wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 04:04 PM EDT

PDB ID	:	5WAU
Title	:	Crystal Structure of CO-bound Cytochrome c Oxidase determined by Synchrotron X-Ray Crystallography at 100 K
Authors	:	Fromme, R.; Ishigami, I.; Yeh, S.Y.; Zatsepin, N.; Grant, T.; Fromme, P.; Rousseau, D.
Deposited on	:	2017-06-27
Resolution	:	1.95 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:

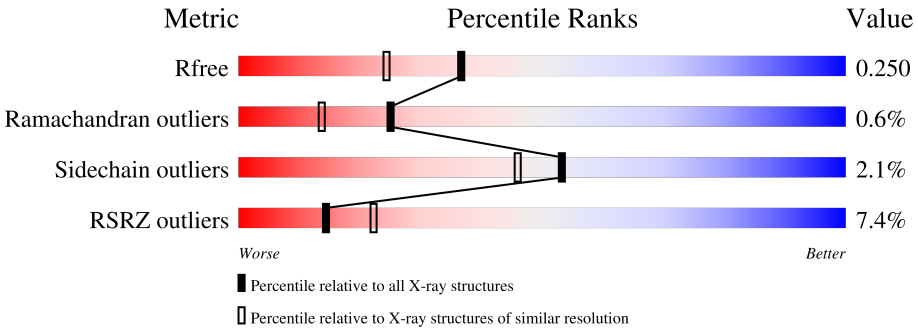
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	514	2% 99% .
1	a	514	2% 98% .
2	B	227	2% 96% .
2	b	227	5% 95% 5%
3	C	261	98% ..
3	c	261	2% 98% ..

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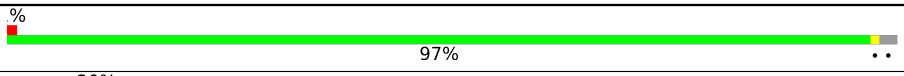
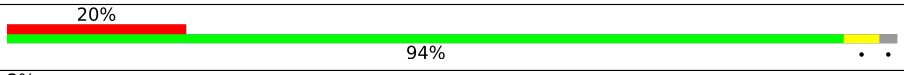
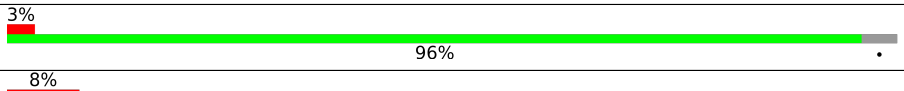
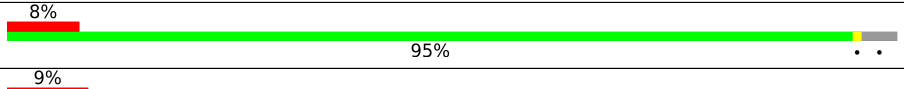
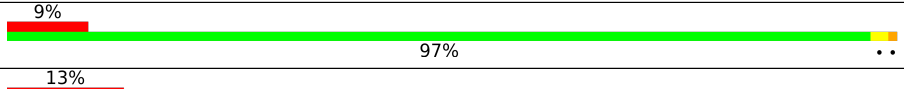
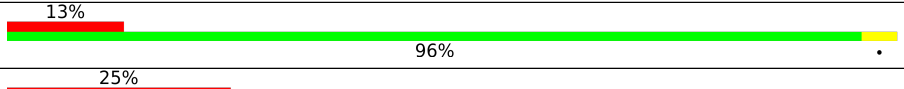
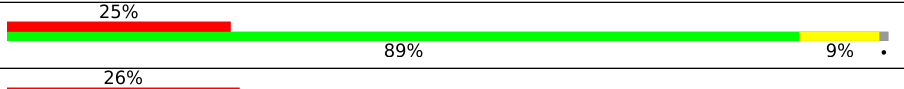
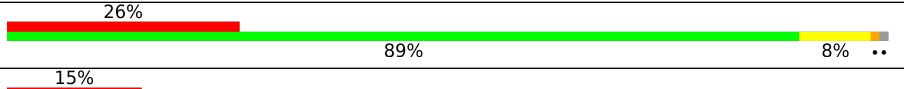
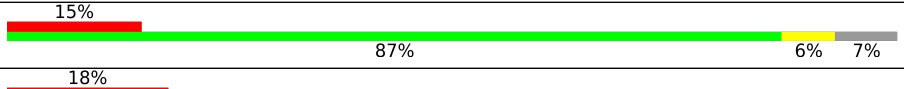
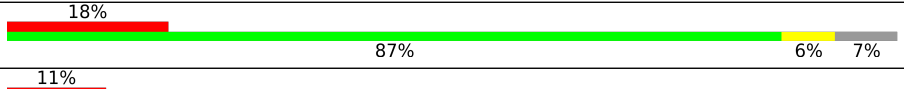
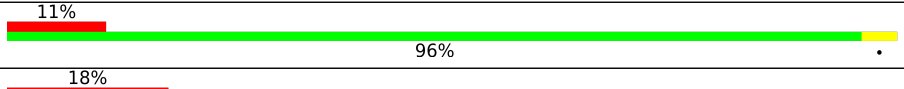
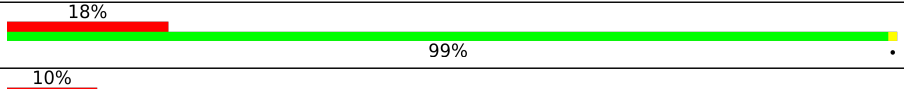
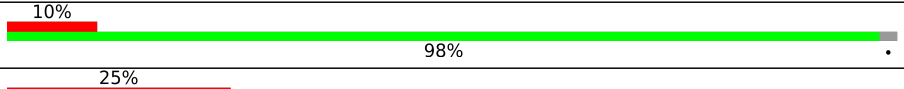
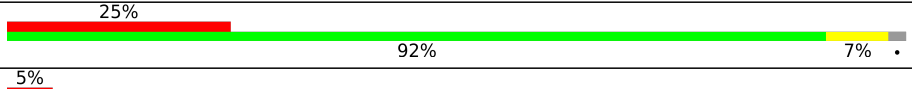
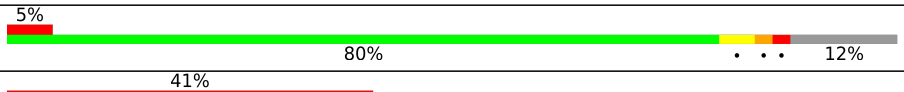
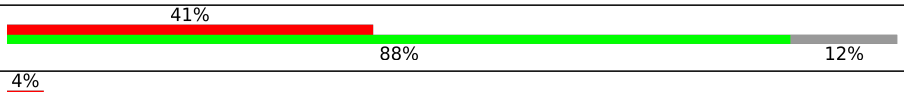
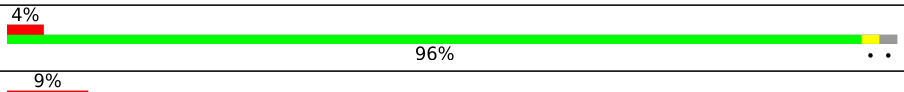
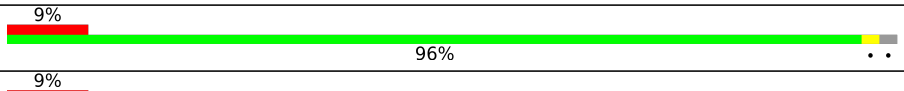
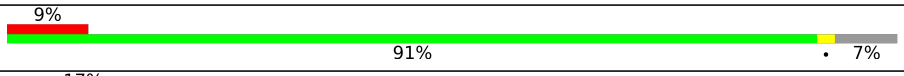
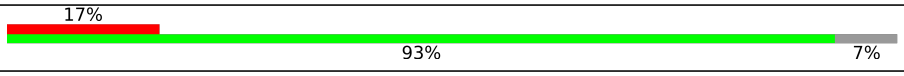
Mol	Chain	Length	Quality of chain
4	D	147	
4	d	147	
5	E	109	
5	e	109	
6	F	98	
6	f	98	
7	G	85	
7	g	85	
8	H	85	
8	h	85	
9	I	73	
9	i	73	
10	J	59	
10	j	59	
11	K	56	
11	k	56	
12	L	47	
12	l	47	
13	M	46	
13	m	46	

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
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-
14	HEA	a	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	a	602	X	-	-	-
18	PGV	a	606	-	-	-	X
23	PEK	C	307	-	-	-	X
25	DMU	C	308	-	-	-	X
7	TPO	g	11	-	-	-	X
9	SAC	i	101	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 32575 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	a	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	b	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	c	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	d	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	e	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	f	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	g	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	h	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	i	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	j	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	k	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

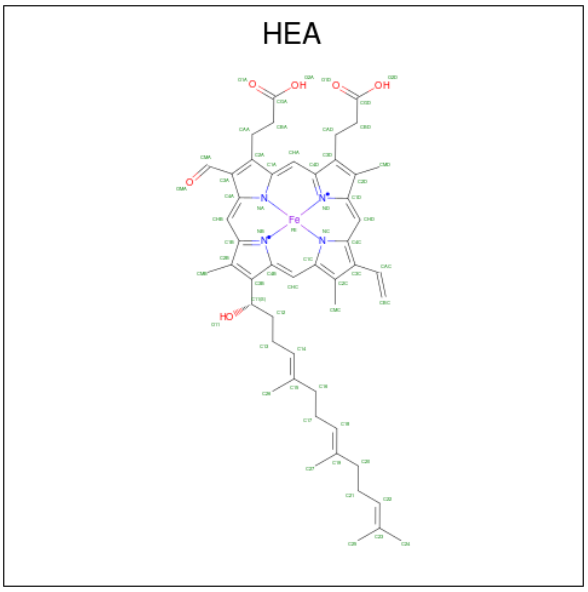
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	l	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	m	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	a	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	a	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	a	1	Total	Cu	0	0
			1	1		

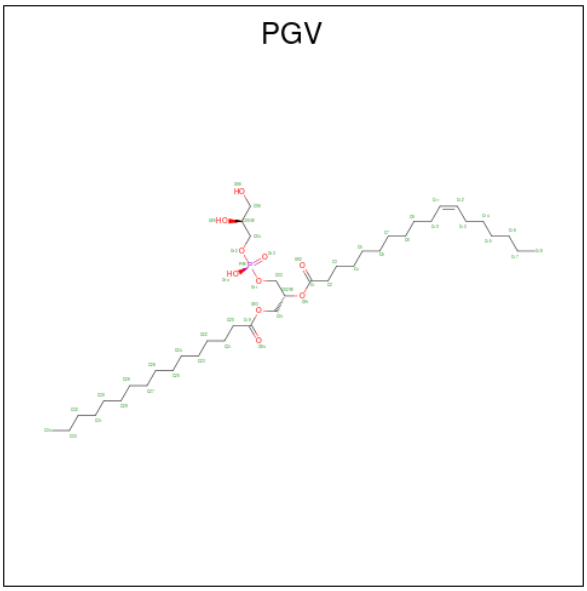
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	a	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

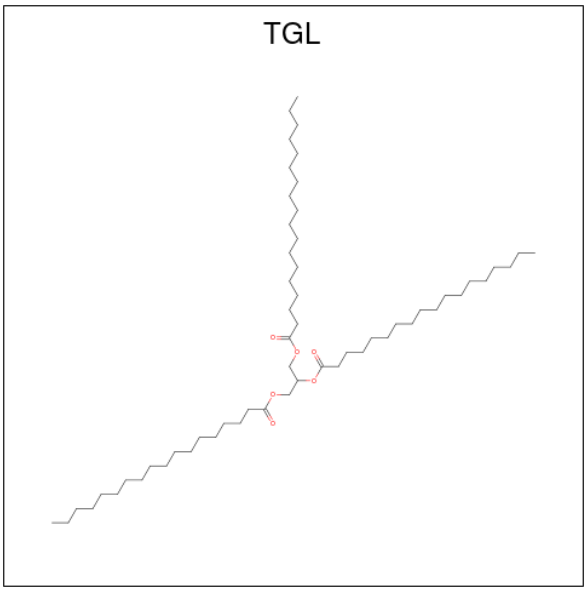
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	a	1	Total Na 1 1	0	0

- Molecule 18 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



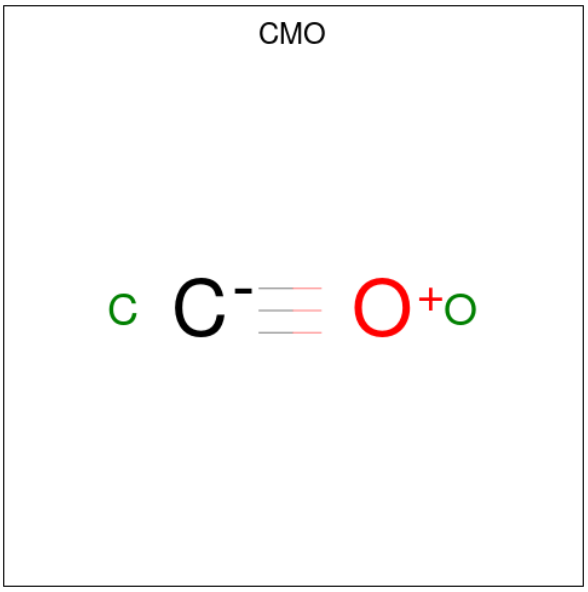
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	a	1	Total C O P 51 40 10 1	0	0
18	a	1	Total C O P 51 40 10 1	0	0
18	c	1	Total C O P 51 40 10 1	0	0
18	c	1	Total C O P 51 40 10 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



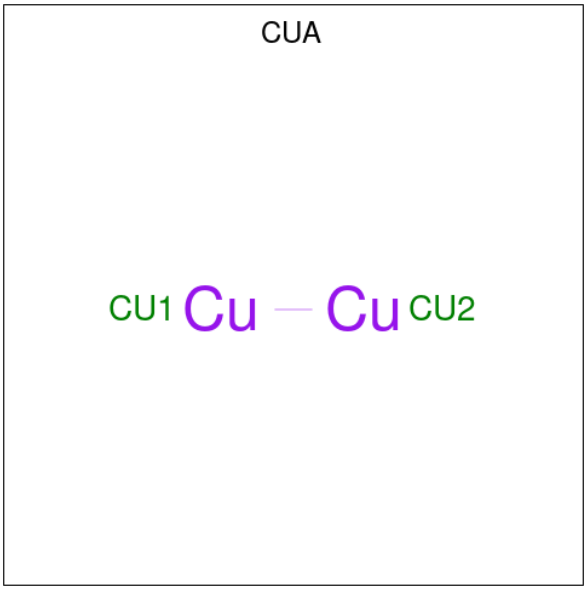
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	b	1	Total C O 63 57 6	0	0
19	d	1	Total C O 63 57 6	0	0
19	l	1	Total C O 63 57 6	0	0

- Molecule 20 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



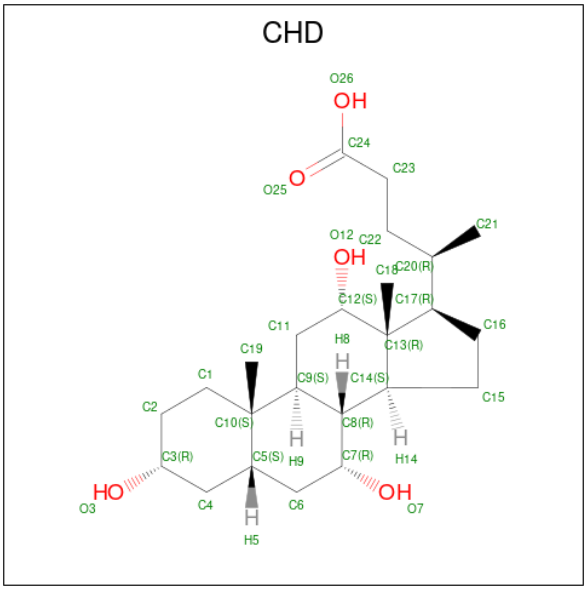
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 2 1 1	0	0
20	a	1	Total C O 2 1 1	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



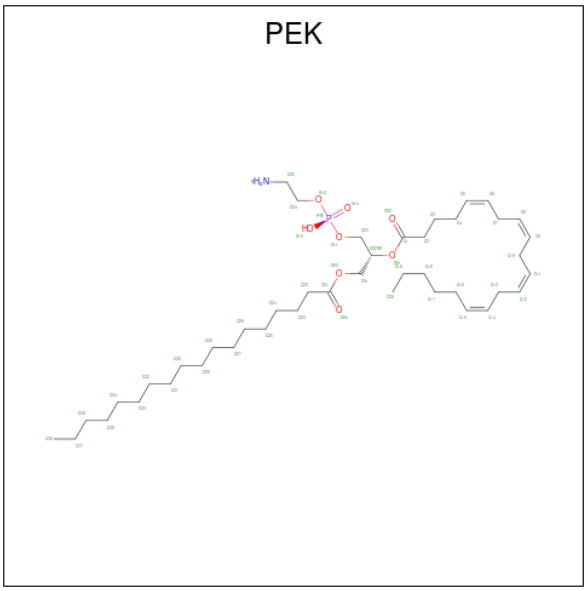
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	b	1	Total Cu 2 2	0	0

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



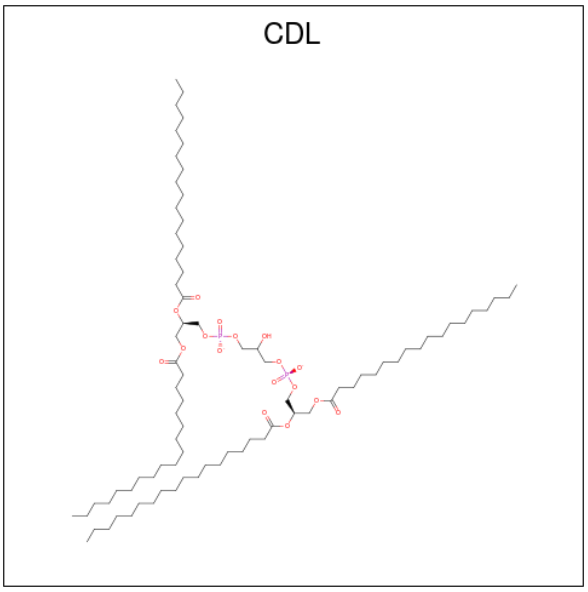
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	c	1	Total C O 29 24 5	0	0
22	c	1	Total C O 29 24 5	0	0
22	j	1	Total C O 29 24 5	0	0

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



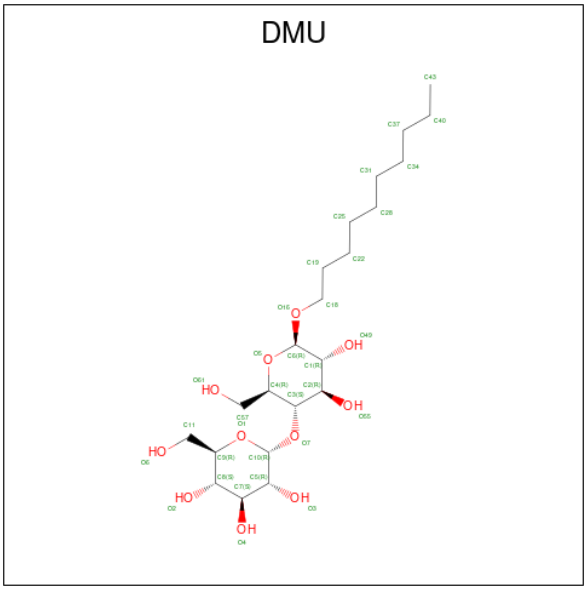
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



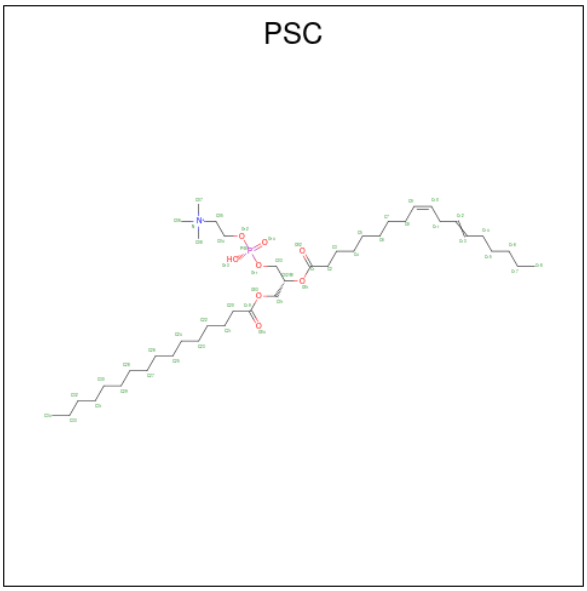
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	C	1	Total	C	O	P	0	0
			100	81	17	2		
24	G	1	Total	C	O	P	0	0
			100	81	17	2		
24	c	1	Total	C	O	P	0	0
			100	81	17	2		
24	g	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C O 33 22 11	0	0
25	M	1	Total C O 33 22 11	0	0
25	c	1	Total C O 33 22 11	0	0
25	m	1	Total C O 33 22 11	0	0

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	E	1	Total C N O P 52 42 1 8 1	0	0
26	b	1	Total C N O P 52 42 1 8 1	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	F	1	Total Zn 1 1	0	0
27	f	1	Total Zn 1 1	0	0

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	243	Total O 243 243	0	0
28	B	180	Total O 180 180	0	0
28	C	122	Total O 122 122	0	0
28	D	125	Total O 125 125	0	0
28	E	100	Total O 100 100	0	0
28	F	104	Total O 104 104	0	0
28	G	57	Total O 57 57	0	0
28	H	57	Total O 57 57	0	0
28	I	33	Total O 33 33	0	0
28	J	36	Total O 36 36	0	0
28	K	41	Total O 41 41	0	0
28	L	47	Total O 47 47	0	0
28	M	29	Total O 29 29	0	0
28	a	187	Total O 187 187	0	0
28	b	109	Total O 109 109	0	0
28	c	96	Total O 96 96	0	0
28	d	37	Total O 37 37	0	0
28	e	56	Total O 56 56	0	0
28	f	62	Total O 62 62	0	0
28	g	27	Total O 27 27	0	0
28	h	36	Total O 36 36	0	0
28	i	23	Total O 23 23	0	0

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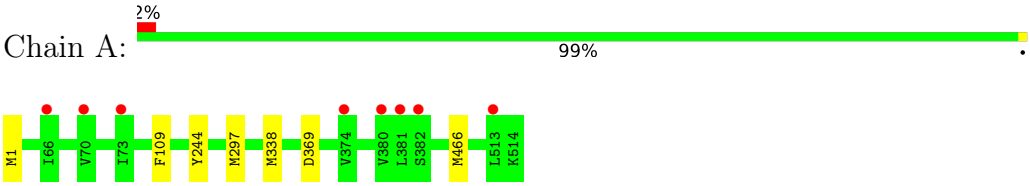
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	j	14	Total O 14 14	0	0
28	k	7	Total O 7 7	0	0
28	l	8	Total O 8 8	0	0
28	m	5	Total O 5 5	0	0

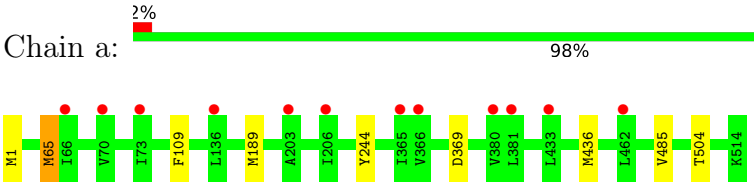
3 Residue-property plots (i)

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.

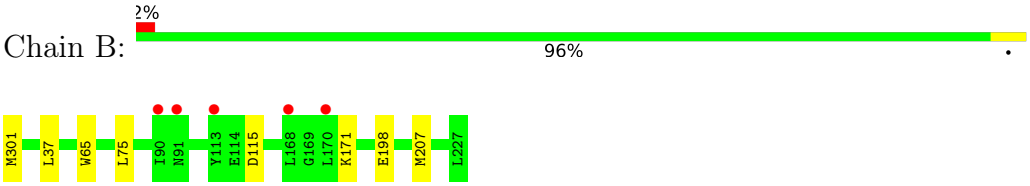
• Molecule 1: Cytochrome c oxidase subunit 1



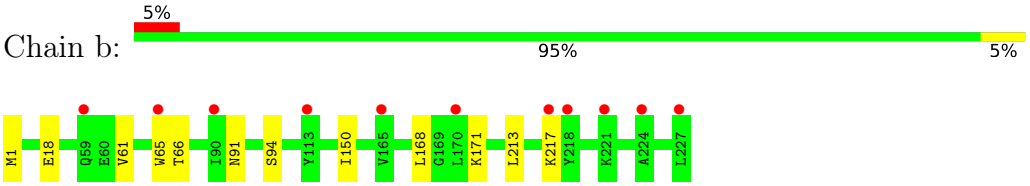
• Molecule 1: Cytochrome c oxidase subunit 1



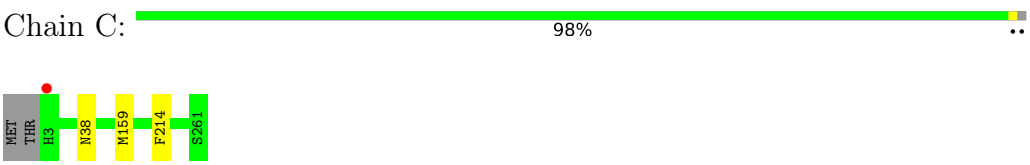
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

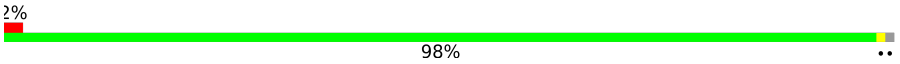


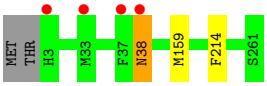
• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 3: Cytochrome c oxidase subunit 3

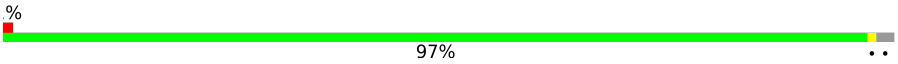
Chain c:

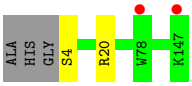




• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

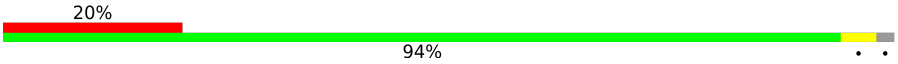
Chain D:

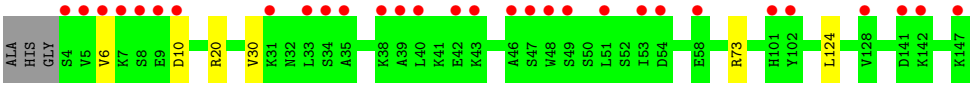




• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

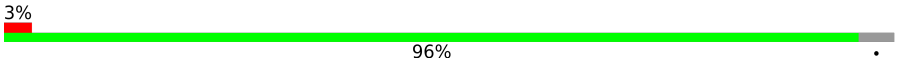
Chain d:

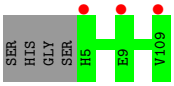




• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

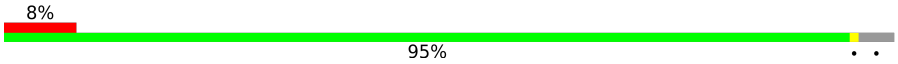
Chain E:

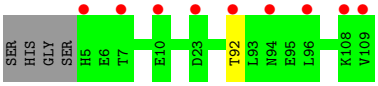




• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

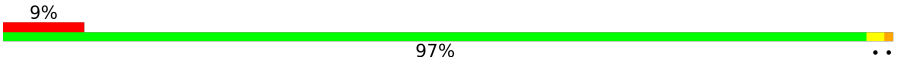
Chain e:

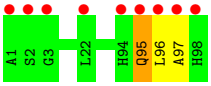




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

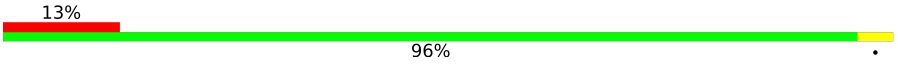
Chain F:

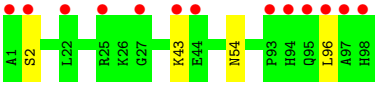




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

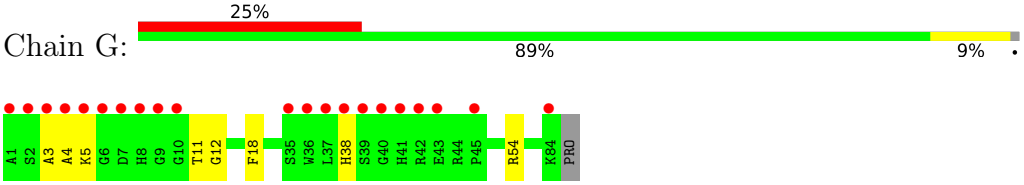
Chain f:





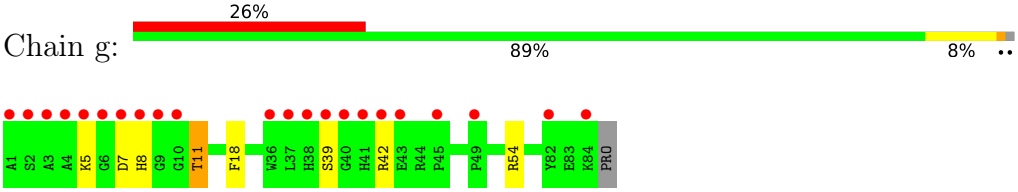
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



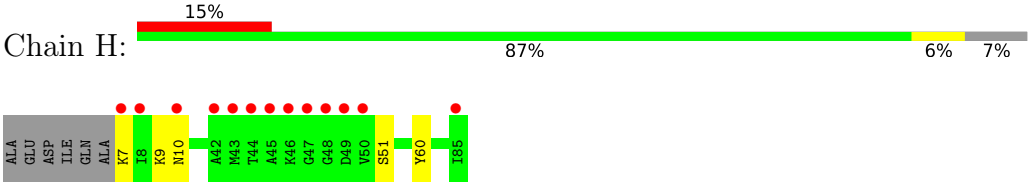
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain g:



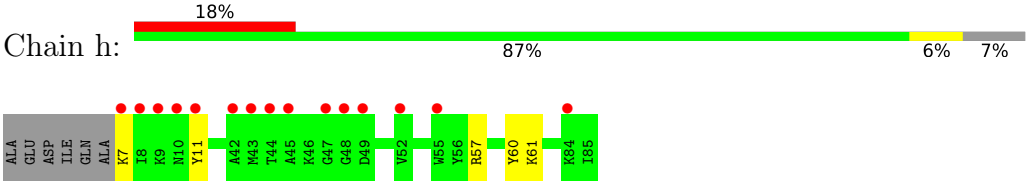
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



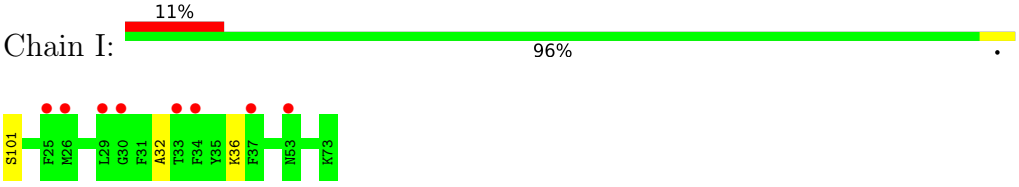
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain h:



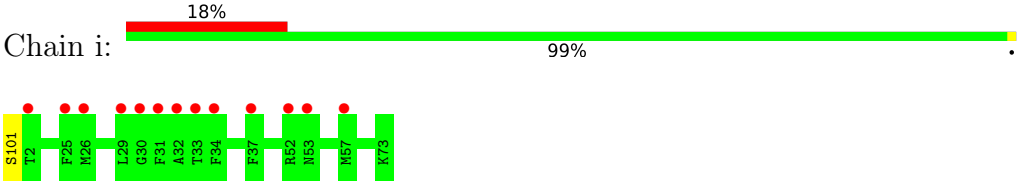
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



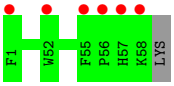
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain i:



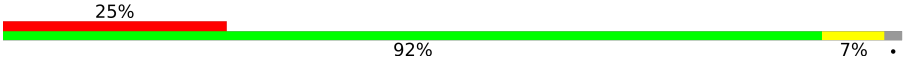
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

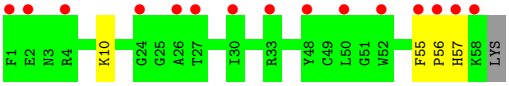
Chain J:



• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

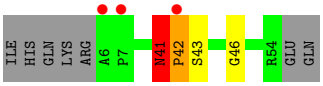
Chain j:





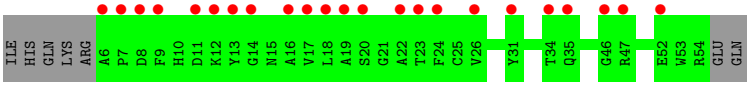
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



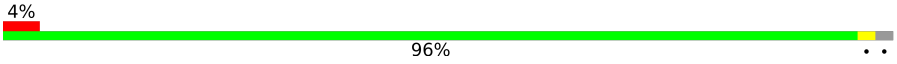
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain k:



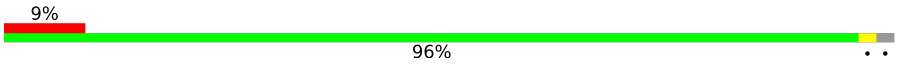
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

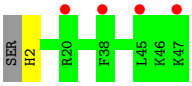
Chain L:



• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

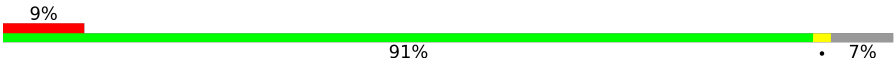
Chain l:

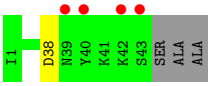




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

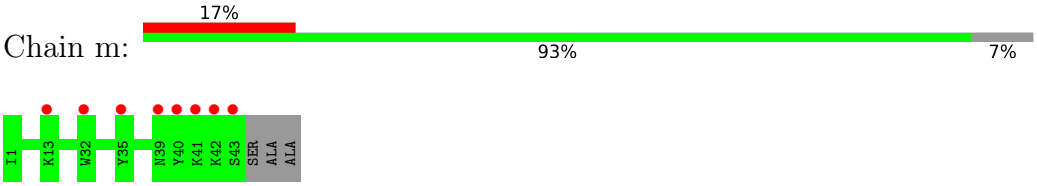
Chain M:





• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain m:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	177.92Å 182.56Å 208.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 1.95 38.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.00-1.95) 94.3 (38.64-1.95)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.217 , 0.244 0.225 , 0.250	Depositor DCC
R_{free} test set	23097 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32575	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: NA, PEK, ZN, CMO, TPO, PGV, CHD, CU, HEA, CUA, FME, DMU, CDL, TGL, PSC, MG, SAC

