wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 03:10 PM EDT

PDB ID	:	4OGQ / pdb_00004ogq
Title	:	Internal Lipid Architecture of the Hetero-Oligomeric Cytochrome b6f Complex
Authors	:	Hasan, S.S.; Cramer, W.A.
Deposited on	:	2014-01-16
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

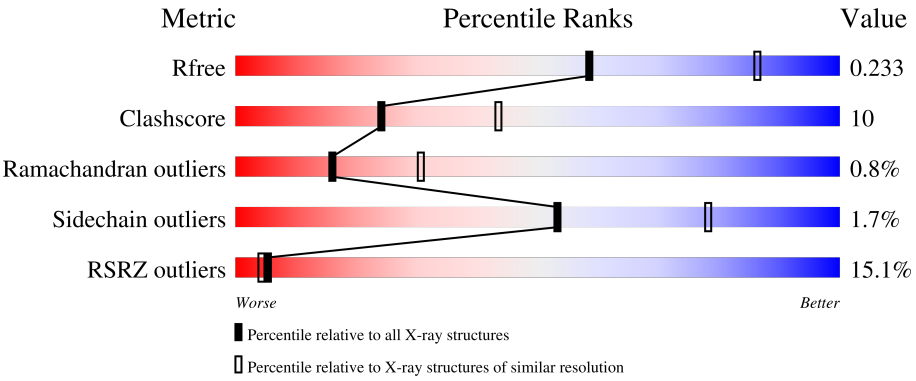
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.50 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.



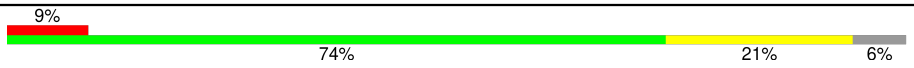
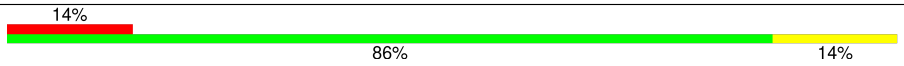
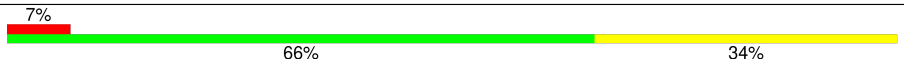
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	A	215	2% 91% 9%
2	B	160	8% 88% 11%
3	C	333	13% 69% 14% 16%
4	D	179	36% 72% 21% 7%
5	E	31	23% 77% 16% 6%

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Mol	Chain	Length	Quality of chain
6	F	34	
7	G	37	
8	H	29	

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
24	1O2	F	103	X	-	-	-
9	HEC	A	301	X	-	-	-
9	HEC	A	302	X	-	-	-
9	HEC	A	303	X	-	-	-
9	HEC	C	301	X	-	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 8396 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 Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1708	1139	271	288	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	S	0	0	0
			1232	825	194	208	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2137	1361	355	415	6			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1250	791	213	240	6			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	31	Total	C	N	O	S	0	0	0
			228	157	35	35	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	32	Total	C	N	O	S	0	0	0
			231	156	36	38	1			

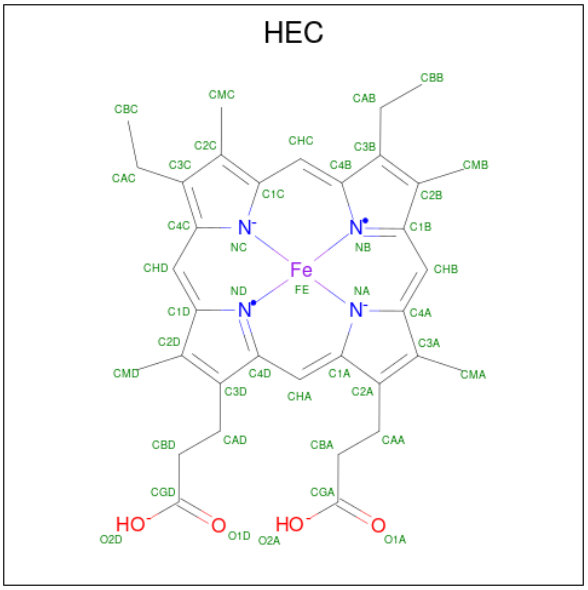
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	37	Total	C	N	O	S	0	0	0
			282	188	44	49	1			

- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

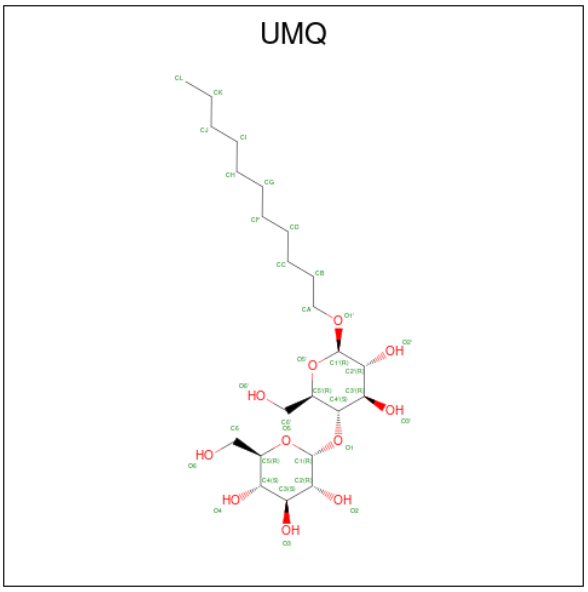
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	29	Total	C	N	O	S	0	0	0
			228	155	36	35	2			

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



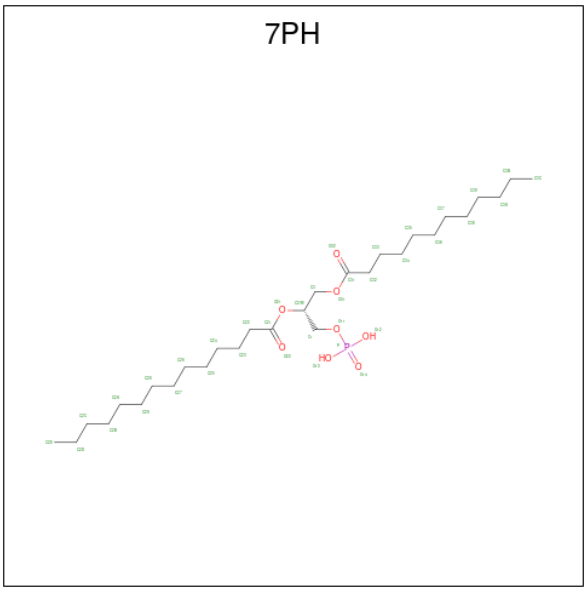
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).



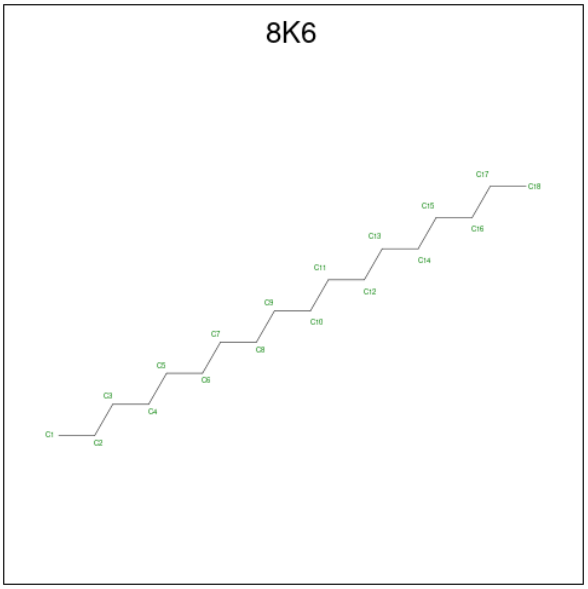
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 34 23 11	0	0
10	B	1	Total C O 34 23 11	0	0
10	B	1	Total C O 34 23 11	0	1
10	D	1	Total C O 34 23 11	0	0
10	G	1	Total C O 34 23 11	0	0

- Molecule 11 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: $C_{29}H_{57}O_8P$).



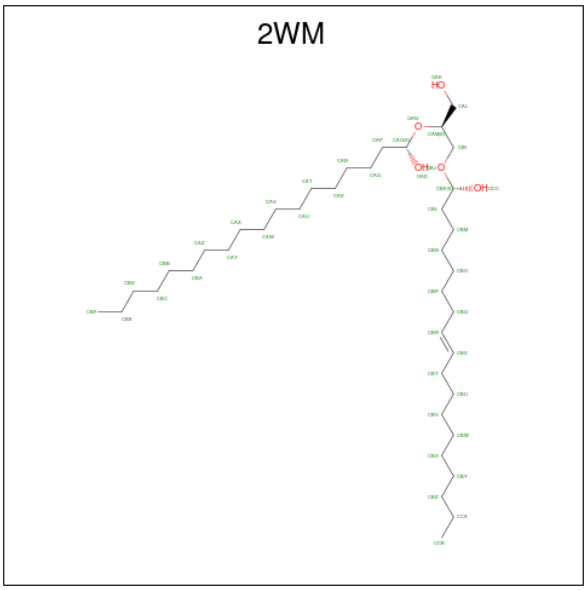
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 32 27 5	0	0
11	B	1	Total C O 32 27 5	0	0
11	C	1	Total C O 32 27 5	0	0
11	D	1	Total C O 32 27 5	0	0
11	F	1	Total C O 32 27 5	0	0

- Molecule 12 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).



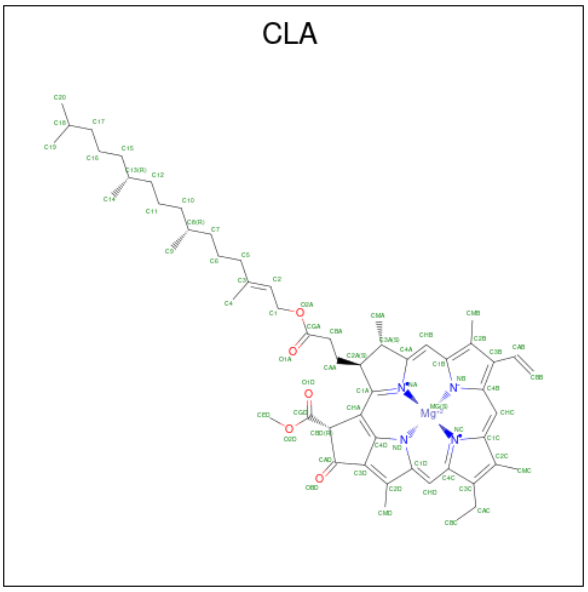
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C 18 18	0	0
12	A	1	Total C 18 18	0	0
12	A	1	Total C 14 14	0	0
12	B	1	Total C 18 18	0	1

- Molecule 13 is (1S,8E)-1-{[(2S)-3-hydroxy-2-{[(1S)-1-hydroxyoctadecyl]oxy}propyl]oxy}octadec-8-en-1-ol (CCD ID: 2WM) (formula: $C_{39}H_{78}O_5$).



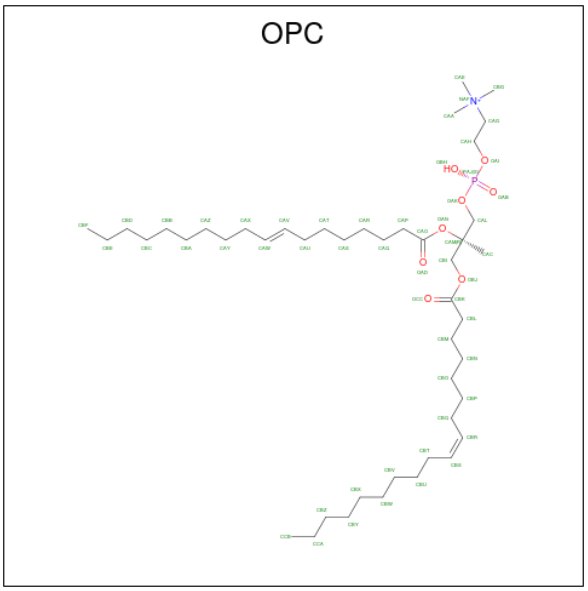
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 44 39 5	0	0

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 15 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: $C_{45}H_{87}NO_8P$).

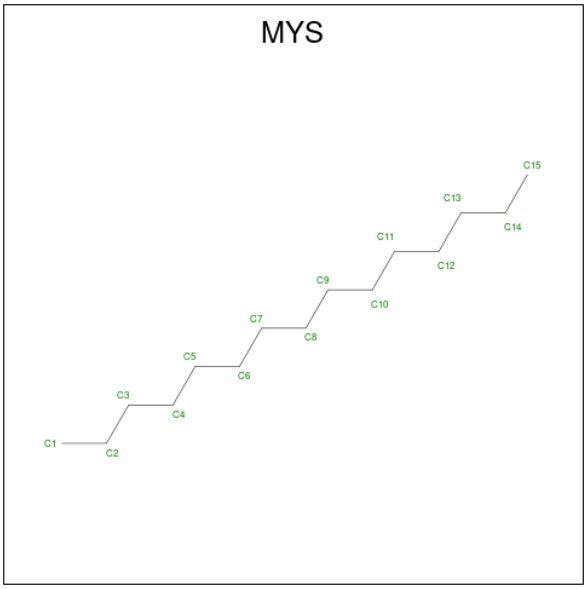


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 16 is CADMIUM ION (CCD ID: CD) (formula: Cd).

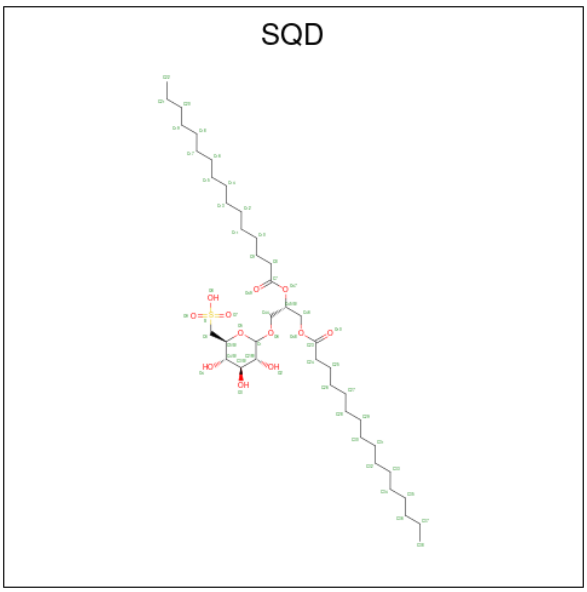
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total Cd 1 1	0	0

- Molecule 17 is PENTADECANE (CCD ID: MYS) (formula: $C_{15}H_{32}$).



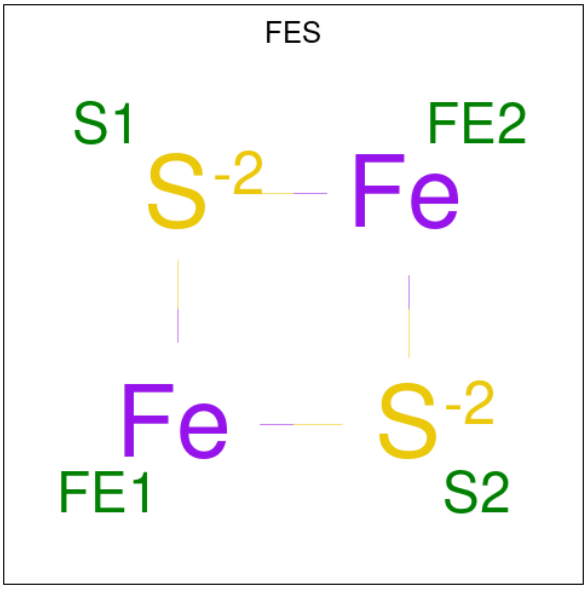
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total C 15 15	0	0

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



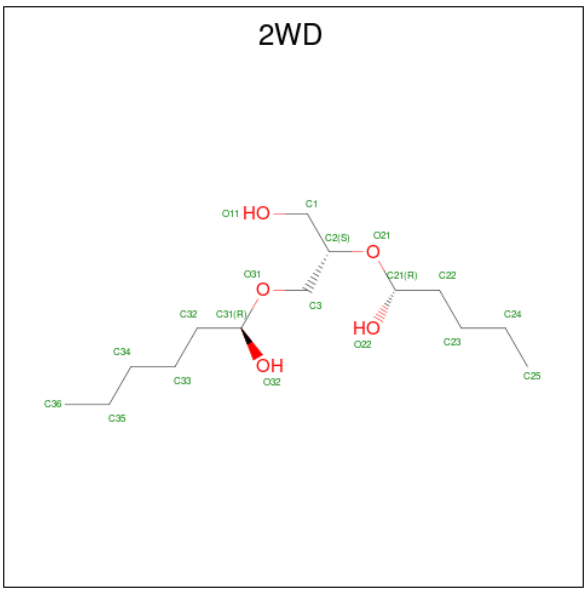
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



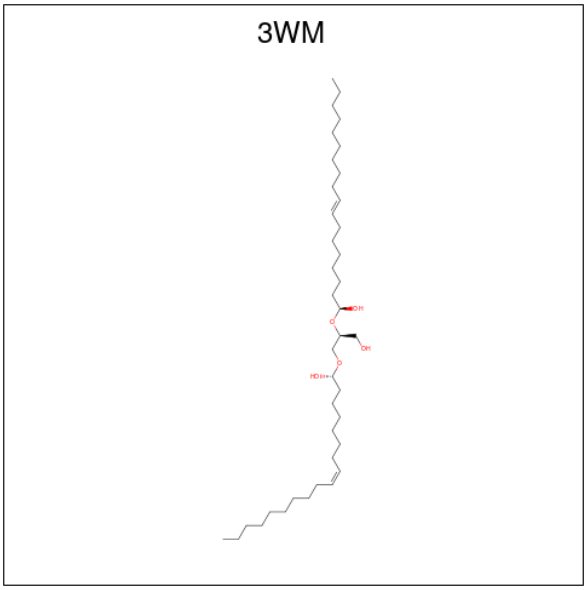
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 20 is (1R)-1-{[(2S)-3-hydroxy-2-{[(1R)-1-hydroxypentyl]oxy}propyl]oxy}hexan-1-ol (CCD ID: 2WD) (formula: $C_{14}H_{30}O_5$).



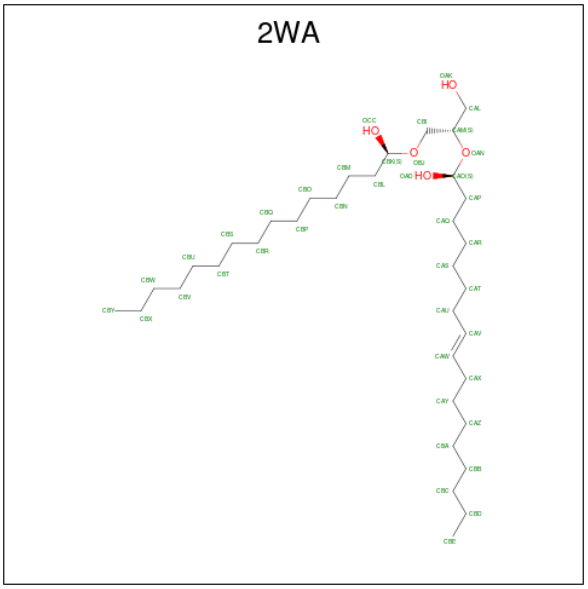
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C O 19 14 5	0	0

- Molecule 21 is (1S,8E,1'R,8'Z)-1,1'-{[(2S)-3-hydroxypropane-1,2-diyl]bis(oxy)}bisoctadec-8-en-1-ol (CCD ID: 3WM) (formula: $C_{39}H_{76}O_5$).



