Full wwPDB X-ray Structure Validation Report ⓘ

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

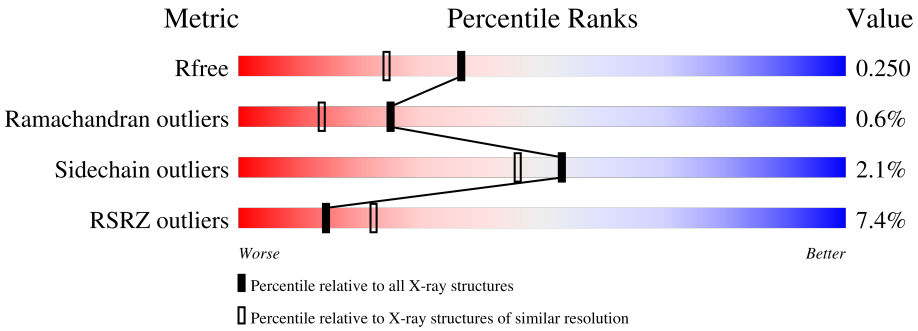
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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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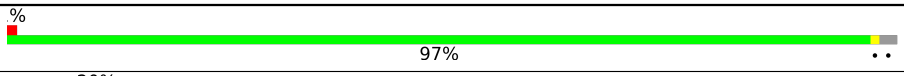
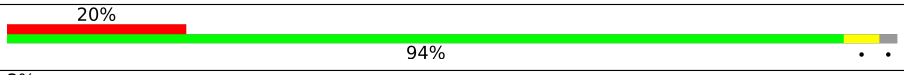
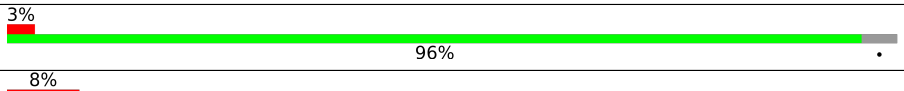
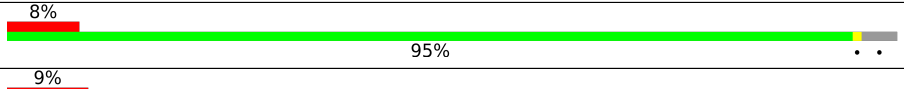
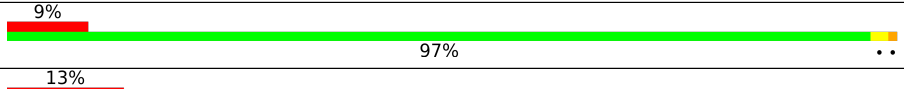
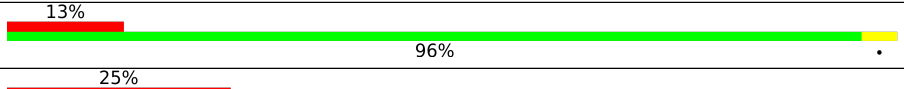
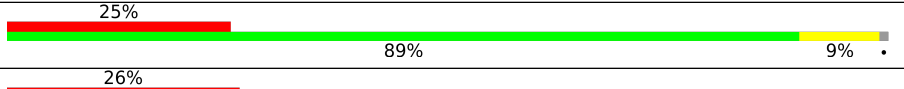
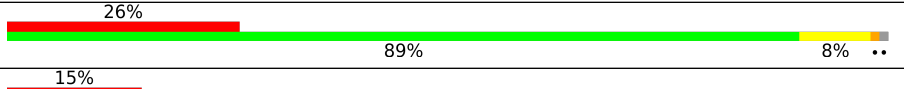
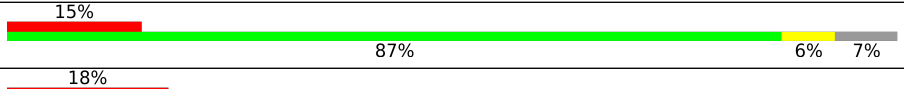
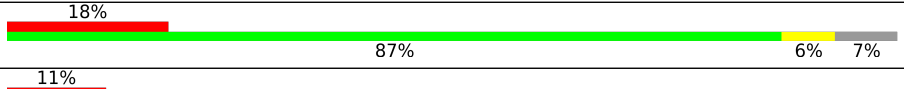
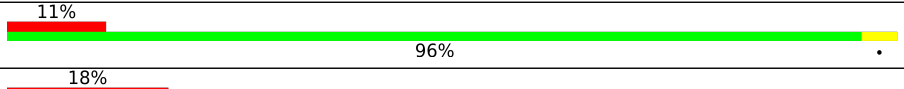
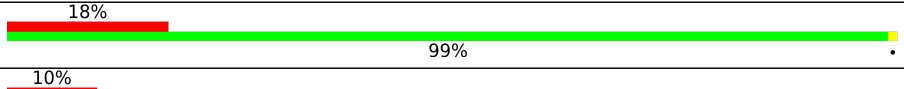
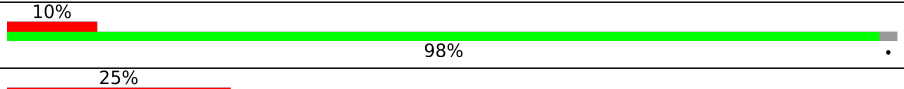
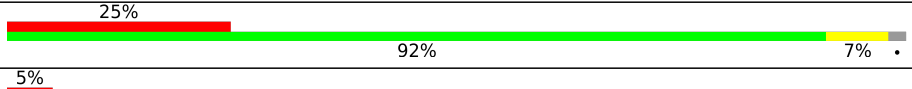
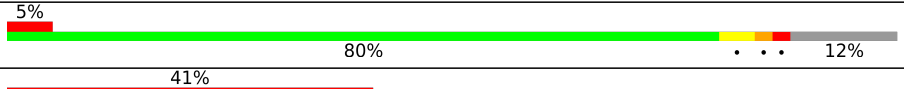
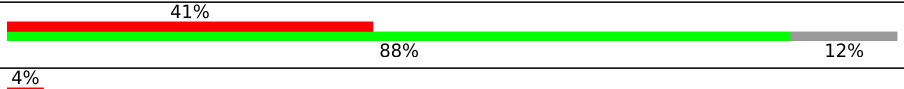
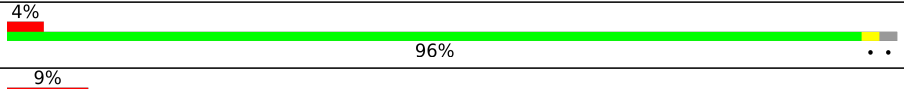
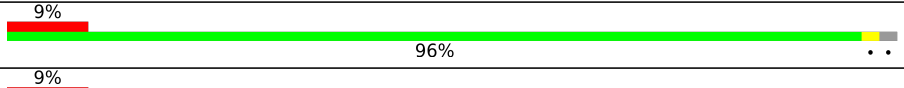
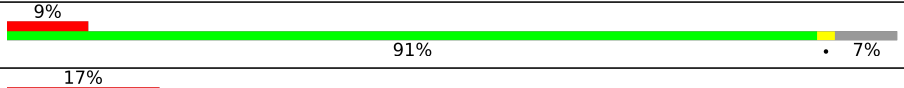
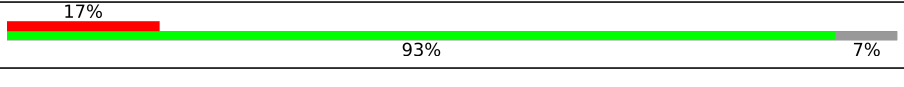
Mol	Chain	Length	Quality of chain
4	D	147	
4	d	147	
5	E	109	
5	e	109	
6	F	98	
6	f	98	
7	G	85	
7	g	85	
8	H	85	
8	h	85	
9	I	73	
9	i	73	
10	J	59	
10	j	59	
11	K	56	
11	k	56	
12	L	47	
12	l	47	
13	M	46	
13	m	46	

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			

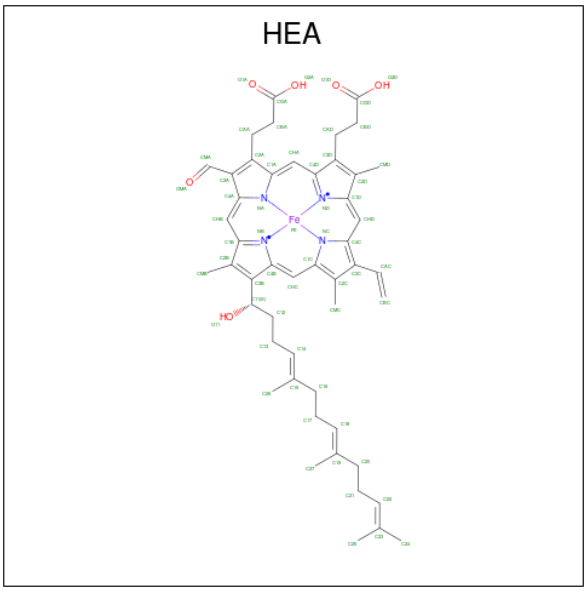
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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		

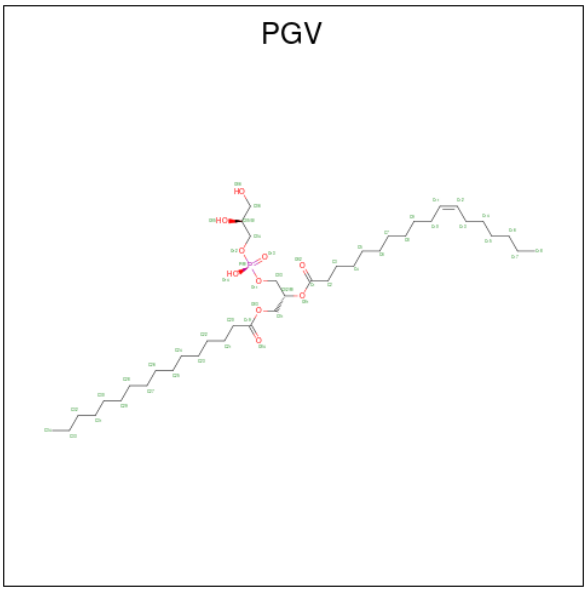
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

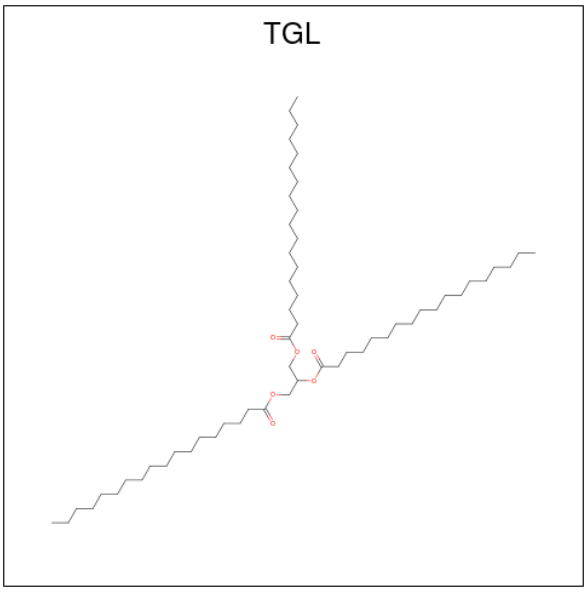
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	a	1	Total Na 1 1	0	0

- 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: $C_{40}H_{77}O_{10}P$).



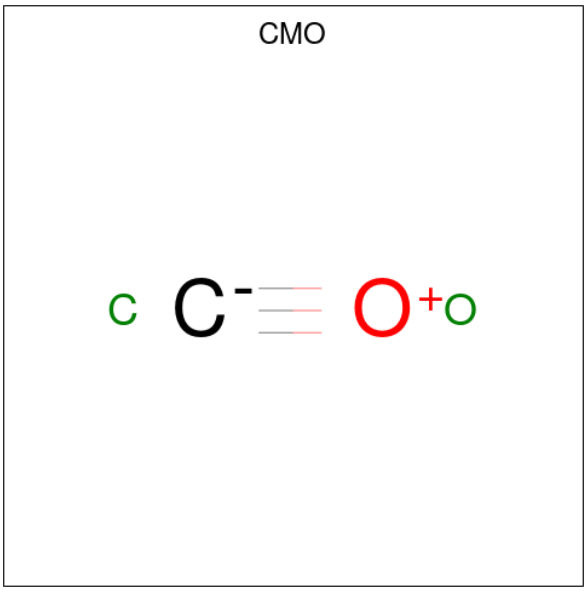
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	a	1	Total C O P 51 40 10 1	0	0
18	a	1	Total C O P 51 40 10 1	0	0
18	c	1	Total C O P 51 40 10 1	0	0
18	c	1	Total C O P 51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

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



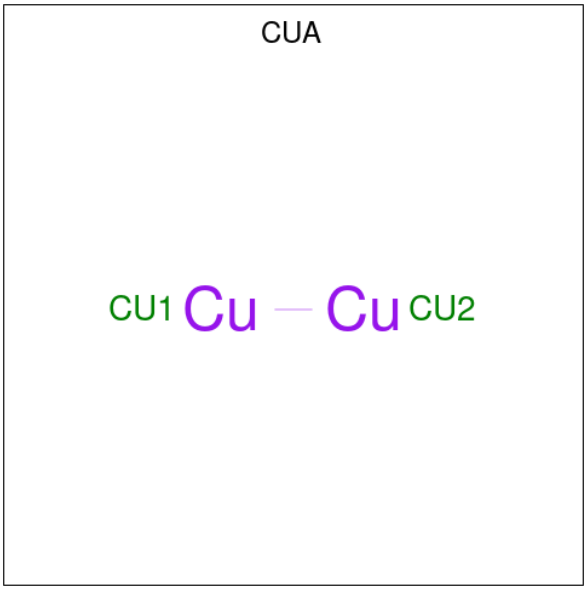
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	b	1	Total C O 63 57 6	0	0
19	d	1	Total C O 63 57 6	0	0
19	l	1	Total C O 63 57 6	0	0

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



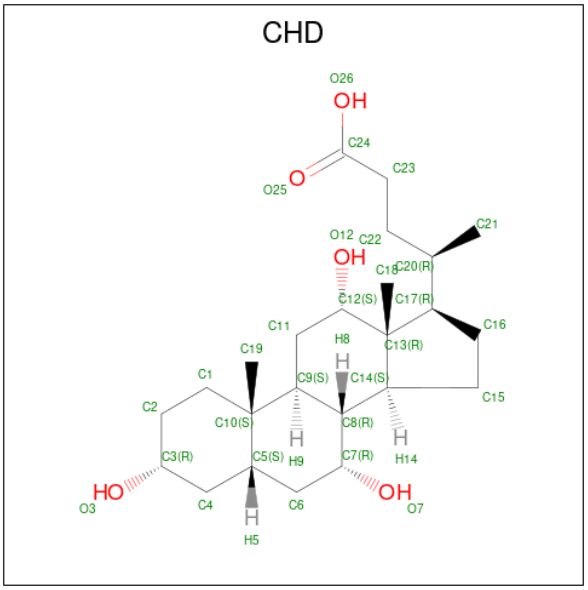
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 2 1 1	0	0
20	a	1	Total C O 2 1 1	0	0

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



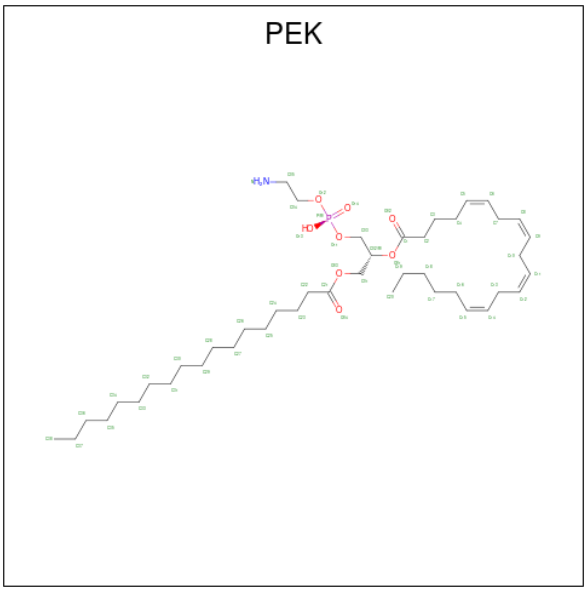
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	b	1	Total Cu 2 2	0	0

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



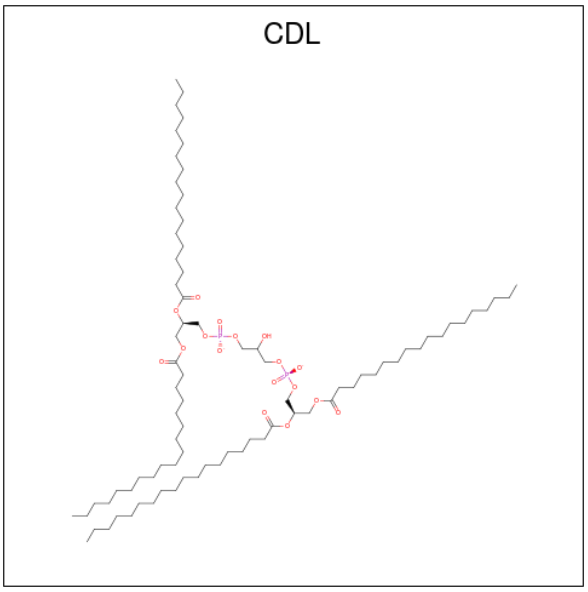
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	c	1	Total C O 29 24 5	0	0
22	c	1	Total C O 29 24 5	0	0
22	j	1	Total C O 29 24 5	0	0

- 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: $C_{43}H_{78}NO_8P$).



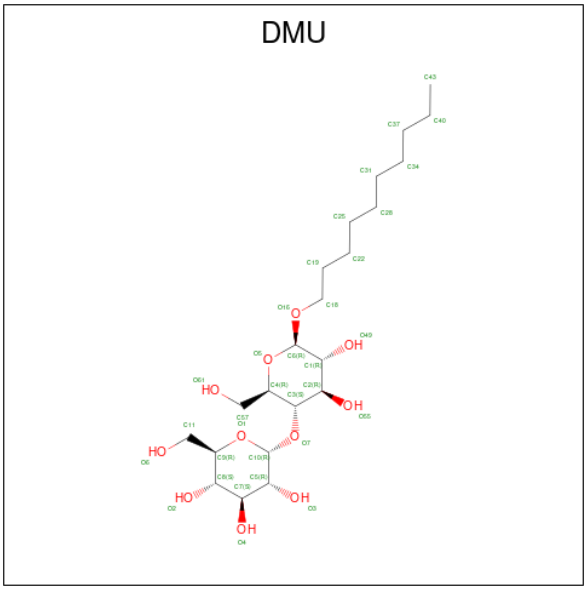
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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



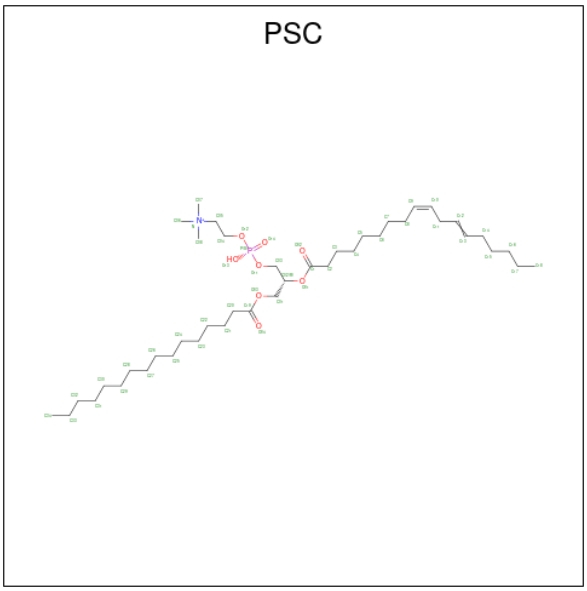
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	C	1	Total	C	O	P	0	0
			100	81	17	2		
24	G	1	Total	C	O	P	0	0
			100	81	17	2		
24	c	1	Total	C	O	P	0	0
			100	81	17	2		
24	g	1	Total	C	O	P	0	0
			100	81	17	2		

- 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

Continued on next page...

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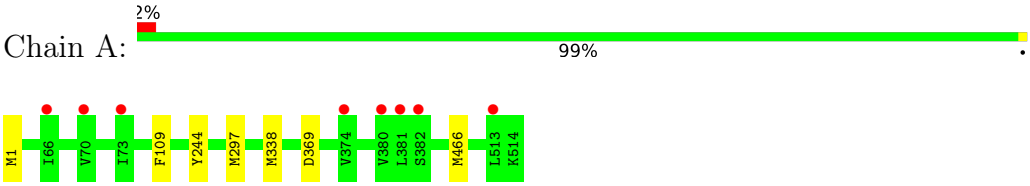
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	j	14	Total O 14 14	0	0
28	k	7	Total O 7 7	0	0
28	l	8	Total O 8 8	0	0
28	m	5	Total O 5 5	0	0

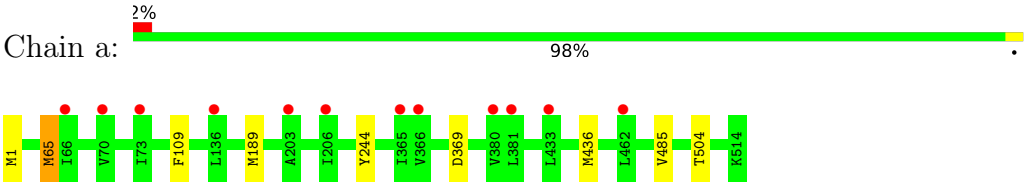
3 Residue-property plots (i)

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.