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	0.52	0/4156	0.68	2/5678 (0.0%)
1	a	0.49	1/4156 (0.0%)	0.66	2/5678 (0.0%)
2	B	0.53	1/1860 (0.1%)	0.77	1/2534 (0.0%)
2	b	0.46	0/1860	0.71	0/2534
3	C	0.45	0/2197	0.62	0/3005
3	c	0.46	0/2197	0.59	0/3005
4	D	0.46	0/1229	0.64	2/1658 (0.1%)
4	d	0.44	0/1229	0.66	1/1658 (0.1%)
5	E	0.46	0/871	0.65	0/1182
5	e	0.42	0/871	0.66	0/1182
6	F	0.51	0/765	0.72	0/1038
6	f	0.43	0/765	0.66	0/1038
7	G	0.48	0/690	0.71	0/937
7	g	0.50	0/690	0.67	0/937
8	H	0.48	0/682	0.72	0/921
8	h	0.44	0/682	0.66	0/921
9	I	0.45	0/605	0.69	0/802
9	i	0.45	0/605	0.66	0/802
10	J	0.43	0/471	0.58	0/636
10	j	0.47	0/471	0.65	0/636
11	K	0.52	0/398	0.83	2/546 (0.4%)
11	k	0.41	0/398	0.57	0/546
12	L	0.48	0/393	0.63	0/526
12	l	0.47	0/393	0.61	0/526
13	M	0.48	0/345	0.63	0/470
13	m	0.43	0/345	0.52	0/470
All	All	0.48	2/29324 (0.0%)	0.67	10/39866 (0.0%)

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
7	g	0	1
10	j	0	1
11	K	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	5.24	1.33	1.23
1	a	244	TYR	CE2-CZ	5.23	1.45	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	207	MET	CG-SD-CE	-6.29	90.14	100.20
4	D	20	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	466	MET	CG-SD-CE	-5.85	90.85	100.20
1	a	244	TYR	CZ-CE2-CD2	-5.80	114.58	119.80
1	a	65	MET	CG-SD-CE	5.78	109.44	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	41	ASN	Peptide
11	K	42	PRO	Peptide
11	K	46	GLY	Peptide
7	g	11	TPO	Peptide
10	j	55	PHE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	512/514 (100%)	497 (97%)	15 (3%)	0	100 100
1	a	512/514 (100%)	499 (98%)	13 (2%)	0	100 100
2	B	225/227 (99%)	218 (97%)	7 (3%)	0	100 100
2	b	225/227 (99%)	215 (96%)	8 (4%)	2 (1%)	17 8
3	C	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	34 22
3	c	257/261 (98%)	250 (97%)	6 (2%)	1 (0%)	34 22
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100 100
4	d	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	22 11
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100 100
5	e	103/109 (94%)	101 (98%)	2 (2%)	0	100 100
6	F	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	4 0
6	f	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	15 6
7	G	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	3 0
7	g	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	13 4
8	H	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	5 1
8	h	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	12 3
9	I	71/73 (97%)	69 (97%)	1 (1%)	1 (1%)	11 3
9	i	71/73 (97%)	68 (96%)	3 (4%)	0	100 100
10	J	56/59 (95%)	56 (100%)	0	0	100 100
10	j	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	8 2
11	K	47/56 (84%)	43 (92%)	1 (2%)	3 (6%)	1 0
11	k	47/56 (84%)	45 (96%)	2 (4%)	0	100 100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
12	l	44/47 (94%)	43 (98%)	1 (2%)	0	100 100
13	M	41/46 (89%)	41 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	m	41/46 (89%)	39 (95%)	2 (5%)	0	100 100
All	All	3504/3614 (97%)	3371 (96%)	112 (3%)	21 (1%)	25 14

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	38	ASN
6	F	95	GLN
6	F	96	LEU
11	K	41	ASN
11	K	42	PRO

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	426/426 (100%)	422 (99%)	4 (1%)	78 77
1	a	426/426 (100%)	419 (98%)	7 (2%)	62 58
2	B	210/210 (100%)	205 (98%)	5 (2%)	49 40
2	b	210/210 (100%)	201 (96%)	9 (4%)	29 16
3	C	224/226 (99%)	222 (99%)	2 (1%)	78 77
3	c	224/226 (99%)	221 (99%)	3 (1%)	69 65
4	D	128/129 (99%)	127 (99%)	1 (1%)	81 80
4	d	128/129 (99%)	124 (97%)	4 (3%)	40 28
5	E	92/95 (97%)	92 (100%)	0	100 100
5	e	92/95 (97%)	91 (99%)	1 (1%)	73 71
6	F	81/81 (100%)	80 (99%)	1 (1%)	71 68
6	f	81/81 (100%)	78 (96%)	3 (4%)	34 22
7	G	67/68 (98%)	63 (94%)	4 (6%)	19 8
7	g	67/68 (98%)	61 (91%)	6 (9%)	9 2
8	H	71/75 (95%)	68 (96%)	3 (4%)	30 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	h	71/75 (95%)	67 (94%)	4 (6%)	21 9
9	I	57/57 (100%)	56 (98%)	1 (2%)	59 53
9	i	57/57 (100%)	57 (100%)	0	100 100
10	J	49/50 (98%)	49 (100%)	0	100 100
10	j	49/50 (98%)	47 (96%)	2 (4%)	30 18
11	K	39/46 (85%)	39 (100%)	0	100 100
11	k	39/46 (85%)	39 (100%)	0	100 100
12	L	39/40 (98%)	38 (97%)	1 (3%)	46 36
12	l	39/40 (98%)	38 (97%)	1 (3%)	46 36
13	M	37/38 (97%)	36 (97%)	1 (3%)	44 34
13	m	37/38 (97%)	37 (100%)	0	100 100
All	All	3040/3082 (99%)	2977 (98%)	63 (2%)	53 46

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	485	VAL
7	g	54	ARG
2	b	168	LEU
7	g	42	ARG
8	h	61	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	56	GLN
13	m	15	GLN
13	m	39	ASN
6	f	54	ASN
10	J	9	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	TPO	G	11	7	8,10,11	1.34	1 (12%)	10,14,16	1.23	2 (20%)
2	FME	B	301	2	8,9,10	0.98	0	7,9,11	3.80	3 (42%)
2	FME	b	1	2	8,9,10	0.63	0	7,9,11	2.22	2 (28%)
9	SAC	i	101	9	7,8,9	1.66	1 (14%)	8,9,11	1.02	0
7	TPO	g	11	7	8,10,11	1.13	1 (12%)	10,14,16	1.08	1 (10%)
1	FME	a	1	1	8,9,10	0.50	0	7,9,11	1.73	1 (14%)
1	FME	A	1	1	8,9,10	0.62	0	7,9,11	2.71	1 (14%)
9	SAC	I	101	9	7,8,9	1.68	1 (14%)	8,9,11	1.90	2 (25%)

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
7	TPO	G	11	7	-	3/9/11/13	-
2	FME	B	301	2	-	1/7/9/11	-
2	FME	b	1	2	-	1/7/9/11	-
9	SAC	i	101	9	-	2/7/8/10	-
7	TPO	g	11	7	-	4/9/11/13	-
1	FME	a	1	1	-	4/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
9	SAC	I	101	9	-	3/7/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	101	SAC	CA-N	4.27	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	101	SAC	CA-N	4.16	1.52	1.46
7	G	11	TPO	P-OG1	3.01	1.65	1.59
7	g	11	TPO	P-OG1	2.03	1.63	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	FME	CA-N-CN	-8.81	109.27	122.82
1	A	1	FME	CA-N-CN	-6.68	112.55	122.82
2	b	1	FME	CA-N-CN	-4.54	115.84	122.82
1	a	1	FME	CA-N-CN	-3.81	116.96	122.82
9	I	101	SAC	CA-N-C1A	3.76	130.09	123.15

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	C-CA-CB-CG
2	B	301	FME	O1-CN-N-CA
7	G	11	TPO	CB-OG1-P-O1P
9	I	101	SAC	CB-CA-N-C1A

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 8 are monoatomic - leaving 46 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	$\#\|Z\|>2$
23	PEK	C	302	-	52,52,52	0.85	2 (3%)	55,57,57	0.95	4 (7%)
20	CMO	A	610	15,14	0,1,1	-	-	-		
22	CHD	J	101	-	32,32,32	0.67	0	51,51,51	2.11	16 (31%)
18	PGV	a	606	-	50,50,50	1.07	2 (4%)	53,56,56	1.17	5 (9%)
24	CDL	g	101	-	99,99,99	1.00	4 (4%)	105,111,111	1.03	6 (5%)
23	PEK	c	305	-	52,52,52	0.99	2 (3%)	55,57,57	0.92	3 (5%)
23	PEK	c	304	-	52,52,52	0.89	2 (3%)	55,57,57	0.84	3 (5%)
24	CDL	G	102	-	99,99,99	1.04	4 (4%)	105,111,111	0.94	6 (5%)
23	PEK	c	301	-	52,52,52	0.99	2 (3%)	55,57,57	0.88	3 (5%)
24	CDL	C	305	-	99,99,99	0.99	4 (4%)	105,111,111	1.00	7 (6%)
14	HEA	a	601	1	57,67,67	2.04	15 (26%)	61,103,103	2.27	20 (32%)
19	TGL	A	608	-	62,62,62	1.10	3 (4%)	65,65,65	0.97	4 (6%)
22	CHD	C	301	-	32,32,32	0.63	0	51,51,51	1.11	4 (7%)
22	CHD	c	308	-	32,32,32	0.51	0	51,51,51	1.06	3 (5%)
25	DMU	c	309	-	34,34,34	0.97	2 (5%)	45,45,45	1.44	6 (13%)
21	CUA	B	401	2	0,1,1	-	-	-		
22	CHD	C	306	-	32,32,32	0.59	0	51,51,51	1.24	6 (11%)
23	PEK	G	101	-	52,52,52	1.01	2 (3%)	55,57,57	1.15	5 (9%)
22	CHD	j	101	-	32,32,32	0.57	0	51,51,51	1.41	10 (19%)
23	PEK	C	307	-	52,52,52	1.02	2 (3%)	55,57,57	0.85	3 (5%)
19	TGL	b	302	-	62,62,62	1.04	3 (4%)	65,65,65	0.95	3 (4%)
25	DMU	M	101	-	34,34,34	0.53	1 (2%)	45,45,45	0.75	0
24	CDL	c	307	-	99,99,99	1.00	4 (4%)	105,111,111	1.03	6 (5%)
14	HEA	A	601	1	57,67,67	1.85	13 (22%)	61,103,103	2.50	26 (42%)
22	CHD	c	303	-	32,32,32	0.62	0	51,51,51	1.05	3 (5%)
18	PGV	C	303	-	50,50,50	0.85	2 (4%)	53,56,56	0.80	1 (1%)
14	HEA	a	602	1,20	57,67,67	2.03	14 (24%)	61,103,103	2.46	22 (36%)
19	TGL	d	201	-	62,62,62	1.10	3 (4%)	65,65,65	1.14	7 (10%)
25	DMU	m	101	-	34,34,34	0.49	0	45,45,45	0.97	3 (6%)
22	CHD	G	103	-	32,32,32	0.66	0	51,51,51	1.11	4 (7%)
14	HEA	A	602	1,20	57,67,67	1.94	11 (19%)	61,103,103	2.69	28 (45%)
20	CMO	a	608	15,14	0,1,1	-	-	-		
22	CHD	B	402	-	32,32,32	0.70	0	51,51,51	1.26	7 (13%)
18	PGV	a	607	-	50,50,50	0.85	2 (4%)	53,56,56	0.75	2 (3%)
26	PSC	E	201	-	51,51,51	1.04	2 (3%)	57,59,59	1.84	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	DMU	C	308	-	34,34,34	0.71	1 (2%)	45,45,45	1.24	6 (13%)
18	PGV	A	606	-	50,50,50	1.03	2 (4%)	53,56,56	0.93	3 (5%)
26	PSC	b	303	-	51,51,51	1.04	2 (3%)	57,59,59	1.79	10 (17%)
19	TGL	l	101	-	62,62,62	1.12	3 (4%)	65,65,65	1.10	5 (7%)
18	PGV	c	302	-	50,50,50	1.06	2 (4%)	53,56,56	1.21	5 (9%)
18	PGV	c	306	-	50,50,50	0.90	2 (4%)	53,56,56	0.81	1 (1%)
19	TGL	D	201	-	62,62,62	1.10	3 (4%)	65,65,65	0.95	4 (6%)
21	CUA	b	301	2	0,1,1	-	-	-		
18	PGV	A	607	-	50,50,50	0.87	2 (4%)	53,56,56	0.85	3 (5%)
19	TGL	A	609	-	62,62,62	1.04	3 (4%)	65,65,65	0.97	5 (7%)
18	PGV	C	304	-	50,50,50	1.07	2 (4%)	53,56,56	0.99	4 (7%)

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
23	PEK	C	302	-	-	21/56/56/56	-
22	CHD	J	101	-	-	5/9/74/74	0/4/4/4
18	PGV	a	606	-	-	28/55/55/55	-
24	CDL	g	101	-	-	58/110/110/110	-
23	PEK	c	305	-	-	25/56/56/56	-
23	PEK	c	304	-	-	16/56/56/56	-
24	CDL	G	102	-	-	57/110/110/110	-
23	PEK	c	301	-	-	24/56/56/56	-
24	CDL	C	305	-	-	51/110/110/110	-
14	HEA	a	601	1	2/2/7/16	4/32/76/76	-
19	TGL	A	608	-	-	32/65/65/65	-
22	CHD	C	301	-	-	0/9/74/74	0/4/4/4
22	CHD	c	308	-	-	2/9/74/74	0/4/4/4
25	DMU	c	309	-	-	7/19/59/59	0/2/2/2
22	CHD	C	306	-	-	2/9/74/74	0/4/4/4
23	PEK	G	101	-	-	26/56/56/56	-
22	CHD	j	101	-	-	8/9/74/74	0/4/4/4
23	PEK	C	307	-	-	18/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	b	302	-	-	33/65/65/65	-
25	DMU	M	101	-	-	6/19/59/59	0/2/2/2
24	CDL	c	307	-	-	54/110/110/110	-
14	HEA	A	601	1	2/2/7/16	5/32/76/76	-
22	CHD	c	303	-	-	2/9/74/74	0/4/4/4
18	PGV	C	303	-	-	13/55/55/55	-
14	HEA	a	602	1,20	2/2/7/16	5/32/76/76	-
19	TGL	d	201	-	-	38/65/65/65	-
25	DMU	m	101	-	-	4/19/59/59	0/2/2/2
22	CHD	G	103	-	-	2/9/74/74	0/4/4/4
14	HEA	A	602	1,20	2/2/7/16	4/32/76/76	-
22	CHD	B	402	-	-	2/9/74/74	0/4/4/4
18	PGV	a	607	-	-	12/55/55/55	-
26	PSC	E	201	-	-	23/55/55/55	-
25	DMU	C	308	-	-	2/19/59/59	0/2/2/2
18	PGV	A	606	-	-	22/55/55/55	-
26	PSC	b	303	-	-	25/55/55/55	-
19	TGL	l	101	-	-	33/65/65/65	-
18	PGV	c	302	-	-	34/55/55/55	-
18	PGV	c	306	-	-	11/55/55/55	-
19	TGL	D	201	-	-	29/65/65/65	-
18	PGV	A	607	-	-	13/55/55/55	-
19	TGL	A	609	-	-	39/65/65/65	-
18	PGV	C	304	-	-	26/55/55/55	-

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	601	HEA	C3B-C2B	5.58	1.47	1.34
14	a	602	HEA	C3A-C2A	5.18	1.47	1.40
14	A	601	HEA	C3B-C2B	5.17	1.46	1.34
26	b	303	PSC	O01-C1	4.91	1.48	1.34
18	a	606	PGV	O01-C1	4.91	1.48	1.34

The worst 5 of 282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	602	HEA	C3D-C4D-ND	6.79	116.93	110.36
26	E	201	PSC	C08-N-C06	-6.59	92.04	108.97
14	A	601	HEA	C3D-C4D-ND	6.51	116.66	110.36
26	b	303	PSC	C08-N-C06	-6.48	92.32	108.97
26	E	201	PSC	C08-N-C07	-6.40	92.52	108.97

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	NB
14	A	601	HEA	ND
14	A	602	HEA	NB
14	A	602	HEA	ND
14	a	601	HEA	NB

5 of 821 torsion outliers are listed below:

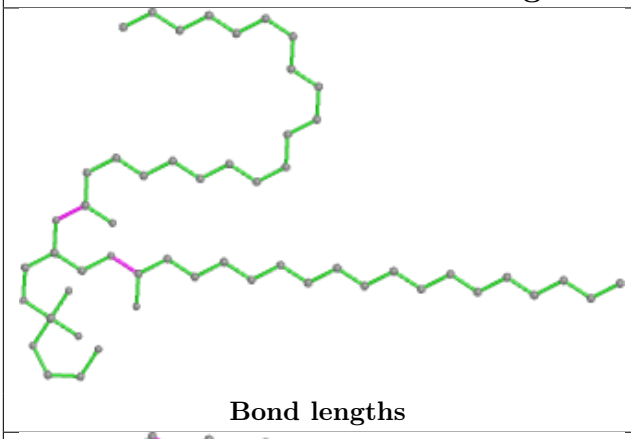
Mol	Chain	Res	Type	Atoms
18	C	304	PGV	C02-C03-O11-P
18	C	304	PGV	O12-C04-C05-C06
18	C	304	PGV	C04-C05-C06-O06
18	a	606	PGV	O02-C1-O01-C02
18	a	606	PGV	C2-C1-O01-C02

There are no ring outliers.

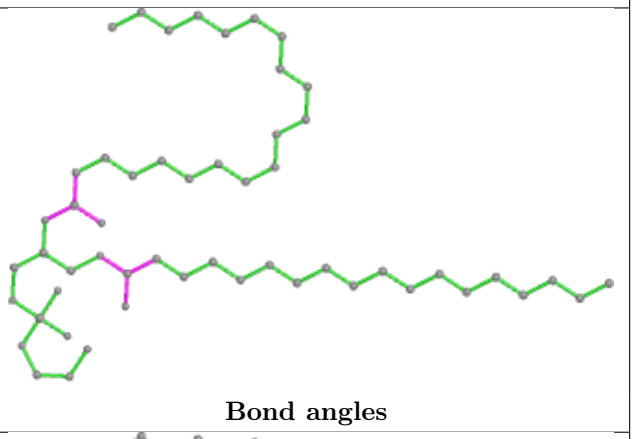
No monomer is involved in short contacts.

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.