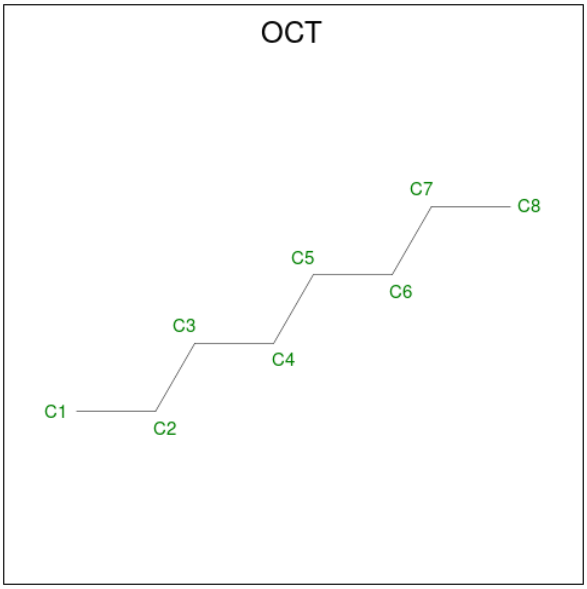
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	E	1	Total C O 44 39 5	0	0

- Molecule 22 is (1S,8E)-1-{[(2S)-1-hydroxy-3-{[(1S)-1-hydroxypentadecyl]oxy}propan-2-yl]oxy}heptadec-8-en-1-ol (CCD ID: 2WA) (formula: $C_{35}H_{70}O_5$).



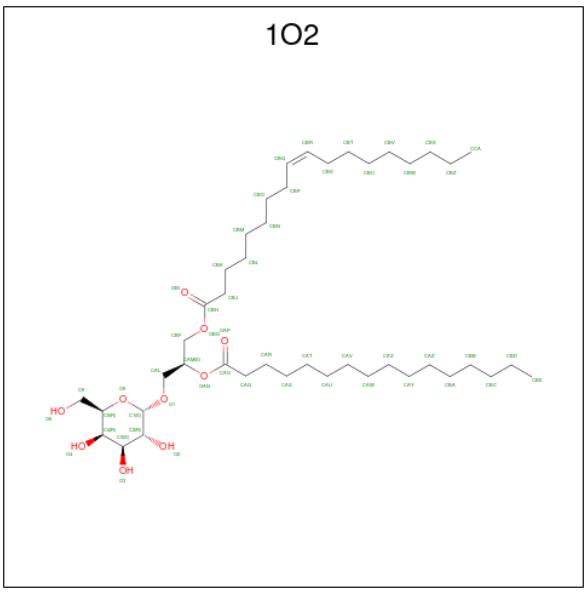
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total C O 40 35 5	0	0

- Molecule 23 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



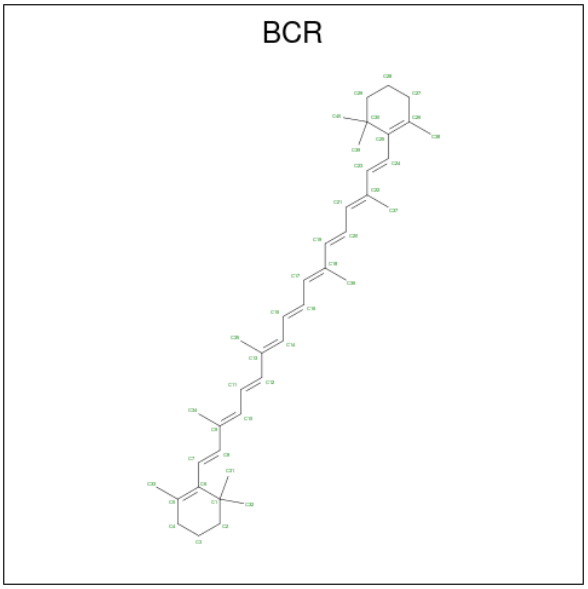
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	F	1	Total C 8 8	0	0

- Molecule 24 is (2S)-3-(alpha-D-galactopyranosyloxy)-2-(hexadecanoyloxy)propyl (9Z)-octadec-9-enoate (CCD ID: 1O2) (formula: $C_{43}H_{80}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	F	1	Total C O 49 39 10	0	0

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	G	1	Total C 40 40	0	0

- Molecule 26 is water.

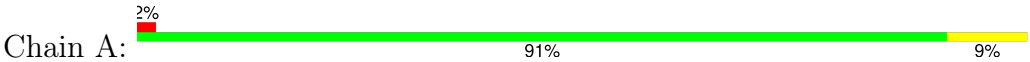
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	21	Total O 21 21	0	0
26	B	25	Total O 25 25	0	0
26	C	38	Total O 38 38	0	0
26	D	1	Total O 1 1	0	0
26	F	1	Total O 1 1	0	0
26	G	7	Total O 7 7	0	0

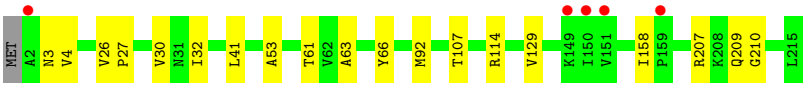
3 Residue-property plots (i)

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: Cytochrome b6

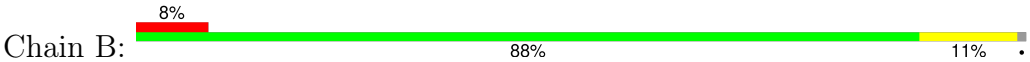
Chain A:

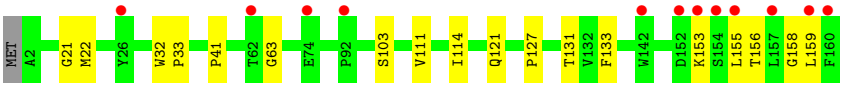




• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:

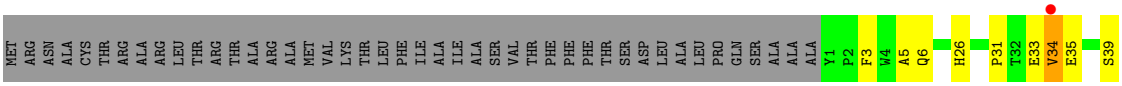


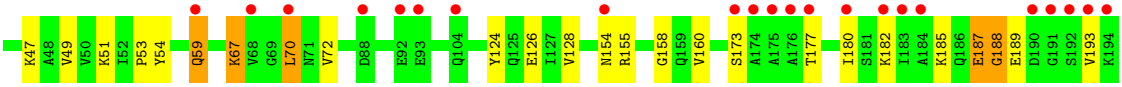


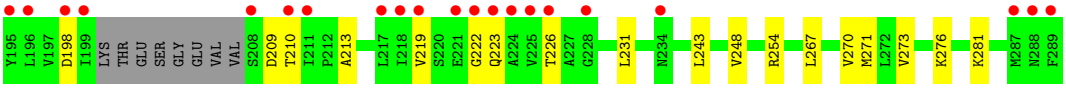
• Molecule 3: Apocytochrome f

Chain C:





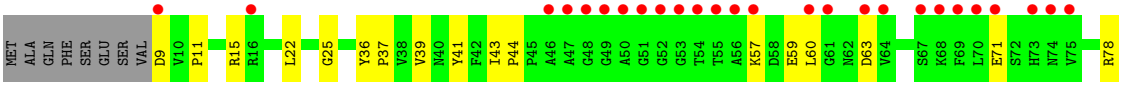


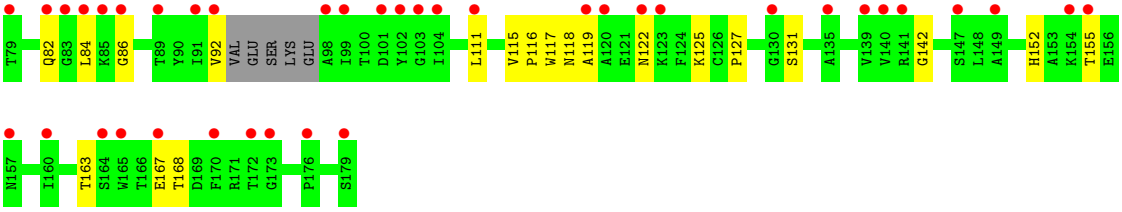


• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1

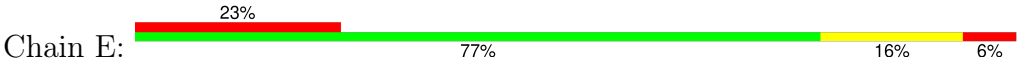
Chain D:

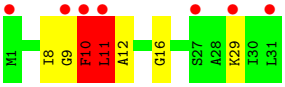






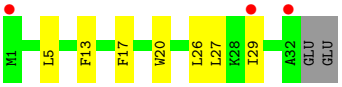
• Molecule 5: Cytochrome b6-f complex subunit 6



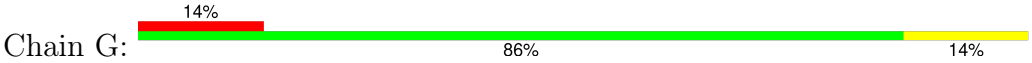


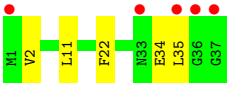
• Molecule 6: Cytochrome b6-f complex subunit 7





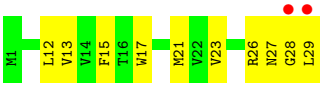
• Molecule 7: Cytochrome b6-f complex subunit 5





• Molecule 8: Cytochrome b6-f complex subunit 8





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	159.23Å 159.23Å 365.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.57 – 2.50 39.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.57-2.50) 89.3 (39.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.201 , 0.232 0.207 , 0.233	Depositor DCC
R_{free} test set	4694 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 91.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, 2WD, OCT, 8K6, 2WM, SQD, 2WA, CLA, 1O2, HEC, CD, OPC, UMQ, 3WM, 7PH, FES, MYS

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	0.33	0/1761	0.79	4/2401 (0.2%)
2	B	0.32	0/1271	0.75	1/1742 (0.1%)
3	C	0.28	0/2182	0.69	0/2972
4	D	0.28	0/1281	0.71	0/1745
5	E	0.36	0/231	1.08	3/309 (1.0%)
6	F	0.25	0/234	0.66	0/315
7	G	0.27	0/287	0.72	0/387
8	H	0.35	0/234	0.66	0/319
All	All	0.30	0/7481	0.74	8/10190 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	10	PHE	N-CA-C	8.31	123.90	113.43
5	E	10	PHE	CA-C-N	6.30	133.04	121.70
5	E	10	PHE	C-N-CA	6.30	133.04	121.70
1	A	158	ILE	CA-C-N	5.66	126.91	119.84
1	A	158	ILE	C-N-CA	5.66	126.91	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	PHE	Peptide

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	1708	0	1721	16	0
2	B	1232	0	1278	16	0
3	C	2137	0	2122	31	0
4	D	1250	0	1208	23	0
5	E	228	0	257	9	0
6	F	231	0	252	8	0
7	G	282	0	303	4	0
8	H	228	0	243	11	0
9	A	129	0	95	6	0
9	C	43	0	31	3	0
10	A	34	0	44	9	0
10	B	68	0	87	17	0
10	D	34	0	44	4	0
10	G	34	0	44	4	0
11	A	32	0	45	1	0
11	B	32	0	45	5	0
11	C	32	0	45	4	0
11	D	32	0	45	1	0
11	F	32	0	45	6	0
12	A	50	0	103	8	0
12	B	18	0	38	3	0
13	A	44	0	78	0	0
14	B	65	0	72	4	0
15	B	54	0	83	5	0
16	C	1	0	0	0	0
17	D	15	0	32	1	0
18	D	54	0	77	2	0
19	D	4	0	0	0	0
20	D	19	0	30	2	0
21	E	44	0	76	9	0
22	F	40	0	70	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	F	8	0	18	0	0
24	F	49	0	69	11	0
25	G	40	0	56	2	0
26	A	21	0	0	0	0
26	B	25	0	0	1	0
26	C	38	0	0	0	0
26	D	1	0	0	0	0
26	F	1	0	0	0	0
26	G	7	0	0	0	0
All	All	8396	0	8756	171	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 171 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)
10:G:101:UMQ:O5'	10:G:101:UMQ:C5'	1.63	1.46
10:A:304:UMQ:O5'	10:A:304:UMQ:C5'	1.63	1.45
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C5'	1.63	1.44
10:B:201:UMQ:C1'	10:B:201:UMQ:O5'	1.69	1.41
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C1'	1.69	1.38

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	212/215 (99%)	202 (95%)	9 (4%)	1 (0%)	24 43
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	277/333 (83%)	249 (90%)	23 (8%)	5 (2%)	6 12
4	D	162/179 (90%)	147 (91%)	15 (9%)	0	100 100
5	E	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3 4
6	F	30/34 (88%)	30 (100%)	0	0	100 100
7	G	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
8	H	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
All	All	929/1018 (91%)	865 (93%)	57 (6%)	7 (1%)	16 31

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	173	SER
1	A	3	ASN
3	C	185	LYS
5	E	11	LEU
3	C	189	GLU

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	A	183/184 (100%)	183 (100%)	0	100 100
2	B	133/134 (99%)	132 (99%)	1 (1%)	73 88
3	C	231/272 (85%)	224 (97%)	7 (3%)	36 64
4	D	133/145 (92%)	129 (97%)	4 (3%)	36 64
5	E	21/21 (100%)	20 (95%)	1 (5%)	23 46
6	F	22/24 (92%)	22 (100%)	0	100 100
7	G	29/29 (100%)	29 (100%)	0	100 100
8	H	24/24 (100%)	24 (100%)	0	100 100
All	All	776/833 (93%)	763 (98%)	13 (2%)	53 78

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	267	LEU
4	D	71	GLU
5	E	11	LEU
4	D	115	VAL
4	D	155	THR

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

Mol	Chain	Res	Type
3	C	154	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\#\|Z\| > 2$
11	7PH	A	305	-	31,31,37	1.29	2 (6%)	33,33,42	1.20	2 (6%)
13	2WM	A	309	-	43,43,43	0.71	2 (4%)	41,45,45	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	UMQ	B	203[B]	-	35,35,35	3.68	17 (48%)	46,46,46	2.11	8 (17%)
14	CLA	B	204	26	69,73,73	1.19	7 (10%)	82,113,113	1.19	5 (6%)
11	7PH	F	104	-	31,31,37	1.30	2 (6%)	33,33,42	1.20	2 (6%)
22	2WA	F	101	-	39,39,39	0.94	1 (2%)	37,41,41	0.54	0
12	8K6	A	306	-	17,17,17	0.07	0	16,16,16	0.85	0
21	3WM	E	101	-	43,43,43	0.79	1 (2%)	41,45,45	0.53	0
11	7PH	B	206	-	31,31,37	1.30	2 (6%)	33,33,42	1.17	2 (6%)
10	UMQ	B	201	-	35,35,35	3.66	17 (48%)	46,46,46	2.12	6 (13%)
10	UMQ	A	304	-	35,35,35	3.67	17 (48%)	46,46,46	2.09	7 (15%)
10	UMQ	G	101	-	35,35,35	3.67	17 (48%)	46,46,46	2.13	6 (13%)
9	HEC	C	301	3	50,50,50	1.90	8 (16%)	68,82,82	1.48	5 (7%)
18	SQD	D	204	-	52,54,54	0.96	3 (5%)	62,65,65	1.41	9 (14%)
9	HEC	A	301	1	50,50,50	1.96	9 (18%)	68,82,82	1.55	7 (10%)
11	7PH	C	303	-	31,31,37	1.29	2 (6%)	33,33,42	1.22	2 (6%)
11	7PH	D	203	-	31,31,37	1.30	2 (6%)	33,33,42	1.14	2 (6%)
17	MYS	D	202	-	14,14,14	0.08	0	13,13,13	0.85	0
23	OCT	F	102	-	7,7,7	0.12	0	6,6,6	0.73	0
25	BCR	G	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
15	OPC	B	205	-	53,53,54	1.05	3 (5%)	59,61,64	1.01	2 (3%)
12	8K6	A	308	-	13,13,17	0.09	0	12,12,16	0.79	0
10	UMQ	D	201	-	35,35,35	3.68	17 (48%)	46,46,46	2.14	9 (19%)
9	HEC	A	303	1,26	50,50,50	2.14	9 (18%)	68,82,82	1.60	7 (10%)
9	HEC	A	302	1	50,50,50	2.00	9 (18%)	68,82,82	1.52	8 (11%)
12	8K6	A	307	-	17,17,17	0.07	0	16,16,16	0.89	0
19	FES	D	205	4	0,4,4	-	-	-		
12	8K6	B	202[A]	-	17,17,17	0.07	0	16,16,16	0.86	0
20	2WD	D	206	-	18,18,18	1.18	1 (5%)	16,20,20	0.52	0
24	1O2	F	103	-	49,49,53	1.46	5 (10%)	57,57,61	1.11	5 (8%)

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
11	7PH	A	305	-	-	14/33/33/39	-
13	2WM	A	309	-	-	26/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	UMQ	B	203[B]	-	-	8/20/60/60	0/2/2/2
14	CLA	B	204	26	-	9/39/115/115	-
11	7PH	F	104	-	-	12/33/33/39	-
22	2WA	F	101	-	-	21/41/41/41	-
12	8K6	A	306	-	-	2/15/15/15	-
21	3WM	E	101	-	-	24/45/45/45	-
11	7PH	B	206	-	-	15/33/33/39	-
10	UMQ	B	201	-	-	3/20/60/60	0/2/2/2
10	UMQ	A	304	-	-	10/20/60/60	0/2/2/2
10	UMQ	G	101	-	-	6/20/60/60	0/2/2/2
9	HEC	C	301	3	1/1/3/7	5/14/54/54	-
18	SQD	D	204	-	-	16/49/69/69	0/1/1/1
9	HEC	A	301	1	1/1/3/7	5/14/54/54	-
11	7PH	C	303	-	-	21/33/33/39	-
11	7PH	D	203	-	-	13/33/33/39	-
17	MYS	D	202	-	-	3/12/12/12	-
23	OCT	F	102	-	-	1/5/5/5	-
25	BCR	G	102	-	-	7/29/63/63	0/2/2/2
15	OPC	B	205	-	-	19/57/57/60	-
12	8K6	A	308	-	-	8/11/11/15	-
10	UMQ	D	201	-	-	7/20/60/60	0/2/2/2
9	HEC	A	303	1,26	1/1/3/7	4/14/54/54	-
9	HEC	A	302	1	1/1/3/7	7/14/54/54	-
12	8K6	A	307	-	-	3/15/15/15	-
19	FES	D	205	4	-	-	0/1/1/1
12	8K6	B	202[A]	-	-	5/15/15/15	-
20	2WD	D	206	-	-	7/20/20/20	-
24	1O2	F	103	-	1/1/8/10	25/44/64/68	0/1/1/1

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	203[B]	UMQ	O5'-C1'	10.69	1.69	1.41
10	D	201	UMQ	O5'-C1'	10.69	1.69	1.41
10	A	304	UMQ	O5'-C1'	10.69	1.69	1.41
10	G	101	UMQ	O5'-C1'	10.69	1.69	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	201	UMQ	O5'-C1'	10.65	1.69	1.41

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	201	UMQ	C1'-O5'-C5'	-9.36	95.44	113.72
10	G	101	UMQ	C1'-O5'-C5'	-9.02	96.10	113.72
10	B	203[B]	UMQ	C1'-O5'-C5'	-8.87	96.41	113.72
10	A	304	UMQ	C1'-O5'-C5'	-8.82	96.50	113.72
10	B	201	UMQ	C1'-O5'-C5'	-8.78	96.57	113.72

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	301	HEC	NA
9	A	302	HEC	NA
9	A	303	HEC	NA
9	C	301	HEC	NA
24	F	103	1O2	C1

5 of 306 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	304	UMQ	O5'-C1'-O1'-CA
10	B	203[B]	UMQ	O5'-C1'-O1'-CA
11	A	305	7PH	O11-C1-C2-C3
11	A	305	7PH	O11-C1-C2-O21
11	B	206	7PH	O11-C1-C2-C3

There are no ring outliers.

