64	123.47
4	A	612	PID	O3-C10-C9	2.03	133.06	130.74
4	D	611	PID	O4-C12-C11	2.01	108.58	107.36
4	D	613	PID	C27-O6-C30	2.01	121.64	117.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	613	PID	C6

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	615	W4O	CFA-CGA-CHA-CIA
5	B	615	W4O	CFB-CGB-CHB-CIB
5	D	615	W4O	CFA-CGA-CHA-CIA
5	A	615	W4O	C2A-C3A-C4A-C5A
5	B	615	W4O	C2A-C3A-C4A-C5A
5	C	615	W4O	C2A-C3A-C4A-C5A
5	D	615	W4O	C2A-C3A-C4A-C5A
5	D	615	W4O	O6E-C5E-C6E-O5E
5	B	615	W4O	O6E-C5E-C6E-O5E
5	A	615	W4O	C4E-C5E-C6E-O5E
5	B	615	W4O	C4E-C5E-C6E-O5E
5	D	615	W4O	C4E-C5E-C6E-O5E
5	A	615	W4O	O6E-C5E-C6E-O5E
5	C	615	W4O	C2D-C1D-O3G-C3G
5	D	615	W4O	C3A-C4A-C5A-C6A
5	B	615	W4O	CFA-CGA-CHA-CIA
5	A	615	W4O	C3A-C4A-C5A-C6A
5	B	615	W4O	C3A-C4A-C5A-C6A
5	C	615	W4O	C1A-C2A-C3A-C4A
5	C	615	W4O	O6D-C1D-O3G-C3G
5	C	615	W4O	C3A-C4A-C5A-C6A
5	A	615	W4O	O6D-C5D-C6D-O5D
3	A	601	CLA	C16-C17-C18-C20
5	C	615	W4O	C4E-C5E-C6E-O5E
5	C	615	W4O	CFA-CGA-CHA-CIA
3	D	601	CLA	CAD-CBD-CGD-O2D
5	A	615	W4O	O6D-C1D-O3G-C3G
5	D	615	W4O	O6D-C5D-C6D-O5D
3	A	601	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
5	A	615	W4O	C4D-C5D-C6D-O5D
5	A	615	W4O	C2D-C1D-O3G-C3G
5	B	615	W4O	C1A-C2A-C3A-C4A
5	D	615	W4O	O6D-C1D-O3G-C3G
5	A	615	W4O	CCA-CDA-CEA-CFA
5	A	615	W4O	CDA-CEA-CFA-CGA
5	B	615	W4O	CCB-CDB-CEB-CFB
5	C	615	W4O	CCA-CDA-CEA-CFA
5	C	615	W4O	CAB-CBB-CCB-CDB
5	C	615	W4O	CCB-CDB-CEB-CFB
5	D	615	W4O	CCA-CDA-CEA-CFA
5	C	615	W4O	O6D-C5D-C6D-O5D
5	B	615	W4O	O2G-C2G-C3G-O3G
3	A	601	CLA	CAD-CBD-CGD-O2D
3	B	601	CLA	CAD-CBD-CGD-O2D
3	C	601	CLA	CAD-CBD-CGD-O2D
3	A	601	CLA	C15-C16-C17-C18
3	A	601	CLA	C13-C15-C16-C17
3	C	601	CLA	CAA-CBA-CGA-O2A

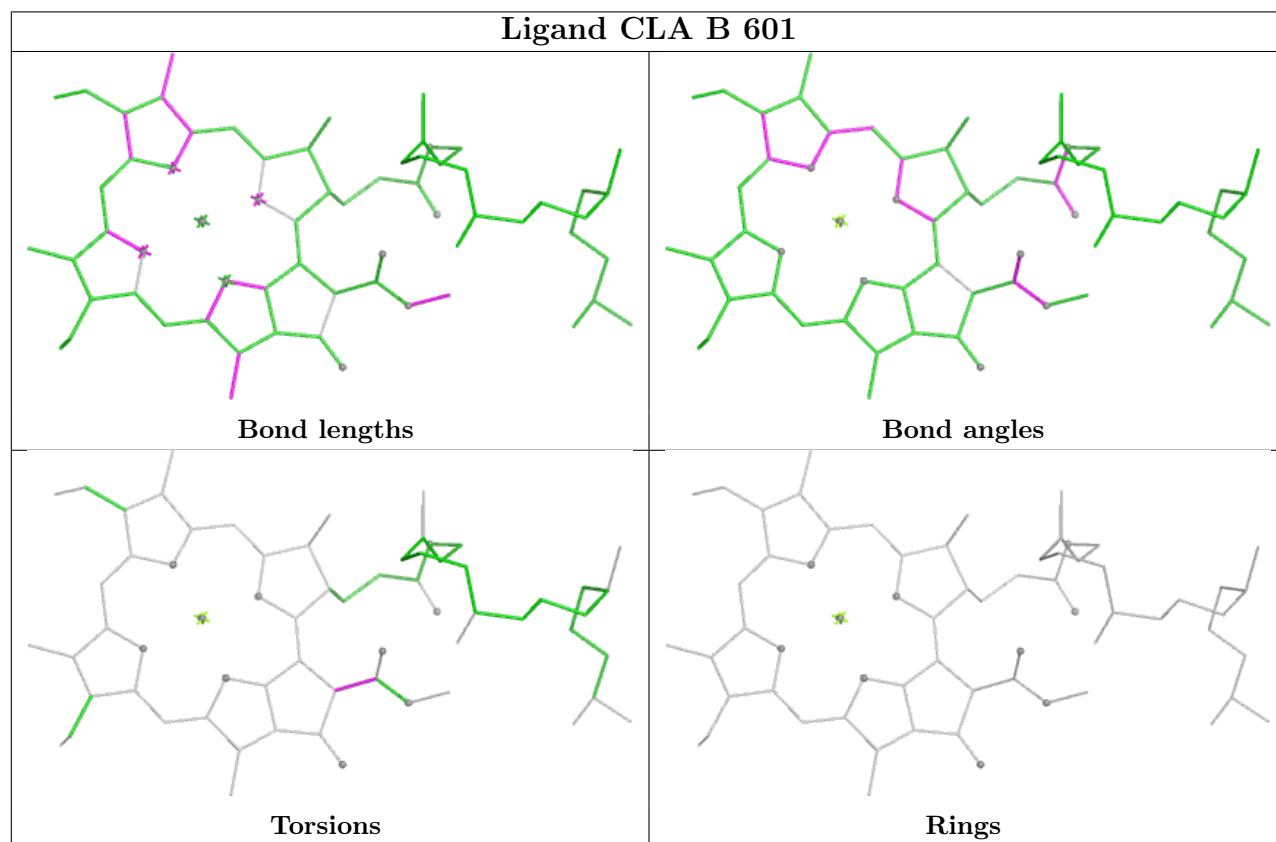
There are no ring outliers.