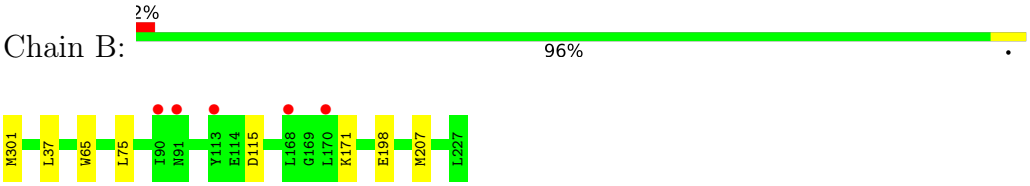
• Molecule 1: Cytochrome c oxidase subunit 1



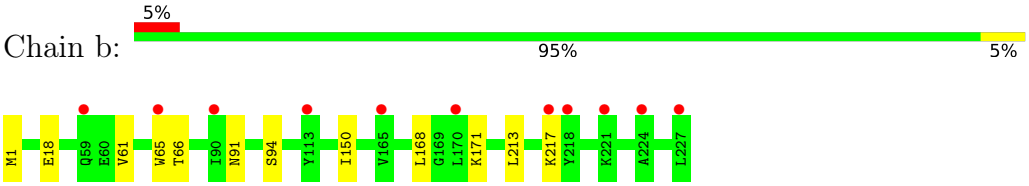
• Molecule 1: Cytochrome c oxidase subunit 1



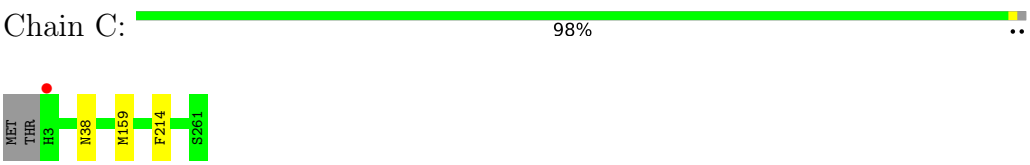
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

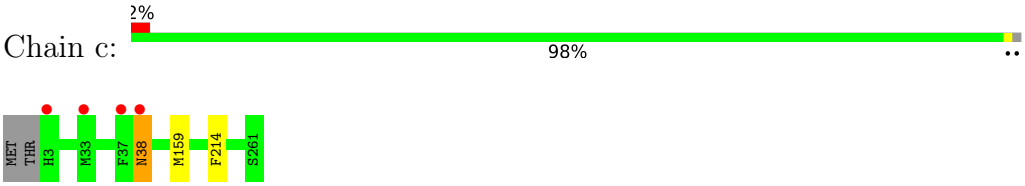


• Molecule 3: Cytochrome c oxidase subunit 3



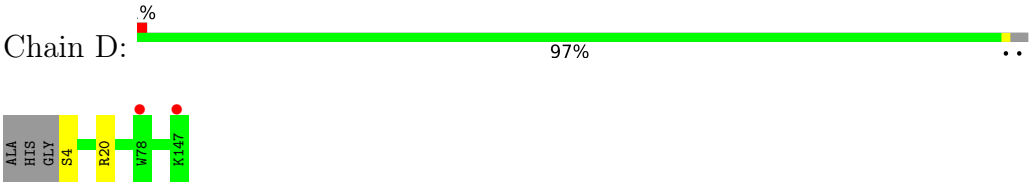
• Molecule 3: Cytochrome c oxidase subunit 3

Chain c:



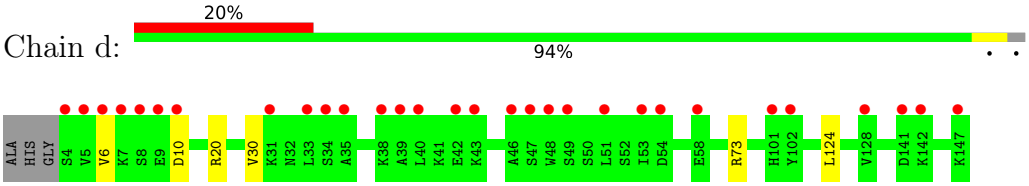
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



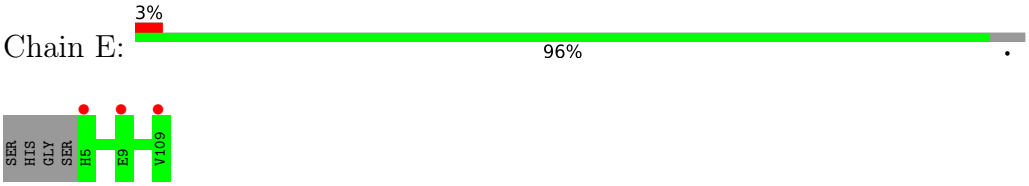
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain d:



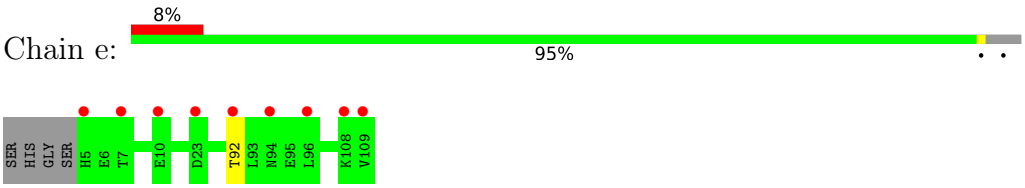
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



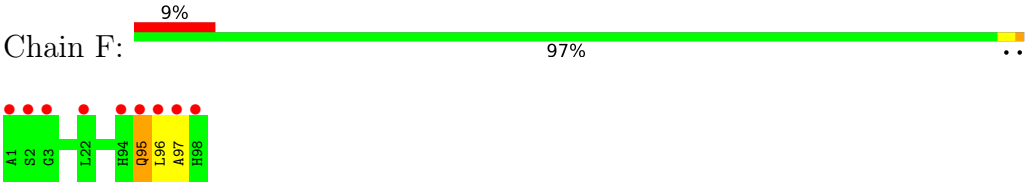
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain e:



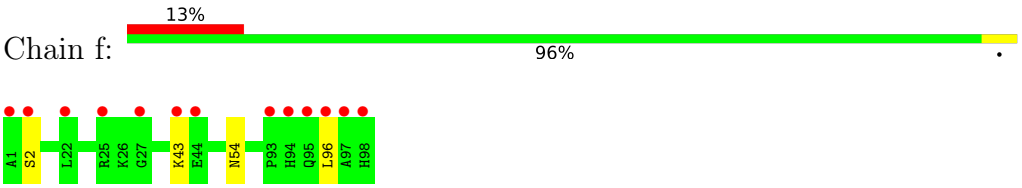
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



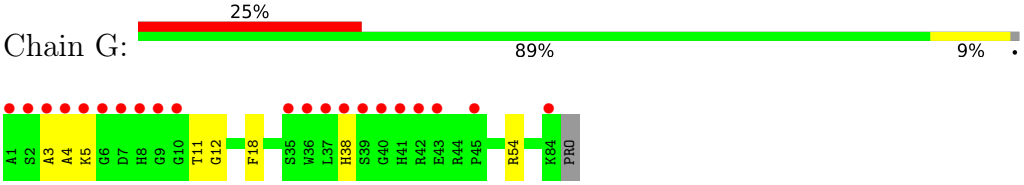
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain f:



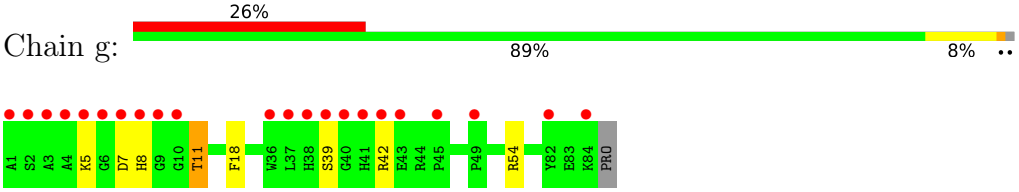
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



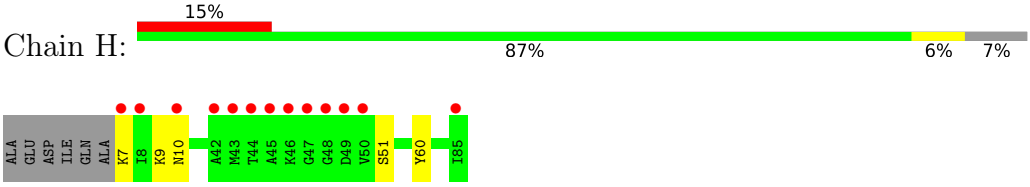
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain g:



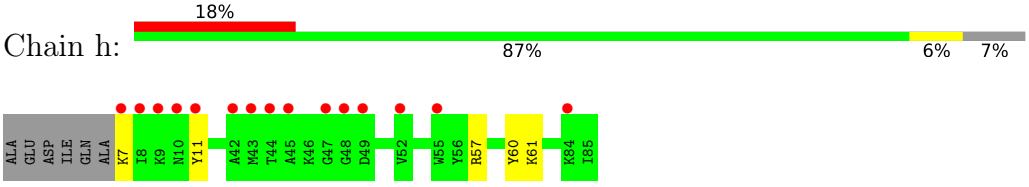
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



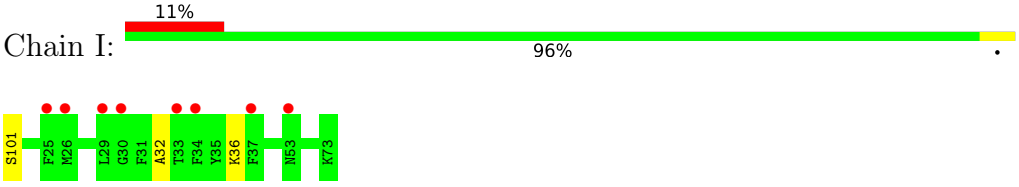
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain h:



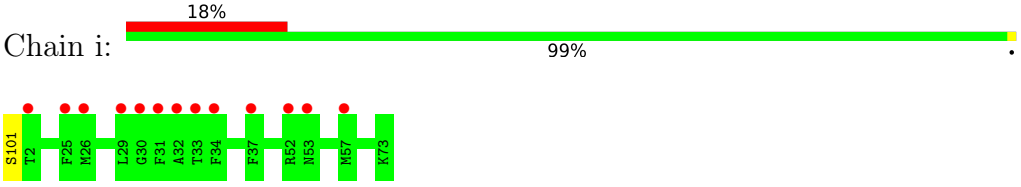
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



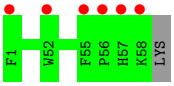
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain i:



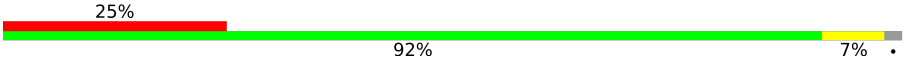
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

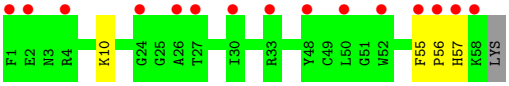
Chain J:



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

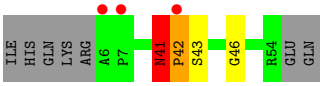
Chain j:





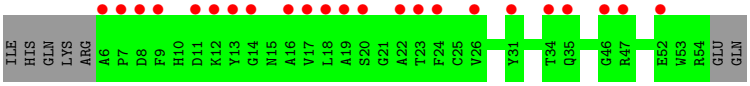
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



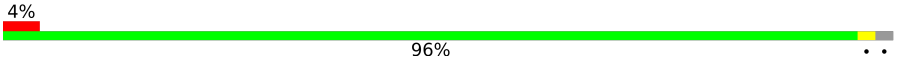
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain k:



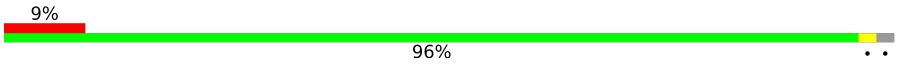
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

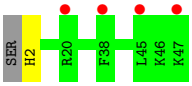
Chain L:



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

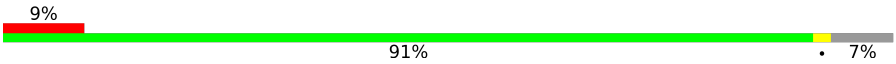
Chain l:

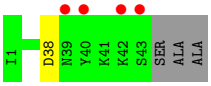




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

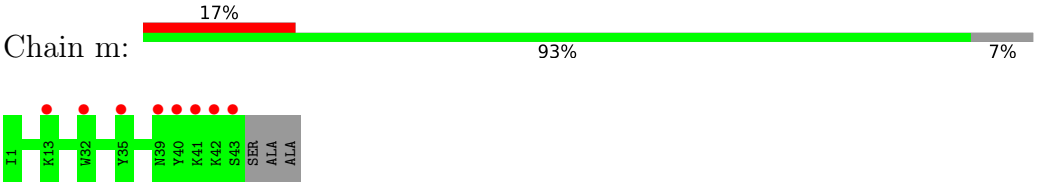
Chain M:





• 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

5.1 Standard geometry

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

All (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
11	K	41	ASN	CB-CA-C	5.39	121.19	110.40
1	A	244	TYR	CZ-CE2-CD2	-5.27	115.06	119.80
4	D	20	ARG	NE-CZ-NH1	5.25	122.93	120.30
11	K	41	ASN	C-N-CD	5.08	139.07	128.40
4	d	20	ARG	NE-CZ-NH1	5.02	122.81	120.30

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

All (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
11	K	43	SER
3	c	38	ASN
4	d	124	LEU
7	G	4	ALA
7	G	12	GLY
8	H	51	SER
9	I	32	ALA
8	h	11	TYR
2	b	91	ASN
10	j	56	PRO
2	b	150	ILE
6	f	2	SER
7	g	8	HIS
6	F	97	ALA
7	G	3	ALA
8	H	10	ASN

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	297	MET
1	A	338	MET
1	A	369	ASP
2	B	37	LEU
2	B	65	TRP

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Mol	Chain	Res	Type
2	B	75	LEU
2	B	115	ASP
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
4	D	4	SER
6	F	95	GLN
7	G	5	LYS
7	G	18	PHE
7	G	38	HIS
7	G	54	ARG
8	H	7	LYS
8	H	9	LYS
8	H	60	TYR
9	I	36	LYS
12	L	47	LYS
13	M	38	ASP
1	a	65	MET
1	a	109	PHE
1	a	189	MET
1	a	369	ASP
1	a	436	MET
1	a	485	VAL
1	a	504	THR
2	b	18	GLU
2	b	61	VAL
2	b	65	TRP
2	b	66	THR
2	b	94	SER
2	b	168	LEU
2	b	171	LYS
2	b	213	LEU
2	b	217	LYS
3	c	38	ASN
3	c	159	MET
3	c	214	PHE
4	d	6	VAL
4	d	10	ASP
4	d	30	VAL
4	d	73	ARG
5	e	92	THR
6	f	43	LYS

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Mol	Chain	Res	Type
6	f	54	ASN
6	f	96	LEU
7	g	5	LYS
7	g	7	ASP
7	g	18	PHE
7	g	39	SER
7	g	42	ARG
7	g	54	ARG
8	h	7	LYS
8	h	57	ARG
8	h	60	TYR
8	h	61	LYS
10	j	10	LYS
10	j	57	HIS
12	l	2	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	256	HIS
1	A	422	ASN
2	B	52	HIS
2	B	102	HIS
4	D	37	GLN
4	D	76	ASN
6	F	80	GLN
10	J	9	GLN
13	M	15	GLN
1	a	216	ASN
2	b	10	GLN
2	b	59	GLN
2	b	103	GLN
3	c	56	GLN
3	c	76	GLN
6	f	54	ASN
13	m	15	GLN
13	m	39	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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
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

All (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
2	B	301	FME	C-CA-N	3.33	115.75	109.73
9	I	101	SAC	CB-CA-N	2.72	116.65	110.55
2	B	301	FME	O1-CN-N	-2.68	118.22	125.27
2	b	1	FME	C-CA-N	2.61	114.45	109.73
7	g	11	TPO	P-OG1-CB	-2.30	116.26	123.21
7	G	11	TPO	P-OG1-CB	-2.09	116.89	123.21
7	G	11	TPO	CG2-CB-CA	-2.08	109.06	113.16

There are no chirality outliers.

All (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
1	a	1	FME	O1-CN-N-CA
1	a	1	FME	N-CA-CB-CG
2	b	1	FME	O1-CN-N-CA
7	g	11	TPO	N-CA-CB-OG1
7	g	11	TPO	CB-OG1-P-O3P
9	i	101	SAC	O-C-CA-CB
9	I	101	SAC	C2A-C1A-N-CA
9	I	101	SAC	OAC-C1A-N-CA
9	i	101	SAC	N-CA-CB-OG
1	A	1	FME	CA-CB-CG-SD
7	g	11	TPO	CB-OG1-P-O1P

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Mol	Chain	Res	Type	Atoms
1	a	1	FME	C-CA-CB-CG
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	CB-OG1-P-O2P
7	G	11	TPO	CB-OG1-P-O3P
1	a	1	FME	CB-CA-N-CN
7	g	11	TPO	O-C-CA-CB

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
14	A	601	HEA	C3D-C2D	4.88	1.47	1.36
18	C	304	PGV	O03-C19	4.87	1.47	1.33
19	A	608	TGL	OG1-CA1	4.86	1.47	1.33
14	A	602	HEA	C3C-C2C	4.84	1.47	1.40
19	l	101	TGL	OG3-CC1	4.83	1.47	1.33
14	A	601	HEA	C3C-C2C	4.83	1.47	1.40
14	a	602	HEA	C3C-C2C	4.83	1.47	1.40
14	a	602	HEA	CHD-C1D	4.81	1.47	1.35
19	l	101	TGL	OG2-CB1	4.81	1.47	1.34
26	E	201	PSC	O01-C1	4.80	1.47	1.34
14	A	602	HEA	CHD-C1D	4.78	1.47	1.35
18	A	606	PGV	O03-C19	4.78	1.47	1.33
18	a	606	PGV	O03-C19	4.77	1.47	1.33
24	G	102	CDL	OB8-CB7	4.75	1.47	1.33
18	c	302	PGV	O01-C1	4.74	1.47	1.34
14	a	601	HEA	C3C-C2C	4.72	1.46	1.40
14	a	602	HEA	C3B-C2B	4.67	1.45	1.34
19	d	201	TGL	OG2-CB1	4.67	1.47	1.34
24	c	307	CDL	OA6-CA5	4.66	1.47	1.34
23	C	307	PEK	O03-C21	4.66	1.47	1.33
23	c	301	PEK	O03-C21	4.63	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	102	CDL	OB6-CB5	4.63	1.47	1.34
14	a	602	HEA	CHC-C4B	4.63	1.46	1.35
23	G	101	PEK	O01-C1	4.61	1.47	1.34
19	D	201	TGL	OG2-CB1	4.59	1.47	1.34
23	C	307	PEK	O01-C1	4.59	1.47	1.34
19	D	201	TGL	OG1-CA1	4.57	1.46	1.33
24	G	102	CDL	OA8-CA7	4.57	1.46	1.33
18	C	304	PGV	O01-C1	4.56	1.47	1.34
23	c	305	PEK	O01-C1	4.56	1.47	1.34
14	A	602	HEA	C3B-C2B	4.55	1.45	1.34
19	A	608	TGL	OG3-CC1	4.54	1.46	1.33
14	a	601	HEA	CHD-C1D	4.54	1.46	1.35
14	A	602	HEA	C3A-C2A	4.53	1.46	1.40
19	l	101	TGL	OG1-CA1	4.53	1.46	1.33
23	c	305	PEK	O03-C21	4.52	1.46	1.33
24	c	307	CDL	OB6-CB5	4.52	1.47	1.34
18	c	302	PGV	O03-C19	4.52	1.46	1.33
24	g	101	CDL	OB6-CB5	4.50	1.47	1.34
24	C	305	CDL	OA6-CA5	4.49	1.47	1.34
19	d	201	TGL	OG1-CA1	4.49	1.46	1.33
24	c	307	CDL	OA8-CA7	4.48	1.46	1.33
23	G	101	PEK	O03-C21	4.47	1.46	1.33
14	A	602	HEA	C3D-C2D	4.46	1.46	1.36
24	g	101	CDL	OB8-CB7	4.46	1.46	1.33
19	D	201	TGL	OG3-CC1	4.46	1.46	1.33
19	b	302	TGL	OG2-CB1	4.46	1.46	1.34
24	g	101	CDL	OA8-CA7	4.44	1.46	1.33
14	a	601	HEA	C3D-C2D	4.44	1.46	1.36
19	A	609	TGL	OG1-CA1	4.43	1.46	1.33
24	C	305	CDL	OA8-CA7	4.43	1.46	1.33
14	a	601	HEA	CHC-C4B	4.43	1.46	1.35
19	b	302	TGL	OG1-CA1	4.42	1.46	1.33
26	b	303	PSC	O03-C19	4.39	1.46	1.33
19	d	201	TGL	OG3-CC1	4.36	1.46	1.33
24	c	307	CDL	OB8-CB7	4.36	1.46	1.33
26	E	201	PSC	O03-C19	4.35	1.46	1.33
24	g	101	CDL	OA6-CA5	4.34	1.46	1.34
24	C	305	CDL	OB8-CB7	4.33	1.46	1.33
19	A	609	TGL	OG2-CB1	4.32	1.46	1.34
23	c	304	PEK	O03-C21	4.32	1.46	1.33
14	a	601	HEA	C3A-C2A	4.30	1.46	1.40
23	c	301	PEK	O01-C1	4.27	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	302	TGL	OG3-CC1	4.25	1.45	1.33
19	A	608	TGL	OG2-CB1	4.23	1.46	1.34
14	A	601	HEA	CHD-C1D	4.23	1.45	1.35
24	C	305	CDL	OB6-CB5	4.22	1.46	1.34
19	A	609	TGL	OG3-CC1	4.21	1.45	1.33
24	G	102	CDL	OA6-CA5	4.21	1.46	1.34
14	A	602	HEA	CHC-C4B	4.10	1.45	1.35
18	c	306	PGV	O01-C1	4.10	1.45	1.34
18	A	606	PGV	O01-C1	4.08	1.45	1.34
14	A	601	HEA	CHC-C4B	4.05	1.45	1.35
18	c	306	PGV	O03-C19	3.82	1.44	1.33
23	C	302	PEK	O03-C21	3.78	1.44	1.33
14	A	602	HEA	C4D-ND	-3.76	1.31	1.38
25	c	309	DMU	O5-C6	3.74	1.51	1.41
18	a	607	PGV	O03-C19	3.73	1.44	1.33
18	C	303	PGV	O01-C1	3.70	1.44	1.34
18	C	303	PGV	O03-C19	3.69	1.44	1.33
14	a	602	HEA	C1B-NB	-3.63	1.31	1.38
18	A	607	PGV	O03-C19	3.63	1.43	1.33
14	A	602	HEA	C1B-NB	-3.62	1.31	1.38
14	a	602	HEA	C3D-C2D	3.61	1.44	1.36
18	a	607	PGV	O01-C1	3.58	1.44	1.34
23	C	302	PEK	O01-C1	3.55	1.44	1.34
14	a	601	HEA	C1D-ND	-3.54	1.34	1.40
23	c	304	PEK	O01-C1	3.49	1.44	1.34
14	a	602	HEA	FE-ND	3.40	2.13	1.96
14	a	601	HEA	C4B-NB	-3.35	1.34	1.40
18	A	607	PGV	O01-C1	3.34	1.43	1.34
14	a	602	HEA	C4D-ND	-3.28	1.32	1.38
14	A	601	HEA	C4B-NB	-3.05	1.35	1.40
14	a	601	HEA	FE-NB	2.92	2.11	1.96
14	a	601	HEA	FE-ND	2.82	2.10	1.96
14	A	601	HEA	C3A-C2A	2.78	1.44	1.40
25	c	309	DMU	O16-C6	2.78	1.44	1.40
14	a	602	HEA	FE-NB	2.77	2.10	1.96
14	A	602	HEA	FE-ND	2.72	2.10	1.96
14	a	601	HEA	C4D-ND	-2.61	1.33	1.38
14	a	602	HEA	C1C-CHC	2.60	1.48	1.41
14	a	601	HEA	C4C-CHD	2.59	1.48	1.41
14	a	602	HEA	C2A-C1A	2.56	1.48	1.42
25	C	308	DMU	O16-C6	2.55	1.44	1.40
14	A	601	HEA	C2A-C1A	2.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	602	HEA	C4B-C3B	2.39	1.48	1.44
14	A	601	HEA	C1D-ND	-2.38	1.36	1.40
14	A	601	HEA	O2D-CGD	-2.37	1.22	1.30
14	a	601	HEA	C2A-C1A	2.37	1.47	1.42
14	A	602	HEA	C2A-C1A	2.35	1.47	1.42
14	a	601	HEA	C1B-NB	-2.32	1.34	1.38
25	M	101	DMU	O16-C6	2.26	1.44	1.40
14	a	602	HEA	C4C-CHD	2.21	1.47	1.41
14	a	601	HEA	C4B-C3B	2.16	1.48	1.44
14	A	601	HEA	C4D-ND	-2.15	1.34	1.38
14	A	601	HEA	FE-ND	2.07	2.07	1.96
14	A	602	HEA	C1C-CHC	2.07	1.46	1.41
14	A	601	HEA	C4C-CHD	2.02	1.46	1.41

