Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2026 – 04:15 am BST

PDB ID	:	2X21 / pdb_00002x21
Title	:	Structure of Peridinin-Chlorophyll-Protein reconstituted with BChl-a
Authors	:	Schulte, T.; Hiller, R.G.; Hofmann, E.
Deposited on	:	2010-01-09
Resolution	:	1.75 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:

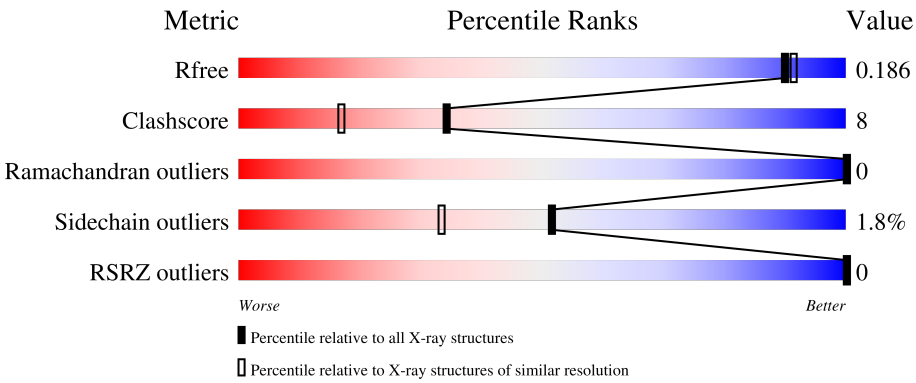
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	151	85% 14% •

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
6	CL	M	1163	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	M	1164	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 1725 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

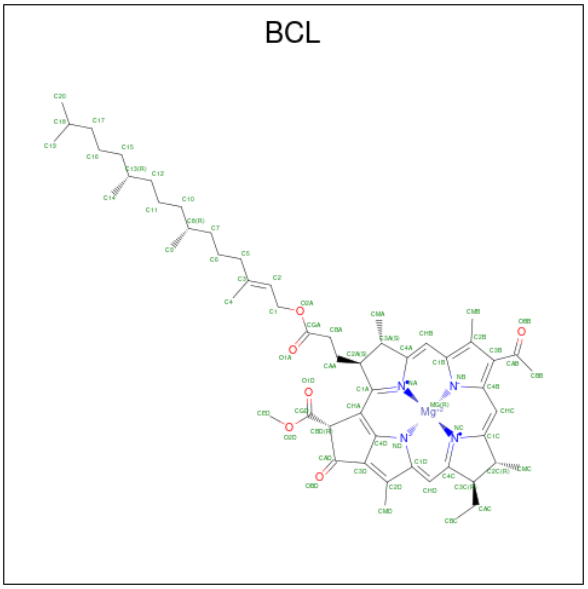
- Molecule 1 is a protein called PERIDININ-CHLOROPHYLL A-BINDING PROTEIN, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	151	1138	720	190	223	5	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	87	SER	ASN	conflict	UNP P80484
M	128	ASN	SER	conflict	UNP P80484

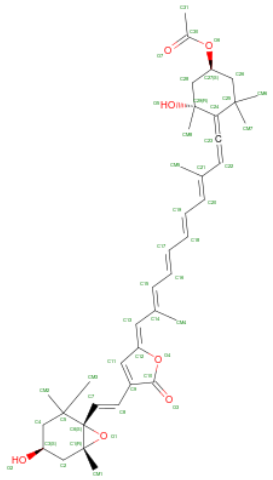
- Molecule 2 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
2	M	1	66	55	1	4	6	0	0

- Molecule 3 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$).

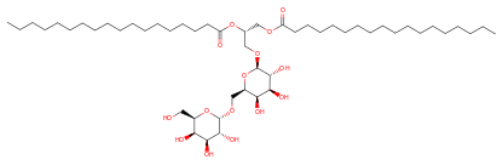
PID



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	M	1	50	42	8	0	1
			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

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

DGD



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	M	1	69	53	16	0	1

- Molecule 5 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
5	M	7	8	8	0	1

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	M	7	7	7	0	0

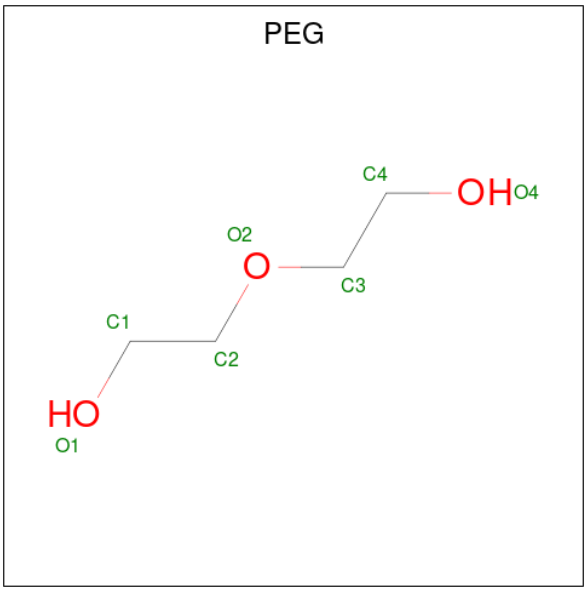
- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	M	4	4	4	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
8	M	1	1	1	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	M	1	7	4	3	0	0

- Molecule 10 is water.

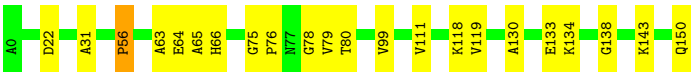
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	M	237	237	237	0	0

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 A-BINDING PROTEIN, CHLOROPLASTIC

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	68.49Å 81.81Å 74.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.01 – 1.75 43.01 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.01-1.75) 99.7 (43.01-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.146 , 0.186 0.146 , 0.186	Depositor DCC
R_{free} test set	1078 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1725	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% 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: PEG, BCL, K, DGD, CL, CD, PID, NA

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	1.74	15/1161 (1.3%)	1.26	2/1568 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	63	ALA	CA-CB	8.05	1.65	1.53
1	M	79	VAL	CA-CB	7.52	1.63	1.54
1	M	119	VAL	CA-C	7.11	1.59	1.52
1	M	130	ALA	CA-CB	6.90	1.64	1.53
1	M	65	ALA	CA-CB	6.55	1.63	1.53
1	M	150	GLN	CD-NE2	6.23	1.46	1.33
1	M	99	VAL	N-CA	5.84	1.51	1.46
1	M	22	ASP	CA-C	5.67	1.59	1.52
1	M	111	VAL	CA-CB	5.56	1.61	1.54
1	M	31	ALA	CA-CB	5.53	1.61	1.53
1	M	80	THR	CA-CB	5.45	1.61	1.53
1	M	138	GLY	N-CA	5.23	1.52	1.45
1	M	56	PRO	CG-CD	5.15	1.68	1.50
1	M	78	GLY	N-CA	5.10	1.52	1.45
1	M	118	LYS	CE-NZ	5.05	1.64	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	75	GLY	CA-C-N	-6.65	113.06	120.45
1	M	75	GLY	C-N-CA	-6.65	113.06	120.45