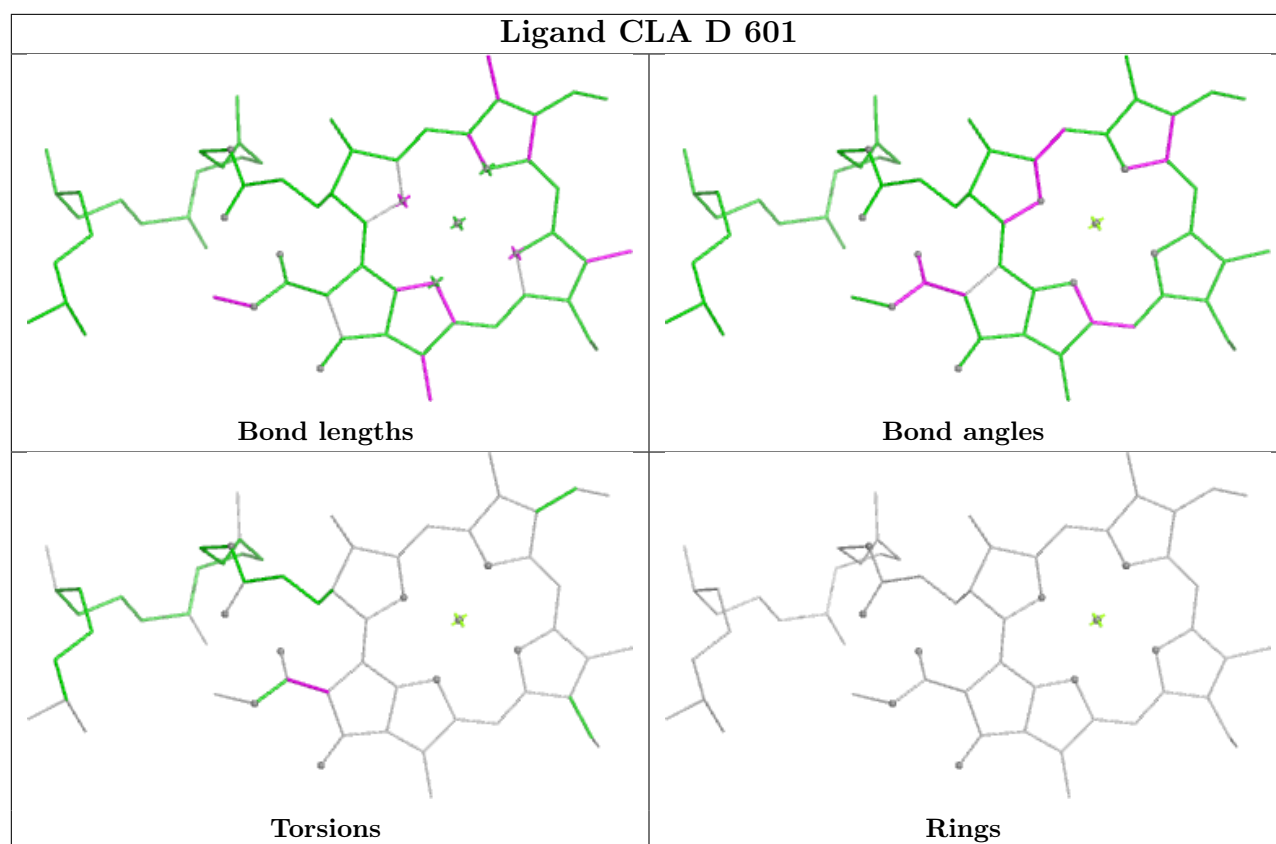
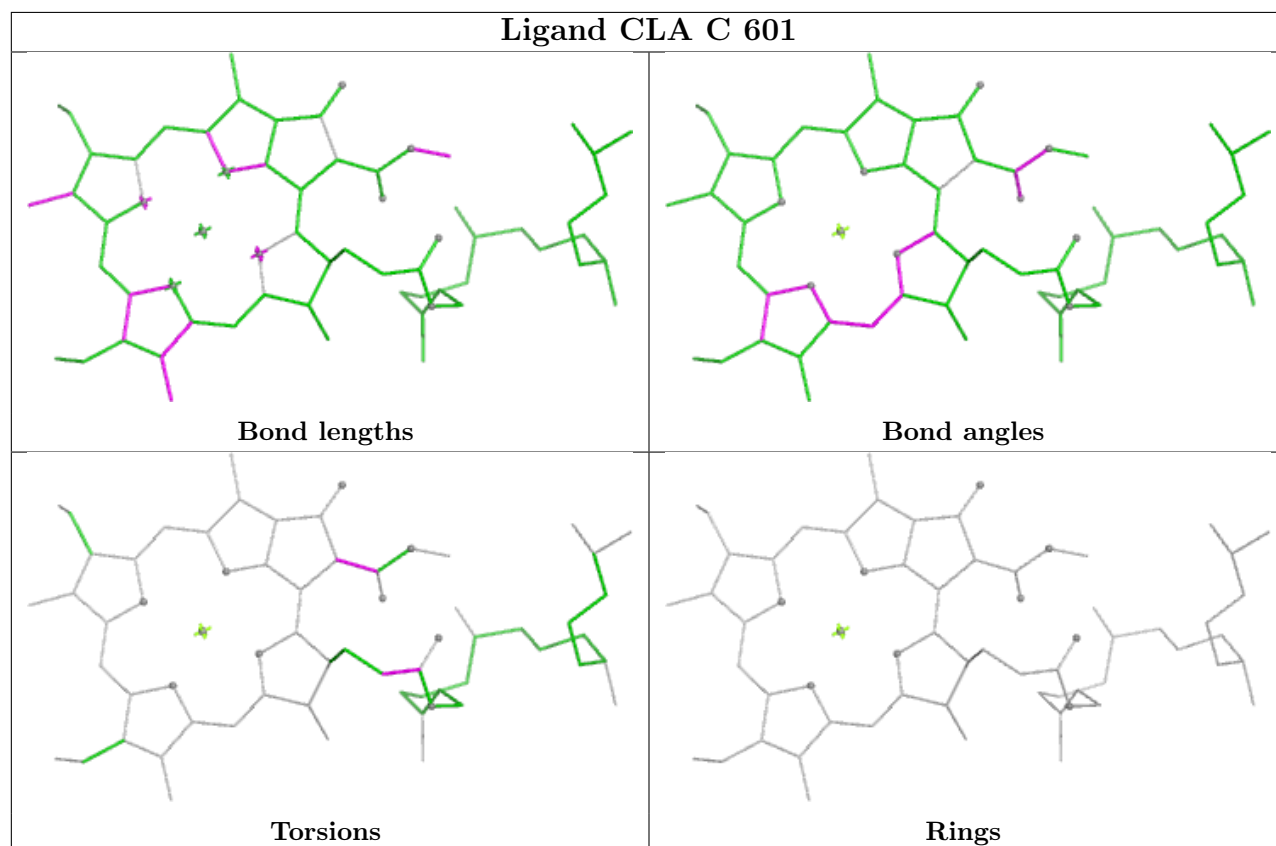
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	614	PID	1	0
4	B	612	PID	1	0
4	C	614	PID	2	0
4	C	613	PID	3	0
4	B	613	PID	1	0
4	D	613	PID	2	0
4	A	613	PID	4	0
4	A	614	PID	2	0
4	D	614	PID	1	0

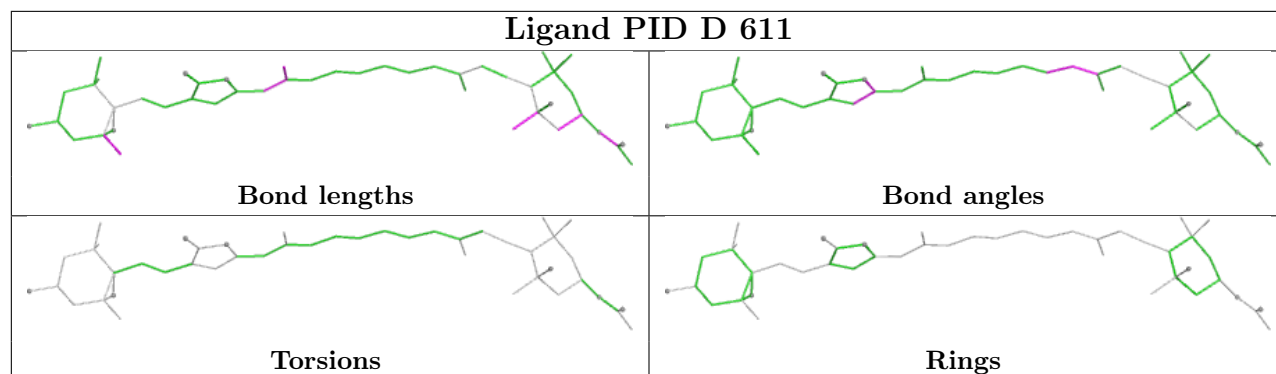
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