25 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	305	7PH	1	0
10	B	203[B]	UMQ	10	0
14	B	204	CLA	4	0
11	F	104	7PH	6	0
22	F	101	2WA	7	0
12	A	306	8K6	2	0
21	E	101	3WM	9	0
11	B	206	7PH	5	0

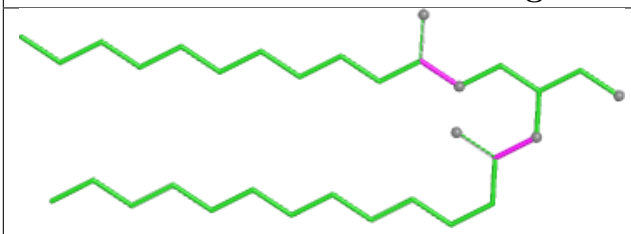
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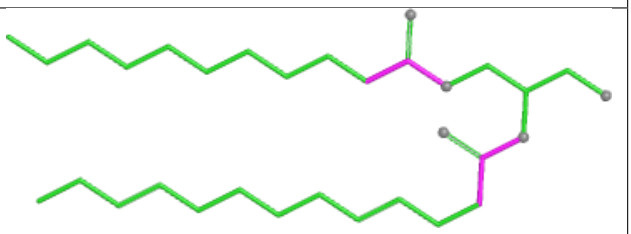
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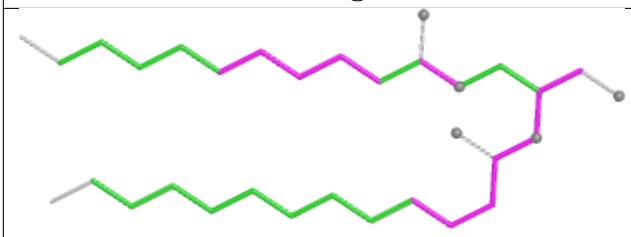
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	201	UMQ	7	0
10	A	304	UMQ	9	0
10	G	101	UMQ	4	0
9	C	301	HEC	3	0
18	D	204	SQD	2	0
11	C	303	7PH	4	0
11	D	203	7PH	1	0
17	D	202	MYS	1	0
25	G	102	BCR	2	0
15	B	205	OPC	5	0
12	A	308	8K6	5	0
10	D	201	UMQ	4	0
9	A	303	HEC	6	0
12	A	307	8K6	2	0
12	B	202[A]	8K6	3	0
20	D	206	2WD	2	0
24	F	103	1O2	11	0

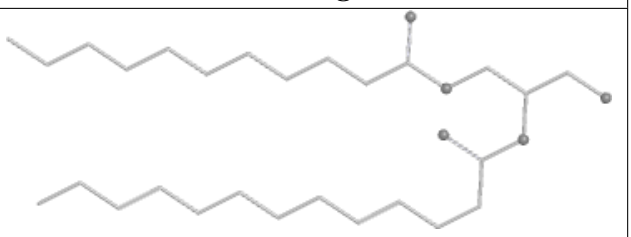
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 7PH A 305

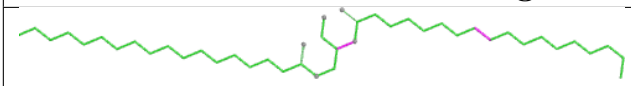

Bond lengths

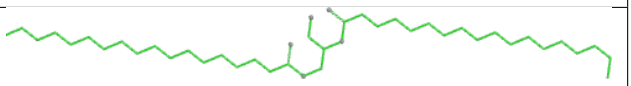

Bond angles

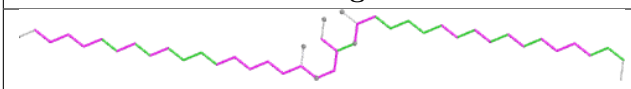

Torsions

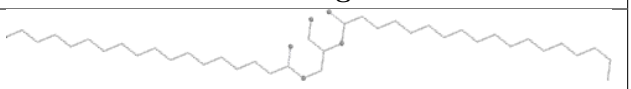

Rings

Ligand 2WM A 309

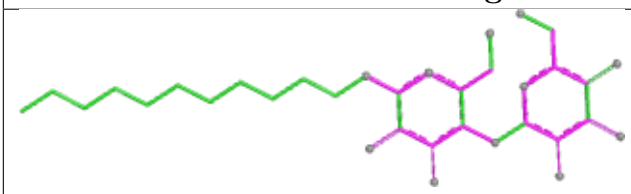

Bond lengths

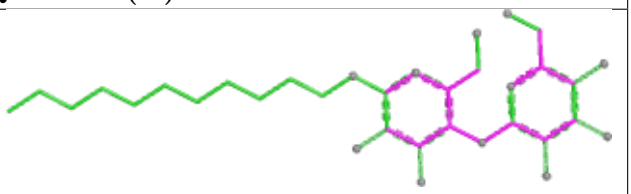

Bond angles

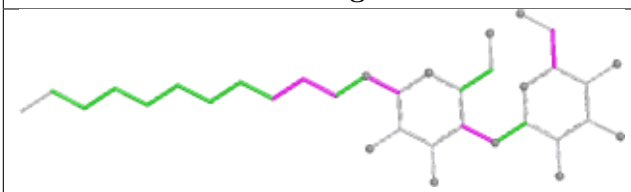

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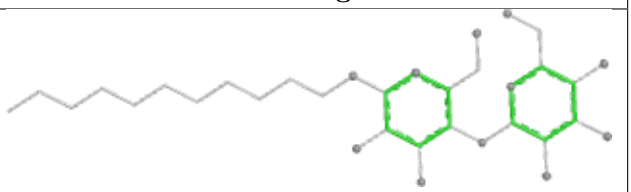

Rings

Ligand UMQ B 203 (B)

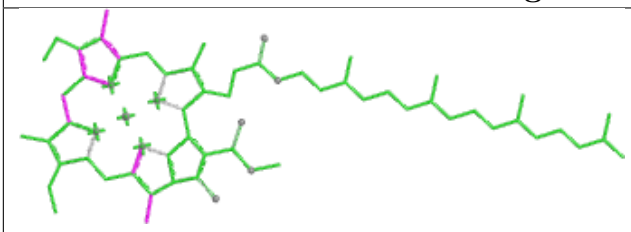

Bond lengths


Bond angles

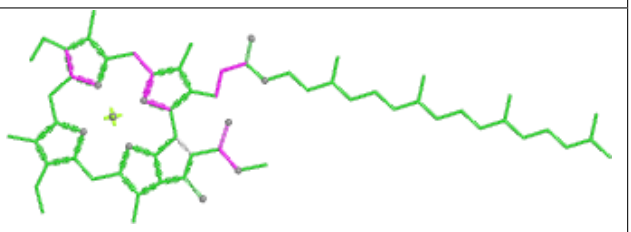

Torsions


Rings

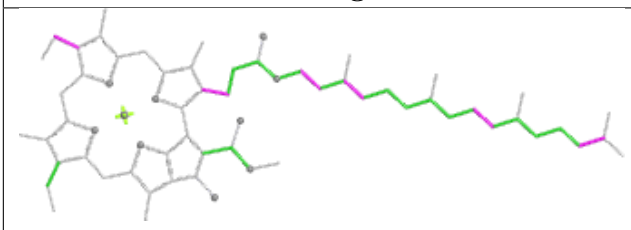
Ligand CLA B 204



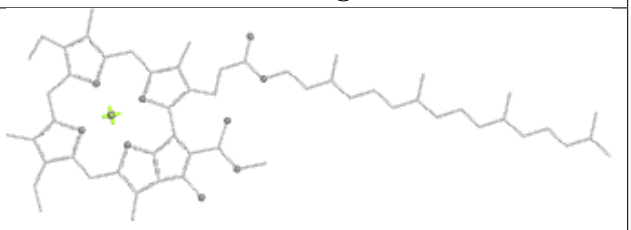
Bond lengths



Bond angles

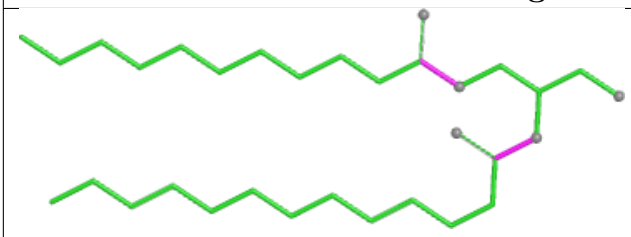


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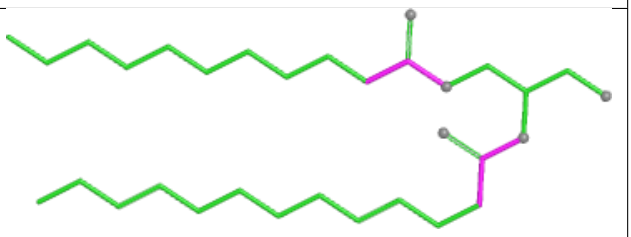


Rings

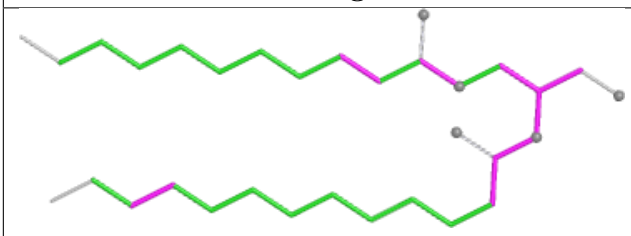
Ligand 7PH F 104



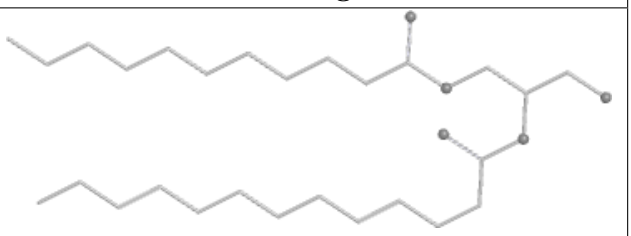
Bond lengths



Bond angles

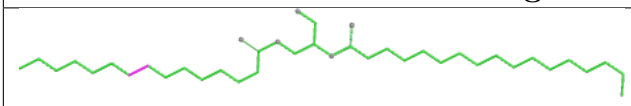


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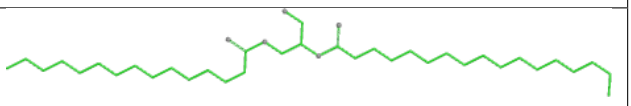


Rings

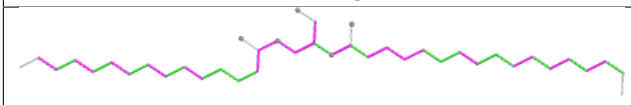
Ligand 2WA F 101



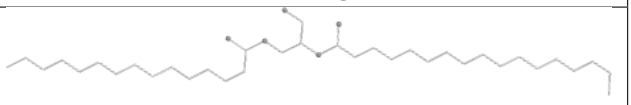
Bond lengths



Bond angles

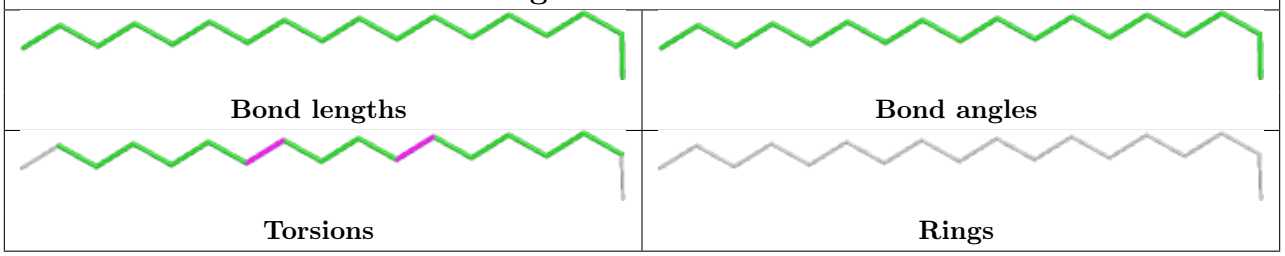


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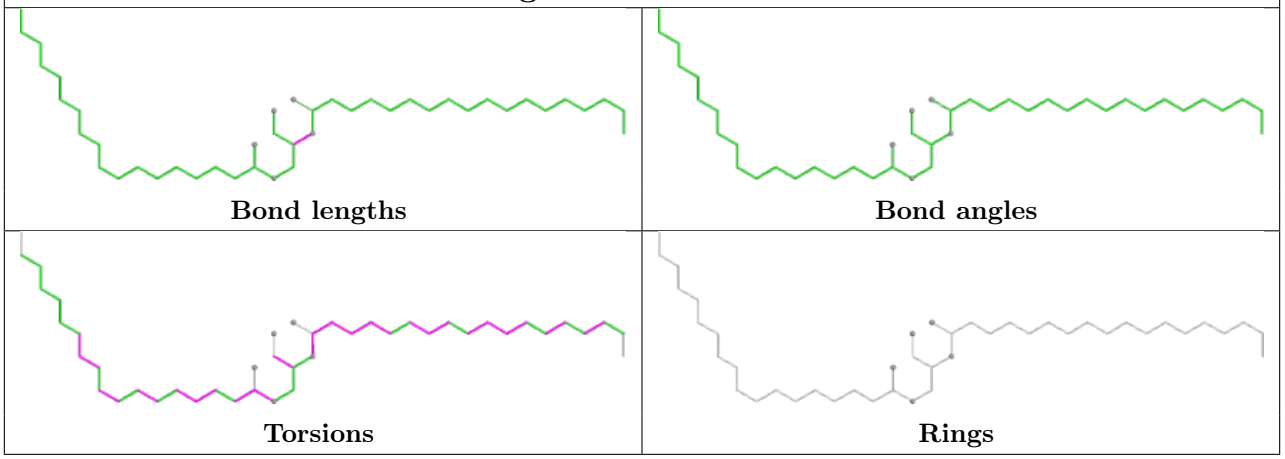


Rings

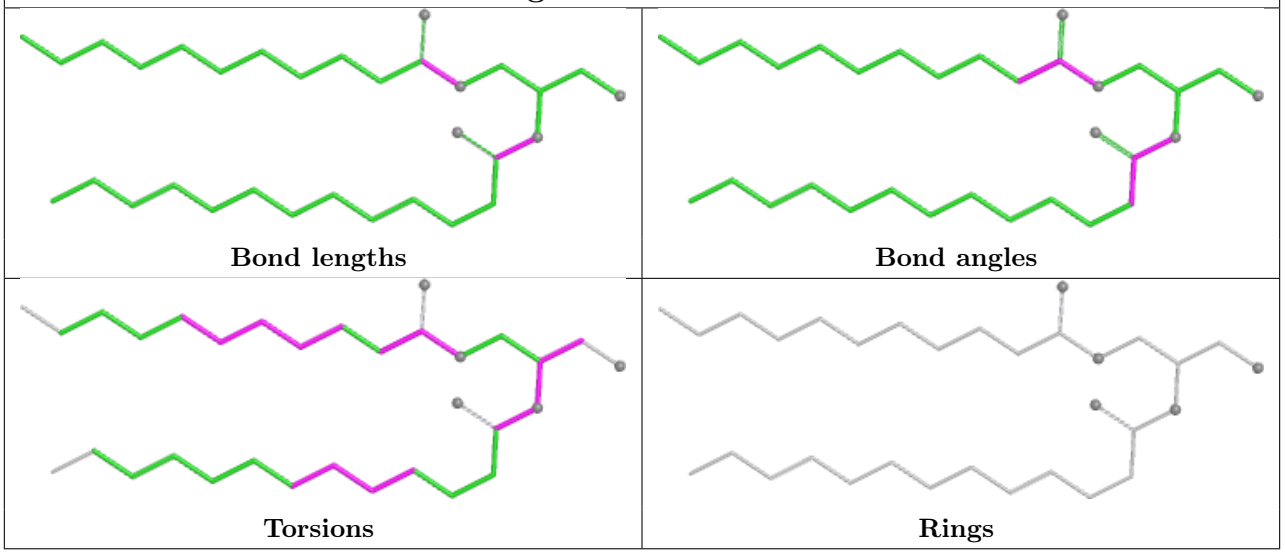
Ligand 8K6 A 306



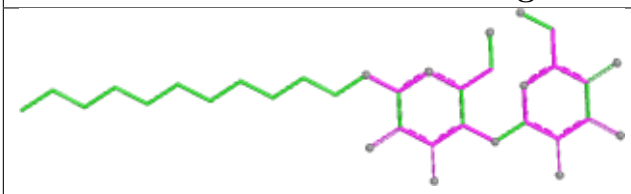
Ligand 3WM E 101



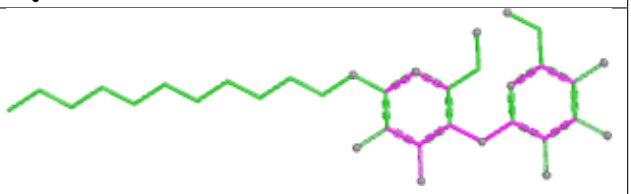
Ligand 7PH B 206



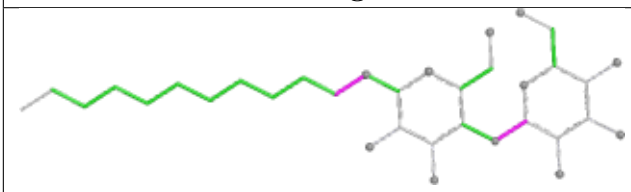
Ligand UMQ B 201



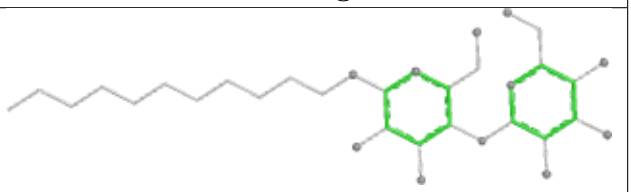
Bond lengths



Bond angles

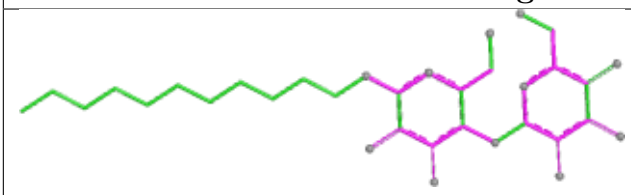


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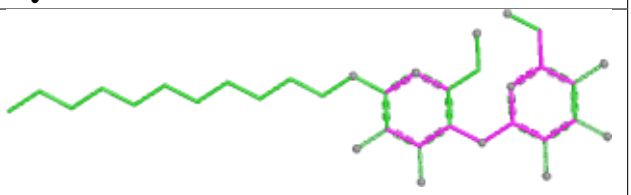


Rings

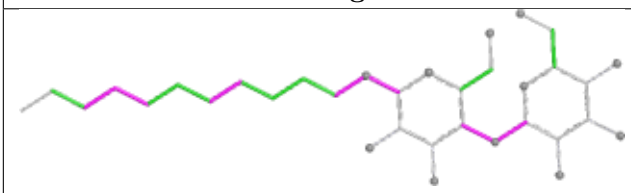
Ligand UMQ A 304



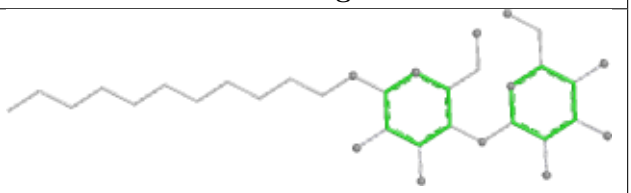
Bond lengths



Bond angles

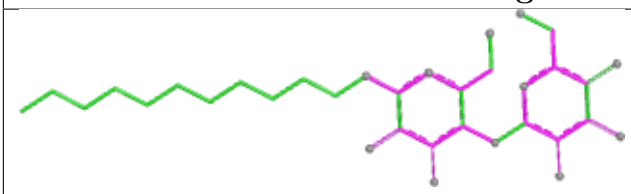


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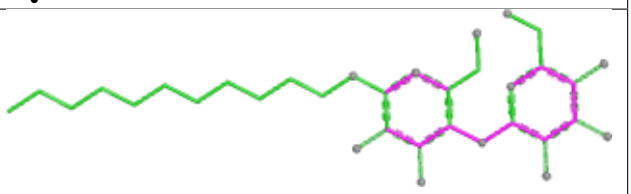