All (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
26	b	303	PSC	C08-N-C07	-6.26	92.88	108.97
14	A	602	HEA	C1D-C2D-C3D	-6.24	100.40	106.96
14	A	602	HEA	C2D-C1D-ND	6.14	117.12	109.84
14	A	602	HEA	C2B-C1B-NB	6.14	117.24	109.88
14	a	601	HEA	C3D-C4D-ND	6.13	116.30	110.36
14	a	602	HEA	CAD-CBD-CGD	-6.08	100.53	113.60
14	a	602	HEA	C3D-C4D-ND	5.87	116.04	110.36
18	a	606	PGV	O01-C1-C2	5.78	123.95	111.50
14	A	601	HEA	C2D-C1D-ND	5.60	116.47	109.84
14	a	602	HEA	C1D-C2D-C3D	-5.57	101.10	106.96
14	a	602	HEA	C2D-C1D-ND	5.54	116.41	109.84
14	A	601	HEA	CMC-C2C-C3C	5.53	135.03	124.68
24	c	307	CDL	OA6-CA5-C11	5.43	123.19	111.50
22	J	101	CHD	C22-C20-C17	5.33	121.30	110.28
18	c	302	PGV	O01-C1-C2	5.29	122.90	111.50
22	J	101	CHD	C6-C7-C8	5.28	117.11	111.48
23	G	101	PEK	O01-C1-C2	5.27	122.87	111.50
14	a	602	HEA	C2B-C1B-NB	5.22	116.13	109.88
14	A	602	HEA	C3B-C4B-NB	5.21	116.02	109.84
19	l	101	TGL	OG2-CB1-CB2	5.19	122.69	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	101	CDL	OB6-CB5-C51	5.10	122.49	111.50
22	J	101	CHD	C13-C17-C20	5.03	125.50	119.50
14	a	601	HEA	C2B-C1B-NB	5.01	115.89	109.88
14	a	601	HEA	C3B-C4B-NB	4.87	115.61	109.84
14	a	602	HEA	C3B-C4B-NB	4.86	115.60	109.84
14	A	601	HEA	C1D-C2D-C3D	-4.83	101.87	106.96
14	A	601	HEA	C2B-C1B-NB	4.83	115.67	109.88
26	E	201	PSC	O01-C1-C2	4.66	121.55	111.50
24	C	305	CDL	OA6-CA5-C11	4.63	121.47	111.50
14	a	601	HEA	C2D-C1D-ND	4.59	115.28	109.84
25	c	309	DMU	O16-C6-C1	4.58	115.45	108.30
14	A	601	HEA	C3B-C4B-NB	4.52	115.19	109.84
14	a	602	HEA	CMC-C2C-C3C	4.51	133.12	124.68
14	A	602	HEA	CMC-C2C-C3C	4.51	133.12	124.68
14	A	602	HEA	CAD-CBD-CGD	-4.44	104.05	113.60
26	E	201	PSC	C07-N-C06	4.37	120.20	108.97
24	c	307	CDL	OB6-CB5-C51	4.36	120.89	111.50
19	d	201	TGL	OG2-CB1-CB2	4.34	120.85	111.50
22	J	101	CHD	C5-C6-C7	4.32	119.23	114.46
14	a	601	HEA	C3C-C4C-NC	4.25	114.70	109.21
14	A	601	HEA	C13-C12-C11	-4.24	107.98	114.35
19	b	302	TGL	OG2-CB1-CB2	4.19	120.53	111.50
24	G	102	CDL	OB6-CB5-C51	4.13	120.41	111.50
14	A	602	HEA	CMD-C2D-C1D	4.08	131.25	125.04
19	A	609	TGL	OG2-CB1-CB2	4.06	120.25	111.50
26	E	201	PSC	C08-N-C05	-4.05	93.33	109.92
19	D	201	TGL	OG2-CB1-CB2	4.02	120.16	111.50
14	a	601	HEA	CMC-C2C-C3C	3.99	132.14	124.68
23	C	302	PEK	O03-C21-C22	3.98	124.39	111.91
24	g	101	CDL	OA6-CA5-C11	3.98	120.07	111.50
26	b	303	PSC	C07-N-C06	3.96	119.15	108.97
14	A	602	HEA	C3C-C4C-NC	3.95	114.32	109.21
18	C	304	PGV	O03-C19-C20	3.91	124.17	111.91
23	c	305	PEK	O01-C1-C2	3.88	119.86	111.50
24	G	102	CDL	OA6-CA5-C11	3.87	119.85	111.50
14	A	601	HEA	C26-C15-C16	3.84	121.74	115.27
23	c	301	PEK	O01-C1-C2	3.80	119.69	111.50
14	a	602	HEA	C3C-C4C-NC	3.77	114.08	109.21
14	a	601	HEA	C1D-C2D-C3D	-3.77	102.99	106.96
14	A	602	HEA	CBA-CAA-C2A	-3.74	106.31	112.60
22	C	306	CHD	C21-C20-C22	-3.72	104.53	110.36
14	a	602	HEA	CBA-CAA-C2A	-3.70	106.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	J	101	CHD	C6-C5-C4	-3.70	106.92	111.19
26	b	303	PSC	C07-N-C05	3.69	125.03	109.92
18	c	302	PGV	O03-C19-C20	3.67	123.42	111.91
14	a	602	HEA	C4B-C3B-C2B	-3.67	101.15	107.41
25	C	308	DMU	C6-O5-C4	3.66	120.88	113.69
14	a	601	HEA	C1B-C2B-C3B	-3.65	102.44	106.80
14	A	601	HEA	C3C-C4C-NC	3.64	113.91	109.21
23	C	307	PEK	O01-C1-C2	3.64	119.34	111.50
14	A	601	HEA	CMD-C2D-C1D	3.61	130.54	125.04
22	J	101	CHD	C6-C5-C10	3.60	116.48	112.66
25	c	309	DMU	C10-O1-C9	3.57	120.70	113.69
14	a	602	HEA	CMD-C2D-C1D	3.55	130.45	125.04
14	a	601	HEA	C13-C12-C11	-3.52	109.07	114.35
23	G	101	PEK	O03-C21-C22	3.50	122.90	111.91
14	A	602	HEA	C4B-NB-C1B	-3.50	101.46	105.07
18	C	304	PGV	O01-C1-C2	3.49	119.03	111.50
14	A	602	HEA	C4B-C3B-C2B	-3.49	101.45	107.41
25	c	309	DMU	O5-C6-C1	3.47	117.70	110.35
14	A	601	HEA	C1B-C2B-C3B	-3.45	102.67	106.80
24	C	305	CDL	OB6-CB5-C51	3.45	118.94	111.50
22	J	101	CHD	C21-C20-C17	-3.43	107.67	112.92
14	a	601	HEA	C4D-C3D-C2D	-3.38	101.97	106.90
18	A	606	PGV	O03-C19-C20	3.38	122.51	111.91
14	A	602	HEA	C1D-ND-C4D	-3.37	101.59	105.07
14	a	601	HEA	C26-C15-C16	3.31	120.84	115.27
14	A	602	HEA	CHD-C1D-C2D	-3.31	117.57	126.72
19	A	608	TGL	OG2-CB1-CB2	3.29	118.59	111.50
19	d	201	TGL	OG3-CC1-CC2	3.29	122.22	111.91
25	c	309	DMU	C18-O16-C6	-3.27	108.41	113.84
24	g	101	CDL	OA8-CA7-C31	3.27	122.17	111.91
18	A	606	PGV	O01-C1-C2	3.26	118.53	111.50
26	b	303	PSC	C08-N-C05	-3.24	96.66	109.92
14	A	601	HEA	CHA-C4D-C3D	-3.21	120.12	124.84
18	c	302	PGV	O03-C19-O04	-3.20	115.51	123.59
14	a	602	HEA	CHD-C1D-C2D	-3.19	117.91	126.72
14	A	601	HEA	CHB-C1B-C2B	-3.16	120.04	124.98
22	j	101	CHD	C21-C20-C17	3.15	117.75	112.92
14	a	601	HEA	CHB-C1B-C2B	-3.15	120.06	124.98
22	B	402	CHD	C17-C13-C14	3.12	103.24	100.09
22	B	402	CHD	C19-C10-C1	-3.12	103.24	108.26
24	C	305	CDL	OA8-CA7-C31	3.11	121.67	111.91
24	G	102	CDL	OB8-CB7-C71	3.10	121.64	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	m	101	DMU	O1-C9-C8	3.05	115.23	109.69
24	C	305	CDL	OB8-CB7-C71	3.05	121.47	111.91
24	g	101	CDL	OB8-CB7-C71	3.04	121.45	111.91
14	a	601	HEA	CHA-C4D-C3D	-3.04	120.37	124.84
18	a	606	PGV	O03-C19-C20	3.03	121.41	111.91
26	b	303	PSC	O01-C1-C2	3.01	117.99	111.50
14	A	602	HEA	C1B-C2B-C3B	-2.99	103.22	106.80
19	A	608	TGL	OG1-CA1-CA2	2.99	121.29	111.91
23	c	304	PEK	O03-C21-C22	2.98	121.25	111.91
14	A	602	HEA	CAD-C3D-C4D	2.97	129.85	124.66
19	A	608	TGL	OG3-CC1-CC2	2.94	121.14	111.91
14	a	601	HEA	C4B-C3B-C2B	-2.93	102.41	107.41
25	c	309	DMU	O1-C10-C5	2.92	116.54	110.35
18	C	304	PGV	O03-C01-C02	2.91	116.89	108.43
24	C	305	CDL	OA6-CA5-OA7	-2.90	116.69	123.70
23	c	305	PEK	O03-C21-C22	2.90	121.01	111.91
14	A	601	HEA	C1D-ND-C4D	-2.90	102.08	105.07
19	D	201	TGL	OG1-CA1-CA2	2.90	121.00	111.91
22	C	306	CHD	C19-C10-C1	-2.88	103.62	108.26
22	G	103	CHD	C22-C20-C17	2.88	116.23	110.28
19	b	302	TGL	OG1-CA1-CA2	2.88	120.93	111.91
18	c	306	PGV	O01-C1-C2	2.88	117.70	111.50
14	a	602	HEA	C1D-ND-C4D	-2.87	102.11	105.07
24	c	307	CDL	OB8-CB7-C71	2.86	120.89	111.91
14	A	601	HEA	C17-C18-C19	-2.85	120.80	127.66
23	c	304	PEK	O01-C1-C2	2.82	117.59	111.50
18	A	607	PGV	O03-C19-C20	2.82	120.75	111.91
19	l	101	TGL	OG1-CA1-CA2	2.82	120.75	111.91
22	J	101	CHD	C5-C4-C3	2.80	116.87	112.76
14	A	602	HEA	CHA-C4D-ND	-2.79	121.39	124.43
22	J	101	CHD	C17-C13-C14	-2.79	97.28	100.09
14	a	602	HEA	CHB-C1B-C2B	-2.78	120.63	124.98
14	A	602	HEA	CHB-C1B-C2B	-2.76	120.66	124.98
14	A	602	HEA	C13-C12-C11	-2.76	110.20	114.35
23	G	101	PEK	O03-C21-O04	-2.75	116.64	123.59
24	c	307	CDL	OA8-CA7-C31	2.75	120.55	111.91
26	b	303	PSC	O03-C19-C20	2.75	120.53	111.91
14	A	601	HEA	C4D-C3D-C2D	-2.74	102.90	106.90
25	C	308	DMU	C10-O1-C9	2.73	119.05	113.69
19	b	302	TGL	OG3-CC1-CC2	2.73	120.47	111.91
25	C	308	DMU	C6-C1-C2	2.72	115.65	110.00
24	C	305	CDL	OB8-CB7-OB9	-2.67	116.84	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	302	PEK	O01-C1-C2	2.67	117.25	111.50
14	A	601	HEA	CAD-C3D-C4D	2.66	129.31	124.66
14	A	601	HEA	OMA-CMA-C3A	-2.66	119.12	124.91
22	j	101	CHD	C6-C5-C4	-2.66	108.13	111.19
19	d	201	TGL	OG1-CA1-CA2	2.66	120.24	111.91
24	G	102	CDL	OA8-CA7-C31	2.63	120.15	111.91
26	E	201	PSC	O03-C19-C20	2.62	120.14	111.91
18	A	607	PGV	O03-C19-O04	-2.62	116.98	123.59
22	c	308	CHD	C6-C5-C4	-2.61	108.18	111.19
19	l	101	TGL	OG3-CC1-CC2	2.61	120.10	111.91
22	c	303	CHD	C19-C10-C1	-2.61	104.06	108.26
22	j	101	CHD	C5-C6-C7	-2.59	111.60	114.46
14	a	602	HEA	CAD-C3D-C4D	2.58	129.16	124.66
26	b	303	PSC	C02-O01-C1	2.57	124.12	117.79
25	m	101	DMU	C7-C8-C9	2.57	114.82	110.24
22	J	101	CHD	O7-C7-C6	-2.57	103.58	109.94
22	j	101	CHD	C9-C10-C5	2.56	112.17	108.58
19	d	201	TGL	CG2-OG2-CB1	2.56	124.09	117.79
22	j	101	CHD	C10-C9-C8	2.55	114.55	111.82
19	d	201	TGL	OG2-CG2-CG1	2.54	117.59	108.40
19	d	201	TGL	OG2-CB1-OB1	-2.53	117.58	123.70
22	G	103	CHD	C19-C10-C1	-2.52	104.21	108.26
14	A	602	HEA	CMB-C2B-C1B	2.52	128.87	125.04
14	A	601	HEA	CBA-CAA-C2A	-2.50	108.40	112.60
26	E	201	PSC	C07-N-C05	2.49	120.10	109.92
22	J	101	CHD	C19-C10-C1	-2.48	104.27	108.26
18	A	606	PGV	O03-C19-O04	-2.48	117.34	123.59
14	A	601	HEA	C4B-C3B-C2B	-2.47	103.19	107.41
22	C	301	CHD	C6-C7-C8	2.47	114.11	111.48
18	a	607	PGV	O01-C1-C2	2.46	116.81	111.50
19	l	101	TGL	CG3-OG3-CC1	2.46	126.22	117.12
24	G	102	CDL	OA6-CA5-OA7	-2.44	117.80	123.70
22	J	101	CHD	C11-C12-C13	2.44	113.75	111.24
14	A	602	HEA	CHC-C4B-C3B	-2.44	119.52	125.80
14	A	601	HEA	C25-C23-C24	2.44	119.99	114.60
22	G	103	CHD	C11-C12-C13	2.43	113.74	111.24
14	a	602	HEA	OMA-CMA-C3A	-2.41	119.66	124.91
22	C	301	CHD	C19-C10-C1	-2.41	104.38	108.26
14	A	601	HEA	CHD-C1D-C2D	-2.41	120.06	126.72
22	B	402	CHD	C14-C13-C12	-2.40	105.17	107.40
23	c	301	PEK	O03-C21-C22	2.38	119.37	111.91
22	c	308	CHD	C19-C10-C1	-2.37	104.44	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	402	CHD	O3-C3-C4	-2.37	105.13	109.85
22	j	101	CHD	O7-C7-C8	2.37	114.72	109.43
22	C	306	CHD	C6-C5-C4	-2.36	108.48	111.19
18	c	302	PGV	C01-O03-C19	2.36	125.85	117.12
19	D	201	TGL	OG2-CB1-OB1	-2.36	118.01	123.70
22	B	402	CHD	C6-C7-C8	2.35	113.99	111.48
22	j	101	CHD	C19-C10-C5	-2.34	106.39	110.36
26	b	303	PSC	O01-C02-C01	2.33	116.86	108.40
19	A	608	TGL	OG1-CA1-OA1	-2.33	117.70	123.59
24	g	101	CDL	OA8-CA7-OA9	-2.33	117.71	123.59
22	c	303	CHD	C18-C13-C12	2.32	111.43	109.07
23	G	101	PEK	O01-C1-O02	-2.32	118.11	123.70
22	j	101	CHD	O7-C7-C6	-2.31	104.21	109.94
23	C	307	PEK	O03-C21-C22	2.31	119.16	111.91
14	a	602	HEA	CHA-C4D-ND	-2.31	121.92	124.43
26	E	201	PSC	O01-C1-O02	-2.30	118.15	123.70
14	A	601	HEA	CAD-CBD-CGD	-2.29	108.67	113.60
22	C	301	CHD	C21-C20-C17	2.27	116.40	112.92
14	a	602	HEA	C1B-C2B-C3B	-2.27	104.09	106.80
22	J	101	CHD	C13-C14-C8	2.27	117.64	114.74
24	G	102	CDL	OB6-CB5-OB7	-2.27	118.22	123.70
23	C	302	PEK	O01-C1-O02	-2.26	118.23	123.70
14	a	602	HEA	CHC-C4B-C3B	-2.26	119.97	125.80
14	A	602	HEA	O2A-CGA-CBA	2.26	121.28	114.03
24	c	307	CDL	OA6-CA5-OA7	-2.25	118.26	123.70
24	C	305	CDL	OA8-CA7-OA9	-2.25	117.92	123.59
19	A	609	TGL	OG2-CB1-OB1	-2.24	118.29	123.70
14	a	601	HEA	OMA-CMA-C3A	-2.24	120.03	124.91
14	A	601	HEA	O11-C11-C12	2.24	115.67	109.42
26	E	201	PSC	C06-N-C05	2.24	119.06	109.92
26	E	201	PSC	O03-C19-O04	-2.23	117.96	123.59
14	a	602	HEA	C25-C23-C24	2.22	119.51	114.60
14	a	602	HEA	C27-C19-C20	2.22	119.00	115.27
19	d	201	TGL	OG3-CC1-OC1	-2.22	117.99	123.59
22	C	306	CHD	C18-C13-C12	2.21	111.32	109.07
24	g	101	CDL	OB6-CB5-OB7	-2.21	118.35	123.70
22	C	306	CHD	C21-C20-C17	2.21	116.31	112.92
24	c	307	CDL	OB8-CB7-OB9	-2.21	118.01	123.59
18	c	302	PGV	O01-C1-O02	-2.20	118.38	123.70
23	C	307	PEK	C01-O03-C21	2.20	125.27	117.12
19	A	609	TGL	CG3-OG3-CC1	2.19	125.25	117.12
25	C	308	DMU	O5-C6-C1	2.19	114.99	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a	607	PGV	O03-C19-C20	2.19	118.78	111.91
14	A	602	HEA	CHB-C1B-NB	-2.19	122.05	124.43
23	C	302	PEK	O03-C21-O04	-2.18	118.08	123.59
23	c	304	PEK	O01-C1-O02	-2.18	118.43	123.70
25	c	309	DMU	C10-C5-C7	2.18	114.53	110.00
22	B	402	CHD	C1-C10-C9	2.17	114.77	111.35
14	a	601	HEA	CHD-C1D-C2D	-2.17	120.71	126.72
23	c	305	PEK	O03-C21-O04	-2.17	118.13	123.59
25	C	308	DMU	O7-C3-C2	2.16	113.04	107.28
14	A	602	HEA	C4D-C3D-C2D	-2.16	103.74	106.90
14	A	602	HEA	O1A-CGA-CBA	-2.16	116.14	123.08
22	G	103	CHD	O26-C24-C23	2.16	120.97	114.03
22	J	101	CHD	C19-C10-C5	-2.16	106.70	110.36
14	A	602	HEA	CHA-C4D-C3D	-2.16	121.67	124.84
14	A	601	HEA	CMC-C2C-C1C	-2.16	125.15	128.46
22	j	101	CHD	C13-C17-C20	2.15	122.06	119.50
14	a	602	HEA	C4B-NB-C1B	-2.15	102.86	105.07
22	J	101	CHD	C9-C10-C5	2.14	111.59	108.58
18	a	606	PGV	O01-C1-O02	-2.14	118.53	123.70
23	G	101	PEK	C2-C3-C4	2.14	117.04	113.23
14	a	601	HEA	C25-C23-C24	2.13	119.32	114.60
22	c	308	CHD	C11-C12-C13	2.13	113.43	111.24
25	C	308	DMU	C2-C3-C4	-2.12	106.07	110.93
22	c	303	CHD	C6-C7-C8	2.11	113.74	111.48
22	B	402	CHD	C11-C12-C13	2.11	113.41	111.24
22	J	101	CHD	C18-C13-C12	-2.10	106.93	109.07
22	C	301	CHD	C18-C13-C12	2.09	111.19	109.07
19	A	609	TGL	OG3-CC1-CC2	2.08	118.44	111.91
14	a	601	HEA	CAA-CBA-CGA	-2.08	107.93	113.76
19	D	201	TGL	OG3-CC1-CC2	2.07	118.41	111.91
18	C	304	PGV	O03-C19-O04	-2.07	118.37	123.59
18	C	303	PGV	O01-C1-C2	2.07	115.96	111.50
22	j	101	CHD	C21-C20-C22	-2.07	107.12	110.36
23	c	301	PEK	C01-O03-C21	2.06	124.73	117.12
26	b	303	PSC	C21-C20-C19	-2.05	106.18	113.62
14	A	601	HEA	CAA-CBA-CGA	-2.05	108.02	113.76
22	C	306	CHD	C10-C9-C8	2.03	114.00	111.82
25	m	101	DMU	O1-C10-C5	-2.03	106.04	110.35
19	l	101	TGL	OG1-CA1-OA1	-2.03	118.46	123.59
19	A	609	TGL	OG1-CA1-CA2	2.03	118.29	111.91
14	a	601	HEA	CHC-C4B-C3B	-2.03	120.57	125.80
18	A	607	PGV	O14-P-O13	2.02	122.24	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	601	HEA	O2D-CGD-CBD	2.02	120.52	114.03
18	a	606	PGV	O03-C01-C02	2.02	114.31	108.43
14	A	602	HEA	C25-C23-C24	2.01	119.05	114.60
14	A	602	HEA	C4D-CHA-C1A	2.01	125.21	122.56
18	a	606	PGV	O03-C19-O04	-2.00	118.53	123.59

All (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
14	a	601	HEA	ND
14	a	602	HEA	NB
14	a	602	HEA	ND