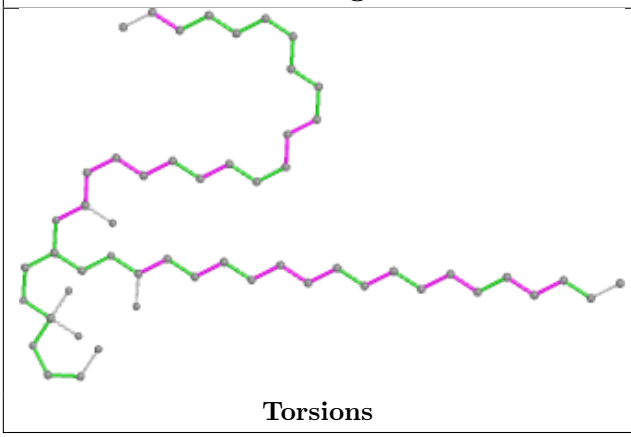
Ligand PEK C 302



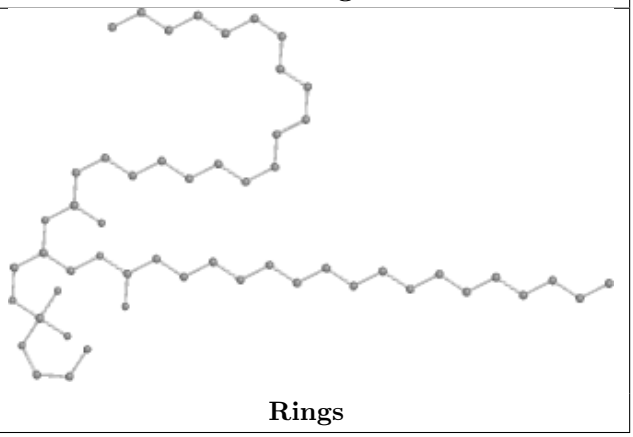
Bond lengths



Bond angles

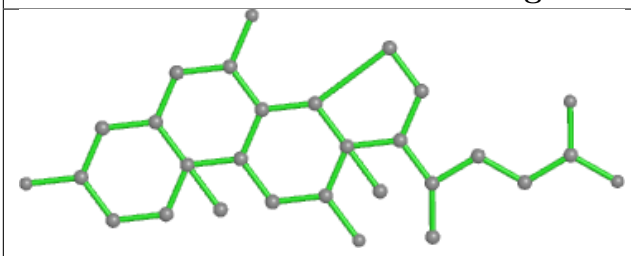


Torsions

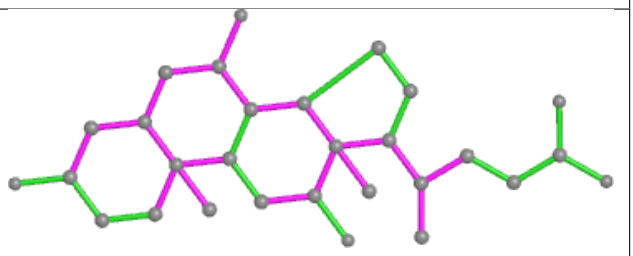


Rings

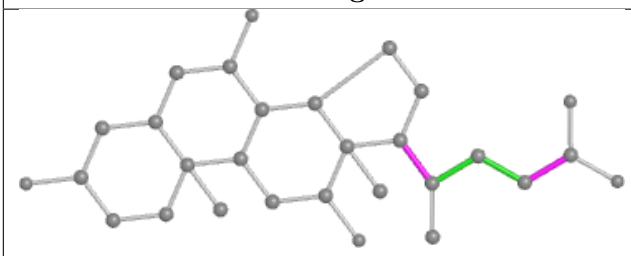
Ligand CHD J 101



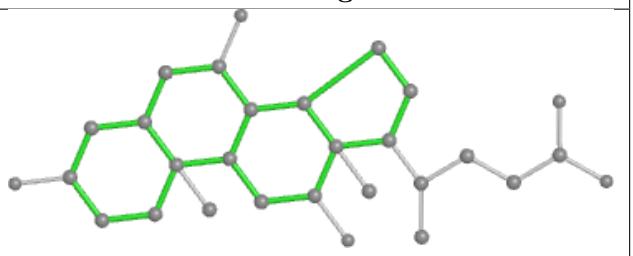
Bond lengths



Bond angles

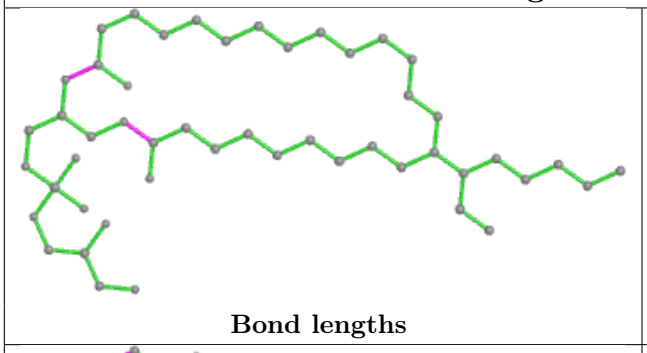


Torsions

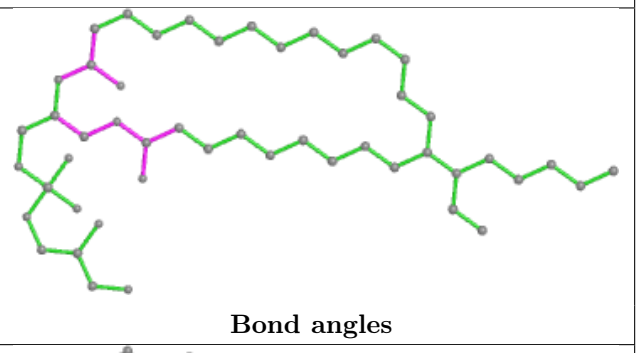


Rings

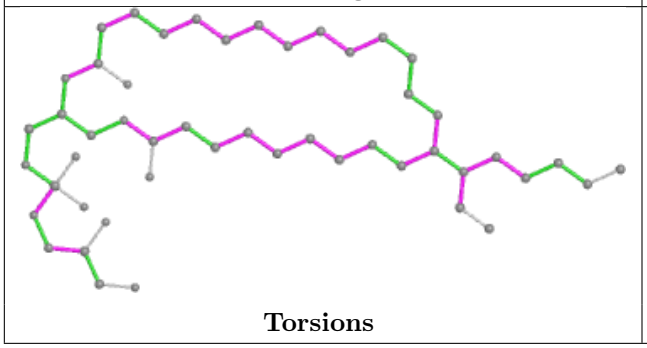
Ligand PGV a 606



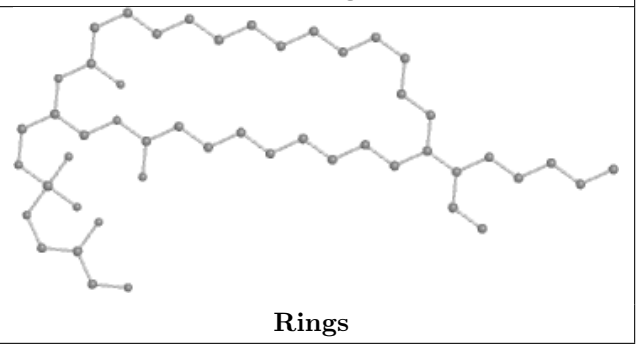
Bond lengths



Bond angles

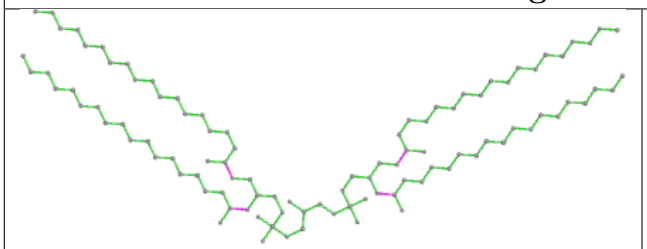


Torsions

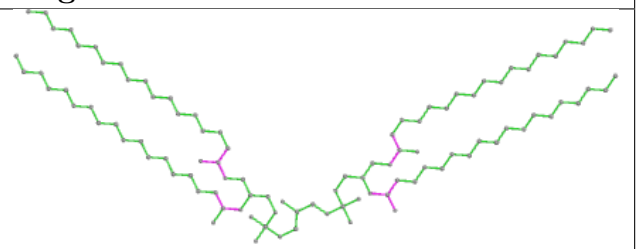


Rings

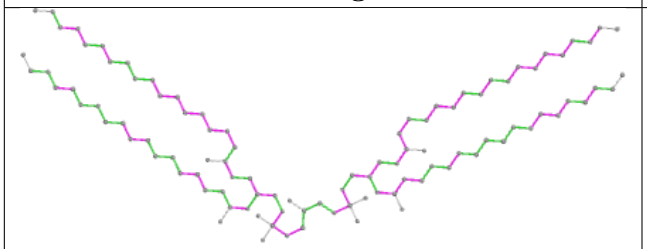
Ligand CDL g 101



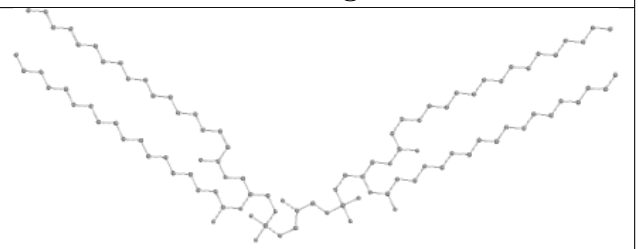
Bond lengths



Bond angles

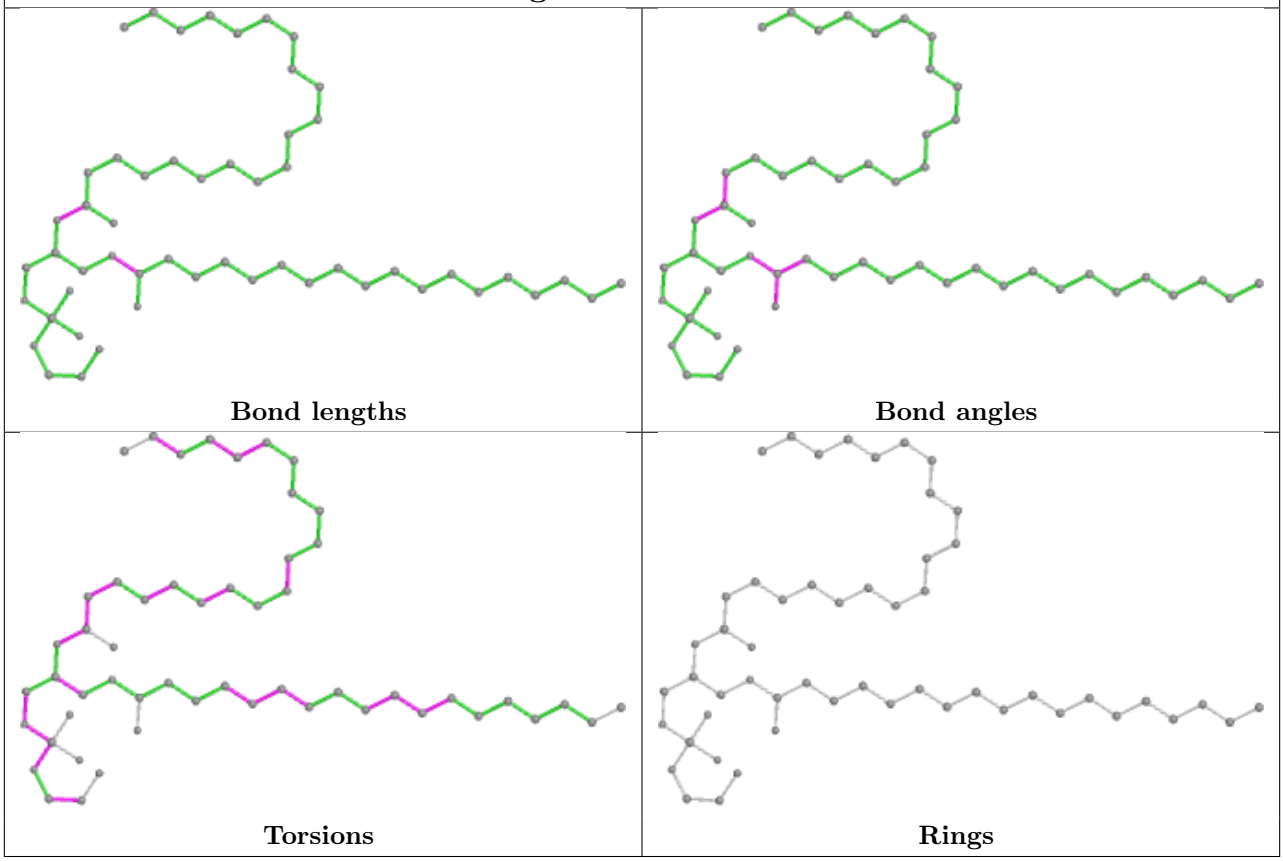


Torsions

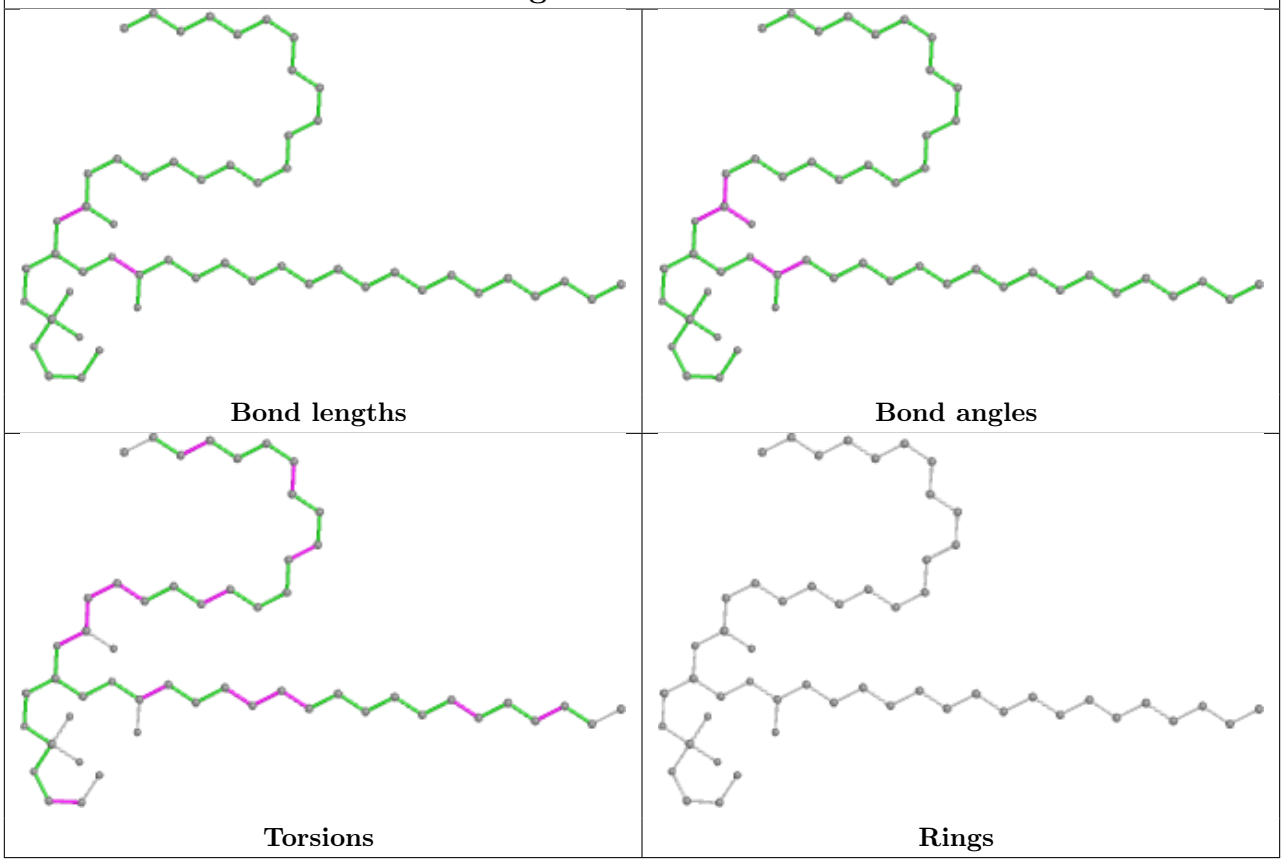


Rings

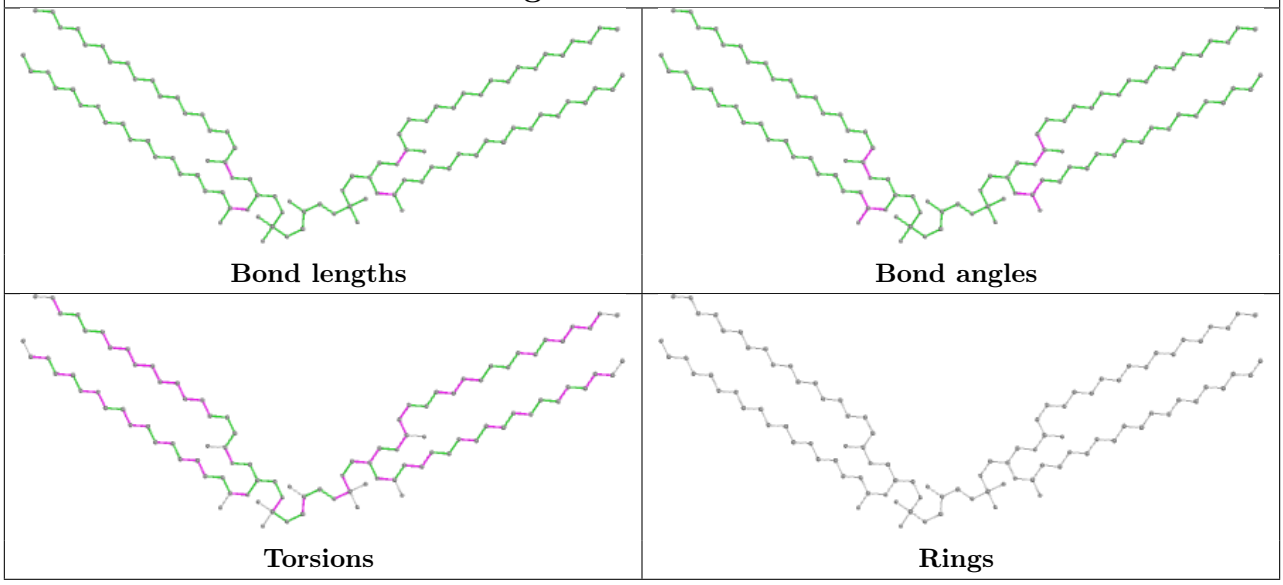
Ligand PEK c 305



Ligand PEK c 304



Ligand CDL G 102



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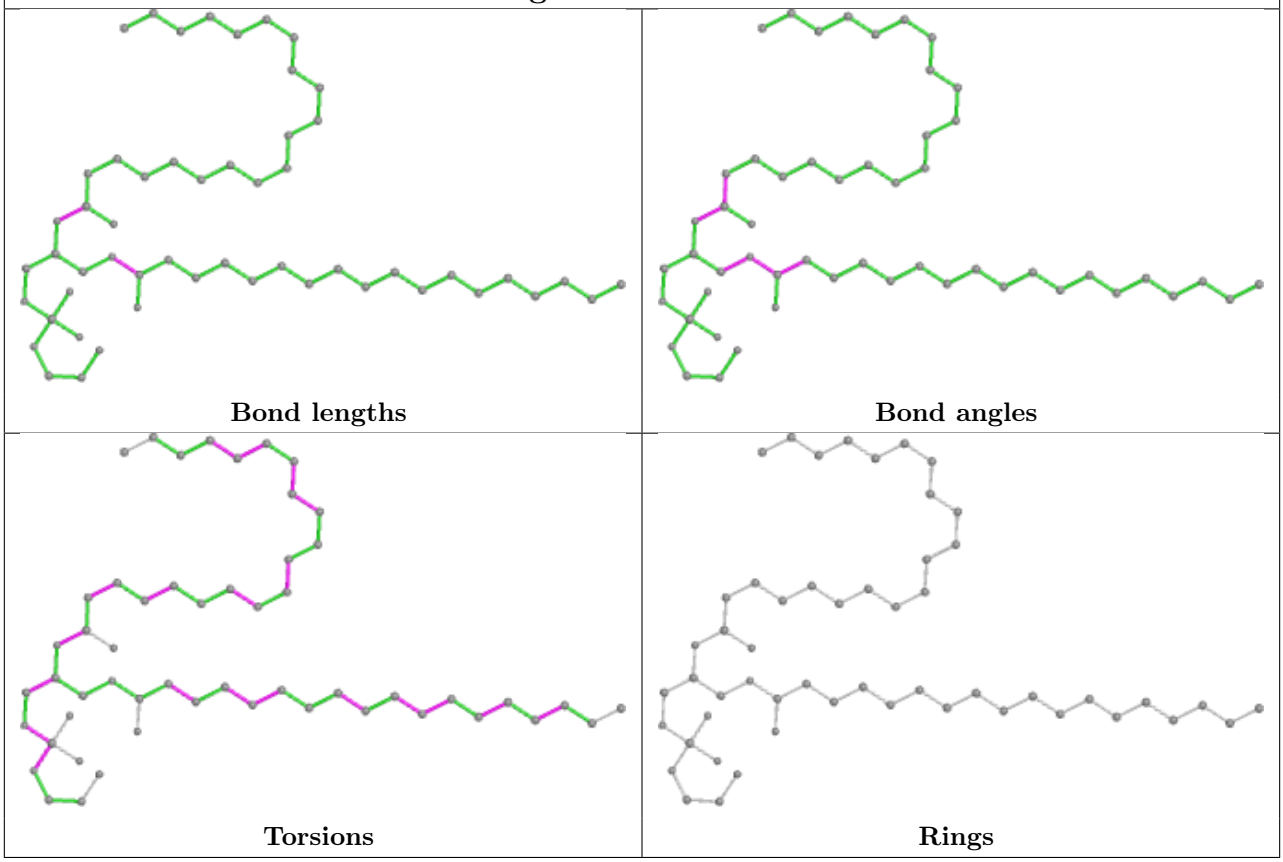

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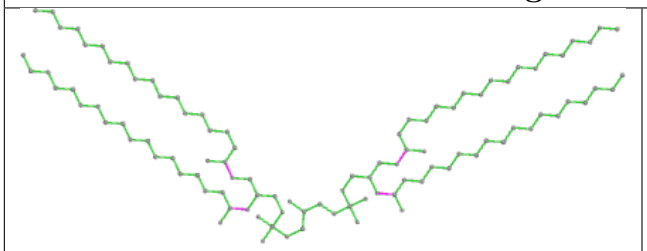
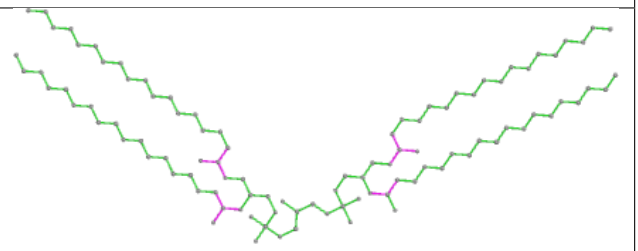
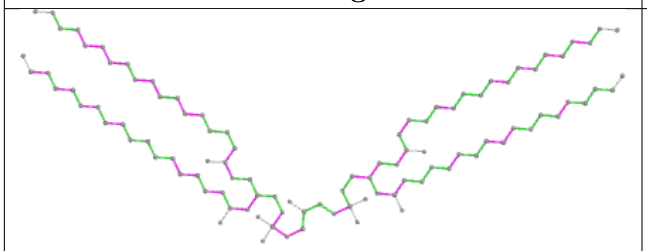


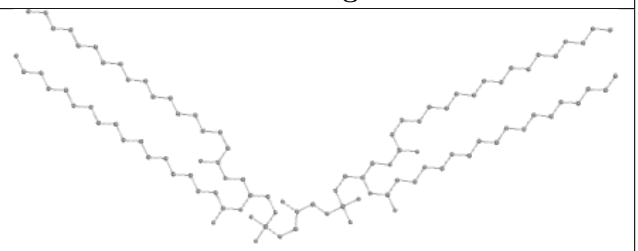
Bond lengths



Bond angles

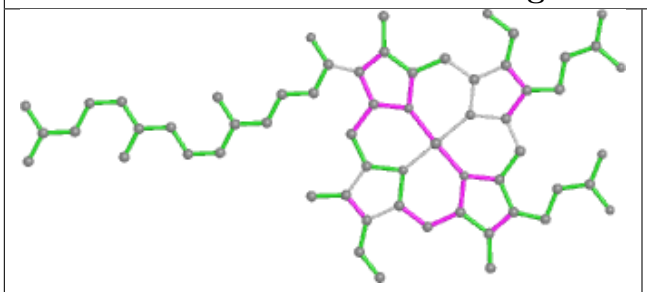


Torsions

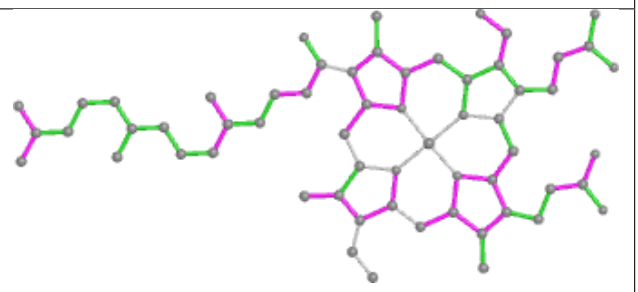


Rings

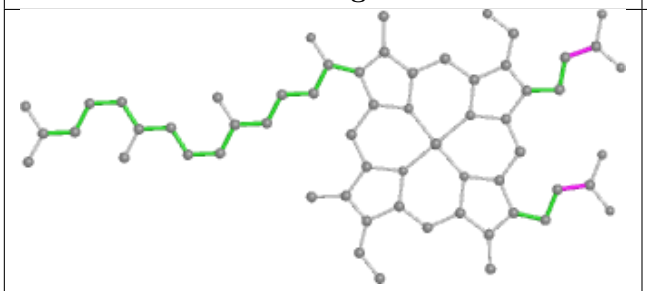
Ligand HEA a 601



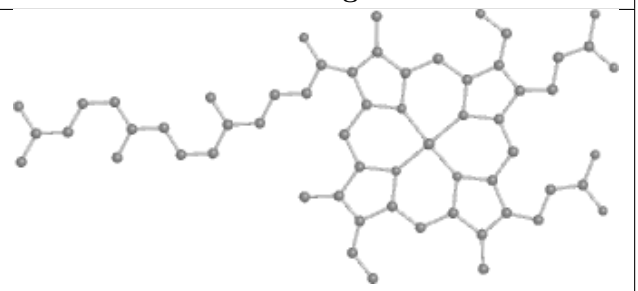
Bond lengths



Bond angles

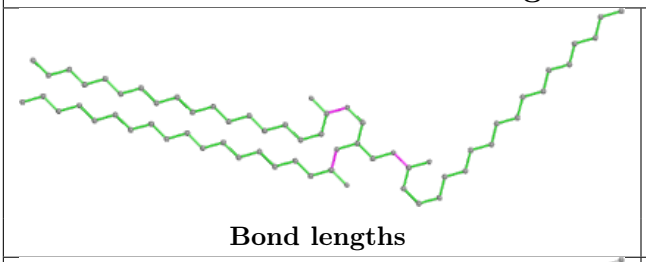


Torsions

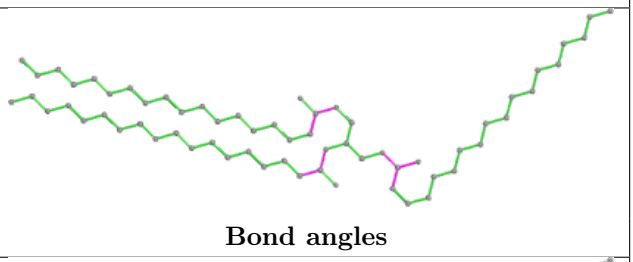


Rings

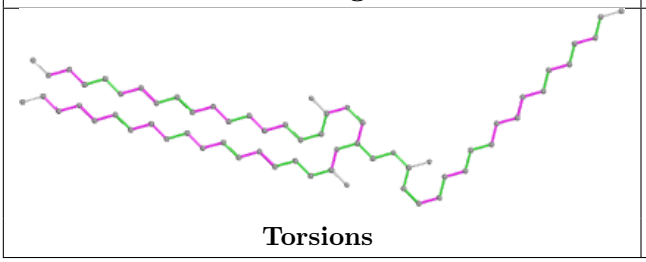
Ligand TGL A 608



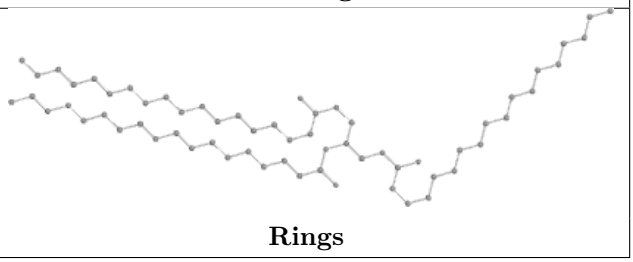
Bond lengths



Bond angles

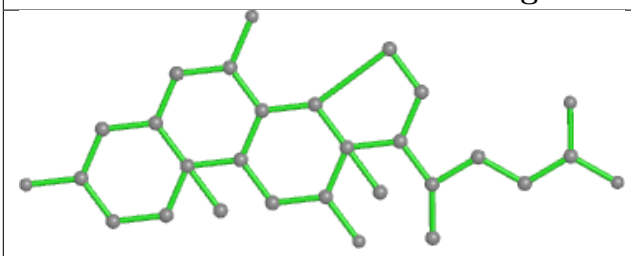


Torsions

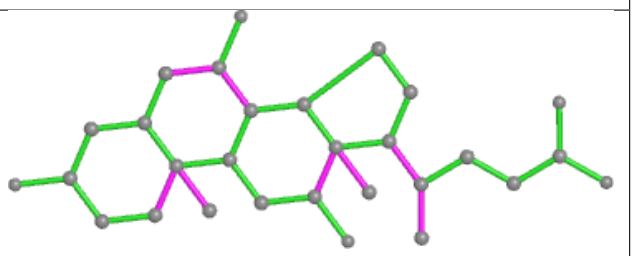


Rings

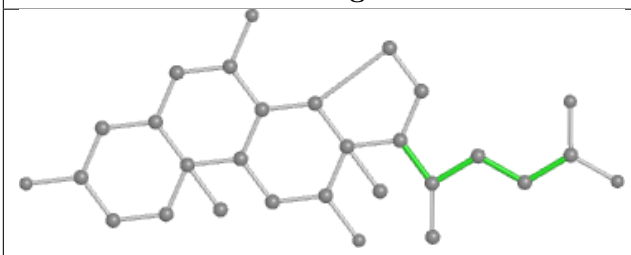
Ligand CHD C 301



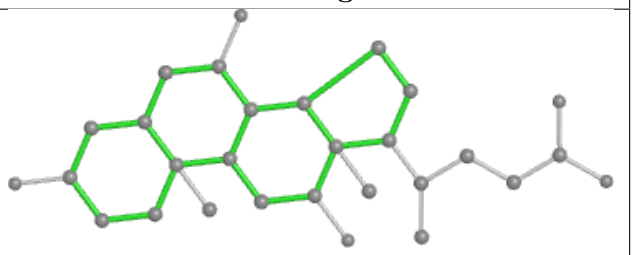
Bond lengths



Bond angles

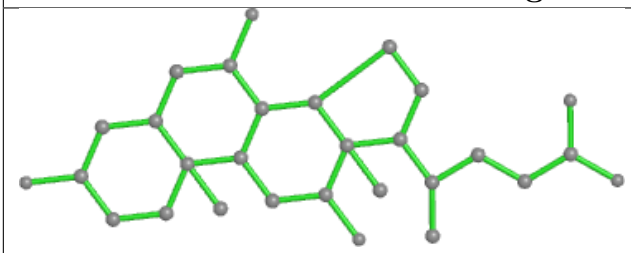


Torsions

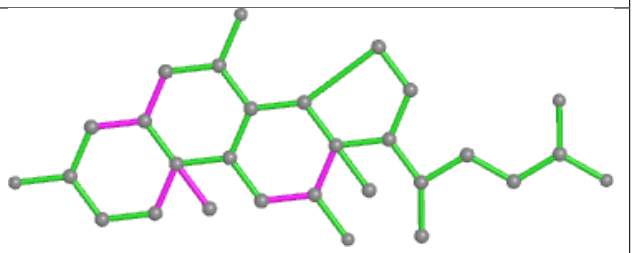


Rings

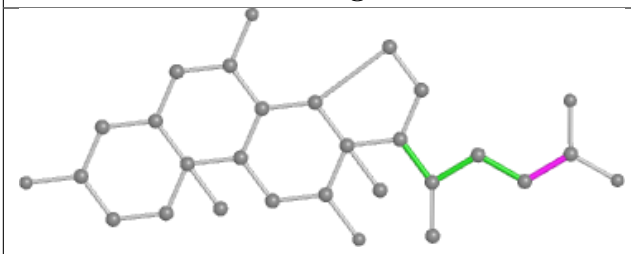
Ligand CHD c 308



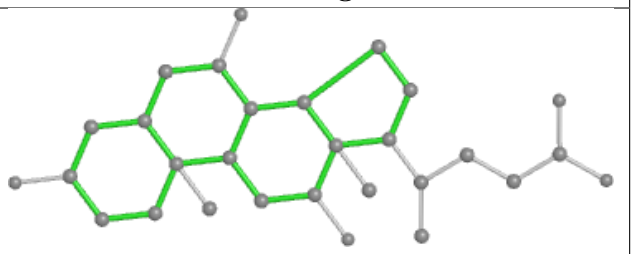
Bond lengths



Bond angles

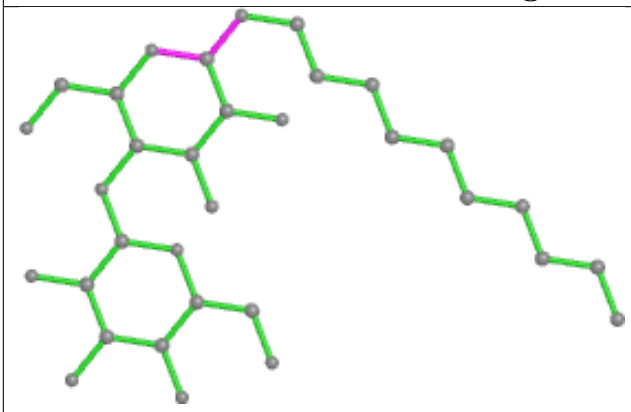


Torsions

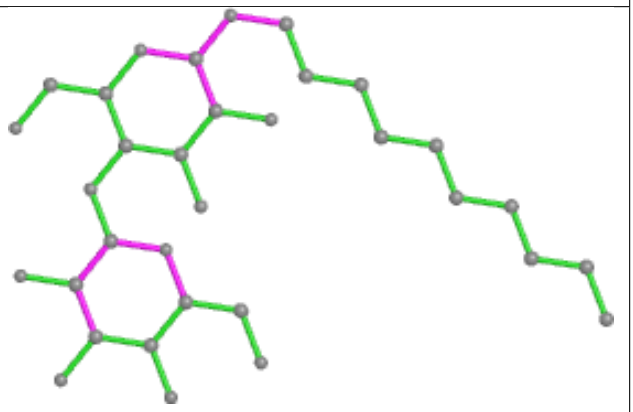


Rings

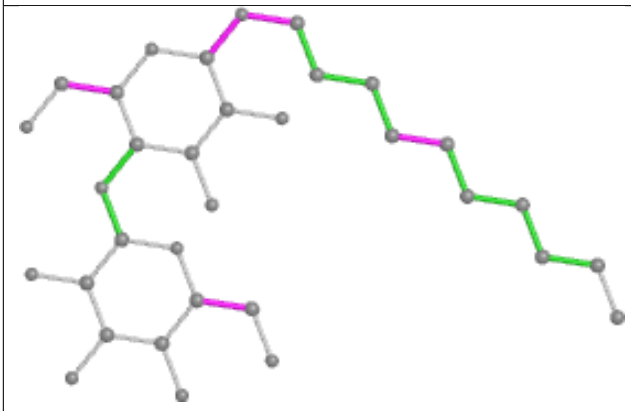
Ligand DMU c 309



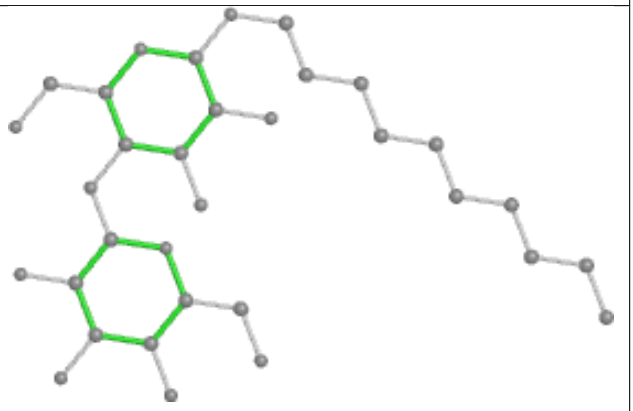
Bond lengths



Bond angles

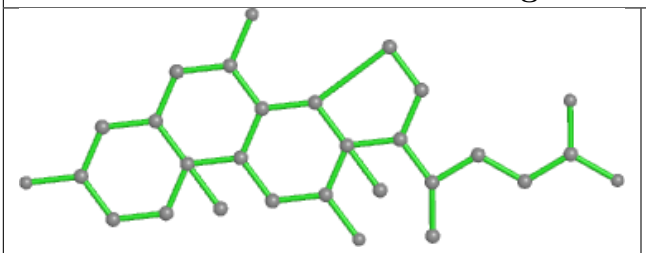


Torsions

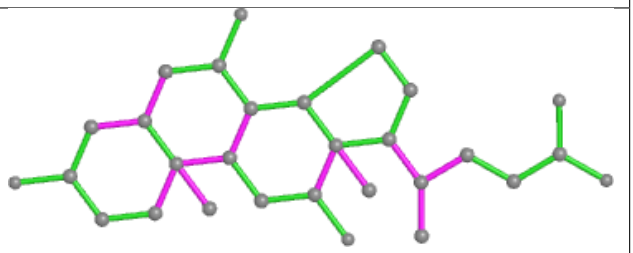


Rings

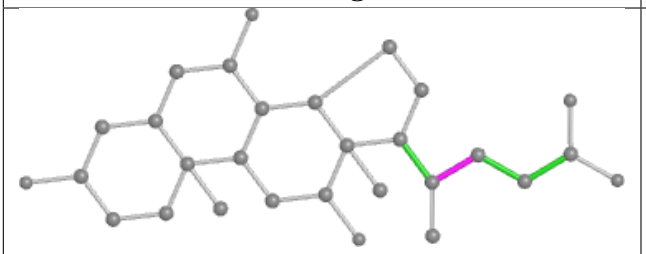
Ligand CHD C 306



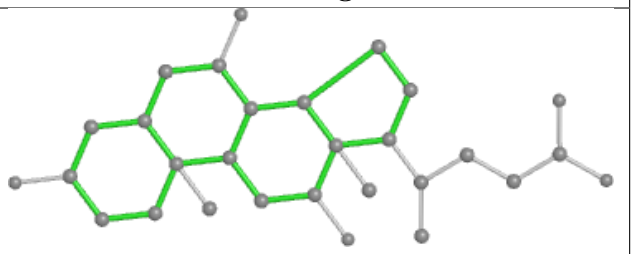
Bond lengths



Bond angles

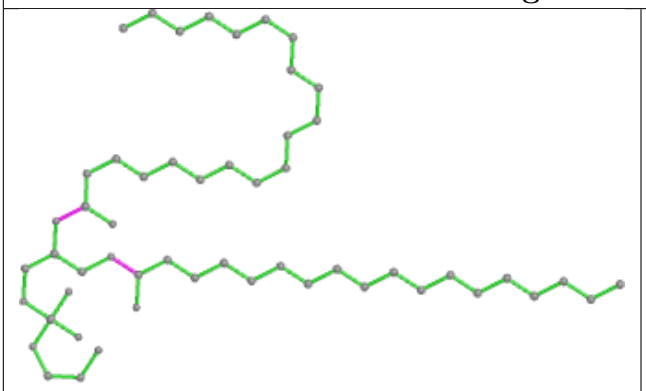


Torsions

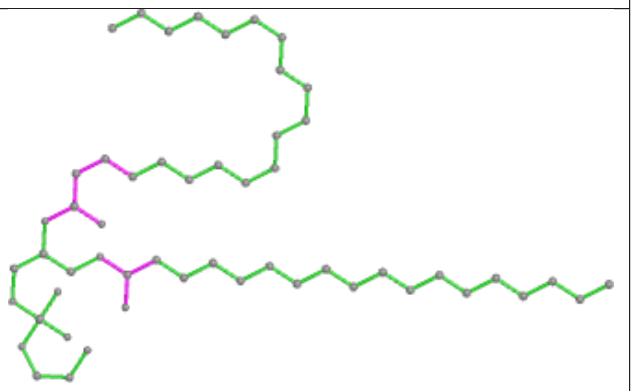


Rings

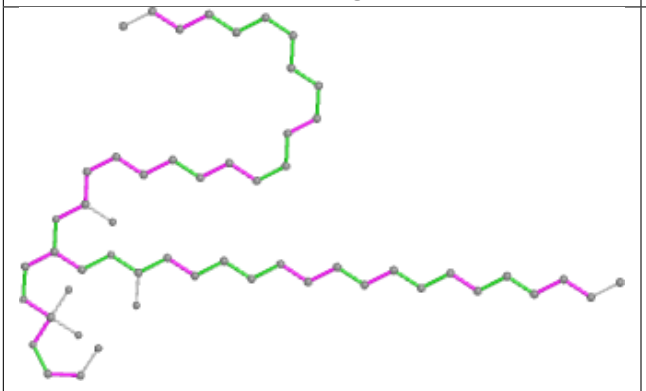
Ligand PEK G 101



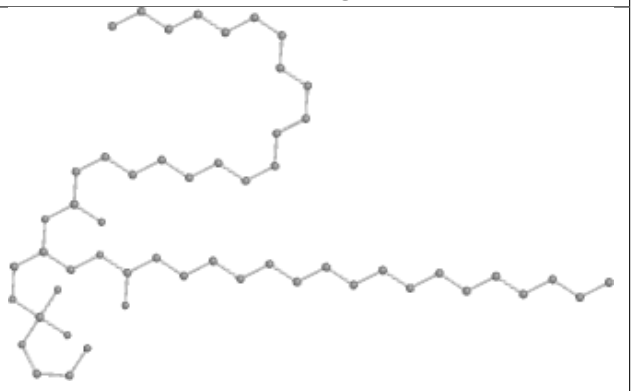
Bond lengths



Bond angles

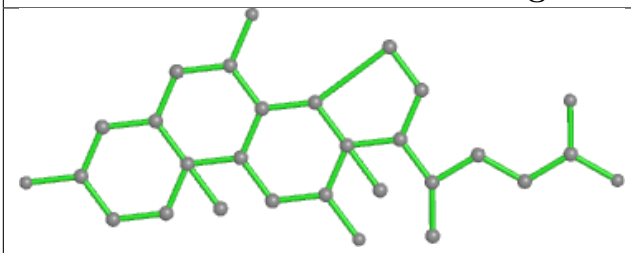


Torsions

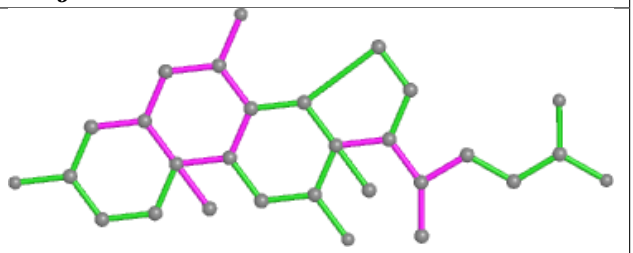


Rings

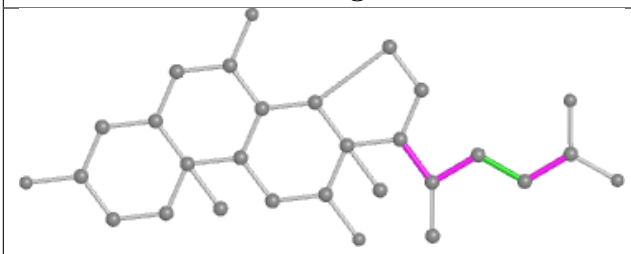
Ligand CHD j 101



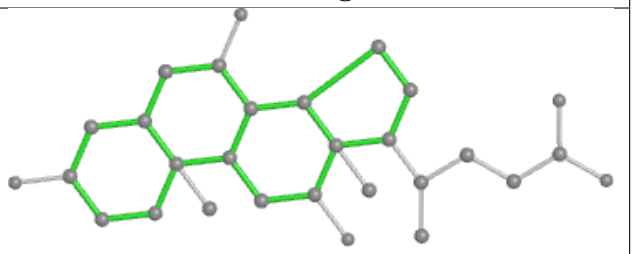
Bond lengths



Bond angles

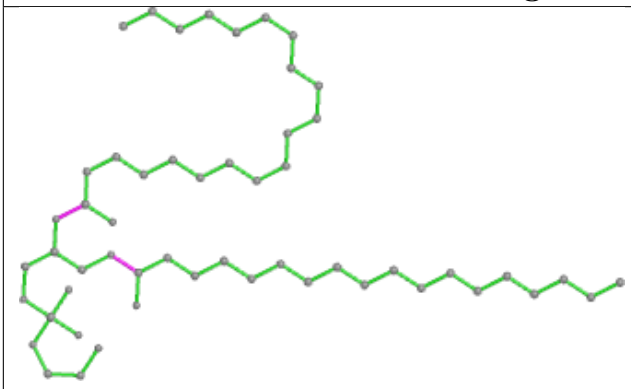


Torsions

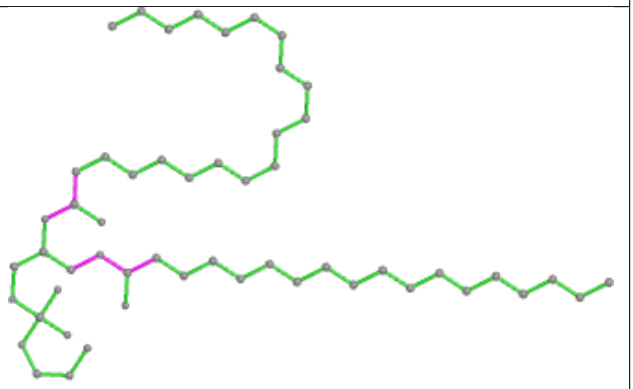


Rings

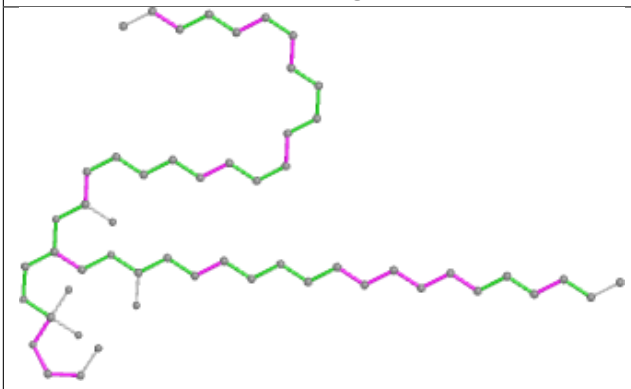
Ligand PEK C 307



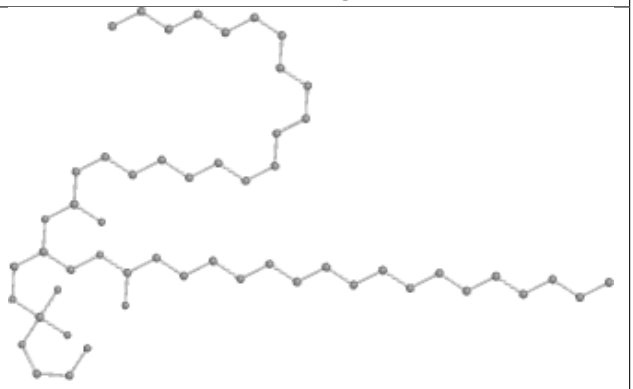
Bond lengths



Bond angles

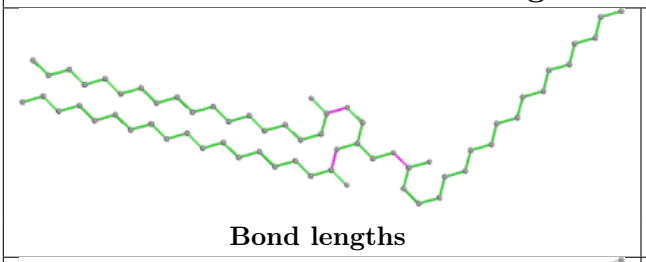


Torsions

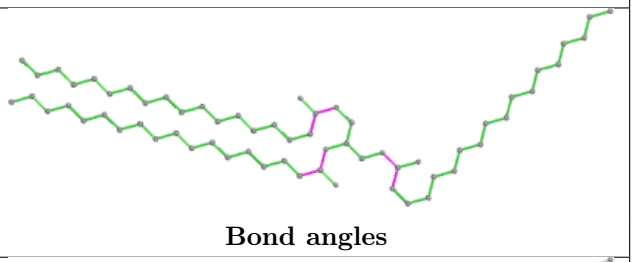


Rings

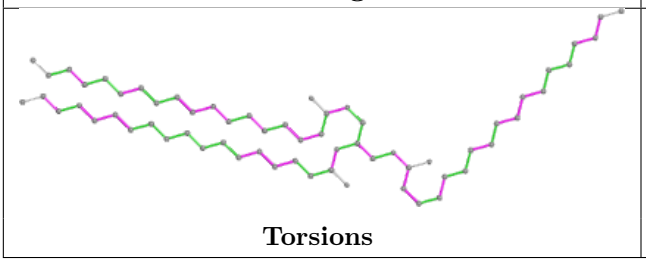
Ligand TGL b 302



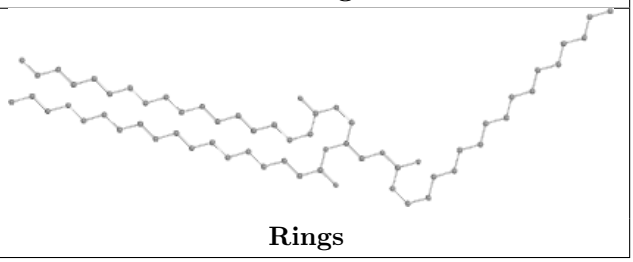
Bond lengths



Bond angles

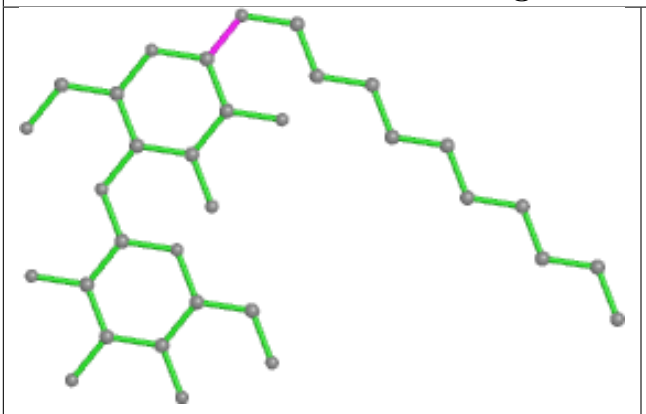


Torsions



Rings

Ligand DMU M 101



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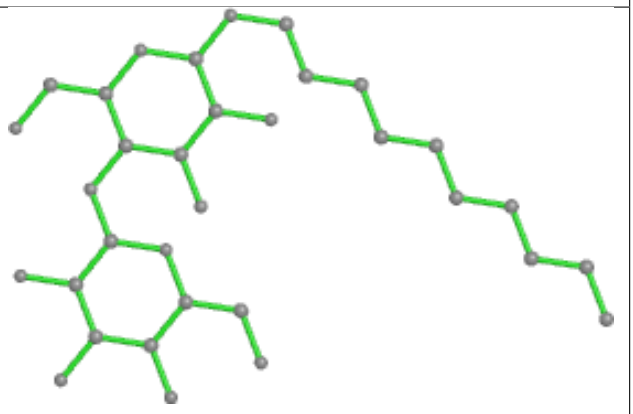
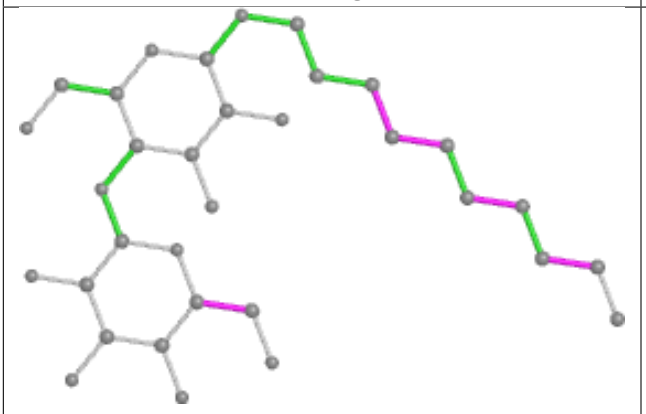
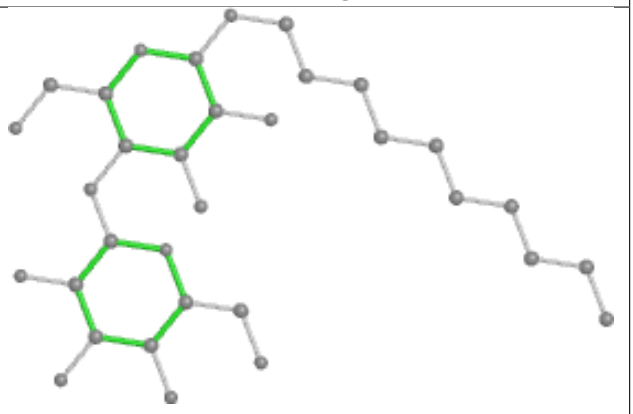