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	1138	0	1144	9	0
2	M	66	0	73	4	0
3	M	188	0	180	3	0
4	M	69	0	10	0	0
5	M	8	0	0	0	0
6	M	7	0	0	7	0
7	M	4	0	0	1	0
8	M	1	0	0	1	0
9	M	7	0	10	1	0
10	M	237	0	0	7	1
All	All	1725	0	1417	19	1

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

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1163:CL:CL	7:M:1168:K:K	1.66	1.39
6:M:1164:CL:CL	8:M:1169:NA:NA	1.68	1.04
1:M:64[A]:GLU:OE1	10:M:2129:HOH:O	1.85	0.94
6:M:1164:CL:CL	10:M:2116:HOH:O	2.26	0.90
1:M:134:LYS:HE3	10:M:2020:HOH:O	1.77	0.85
6:M:1160:CL:CL	10:M:2014:HOH:O	2.45	0.71
1:M:133:GLU:OE2	6:M:1163:CL:CL	2.51	0.65
9:M:1170:PEG:H42	10:M:2157:HOH:O	2.05	0.56
1:M:133:GLU:CD	6:M:1163:CL:CL	2.88	0.54
2:M:601:BCL:H202	2:M:601:BCL:CED	2.38	0.54
1:M:133:GLU:OE1	6:M:1163:CL:CL	2.63	0.52
1:M:76:PRO:O	10:M:2141:HOH:O	2.19	0.52
1:M:64[A]:GLU:CD	10:M:2128:HOH:O	2.59	0.46
1:M:66:HIS:CG	2:M:601:BCL:HMC3	2.54	0.43
2:M:601:BCL:H202	2:M:601:BCL:HED1	2.01	0.42
1:M:66:HIS:CD2	2:M:601:BCL:CHC	3.03	0.41

All (1) 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)
10:M:2001:HOH:O	10:M:2142:HOH:O[8_555]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	152/151 (101%)	151 (99%)	1 (1%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	117/114 (103%)	115 (98%)	2 (2%)	53 36

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	56	PRO
1	M	143	LYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 20 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PID	M	611[A]	-	41,49,49	1.80	13 (31%)	49,76,76	3.40	21 (42%)
3	PID	M	611[B]	-	41,49,49	1.73	11 (26%)	49,76,76	3.35	21 (42%)
3	PID	M	614	-	41,49,49	1.54	10 (24%)	49,76,76	3.16	18 (36%)
3	PID	M	613	-	41,49,49	1.61	10 (24%)	49,76,76	3.51	21 (42%)
4	DGD	M	615[B]	-	67,67,67	1.05	4 (5%)	81,81,81	1.41	9 (11%)
9	PEG	M	1170	-	6,6,6	1.02	0	5,5,5	0.65	0
4	DGD	M	615[A]	-	67,67,67	1.05	4 (5%)	81,81,81	1.41	9 (11%)
2	BCL	M	601	10	69,74,74	1.75	12 (17%)	83,115,115	1.83	16 (19%)
3	PID	M	612	-	41,49,49	1.61	9 (21%)	49,76,76	3.30	21 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PID	M	611[A]	-	-	0/24/93/93	0/4/4/4
3	PID	M	611[B]	-	-	0/24/93/93	0/4/4/4
3	PID	M	614	-	-	0/24/93/93	0/4/4/4
3	PID	M	613	-	-	0/24/93/93	0/4/4/4
4	DGD	M	615[B]	-	-	27/55/95/95	0/2/2/2
9	PEG	M	1170	-	-	2/4/4/4	-
4	DGD	M	615[A]	-	-	28/55/95/95	0/2/2/2
2	BCL	M	601	10	-	3/41/137/137	-
3	PID	M	612	-	-	0/24/93/93	0/4/4/4

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	601	BCL	OBD-CAD	5.45	1.31	1.22
2	M	601	BCL	CHD-C1D	5.25	1.48	1.38
3	M	611[A]	PID	C13-C12	4.79	1.49	1.36
3	M	611[B]	PID	C13-C12	4.79	1.49	1.36
2	M	601	BCL	CHB-C1B	4.44	1.49	1.39
4	M	615[A]	DGD	O2G-C1B	4.23	1.46	1.34
4	M	615[B]	DGD	O2G-C1B	4.23	1.46	1.34
3	M	613	PID	C26-C27	3.97	1.59	1.51
3	M	613	PID	C13-C12	3.91	1.47	1.36
3	M	612	PID	C13-C12	3.88	1.47	1.36
2	M	601	BCL	CMB-C2B	3.85	1.59	1.50
2	M	601	BCL	C3D-C4D	-3.83	1.35	1.44
3	M	611[A]	PID	O6-C30	3.71	1.43	1.35
3	M	611[B]	PID	O6-C30	3.71	1.43	1.35
3	M	612	PID	C2-C1	3.70	1.57	1.52
4	M	615[A]	DGD	O5D-C1E	3.58	1.46	1.40
4	M	615[B]	DGD	O5D-C1E	3.58	1.46	1.40
2	M	601	BCL	CHC-C4B	3.42	1.47	1.39
3	M	612	PID	O3-C10	3.39	1.28	1.21
2	M	601	BCL	O2D-CGD	3.28	1.41	1.33
2	M	601	BCL	O2A-CGA	3.27	1.42	1.33
3	M	613	PID	O6-C30	3.07	1.42	1.35
3	M	614	PID	O4-C12	-3.05	1.32	1.38
3	M	614	PID	C13-C12	3.04	1.44	1.36
3	M	613	PID	O3-C10	2.93	1.27	1.21
3	M	611[A]	PID	O3-C10	2.86	1.27	1.21
3	M	611[B]	PID	O3-C10	2.86	1.27	1.21
3	M	614	PID	O3-C10	2.84	1.27	1.21
3	M	614	PID	C2-C1	2.77	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	611[A]	PID	O4-C10	-2.74	1.33	1.39
3	M	611[B]	PID	O4-C10	-2.74	1.33	1.39
3	M	612	PID	O6-C30	2.70	1.41	1.35
2	M	601	BCL	OBB-CAB	2.66	1.29	1.23
3	M	611[A]	PID	C15-C14	2.55	1.39	1.35
3	M	611[B]	PID	C15-C14	2.55	1.39	1.35
2	M	601	BCL	CAC-C3C	2.55	1.59	1.54
3	M	613	PID	CM8-C29	-2.52	1.48	1.52
3	M	613	PID	C2-C1	2.51	1.55	1.52
3	M	614	PID	C23-C22	-2.49	1.27	1.32
3	M	612	PID	C13-C14	2.44	1.50	1.45
3	M	611[A]	PID	C19-C20	2.41	1.50	1.43
3	M	611[B]	PID	C19-C20	2.41	1.50	1.43
4	M	615[A]	DGD	O1G-C1A	2.40	1.40	1.33
4	M	615[B]	DGD	O1G-C1A	2.40	1.40	1.33
3	M	611[A]	PID	C28-C27	2.40	1.56	1.51
3	M	611[B]	PID	C28-C27	2.40	1.56	1.51
3	M	614	PID	C15-C14	2.36	1.38	1.35
3	M	611[A]	PID	C17-C16	2.33	1.42	1.36
3	M	611[B]	PID	C17-C16	2.33	1.42	1.36
3	M	611[A]	PID	C19-C18	2.30	1.42	1.36
3	M	611[B]	PID	C19-C18	2.30	1.42	1.36
3	M	614	PID	CM3-C5	2.29	1.58	1.53
3	M	612	PID	C8-C9	2.25	1.51	1.46
3	M	613	PID	C8-C9	2.24	1.51	1.46
3	M	613	PID	C18-C17	2.23	1.50	1.44
3	M	614	PID	CM8-C29	2.21	1.56	1.52
3	M	614	PID	O6-C30	2.19	1.40	1.35
3	M	614	PID	C20-C21	2.17	1.38	1.35
3	M	611[A]	PID	C20-C21	2.17	1.38	1.35
3	M	611[B]	PID	C20-C21	2.17	1.38	1.35
2	M	601	BCL	C6-C5	2.16	1.60	1.52
3	M	613	PID	CM5-C21	2.10	1.55	1.50
2	M	601	BCL	O1A-CGA	2.09	1.28	1.22
3	M	611[A]	PID	C2-C1	2.09	1.55	1.52
3	M	611[A]	PID	C4-C5	-2.07	1.51	1.54
3	M	612	PID	C2-C3	2.06	1.55	1.52
3	M	611[A]	PID	C18-C17	2.04	1.50	1.44
3	M	611[B]	PID	C18-C17	2.04	1.50	1.44
3	M	613	PID	C19-C20	2.04	1.49	1.43
3	M	612	PID	C11-C12	-2.04	1.40	1.44
3	M	612	PID	CM8-C29	2.02	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	615[A]	DGD	O6D-C1D	2.00	1.46	1.41
4	M	615[B]	DGD	O6D-C1D	2.00	1.46	1.41