Rings

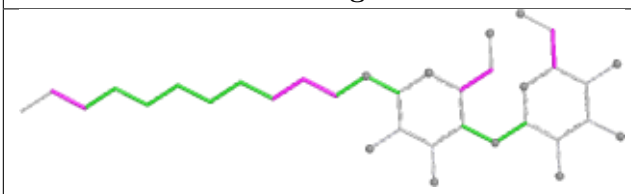
Ligand UMQ G 101



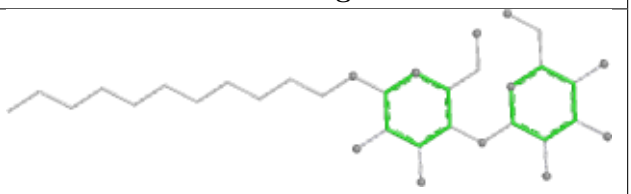
Bond lengths



Bond angles

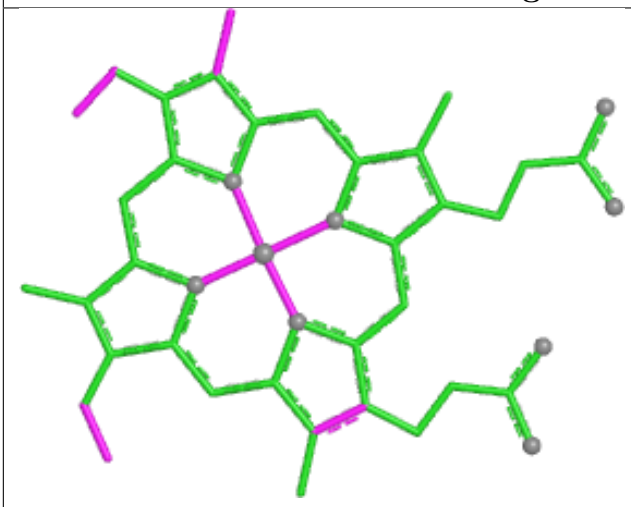


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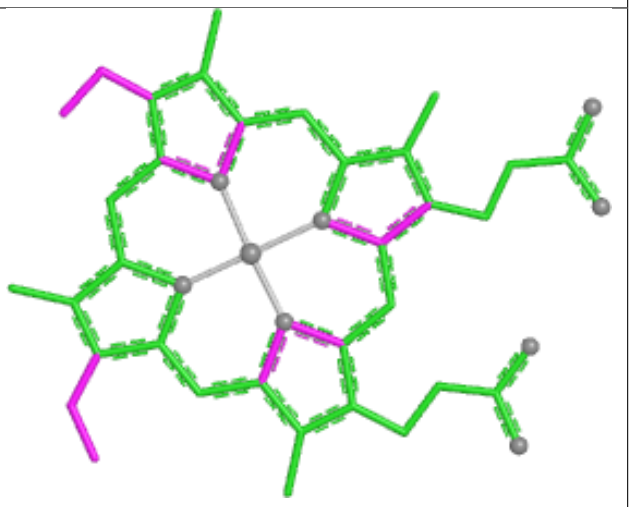


Rings

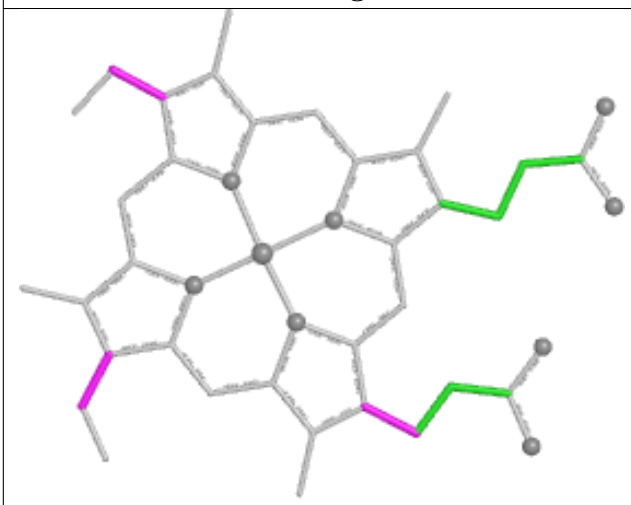
Ligand HEC C 301



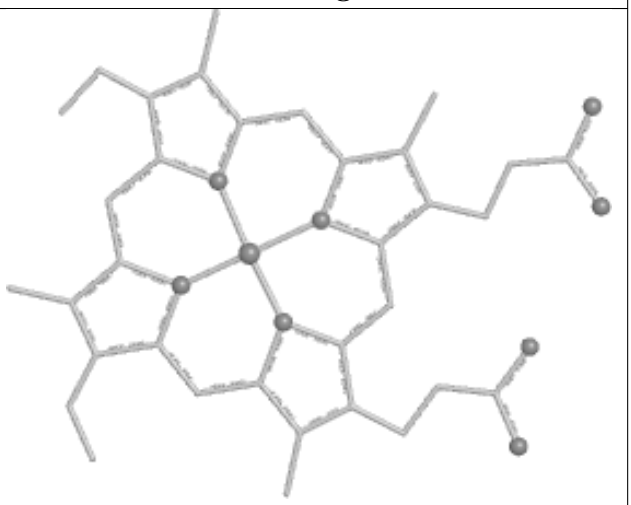
Bond lengths



Bond angles

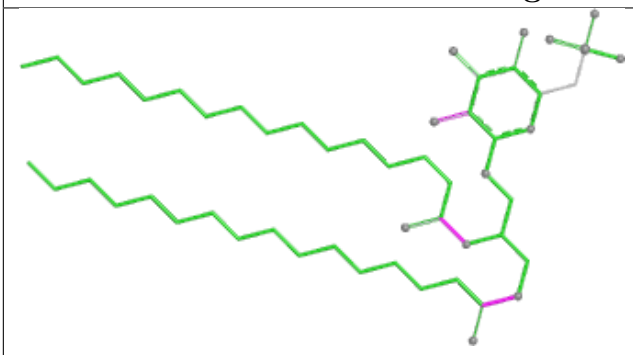


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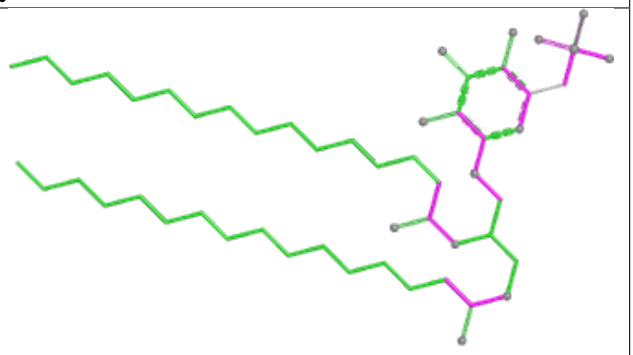


Rings

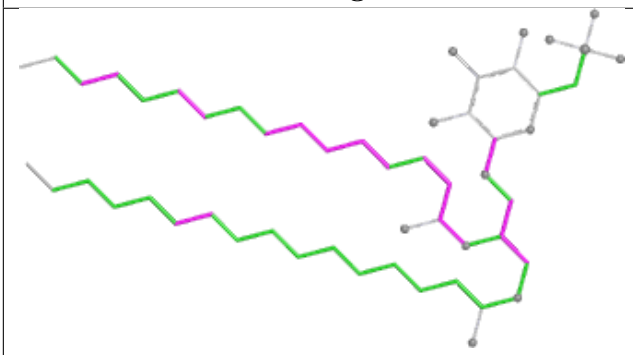
Ligand SQD D 204



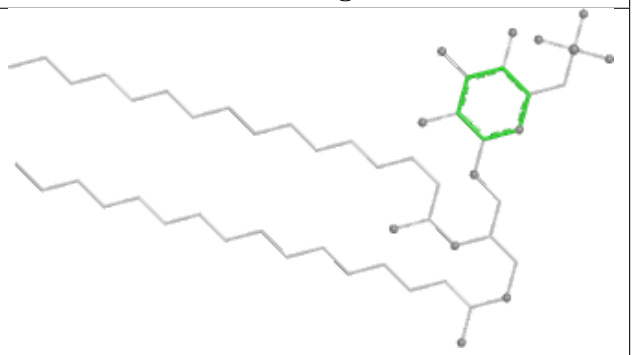
Bond lengths



Bond angles

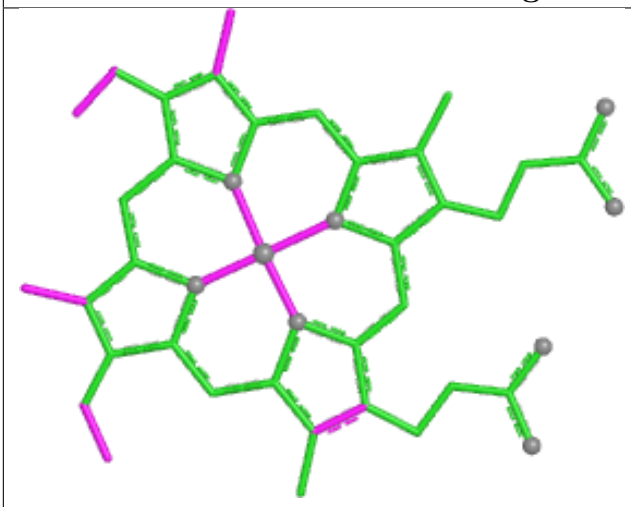


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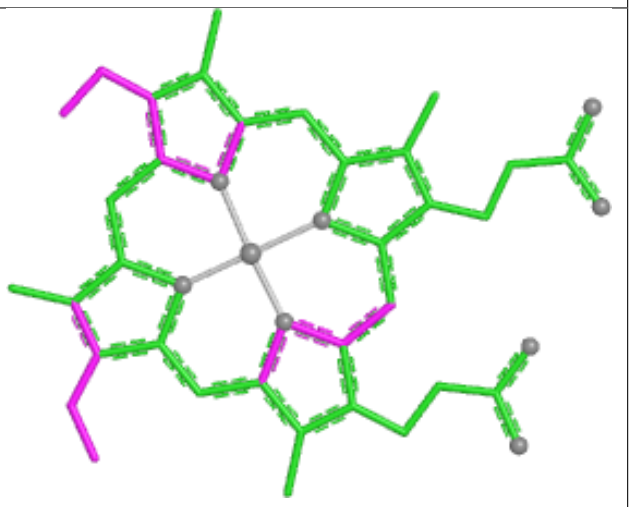


Rings

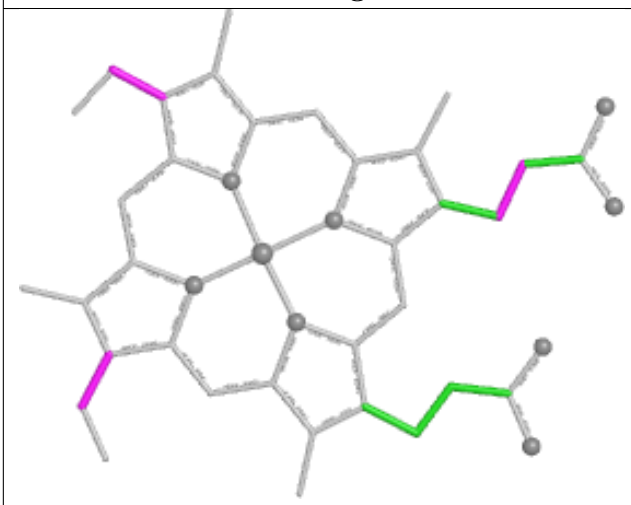
Ligand HEC A 301



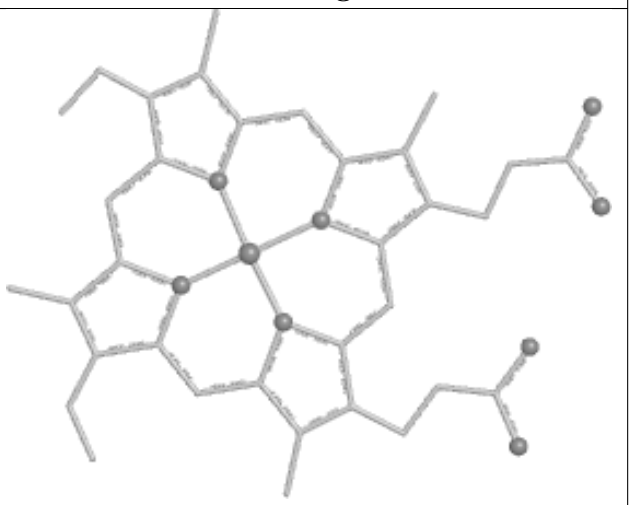
Bond lengths



Bond angles

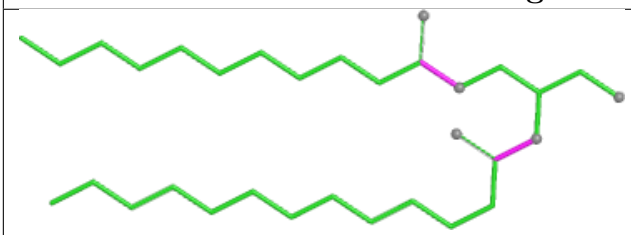


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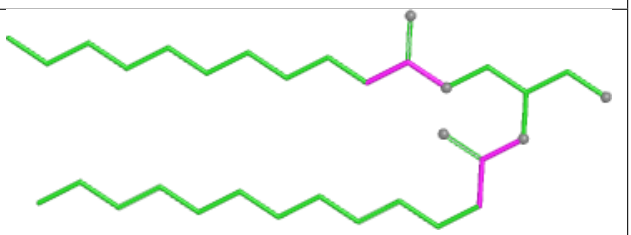


Rings

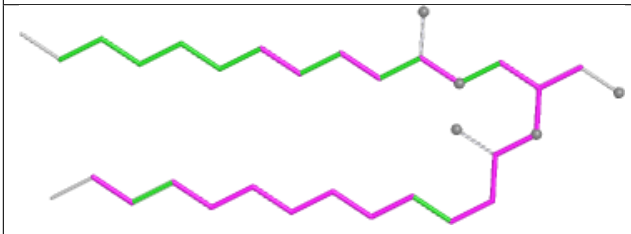
Ligand 7PH C 303



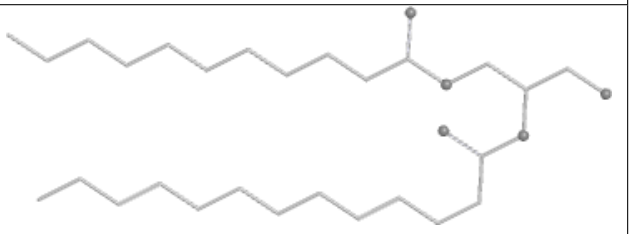
Bond lengths



Bond angles

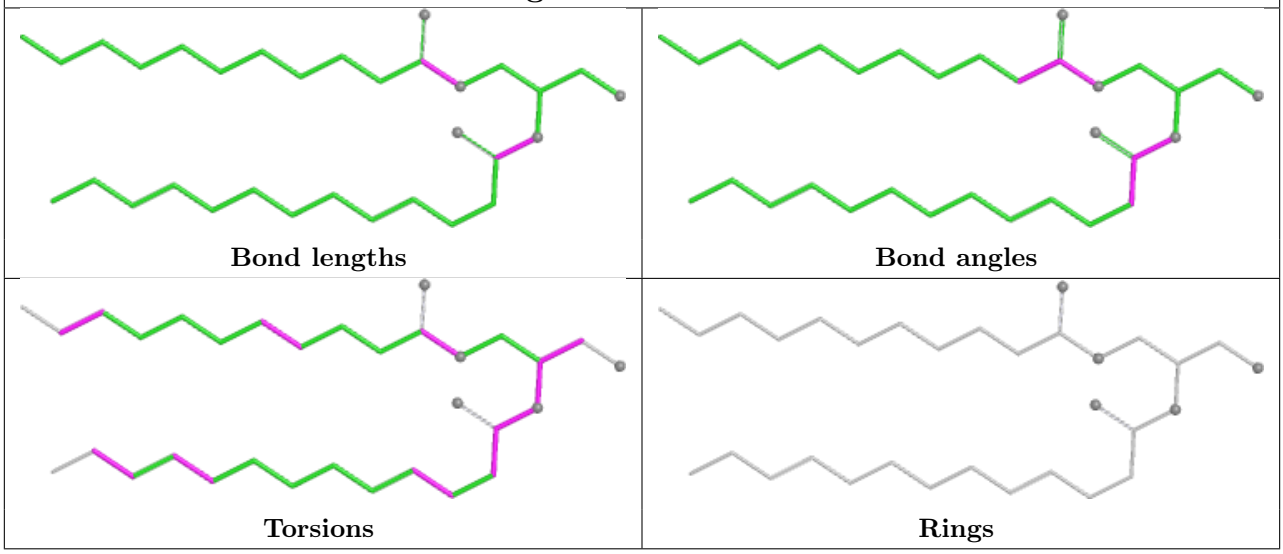


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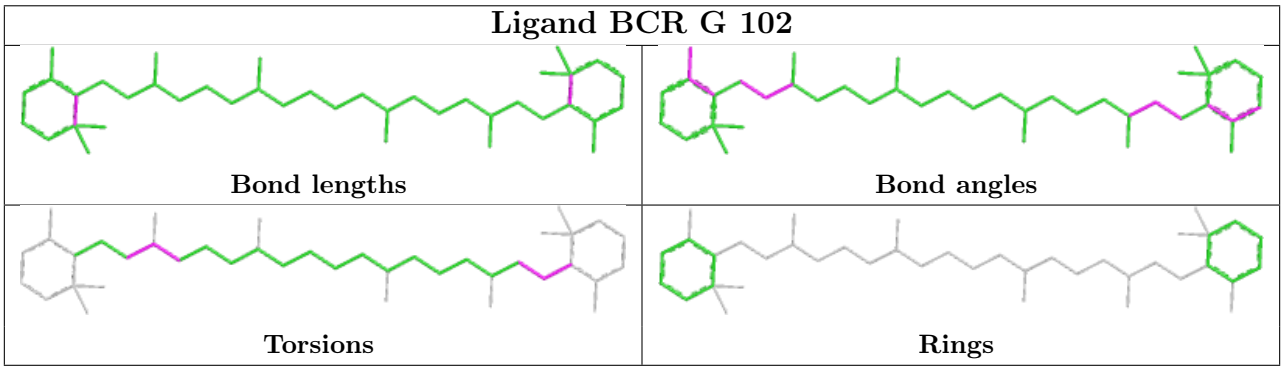


Rings

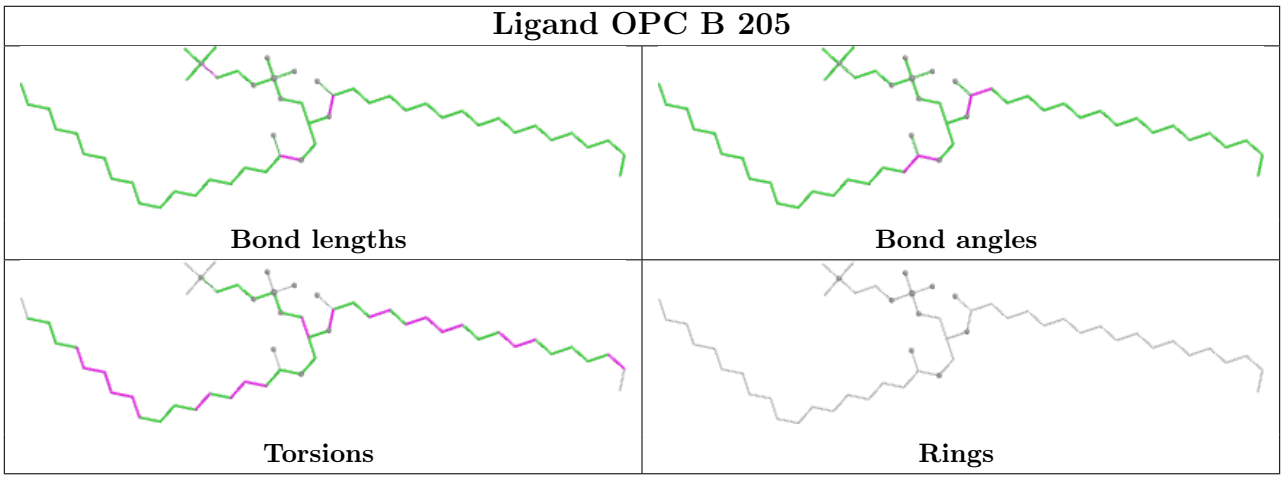
Ligand 7PH D 203



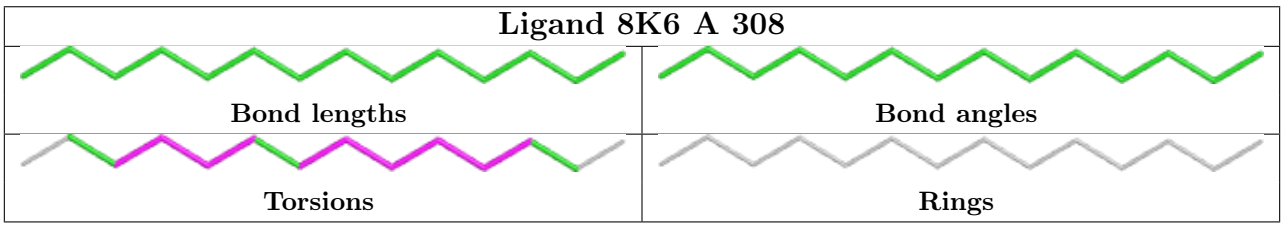
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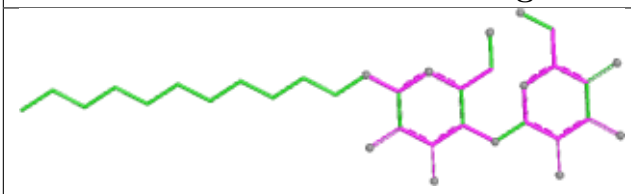
Ligand OPC B 205