Bond angles

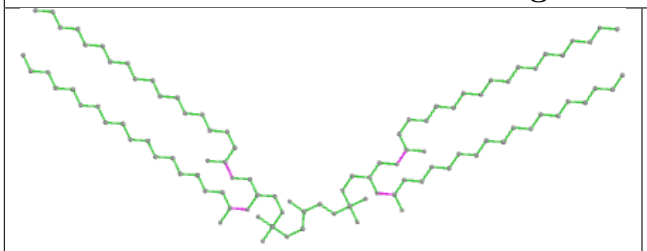


Torsions

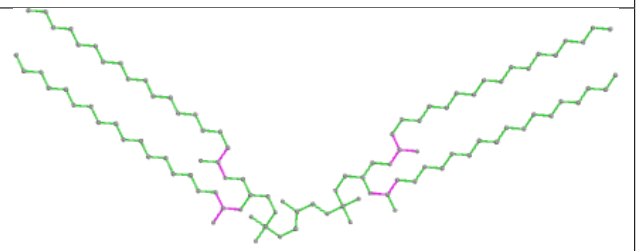


Rings

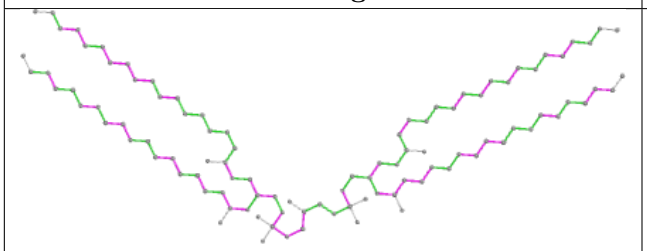
Ligand CDL c 307



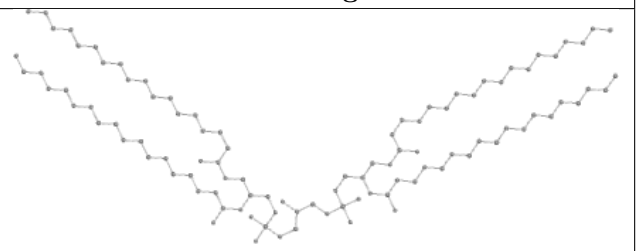
Bond lengths



Bond angles

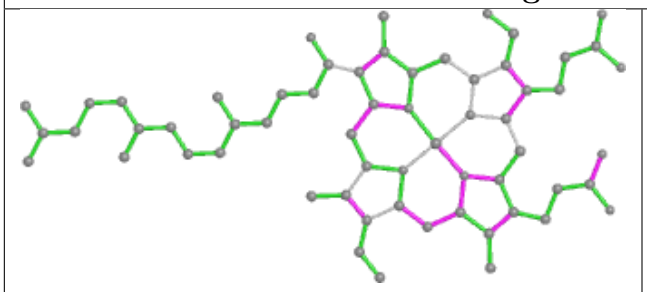


Torsions

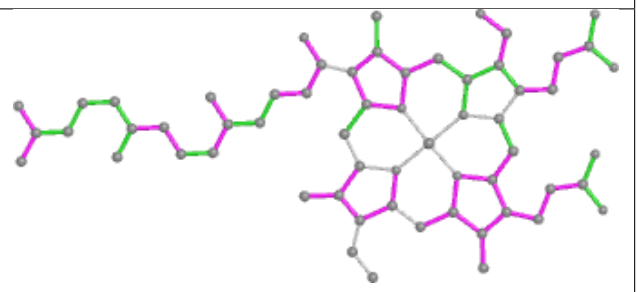


Rings

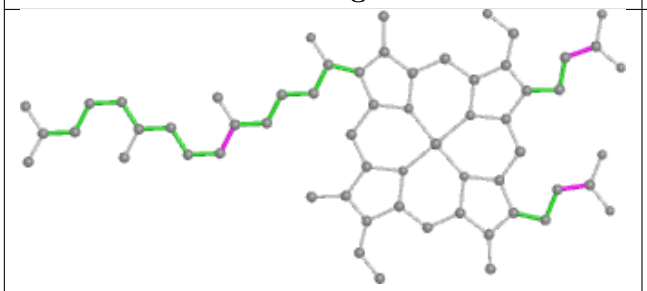
Ligand HEA A 601



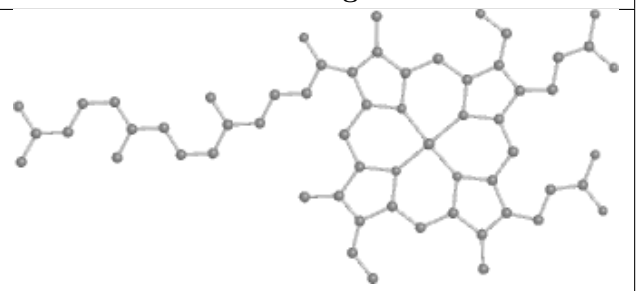
Bond lengths



Bond angles

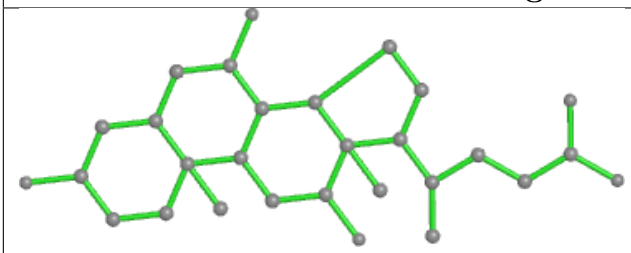


Torsions



Rings

Ligand CHD c 303



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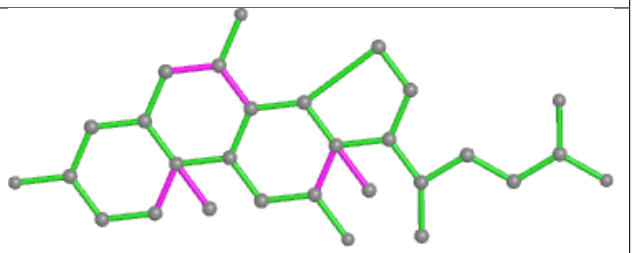
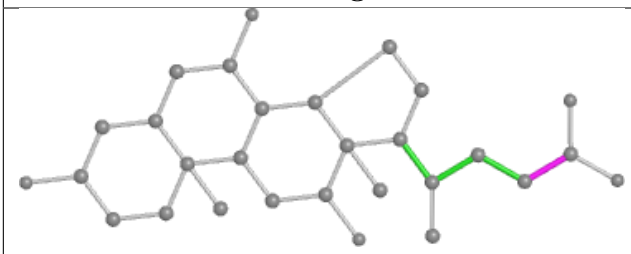
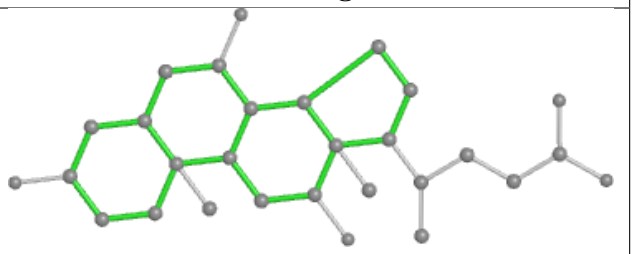


Bond angles

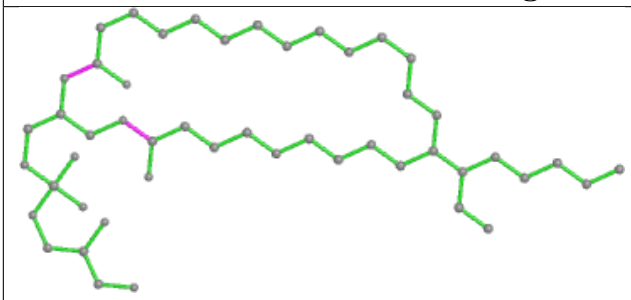


Torsions

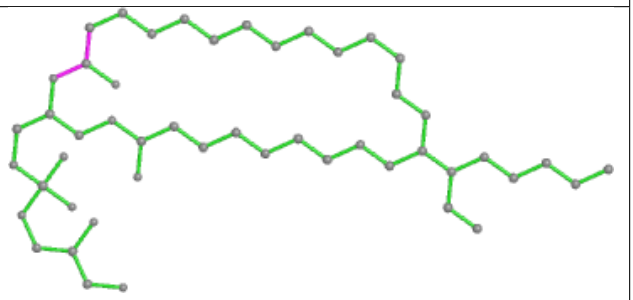


Rings

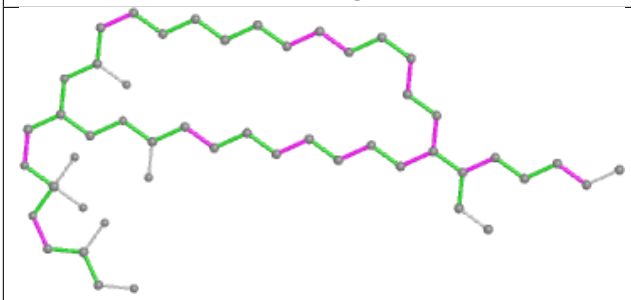
Ligand PGV C 303



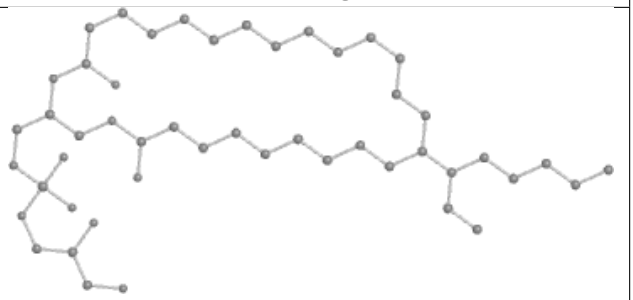
Bond lengths



Bond angles

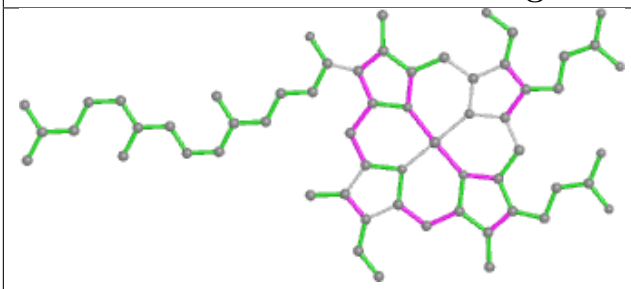


Torsions



Rings

Ligand HEA a 602



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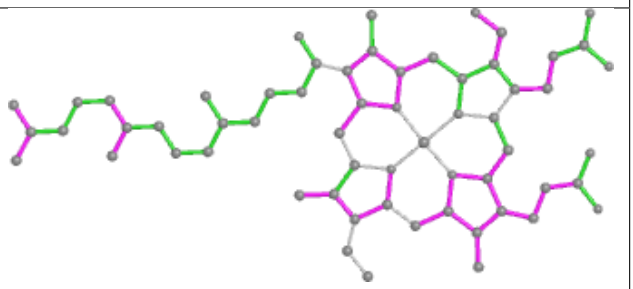
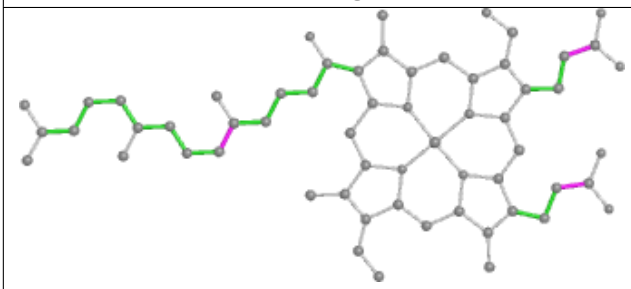
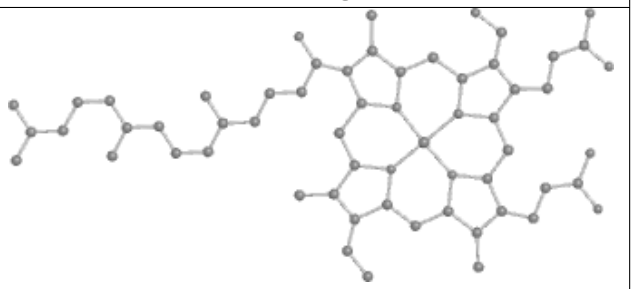


Bond angles

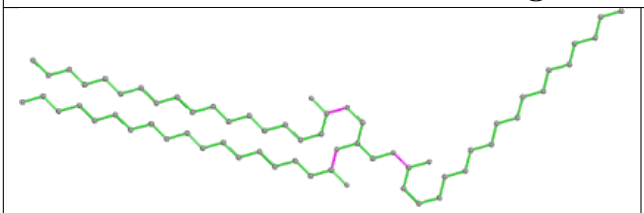


Torsions



Rings

Ligand TGL d 201



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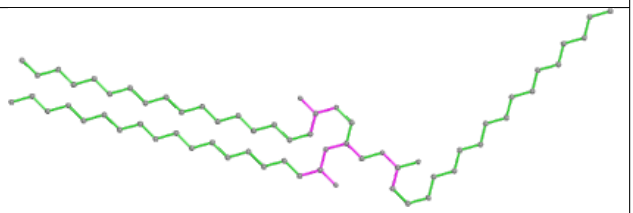
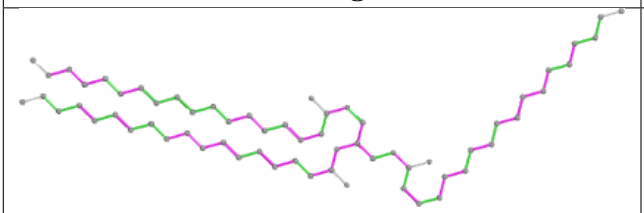
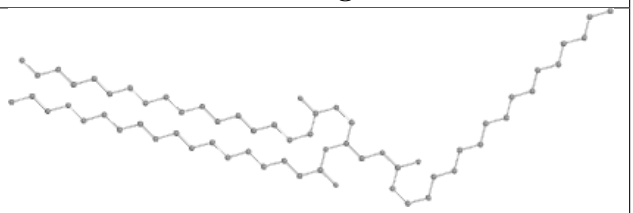


Bond angles

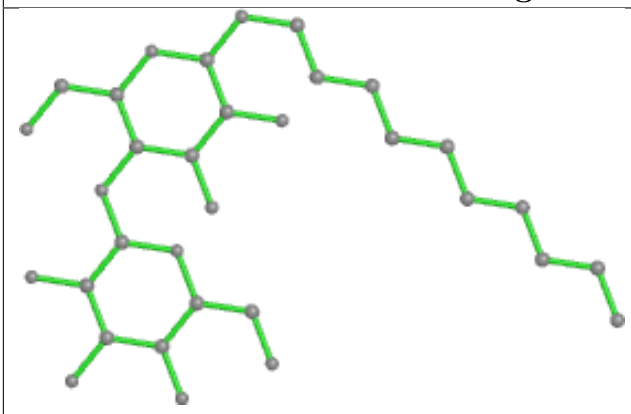


Torsions

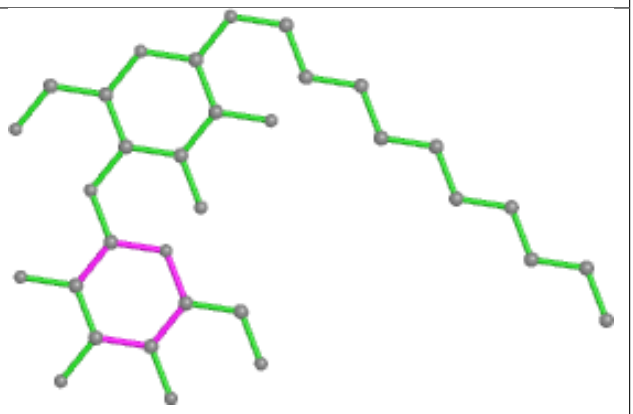


Rings

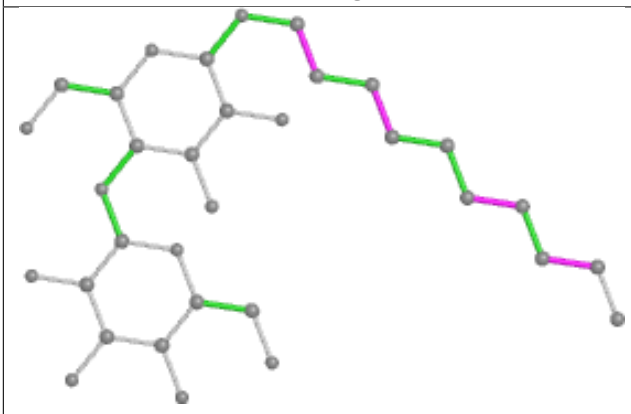
Ligand DMU m 101



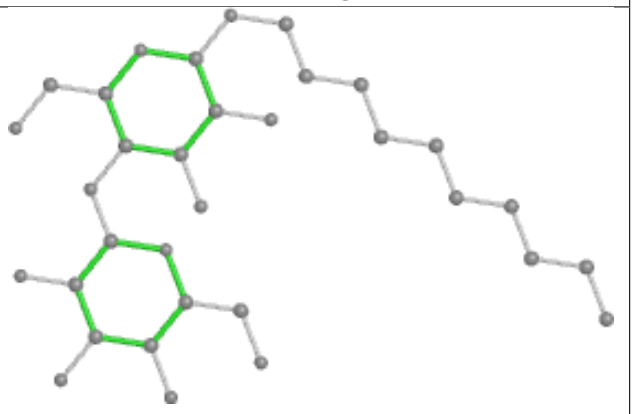
Bond lengths



Bond angles

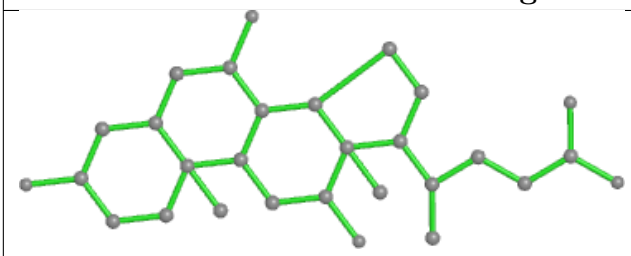


Torsions

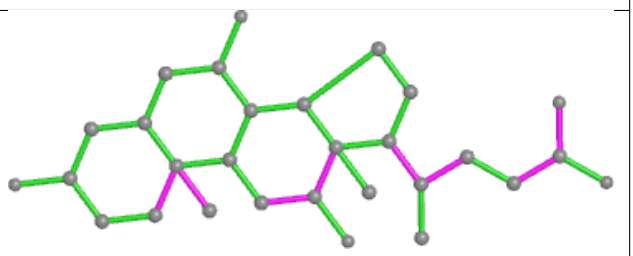


Rings

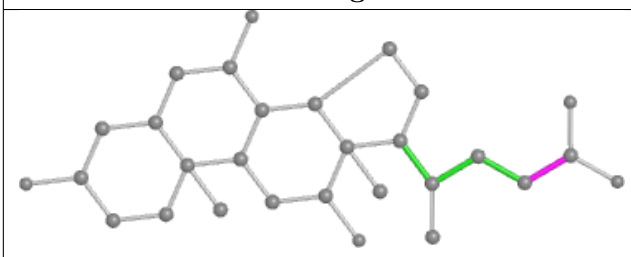
Ligand CHD G 103



Bond lengths



Bond angles



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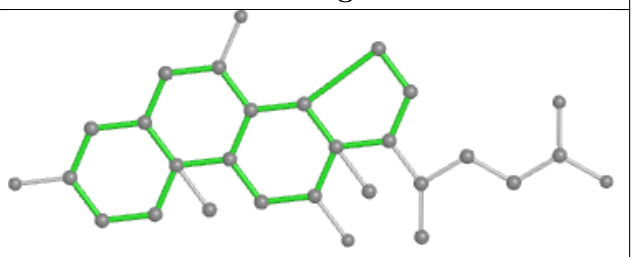
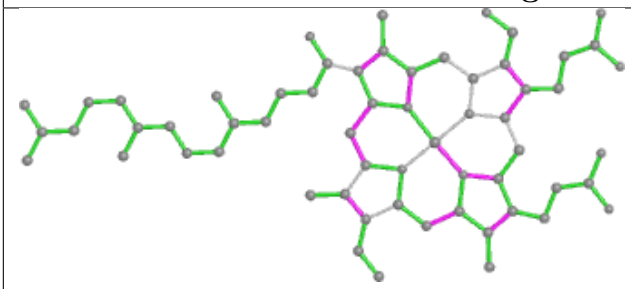
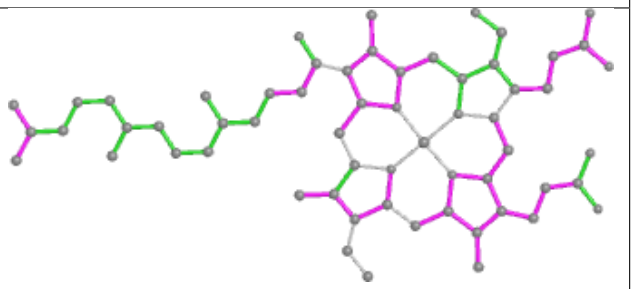