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	613	PID	O4-C12-C11	14.51	116.15	107.36
3	M	612	PID	O4-C12-C11	14.45	116.12	107.36
3	M	611[A]	PID	O4-C12-C11	14.25	116.00	107.36
3	M	611[B]	PID	O4-C12-C11	14.25	116.00	107.36
3	M	614	PID	O4-C12-C11	13.77	115.71	107.36
3	M	613	PID	C12-O4-C10	-10.65	102.11	107.65
2	M	601	BCL	C2B-C1B-NB	8.12	115.67	110.23
3	M	611[A]	PID	C12-O4-C10	-7.79	103.60	107.65
3	M	611[B]	PID	C12-O4-C10	-7.79	103.60	107.65
3	M	612	PID	CM7-C25-C24	6.78	116.54	110.47
3	M	614	PID	C12-O4-C10	-6.55	104.24	107.65
3	M	614	PID	O1-C1-C2	5.81	117.75	113.38
3	M	611[A]	PID	CM3-C5-C4	-5.69	99.10	108.98
3	M	611[A]	PID	O3-C10-C9	-5.62	124.34	130.74
3	M	611[B]	PID	O3-C10-C9	-5.62	124.34	130.74
3	M	611[B]	PID	O1-C1-C2	5.60	117.59	113.38
3	M	613	PID	C6-C7-C8	-5.48	114.41	125.99
3	M	612	PID	C12-O4-C10	-5.44	104.82	107.65
4	M	615[A]	DGD	O2E-C2E-C3E	-5.36	97.97	110.35
4	M	615[B]	DGD	O2E-C2E-C3E	-5.36	97.97	110.35
3	M	611[A]	PID	O1-C1-CM1	5.23	121.32	115.06
3	M	611[B]	PID	O1-C1-CM1	5.23	121.32	115.06
3	M	614	PID	CM1-C1-C2	5.10	120.02	114.28
3	M	612	PID	O1-C1-C2	5.09	117.21	113.38
3	M	611[A]	PID	CM2-C5-C4	5.03	117.73	108.98
3	M	613	PID	O1-C1-CM1	4.97	121.02	115.06
2	M	601	BCL	CHB-C1B-NB	-4.86	119.11	124.26
3	M	612	PID	O1-C1-CM1	4.83	120.84	115.06
3	M	611[A]	PID	C6-C7-C8	-4.82	115.81	125.99
3	M	611[B]	PID	C6-C7-C8	-4.82	115.81	125.99
3	M	612	PID	C28-C27-C26	4.79	118.23	109.88
3	M	611[A]	PID	C18-C19-C20	-4.73	113.78	123.47
3	M	611[B]	PID	C18-C19-C20	-4.73	113.78	123.47
3	M	613	PID	C19-C20-C21	-4.51	120.87	127.31
3	M	613	PID	C18-C17-C16	-4.50	114.80	124.81
3	M	612	PID	C17-C16-C15	-4.49	114.28	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	601	BCL	CHD-C1D-ND	-4.46	120.35	124.45
3	M	613	PID	O4-C10-C9	4.45	111.76	108.04
3	M	611[A]	PID	C11-C12-C13	-4.38	118.66	128.34
3	M	611[B]	PID	C11-C12-C13	-4.38	118.66	128.34
3	M	614	PID	O3-C10-C9	-4.26	125.89	130.74
3	M	612	PID	C1-C2-C3	-4.25	104.35	112.75
3	M	612	PID	CM3-C5-CM2	4.17	113.51	107.37
3	M	614	PID	C18-C17-C16	-4.15	115.58	124.81
4	M	615[A]	DGD	O1G-C1A-O1A	-4.03	113.43	123.59
4	M	615[B]	DGD	O1G-C1A-O1A	-4.03	113.43	123.59
3	M	613	PID	CM6-C25-C24	4.02	114.07	110.47
3	M	611[B]	PID	O2-C3-C4	-4.01	101.83	109.80
3	M	611[A]	PID	O1-C1-C2	3.99	116.38	113.38
3	M	613	PID	CM1-C1-C6	-3.87	115.77	122.26
2	M	601	BCL	C4-C3-C5	3.85	121.75	115.27
3	M	614	PID	CM1-C1-C6	-3.85	115.81	122.26
3	M	614	PID	O4-C10-C9	3.84	111.25	108.04
3	M	612	PID	C11-C12-C13	-3.81	119.91	128.34
3	M	614	PID	C16-C15-C14	-3.80	121.88	127.31
4	M	615[A]	DGD	O3G-C1D-C2D	-3.67	102.58	108.30
4	M	615[B]	DGD	O3G-C1D-C2D	-3.67	102.58	108.30
3	M	611[A]	PID	C18-C17-C16	-3.62	116.74	124.81
3	M	611[B]	PID	C18-C17-C16	-3.62	116.74	124.81
3	M	612	PID	CM3-C5-C4	-3.59	102.74	108.98
3	M	612	PID	C8-C9-C11	-3.57	120.52	127.37
2	M	601	BCL	C4D-C3D-CAD	-3.53	103.93	108.10
2	M	601	BCL	C1C-NC-C4C	-3.48	105.14	106.71
3	M	611[A]	PID	CM7-C25-C24	3.47	113.57	110.47
3	M	611[B]	PID	CM7-C25-C24	3.47	113.57	110.47
3	M	611[A]	PID	C8-C9-C11	-3.40	120.83	127.37
3	M	611[B]	PID	C8-C9-C11	-3.40	120.83	127.37
2	M	601	BCL	CHB-C4A-NA	3.40	129.21	124.51
3	M	613	PID	C11-C12-C13	-3.37	120.88	128.34
3	M	613	PID	CM7-C25-C24	3.36	113.48	110.47
3	M	614	PID	C6-C7-C8	-3.36	118.89	125.99
3	M	611[B]	PID	CM3-C5-C4	3.31	114.74	108.98
3	M	614	PID	CM3-C5-CM2	-3.31	102.48	107.37
4	M	615[A]	DGD	O1G-C1A-C2A	3.31	122.29	111.91
4	M	615[B]	DGD	O1G-C1A-C2A	3.31	122.29	111.91
3	M	614	PID	C17-C16-C15	-3.18	116.97	123.47
3	M	613	PID	C4-C3-C2	3.17	116.90	110.77
3	M	613	PID	CM1-C1-C2	3.16	117.83	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	613	PID	O1-C1-C6	-3.14	56.36	58.96
3	M	613	PID	C17-C18-C19	-3.10	117.92	124.81
3	M	614	PID	O1-C1-C6	-3.08	56.41	58.96
3	M	614	PID	C11-C12-C13	-3.07	121.55	128.34
2	M	601	BCL	CAA-CBA-CGA	-3.05	104.35	113.25
3	M	612	PID	CM1-C1-C6	-3.04	117.17	122.26
3	M	611[A]	PID	C1-C2-C3	2.91	118.50	112.75
3	M	613	PID	O3-C10-C9	-2.88	127.46	130.74
2	M	601	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
3	M	613	PID	O6-C30-O7	-2.75	117.50	122.96
3	M	611[A]	PID	O4-C10-O3	2.73	125.38	120.12
3	M	611[B]	PID	O4-C10-O3	2.73	125.38	120.12
3	M	612	PID	C18-C19-C20	-2.69	117.97	123.47
3	M	612	PID	C17-C18-C19	-2.68	118.86	124.81
3	M	613	PID	CM4-C14-C15	2.68	126.67	122.92
4	M	615[A]	DGD	C4D-C3D-C2D	2.66	115.47	110.82
4	M	615[B]	DGD	C4D-C3D-C2D	2.66	115.47	110.82
2	M	601	BCL	CHA-C1A-NA	-2.65	120.34	126.40
3	M	613	PID	O6-C27-C28	-2.64	101.01	107.59
2	M	601	BCL	CMC-C2C-C1C	2.63	118.85	111.77
3	M	611[A]	PID	O4-C10-C9	2.63	110.24	108.04
3	M	611[B]	PID	O4-C10-C9	2.63	110.24	108.04
4	M	615[A]	DGD	O4D-C4D-C5D	2.59	115.72	109.30
4	M	615[B]	DGD	O4D-C4D-C5D	2.59	115.72	109.30
3	M	614	PID	CM6-C25-C24	-2.58	108.17	110.47
3	M	611[A]	PID	O1-C1-C6	-2.52	56.88	58.96
3	M	611[B]	PID	O1-C1-C6	-2.52	56.88	58.96
3	M	612	PID	CM2-C5-C6	-2.50	103.30	110.05
3	M	613	PID	CM5-C21-C20	2.49	126.41	122.92
3	M	612	PID	CM4-C14-C13	2.46	124.73	119.05
3	M	614	PID	O2-C3-C4	-2.45	104.93	109.80
2	M	601	BCL	CAC-C3C-C2C	2.43	120.32	114.26
3	M	611[B]	PID	CM2-C5-C4	-2.40	104.82	108.98
2	M	601	BCL	O2D-CGD-CBD	2.35	115.44	111.27
3	M	611[A]	PID	C28-C27-C26	2.28	113.86	109.88
3	M	611[B]	PID	C28-C27-C26	2.28	113.86	109.88
4	M	615[B]	DGD	O6E-C5E-C6E	2.26	112.06	106.44
3	M	612	PID	C19-C20-C21	-2.24	124.11	127.31
3	M	611[A]	PID	C17-C18-C19	-2.19	119.93	124.81
3	M	611[B]	PID	C17-C18-C19	-2.19	119.93	124.81
3	M	612	PID	C4-C3-C2	-2.16	106.59	110.77
3	M	614	PID	C29-C24-C25	-2.15	117.56	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	601	BCL	CHC-C4B-C3B	-2.14	124.73	132.35
4	M	615[A]	DGD	O6E-C5E-C6E	2.11	111.68	106.44
4	M	615[A]	DGD	O5D-C1E-C2E	-2.11	105.01	108.30
4	M	615[B]	DGD	O5D-C1E-C2E	-2.11	105.01	108.30
3	M	614	PID	O6-C27-C26	-2.10	102.36	107.59
3	M	613	PID	CM3-C5-CM2	-2.08	104.30	107.37
4	M	615[A]	DGD	CCB-CBB-CAB	2.03	124.72	114.42
4	M	615[B]	DGD	CCB-CBB-CAB	2.03	124.72	114.42
2	M	601	BCL	O2D-CGD-O1D	-2.03	119.87	123.84
3	M	611[A]	PID	O6-C30-O7	-2.03	118.94	122.96
3	M	611[B]	PID	O6-C30-O7	-2.03	118.94	122.96
3	M	612	PID	O6-C30-C31	2.02	114.81	111.09
2	M	601	BCL	C20-C18-C19	2.02	119.82	110.51
3	M	611[A]	PID	CM4-C14-C13	2.01	123.70	119.05
3	M	611[B]	PID	CM4-C14-C13	2.01	123.70	119.05
3	M	612	PID	O6-C27-C28	-2.00	102.60	107.59