All (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
18	c	302	PGV	C03-O11-P-O14
18	c	302	PGV	O12-C04-C05-C06
18	c	302	PGV	O04-C19-O03-C01
18	c	302	PGV	C20-C19-O03-C01
19	D	201	TGL	CB2-CB1-OG2-CG2
19	d	201	TGL	CB2-CB1-OG2-CG2
23	C	307	PEK	O12-C04-C05-N
23	G	101	PEK	C03-O11-P-O13
23	G	101	PEK	C2-C1-O01-C02
23	G	101	PEK	C6-C7-C8-C9
23	c	305	PEK	C03-O11-P-O14
23	c	305	PEK	C04-O12-P-O13
24	C	305	CDL	C1-CA2-OA2-PA1
24	C	305	CDL	CA2-OA2-PA1-OA3
24	C	305	CDL	C11-CA5-OA6-CA4
24	G	102	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
24	G	102	CDL	CA3-OA5-PA1-OA4
24	G	102	CDL	OA7-CA5-OA6-CA4
24	G	102	CDL	C11-CA5-OA6-CA4
24	G	102	CDL	CB3-OB5-PB2-OB4
24	G	102	CDL	C51-CB5-OB6-CB4
24	c	307	CDL	C1-CA2-OA2-PA1
24	c	307	CDL	CA2-OA2-PA1-OA4
24	c	307	CDL	CA3-OA5-PA1-OA2
24	c	307	CDL	CA3-OA5-PA1-OA3
24	c	307	CDL	CA3-OA5-PA1-OA4
24	c	307	CDL	OA7-CA5-OA6-CA4
24	c	307	CDL	C11-CA5-OA6-CA4
24	c	307	CDL	CB3-OB5-PB2-OB3
24	g	101	CDL	OA7-CA5-OA6-CA4
24	g	101	CDL	C11-CA5-OA6-CA4
24	g	101	CDL	CB2-OB2-PB2-OB3
25	c	309	DMU	C1-C6-O16-C18
25	c	309	DMU	O5-C6-O16-C18
26	E	201	PSC	C04-O12-P-O14
26	E	201	PSC	C2-C1-O01-C02
26	b	303	PSC	C01-C02-O01-C1
26	b	303	PSC	O12-C04-C05-N
26	b	303	PSC	O04-C19-O03-C01
26	b	303	PSC	C20-C19-O03-C01
19	b	302	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	CA2-CA1-OG1-CG1
19	A	608	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	OA1-CA1-OG1-CG1
19	d	201	TGL	OA1-CA1-OG1-CG1
24	g	101	CDL	OA9-CA7-OA8-CA6
18	c	302	PGV	O02-C1-O01-C02
19	A	608	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	OB1-CB1-OG2-CG2
19	d	201	TGL	OB1-CB1-OG2-CG2
23	c	305	PEK	O02-C1-O01-C02
24	C	305	CDL	OA7-CA5-OA6-CA4
24	G	102	CDL	OB7-CB5-OB6-CB4
26	E	201	PSC	O02-C1-O01-C02
19	A	608	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CC2-CC1-OG3-CG3
19	b	302	TGL	CC2-CC1-OG3-CG3
19	d	201	TGL	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
24	G	102	CDL	C71-CB7-OB8-CB6
24	g	101	CDL	C31-CA7-OA8-CA6
19	A	608	TGL	CB2-CB1-OG2-CG2
23	c	305	PEK	C2-C1-O01-C02
19	D	201	TGL	OC1-CC1-OG3-CG3
24	C	305	CDL	C31-CA7-OA8-CA6
24	g	101	CDL	C71-CB7-OB8-CB6
23	G	101	PEK	O02-C1-O01-C02
18	a	606	PGV	O04-C19-O03-C01
24	C	305	CDL	OA9-CA7-OA8-CA6
24	G	102	CDL	OB9-CB7-OB8-CB6
24	g	101	CDL	OB9-CB7-OB8-CB6
18	C	304	PGV	O12-C04-C05-O05
18	a	606	PGV	O12-C04-C05-O05
18	c	302	PGV	O12-C04-C05-O05
24	G	102	CDL	O1-C1-CA2-OA2
24	C	305	CDL	C71-CB7-OB8-CB6
26	E	201	PSC	C20-C19-O03-C01
18	c	302	PGV	C2-C1-O01-C02
19	l	101	TGL	CA3-CA4-CA5-CA6
18	c	306	PGV	C27-C28-C29-C30
25	C	308	DMU	O6-C11-C9-O1
19	d	201	TGL	CA1-CA2-CA3-CA4
18	A	607	PGV	C29-C30-C31-C32
19	d	201	TGL	C13-C14-C29-C30
18	a	606	PGV	C20-C19-O03-C01
25	M	101	DMU	O6-C11-C9-O1
25	c	309	DMU	O5-C4-C57-O61
24	C	305	CDL	OB9-CB7-OB8-CB6
26	E	201	PSC	O04-C19-O03-C01
19	d	201	TGL	CC1-CC2-CC3-CC4
22	C	306	CHD	C17-C20-C22-C23
22	j	101	CHD	C17-C20-C22-C23
18	a	606	PGV	O12-C04-C05-C06
22	C	306	CHD	C21-C20-C22-C23
25	M	101	DMU	O6-C11-C9-C8
25	c	309	DMU	C3-C4-C57-O61
24	G	102	CDL	CB5-C51-C52-C53
24	g	101	CDL	OA6-CA4-CA6-OA8
18	C	304	PGV	C1-C2-C3-C4
24	G	102	CDL	C31-CA7-OA8-CA6
24	G	102	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
23	G	101	PEK	C21-C22-C23-C24
24	g	101	CDL	CA7-C31-C32-C33
24	g	101	CDL	CB7-C71-C72-C73
22	J	101	CHD	C13-C17-C20-C22
23	C	302	PEK	C1-C2-C3-C4
23	c	305	PEK	C1-C2-C3-C4
24	C	305	CDL	CB7-C71-C72-C73
24	G	102	CDL	CB7-C71-C72-C73
24	c	307	CDL	CB7-C71-C72-C73
26	b	303	PSC	C19-C20-C21-C22
22	j	101	CHD	C21-C20-C22-C23
18	A	606	PGV	C2-C1-O01-C02
19	b	302	TGL	CA1-CA2-CA3-CA4
19	b	302	TGL	CC1-CC2-CC3-CC4
22	J	101	CHD	C16-C17-C20-C21
24	G	102	CDL	OA9-CA7-OA8-CA6
24	C	305	CDL	C51-CB5-OB6-CB4
18	c	302	PGV	C6-C7-C8-C9
18	A	606	PGV	C03-O11-P-O12
18	C	304	PGV	C03-O11-P-O12
18	c	302	PGV	C03-O11-P-O12
23	c	305	PEK	C04-O12-P-O11
24	C	305	CDL	CA3-OA5-PA1-OA2
24	C	305	CDL	CB2-OB2-PB2-OB5
24	G	102	CDL	CA3-OA5-PA1-OA2
24	G	102	CDL	CB3-OB5-PB2-OB2
24	c	307	CDL	CA2-OA2-PA1-OA5
26	b	303	PSC	C03-O11-P-O12
24	g	101	CDL	CB5-C51-C52-C53
22	J	101	CHD	C13-C17-C20-C21
18	A	606	PGV	O02-C1-O01-C02
24	C	305	CDL	OB7-CB5-OB6-CB4
24	c	307	CDL	C31-CA7-OA8-CA6
19	A	609	TGL	C11-C12-C13-C14
19	A	609	TGL	CB2-CB1-OG2-CG2
23	c	301	PEK	C2-C1-O01-C02
19	A	609	TGL	C12-C13-C14-C29
19	A	609	TGL	CC9-C15-C16-C17
19	A	609	TGL	C16-C17-C18-C19
19	l	101	TGL	CC4-CC5-CC6-CC7
24	c	307	CDL	C63-C64-C65-C66
24	g	101	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
25	m	101	DMU	C19-C22-C25-C28
18	A	607	PGV	C6-C7-C8-C9
18	a	606	PGV	C7-C8-C9-C10
18	a	606	PGV	C26-C27-C28-C29
19	A	609	TGL	C10-C11-C12-C13
19	A	609	TGL	C16-C15-CC9-CC8
19	d	201	TGL	CA4-CA5-CA6-CA7
23	C	302	PEK	C30-C31-C32-C33
23	c	305	PEK	C28-C29-C30-C31
24	G	102	CDL	C79-C80-C81-C82
24	G	102	CDL	C83-C84-C85-C86
19	d	201	TGL	CG1-CG2-OG2-CB1
19	A	609	TGL	OB1-CB1-OG2-CG2
23	c	301	PEK	O02-C1-O01-C02
24	C	305	CDL	C41-C42-C43-C44
24	C	305	CDL	C53-C54-C55-C56
24	C	305	CDL	C57-C58-C59-C60
24	c	307	CDL	C39-C40-C41-C42
24	c	307	CDL	C78-C79-C80-C81
18	A	607	PGV	C4-C5-C6-C7
19	b	302	TGL	C16-C17-C18-C19
19	d	201	TGL	C23-C24-C25-C26
23	c	301	PEK	C29-C30-C31-C32
24	G	102	CDL	C14-C15-C16-C17
24	G	102	CDL	C19-C20-C21-C22
25	C	308	DMU	O6-C11-C9-C8
18	c	302	PGV	C23-C24-C25-C26
18	c	302	PGV	C24-C25-C26-C27
23	G	101	PEK	C28-C29-C30-C31
24	G	102	CDL	C22-C23-C24-C25
19	A	609	TGL	CC1-CC2-CC3-CC4
19	D	201	TGL	CA1-CA2-CA3-CA4
18	c	302	PGV	C20-C21-C22-C23
19	D	201	TGL	CA9-C20-C21-C22
24	c	307	CDL	OA9-CA7-OA8-CA6
18	A	606	PGV	C5-C6-C7-C8
19	A	608	TGL	CB7-CB8-CB9-C10
19	d	201	TGL	C16-C17-C18-C19
19	b	302	TGL	CA3-CA4-CA5-CA6
19	b	302	TGL	CB2-CB3-CB4-CB5
19	b	302	TGL	CB3-CB4-CB5-CB6
19	l	101	TGL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	l	101	TGL	CC5-CC6-CC7-CC8
19	l	101	TGL	C17-C18-C19-C33
23	c	305	PEK	C25-C26-C27-C28
24	C	305	CDL	C61-C62-C63-C64
18	C	304	PGV	C7-C8-C9-C10
19	A	608	TGL	C19-C33-C34-C35
23	C	302	PEK	C22-C23-C24-C25
24	G	102	CDL	C75-C76-C77-C78
18	A	606	PGV	C7-C8-C9-C10
18	C	304	PGV	C30-C31-C32-C33
19	D	201	TGL	CA4-CA5-CA6-CA7
19	D	201	TGL	C24-C25-C26-C27
23	C	307	PEK	C29-C30-C31-C32
24	c	307	CDL	C11-C12-C13-C14
18	c	306	PGV	C19-C20-C21-C22
19	A	608	TGL	C24-C25-C26-C27
23	c	304	PEK	C24-C25-C26-C27
23	c	305	PEK	C29-C30-C31-C32
24	G	102	CDL	C37-C38-C39-C40
24	c	307	CDL	C74-C75-C76-C77
24	g	101	CDL	C22-C23-C24-C25
25	M	101	DMU	C28-C31-C34-C37
26	E	201	PSC	C04-C05-N-C06
24	G	102	CDL	C11-C12-C13-C14
18	c	302	PGV	C5-C6-C7-C8
19	D	201	TGL	C18-C19-C33-C34
19	d	201	TGL	C21-C20-CA9-CA8
23	C	307	PEK	C31-C32-C33-C34
23	c	301	PEK	C34-C35-C36-C37
24	c	307	CDL	C35-C36-C37-C38
18	a	607	PGV	C19-C20-C21-C22
18	C	304	PGV	C20-C21-C22-C23
23	c	304	PEK	C34-C35-C36-C37
19	l	101	TGL	CA2-CA1-OG1-CG1
19	A	609	TGL	CA9-C20-C21-C22
19	D	201	TGL	C11-C12-C13-C14
24	G	102	CDL	C40-C41-C42-C43
24	G	102	CDL	C54-C55-C56-C57
24	g	101	CDL	C31-C32-C33-C34
25	c	309	DMU	C19-C18-O16-C6
18	C	304	PGV	C13-C14-C15-C16
18	C	304	PGV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
18	C	304	PGV	C27-C28-C29-C30
19	A	608	TGL	C16-C17-C18-C19
19	A	608	TGL	CA9-C20-C21-C22
19	A	609	TGL	CB2-CB3-CB4-CB5
23	c	301	PEK	C24-C25-C26-C27
24	C	305	CDL	C40-C41-C42-C43
26	E	201	PSC	C21-C22-C23-C24
18	c	302	PGV	C7-C8-C9-C10
19	d	201	TGL	CA6-CA7-CA8-CA9
23	G	101	PEK	C16-C17-C18-C19
24	c	307	CDL	C40-C41-C42-C43
18	c	306	PGV	C7-C8-C9-C10
19	D	201	TGL	CA2-CA3-CA4-CA5
24	g	101	CDL	C80-C81-C82-C83
26	E	201	PSC	C2-C3-C4-C5
18	A	607	PGV	C19-C20-C21-C22
19	l	101	TGL	C15-C16-C17-C18
19	b	302	TGL	CA2-CA1-OG1-CG1
19	l	101	TGL	CB2-CB1-OG2-CG2
18	a	606	PGV	C3-C4-C5-C6
24	c	307	CDL	C54-C55-C56-C57
25	c	309	DMU	C22-C25-C28-C31
18	C	304	PGV	O05-C05-C06-O06
18	c	302	PGV	C14-C15-C16-C17
23	C	302	PEK	C31-C32-C33-C34
23	c	305	PEK	C30-C31-C32-C33
24	g	101	CDL	C16-C17-C18-C19
26	E	201	PSC	C23-C24-C25-C26
18	A	606	PGV	C11-C10-C9-C8
18	A	606	PGV	C12-C13-C14-C15
18	A	607	PGV	C12-C13-C14-C15
24	c	307	CDL	C43-C44-C45-C46
24	c	307	CDL	C56-C57-C58-C59
23	C	307	PEK	C27-C28-C29-C30
19	b	302	TGL	CA9-C20-C21-C22
23	C	302	PEK	C26-C27-C28-C29
19	l	101	TGL	OB1-CB1-OG2-CG2
18	C	303	PGV	C7-C8-C9-C10
19	b	302	TGL	C20-C21-C22-C23
19	d	201	TGL	CB7-CB8-CB9-C10
19	d	201	TGL	CA9-C20-C21-C22
19	b	302	TGL	C16-C15-CC9-CC8