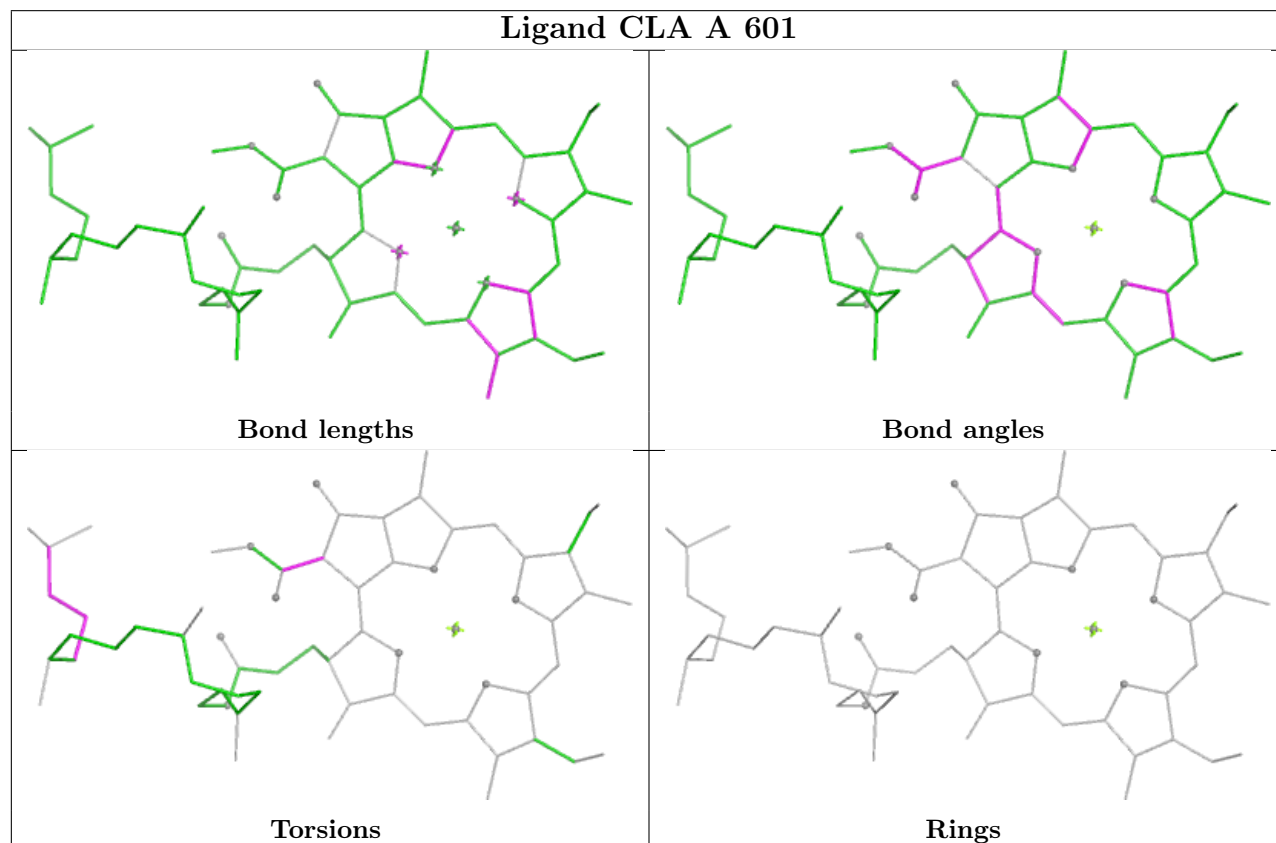




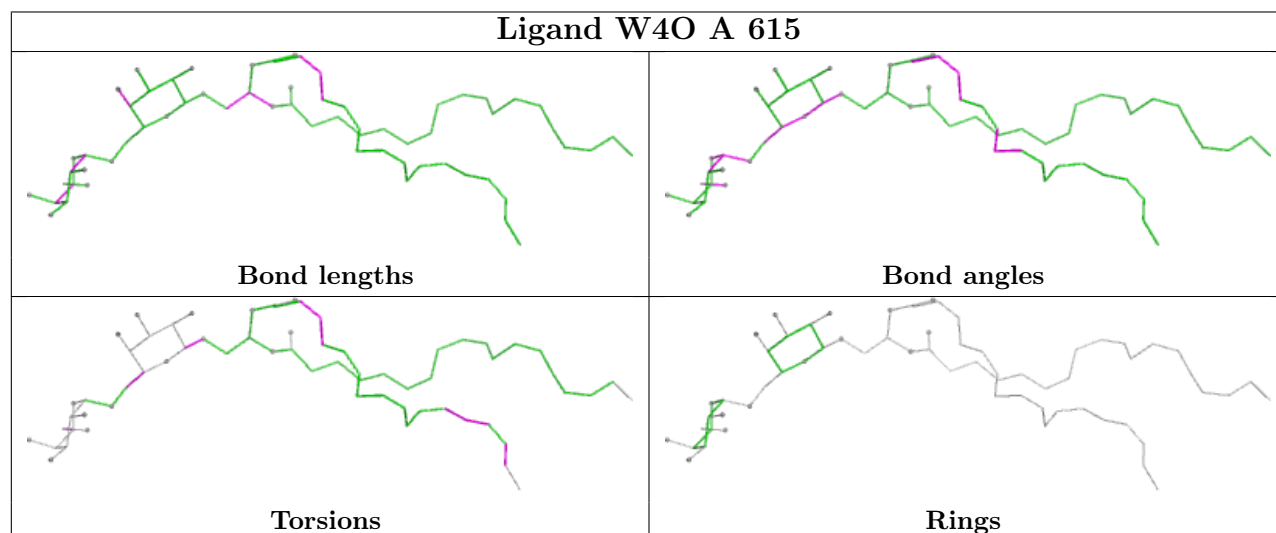
Ligand PID D 611



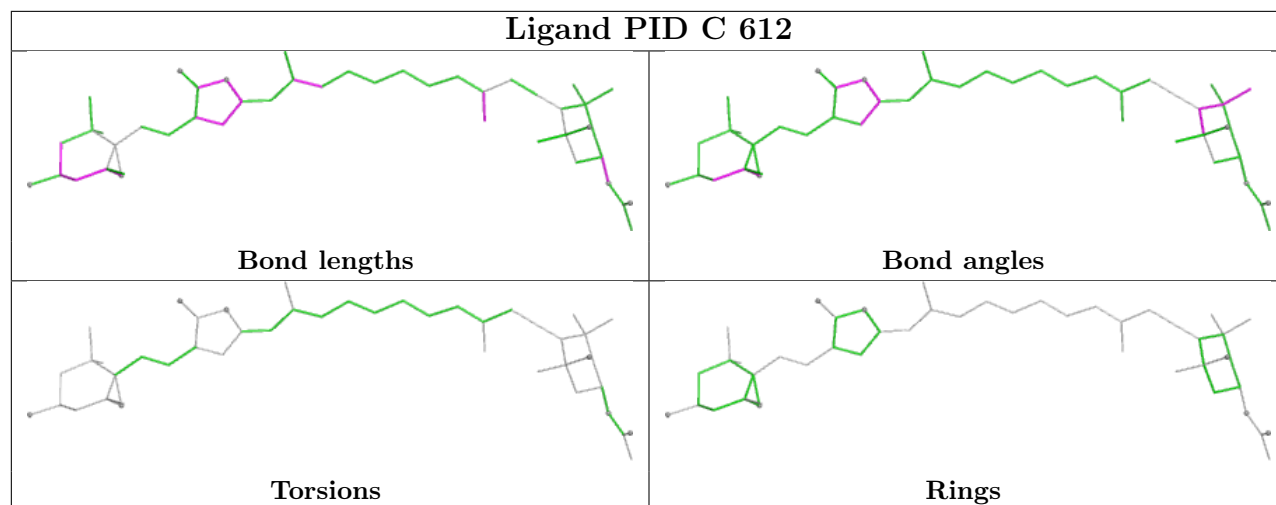
Ligand CLA A 601



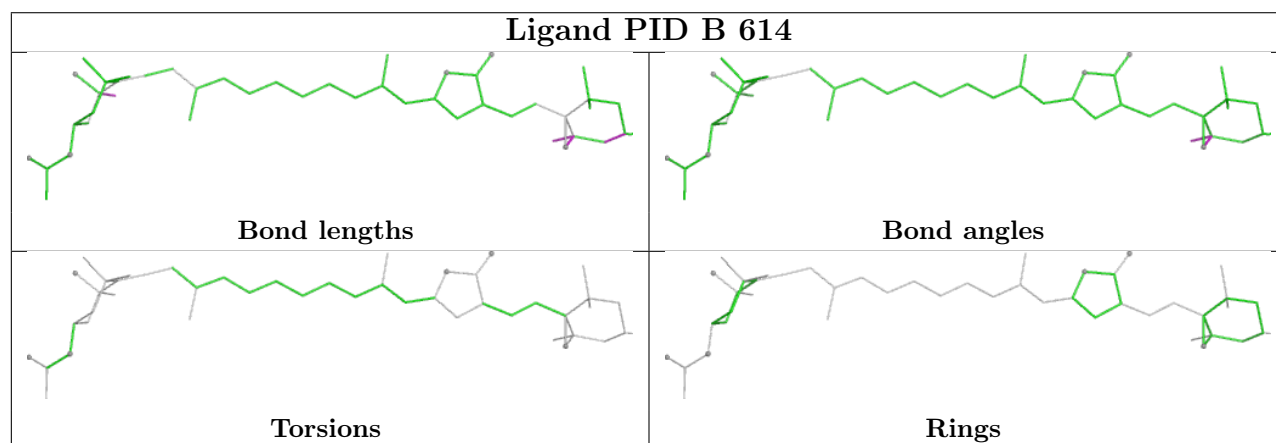
Ligand W4O A 615



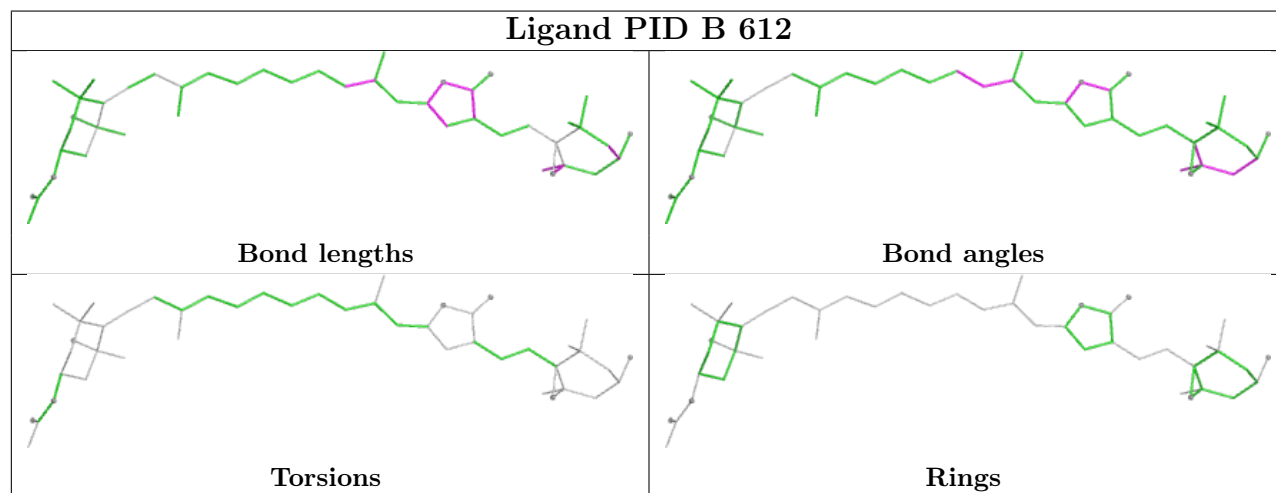
Ligand PID C 612

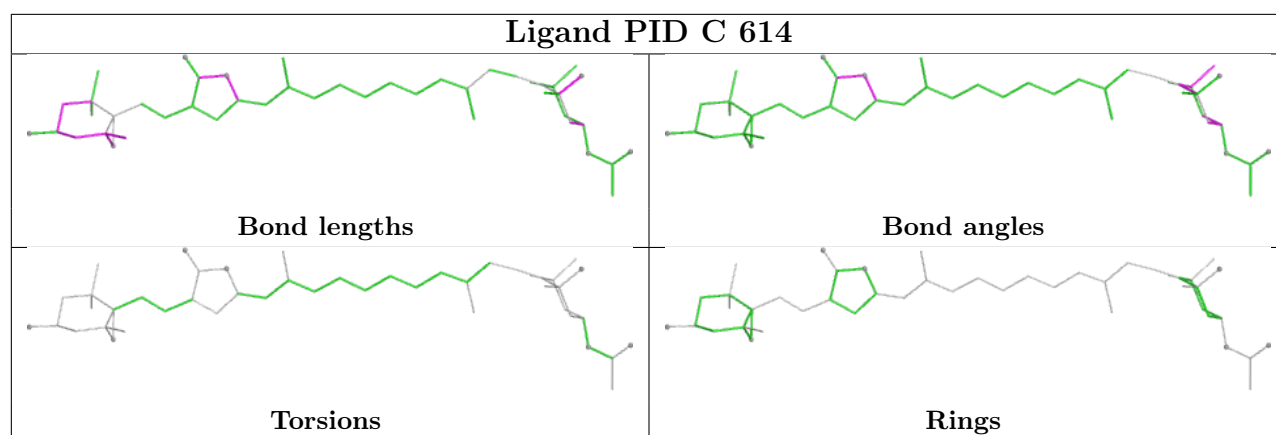
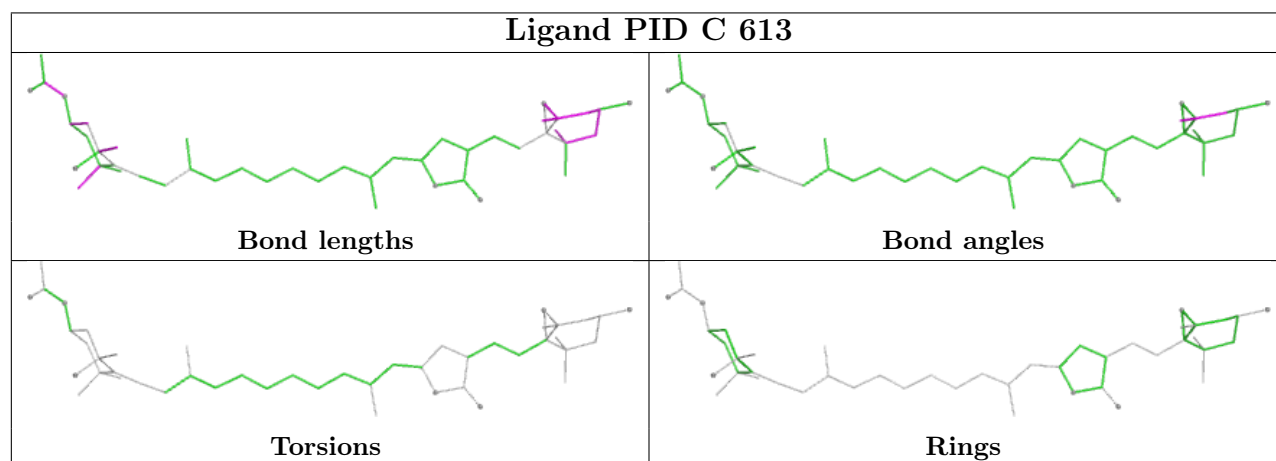
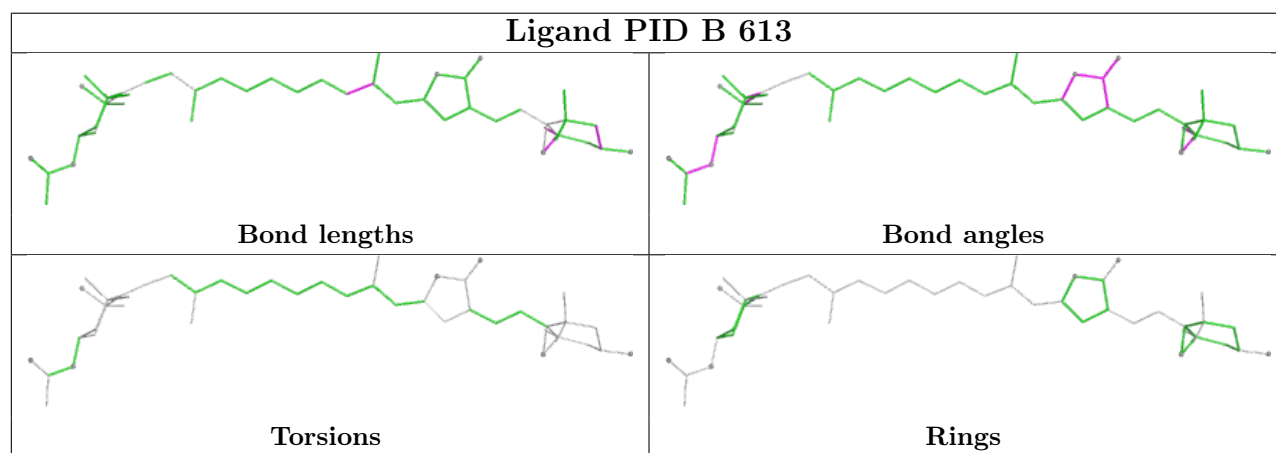