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	615[A]	DGD	CAB-CBB-CCB-CDB
4	M	615[B]	DGD	CAB-CBB-CCB-CDB
4	M	615[A]	DGD	O6E-C5E-C6E-O5E
4	M	615[A]	DGD	CCB-CDB-CEB-CFB
4	M	615[B]	DGD	CCB-CDB-CEB-CFB
4	M	615[A]	DGD	C7B-C8B-C9B-CAB
4	M	615[B]	DGD	C7B-C8B-C9B-CAB
4	M	615[A]	DGD	C1A-C2A-C3A-C4A
4	M	615[B]	DGD	C1A-C2A-C3A-C4A
4	M	615[A]	DGD	C3B-C4B-C5B-C6B
4	M	615[B]	DGD	C3B-C4B-C5B-C6B
4	M	615[A]	DGD	C6A-C7A-C8A-C9A
4	M	615[B]	DGD	C6A-C7A-C8A-C9A
4	M	615[A]	DGD	C5B-C6B-C7B-C8B
4	M	615[B]	DGD	C5B-C6B-C7B-C8B
4	M	615[A]	DGD	CCA-CDA-CEA-CFA
4	M	615[B]	DGD	CCA-CDA-CEA-CFA
4	M	615[A]	DGD	C2A-C3A-C4A-C5A
4	M	615[A]	DGD	CDB-CEB-CFB-CGB
4	M	615[B]	DGD	C2A-C3A-C4A-C5A
4	M	615[B]	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
4	M	615[B]	DGD	O6E-C5E-C6E-O5E
4	M	615[A]	DGD	C5A-C6A-C7A-C8A
4	M	615[B]	DGD	C5A-C6A-C7A-C8A
2	M	601	BCL	C16-C17-C18-C19
4	M	615[A]	DGD	CFB-CGB-CHB-CIB
4	M	615[B]	DGD	CFB-CGB-CHB-CIB
4	M	615[A]	DGD	CEB-CFB-CGB-CHB
4	M	615[B]	DGD	CEB-CFB-CGB-CHB
4	M	615[A]	DGD	C4A-C5A-C6A-C7A
4	M	615[B]	DGD	C4A-C5A-C6A-C7A
4	M	615[A]	DGD	C7A-C8A-C9A-CAA
4	M	615[B]	DGD	C7A-C8A-C9A-CAA
4	M	615[A]	DGD	C4B-C5B-C6B-C7B
4	M	615[B]	DGD	C4B-C5B-C6B-C7B
2	M	601	BCL	C16-C17-C18-C20
9	M	1170	PEG	O1-C1-C2-O2
2	M	601	BCL	CAD-CBD-CGD-O2D
4	M	615[A]	DGD	C8A-C9A-CAA-CBA
4	M	615[B]	DGD	C8A-C9A-CAA-CBA
9	M	1170	PEG	C4-C3-O2-C2
4	M	615[A]	DGD	CBB-CCB-CDB-CEB
4	M	615[B]	DGD	CBB-CCB-CDB-CEB
4	M	615[A]	DGD	CBA-CCA-CDA-CEA
4	M	615[B]	DGD	CBA-CCA-CDA-CEA
4	M	615[A]	DGD	C4D-C5D-C6D-O5D
4	M	615[B]	DGD	C4D-C5D-C6D-O5D
4	M	615[A]	DGD	C9B-CAB-CBB-CCB
4	M	615[B]	DGD	C9B-CAB-CBB-CCB
4	M	615[A]	DGD	C4E-C5E-C6E-O5E
4	M	615[A]	DGD	C9A-CAA-CBA-CCA
4	M	615[B]	DGD	C9A-CAA-CBA-CCA
4	M	615[A]	DGD	CDA-CEA-CFA-CGA
4	M	615[B]	DGD	CDA-CEA-CFA-CGA
4	M	615[A]	DGD	O6D-C5D-C6D-O5D
4	M	615[B]	DGD	O6D-C5D-C6D-O5D
4	M	615[A]	DGD	O2G-C1B-C2B-C3B
4	M	615[B]	DGD	O2G-C1B-C2B-C3B
4	M	615[A]	DGD	O1B-C1B-C2B-C3B
4	M	615[B]	DGD	O1B-C1B-C2B-C3B