Rings

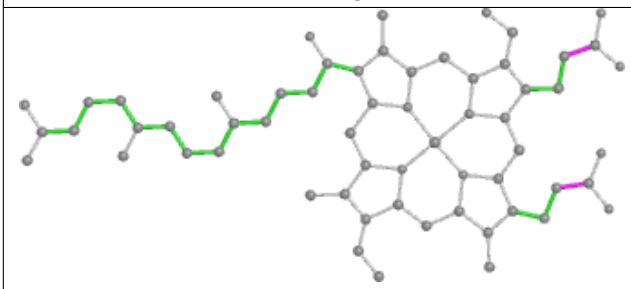
Ligand HEA A 602



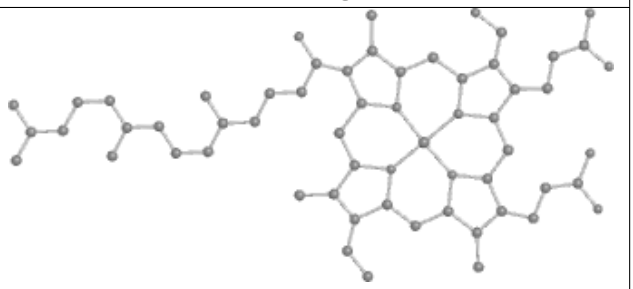
Bond lengths



Bond angles

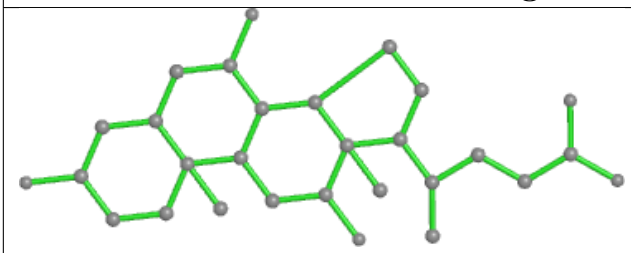


Torsions

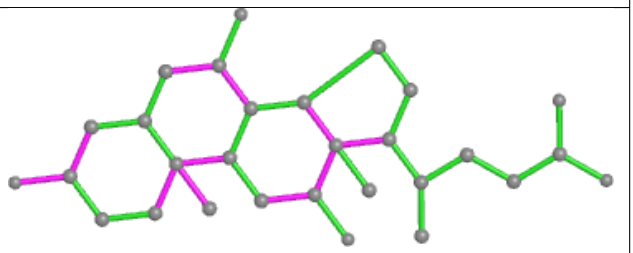


Rings

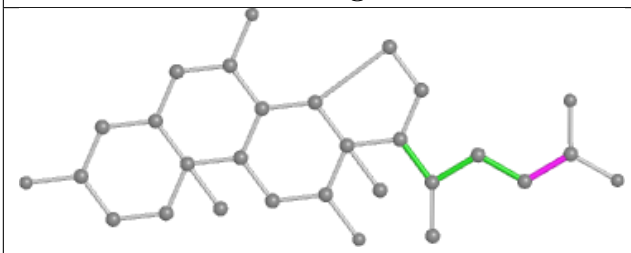
Ligand CHD B 402



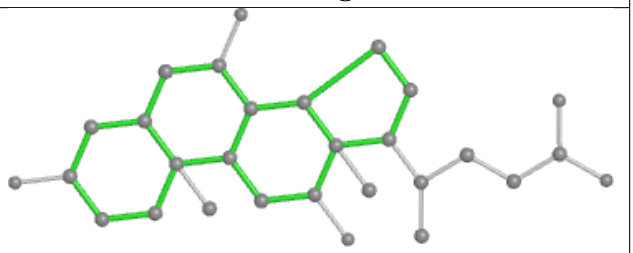
Bond lengths



Bond angles

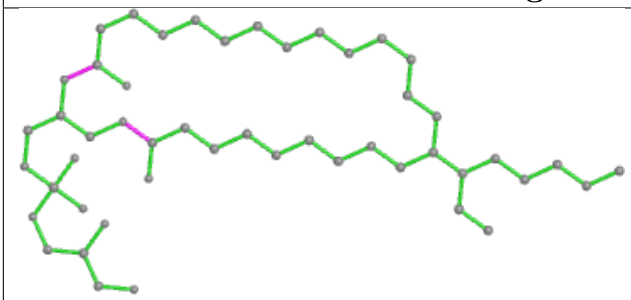


Torsions

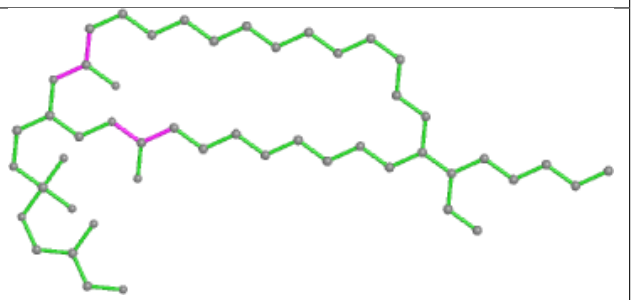


Rings

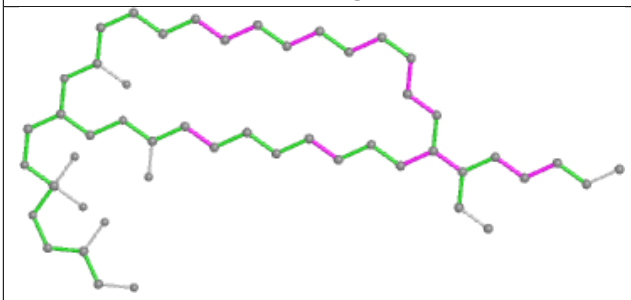
Ligand PGV a 607



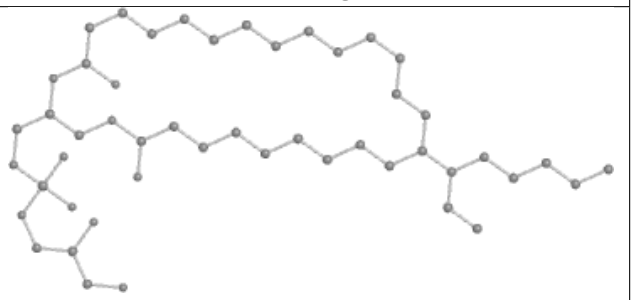
Bond lengths



Bond angles

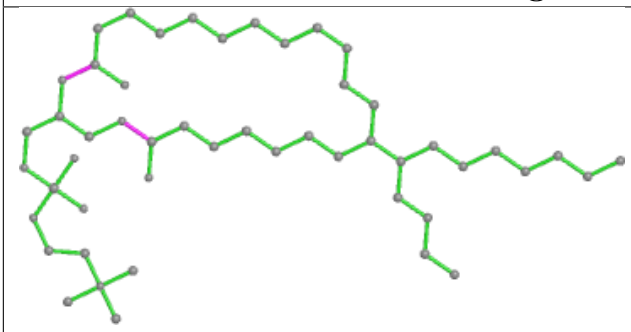


Torsions

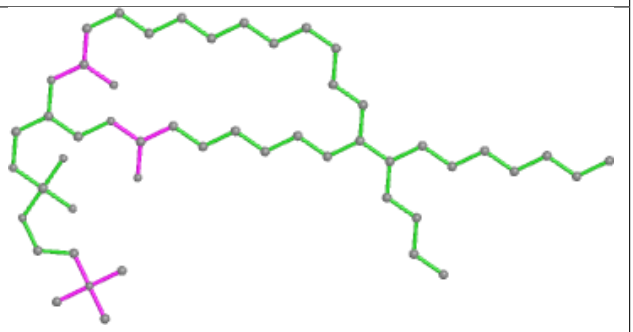


Rings

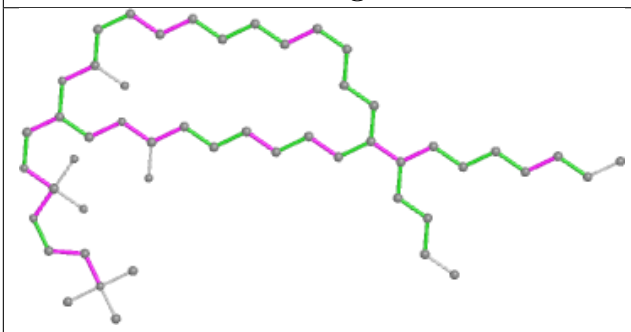
Ligand PSC E 201



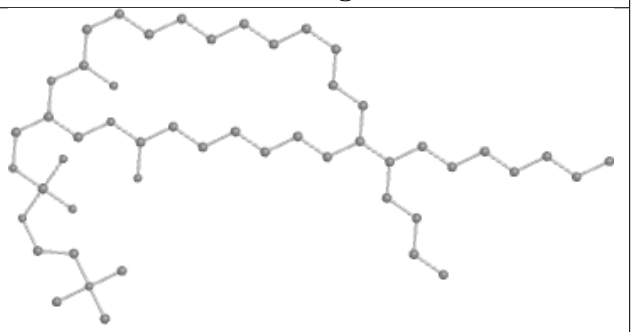
Bond lengths



Bond angles

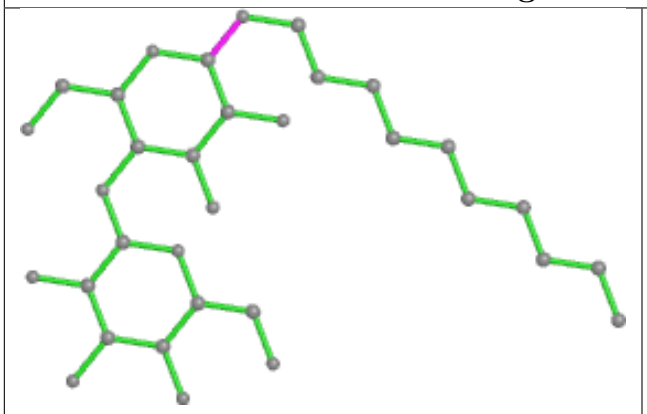


Torsions

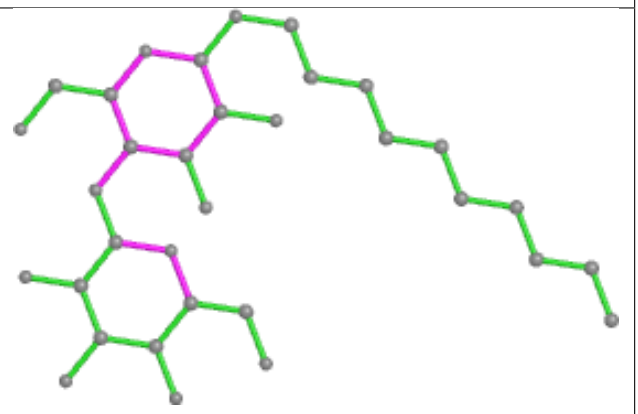


Rings

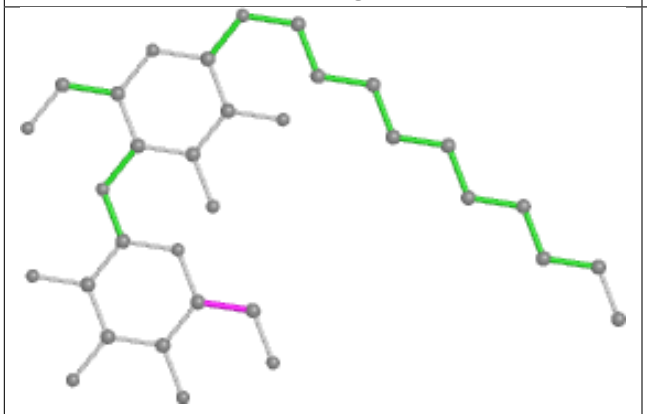
Ligand DMU C 308



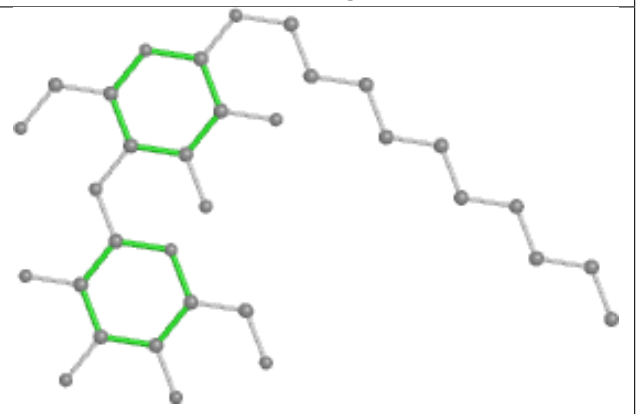
Bond lengths



Bond angles

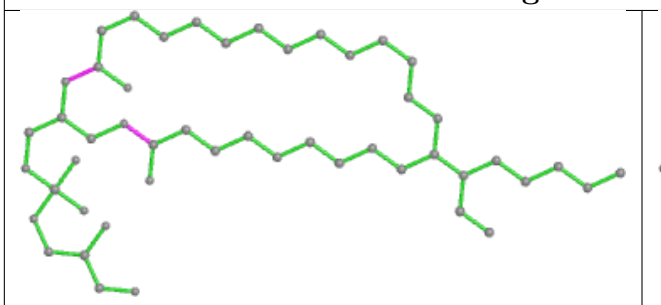


Torsions

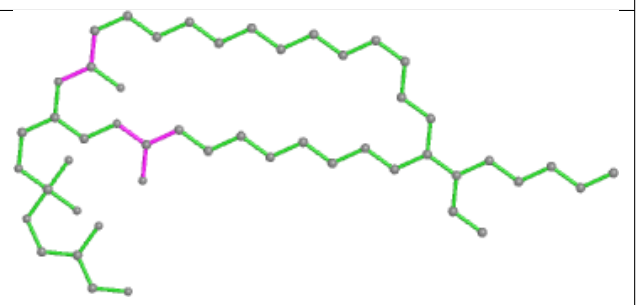


Rings

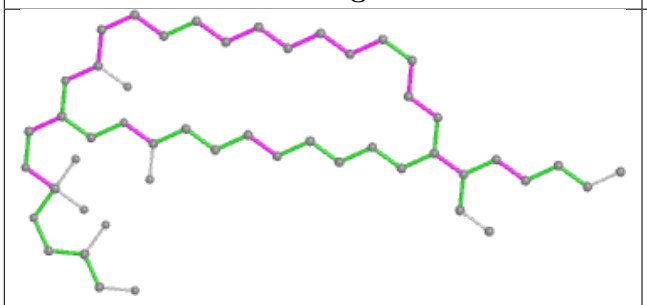
Ligand PGV A 606



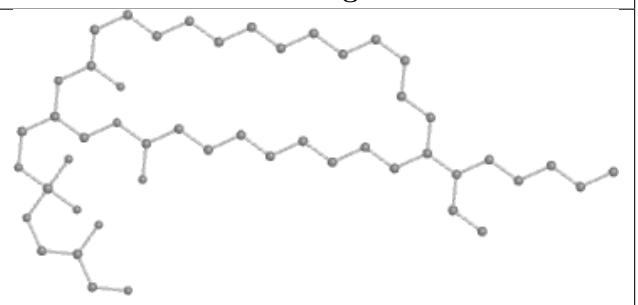
Bond lengths



Bond angles

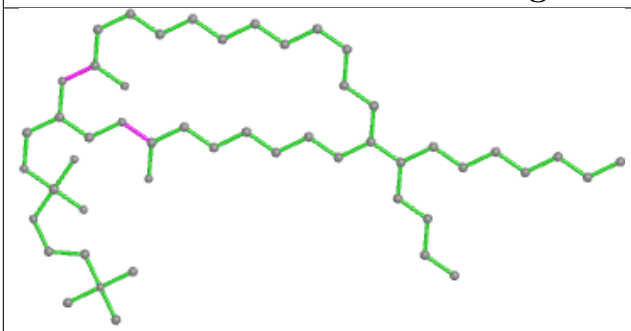


Torsions

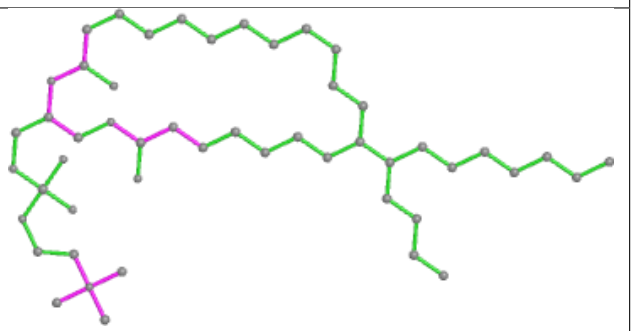


Rings

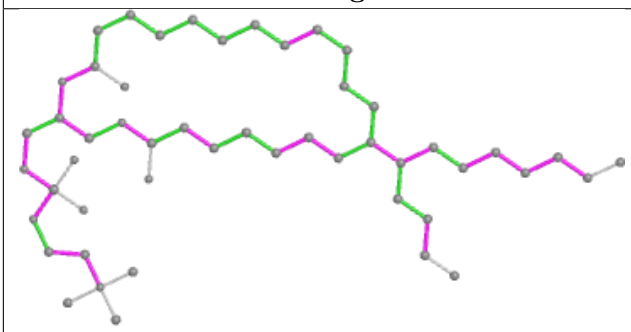
Ligand PSC b 303



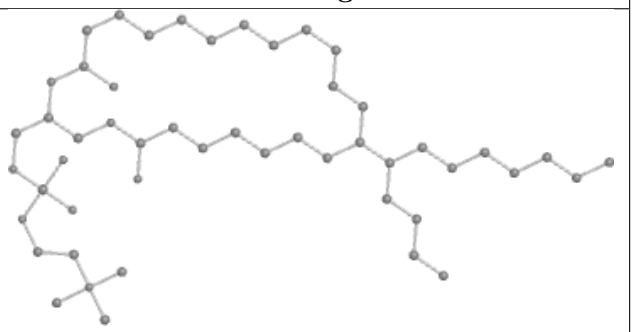
Bond lengths



Bond angles

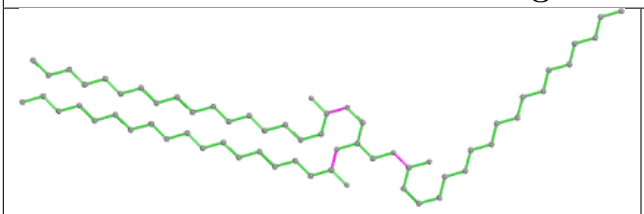


Torsions

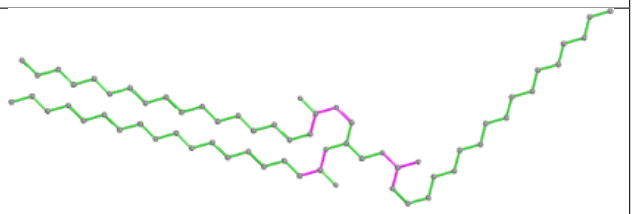


Rings

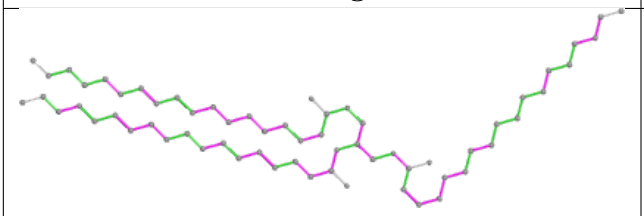
Ligand TGL l 101



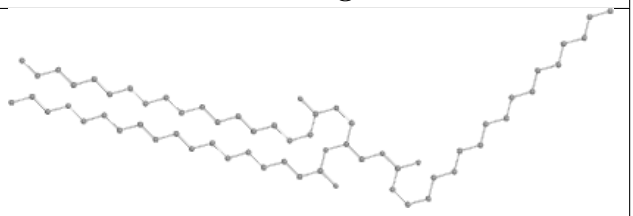
Bond lengths



Bond angles

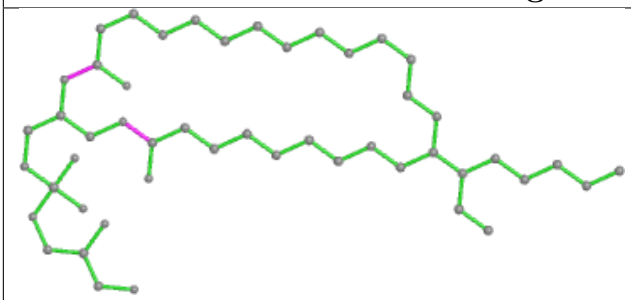


Torsions

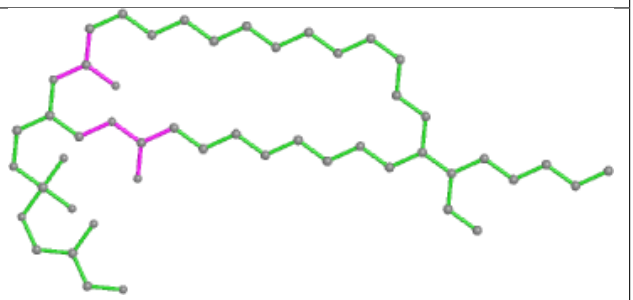


Rings

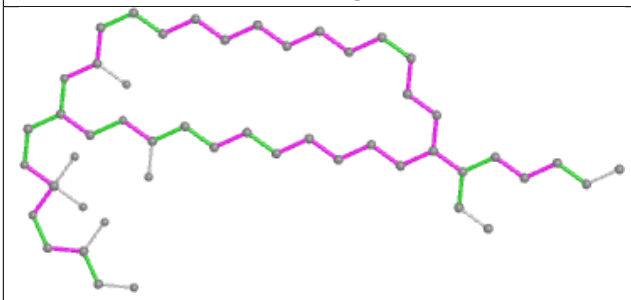
Ligand PGV c 302



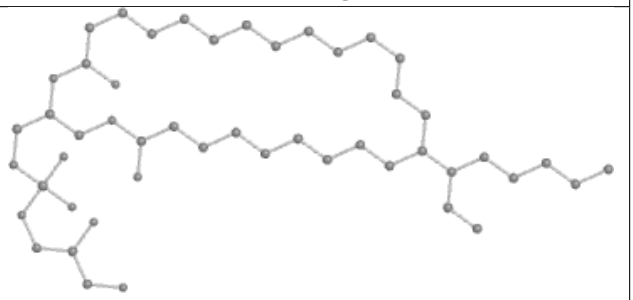
Bond lengths



Bond angles

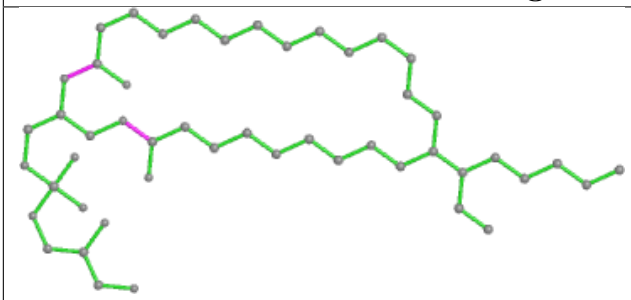


Torsions

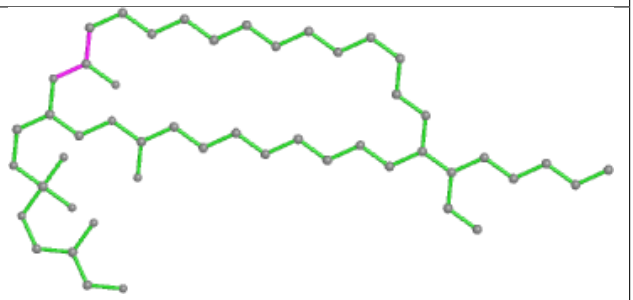


Rings

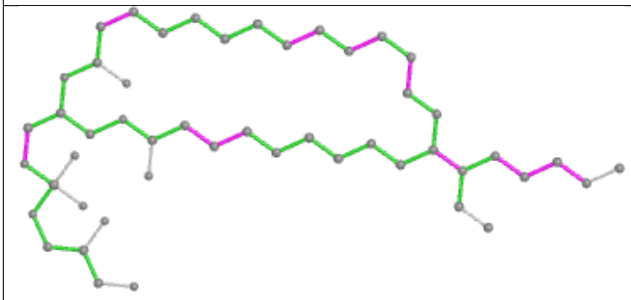
Ligand PGV c 306



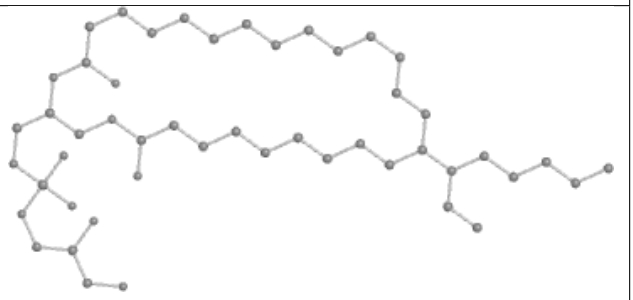
Bond lengths



Bond angles

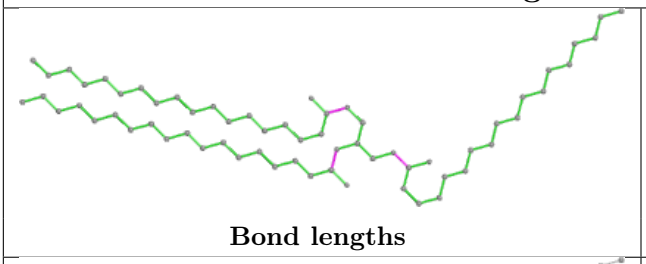


Torsions

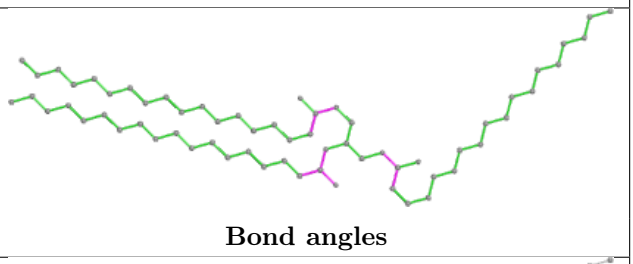


Rings

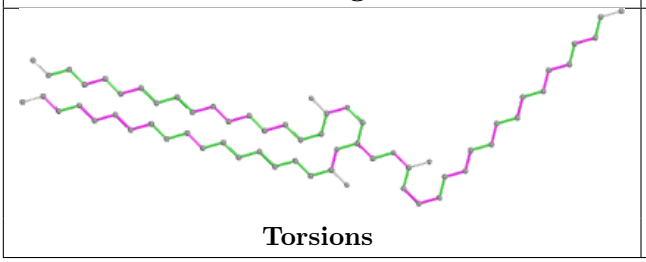
Ligand TGL D 201



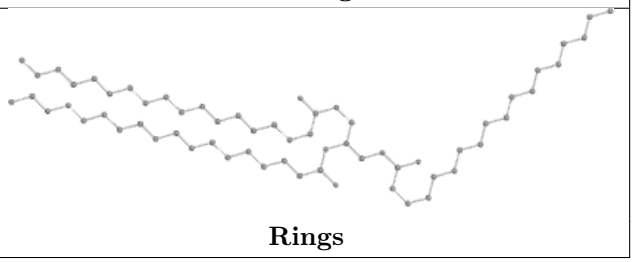
Bond lengths



Bond angles

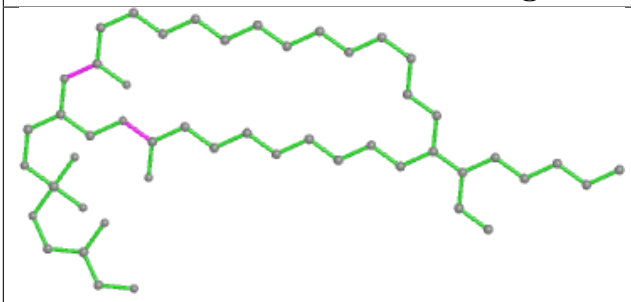


Torsions

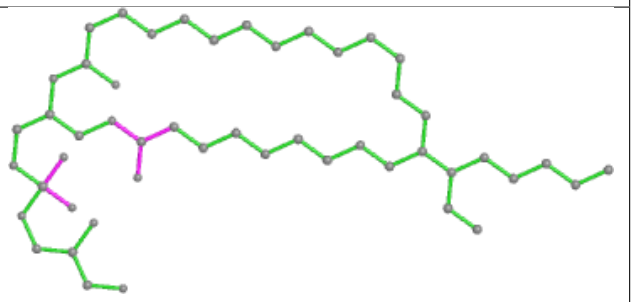


Rings

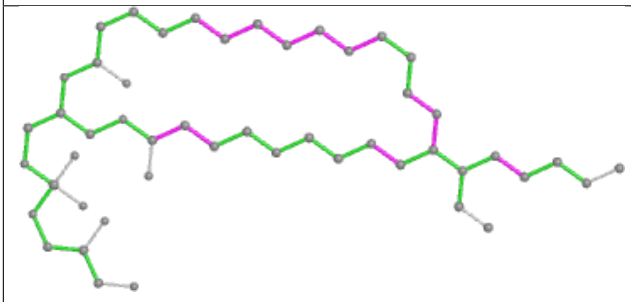
Ligand PGV A 607



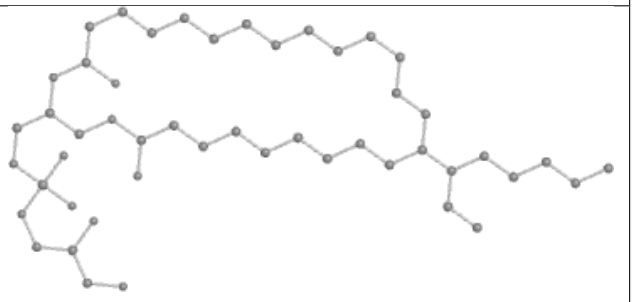
Bond lengths



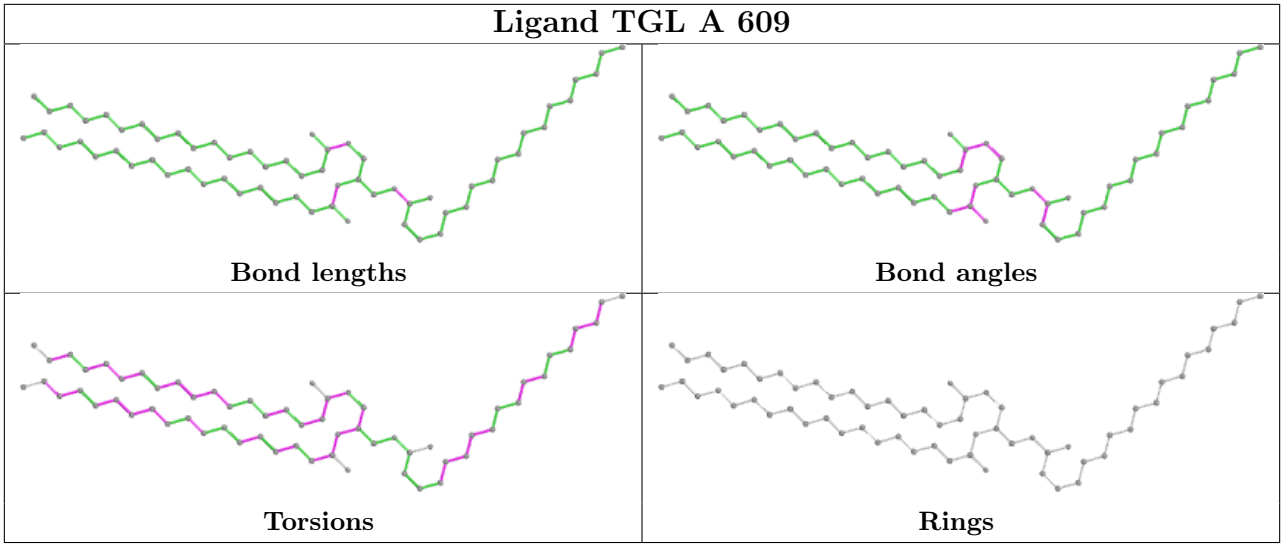
Bond angles

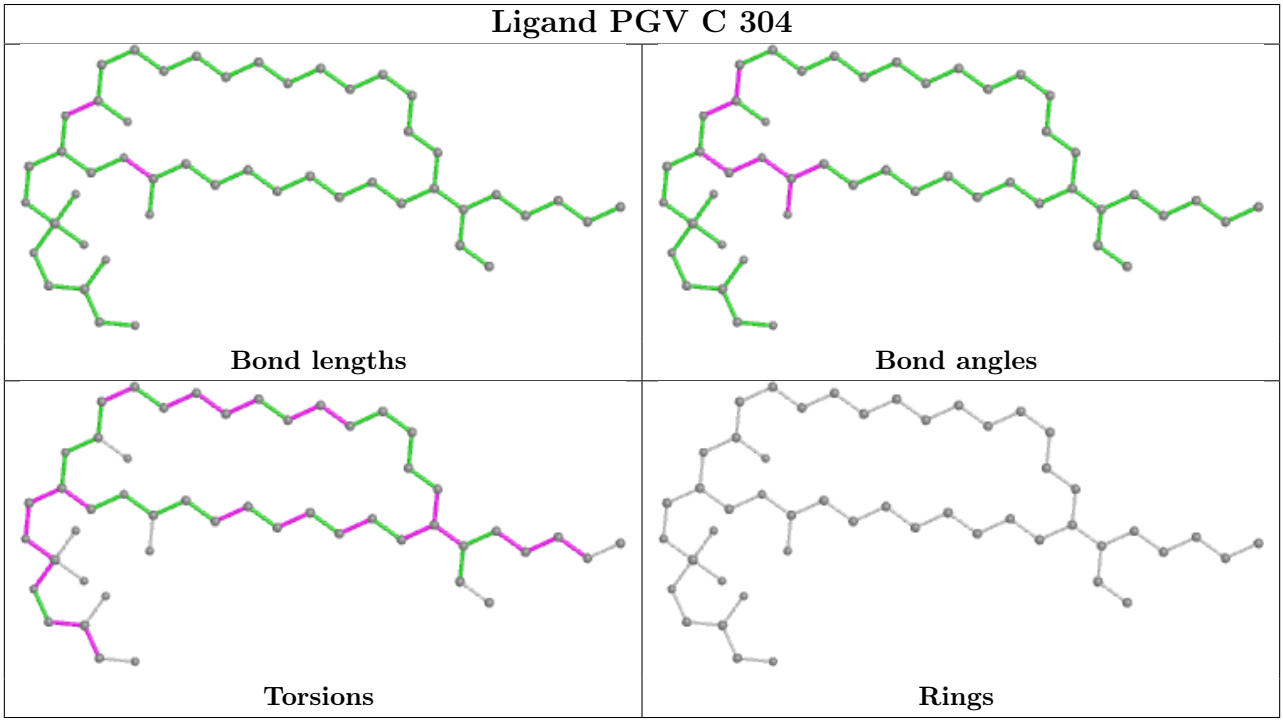


Torsions



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	513/514 (99%)	0.23	8 (1%) 72 79	21, 27, 36, 72	0
1	a	513/514 (99%)	0.39	12 (2%) 60 69	27, 39, 52, 76	0
2	B	226/227 (99%)	0.01	5 (2%) 62 70	23, 34, 55, 89	0
2	b	226/227 (99%)	0.43	11 (4%) 29 39	35, 45, 70, 104	0
3	C	259/261 (99%)	-0.21	1 (0%) 92 95	26, 32, 44, 79	0
3	c	259/261 (99%)	-0.07	4 (1%) 73 81	30, 39, 55, 79	0
4	D	144/147 (97%)	-0.07	2 (1%) 75 82	29, 37, 53, 77	0
4	d	144/147 (97%)	1.37	30 (20%) 1 1	46, 58, 90, 147	0
5	E	105/109 (96%)	0.00	3 (2%) 51 60	32, 40, 60, 107	0
5	e	105/109 (96%)	0.63	9 (8%) 10 16	39, 51, 70, 105	0
6	F	98/98 (100%)	0.85	9 (9%) 9 14	27, 38, 87, 129	0
6	f	98/98 (100%)	1.15	13 (13%) 3 5	34, 48, 103, 143	0
7	G	83/85 (97%)	1.08	21 (25%) 0 0	30, 40, 106, 141	0
7	g	83/85 (97%)	1.21	22 (26%) 0 0	32, 49, 103, 118	0
8	H	79/85 (92%)	0.75	13 (16%) 1 2	29, 42, 89, 120	0
8	h	79/85 (92%)	1.06	15 (18%) 1 1	40, 52, 97, 116	0
9	I	72/73 (98%)	0.44	8 (11%) 5 8	32, 45, 63, 75	0
9	i	72/73 (98%)	0.98	13 (18%) 1 1	37, 54, 73, 90	0
10	J	58/59 (98%)	0.45	6 (10%) 6 10	30, 42, 64, 110	0
10	j	58/59 (98%)	1.25	15 (25%) 0 0	42, 53, 77, 130	0
11	K	49/56 (87%)	0.49	3 (6%) 21 29	31, 41, 58, 73	0
11	k	49/56 (87%)	1.91	23 (46%) 0 0	53, 60, 79, 91	0
12	L	46/47 (97%)	0.01	2 (4%) 35 45	28, 34, 54, 88	0
12	l	46/47 (97%)	0.56	4 (8%) 10 16	44, 52, 72, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.25	4 (9%) 8 14	31, 35, 62, 88	0
13	m	43/46 (93%)	1.23	8 (18%) 1 1	47, 57, 87, 117	0
All	All	3550/3614 (98%)	0.43	264 (7%) 14 22	21, 40, 73, 147	0

The worst 5 of 264 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	f	97	ALA	17.9
4	d	4	SER	17.6
6	f	96	LEU	17.0
6	F	96	LEU	15.7
4	d	5	VAL	15.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	g	11	11/12	0.29	0.46	88,116,130,131	0
7	TPO	G	11	11/12	0.56	0.31	64,95,111,114	0
9	SAC	i	101	9/10	0.60	0.48	100,104,108,108	0
9	SAC	I	101	9/10	0.85	0.23	64,68,76,79	0
1	FME	A	1	10/11	0.91	0.23	39,49,82,85	0
1	FME	a	1	10/11	0.92	0.21	55,69,82,85	0
2	FME	B	301	10/11	0.94	0.16	30,33,43,46	0
2	FME	b	1	10/11	0.96	0.16	45,47,58,59	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	DMU	c	309	33/33	0.27	0.38	100,119,130,133	0
25	DMU	C	308	33/33	0.29	0.42	70,94,111,112	0
18	PGV	a	606	51/51	0.43	0.43	62,89,129,134	0
23	PEK	C	307	53/53	0.44	0.41	59,86,146,157	0
19	TGL	l	101	63/63	0.45	0.36	63,80,110,114	0
23	PEK	c	305	53/53	0.51	0.34	63,90,111,120	0
26	PSC	b	303	52/52	0.51	0.38	53,96,136,144	0
23	PEK	G	101	53/53	0.54	0.33	61,84,119,130	0
18	PGV	c	302	51/51	0.55	0.31	63,84,114,117	0
24	CDL	c	307	100/100	0.56	0.34	62,96,126,135	0
19	TGL	b	302	63/63	0.57	0.33	68,86,96,97	0
19	TGL	d	201	63/63	0.57	0.27	67,81,103,111	0
19	TGL	A	609	63/63	0.59	0.30	50,68,89,94	0
24	CDL	G	102	100/100	0.60	0.34	62,96,130,139	0
24	CDL	C	305	100/100	0.60	0.34	53,87,111,114	0
24	CDL	g	101	100/100	0.60	0.30	66,102,140,149	0
19	TGL	D	201	63/63	0.61	0.30	61,78,87,94	0
23	PEK	c	301	53/53	0.62	0.31	58,93,150,158	0
18	PGV	A	606	51/51	0.65	0.34	48,77,123,129	0
18	PGV	C	304	51/51	0.65	0.24	64,90,105,109	0
26	PSC	E	201	52/52	0.67	0.34	53,101,160,171	0
19	TGL	A	608	63/63	0.67	0.30	55,79,96,100	0
16	MG	a	604	1/1	0.70	0.21	47,47,47,47	0
22	CHD	J	101	29/29	0.75	0.32	64,70,84,86	0
25	DMU	m	101	33/33	0.76	0.25	70,81,91,94	0
22	CHD	j	101	29/29	0.78	0.33	86,90,99,103	0
25	DMU	M	101	33/33	0.84	0.19	39,48,58,63	0
20	CMO	a	608	2/2	0.89	0.24	65,65,65,69	0
22	CHD	c	308	29/29	0.90	0.20	59,62,68,69	0
22	CHD	C	306	29/29	0.91	0.19	50,54,62,64	0
17	NA	a	605	1/1	0.91	0.06	48,48,48,48	0
23	PEK	c	304	53/53	0.93	0.22	41,63,99,101	0
17	NA	A	605	1/1	0.93	0.10	28,28,28,28	0
21	CUA	b	301	2/2	0.94	0.07	36,36,36,38	0
18	PGV	c	306	51/51	0.94	0.19	32,46,82,85	0
22	CHD	G	103	29/29	0.95	0.09	32,35,38,41	0
22	CHD	B	402	29/29	0.95	0.12	31,32,36,41	0
23	PEK	C	302	53/53	0.95	0.22	31,53,83,89	0
14	HEA	a	601	60/60	0.96	0.18	32,37,55,62	0
14	HEA	a	602	60/60	0.96	0.16	29,32,40,43	0
22	CHD	c	303	29/29	0.96	0.08	34,36,40,41	0
18	PGV	a	607	51/51	0.96	0.20	32,48,74,83	0

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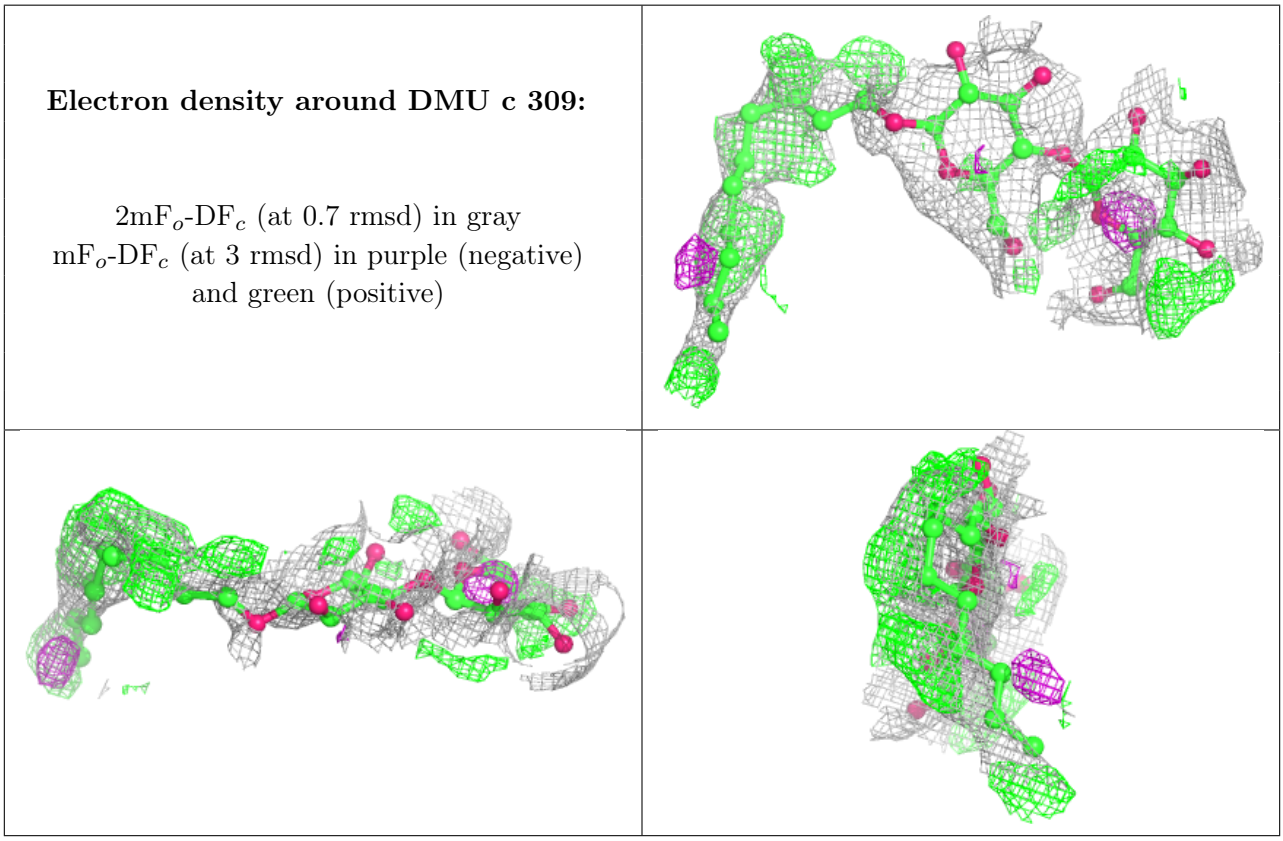
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	PGV	A	607	51/51	0.96	0.18	25,42,65,69	0
22	CHD	C	301	29/29	0.96	0.06	31,34,36,38	0
18	PGV	C	303	51/51	0.96	0.17	27,39,70,76	0
20	CMO	A	610	2/2	0.97	0.15	46,46,46,46	0
16	MG	A	604	1/1	0.97	0.09	27,27,27,27	0
14	HEA	A	602	60/60	0.97	0.14	22,24,33,35	0
21	CUA	B	401	2/2	0.98	0.06	24,24,24,24	0
14	HEA	A	601	60/60	0.98	0.15	21,23,45,50	0
15	CU	a	603	1/1	0.99	0.10	34,34,34,34	0
27	ZN	F	101	1/1	0.99	0.04	33,33,33,33	0
27	ZN	f	101	1/1	0.99	0.06	41,41,41,41	0
15	CU	A	603	1/1	1.00	0.07	25,25,25,25	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.