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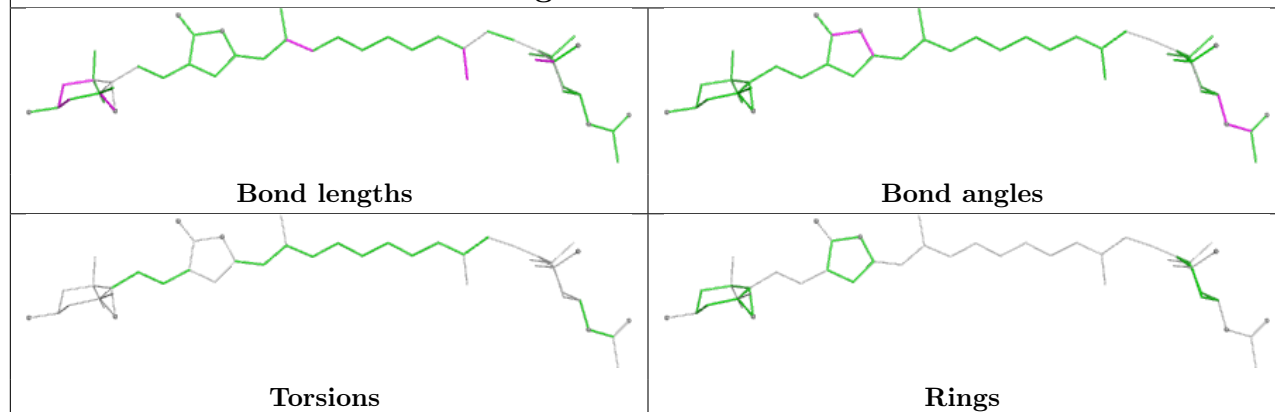


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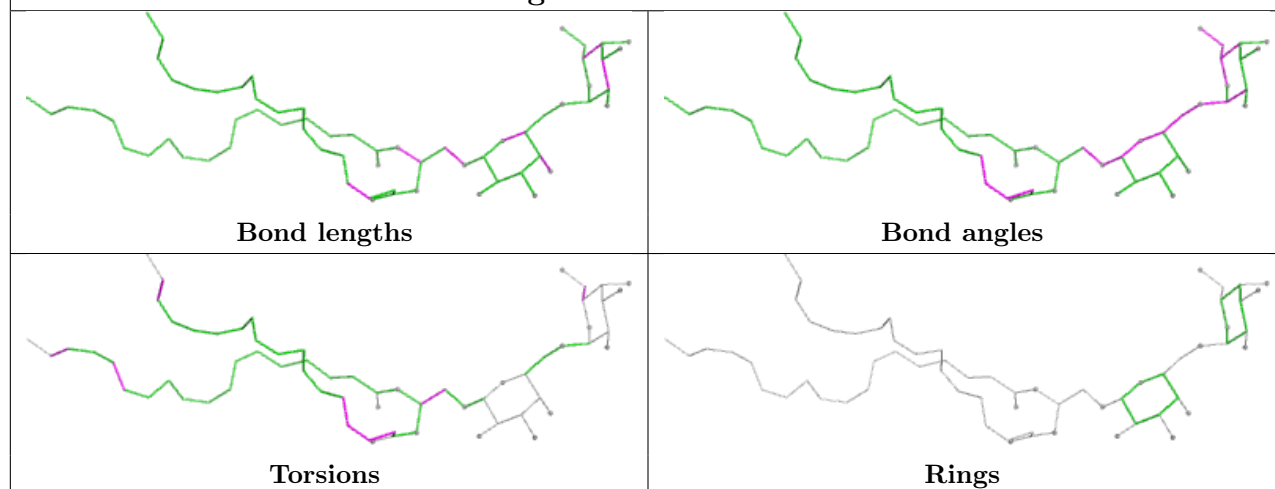