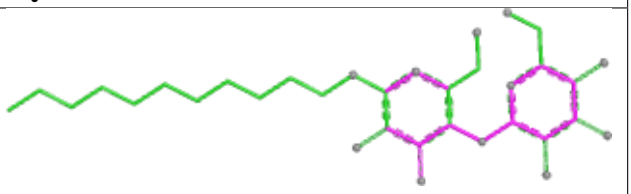
Ligand 8K6 A 308



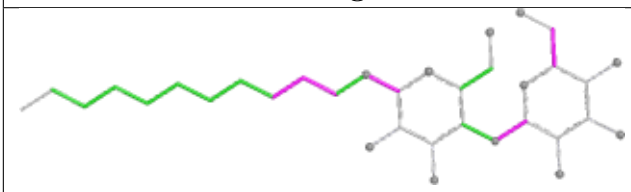
Ligand UMQ D 201



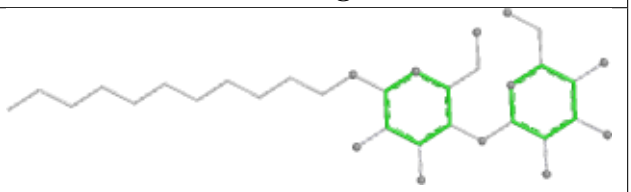
Bond lengths



Bond angles

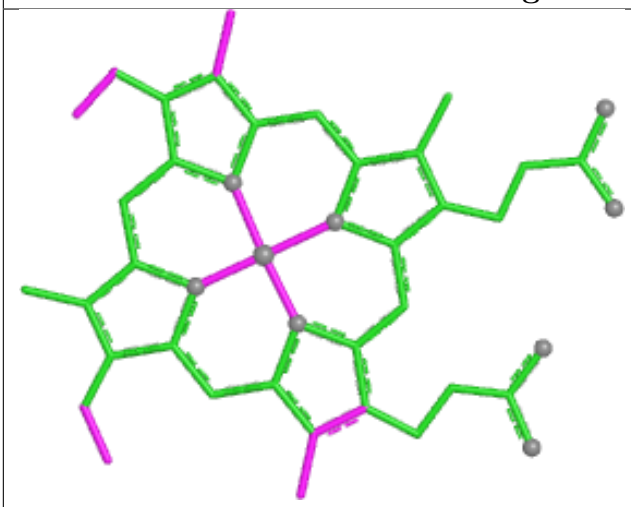


Torsions

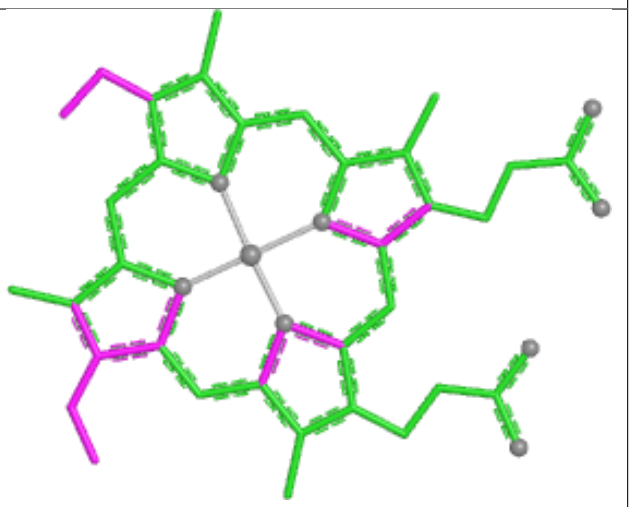


Rings

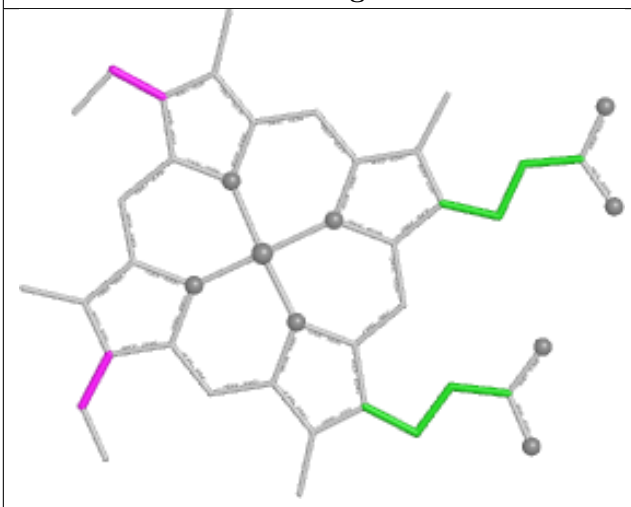
Ligand HEC A 303



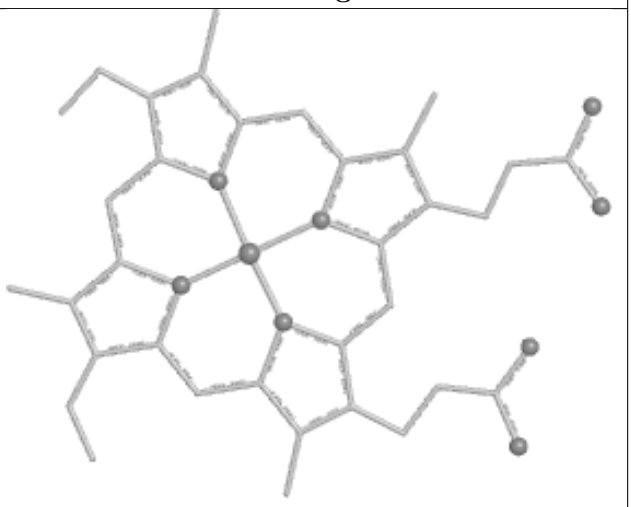
Bond lengths



Bond angles

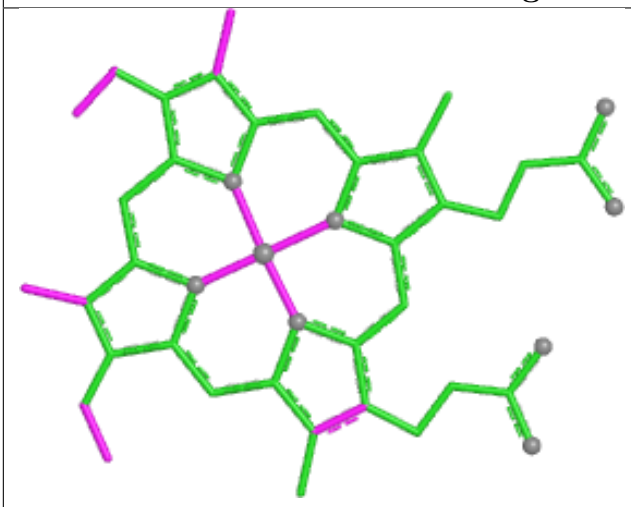


Torsions

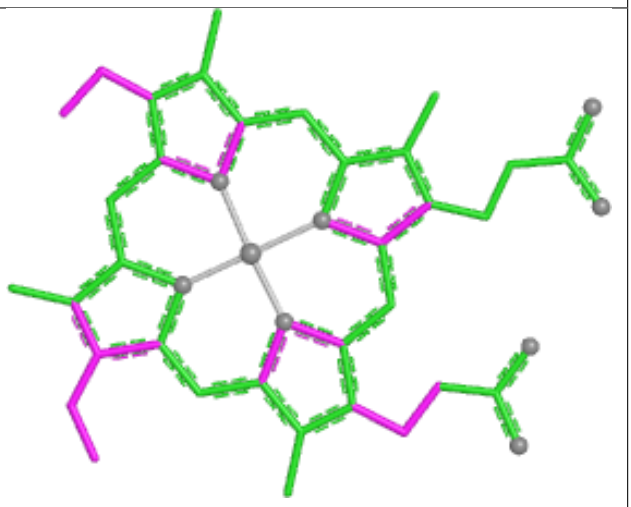


Rings

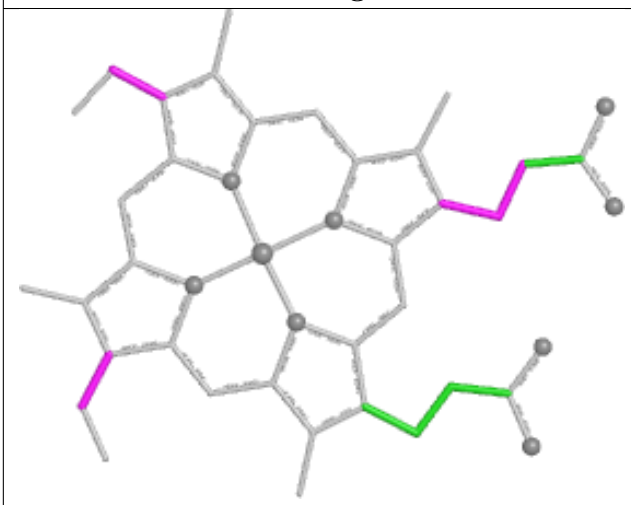
Ligand HEC A 302



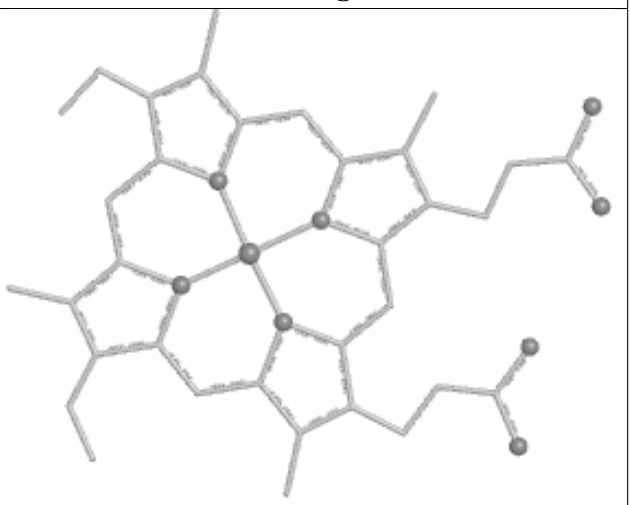
Bond lengths



Bond angles



Torsions



Rings

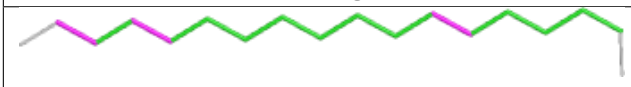
Ligand 8K6 A 307



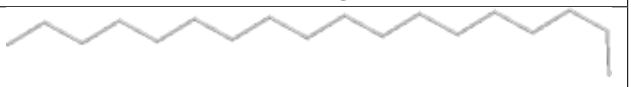
Bond lengths



Bond angles

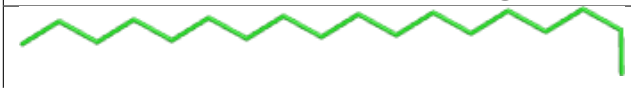


Torsions

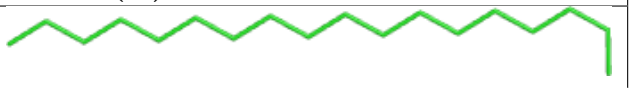


Rings

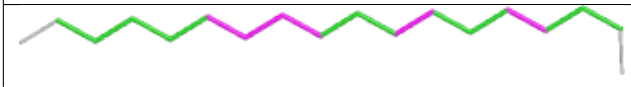
Ligand 8K6 B 202 (A)



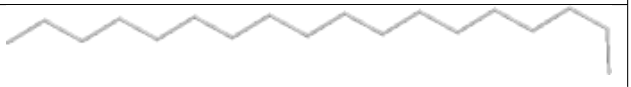
Bond lengths



Bond angles

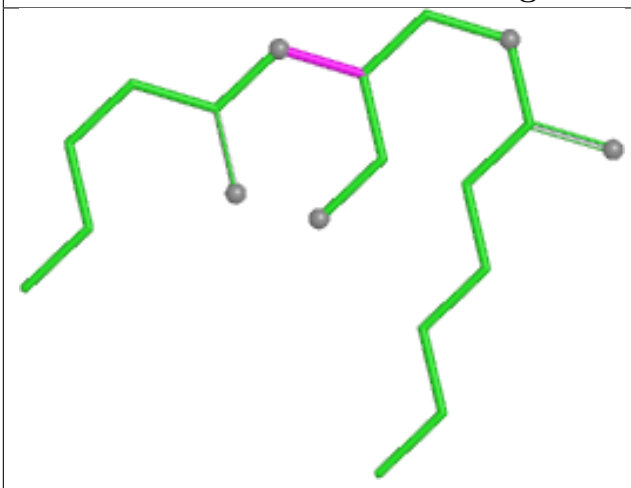


Torsions

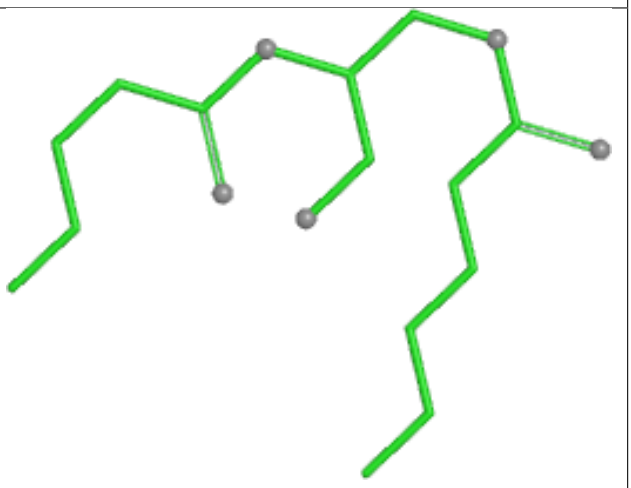


Rings

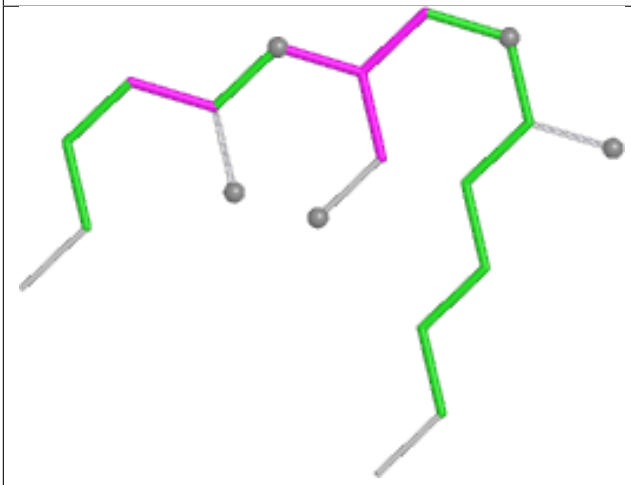
Ligand 2WD D 206



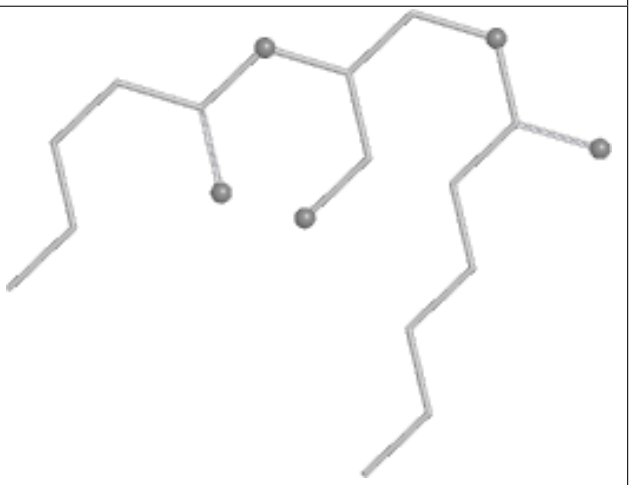
Bond lengths



Bond angles

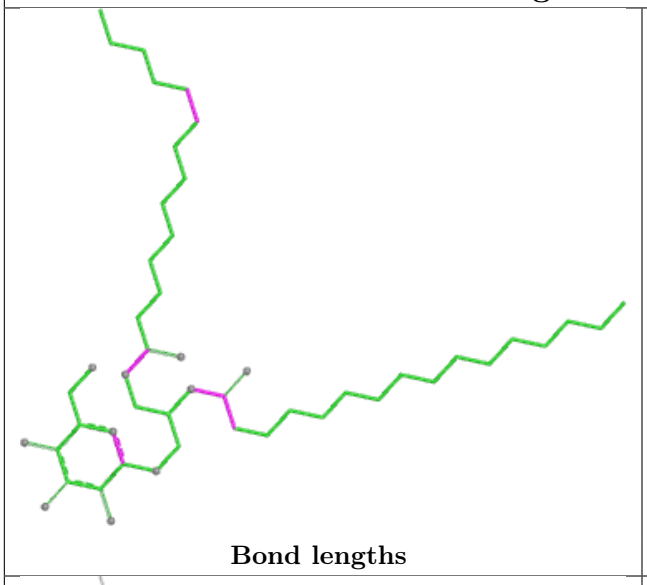


Torsions

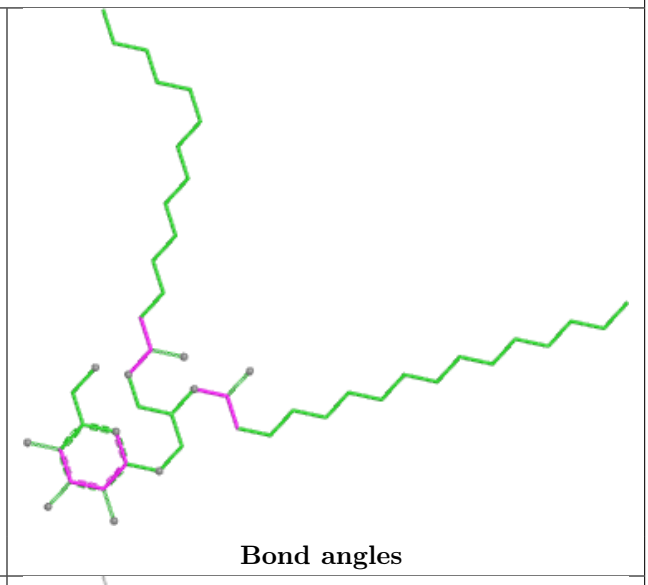


Rings

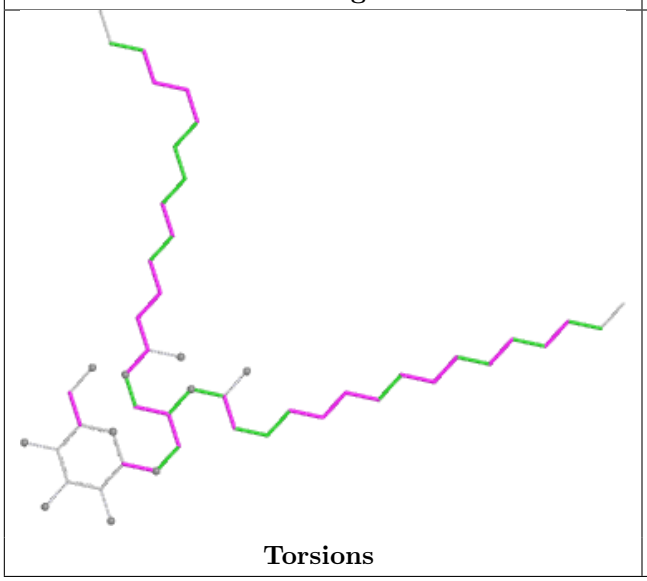
Ligand 1O2 F 103



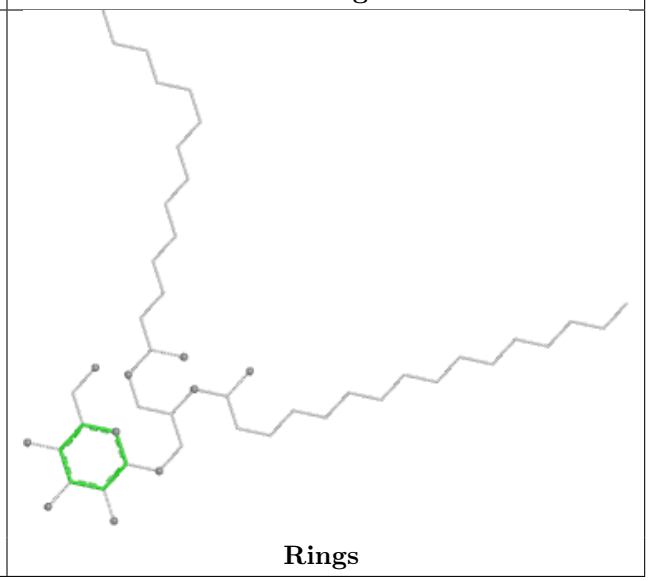
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	214/215 (99%)	-0.03	5 (2%) 61 57	43, 59, 97, 186	0
2	B	159/160 (99%)	0.30	12 (7%) 20 18	52, 77, 124, 195	0
3	C	281/333 (84%)	0.76	44 (15%) 5 4	57, 85, 191, 249	0
4	D	166/179 (92%)	1.92	65 (39%) 1 0	50, 145, 205, 239	0
5	E	31/31 (100%)	1.11	7 (22%) 2 2	81, 98, 123, 153	0
6	F	32/34 (94%)	0.72	3 (9%) 14 12	69, 87, 131, 169	0
7	G	37/37 (100%)	0.64	5 (13%) 7 5	57, 74, 144, 155	0
8	H	29/29 (100%)	0.29	2 (6%) 23 20	59, 71, 100, 144	0
All	All	949/1018 (93%)	0.70	143 (15%) 5 4	43, 81, 185, 249	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	98	ALA	11.5
4	D	50	ALA	9.1
4	D	99	ILE	7.7
3	C	192	SER	6.6
5	E	10	PHE	6.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