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Mol	Chain	Res	Type	Atoms
18	C	304	PGV	C29-C30-C31-C32
18	c	302	PGV	C4-C5-C6-C7
24	C	305	CDL	C36-C37-C38-C39
23	c	304	PEK	C1-C2-C3-C4
19	d	201	TGL	C18-C19-C33-C34
19	b	302	TGL	OA1-CA1-OG1-CG1
19	l	101	TGL	OA1-CA1-OG1-CG1
18	C	304	PGV	C11-C10-C9-C8
19	A	609	TGL	C23-C24-C25-C26
19	D	201	TGL	C21-C22-C23-C24
18	a	607	PGV	C7-C8-C9-C10
19	d	201	TGL	C11-C12-C13-C14
19	l	101	TGL	CA2-CA3-CA4-CA5
24	C	305	CDL	C79-C80-C81-C82
24	G	102	CDL	C56-C57-C58-C59
18	C	303	PGV	C19-C20-C21-C22
19	A	609	TGL	CB4-CB5-CB6-CB7
19	l	101	TGL	CB6-CB7-CB8-CB9
19	l	101	TGL	CC3-CC4-CC5-CC6
19	A	608	TGL	C13-C14-C29-C30
23	c	301	PEK	C23-C24-C25-C26
18	C	304	PGV	C4-C5-C6-C7
19	A	608	TGL	CC4-CC5-CC6-CC7
19	l	101	TGL	CA4-CA5-CA6-CA7
19	l	101	TGL	CB3-CB4-CB5-CB6
24	G	102	CDL	C32-C33-C34-C35
24	g	101	CDL	C35-C36-C37-C38
24	C	305	CDL	CA5-C11-C12-C13
24	g	101	CDL	C51-CB5-OB6-CB4
24	c	307	CDL	OB7-CB5-OB6-CB4
19	b	302	TGL	OG1-CG1-CG2-OG2
19	l	101	TGL	OG1-CG1-CG2-OG2
23	c	305	PEK	O03-C01-C02-O01
19	A	608	TGL	CB6-CB7-CB8-CB9
19	D	201	TGL	C16-C17-C18-C19
23	C	307	PEK	C28-C29-C30-C31
24	G	102	CDL	C33-C34-C35-C36
24	G	102	CDL	C58-C59-C60-C61
18	A	607	PGV	C11-C10-C9-C8
18	C	303	PGV	C11-C10-C9-C8
23	c	305	PEK	C15-C16-C17-C18
18	c	306	PGV	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
19	l	101	TGL	C14-C29-C30-C31
24	g	101	CDL	C36-C37-C38-C39
24	G	102	CDL	C34-C35-C36-C37
18	C	304	PGV	C3-C4-C5-C6
18	c	302	PGV	C29-C30-C31-C32
24	C	305	CDL	C56-C57-C58-C59
24	G	102	CDL	C81-C82-C83-C84
26	b	303	PSC	C22-C23-C24-C25
23	c	304	PEK	C2-C1-O01-C02
24	c	307	CDL	C51-CB5-OB6-CB4
19	A	609	TGL	CA6-CA7-CA8-CA9
19	A	609	TGL	C17-C18-C19-C33
18	c	302	PGV	C04-O12-P-O11
23	G	101	PEK	C03-O11-P-O12
23	c	305	PEK	C03-O11-P-O12
18	a	607	PGV	C5-C6-C7-C8
26	b	303	PSC	C23-C24-C25-C26
19	d	201	TGL	CC2-CC1-OG3-CG3
24	c	307	CDL	OA5-CA3-CA4-CA6
22	j	101	CHD	C13-C17-C20-C21
19	l	101	TGL	C11-C12-C13-C14
18	C	303	PGV	C24-C25-C26-C27
19	d	201	TGL	CB6-CB7-CB8-CB9
24	C	305	CDL	C34-C35-C36-C37
24	G	102	CDL	C20-C21-C22-C23
19	l	101	TGL	CC1-CC2-CC3-CC4
23	C	307	PEK	C22-C23-C24-C25
24	g	101	CDL	C73-C74-C75-C76
18	a	606	PGV	C22-C23-C24-C25
24	c	307	CDL	C81-C82-C83-C84
18	a	607	PGV	C23-C24-C25-C26
18	C	304	PGV	O03-C01-C02-C03
19	D	201	TGL	OG1-CG1-CG2-CG3
19	b	302	TGL	OG1-CG1-CG2-CG3
19	d	201	TGL	OG1-CG1-CG2-CG3
19	d	201	TGL	CG1-CG2-CG3-OG3
24	C	305	CDL	CB3-CB4-CB6-OB8
24	g	101	CDL	CA3-CA4-CA6-OA8
24	g	101	CDL	C42-C43-C44-C45
18	A	606	PGV	C2-C3-C4-C5
19	D	201	TGL	CC6-CC7-CC8-CC9
19	l	101	TGL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	c	305	PEK	C23-C24-C25-C26
18	A	606	PGV	C29-C30-C31-C32
18	a	607	PGV	C29-C30-C31-C32
19	D	201	TGL	CC5-CC6-CC7-CC8
24	c	307	CDL	C64-C65-C66-C67
18	c	302	PGV	C30-C31-C32-C33
23	G	101	PEK	C34-C35-C36-C37
18	a	606	PGV	C4-C5-C6-C7
19	b	302	TGL	CC2-CC3-CC4-CC5
23	C	302	PEK	C2-C3-C4-C5
23	G	101	PEK	C2-C3-C4-C5
23	c	301	PEK	C15-C16-C17-C18
23	c	304	PEK	C2-C3-C4-C5
18	A	606	PGV	C14-C15-C16-C17
19	A	608	TGL	CA7-CA8-CA9-C20
19	d	201	TGL	CB5-CB6-CB7-CB8
24	C	305	CDL	C83-C84-C85-C86
24	c	307	CDL	C55-C56-C57-C58
24	g	101	CDL	C53-C54-C55-C56
23	C	302	PEK	C17-C18-C19-C20
26	b	303	PSC	C28-C29-C30-C31
23	G	101	PEK	C25-C26-C27-C28
18	C	303	PGV	C22-C23-C24-C25
19	A	608	TGL	C15-C16-C17-C18
19	D	201	TGL	CB7-CB8-CB9-C10
19	b	302	TGL	C11-C12-C13-C14
24	g	101	CDL	C72-C73-C74-C75
19	d	201	TGL	OC1-CC1-OG3-CG3
26	b	303	PSC	C04-C05-N-C07
18	A	606	PGV	C4-C5-C6-C7
19	D	201	TGL	C12-C13-C14-C29
19	b	302	TGL	C13-C14-C29-C30
18	c	302	PGV	C12-C13-C14-C15
19	d	201	TGL	CC4-CC5-CC6-CC7
24	g	101	CDL	C76-C77-C78-C79
18	C	304	PGV	O03-C01-C02-O01
19	A	608	TGL	C29-C30-C31-C32
19	d	201	TGL	CA3-CA4-CA5-CA6
19	d	201	TGL	C21-C22-C23-C24
23	G	101	PEK	C17-C18-C19-C20
24	g	101	CDL	OB7-CB5-OB6-CB4
18	C	304	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
19	A	609	TGL	CC3-CC4-CC5-CC6
23	C	302	PEK	C34-C35-C36-C37
26	b	303	PSC	C15-C16-C17-C18
26	b	303	PSC	C31-C32-C33-C34
24	C	305	CDL	C24-C25-C26-C27
18	c	302	PGV	C22-C23-C24-C25
19	A	609	TGL	C20-C21-C22-C23
19	D	201	TGL	C13-C14-C29-C30
19	d	201	TGL	CB3-CB4-CB5-CB6
24	c	307	CDL	C20-C21-C22-C23
18	c	302	PGV	C9-C10-C11-C12
24	G	102	CDL	C24-C25-C26-C27
18	A	606	PGV	C01-C02-C03-O11
23	G	101	PEK	C01-C02-C03-O11
23	c	301	PEK	C01-C02-C03-O11
24	C	305	CDL	OB5-CB3-CB4-CB6
24	g	101	CDL	OA5-CA3-CA4-CA6
24	g	101	CDL	OB5-CB3-CB4-CB6
24	c	307	CDL	C18-C19-C20-C21
23	G	101	PEK	O12-C04-C05-N
23	c	304	PEK	O12-C04-C05-N
23	c	305	PEK	O12-C04-C05-N
18	a	606	PGV	C13-C14-C15-C16
24	g	101	CDL	C43-C44-C45-C46
19	l	101	TGL	CB1-CB2-CB3-CB4
25	m	101	DMU	C34-C37-C40-C43
19	b	302	TGL	C25-C26-C27-C28
19	A	608	TGL	CB9-C10-C11-C12
19	A	608	TGL	CA4-CA5-CA6-CA7
23	c	305	PEK	C02-C03-O11-P
23	G	101	PEK	C26-C27-C28-C29
24	g	101	CDL	C32-C33-C34-C35
18	c	306	PGV	C31-C32-C33-C34
24	c	307	CDL	C23-C24-C25-C26
19	A	609	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CA7-CA8-CA9-C20
19	l	101	TGL	CB9-C10-C11-C12
24	C	305	CDL	C13-C14-C15-C16
19	A	608	TGL	CG1-CG2-CG3-OG3
19	l	101	TGL	OG1-CG1-CG2-CG3
23	c	305	PEK	O03-C01-C02-C03
24	G	102	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
23	c	304	PEK	O02-C1-O01-C02
24	C	305	CDL	C37-C38-C39-C40
23	c	304	PEK	C23-C24-C25-C26
18	a	606	PGV	C24-C25-C26-C27
18	C	303	PGV	C1-C2-C3-C4
19	d	201	TGL	C33-C34-C35-C36
18	C	303	PGV	C13-C14-C15-C16
18	A	607	PGV	C5-C6-C7-C8
19	D	201	TGL	CA5-CA6-CA7-CA8
23	C	302	PEK	C11-C10-C9-C8
23	C	302	PEK	C9-C10-C11-C12
23	C	307	PEK	C5-C6-C7-C8
23	C	307	PEK	C12-C13-C14-C15
23	G	101	PEK	C5-C6-C7-C8
23	G	101	PEK	C9-C10-C11-C12
23	c	301	PEK	C11-C10-C9-C8
23	c	301	PEK	C11-C12-C13-C14
23	c	301	PEK	C12-C13-C14-C15
23	c	304	PEK	C12-C13-C14-C15
23	c	305	PEK	C5-C6-C7-C8
23	c	301	PEK	C1-C2-C3-C4
23	G	101	PEK	C35-C36-C37-C38
24	g	101	CDL	C63-C64-C65-C66
18	A	606	PGV	O01-C02-C03-O11
24	c	307	CDL	OA5-CA3-CA4-OA6
24	g	101	CDL	OA5-CA3-CA4-OA6
18	c	306	PGV	C29-C30-C31-C32
19	A	609	TGL	CA5-CA6-CA7-CA8
19	d	201	TGL	CC5-CC6-CC7-CC8
18	c	302	PGV	O03-C01-C02-O01
19	A	608	TGL	OG2-CG2-CG3-OG3
19	d	201	TGL	OG2-CG2-CG3-OG3
26	b	303	PSC	O03-C01-C02-O01
19	A	609	TGL	C29-C30-C31-C32
19	l	101	TGL	C25-C26-C27-C28
24	C	305	CDL	C33-C34-C35-C36
24	C	305	CDL	C81-C82-C83-C84
26	b	303	PSC	O02-C1-O01-C02
18	c	302	PGV	C27-C28-C29-C30
19	D	201	TGL	C22-C23-C24-C25
24	G	102	CDL	C61-C62-C63-C64
24	g	101	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
24	g	101	CDL	C1-CA2-OA2-PA1
18	a	606	PGV	C11-C10-C9-C8
19	l	101	TGL	CC6-CC7-CC8-CC9
19	b	302	TGL	C12-C13-C14-C29
19	b	302	TGL	CC7-CC8-CC9-C15
23	C	307	PEK	C30-C31-C32-C33
23	G	101	PEK	C31-C32-C33-C34
23	C	302	PEK	C2-C1-O01-C02
26	b	303	PSC	C2-C1-O01-C02
23	C	302	PEK	C28-C29-C30-C31
24	G	102	CDL	C84-C85-C86-C87
19	D	201	TGL	CC3-CC4-CC5-CC6
19	b	302	TGL	C21-C20-CA9-CA8
19	A	609	TGL	C14-C29-C30-C31
24	c	307	CDL	C51-C52-C53-C54
18	A	607	PGV	C7-C8-C9-C10
18	a	606	PGV	C28-C29-C30-C31
18	C	304	PGV	C24-C25-C26-C27
18	C	304	PGV	C31-C32-C33-C34
24	c	307	CDL	C42-C43-C44-C45
23	c	304	PEK	C25-C26-C27-C28
18	c	306	PGV	C02-C03-O11-P
24	c	307	CDL	CA3-CA4-CA6-OA8
24	c	307	CDL	CB3-CB4-CB6-OB8
23	G	101	PEK	O01-C02-C03-O11
23	c	301	PEK	O01-C02-C03-O11
24	C	305	CDL	OB5-CB3-CB4-OB6
26	E	201	PSC	O01-C02-C03-O11
19	d	201	TGL	C11-C10-CB9-CB8
23	c	305	PEK	C24-C25-C26-C27
24	c	307	CDL	C17-C18-C19-C20
23	C	302	PEK	C24-C25-C26-C27
19	b	302	TGL	C19-C33-C34-C35
19	d	201	TGL	OG1-CG1-CG2-OG2
19	l	101	TGL	OG2-CG2-CG3-OG3
23	C	307	PEK	O03-C01-C02-O01
24	G	102	CDL	OB6-CB4-CB6-OB8
24	g	101	CDL	OB6-CB4-CB6-OB8
19	A	609	TGL	OC1-CC1-OG3-CG3
24	C	305	CDL	C77-C78-C79-C80
18	c	302	PGV	C11-C10-C9-C8
19	b	302	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
23	C	302	PEK	O02-C1-O01-C02
24	c	307	CDL	C37-C38-C39-C40
19	A	609	TGL	C24-C25-C26-C27
19	D	201	TGL	C10-C11-C12-C13
24	G	102	CDL	C35-C36-C37-C38
19	l	101	TGL	CC7-CC8-CC9-C15
23	c	304	PEK	C16-C17-C18-C19
25	c	309	DMU	O6-C11-C9-O1
25	m	101	DMU	O16-C18-C19-C22
19	l	101	TGL	CB4-CB5-CB6-CB7
18	C	304	PGV	C04-O12-P-O11
24	C	305	CDL	CA2-OA2-PA1-OA5
24	g	101	CDL	CA2-OA2-PA1-OA5
18	C	303	PGV	C02-C03-O11-P
18	A	606	PGV	C03-O11-P-O13
18	C	304	PGV	C03-O11-P-O13
18	c	302	PGV	C04-O12-P-O14
23	G	101	PEK	C03-O11-P-O14
24	C	305	CDL	CA3-OA5-PA1-OA3
24	C	305	CDL	CA3-OA5-PA1-OA4
24	C	305	CDL	CB2-OB2-PB2-OB3
24	C	305	CDL	CB2-OB2-PB2-OB4
24	c	307	CDL	CA2-OA2-PA1-OA3
26	b	303	PSC	C03-O11-P-O13
26	E	201	PSC	C01-C02-C03-O11
19	b	302	TGL	CA6-CA7-CA8-CA9
23	C	307	PEK	C05-C04-O12-P
18	A	606	PGV	C1-C2-C3-C4
23	c	301	PEK	C21-C22-C23-C24
18	c	302	PGV	C3-C4-C5-C6
22	j	101	CHD	C16-C17-C20-C22
18	a	606	PGV	C20-C21-C22-C23
19	A	608	TGL	C21-C20-CA9-CA8
24	g	101	CDL	OB5-CB3-CB4-OB6
19	D	201	TGL	CC7-CC8-CC9-C15
23	c	301	PEK	C30-C31-C32-C33
24	g	101	CDL	C17-C18-C19-C20
19	l	101	TGL	OG2-CB1-CB2-CB3
18	a	607	PGV	C4-C5-C6-C7
19	b	302	TGL	CB2-CB1-OG2-CG2
24	g	101	CDL	C12-C13-C14-C15
23	c	304	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
18	c	302	PGV	O03-C01-C02-C03
26	E	201	PSC	O12-C04-C05-N
19	D	201	TGL	OG1-CG1-CG2-OG2
24	c	307	CDL	OB6-CB4-CB6-OB8
19	d	201	TGL	CB2-CB3-CB4-CB5
24	g	101	CDL	C61-C62-C63-C64
24	C	305	CDL	C42-C43-C44-C45
18	C	303	PGV	C28-C29-C30-C31
19	d	201	TGL	CC2-CC3-CC4-CC5
24	G	102	CDL	C74-C75-C76-C77
18	c	306	PGV	C20-C21-C22-C23
19	A	608	TGL	CC6-CC7-CC8-CC9
18	a	607	PGV	C30-C31-C32-C33
24	g	101	CDL	C33-C34-C35-C36
23	C	302	PEK	O03-C21-C22-C23
23	C	302	PEK	C33-C34-C35-C36
19	A	608	TGL	C22-C23-C24-C25
19	A	609	TGL	CG1-CG2-OG2-CB1
18	A	606	PGV	C21-C22-C23-C24
19	l	101	TGL	CA6-CA7-CA8-CA9
18	a	606	PGV	C5-C6-C7-C8
19	A	609	TGL	CA3-CA4-CA5-CA6
24	C	305	CDL	C12-C13-C14-C15
19	A	608	TGL	CC7-CC8-CC9-C15
19	b	302	TGL	C29-C30-C31-C32
24	C	305	CDL	OB6-CB4-CB6-OB8
18	a	606	PGV	C04-O12-P-O11
23	C	307	PEK	C04-O12-P-O11
23	G	101	PEK	C04-O12-P-O11
23	c	301	PEK	C03-O11-P-O12
23	c	301	PEK	C04-O12-P-O11
24	G	102	CDL	CB2-OB2-PB2-OB5
24	c	307	CDL	CB3-OB5-PB2-OB2
24	g	101	CDL	CA3-OA5-PA1-OA2
24	g	101	CDL	CB2-OB2-PB2-OB5
24	g	101	CDL	CB3-OB5-PB2-OB2
26	E	201	PSC	C03-O11-P-O12
26	E	201	PSC	C04-O12-P-O11
26	b	303	PSC	C04-O12-P-O11
19	l	101	TGL	CG1-CG2-CG3-OG3
26	b	303	PSC	O03-C01-C02-C03
19	d	201	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
24	g	101	CDL	C59-C60-C61-C62
18	C	303	PGV	C31-C32-C33-C34
25	m	101	DMU	C28-C31-C34-C37
19	D	201	TGL	C29-C30-C31-C32
19	A	609	TGL	C33-C34-C35-C36
23	c	305	PEK	C17-C18-C19-C20
26	E	201	PSC	C7-C8-C9-C10
24	c	307	CDL	C14-C15-C16-C17
19	l	101	TGL	CA1-CA2-CA3-CA4
18	a	607	PGV	C12-C13-C14-C15
14	A	602	HEA	CAA-CBA-CGA-O1A
18	a	607	PGV	C27-C28-C29-C30
24	c	307	CDL	C60-C61-C62-C63
23	G	101	PEK	C3-C4-C5-C6
14	A	601	HEA	CAD-CBD-CGD-O1D
22	c	308	CHD	C22-C23-C24-O25
19	A	609	TGL	C25-C26-C27-C28
19	A	608	TGL	C12-C13-C14-C29
25	M	101	DMU	C19-C22-C25-C28
24	c	307	CDL	C38-C39-C40-C41
18	a	606	PGV	C15-C16-C17-C18
22	j	101	CHD	C22-C23-C24-O25
22	B	402	CHD	C22-C23-C24-O25
19	A	608	TGL	CA2-CA3-CA4-CA5
18	C	303	PGV	C05-C04-O12-P
26	b	303	PSC	C02-C03-O11-P
24	g	101	CDL	C74-C75-C76-C77
25	M	101	DMU	C22-C25-C28-C31
26	b	303	PSC	C30-C31-C32-C33
14	a	601	HEA	CAD-CBD-CGD-O1D
19	A	609	TGL	CC7-CC8-CC9-C15
23	C	307	PEK	C17-C18-C19-C20
24	G	102	CDL	C39-C40-C41-C42
19	A	609	TGL	C18-C19-C33-C34
24	g	101	CDL	CB3-CB4-CB6-OB8
22	J	101	CHD	C22-C23-C24-O25
23	C	307	PEK	C34-C35-C36-C37
24	C	305	CDL	CA3-CA4-OA6-CA5
24	C	305	CDL	CA6-CA4-OA6-CA5
26	b	303	PSC	C26-C27-C28-C29
26	E	201	PSC	C12-C13-C14-C15
23	C	302	PEK	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	C	307	PEK	C11-C10-C9-C8
23	c	301	PEK	C6-C7-C8-C9
23	c	304	PEK	C5-C6-C7-C8
23	c	304	PEK	C9-C10-C11-C12
23	c	305	PEK	C11-C10-C9-C8
22	G	103	CHD	C22-C23-C24-O26
24	C	305	CDL	C22-C23-C24-C25
22	G	103	CHD	C22-C23-C24-O25
24	G	102	CDL	C12-C13-C14-C15
18	C	304	PGV	C01-C02-C03-O11
14	a	601	HEA	CAD-CBD-CGD-O2D
22	B	402	CHD	C22-C23-C24-O26
18	A	607	PGV	C25-C26-C27-C28
14	A	601	HEA	CAD-CBD-CGD-O2D
19	b	302	TGL	CC6-CC7-CC8-CC9
24	G	102	CDL	C16-C17-C18-C19
24	g	101	CDL	C60-C61-C62-C63
18	c	302	PGV	C13-C14-C15-C16
19	b	302	TGL	CB4-CB5-CB6-CB7
23	c	301	PEK	C27-C28-C29-C30
24	G	102	CDL	C64-C65-C66-C67
14	A	602	HEA	CAA-CBA-CGA-O2A
14	a	602	HEA	CAD-CBD-CGD-O2D
22	c	308	CHD	C22-C23-C24-O26
22	j	101	CHD	C22-C23-C24-O26
24	g	101	CDL	C11-C12-C13-C14
24	C	305	CDL	C39-C40-C41-C42
26	E	201	PSC	C30-C31-C32-C33
24	G	102	CDL	C36-C37-C38-C39
18	A	606	PGV	O04-C19-O03-C01
23	c	301	PEK	C32-C33-C34-C35
14	a	602	HEA	CAA-CBA-CGA-O1A
24	C	305	CDL	C32-C31-CA7-OA8
18	a	607	PGV	C26-C27-C28-C29
23	C	307	PEK	O03-C01-C02-C03
14	A	602	HEA	CAD-CBD-CGD-O1D
24	C	305	CDL	C20-C21-C22-C23
26	E	201	PSC	C26-C27-C28-C29
24	G	102	CDL	OB5-CB3-CB4-OB6
23	G	101	PEK	C1-C2-C3-C4
24	G	102	CDL	C38-C39-C40-C41
22	J	101	CHD	C22-C23-C24-O26

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Mol	Chain	Res	Type	Atoms
24	g	101	CDL	C52-C51-CB5-OB6
24	G	102	CDL	C44-C45-C46-C47
18	A	607	PGV	C13-C14-C15-C16
19	A	608	TGL	CB4-CB5-CB6-CB7
23	c	304	PEK	O03-C21-C22-C23
19	l	101	TGL	C24-C25-C26-C27
18	A	606	PGV	C20-C19-O03-C01
18	a	607	PGV	C11-C12-C13-C14
14	A	602	HEA	CAD-CBD-CGD-O2D
19	A	609	TGL	OG2-CB1-CB2-CB3
19	A	609	TGL	CB9-C10-C11-C12
24	C	305	CDL	C18-C19-C20-C21
24	c	307	CDL	C76-C77-C78-C79
23	c	301	PEK	C14-C15-C16-C17
24	C	305	CDL	C52-C51-CB5-OB6
24	g	101	CDL	C72-C71-CB7-OB8
14	A	601	HEA	C26-C15-C16-C17
24	g	101	CDL	C40-C41-C42-C43
18	A	607	PGV	C9-C10-C11-C12
18	C	303	PGV	C11-C12-C13-C14
18	c	302	PGV	C11-C12-C13-C14
18	c	306	PGV	C9-C10-C11-C12
26	b	303	PSC	C12-C13-C14-C15
24	G	102	CDL	C17-C18-C19-C20
23	C	302	PEK	C25-C26-C27-C28
18	A	606	PGV	C6-C7-C8-C9
18	c	302	PGV	O01-C1-C2-C3
19	d	201	TGL	OG2-CB1-CB2-CB3
18	a	606	PGV	C6-C7-C8-C9
26	E	201	PSC	C3-C4-C5-C6
24	c	307	CDL	C12-C11-CA5-OA6
19	A	608	TGL	C10-C11-C12-C13
24	g	101	CDL	C81-C82-C83-C84
23	c	305	PEK	C3-C4-C5-C6
19	A	608	TGL	C20-C21-C22-C23
24	g	101	CDL	C79-C80-C81-C82
24	C	305	CDL	C73-C74-C75-C76
19	b	302	TGL	OG1-CA1-CA2-CA3
18	c	306	PGV	C30-C31-C32-C33
18	A	606	PGV	C9-C10-C11-C12
18	a	607	PGV	C9-C10-C11-C12
23	c	301	PEK	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	E	201	PSC	O03-C19-C20-C21
24	g	101	CDL	C84-C85-C86-C87
19	A	609	TGL	CB7-CB8-CB9-C10
23	G	101	PEK	O03-C01-C02-O01
18	A	606	PGV	C11-C12-C13-C14
23	C	307	PEK	C14-C15-C16-C17
19	A	608	TGL	CB3-CB4-CB5-CB6
19	A	609	TGL	OG3-CC1-CC2-CC3
23	c	305	PEK	O01-C1-C2-C3
24	G	102	CDL	C72-C71-CB7-OB8
14	a	602	HEA	CAA-CBA-CGA-O2A
14	a	602	HEA	CAD-CBD-CGD-O1D
18	c	306	PGV	C11-C12-C13-C14
26	b	303	PSC	C7-C8-C9-C10
19	A	609	TGL	OB1-CB1-CB2-CB3
24	g	101	CDL	C72-C71-CB7-OB9
19	b	302	TGL	C24-C25-C26-C27
18	C	303	PGV	C26-C27-C28-C29
18	C	304	PGV	C5-C6-C7-C8
24	g	101	CDL	C34-C35-C36-C37
18	a	606	PGV	C9-C10-C11-C12
18	a	606	PGV	C29-C30-C31-C32
24	C	305	CDL	C52-C51-CB5-OB7
19	A	608	TGL	C14-C29-C30-C31
19	d	201	TGL	C19-C33-C34-C35
24	G	102	CDL	C82-C83-C84-C85
24	c	307	CDL	C13-C14-C15-C16
24	G	102	CDL	C63-C64-C65-C66
26	E	201	PSC	O04-C19-C20-C21
23	c	305	PEK	C14-C15-C16-C17
24	c	307	CDL	C12-C11-CA5-OA7
22	c	303	CHD	C22-C23-C24-O26
19	A	609	TGL	CG1-CG2-CG3-OG3
24	c	307	CDL	C52-C51-CB5-OB6
26	E	201	PSC	C02-C01-O03-C19
24	c	307	CDL	C82-C83-C84-C85
18	a	606	PGV	O03-C19-C20-C21
14	A	601	HEA	CAA-CBA-CGA-O2A
19	A	609	TGL	CC6-CC7-CC8-CC9
18	a	606	PGV	C04-O12-P-O13
23	c	301	PEK	C03-O11-P-O14
23	c	301	PEK	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
24	G	102	CDL	CB2-OB2-PB2-OB3
24	g	101	CDL	CB3-OB5-PB2-OB3
26	E	201	PSC	C03-O11-P-O14
26	b	303	PSC	C04-O12-P-O14
18	a	606	PGV	C1-C2-C3-C4
24	G	102	CDL	C51-C52-C53-C54
18	a	606	PGV	C23-C24-C25-C26
18	c	302	PGV	O02-C1-C2-C3
23	C	302	PEK	O01-C1-C2-C3
19	d	201	TGL	OB1-CB1-CB2-CB3
19	A	608	TGL	C33-C34-C35-C36
18	a	606	PGV	C21-C22-C23-C24
19	b	302	TGL	OA1-CA1-CA2-CA3
19	A	608	TGL	CC3-CC4-CC5-CC6
19	A	609	TGL	CA4-CA5-CA6-CA7
22	c	303	CHD	C22-C23-C24-O25
19	A	609	TGL	CG3-CG2-OG2-CB1
23	c	305	PEK	O02-C1-C2-C3
26	b	303	PSC	C29-C30-C31-C32
23	c	304	PEK	O01-C1-C2-C3
24	c	307	CDL	CB5-C51-C52-C53
24	c	307	CDL	C52-C51-CB5-OB7
22	j	101	CHD	C13-C17-C20-C22
18	A	607	PGV	O03-C19-C20-C21
18	c	302	PGV	C25-C26-C27-C28
19	A	609	TGL	OC1-CC1-CC2-CC3
24	c	307	CDL	CB2-C1-CA2-OA2
19	b	302	TGL	CC4-CC5-CC6-CC7
14	a	602	HEA	C26-C15-C16-C17
14	A	601	HEA	CAA-CBA-CGA-O1A
14	a	601	HEA	CAA-CBA-CGA-O1A
18	A	606	PGV	O01-C1-C2-C3
23	C	302	PEK	C3-C4-C5-C6
18	a	606	PGV	O04-C19-C20-C21
23	C	302	PEK	O02-C1-C2-C3
23	C	307	PEK	O01-C1-C2-C3
23	G	101	PEK	O01-C1-C2-C3
24	G	102	CDL	C72-C71-CB7-OB9
25	M	101	DMU	C34-C37-C40-C43
22	j	101	CHD	C16-C17-C20-C21
24	c	307	CDL	O1-C1-CA2-OA2
18	A	607	PGV	O04-C19-C20-C21

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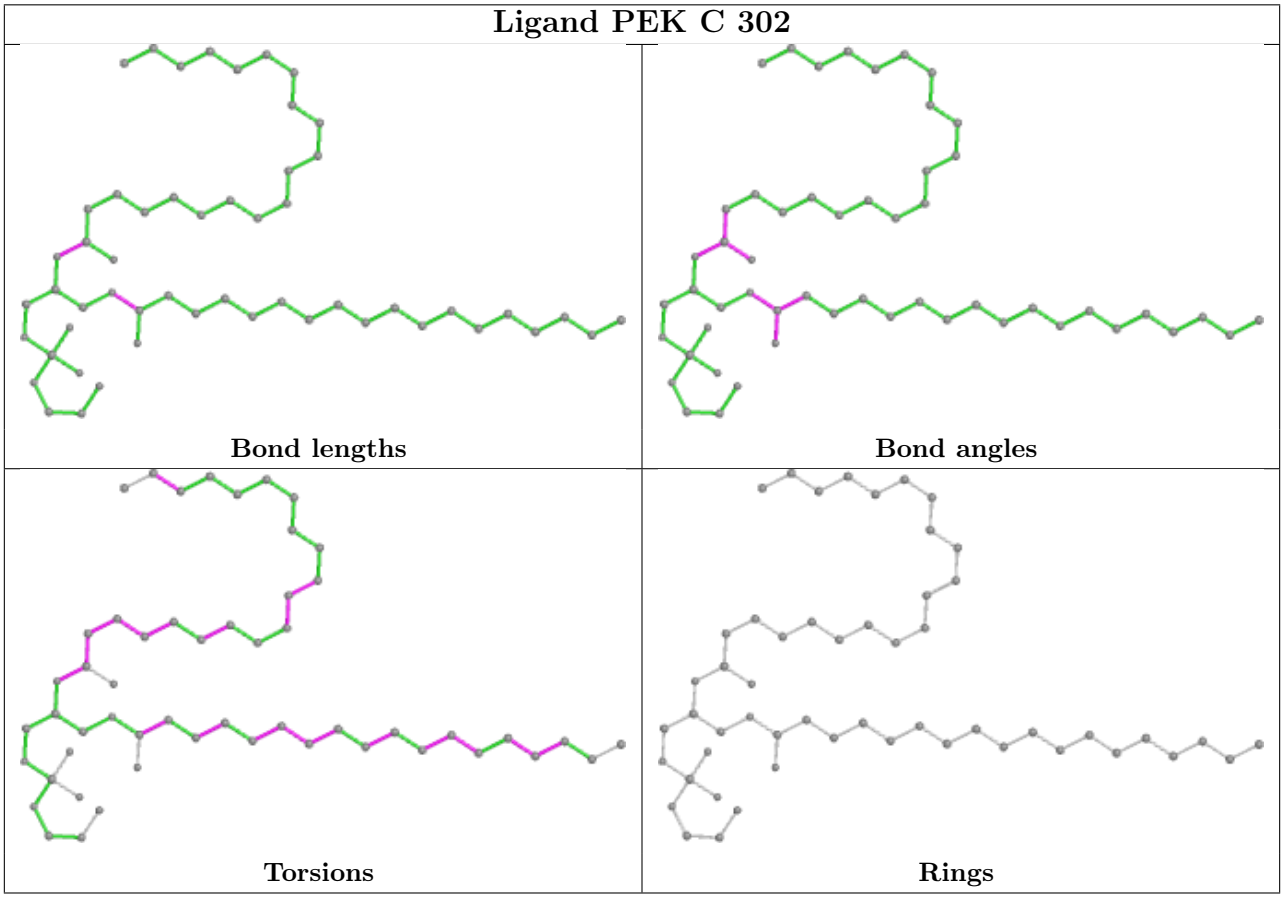
Mol	Chain	Res	Type	Atoms
14	a	601	HEA	CAA-CBA-CGA-O2A
18	c	302	PGV	C26-C27-C28-C29

There are no ring outliers.