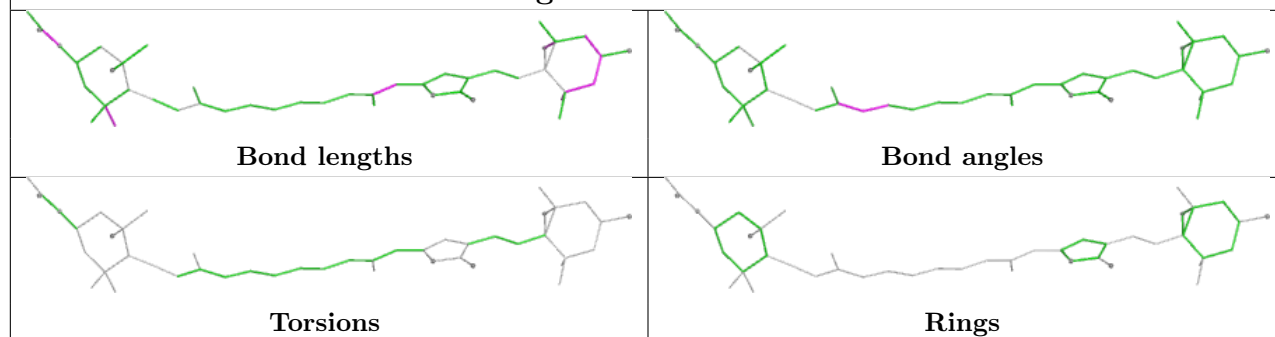
Ligand PID D 613



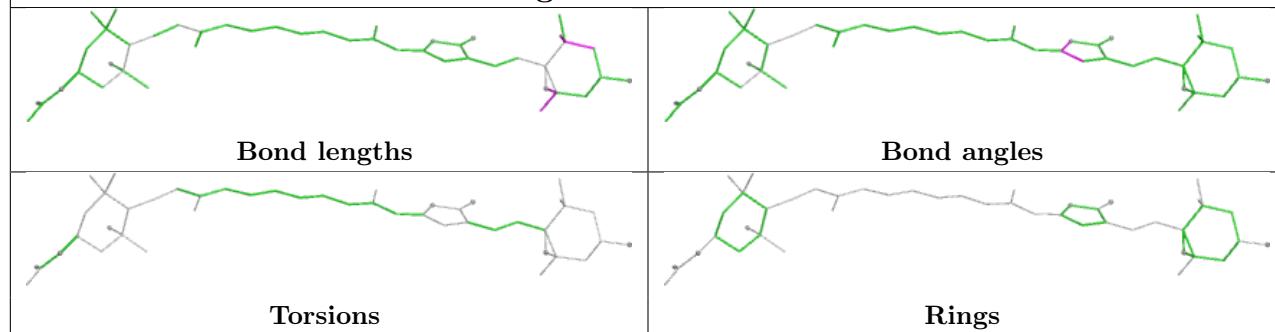
Ligand W4O B 615

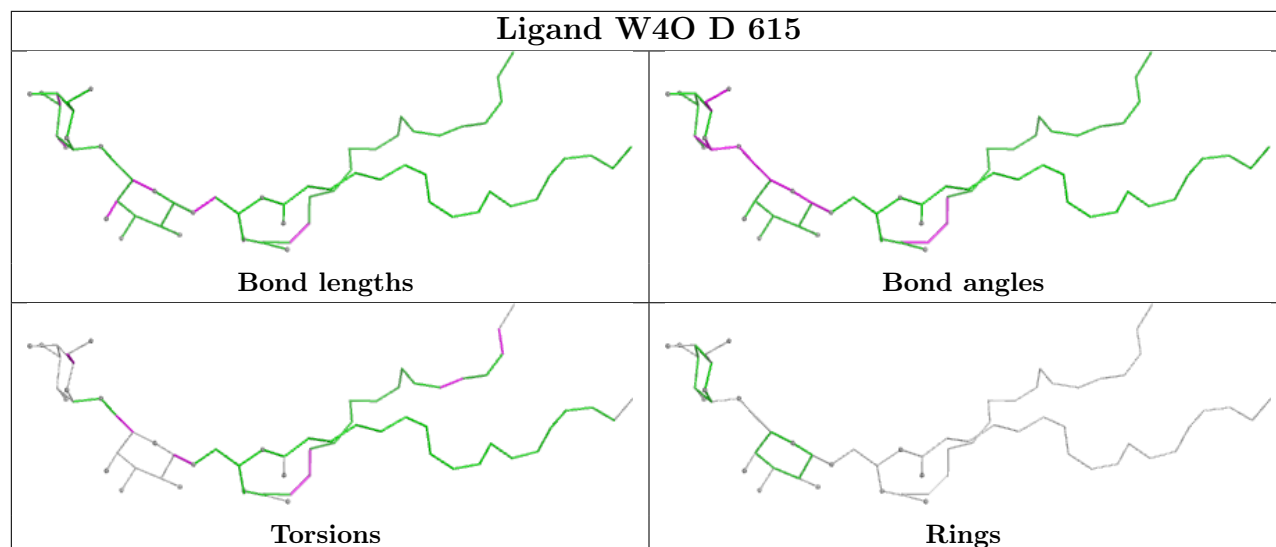
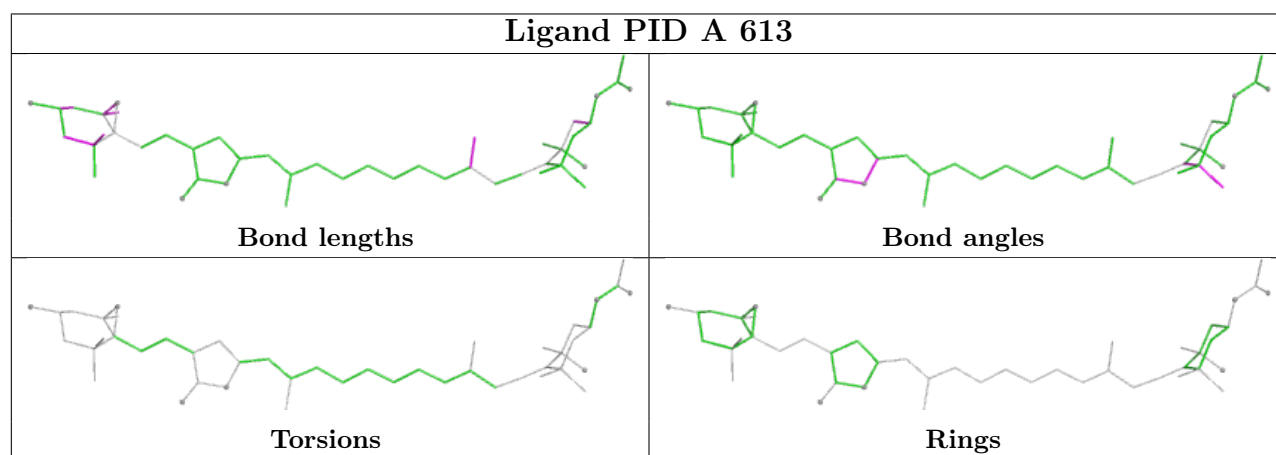
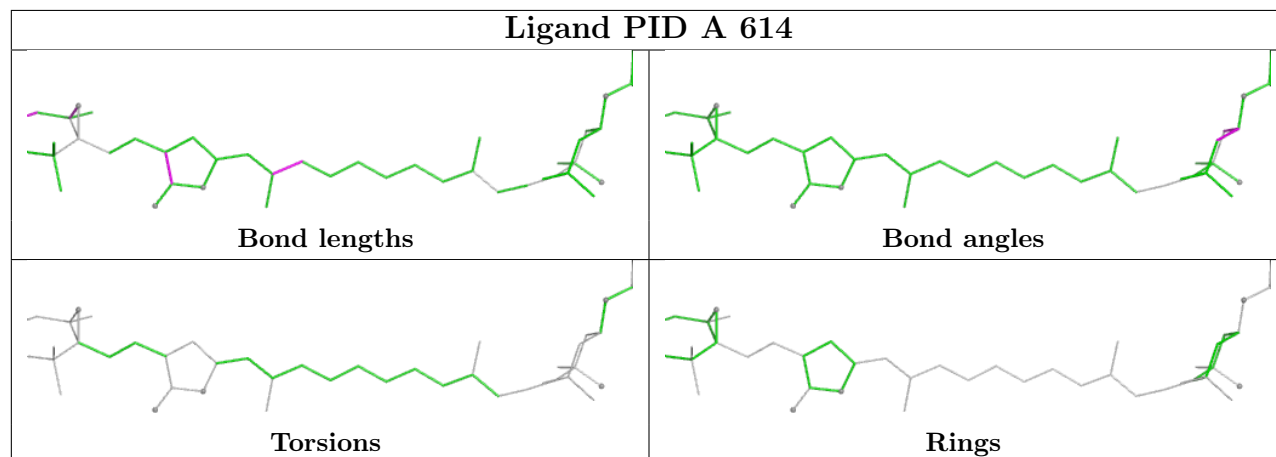


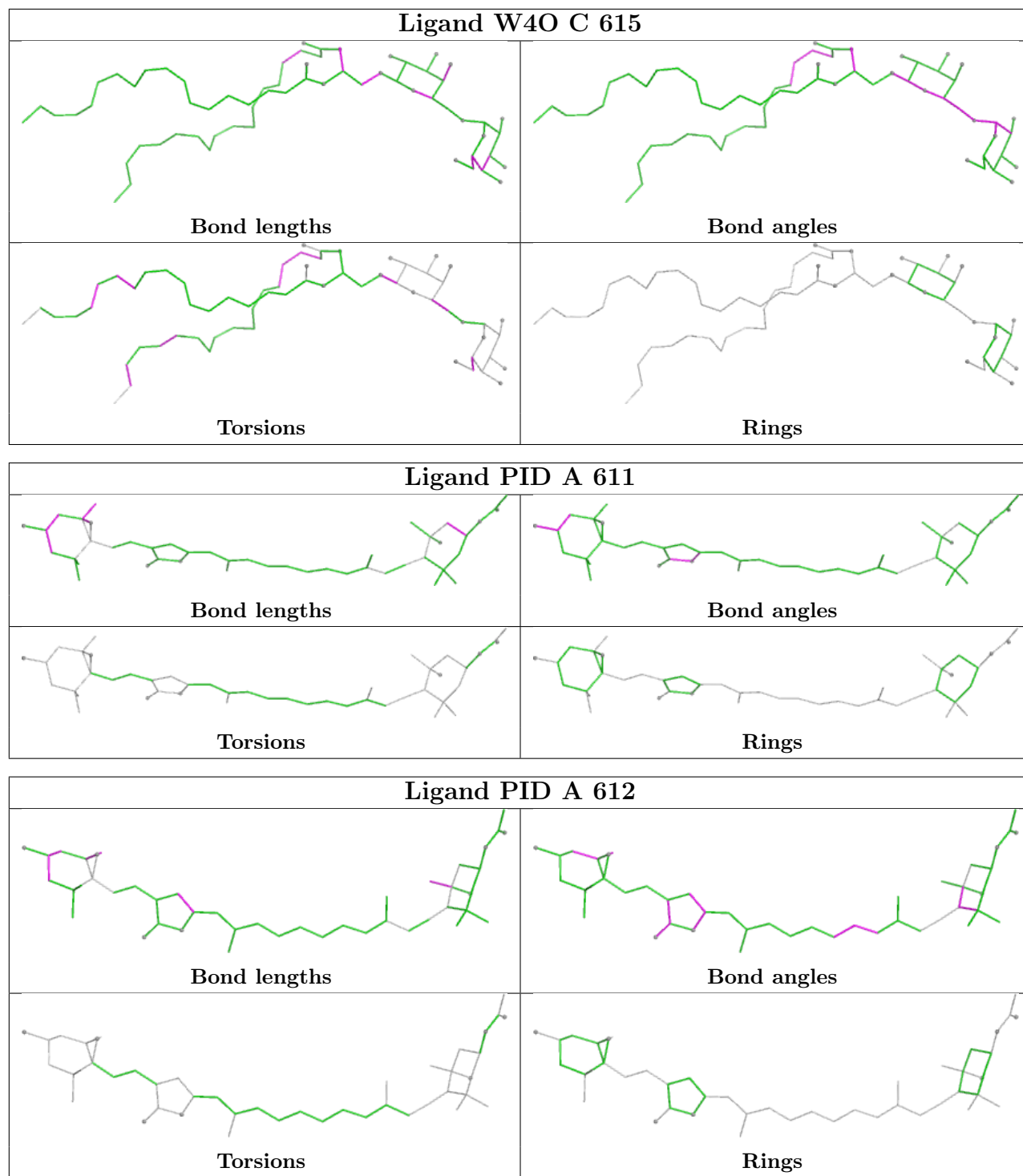
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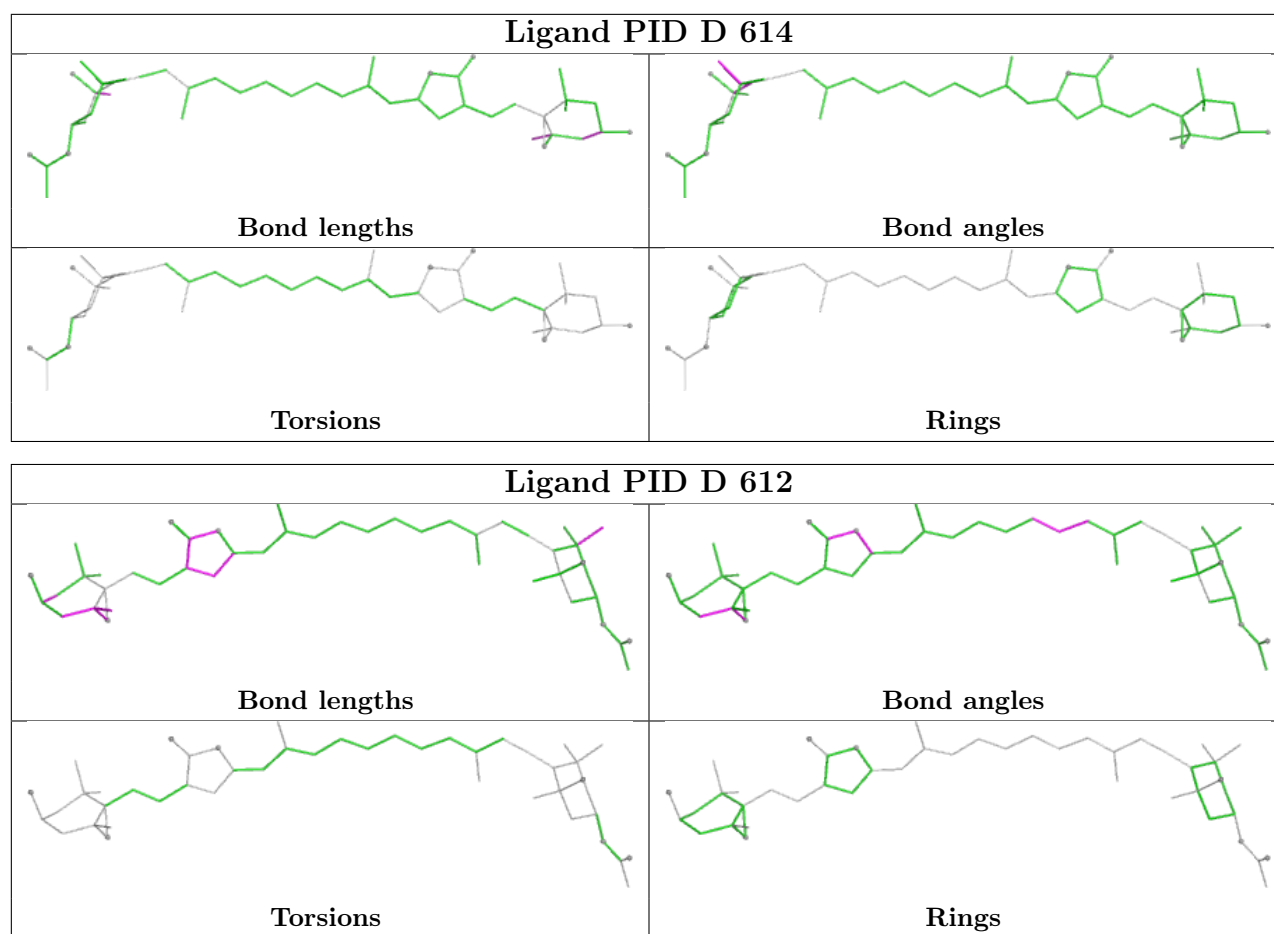