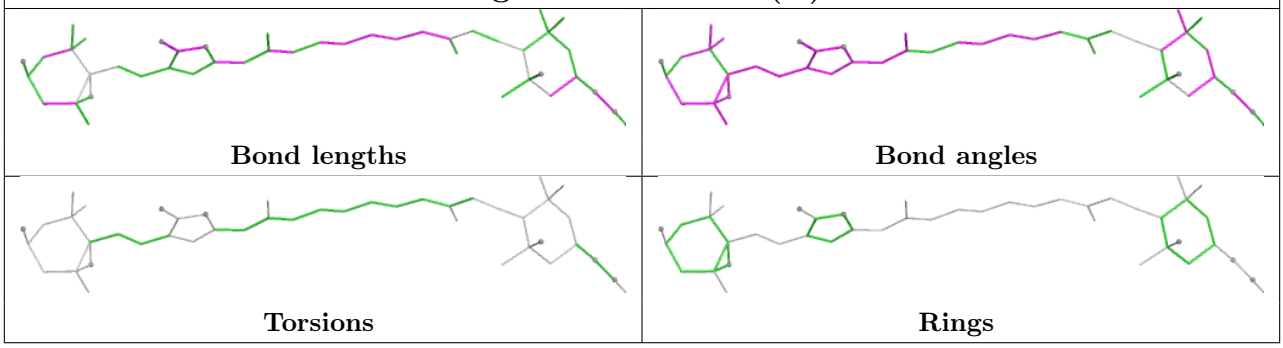
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	613	PID	1	0
9	M	1170	PEG	1	0
2	M	601	BCL	4	0
3	M	612	PID	2	0

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

Ligand PID M 611 (A)



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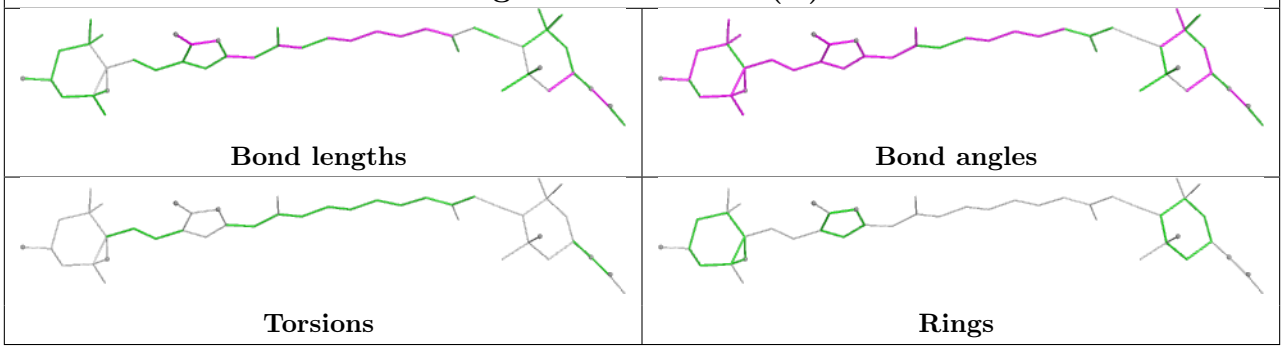

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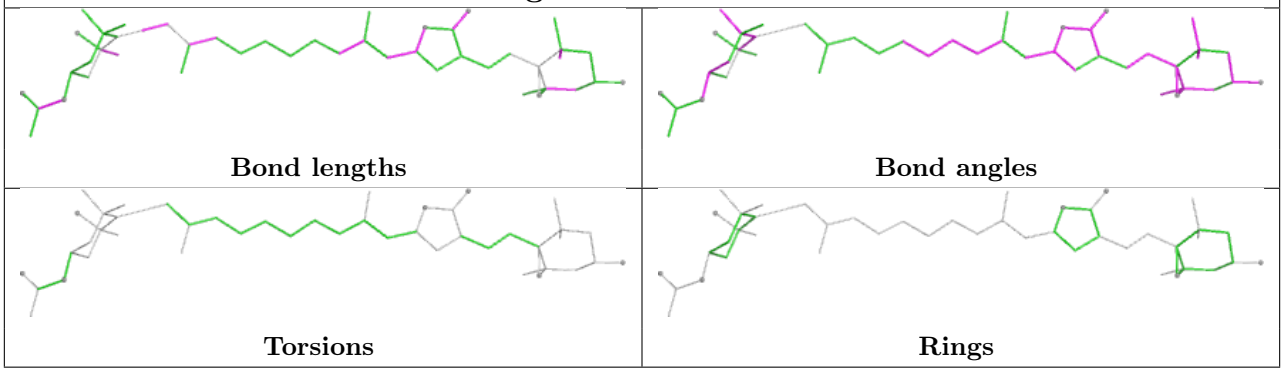