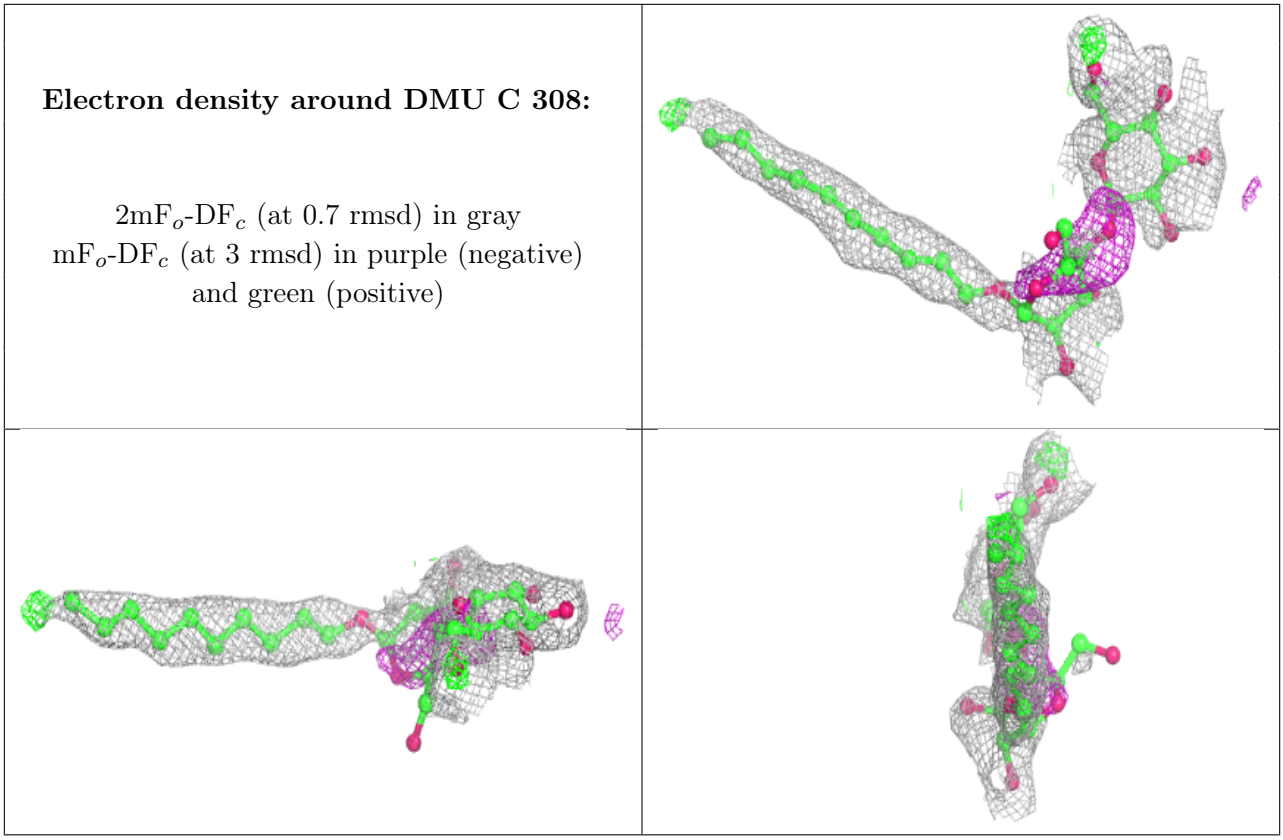
Electron density around DMU c 309:

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



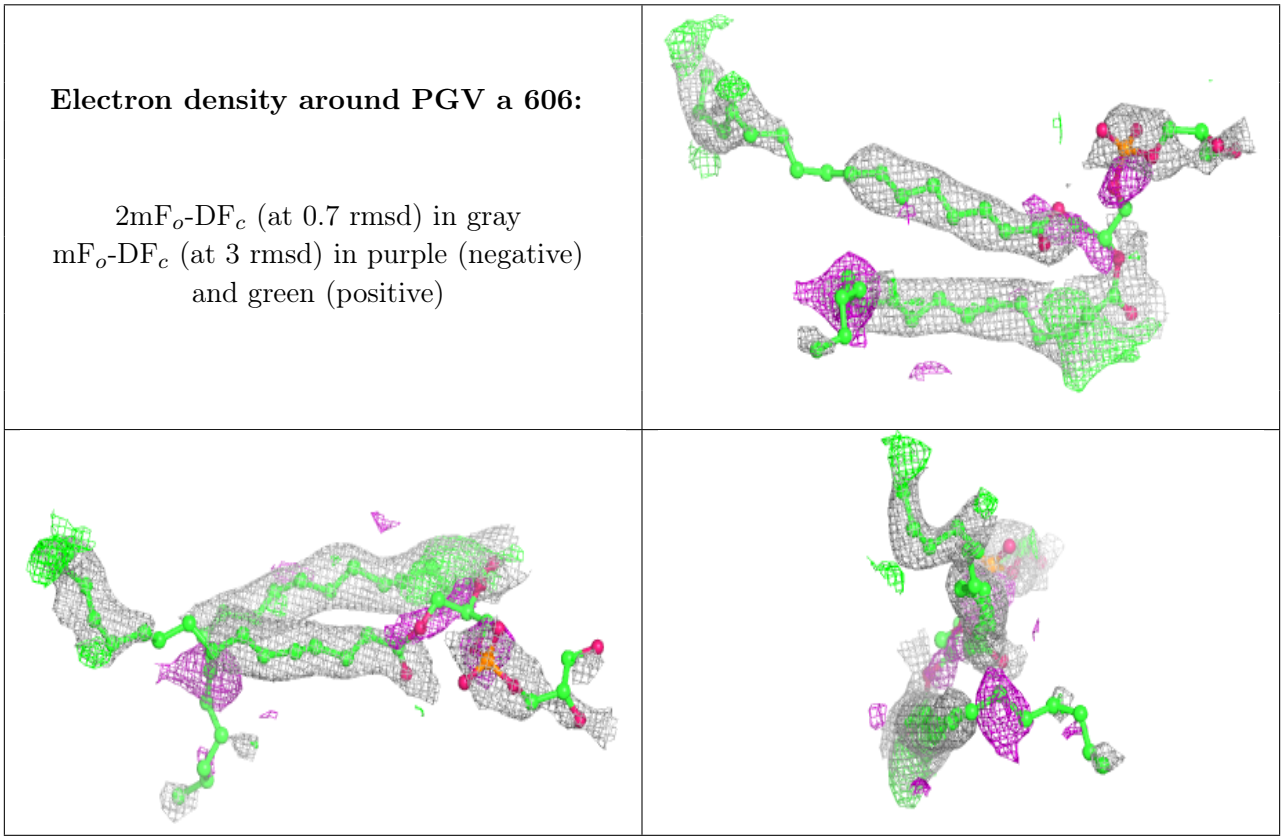
Electron density around DMU C 308:

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



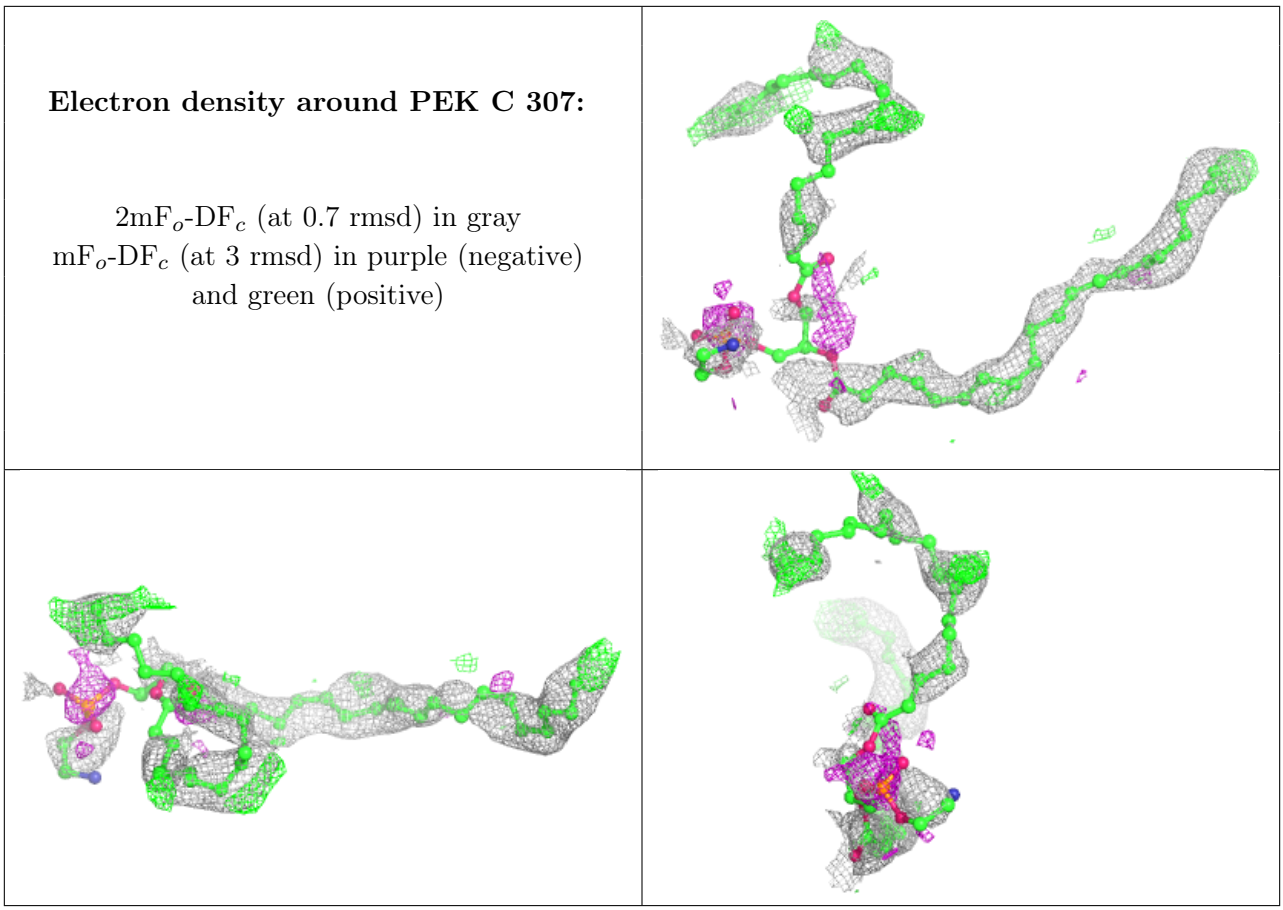
Electron density around PGV a 606:

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



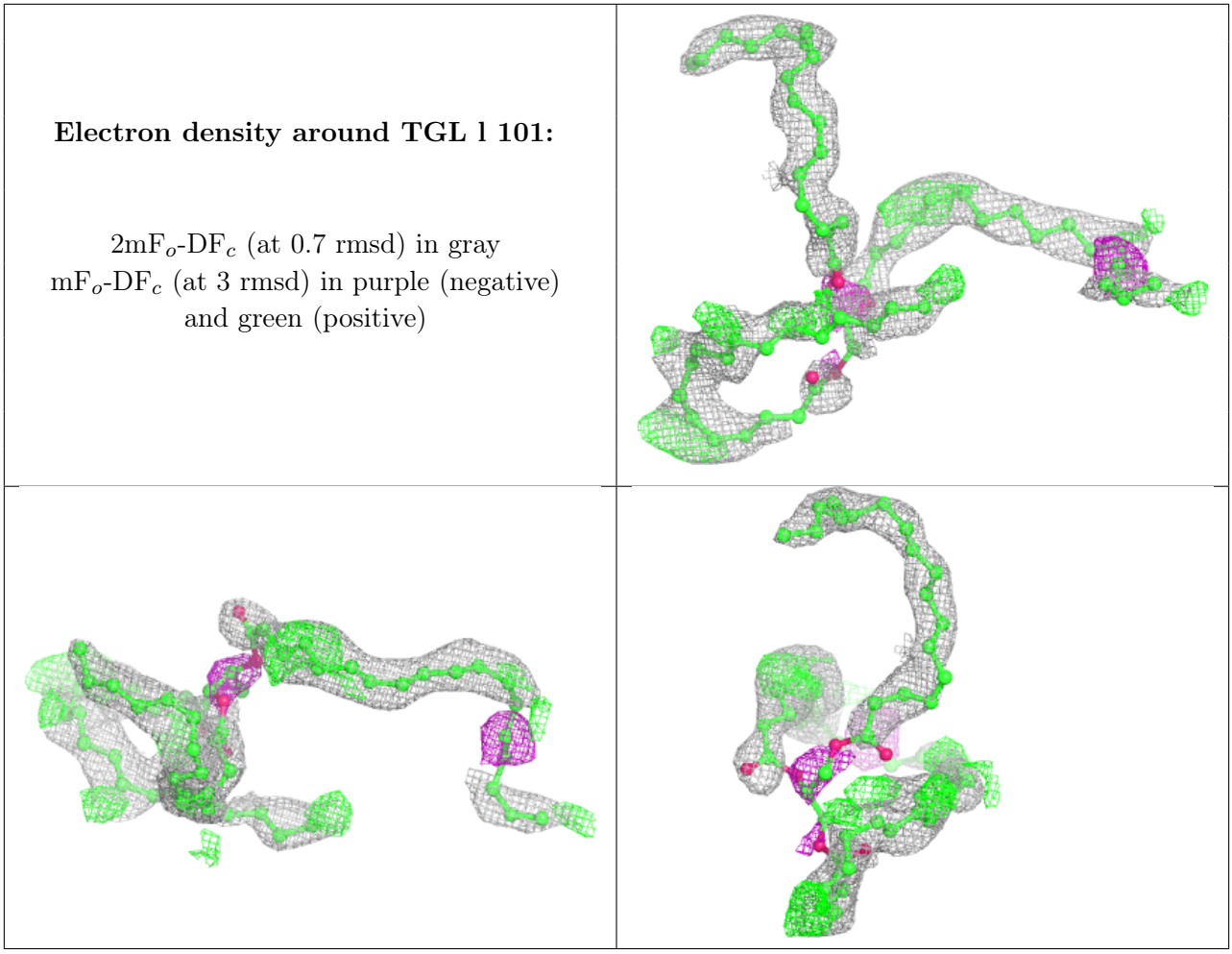
Electron density around PEK C 307:

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



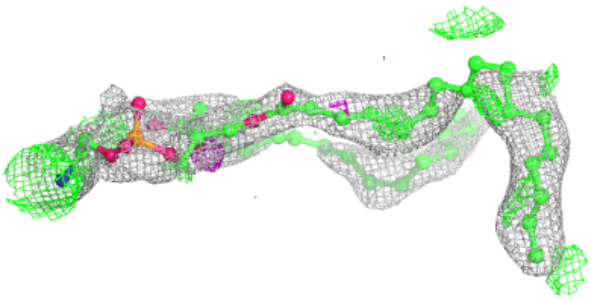
Electron density around TGL l 101:

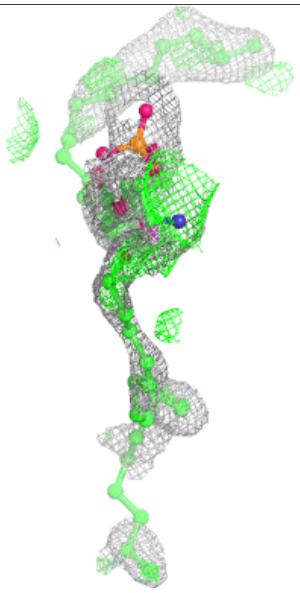
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PEK c 305:

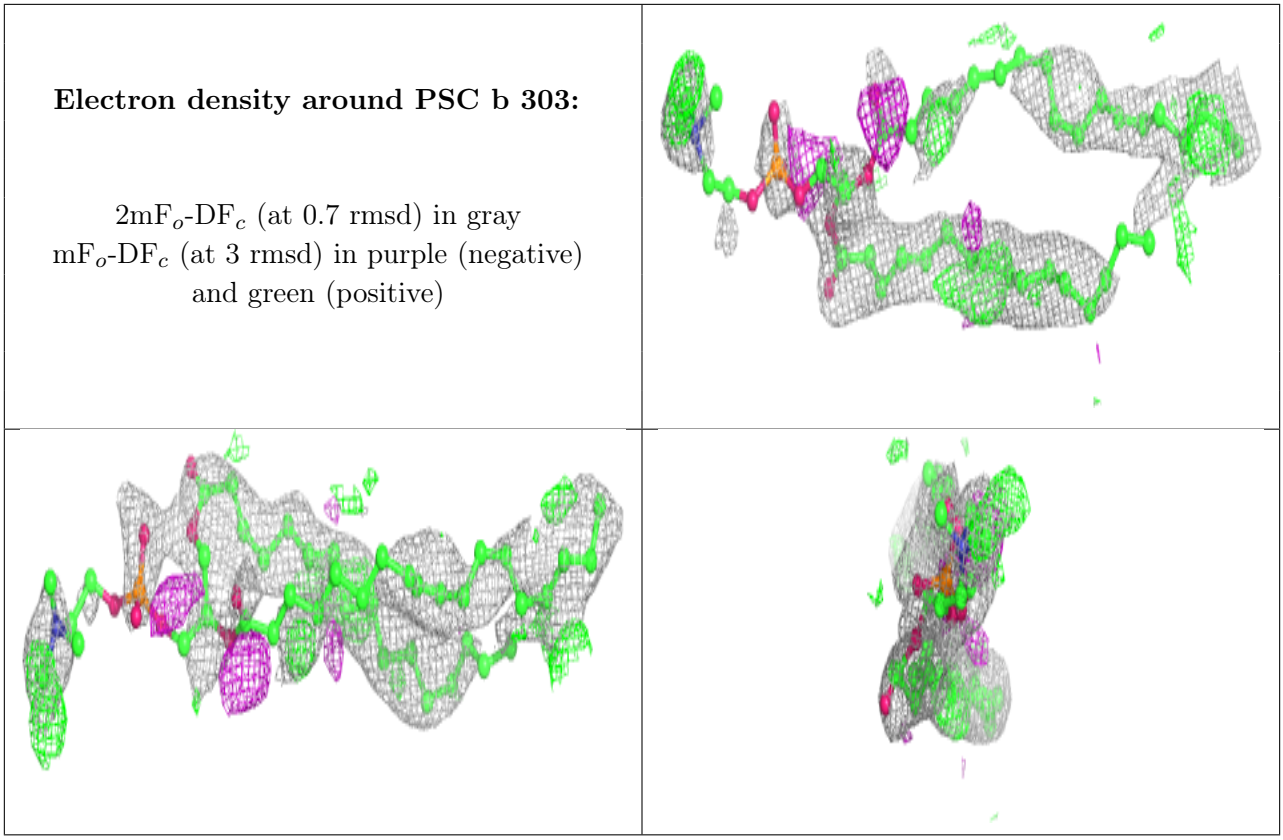
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





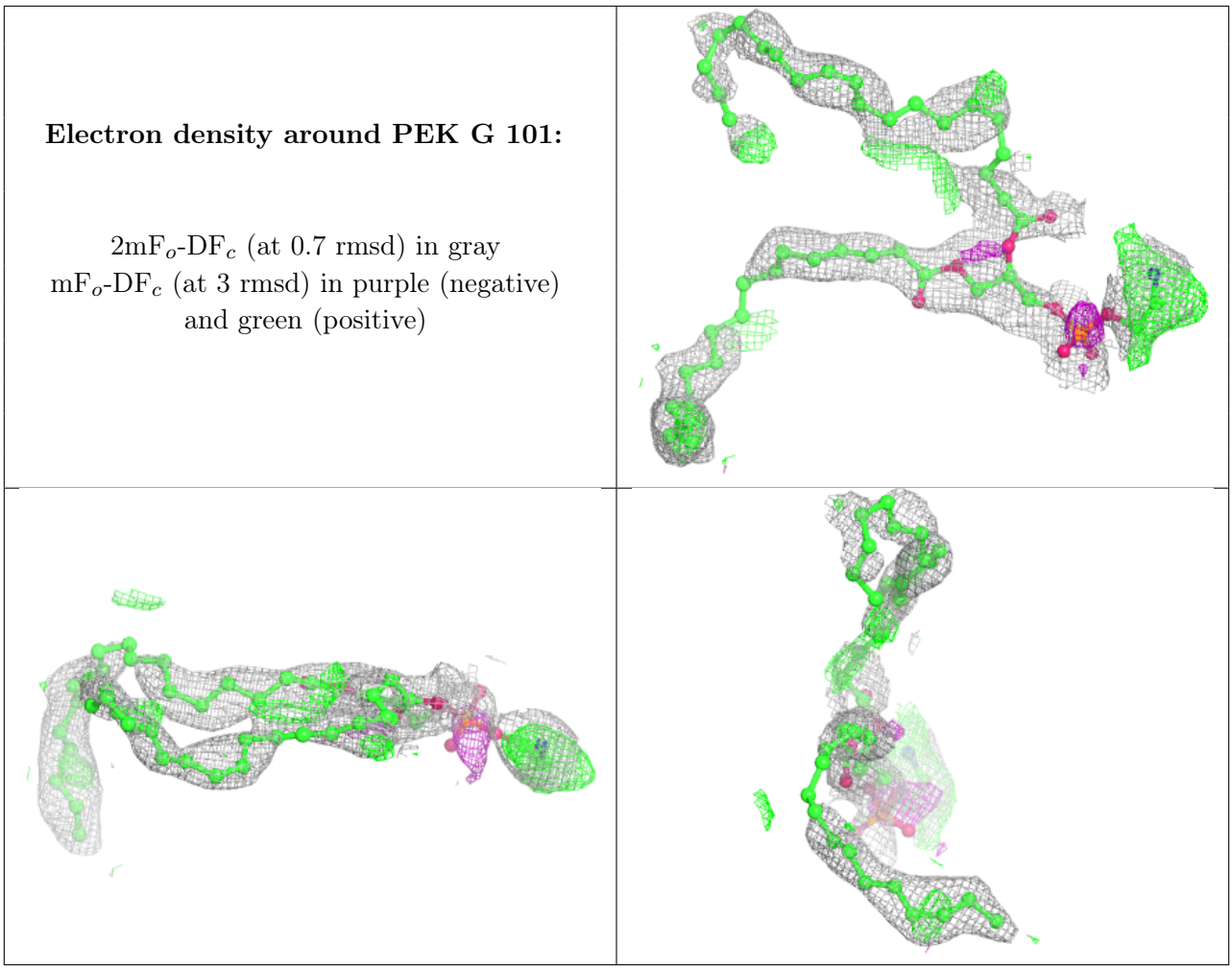
Electron density around PSC b 303:

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



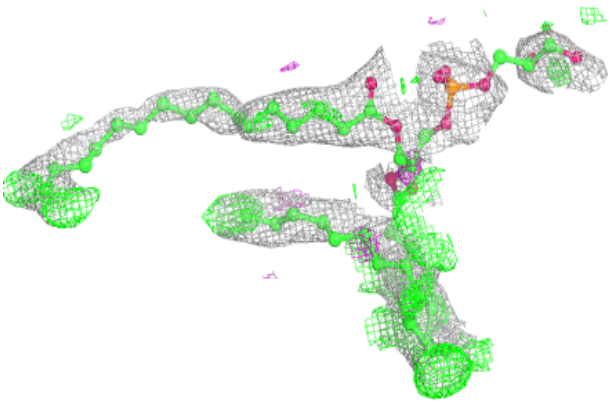
Electron density around PEK G 101:

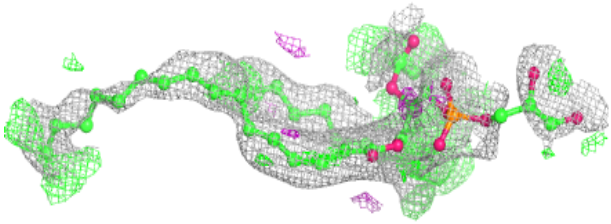
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

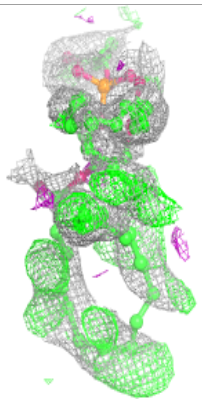


Electron density around PGV c 302:

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

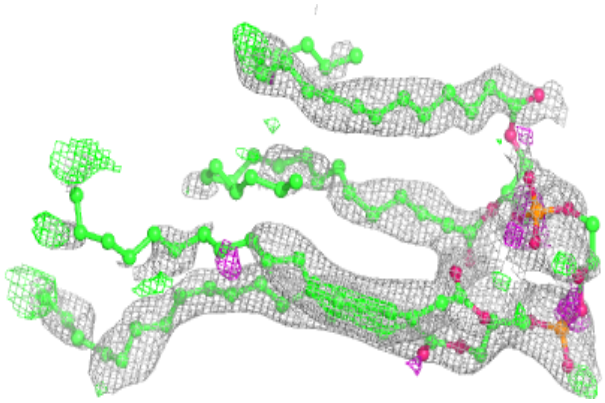


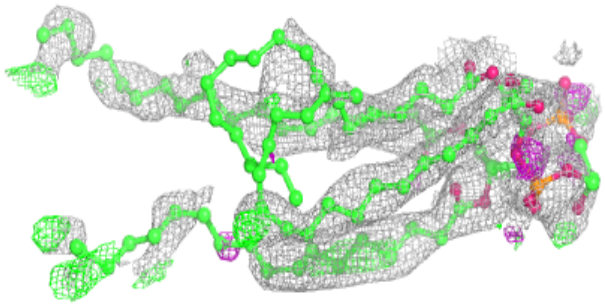


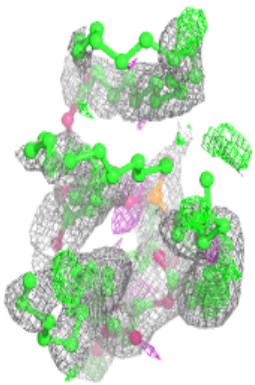


Electron density around CDL c 307:

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

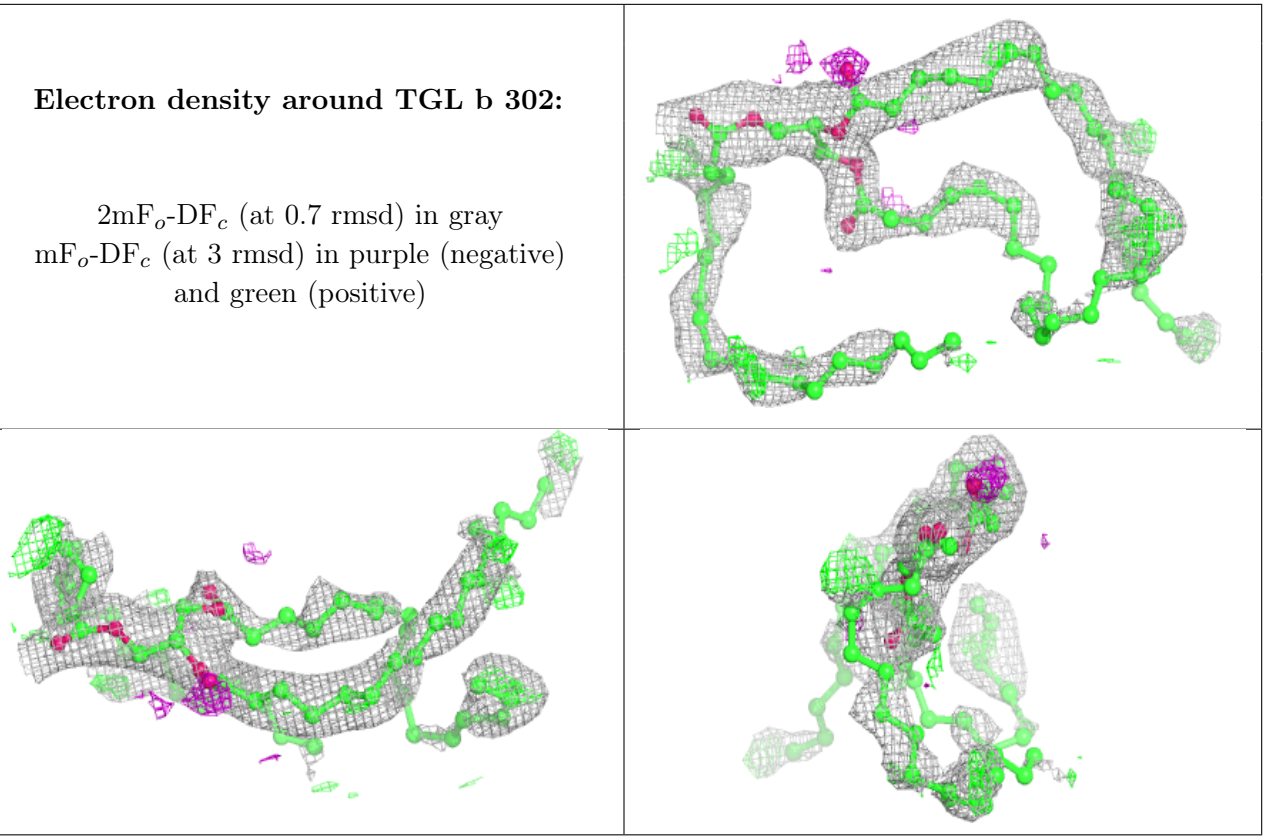






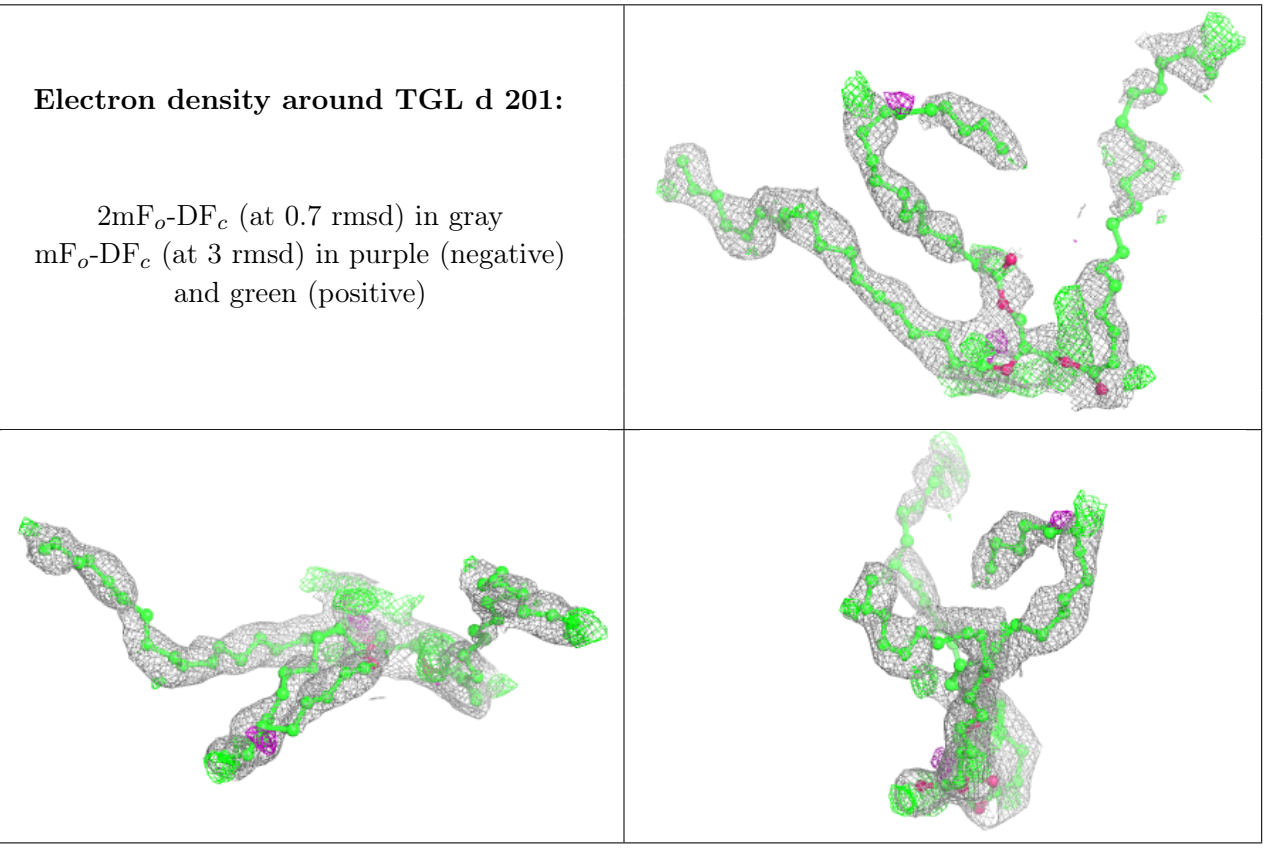
Electron density around TGL b 302:

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



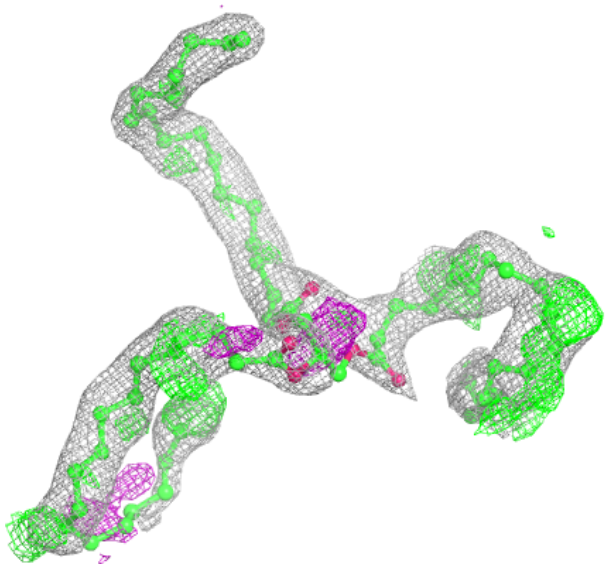
Electron density around TGL d 201:

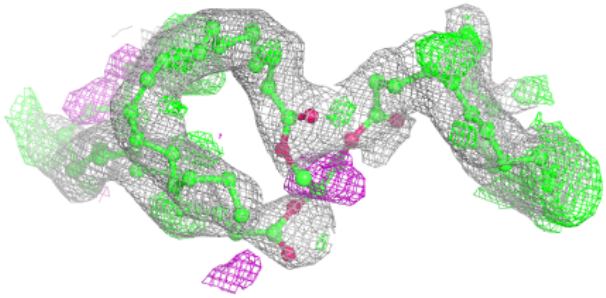
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