Ligand PID B 611









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	148/149 (99%)	-1.35	0 100 100	6, 10, 17, 24	1 (0%)
1	C	148/149 (99%)	-1.20	0 100 100	7, 13, 20, 27	2 (1%)
2	B	148/149 (99%)	-1.32	0 100 100	5, 10, 17, 25	8 (5%)
2	D	148/149 (99%)	-1.18	0 100 100	7, 14, 21, 28	4 (2%)
All	All	592/596 (99%)	-1.26	0 100 100	5, 12, 20, 28	15 (2%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HYP	A	32	8/9	1.00	0.02	10,11,13,13	0
1	HYP	C	32	8/9	1.00	0.02	10,12,14,14	0
2	HYP	B	32	8/9	1.00	0.01	8,10,10,11	0
2	HYP	D	32	8/9	1.00	0.02	11,12,14,14	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

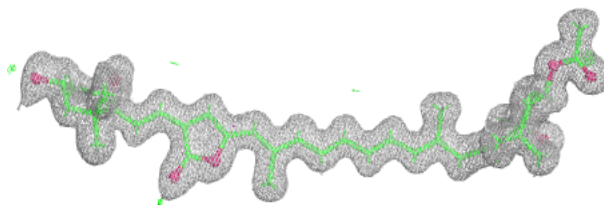
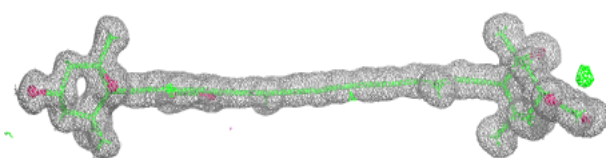
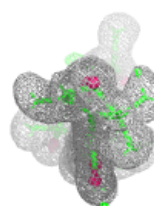
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PID	D	613	46/46	0.99	0.03	8,12,23,24	0
5	W4O	A	615	66/66	0.99	0.04	9,13,41,49	0
5	W4O	C	615	66/66	0.99	0.04	10,14,46,57	0
5	W4O	D	615	66/66	0.99	0.03	9,14,34,42	0
7	PO4	A	608	5/5	0.99	0.04	13,15,18,18	0
8	CL	B	608	1/1	0.99	0.04	33,33,33,33	0
4	PID	A	613	46/46	1.00	0.02	7,9,14,15	0
4	PID	A	614	46/46	1.00	0.02	6,8,10,12	0
4	PID	B	611	46/46	1.00	0.02	6,9,12,14	0
4	PID	B	612	46/46	1.00	0.02	6,8,12,15	0
4	PID	B	613	46/46	1.00	0.02	6,9,17,19	0
4	PID	B	614	46/46	1.00	0.02	7,8,10,12	0
4	PID	C	611	46/46	1.00	0.02	8,11,15,18	0
4	PID	C	612	46/46	1.00	0.02	7,10,13,14	0
4	PID	C	613	46/46	1.00	0.02	7,10,19,21	0
4	PID	C	614	46/46	1.00	0.02	8,11,13,16	0
4	PID	D	611	46/46	1.00	0.02	8,11,18,21	0
4	PID	D	612	46/46	1.00	0.02	7,10,15,17	0
3	CLA	A	601	65/65	1.00	0.02	6,8,14,17	0
4	PID	D	614	46/46	1.00	0.02	8,11,18,22	0
3	CLA	B	601	65/65	1.00	0.02	6,8,11,13	0
5	W4O	B	615	66/66	1.00	0.03	8,11,29,36	0
3	CLA	C	601	65/65	1.00	0.02	8,10,14,17	0
3	CLA	D	601	65/65	1.00	0.02	7,11,16,17	0
6	K	A	607	1/1	1.00	0.09	17,17,17,17	0
6	K	B	607	1/1	1.00	0.12	13,13,13,13	0
4	PID	A	611	46/46	1.00	0.02	6,8,14,17	0
4	PID	A	612	46/46	1.00	0.01	6,8,12,12	0

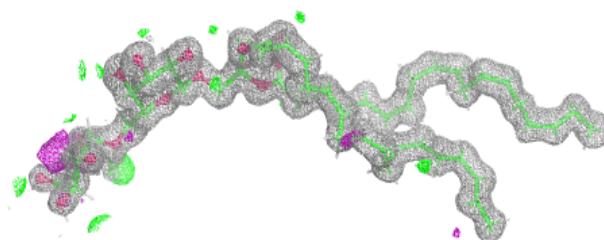
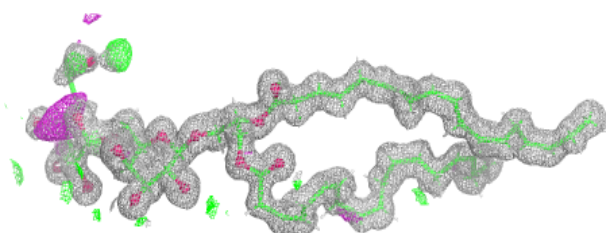
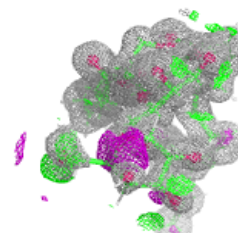
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PID D 613:

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

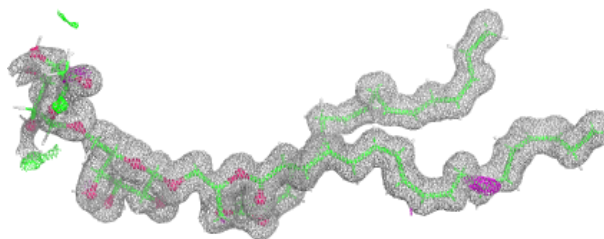
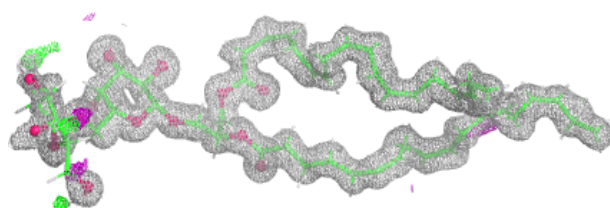
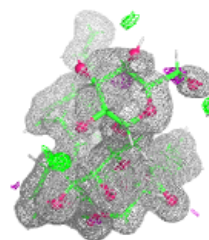
**Electron density around W4O A 615:**

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

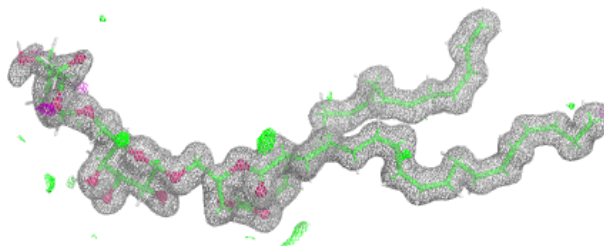
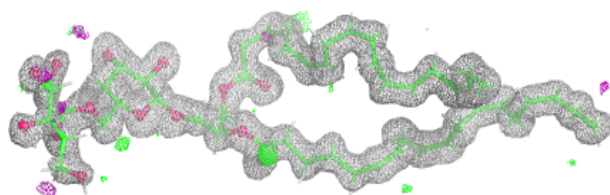
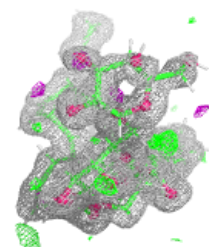


Electron density around W4O C 615:

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

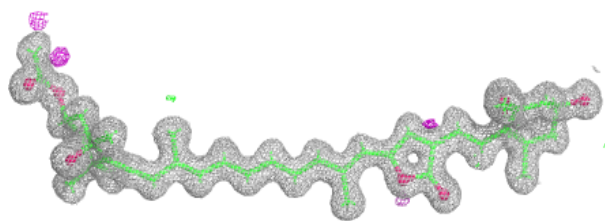
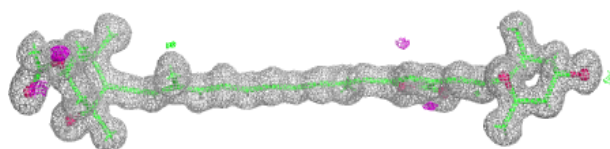
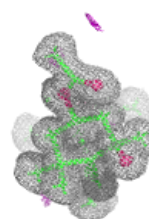
**Electron density around W4O D 615:**