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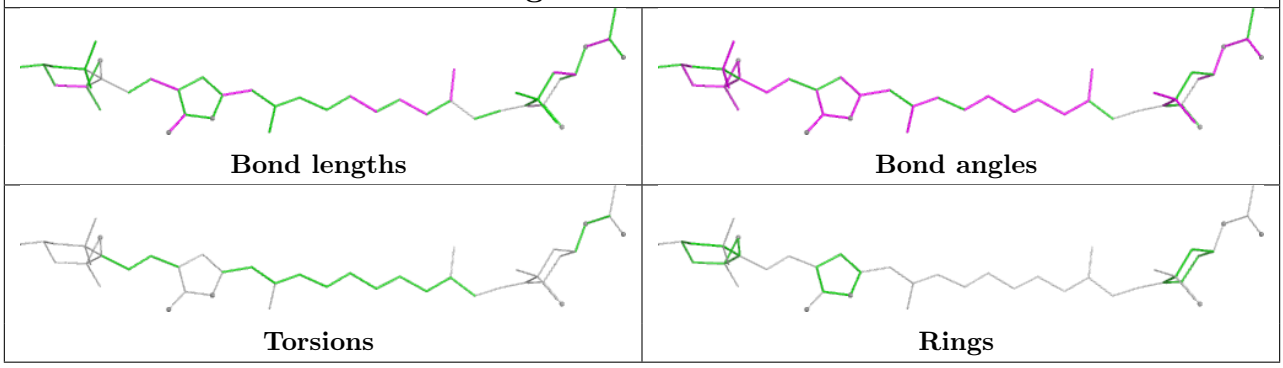
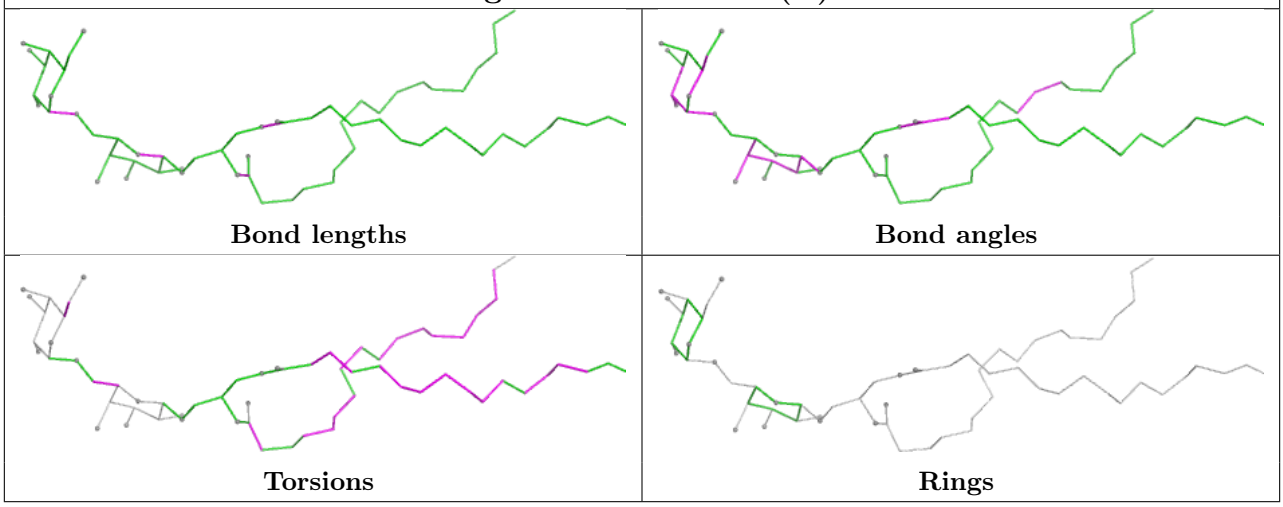
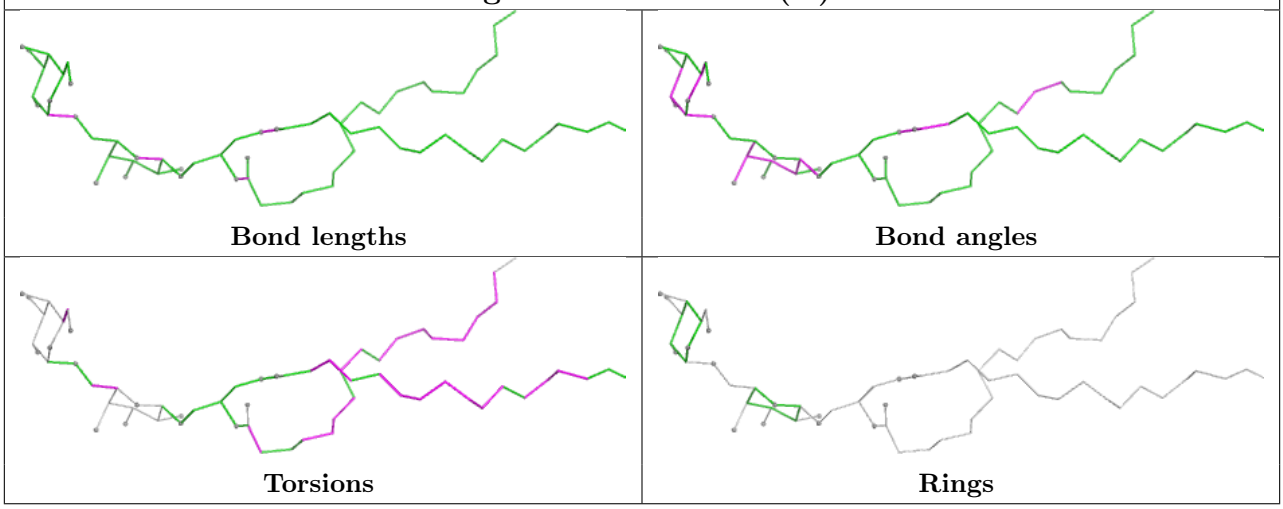


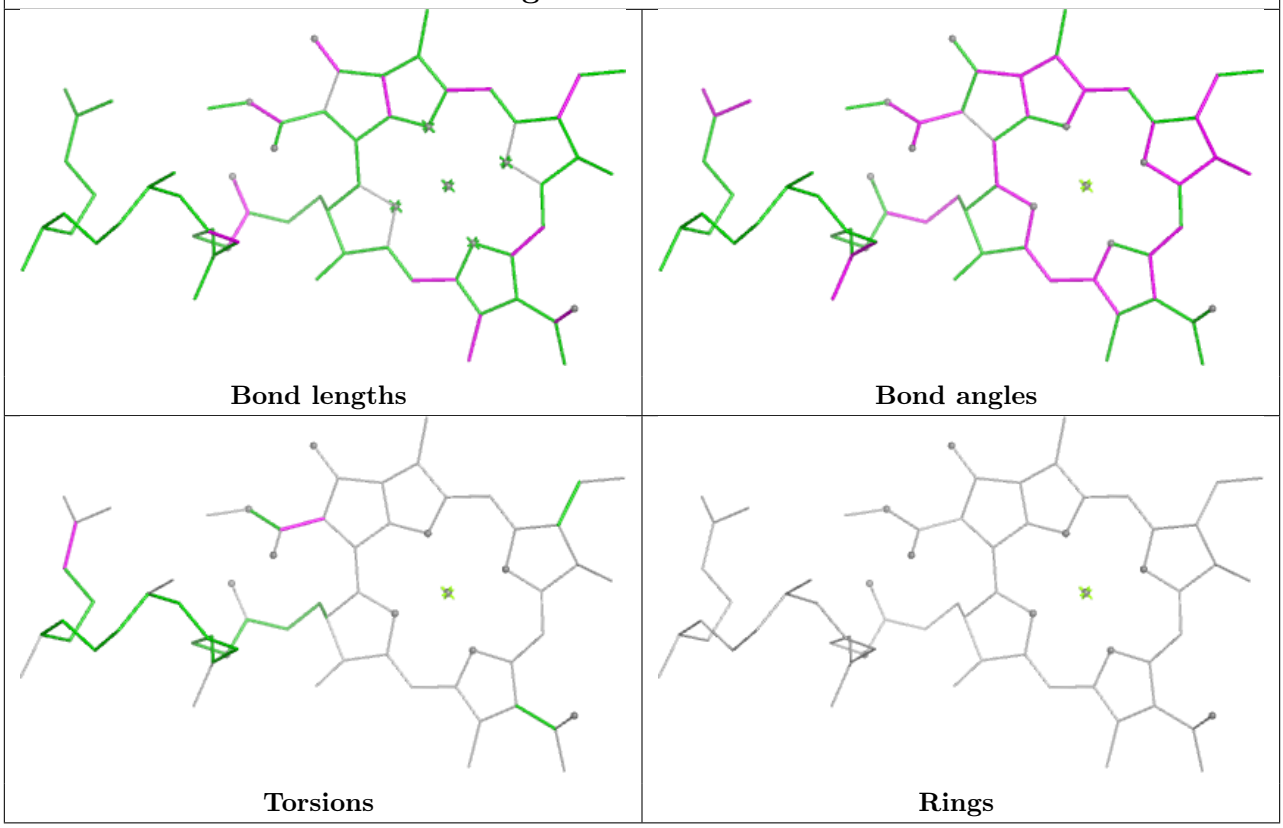
Ligand DGD M 615 (B)