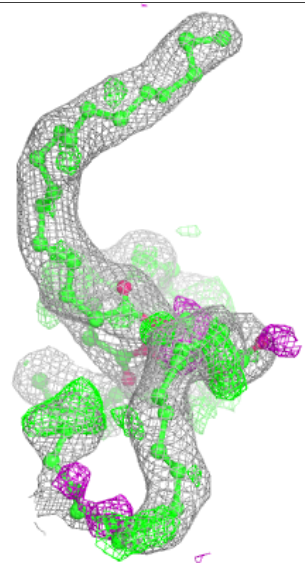


Electron density around TGL A 609:

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

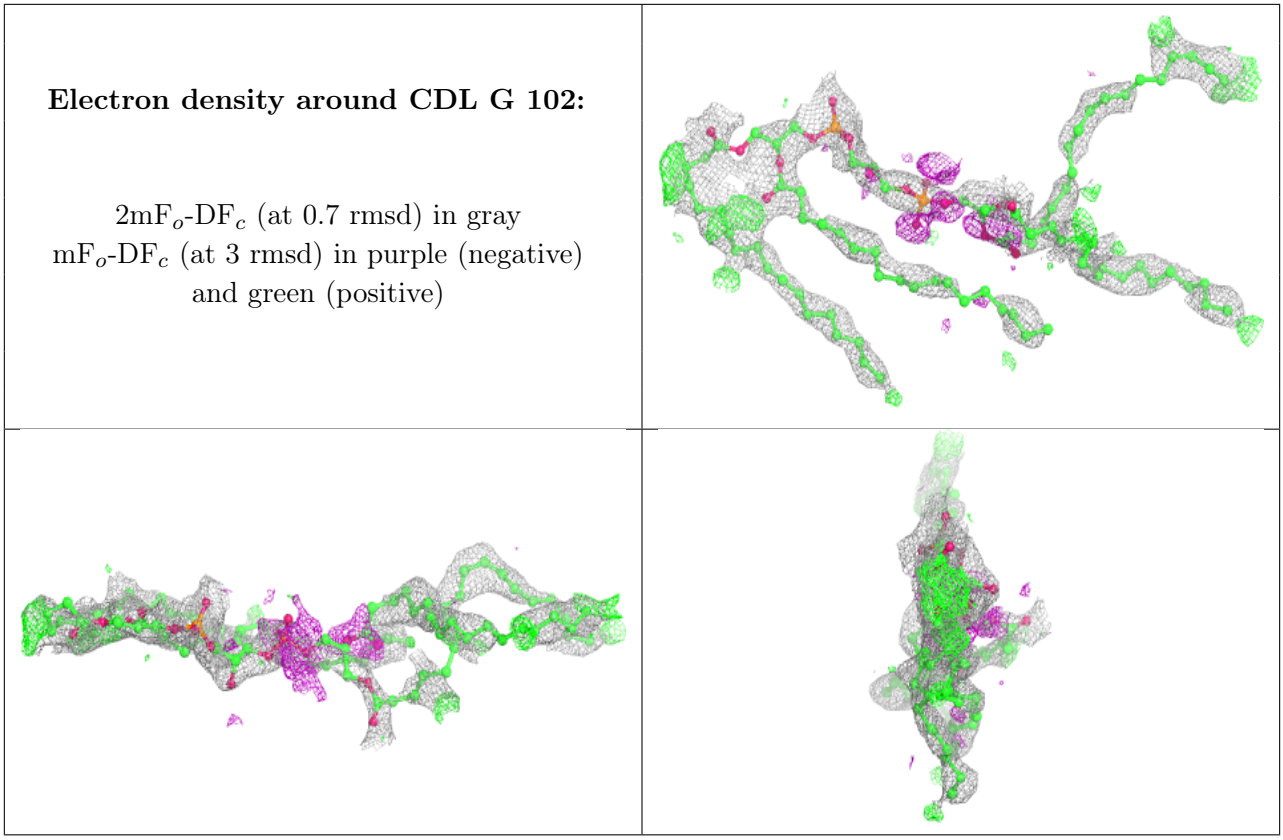






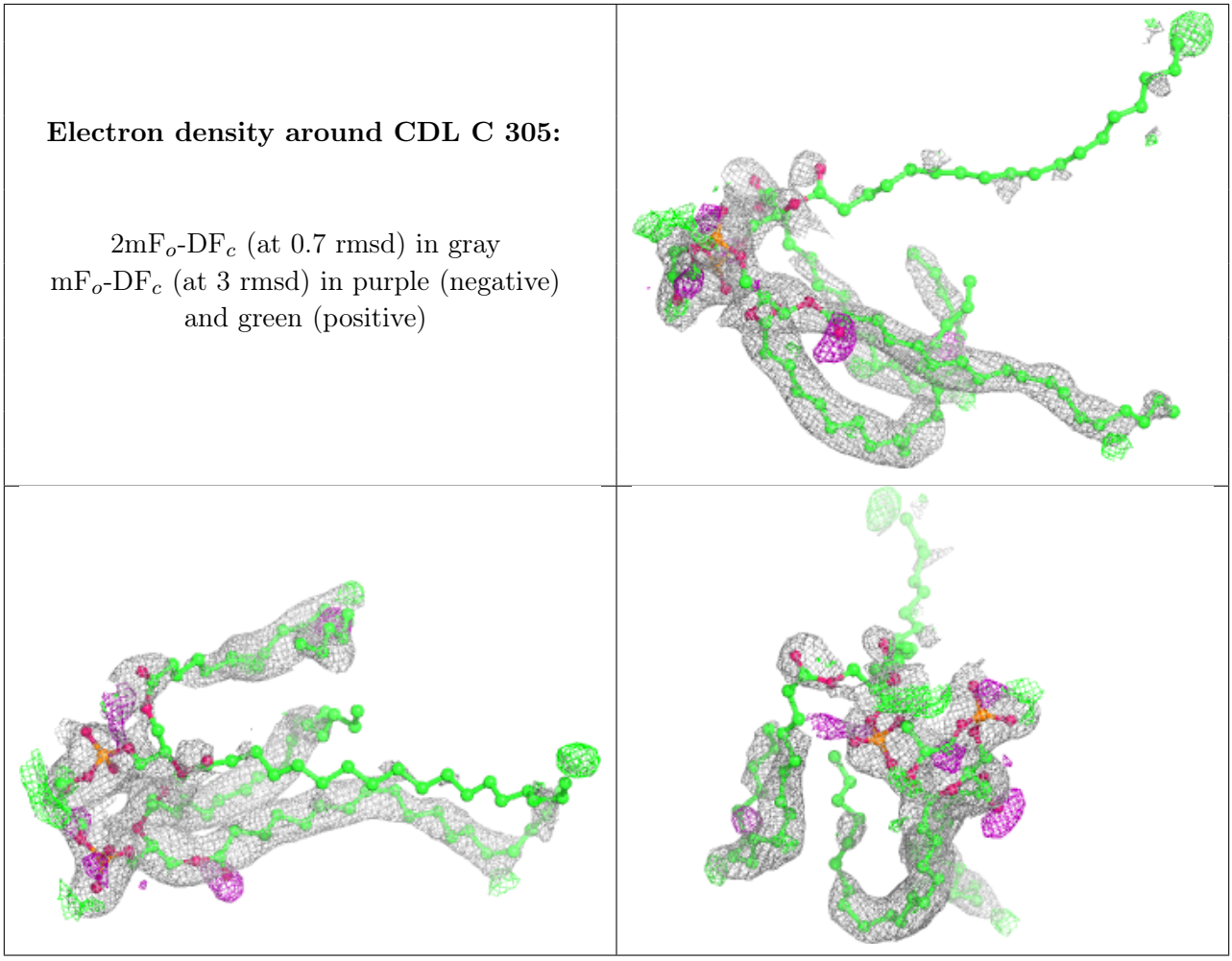
Electron density around CDL G 102:

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



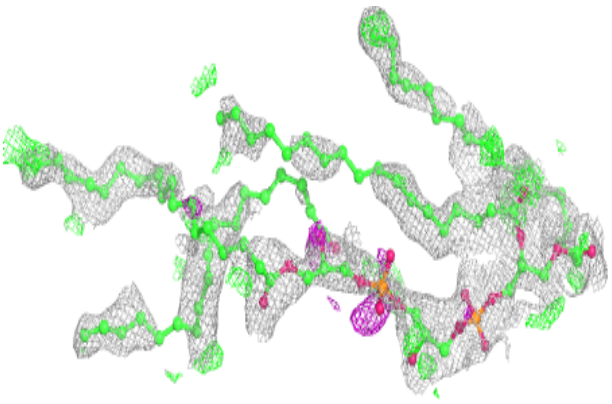
Electron density around CDL C 305:

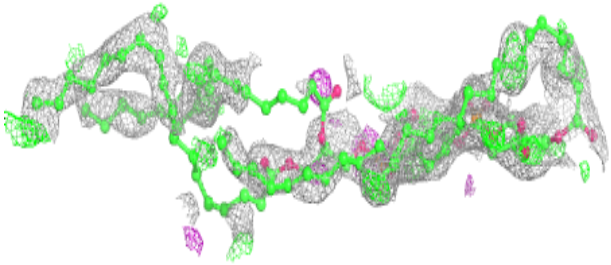
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

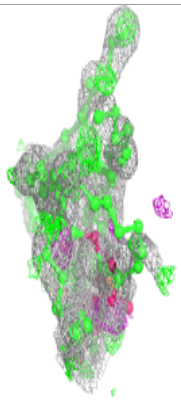


Electron density around CDL g 101:

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

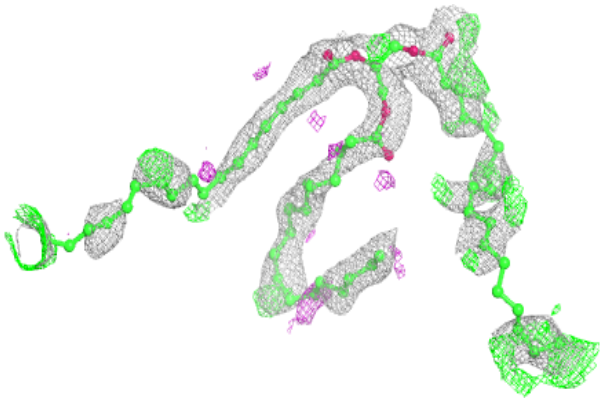


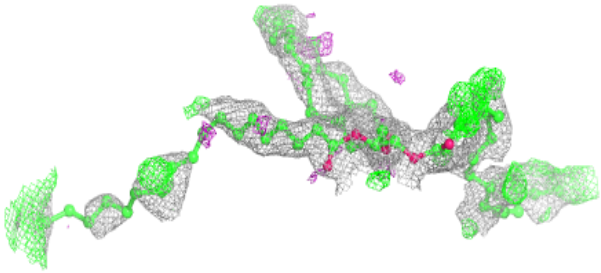


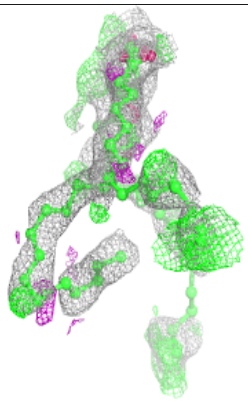


Electron density around TGL D 201:

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

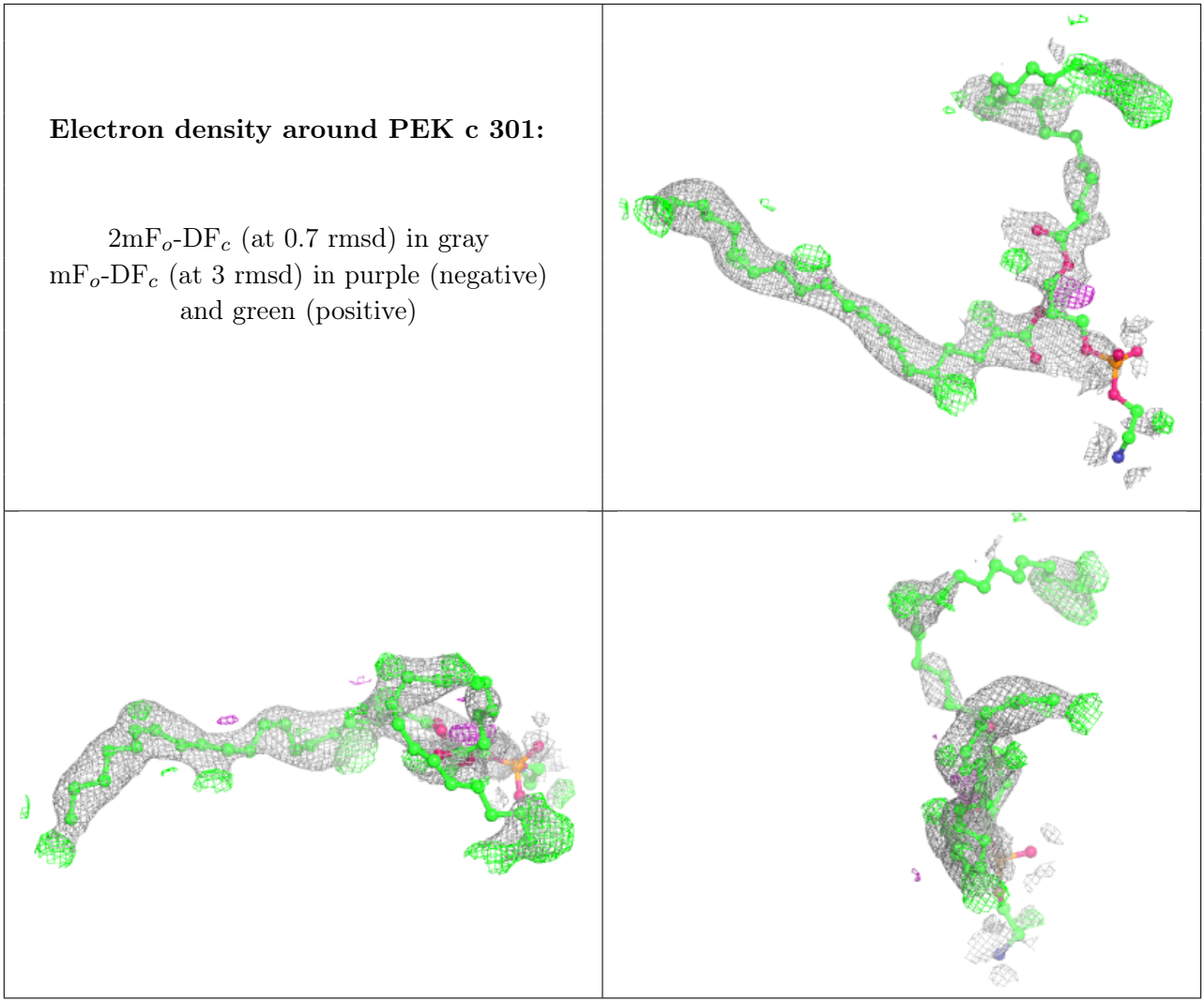






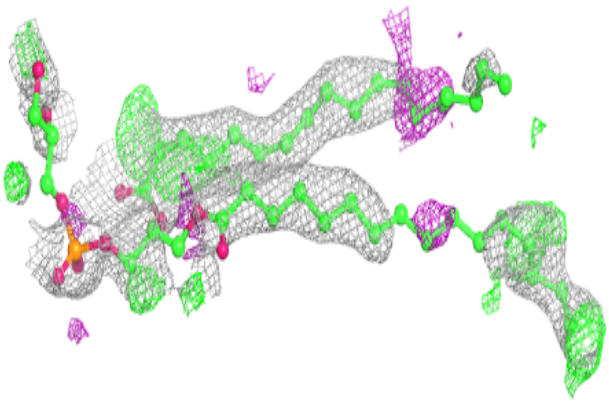
Electron density around PEK c 301:

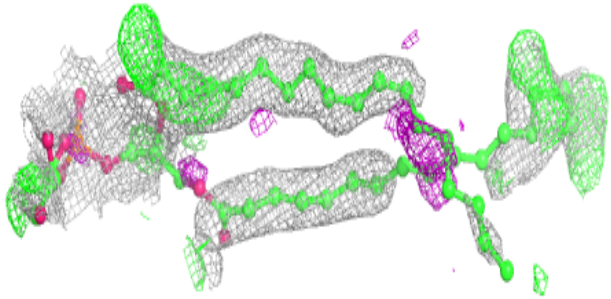
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

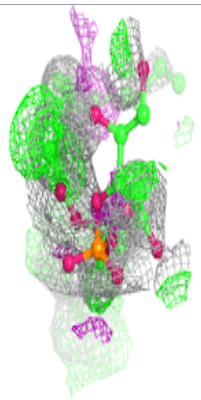


Electron density around PGV A 606:

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

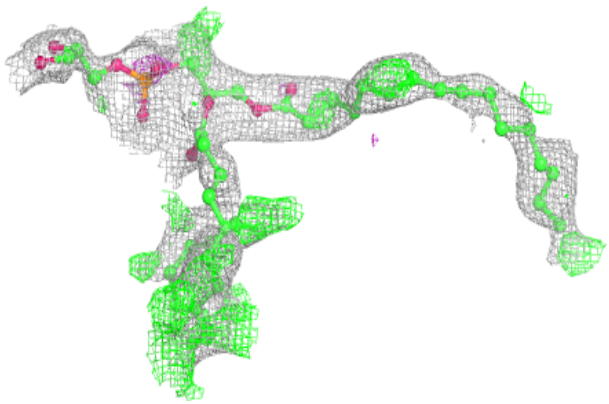


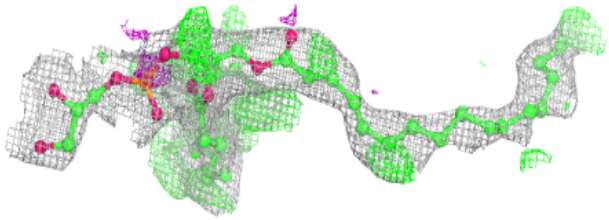


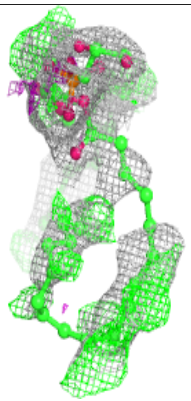


Electron density around PGV C 304:

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

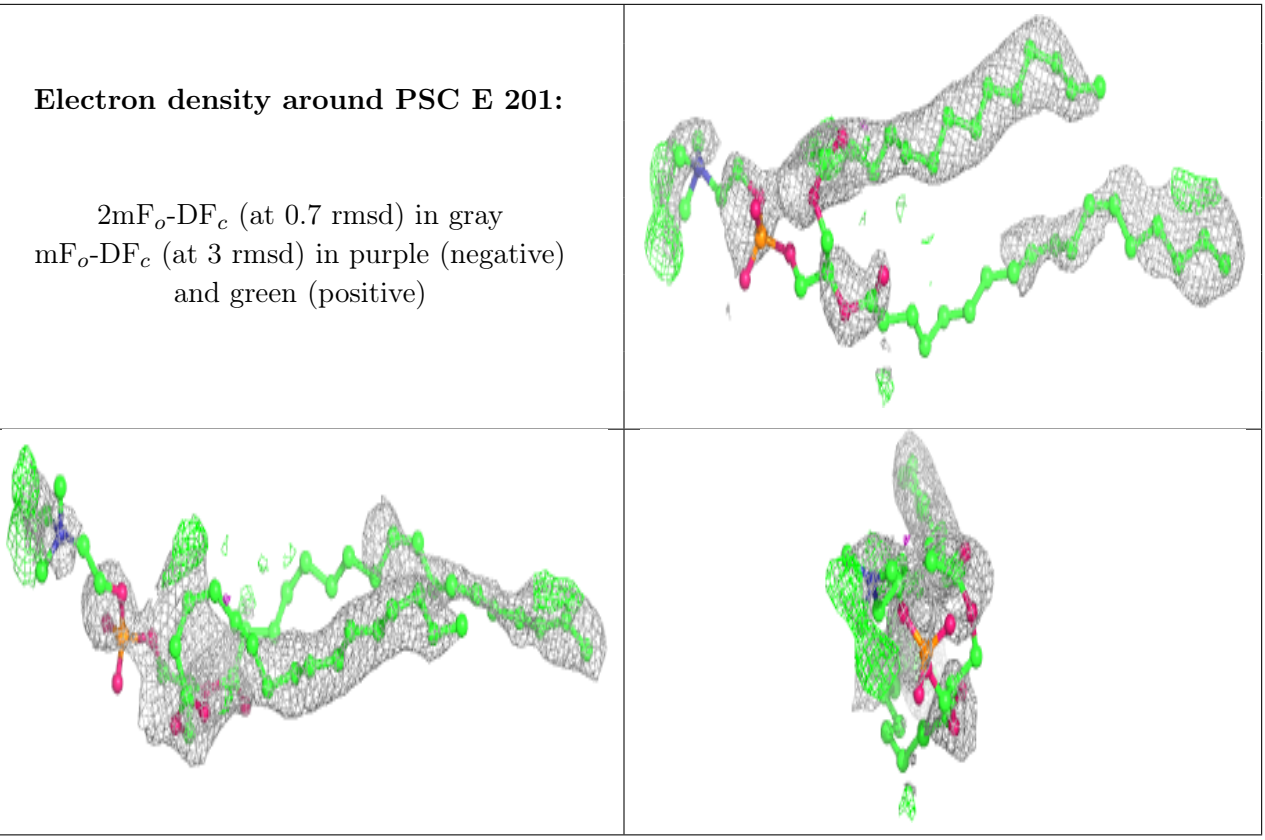






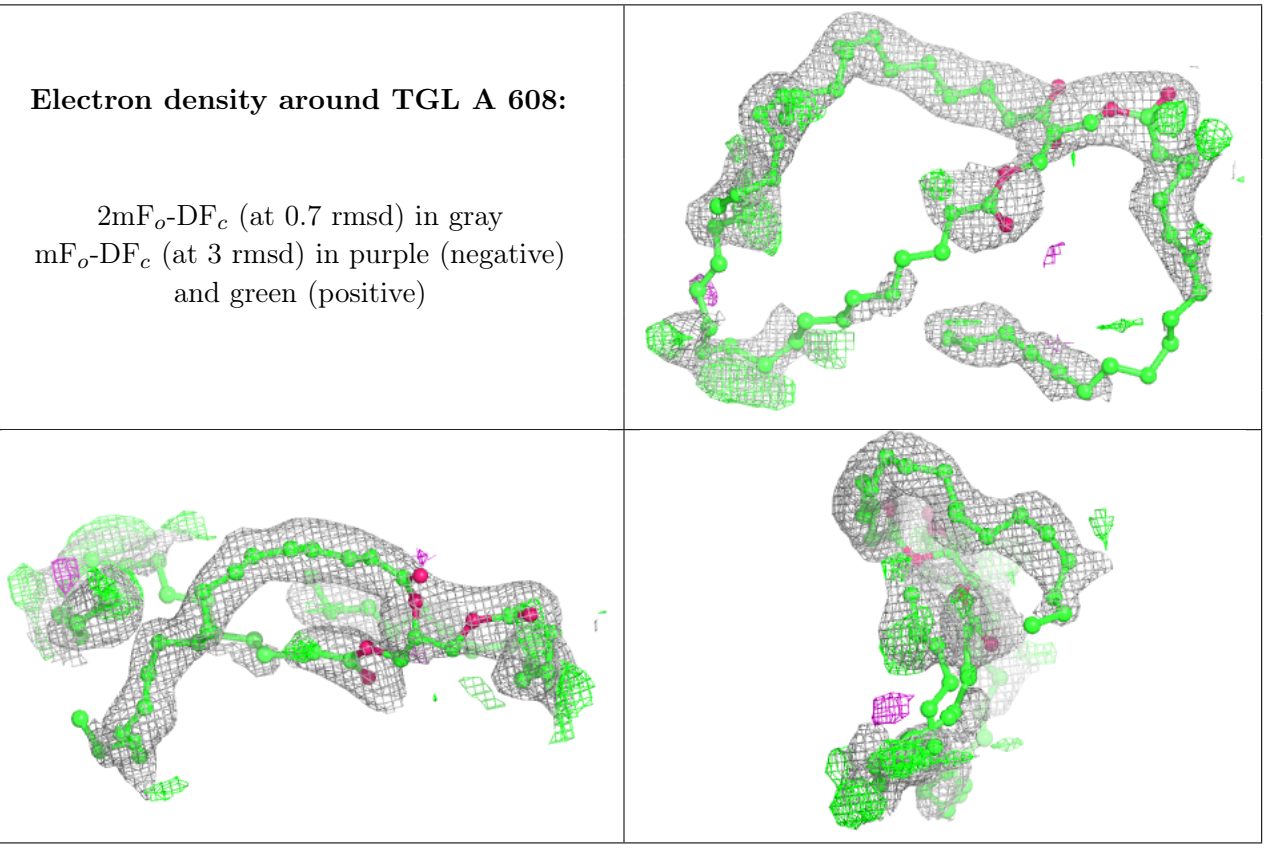
Electron density around PSC E 201:

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



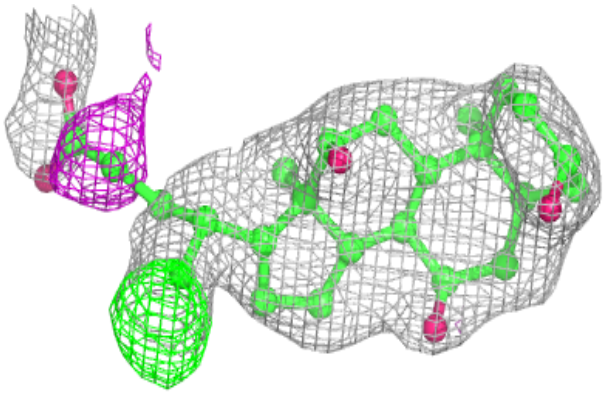
Electron density around TGL A 608:

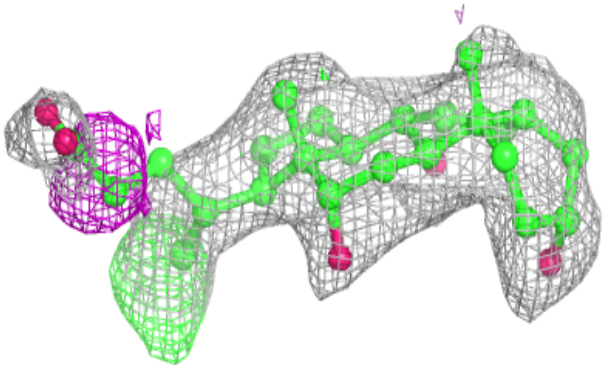
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

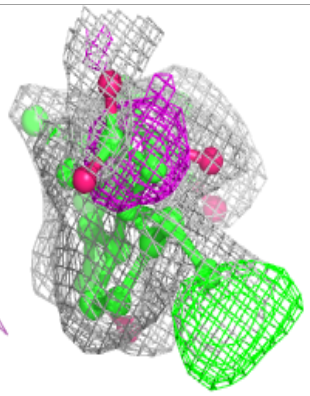


Electron density around CHD J 101:

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

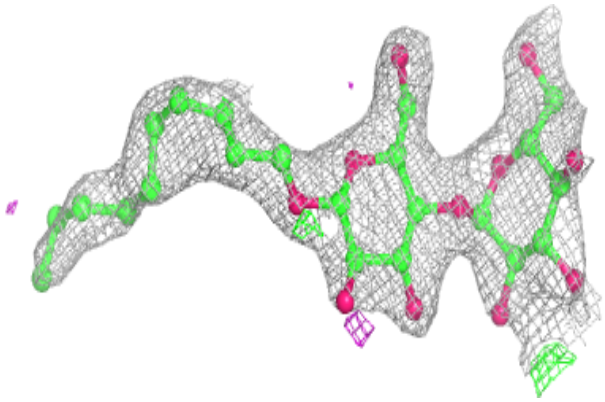


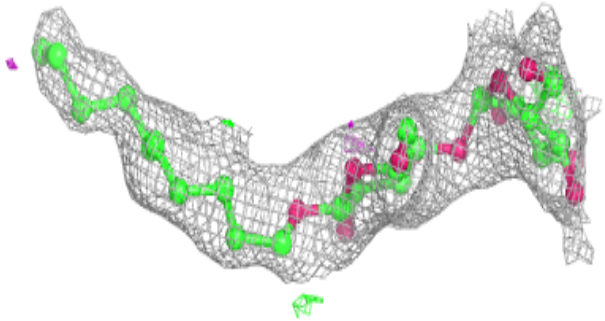


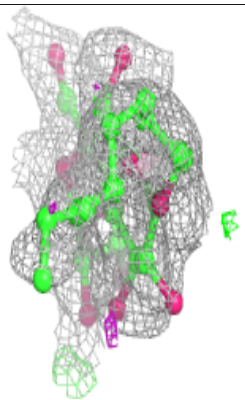


Electron density around DMU m 101:

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

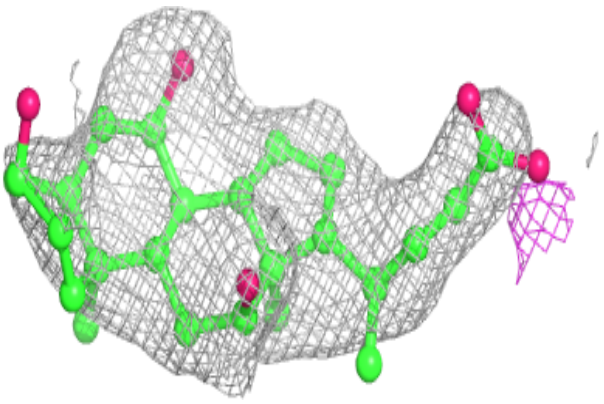


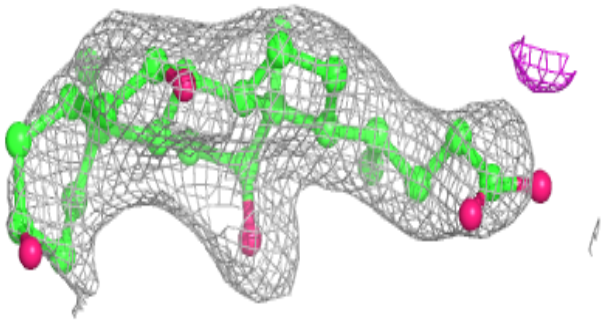


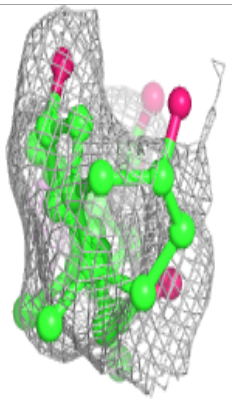


Electron density around CHD j 101:

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

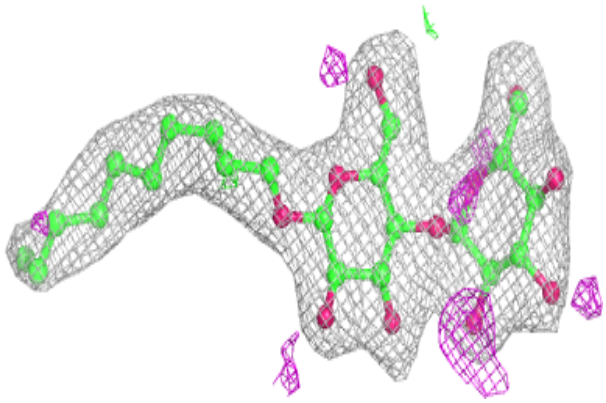


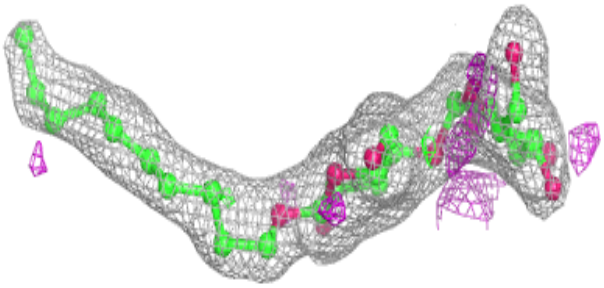


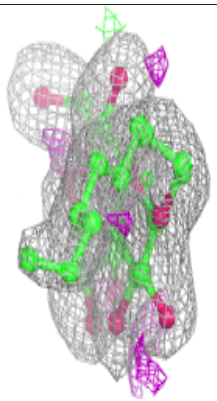


Electron density around DMU M 101:

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

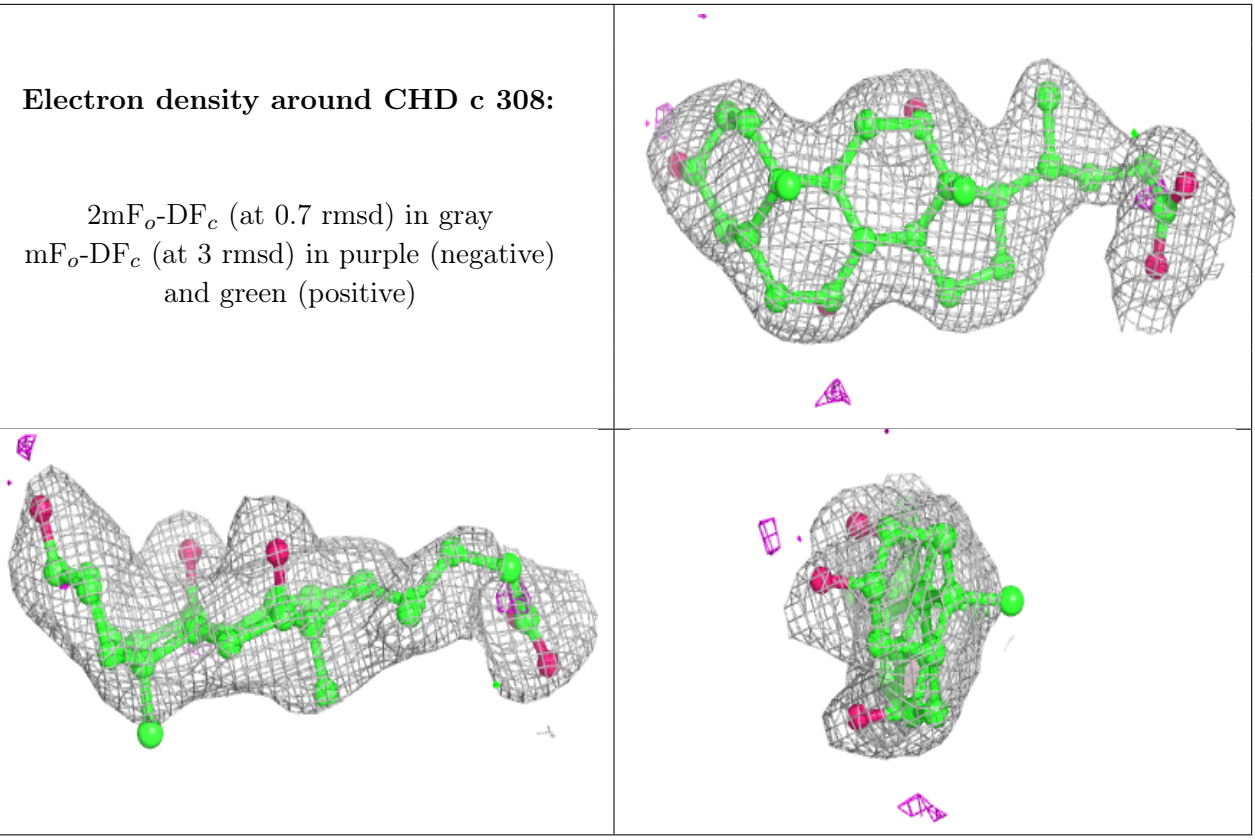






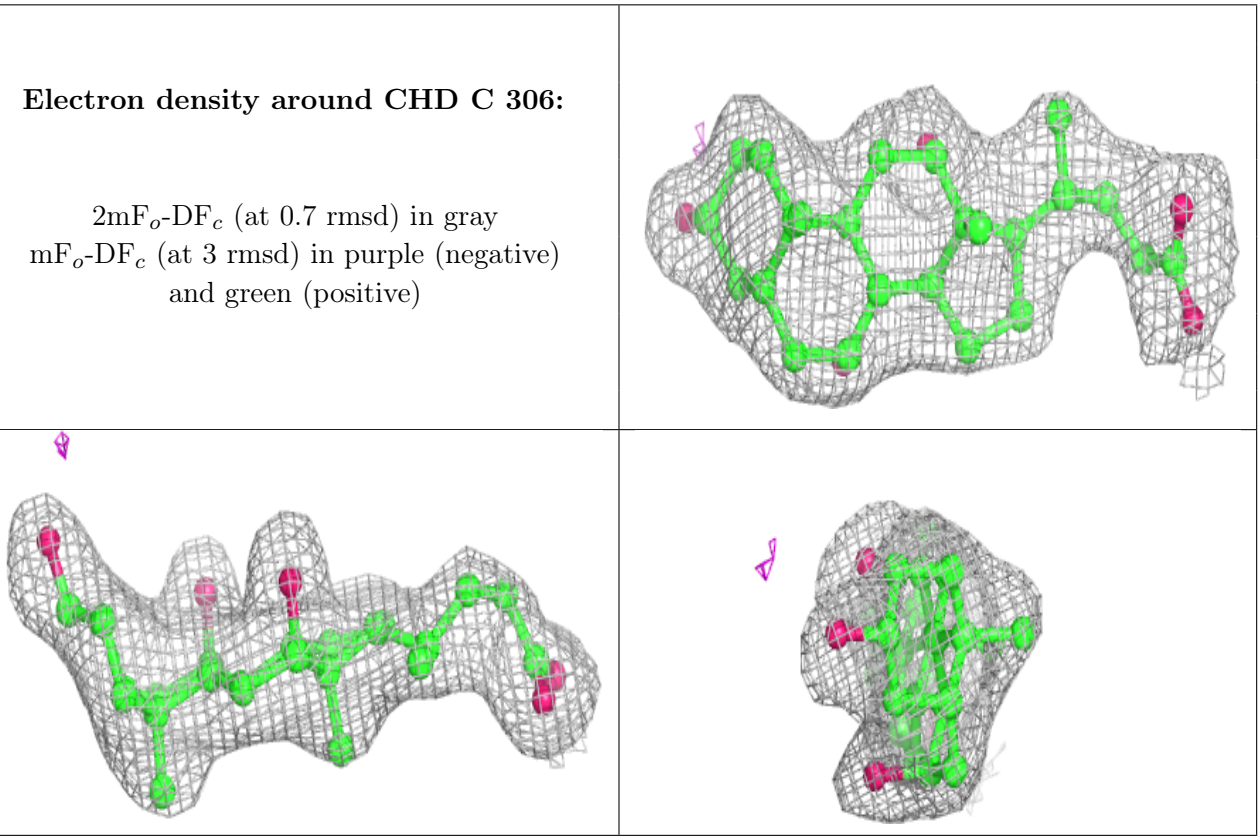
Electron density around CHD c 308:

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



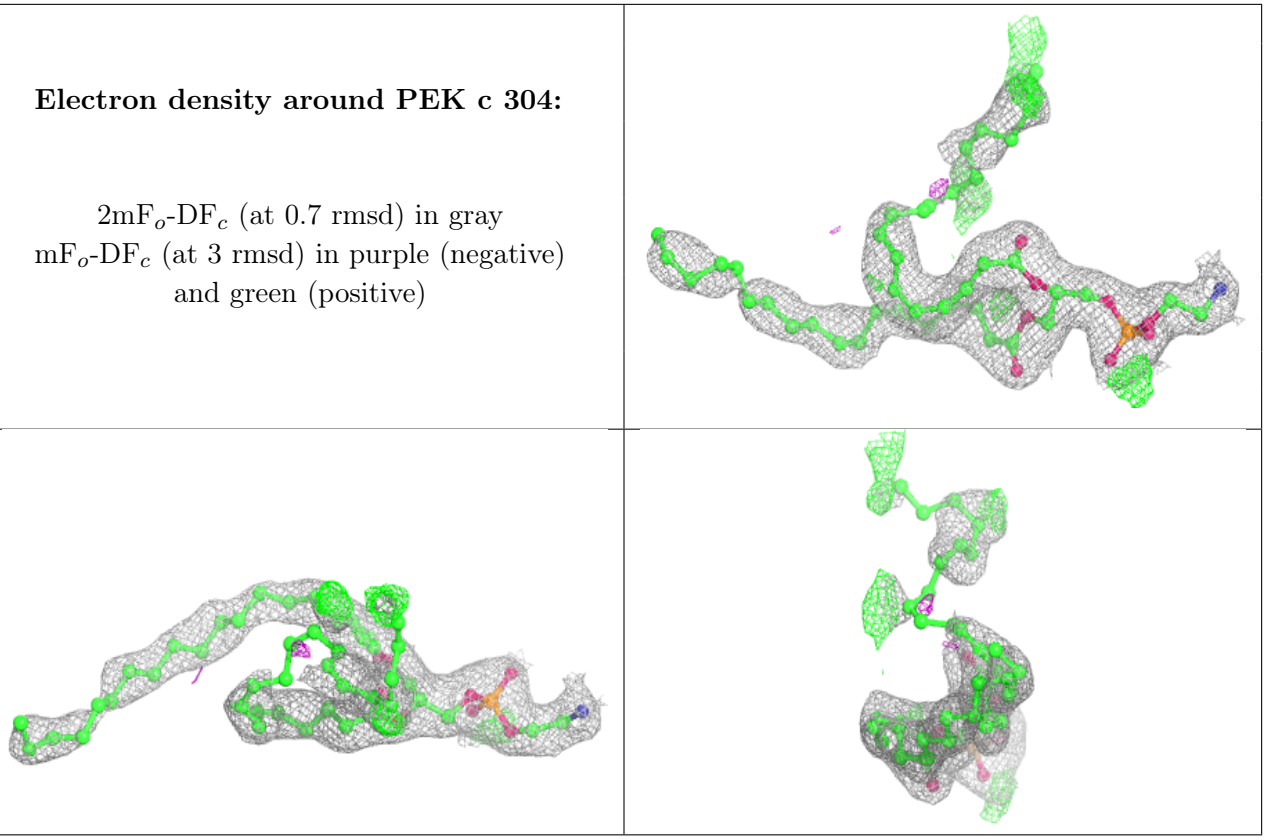
Electron density around CHD C 306:

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



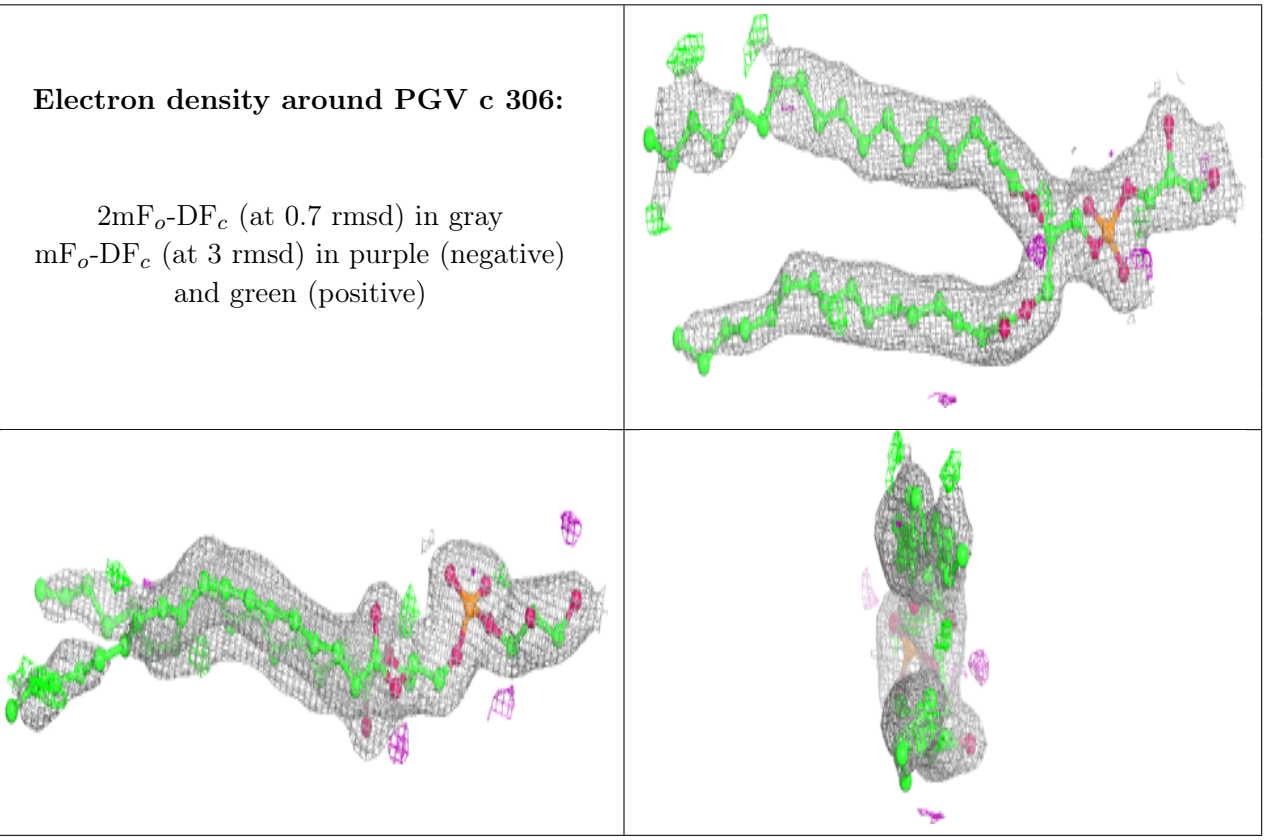
Electron density around PEK c 304:

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



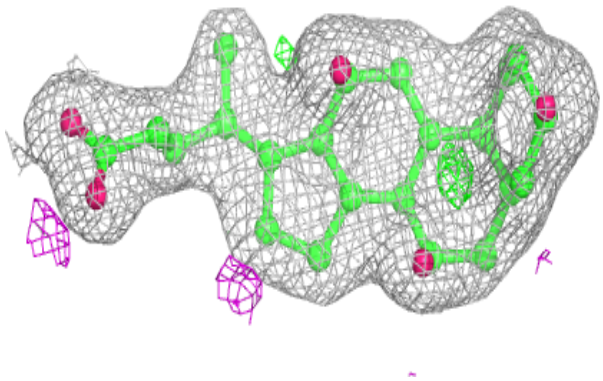
Electron density around PGV c 306:

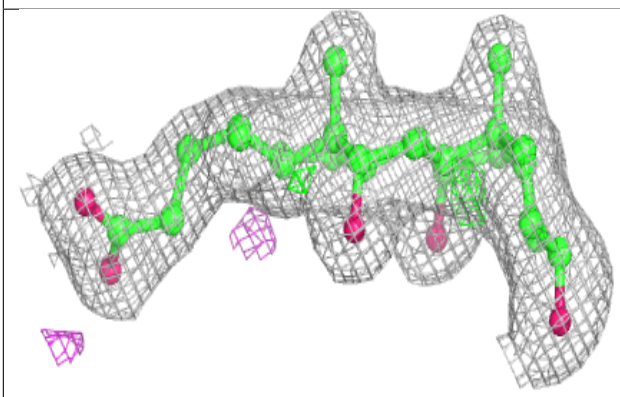
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

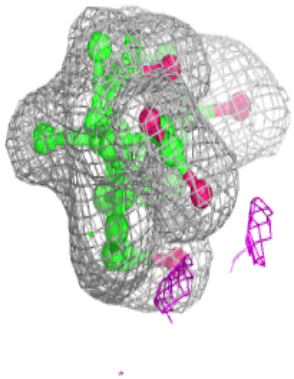


Electron density around CHD G 103:

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

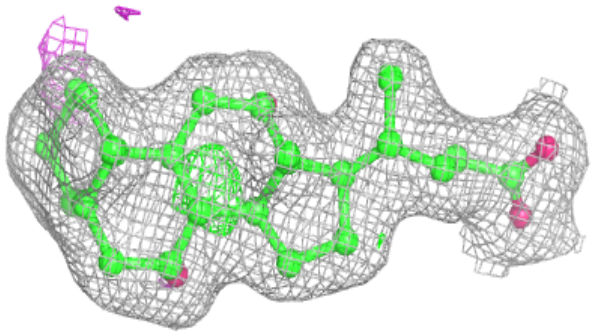


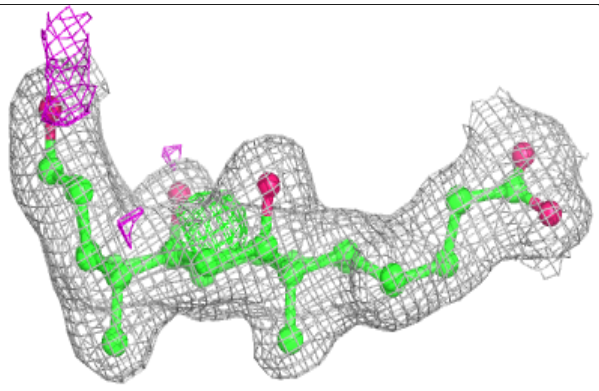


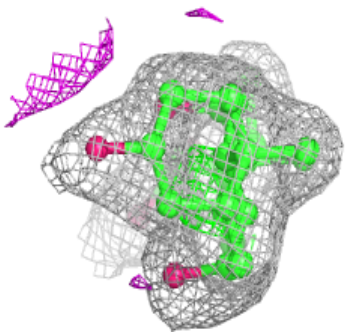


Electron density around CHD B 402:

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

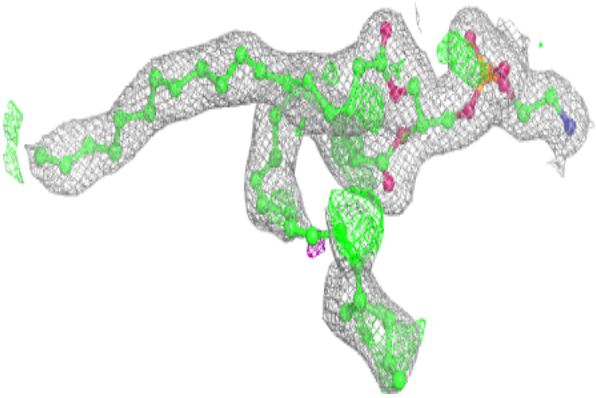


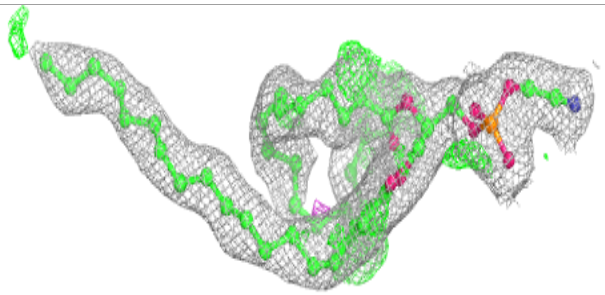


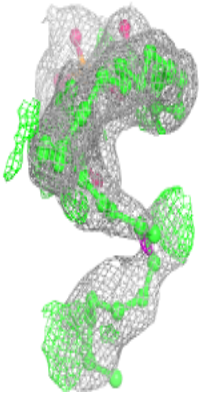


Electron density around PEK C 302:

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

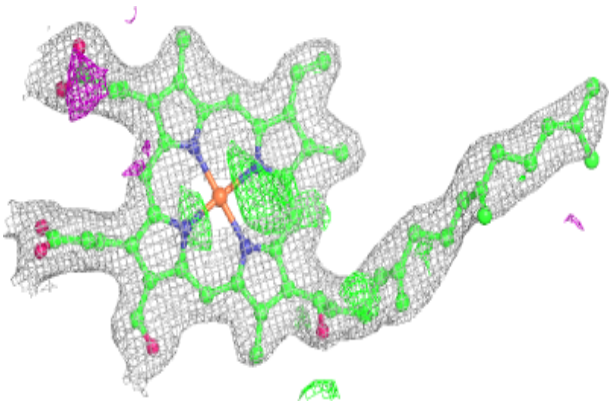


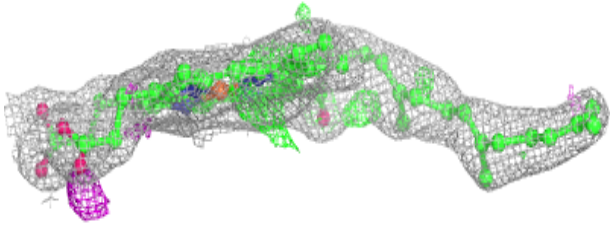


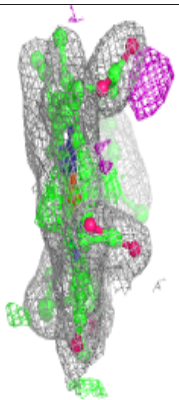


Electron density around HEA a 601:

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

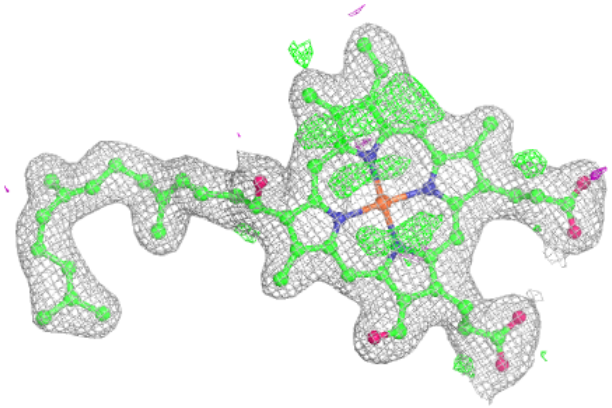


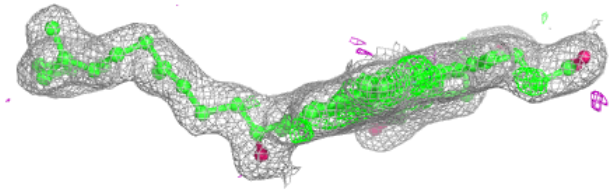


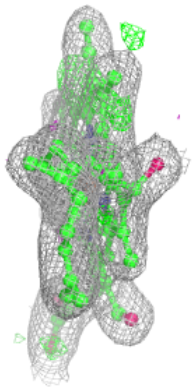


Electron density around HEA a 602:

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

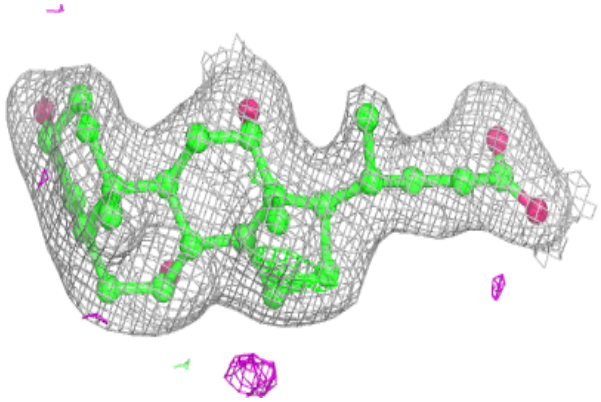


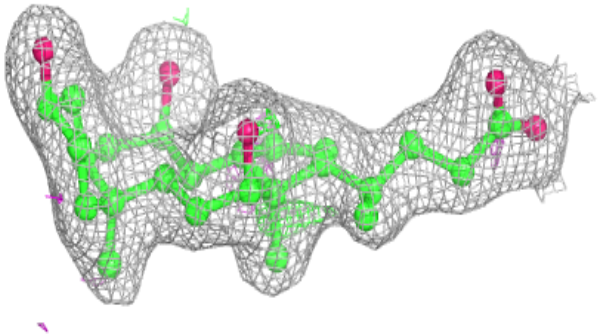


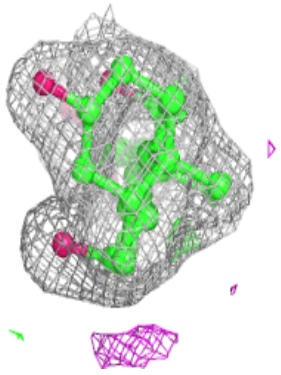


Electron density around CHD c 303:

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

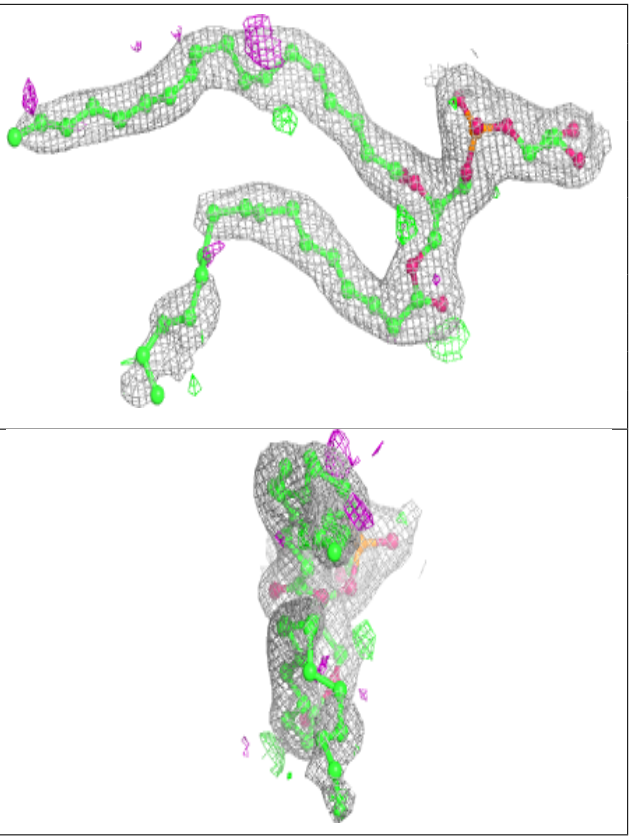


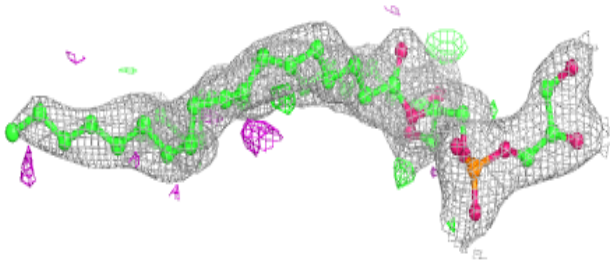




Electron density around PGV a 607:

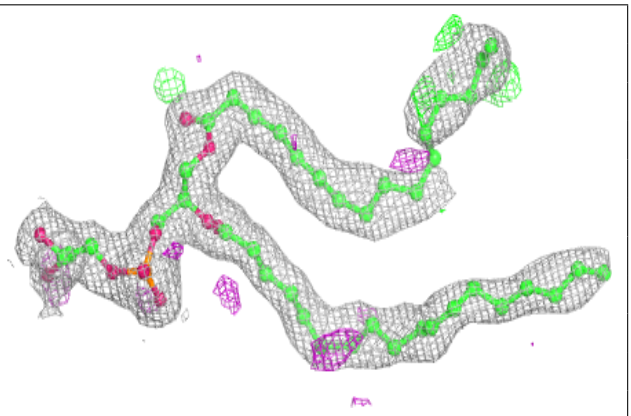
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

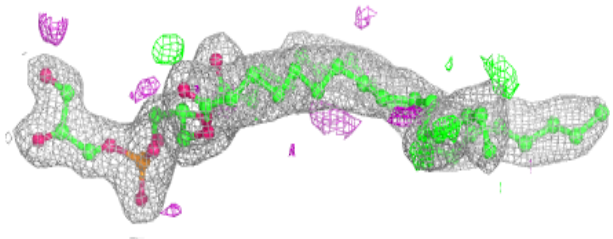


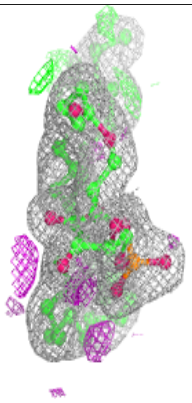


Electron density around PGV A 607:

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

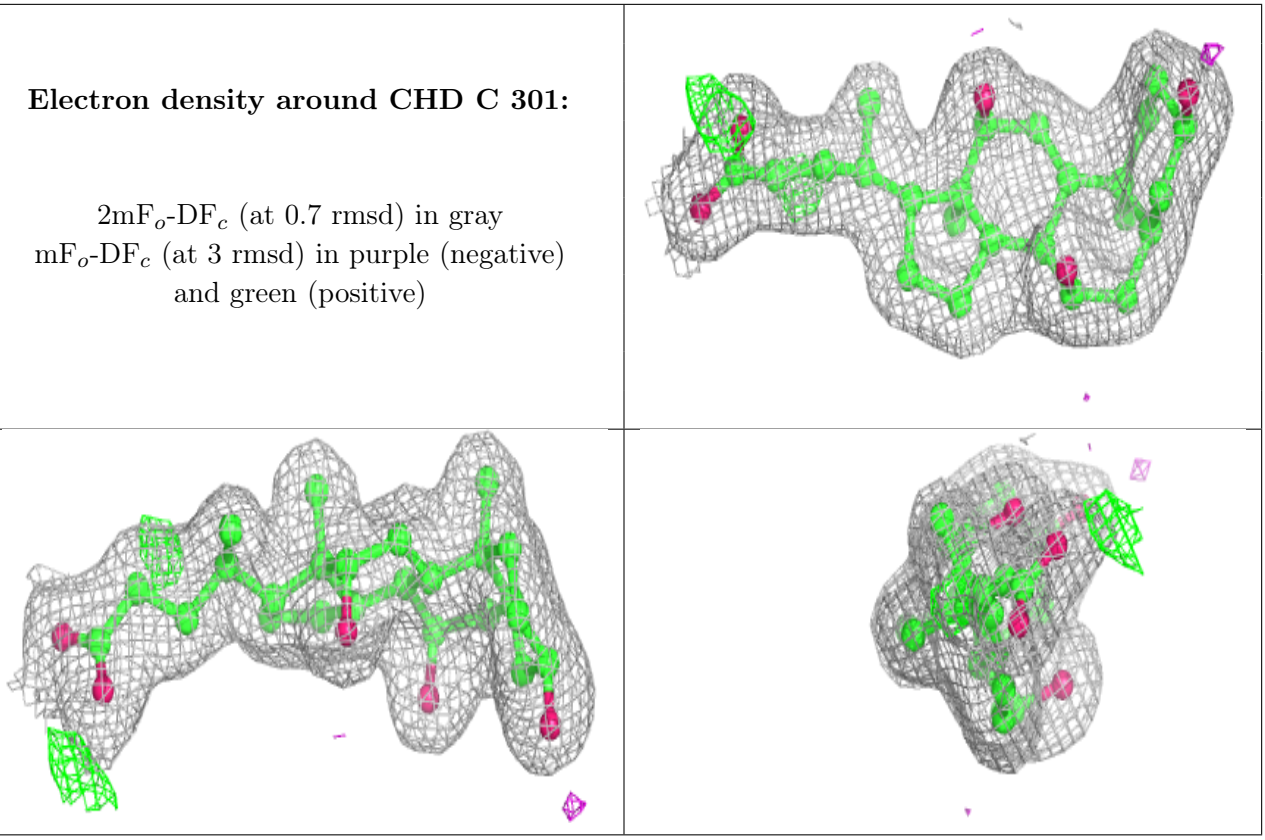






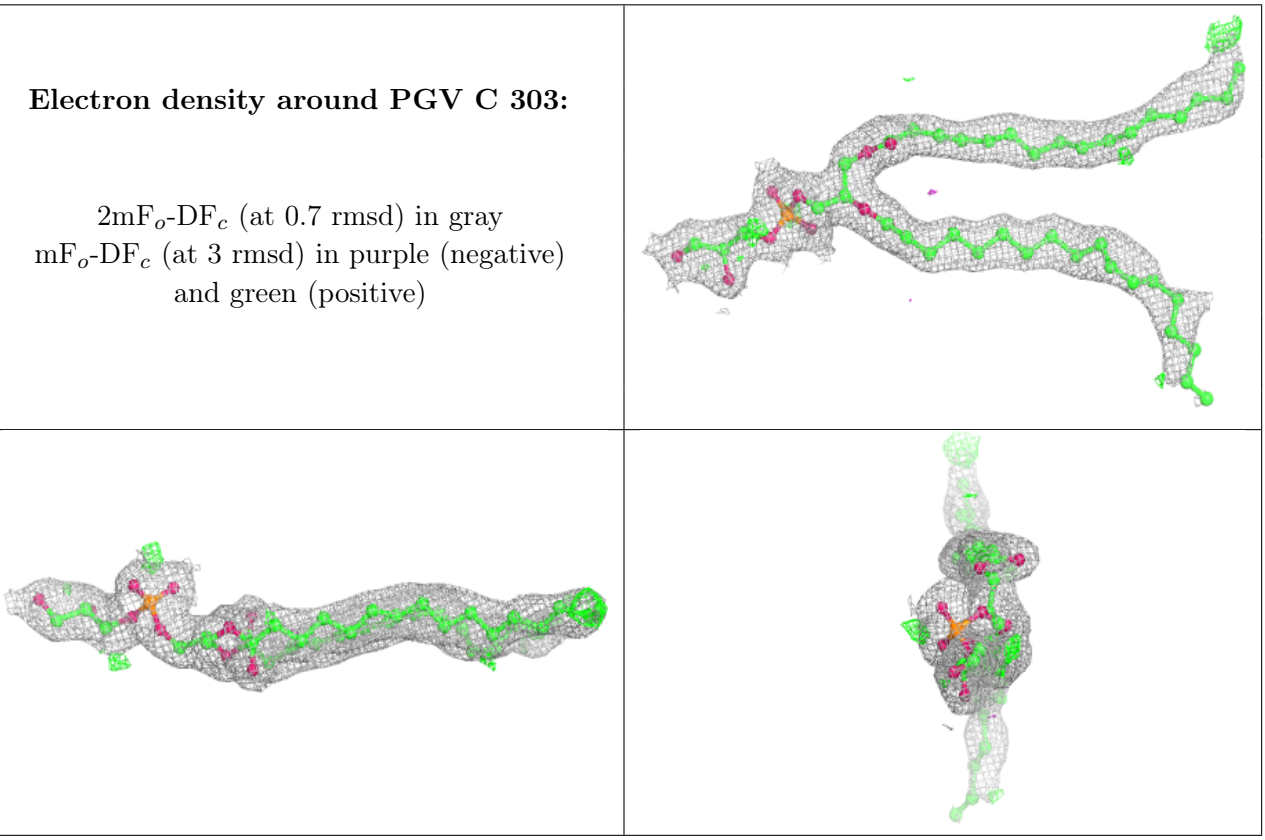
Electron density around CHD C 301:

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



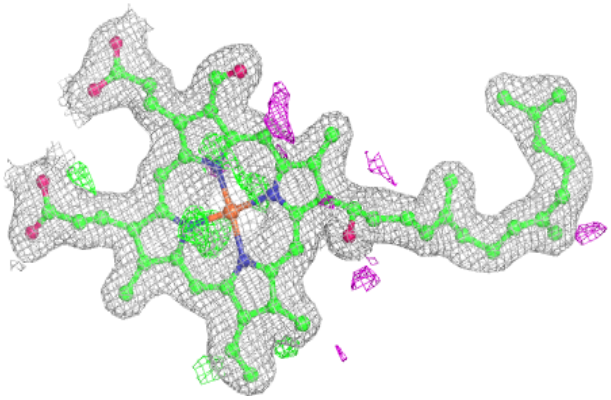
Electron density around PGV C 303:

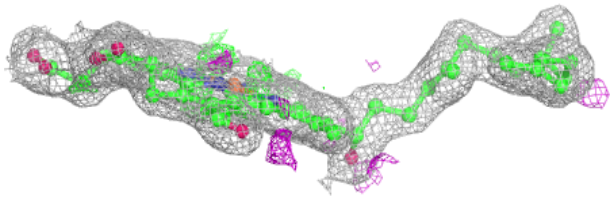
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

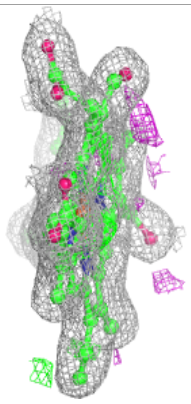


Electron density around HEA A 602:

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

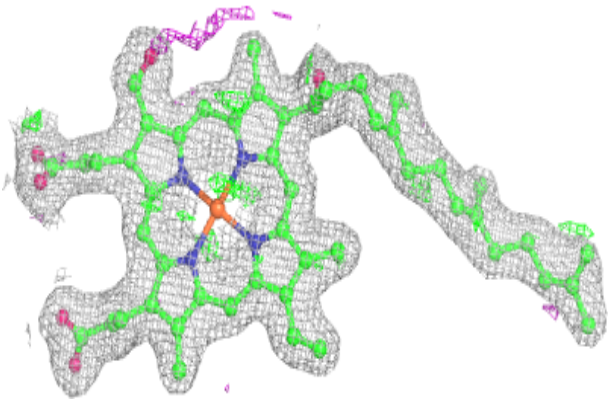


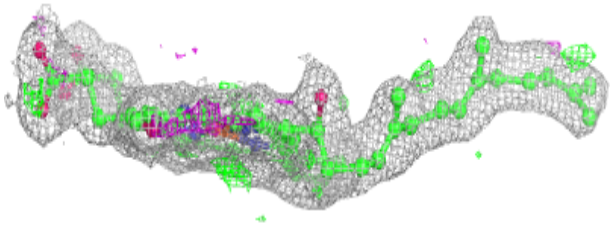


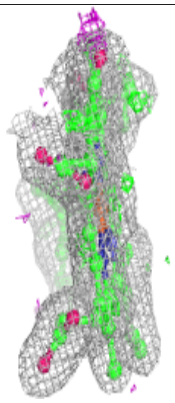


Electron density around HEA A 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.