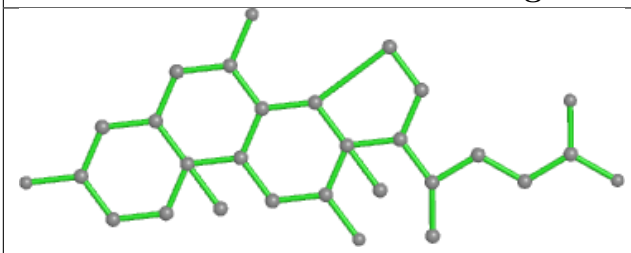
No monomer is involved in short contacts.

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.

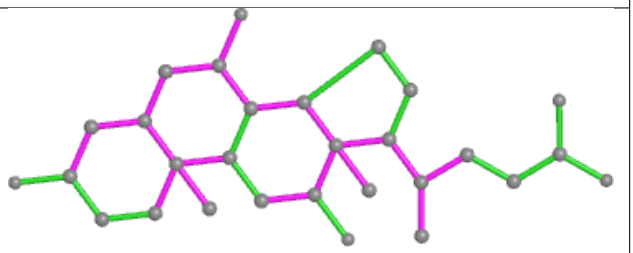
Ligand PEK C 302



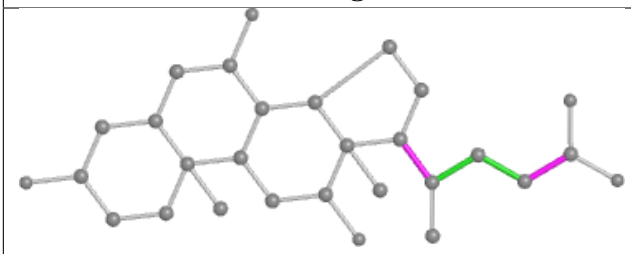
Ligand CHD J 101



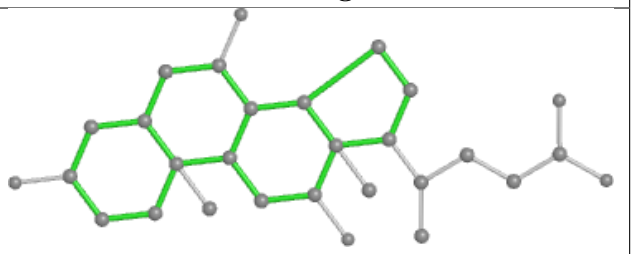
Bond lengths



Bond angles

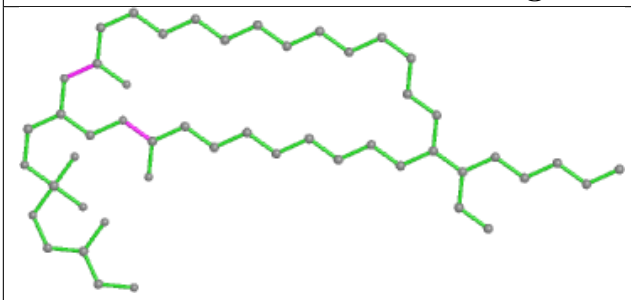


Torsions

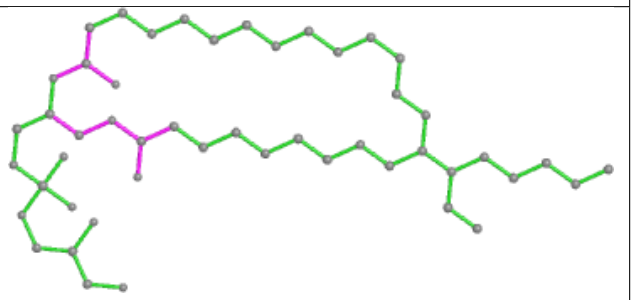


Rings

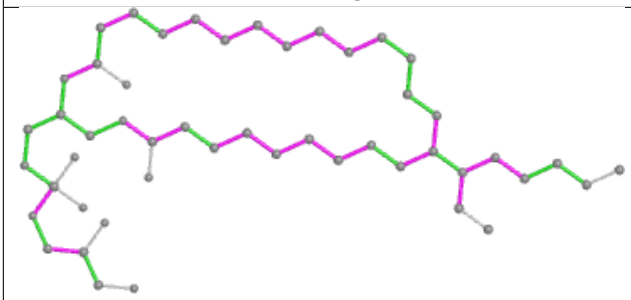
Ligand PGV a 606



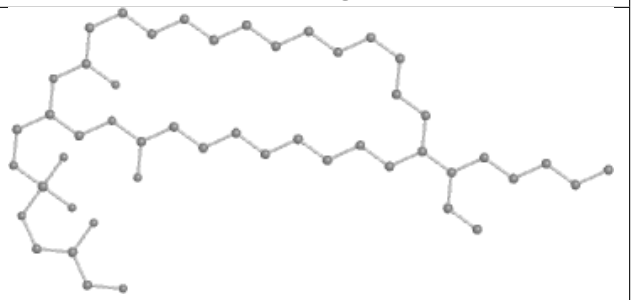
Bond lengths



Bond angles

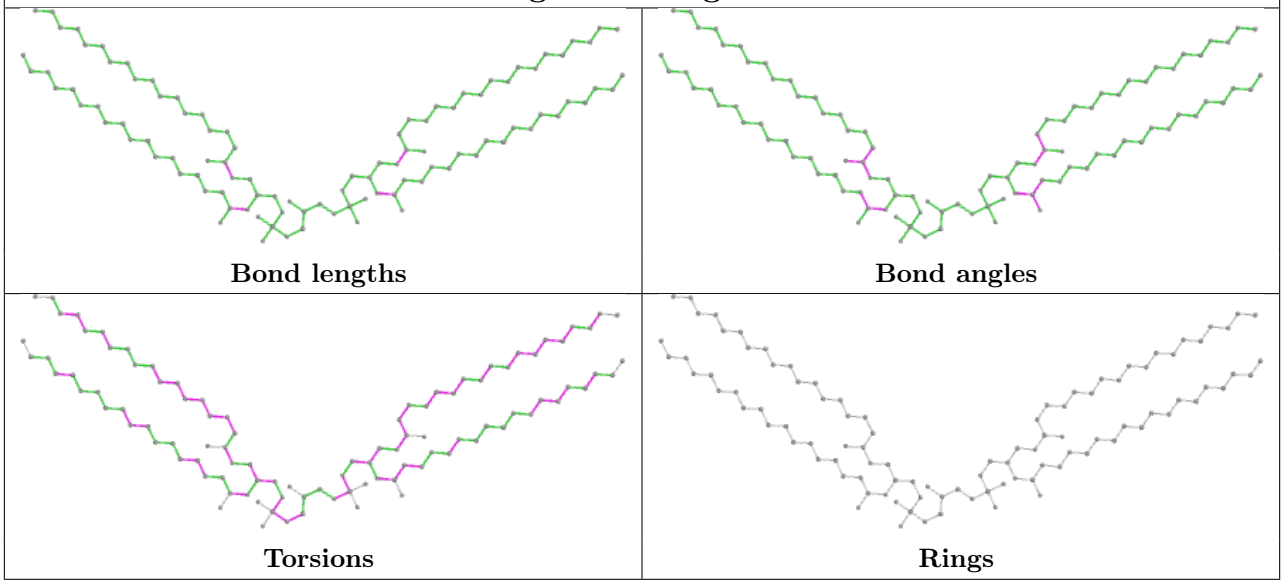


Torsions

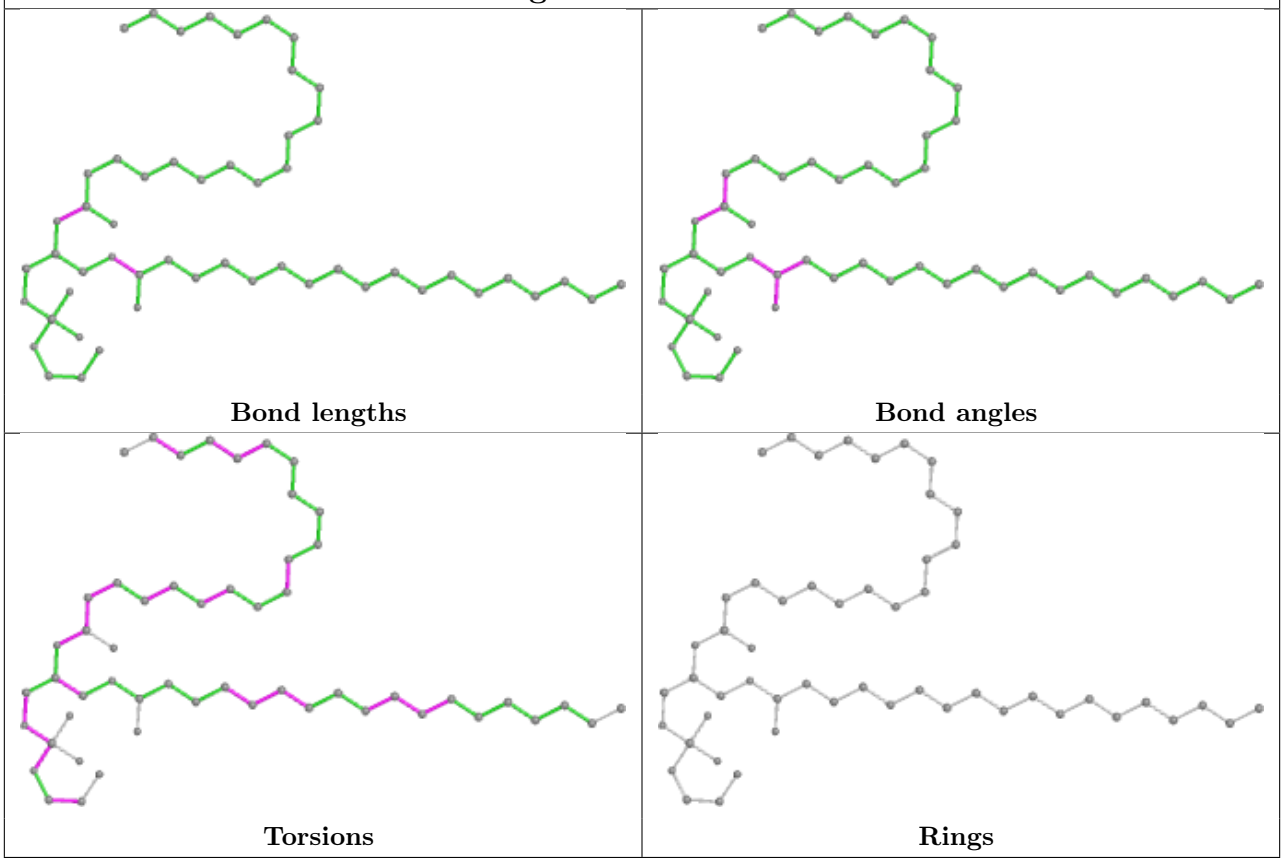


Rings

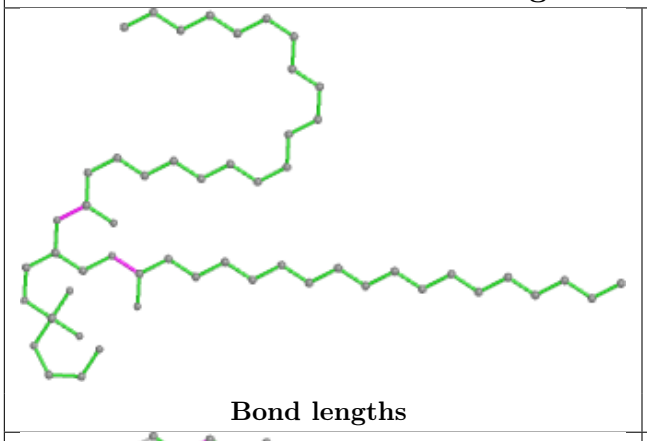
Ligand CDL g 101



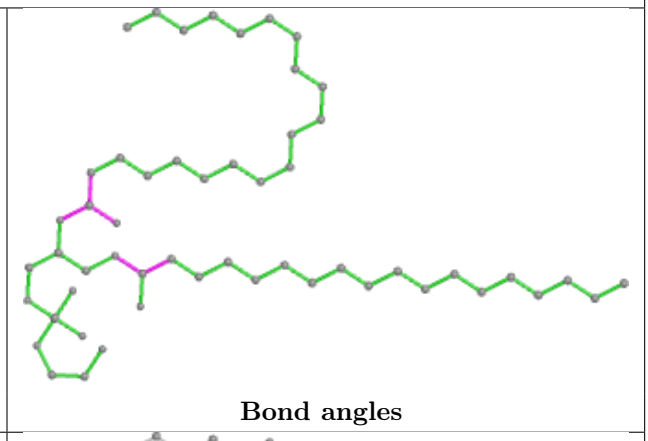
Ligand PEK c 305



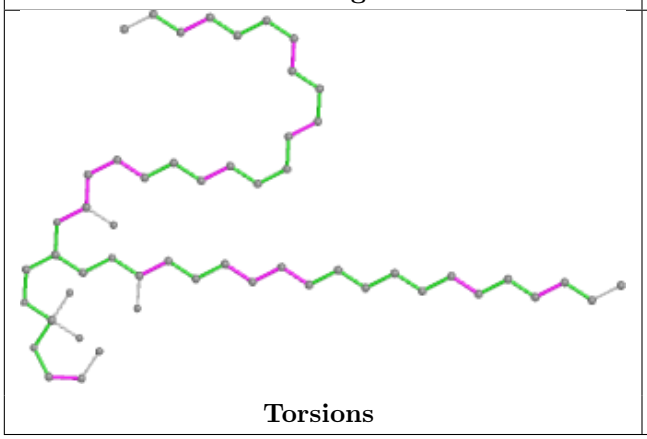
Ligand PEK c 304



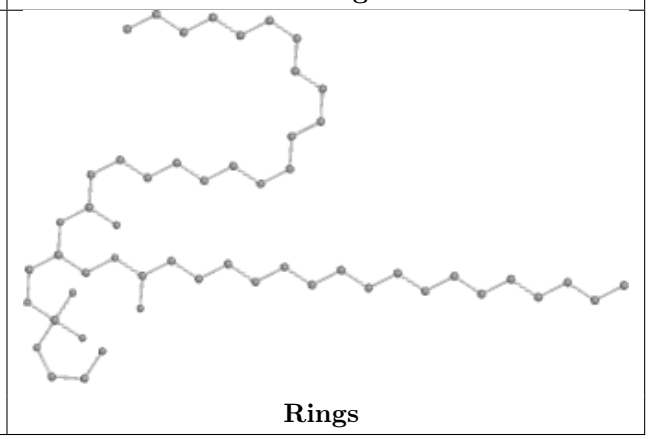
Bond lengths



Bond angles

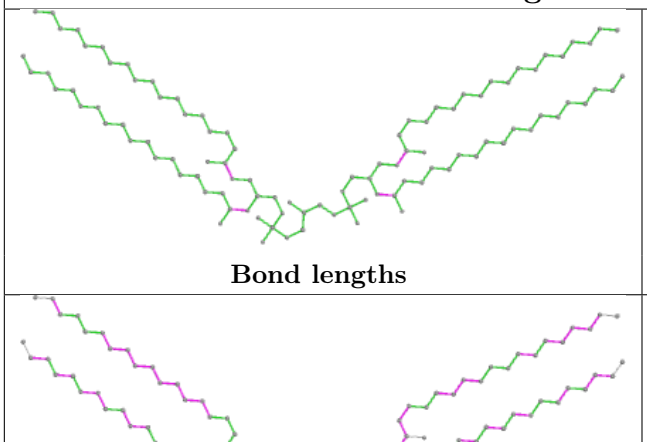


Torsions

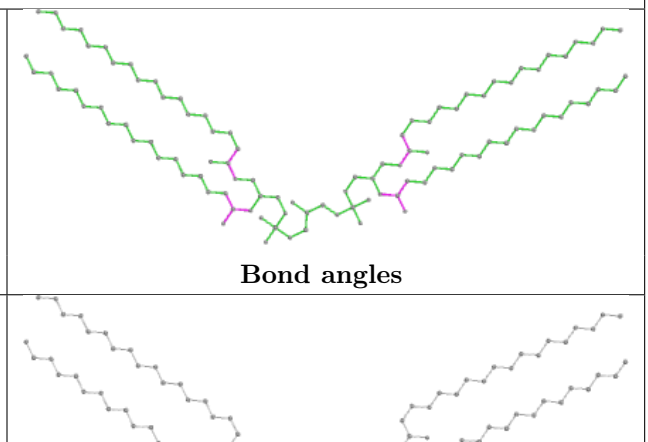


Rings

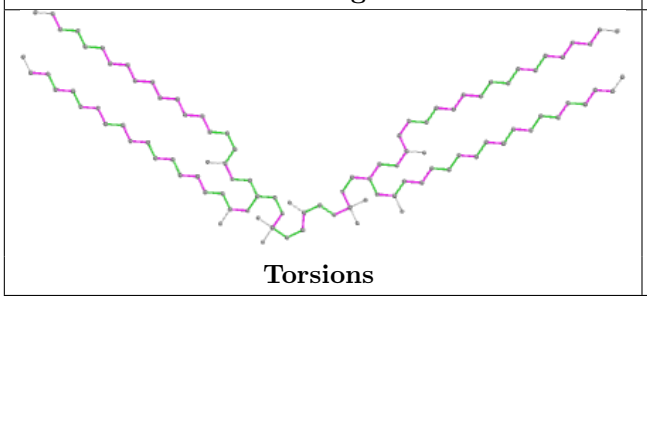
Ligand CDL G 102



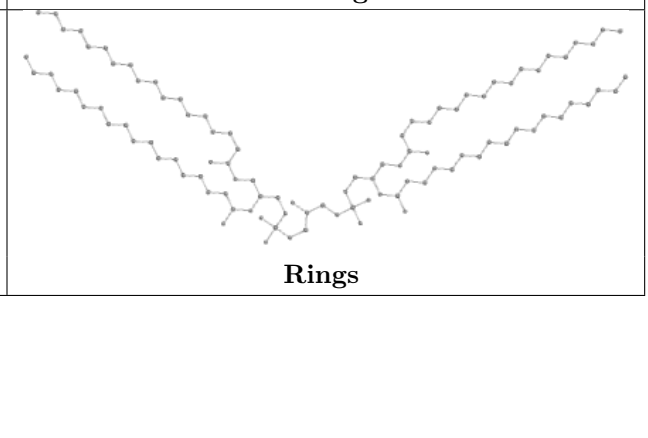
Bond lengths



Bond angles

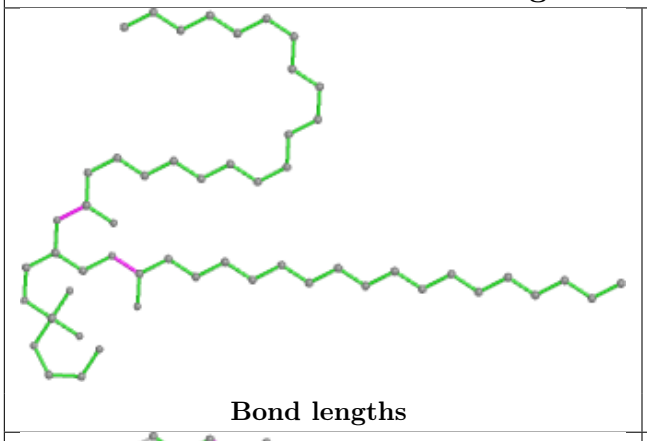


Torsions

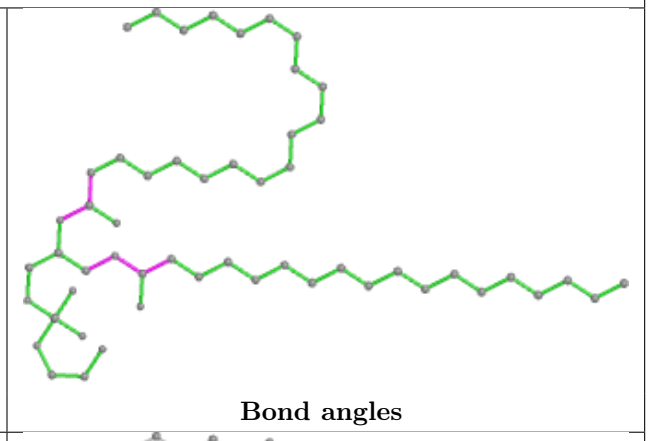


Rings

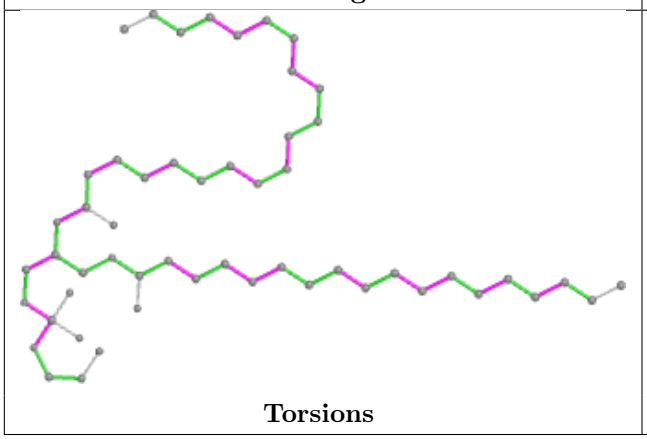
Ligand PEK c 301



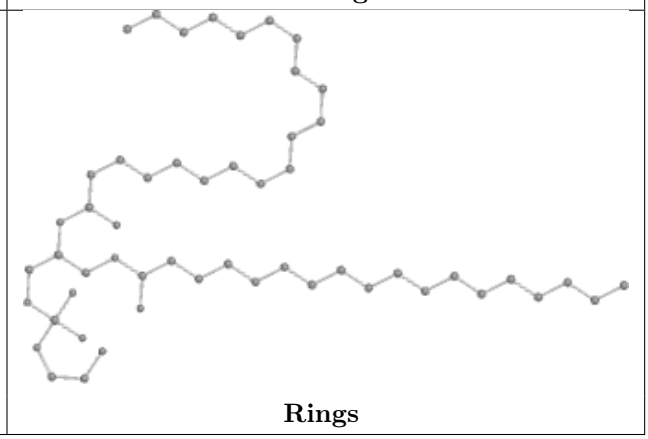
Bond lengths



Bond angles

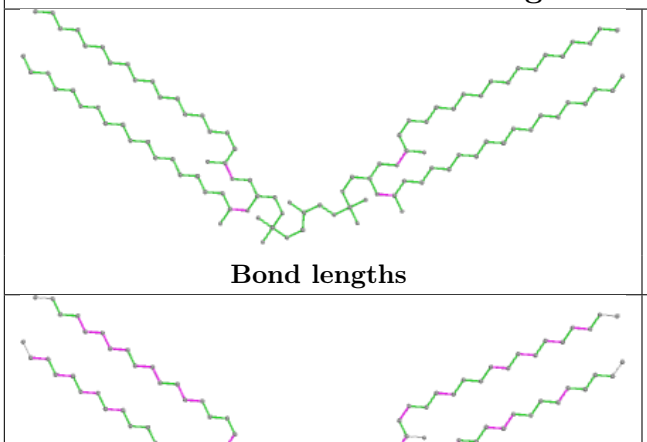


Torsions

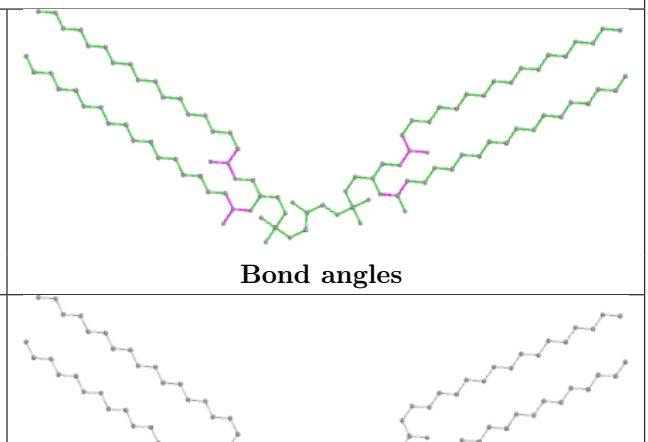


Rings

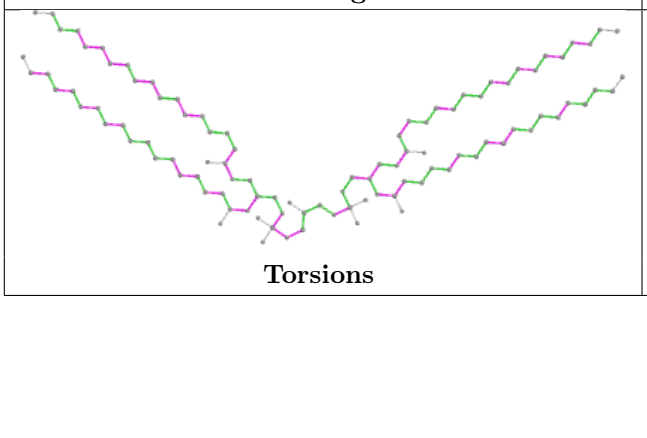
Ligand CDL C 305