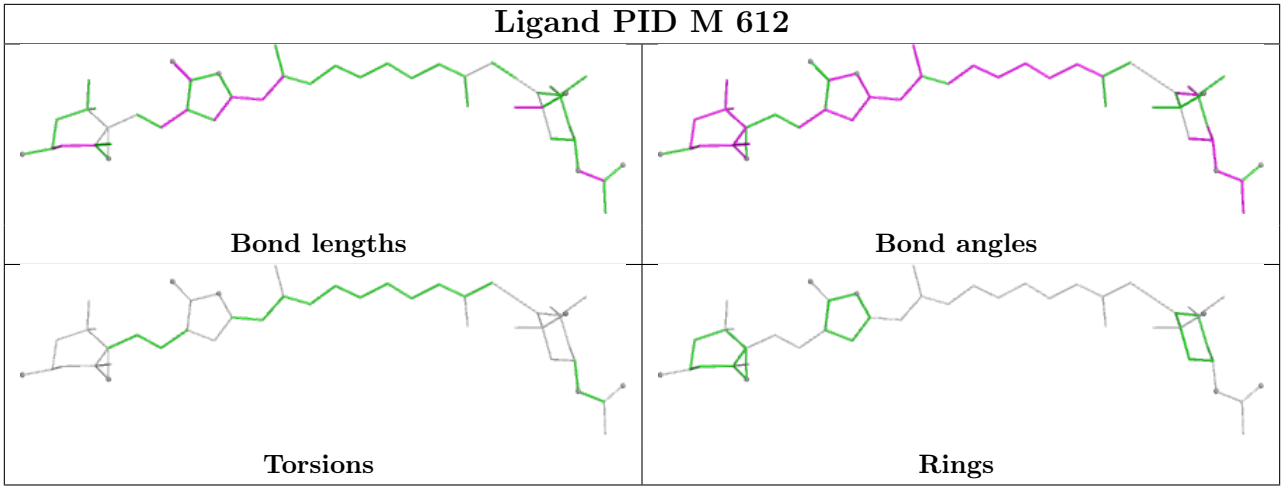


Ligand DGD M 615 (A)



Ligand BCL M 601





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	151/151 (100%)	-0.69	0 100 100	4, 11, 22, 27	3 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PEG	M	1170	7/7	0.75	0.17	34,37,39,41	0
6	CL	M	1163	1/1	0.89	0.11	26,26,26,26	1
7	K	M	1167	1/1	0.92	0.13	46,46,46,46	0
6	CL	M	1159	1/1	0.93	0.11	16,16,16,16	1
6	CL	M	1164	1/1	0.93	0.15	44,44,44,44	0
7	K	M	1166	1/1	0.94	0.08	39,39,39,39	0
4	DGD	M	615[B]	66/66	0.94	0.10	11,26,44,48	3
4	DGD	M	615[A]	66/66	0.94	0.10	11,27,44,48	3
6	CL	M	1160	1/1	0.95	0.12	19,19,19,19	1

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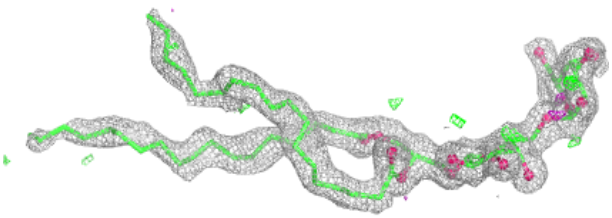
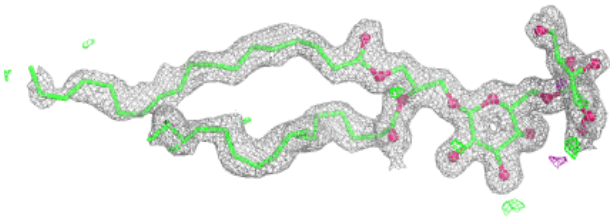
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PID	M	612	46/46	0.95	0.07	10,14,29,38	0
7	K	M	1168	1/1	0.96	0.05	28,28,28,28	0
3	PID	M	611[B]	46/46	0.97	0.05	7,11,15,19	4
2	BCL	M	601	66/66	0.97	0.05	6,10,15,20	0
8	NA	M	1169	1/1	0.97	0.08	26,26,26,26	0
3	PID	M	611[A]	46/46	0.97	0.05	7,11,15,19	4
5	CD	M	1155	1/1	0.98	0.03	17,17,17,17	1
3	PID	M	613	46/46	0.98	0.04	6,9,17,21	0
7	K	M	1165	1/1	0.98	0.08	25,25,25,25	0
3	PID	M	614	46/46	0.98	0.04	6,9,13,19	0
6	CL	M	1161	1/1	0.99	0.03	12,12,12,12	0
5	CD	M	1156	1/1	0.99	0.03	20,20,20,20	1
6	CL	M	1158	1/1	0.99	0.04	16,16,16,16	0
5	CD	M	1157	1/1	1.00	0.03	10,10,10,10	1
5	CD	M	1152[B]	1/1	1.00	0.02	11,11,11,11	1
5	CD	M	1153	1/1	1.00	0.01	12,12,12,12	0
5	CD	M	1154	1/1	1.00	0.02	15,15,15,15	1
5	CD	M	1151	1/1	1.00	0.02	9,9,9,9	0
6	CL	M	1162	1/1	1.00	0.02	19,19,19,19	0
5	CD	M	1152[A]	1/1	1.00	0.02	9,9,9,9	1

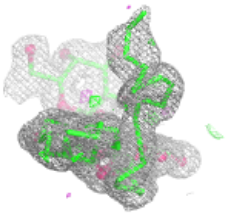
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD M 615 (B):