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

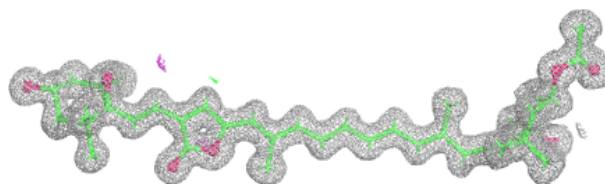
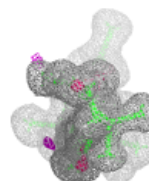


Electron density around PID A 613:

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

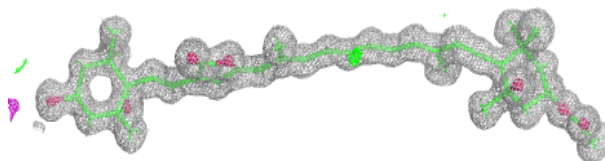
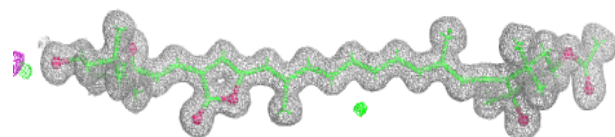
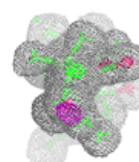
**Electron density around PID A 614:**

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

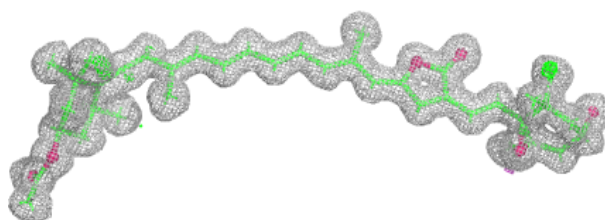
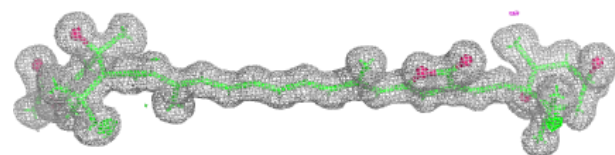
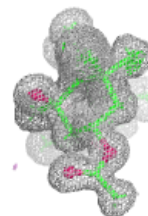


Electron density around PID B 611:

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

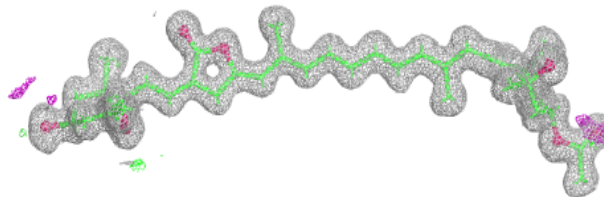
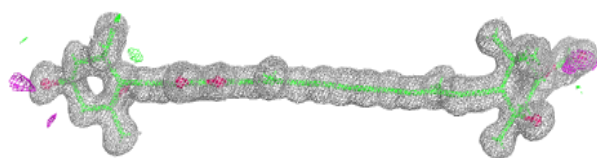
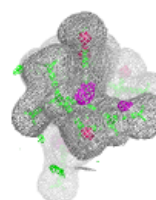
**Electron density around PID B 612:**

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

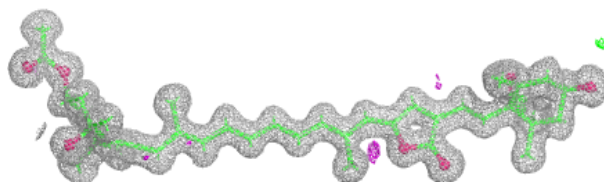
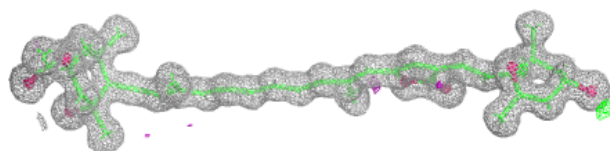
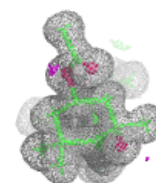


Electron density around PID B 613:

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

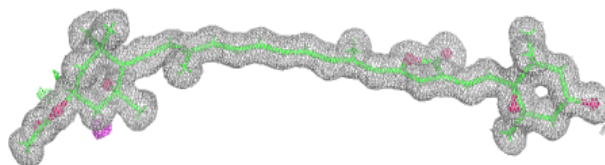
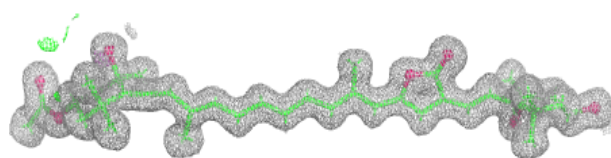
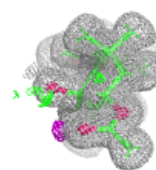
**Electron density around PID B 614:**

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

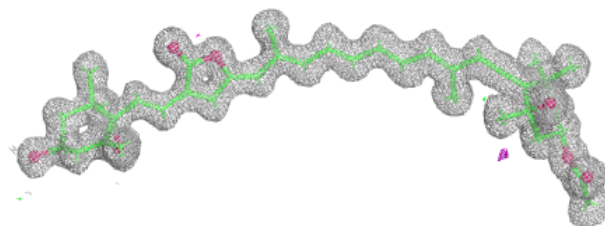
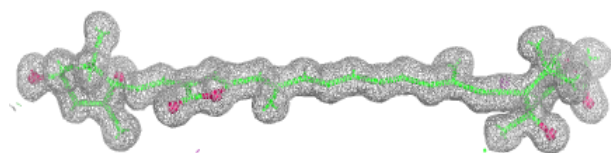
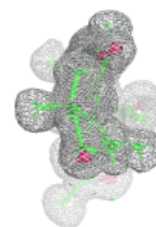


Electron density around PID C 611:

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

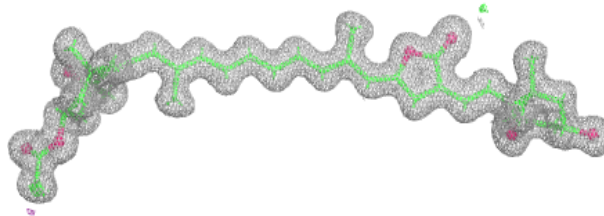
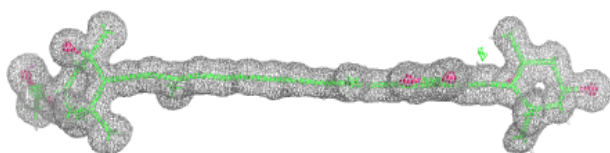
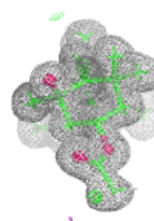
**Electron density around PID C 612:**

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

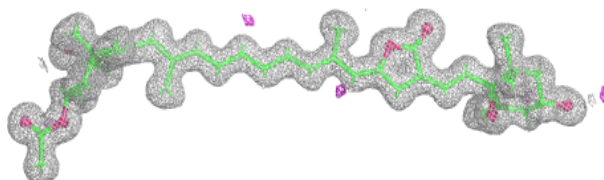
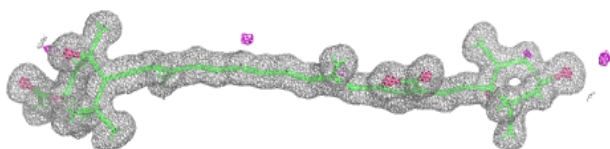
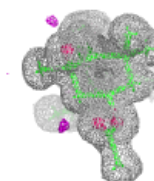


Electron density around PID C 613:

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

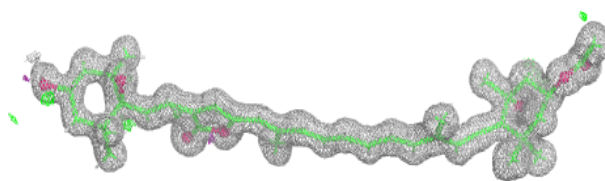
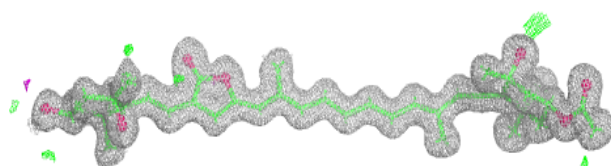
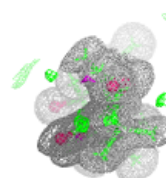
**Electron density around PID C 614:**

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

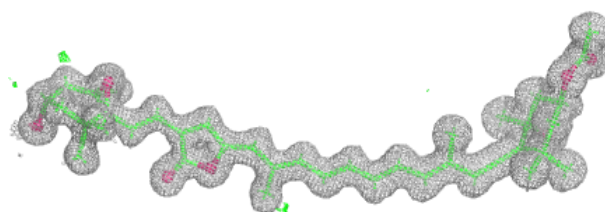
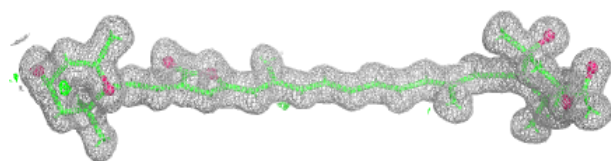
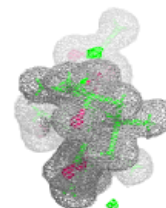


Electron density around PID D 611:

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

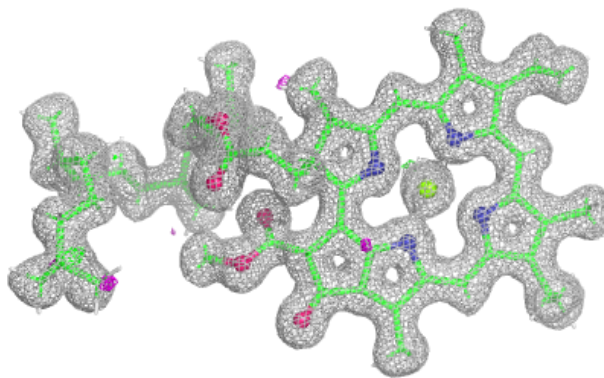
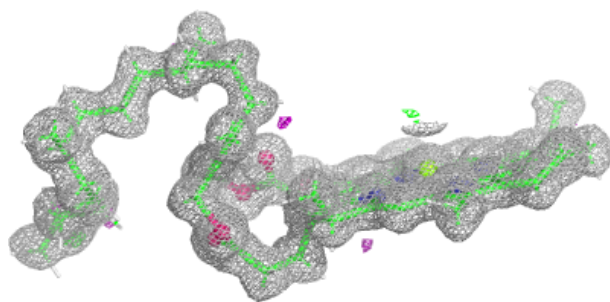
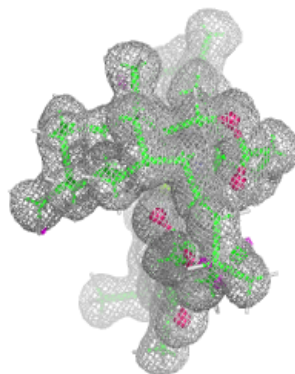
**Electron density around PID D 612:**

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

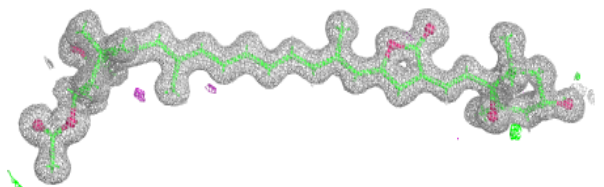
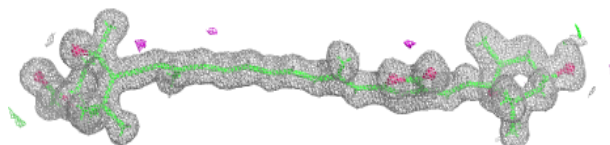
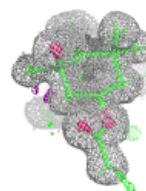


Electron density around CLA A 601:

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

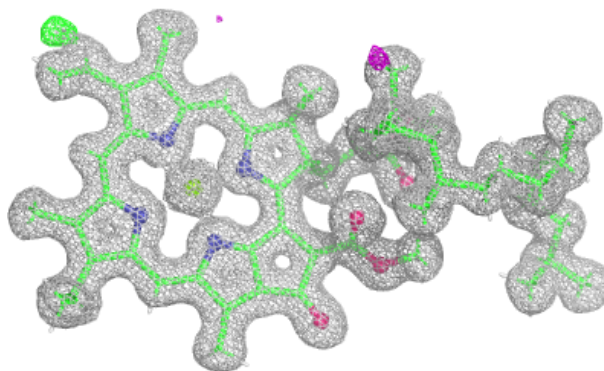
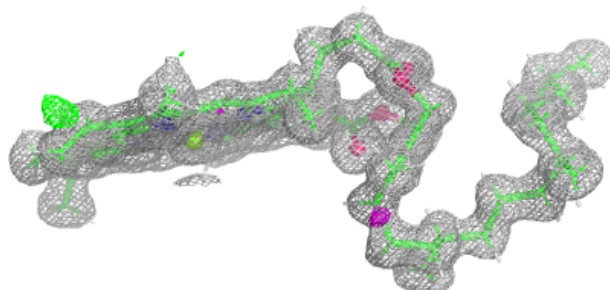
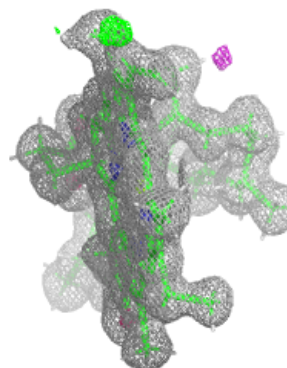
**Electron density around PID D 614:**

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

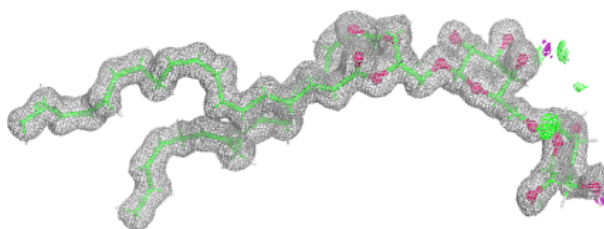
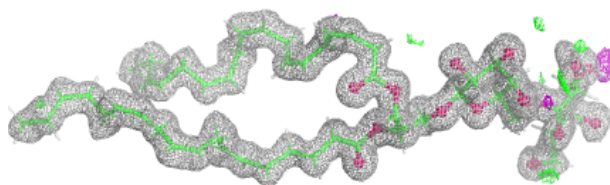
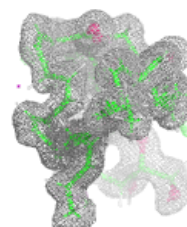


Electron density around CLA B 601:

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

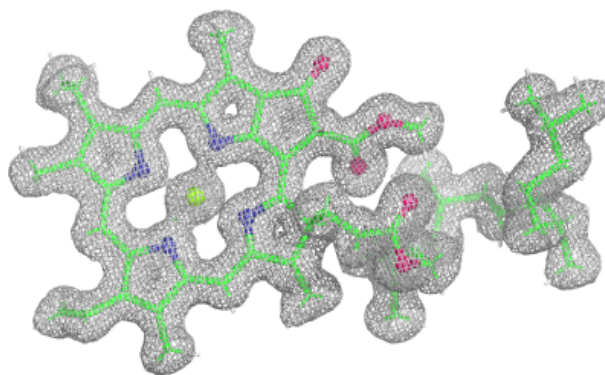
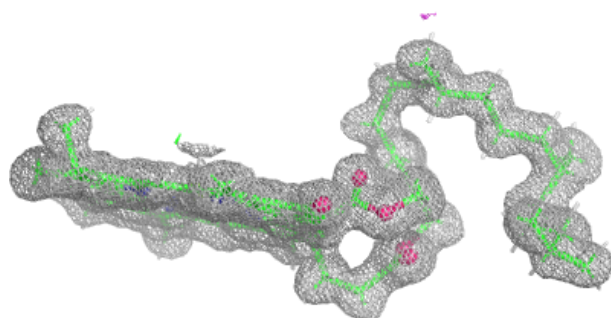
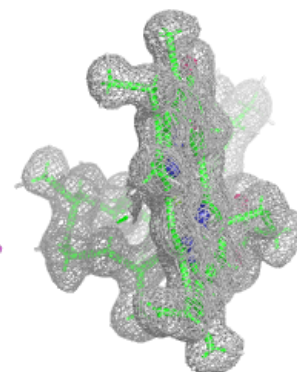
**Electron density around W4O B 615:**

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

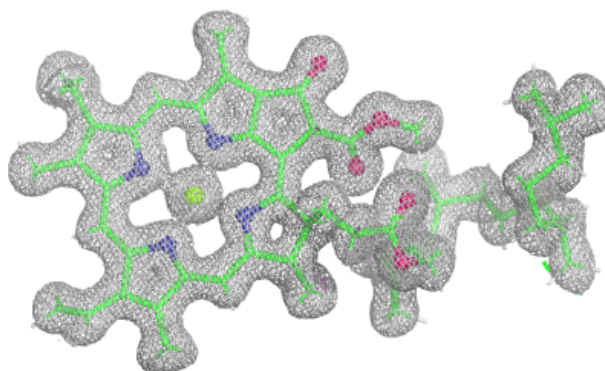
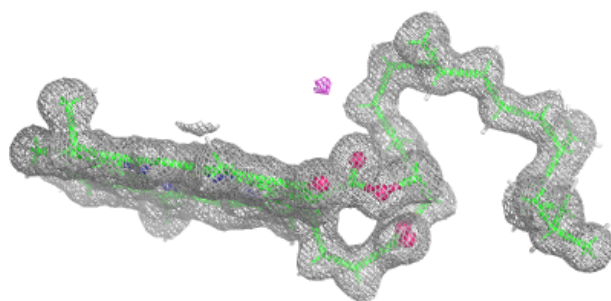
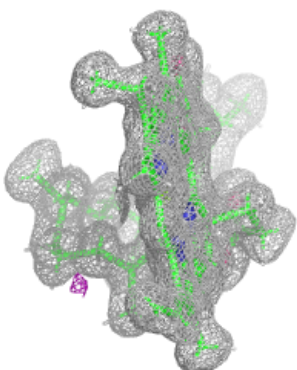


Electron density around CLA C 601:

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

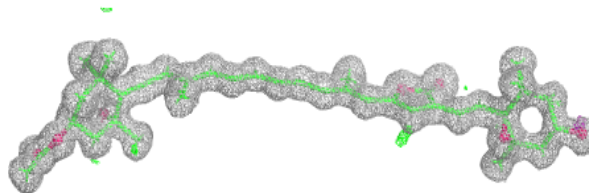
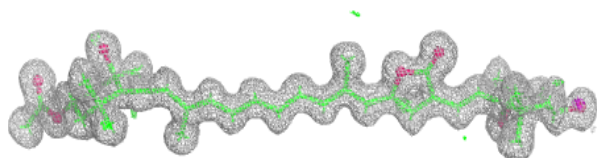
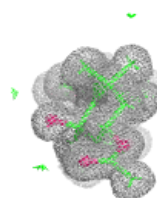
**Electron density around CLA D 601:**

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

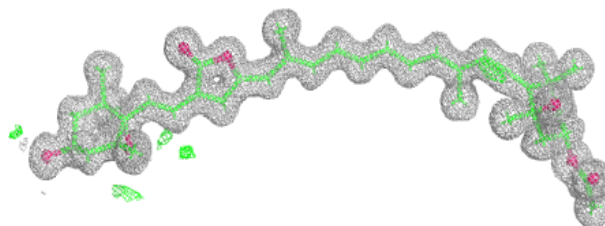
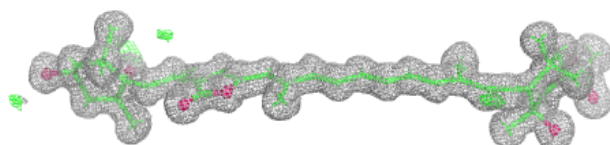
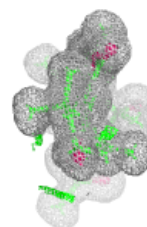


Electron density around PID A 611:

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

**Electron density around PID A 612:**

$2mF_o-DF_c$ (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.