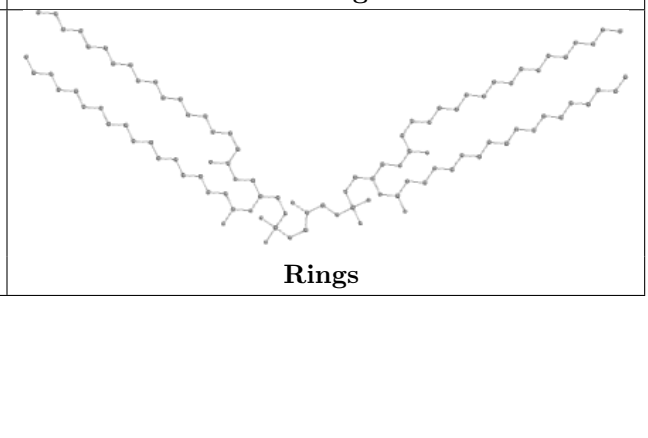
Bond lengths



Bond angles

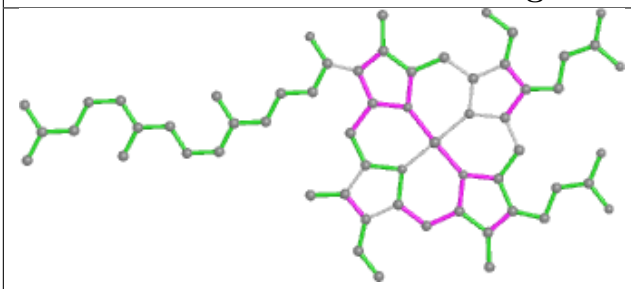


Torsions

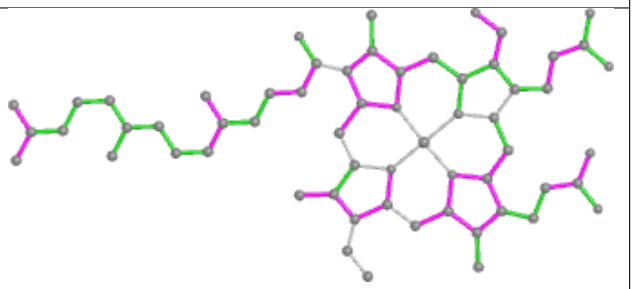


Rings

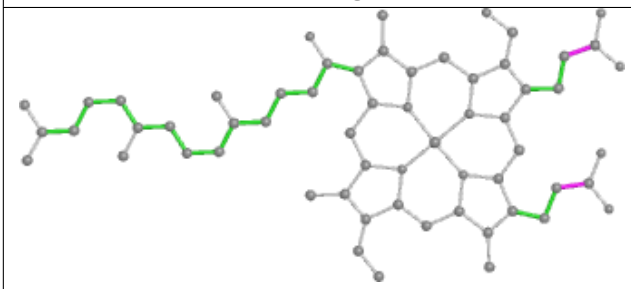
Ligand HEA a 601



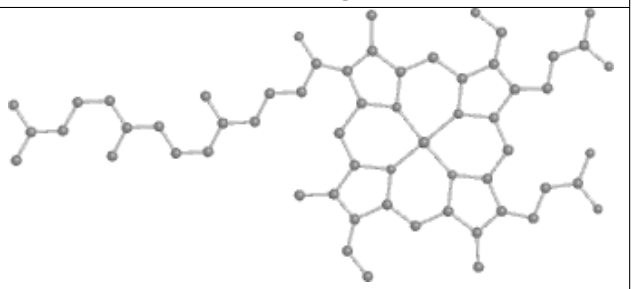
Bond lengths



Bond angles

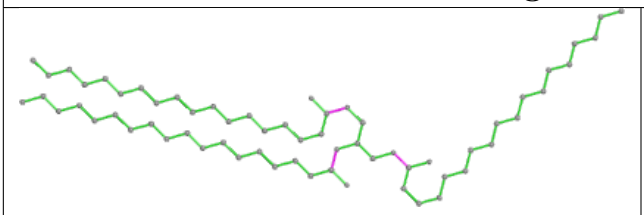


Torsions

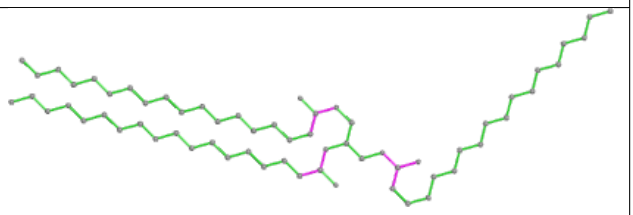


Rings

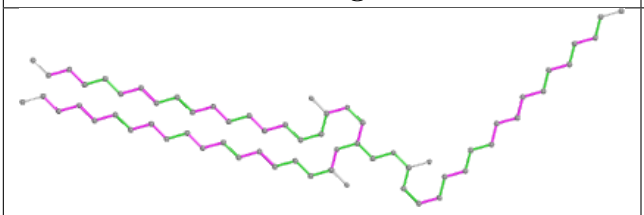
Ligand TGL A 608



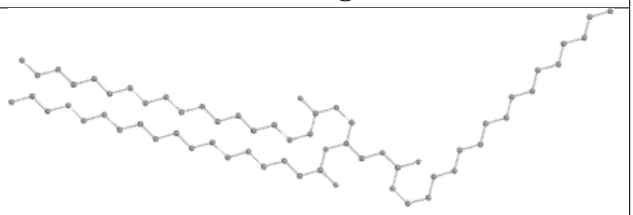
Bond lengths



Bond angles

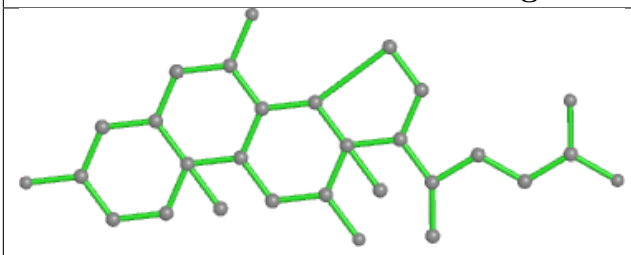


Torsions

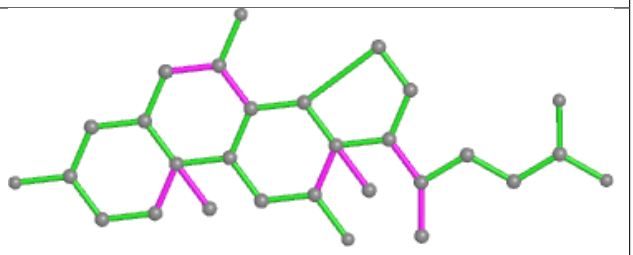


Rings

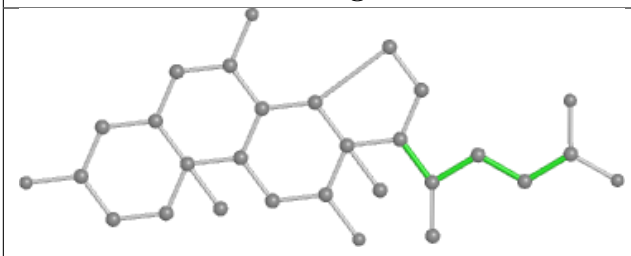
Ligand CHD C 301



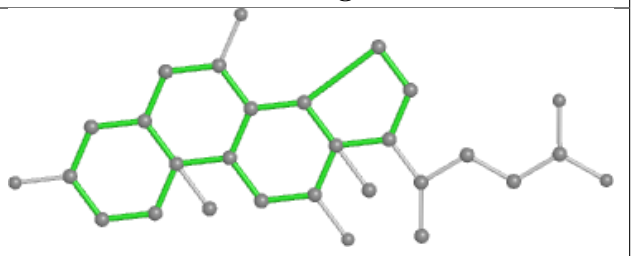
Bond lengths



Bond angles

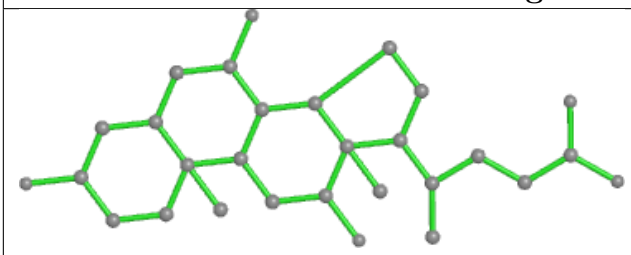


Torsions

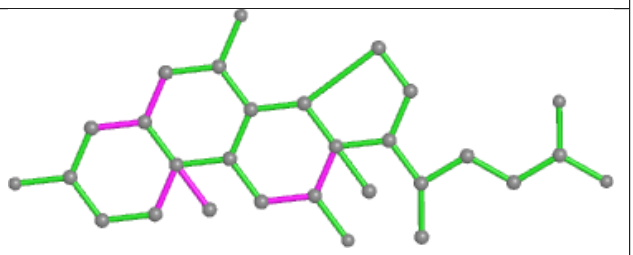


Rings

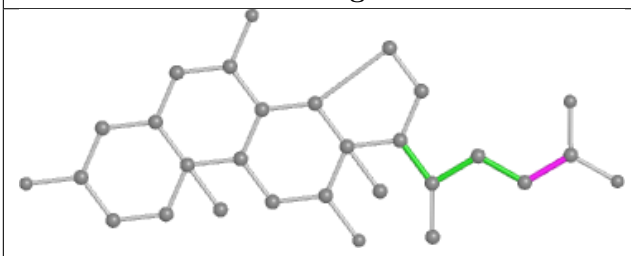
Ligand CHD c 308



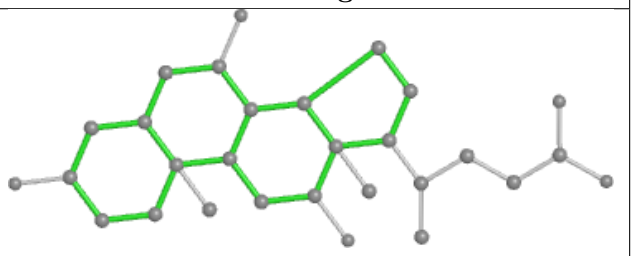
Bond lengths



Bond angles

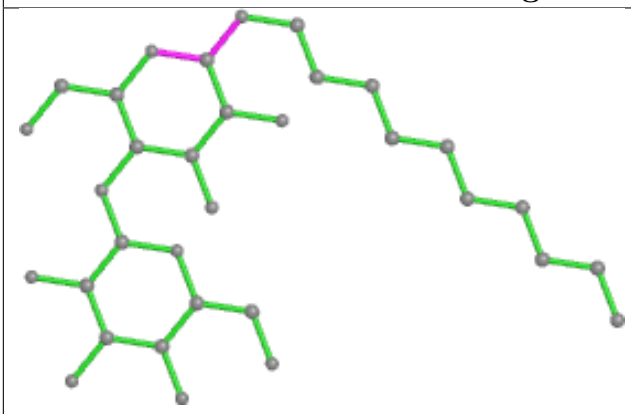


Torsions

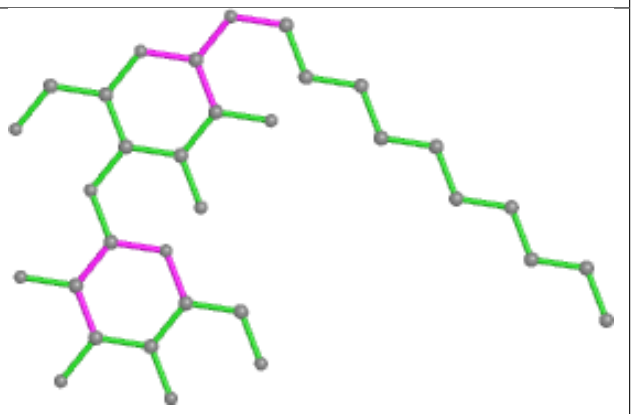


Rings

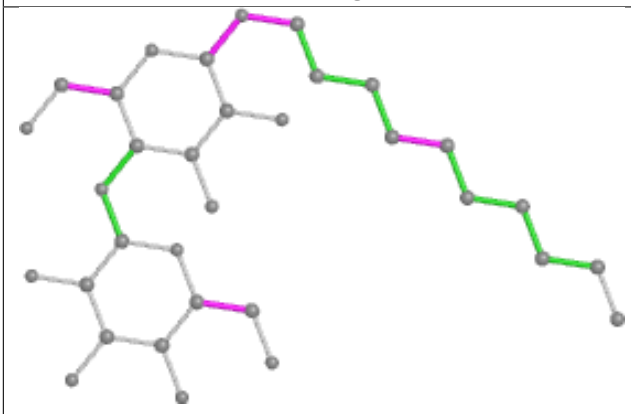
Ligand DMU c 309



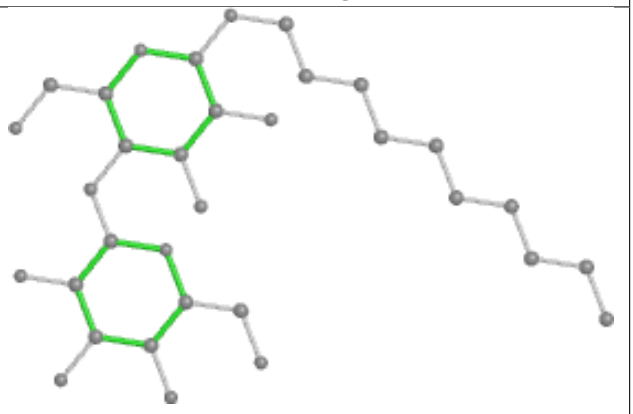
Bond lengths



Bond angles

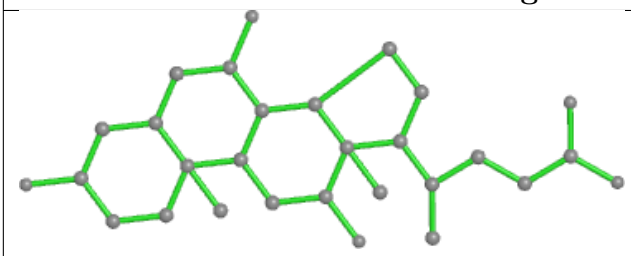


Torsions

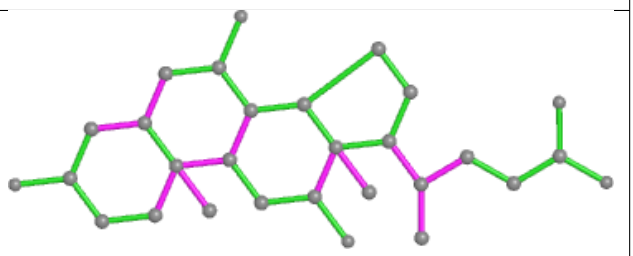


Rings

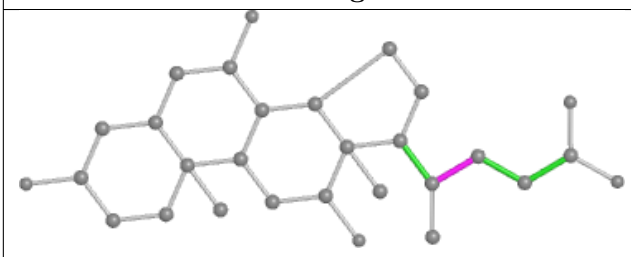
Ligand CHD C 306



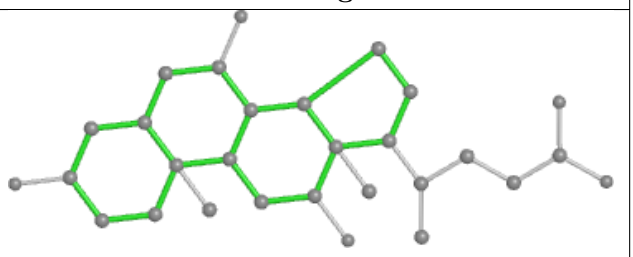
Bond lengths



Bond angles

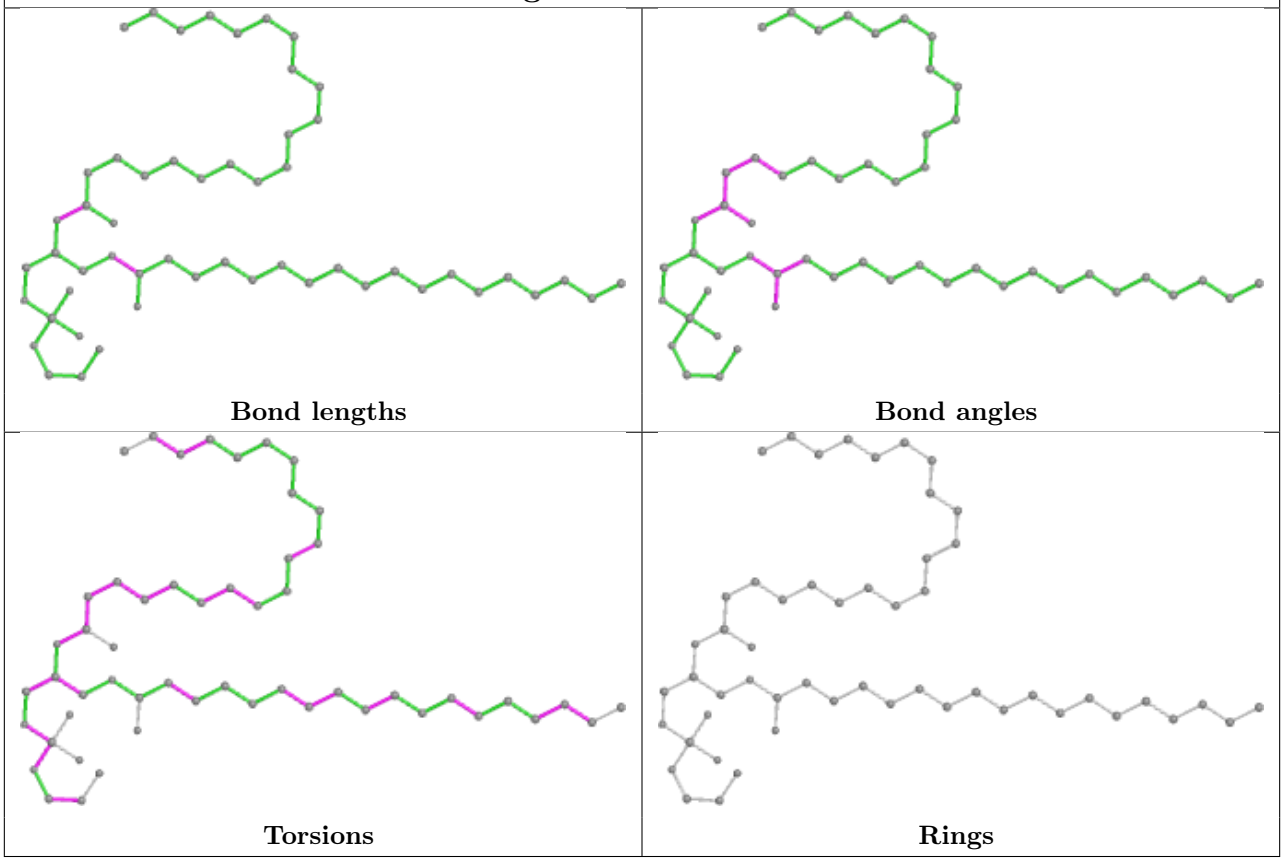


Torsions

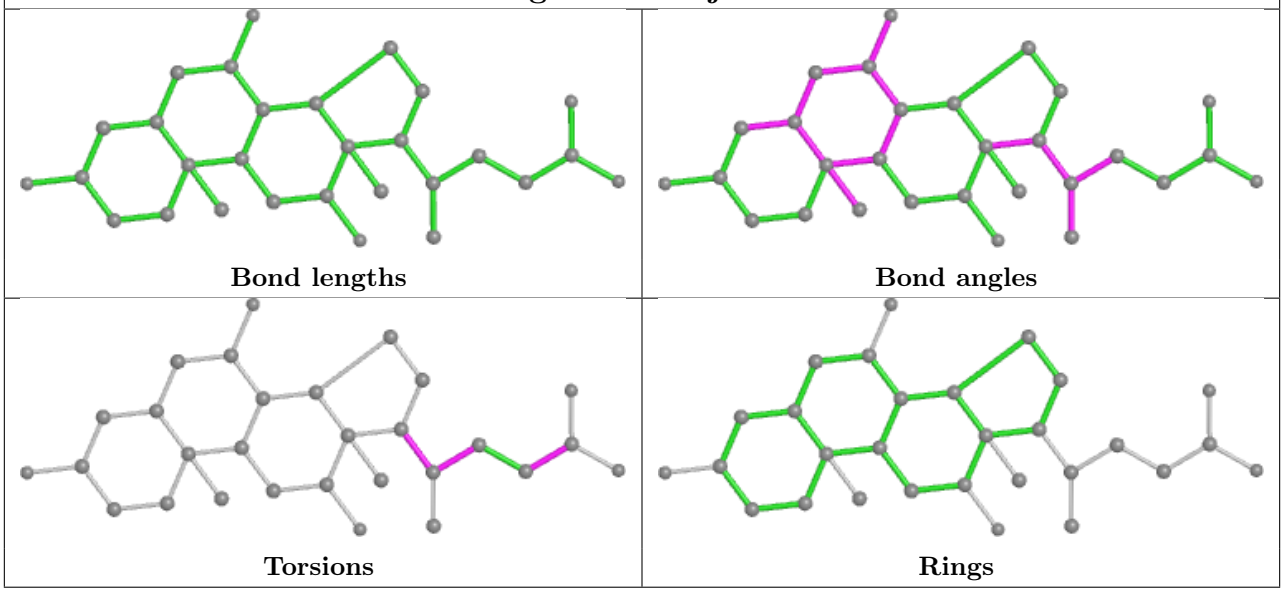


Rings