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

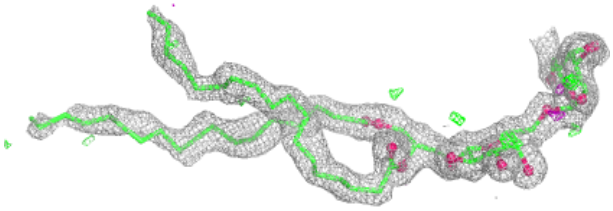


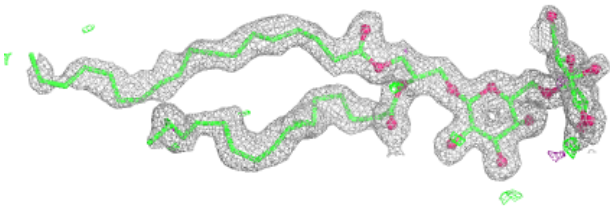


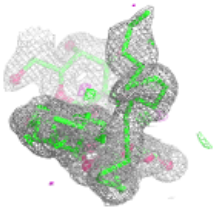


Electron density around DGD M 615 (A):

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

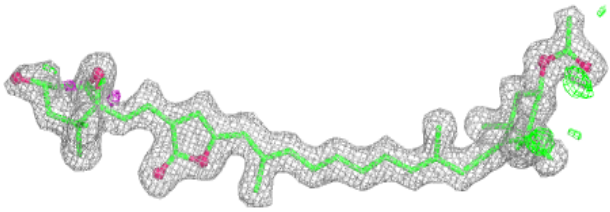


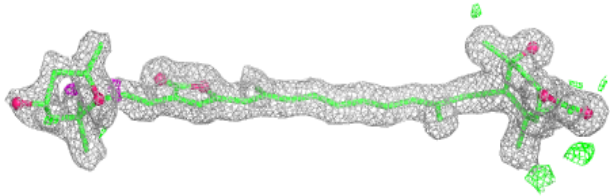


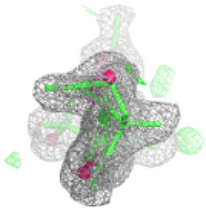


Electron density around PID M 612:

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

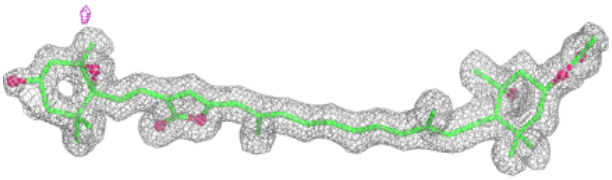


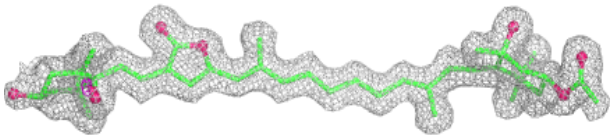


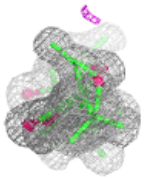


Electron density around PID M 611 (B):

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

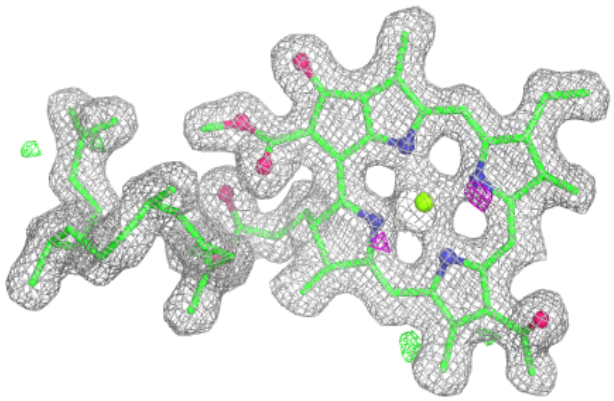


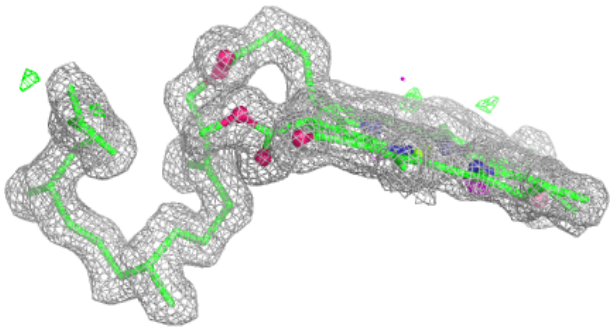




Electron density around BCL M 601:

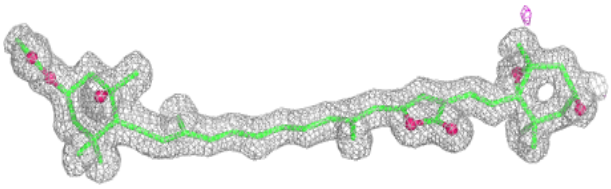
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

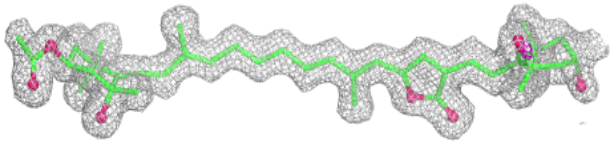


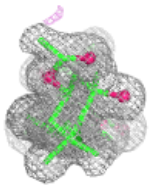


Electron density around PID M 611 (A):

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

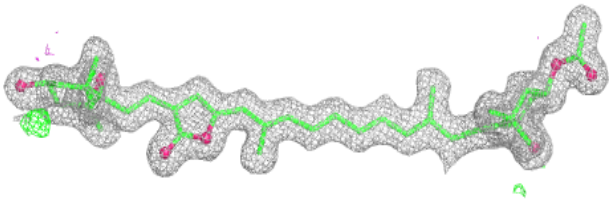


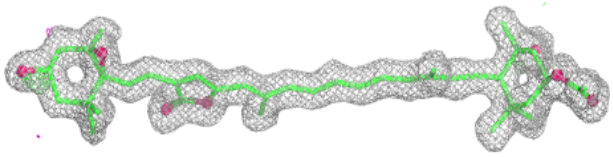


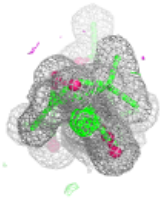


Electron density around PID M 613:

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

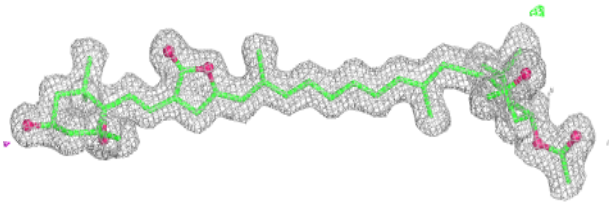


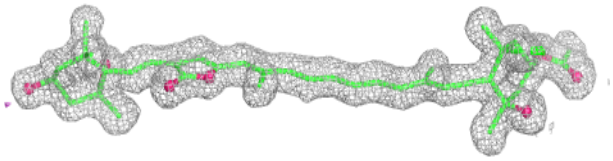


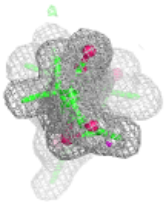


Electron density around PID M 614:

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







6.5 Other polymers (i)

There are no such residues in this entry.