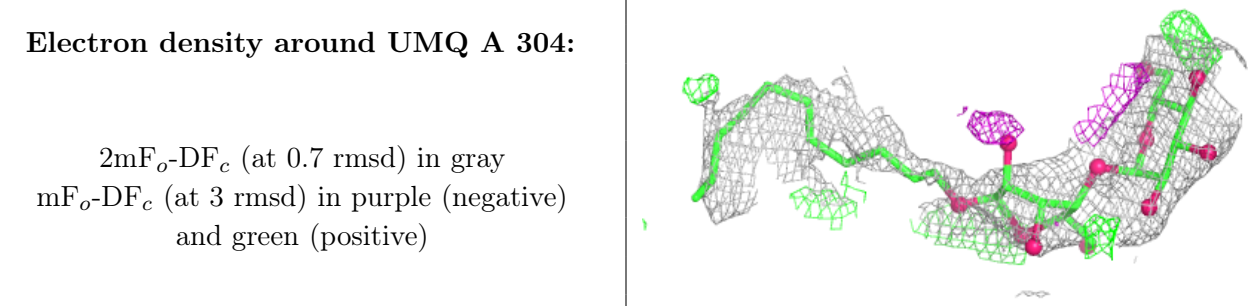
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

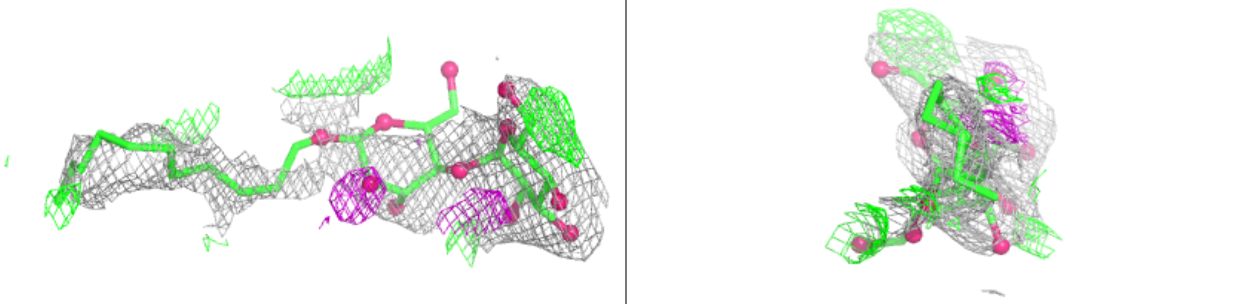
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	UMQ	A	304	34/34	0.68	0.25	127,146,201,254	0
10	UMQ	G	101	34/34	0.72	0.20	81,173,199,284	0
20	2WD	D	206	19/19	0.72	0.26	75,123,142,145	0
23	OCT	F	102	8/8	0.74	0.29	101,106,110,116	0
10	UMQ	D	201	34/34	0.78	0.22	102,210,248,264	0
11	7PH	B	206	32/38	0.81	0.23	77,132,182,184	0
11	7PH	C	303	32/38	0.81	0.26	73,117,149,150	0
24	1O2	F	103	49/53	0.81	0.20	80,127,216,220	0
12	8K6	A	306	18/18	0.82	0.23	93,113,147,148	0
13	2WM	A	309	44/44	0.83	0.22	70,96,152,158	0
12	8K6	A	307	18/18	0.84	0.21	76,108,124,127	0
12	8K6	B	202[A]	18/18	0.84	0.24	47,102,122,122	18
11	7PH	F	104	32/38	0.84	0.21	81,101,172,175	0
12	8K6	A	308	14/18	0.85	0.21	62,82,95,99	0
11	7PH	A	305	32/38	0.85	0.24	93,126,189,190	0
10	UMQ	B	201	34/34	0.85	0.18	64,114,151,224	0
18	SQD	D	204	54/54	0.86	0.20	73,116,159,177	0
10	UMQ	B	203[B]	34/34	0.86	0.28	80,103,132,144	34
17	MYS	D	202	15/15	0.88	0.22	93,107,121,126	0
16	CD	C	302	1/1	0.89	0.11	136,136,136,136	1
11	7PH	D	203	32/38	0.89	0.16	54,81,153,157	0
22	2WA	F	101	40/40	0.90	0.20	70,111,169,182	0
15	OPC	B	205	54/55	0.92	0.17	55,92,121,137	0
25	BCR	G	102	40/40	0.92	0.15	49,74,116,122	0
21	3WM	E	101	44/44	0.93	0.17	60,97,122,125	0
14	CLA	B	204	65/65	0.94	0.12	59,79,107,117	0
9	HEC	C	301	43/43	0.98	0.12	46,69,96,113	0
9	HEC	A	302	43/43	0.98	0.09	34,57,71,76	0
9	HEC	A	303	43/43	0.98	0.09	47,66,85,95	0
9	HEC	A	301	43/43	0.99	0.09	31,50,65,78	0
19	FES	D	205	4/4	0.99	0.07	96,97,100,102	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 UMQ A 304:

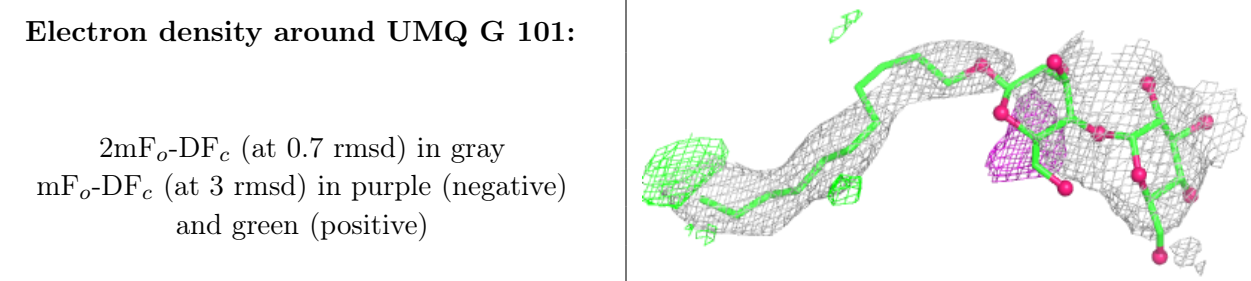
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

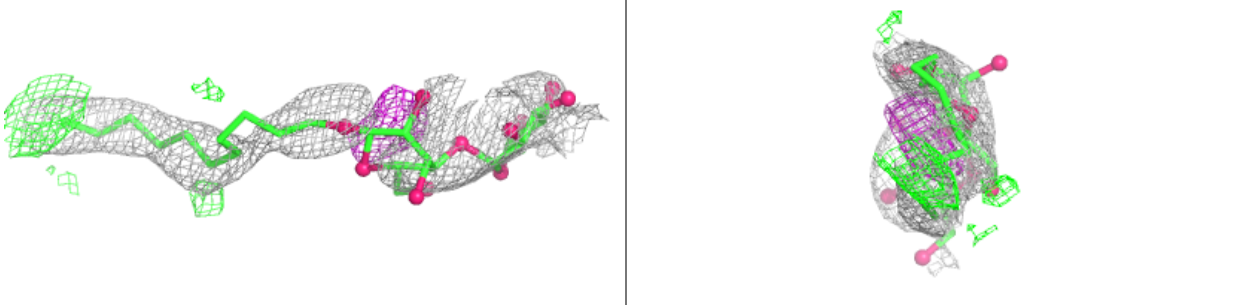




Electron density around UMQ G 101:

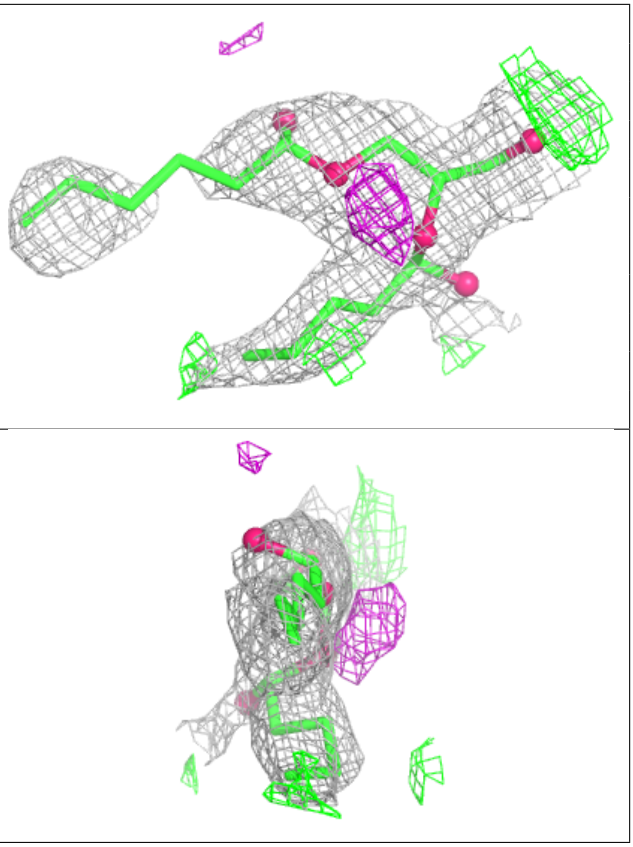
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





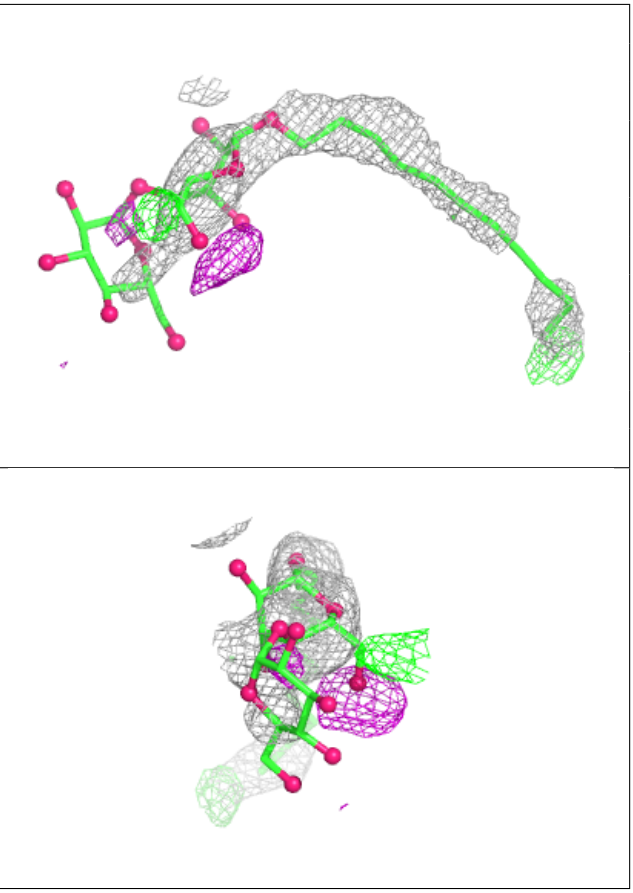
Electron density around 2WD D 206:

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



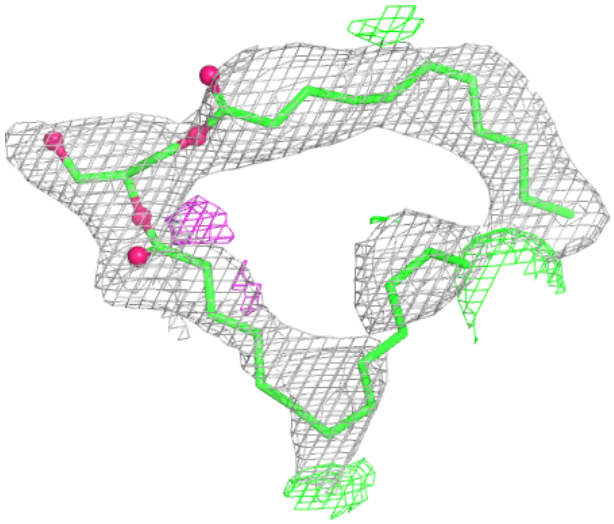
Electron density around UMQ D 201:

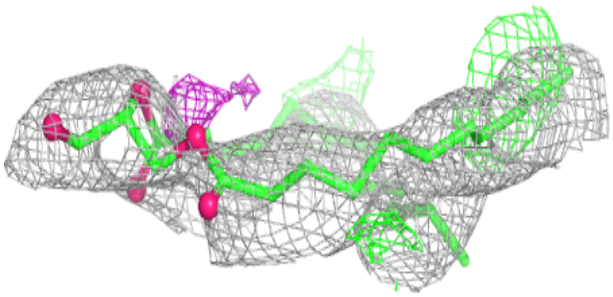
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

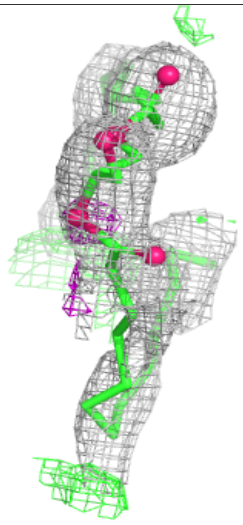


Electron density around 7PH B 206:

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

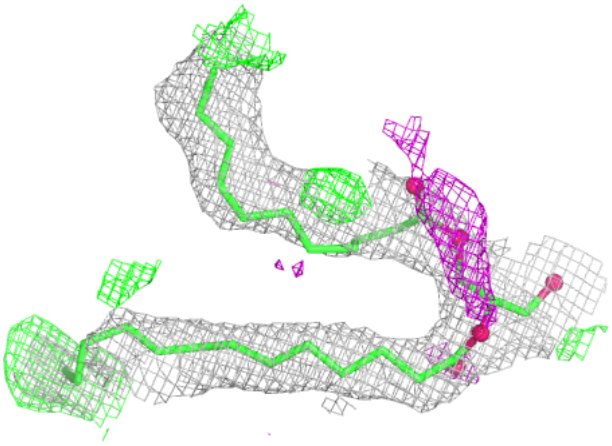


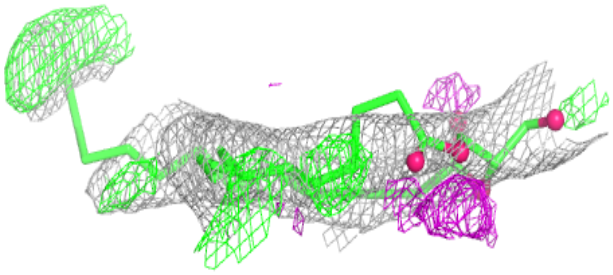


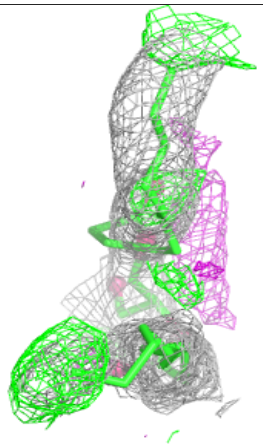


Electron density around 7PH C 303:

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

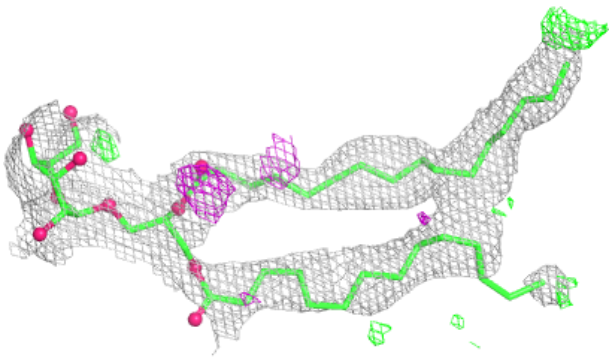


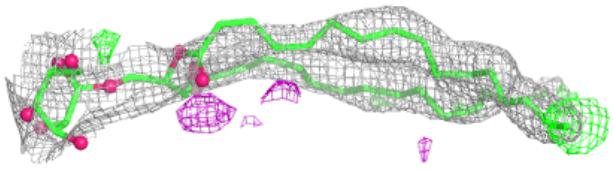


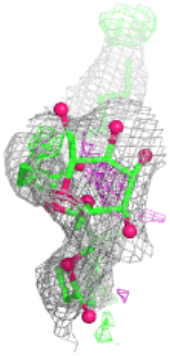


Electron density around 1O2 F 103:

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

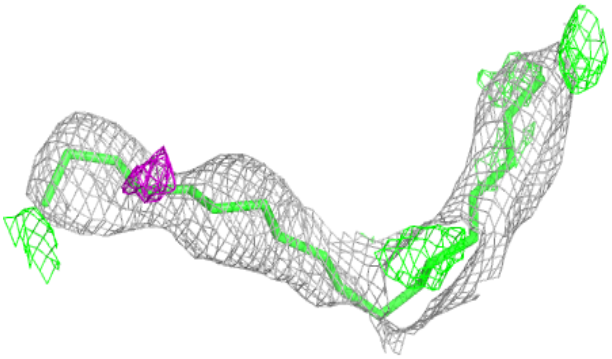


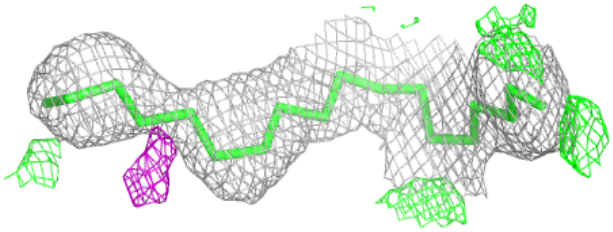


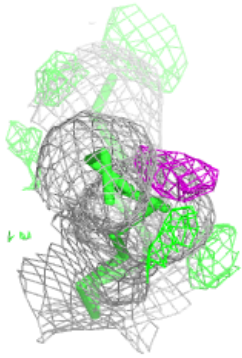


Electron density around 8K6 A 306:

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

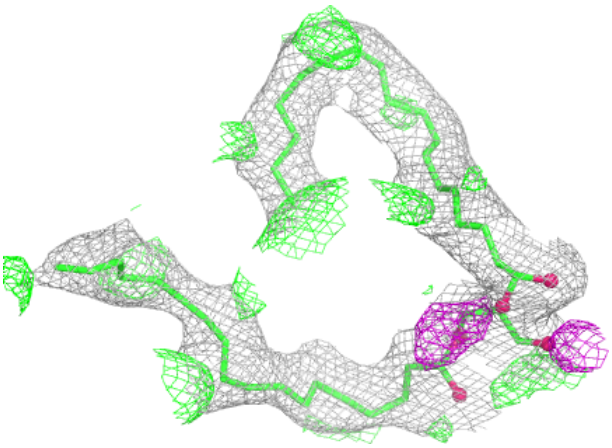


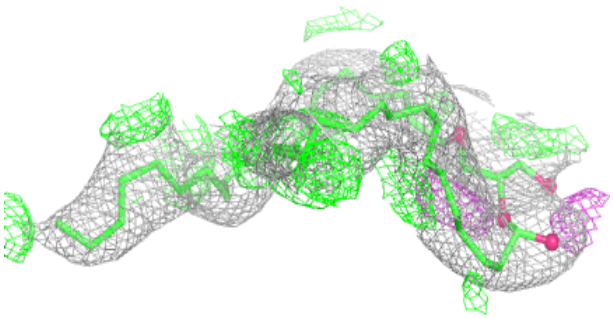


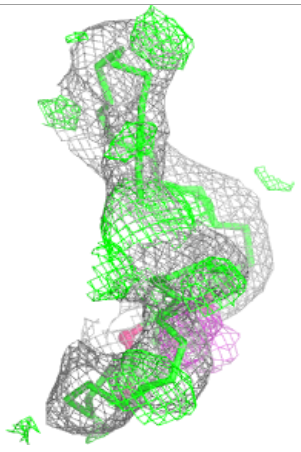


Electron density around 2WM A 309:

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

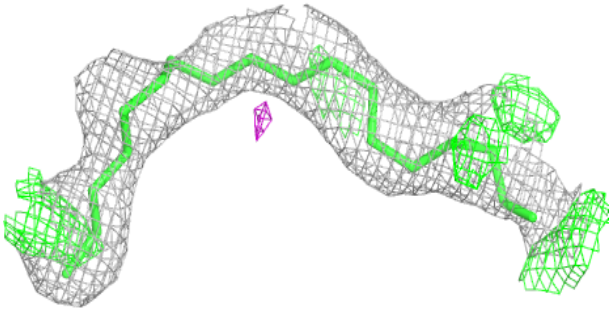


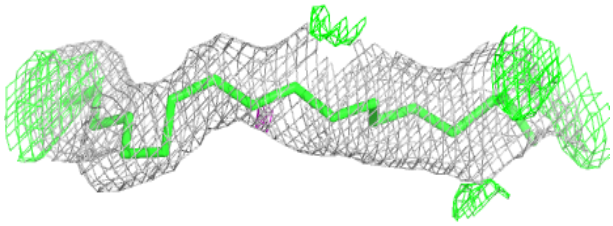


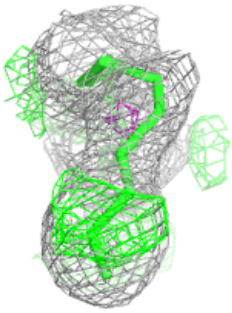


Electron density around 8K6 A 307:

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

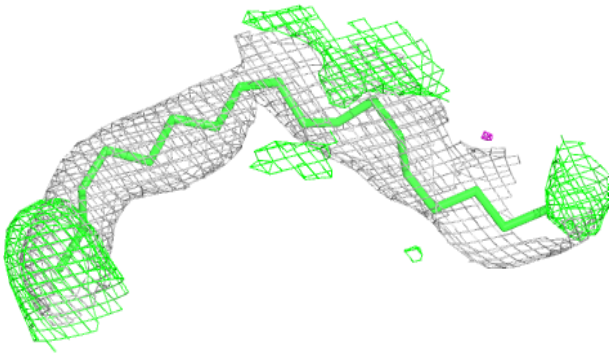


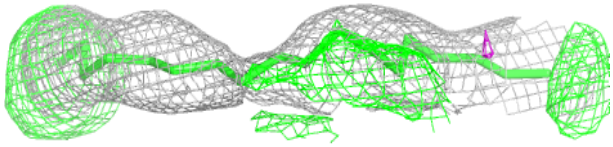


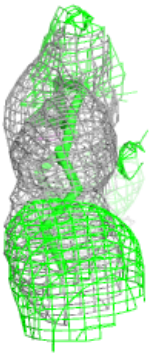


Electron density around 8K6 B 202 (A):

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

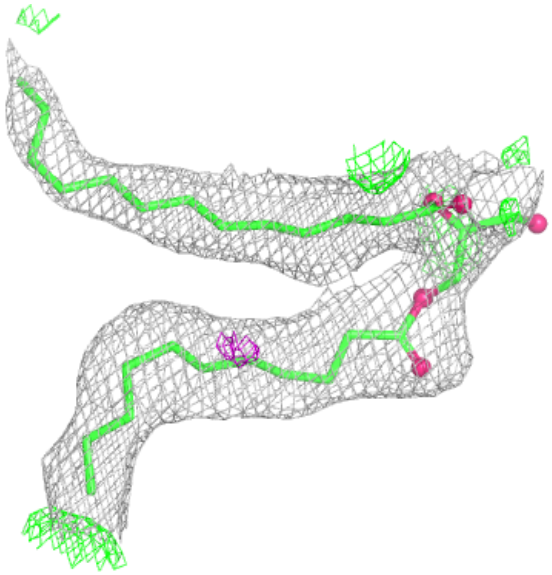


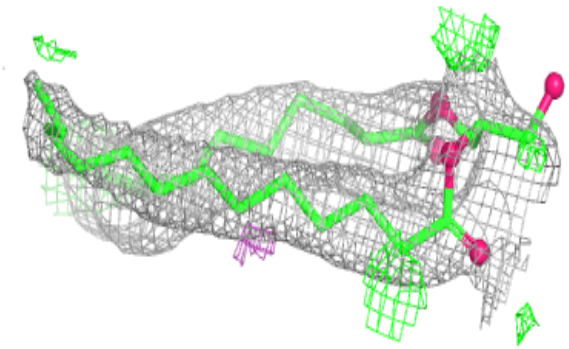


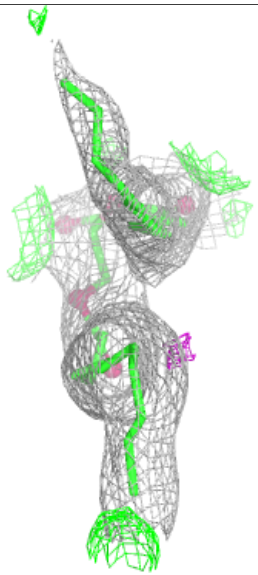


Electron density around 7PH F 104:

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

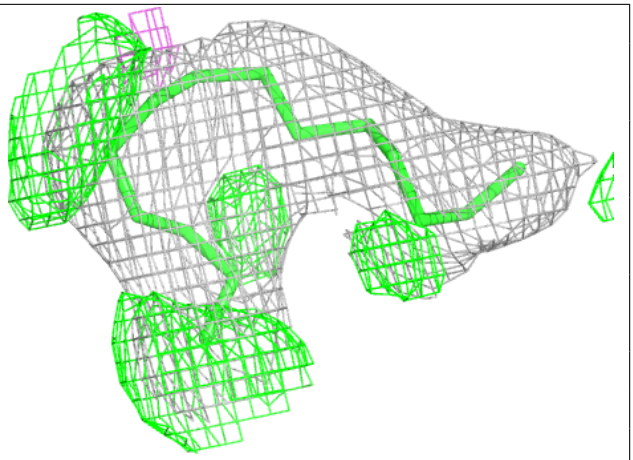


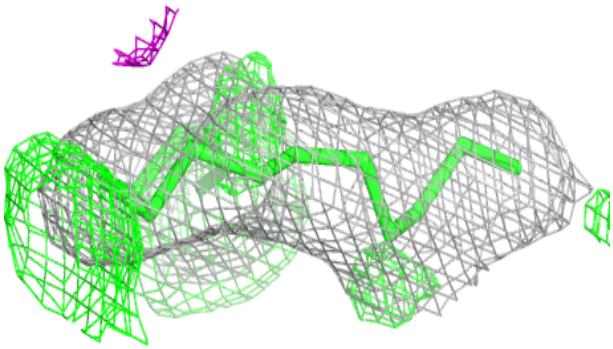


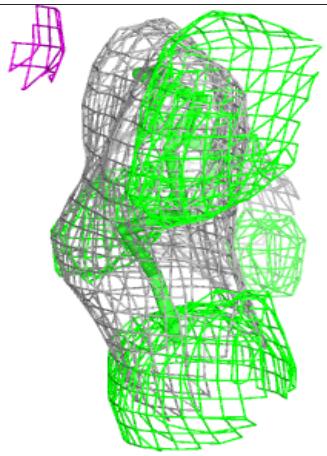


Electron density around 8K6 A 308:

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

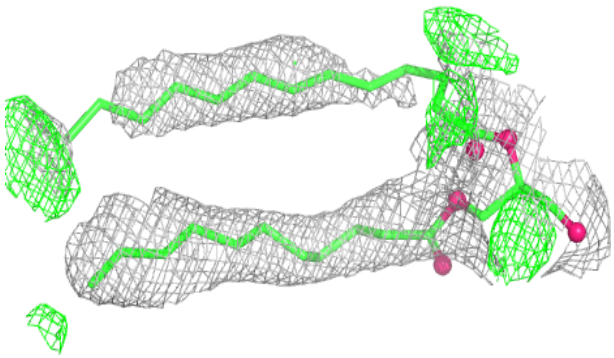


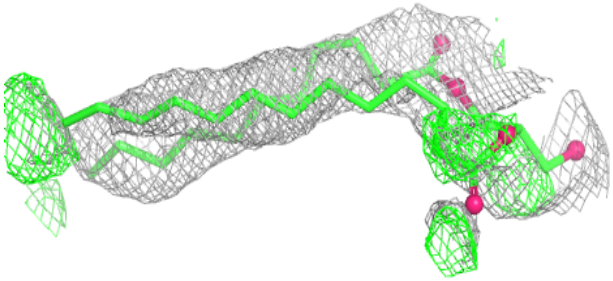


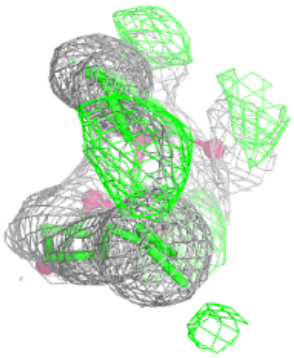


Electron density around 7PH A 305:

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

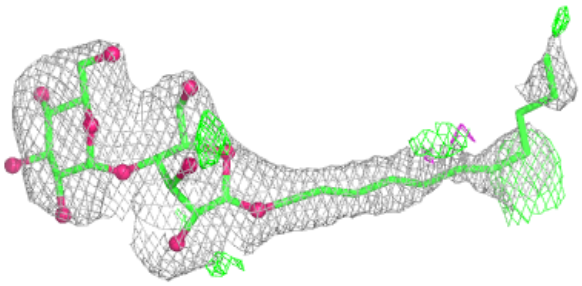


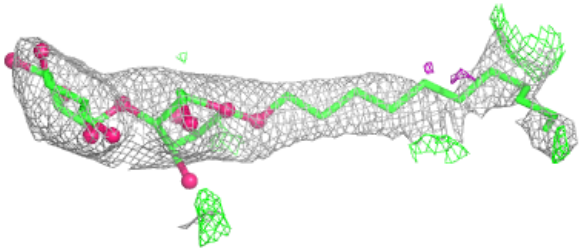


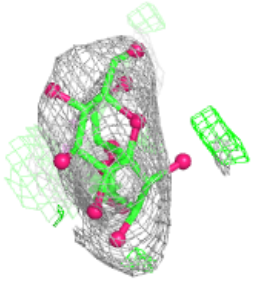


Electron density around UMQ B 201:

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

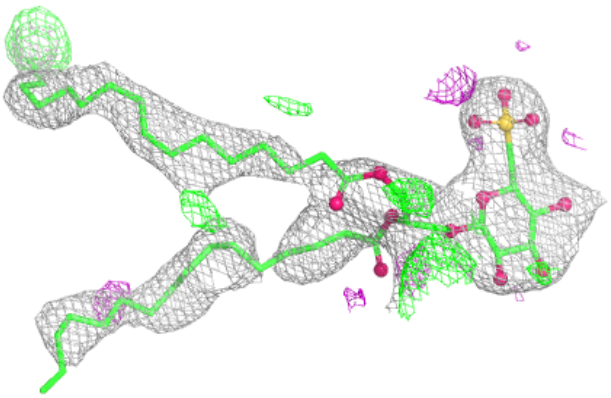


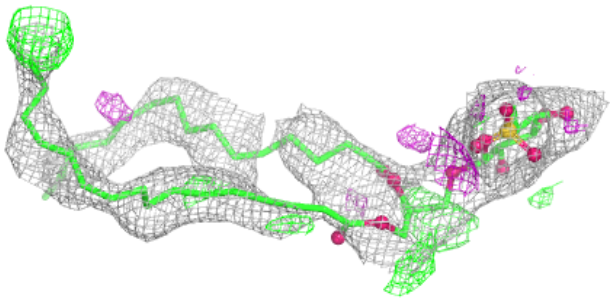


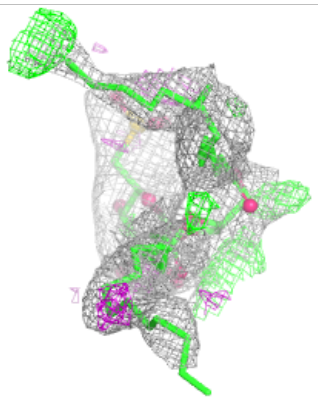


Electron density around SQD D 204:

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

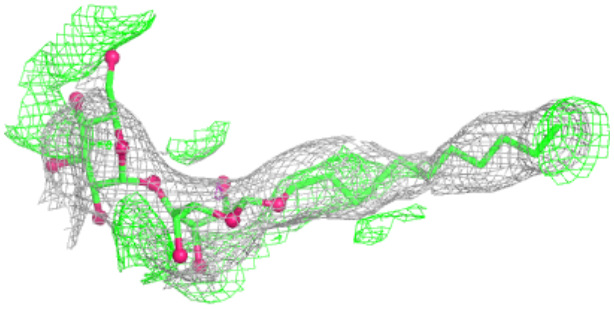


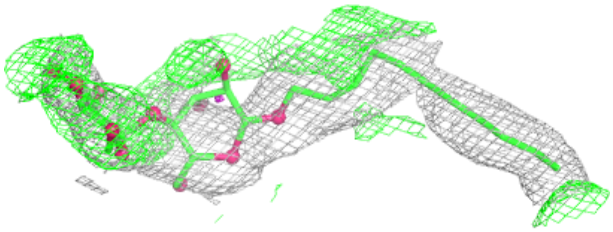


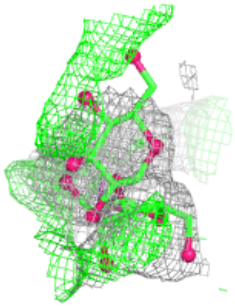


Electron density around UMQ B 203 (B):

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

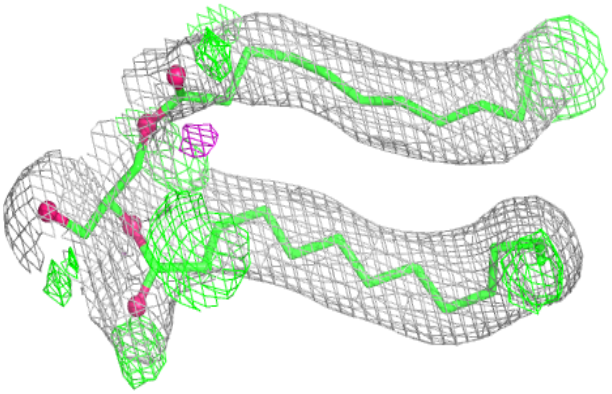


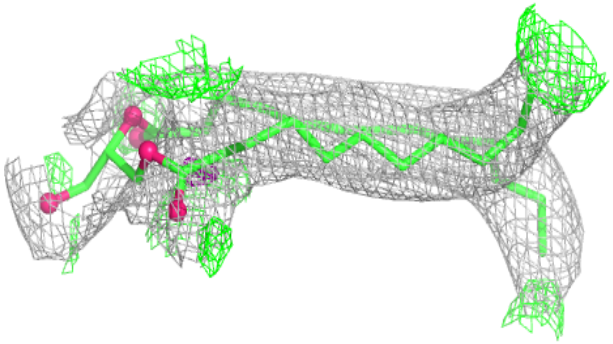


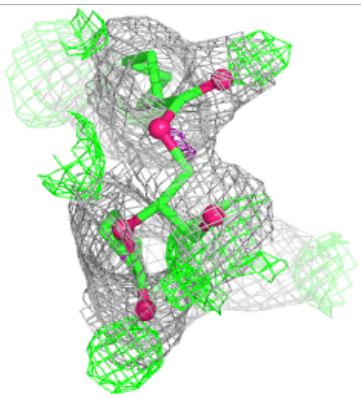


Electron density around 7PH D 203:

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

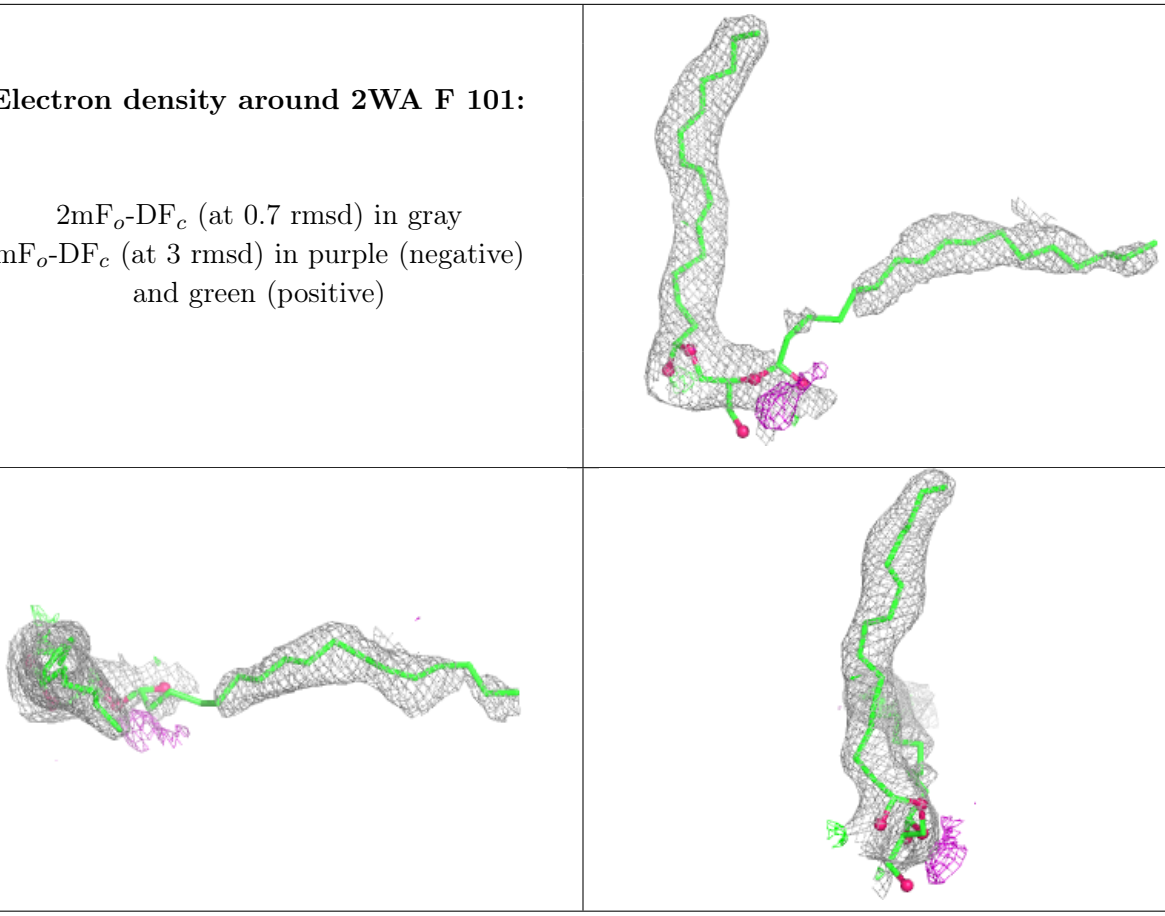






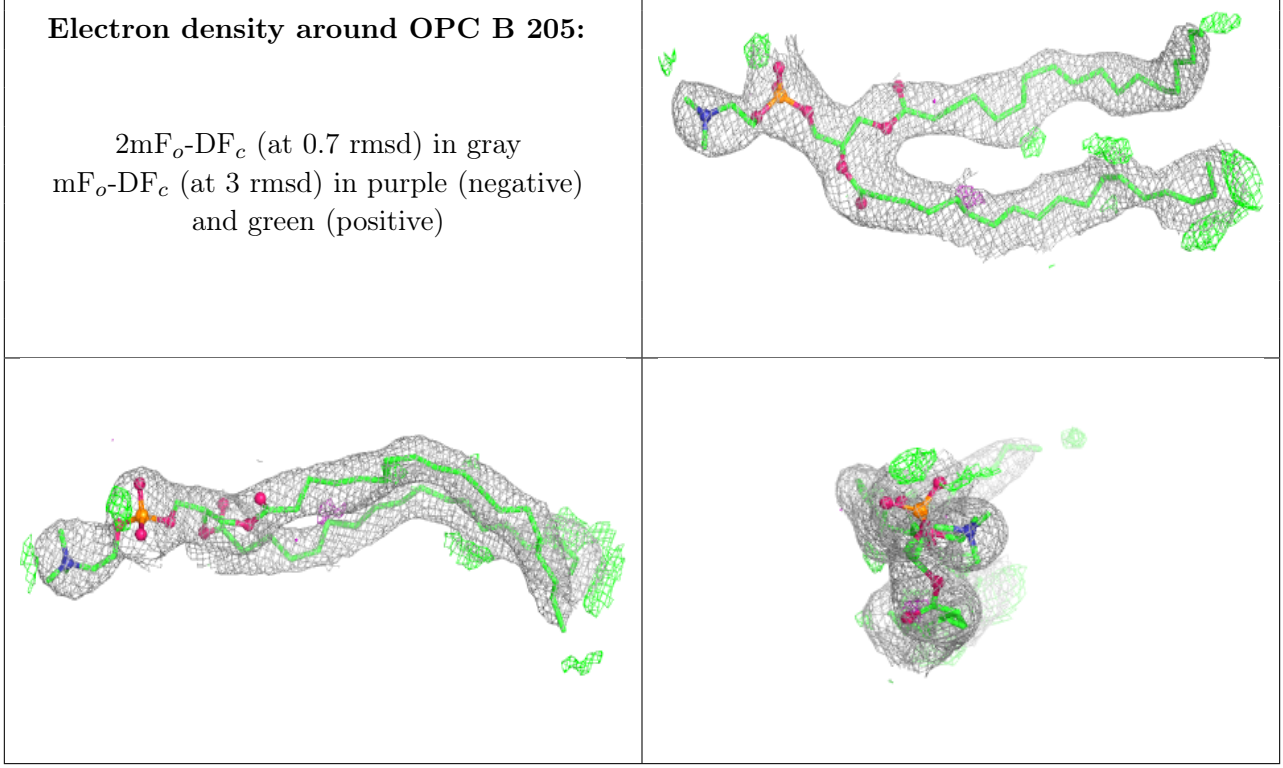
Electron density around 2WA F 101:

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



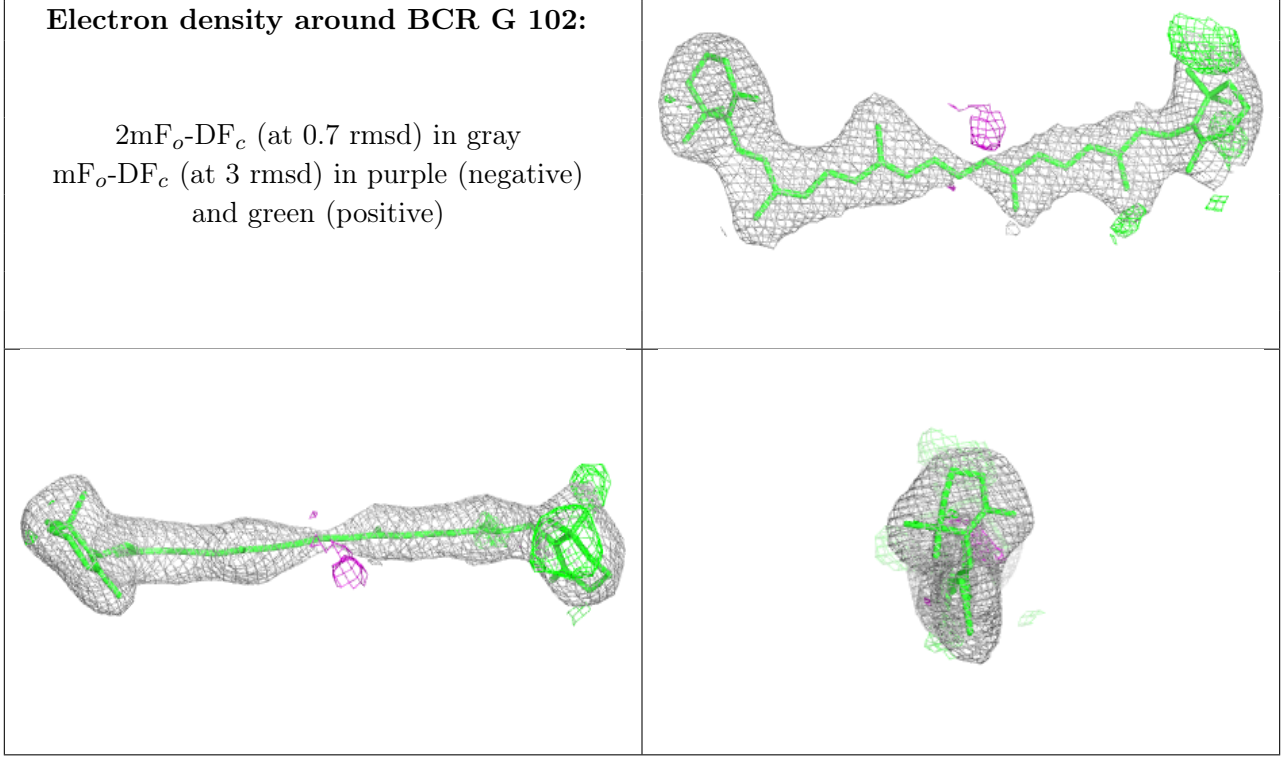
Electron density around OPC B 205:

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



Electron density around BCR G 102:

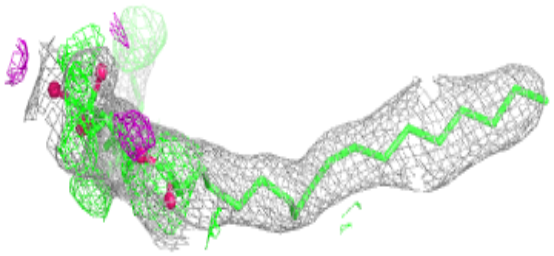
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

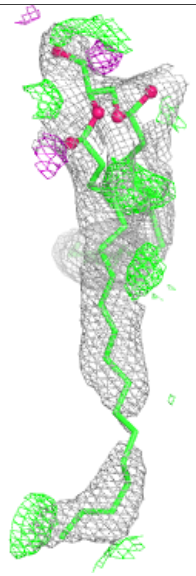


Electron density around 3WM E 101:

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

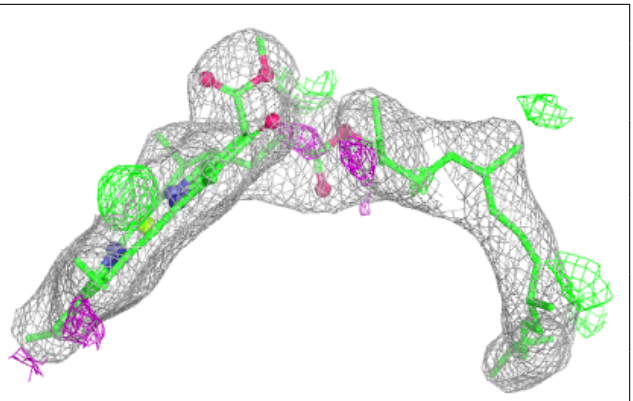


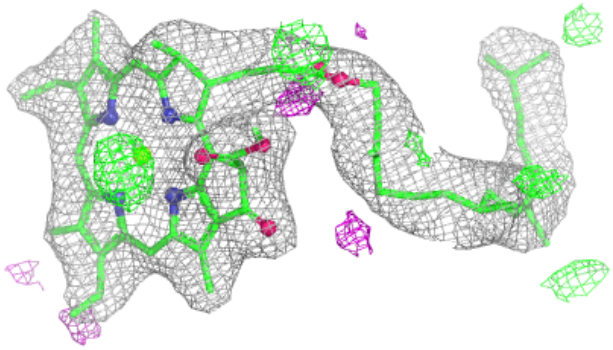


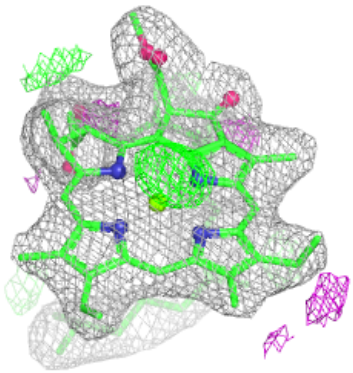


Electron density around CLA B 204:

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

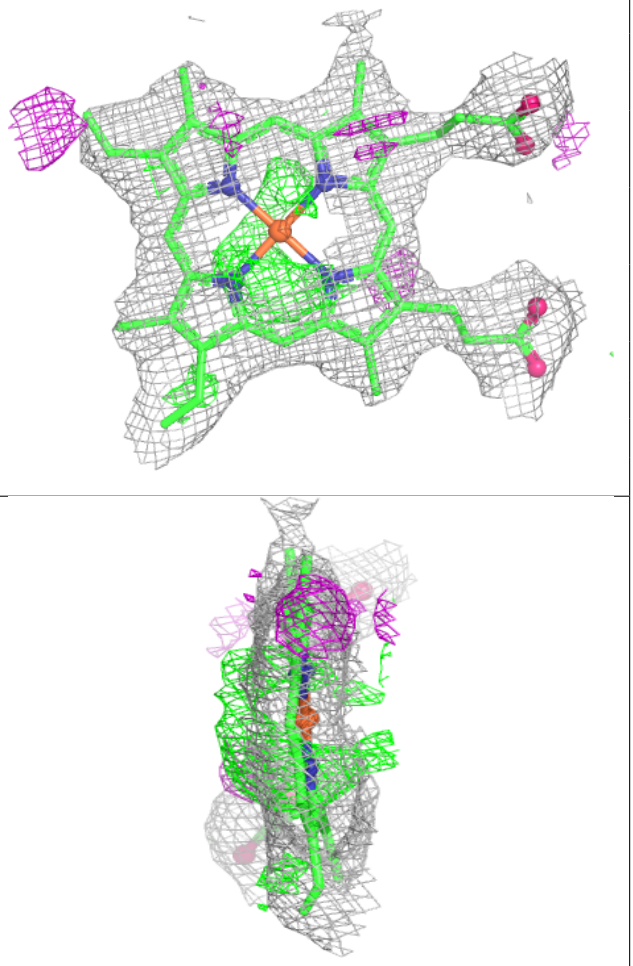


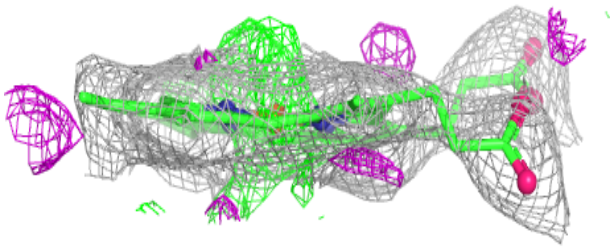




Electron density around HEC C 301:

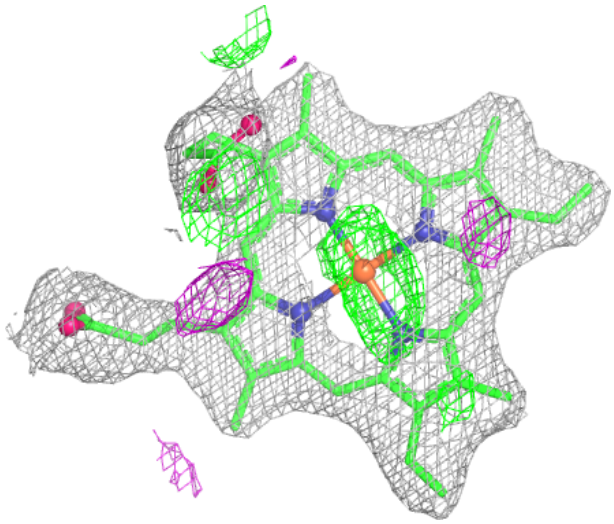
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

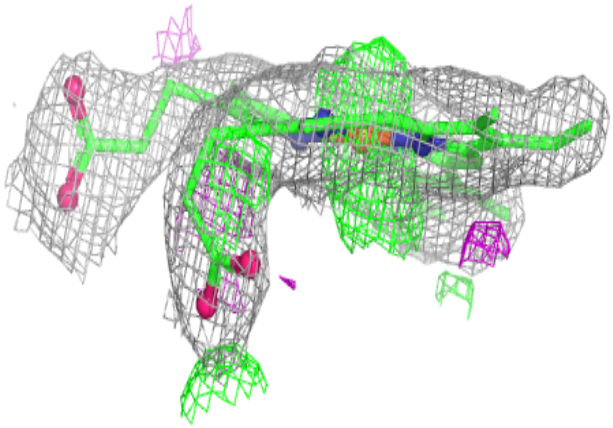


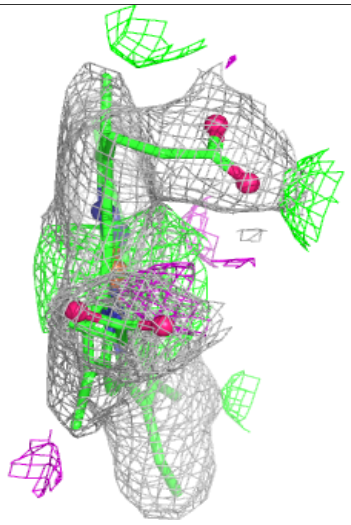


Electron density around HEC A 302:

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

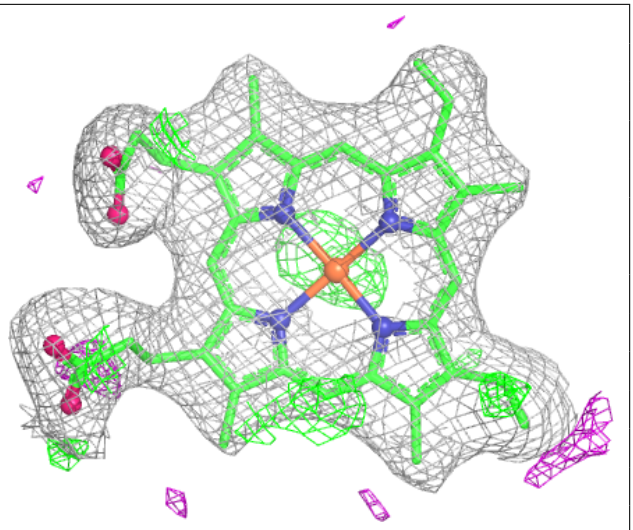


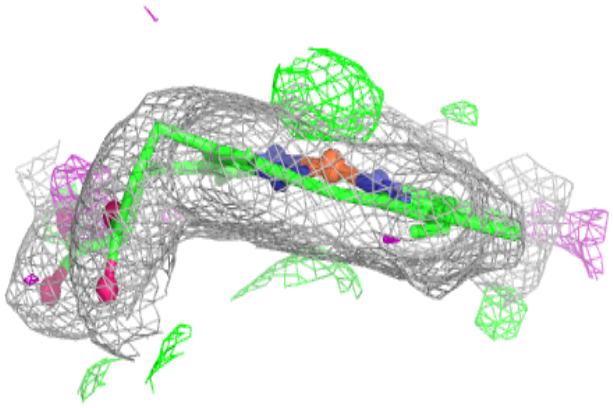


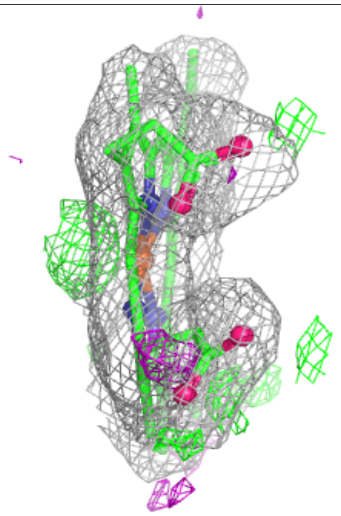


Electron density around HEC A 303:

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

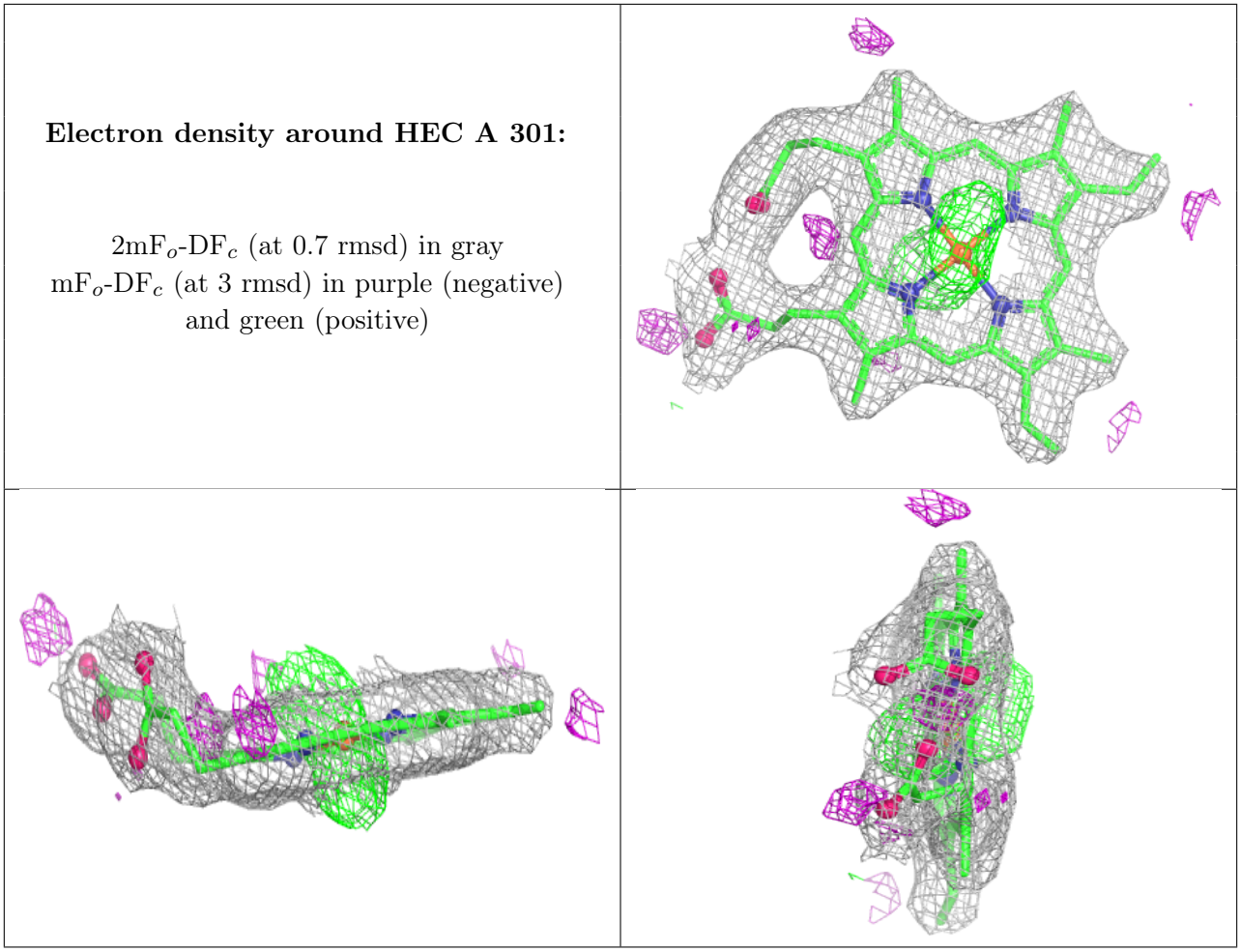






Electron density around HEC A 301:

$2mF_o$-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.