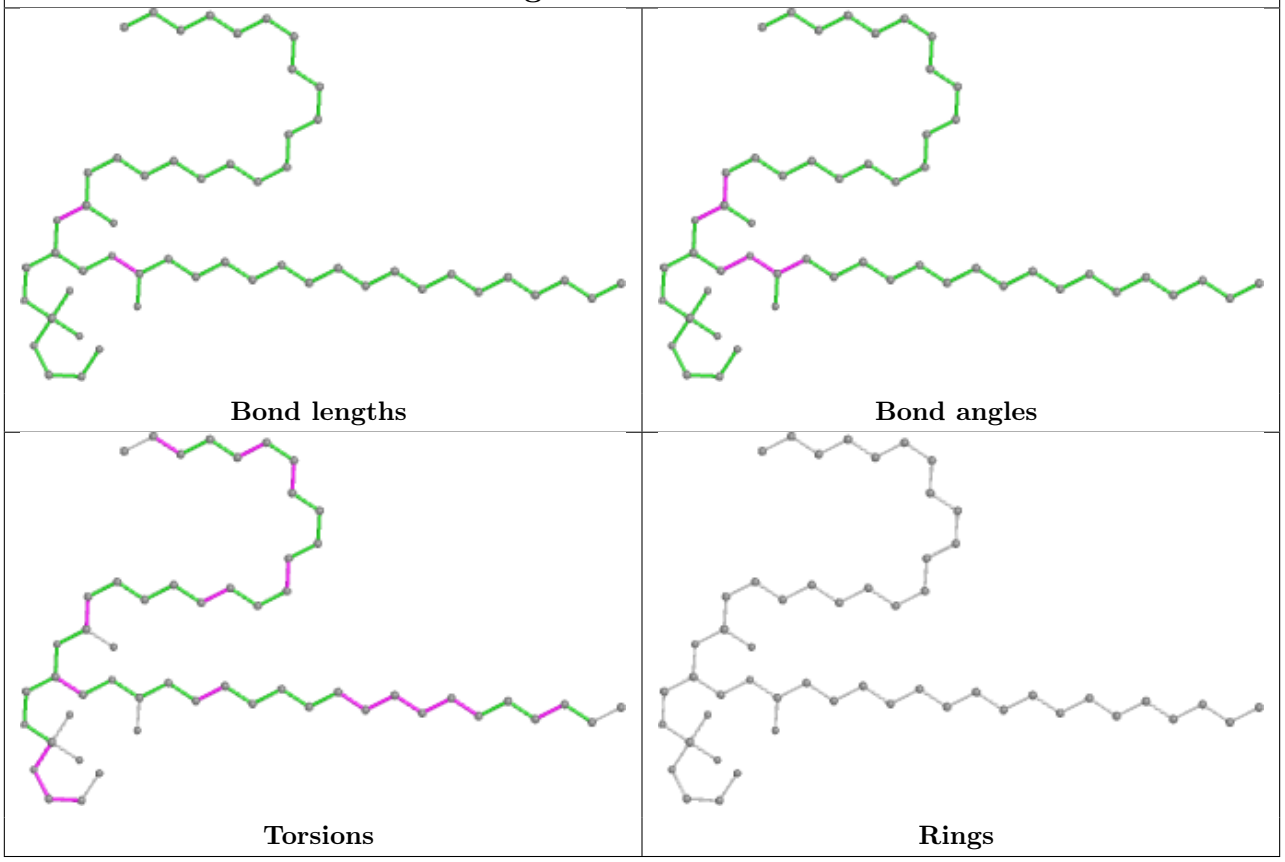
Ligand PEK G 101



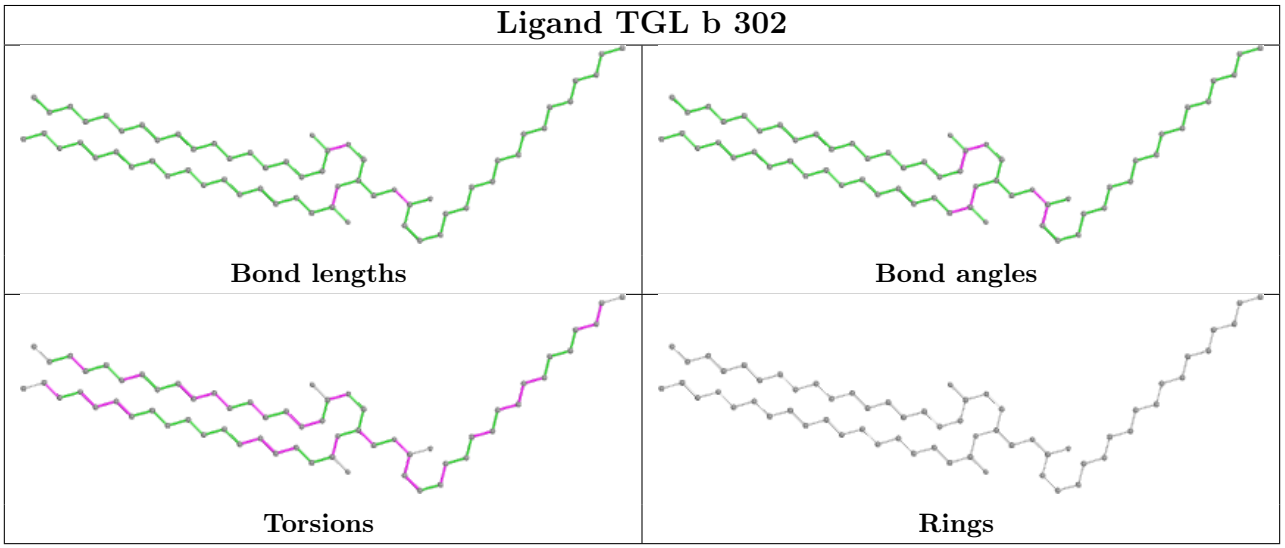
Ligand CHD j 101



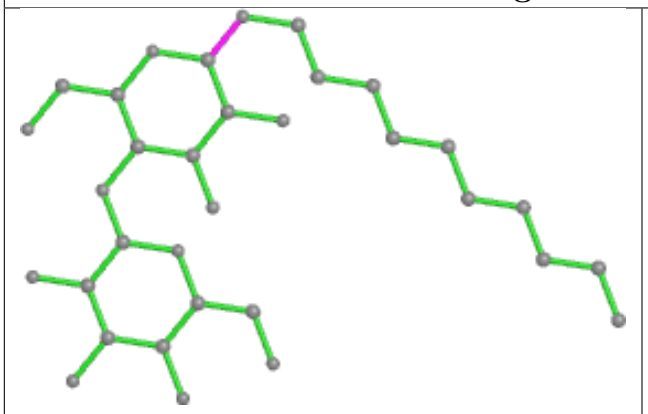
Ligand PEK C 307



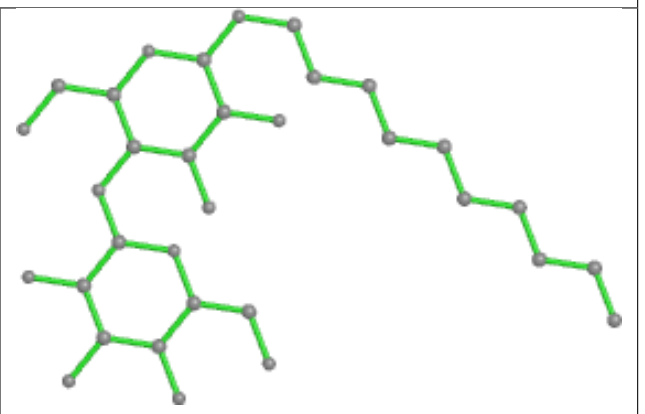
Ligand TGL b 302



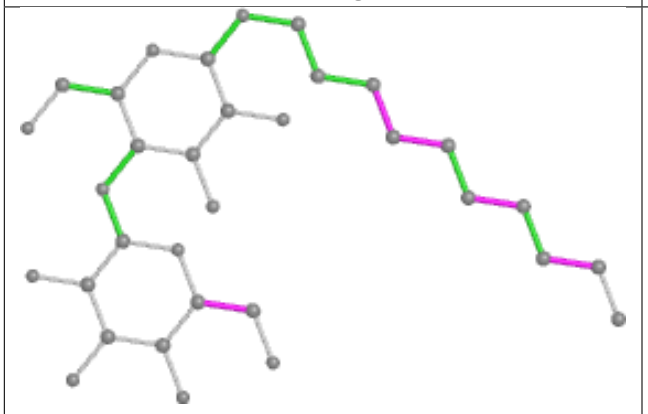
Ligand DMU M 101



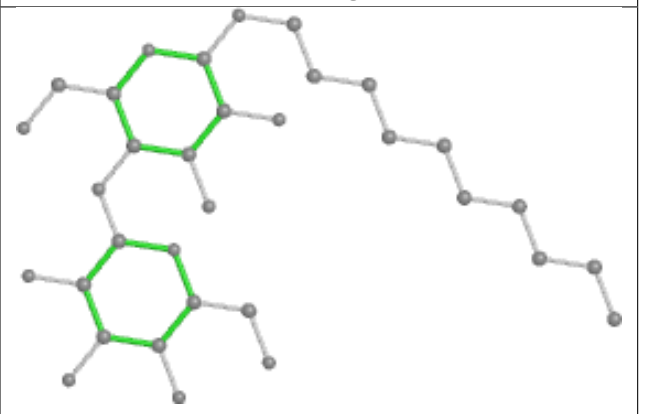
Bond lengths



Bond angles

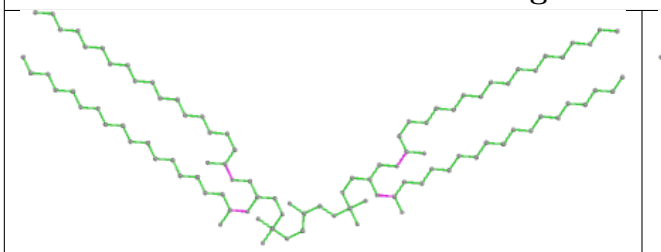


Torsions

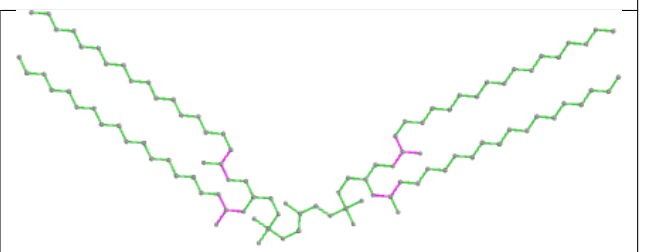


Rings

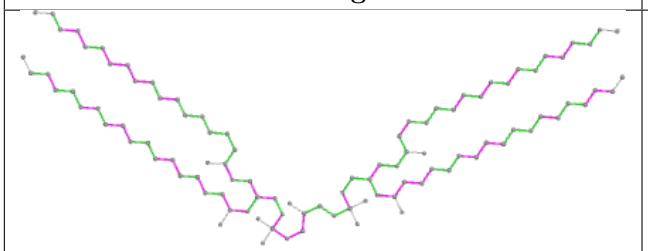
Ligand CDL c 307



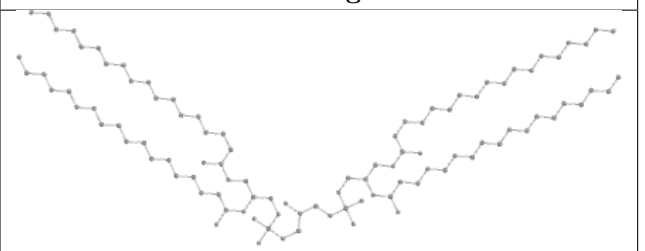
Bond lengths



Bond angles

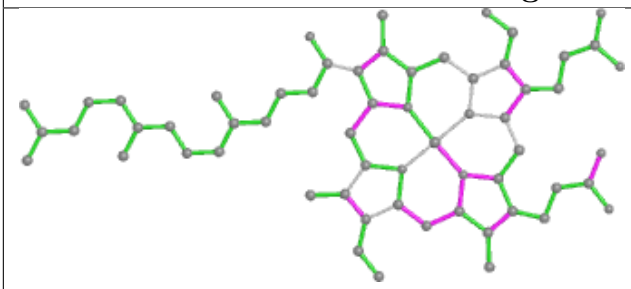


Torsions

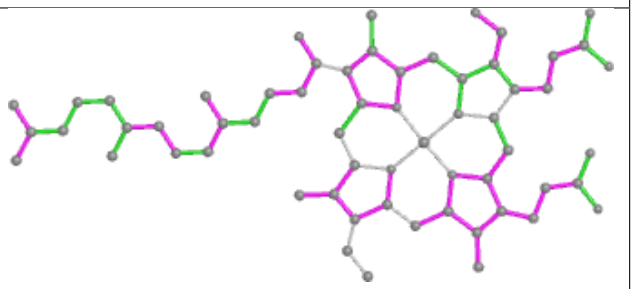


Rings

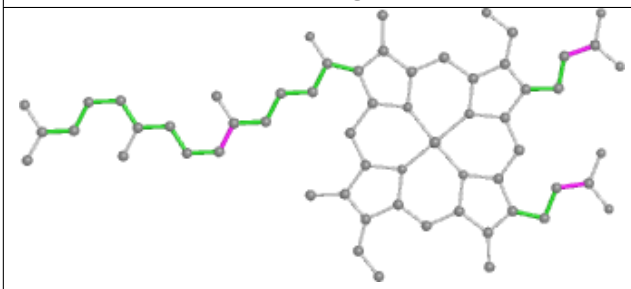
Ligand HEA A 601



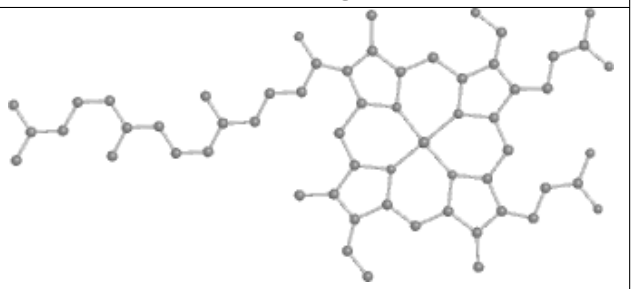
Bond lengths



Bond angles

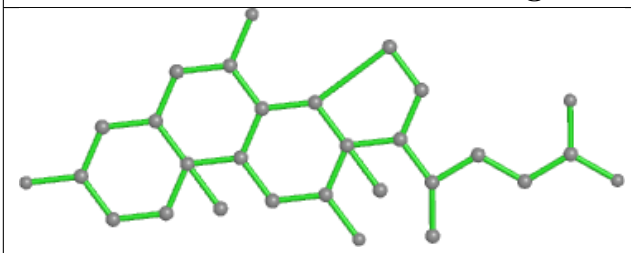


Torsions

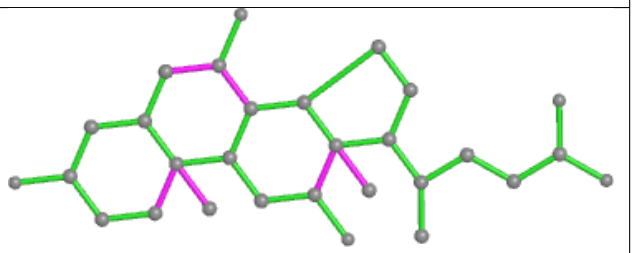


Rings

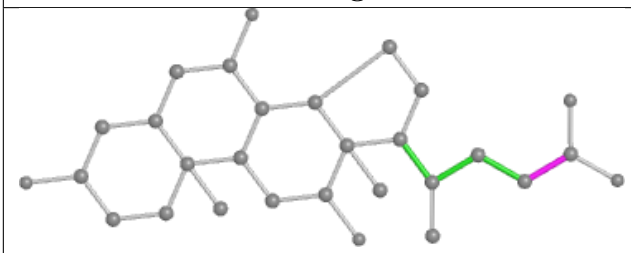
Ligand CHD c 303



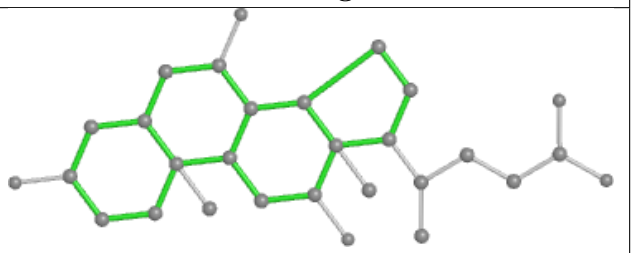
Bond lengths



Bond angles

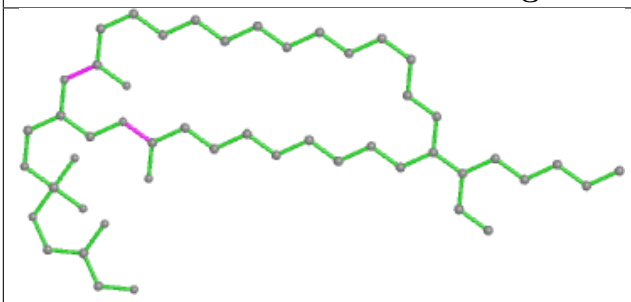


Torsions

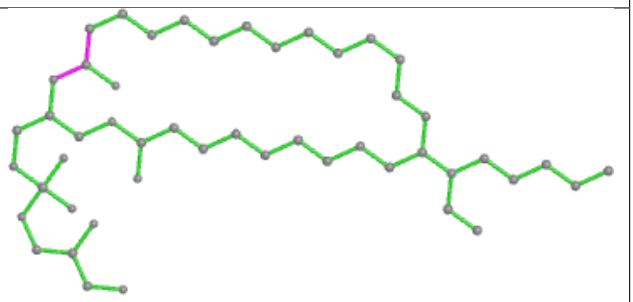


Rings

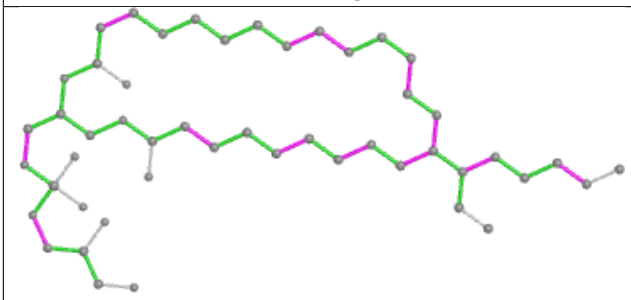
Ligand PGV C 303



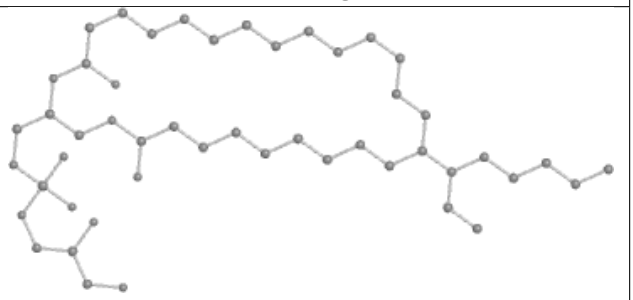
Bond lengths



Bond angles

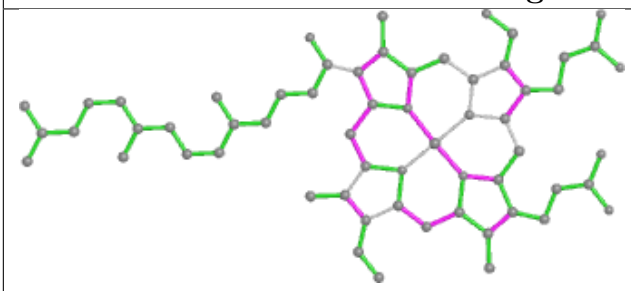


Torsions



Rings

Ligand HEA a 602



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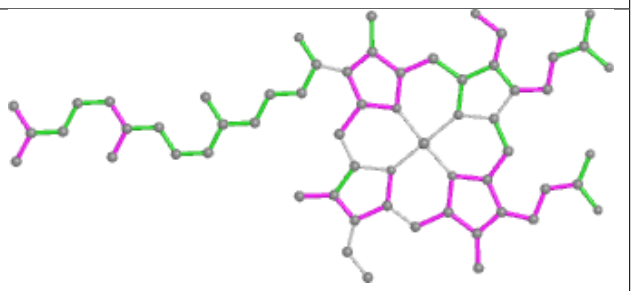
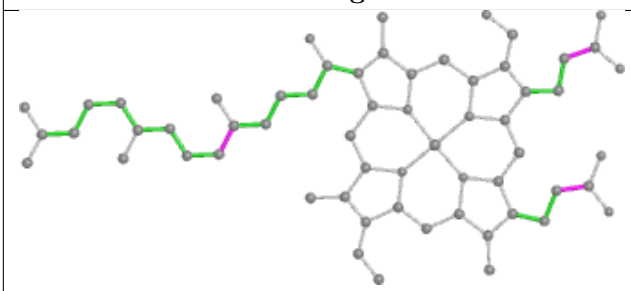
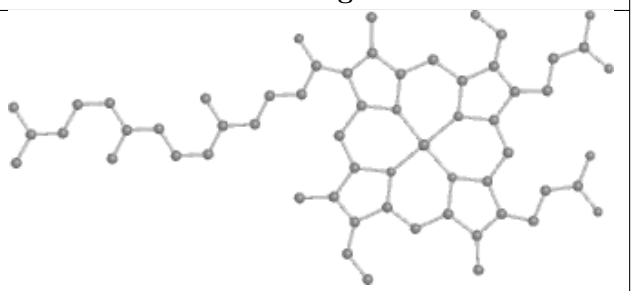


Bond angles

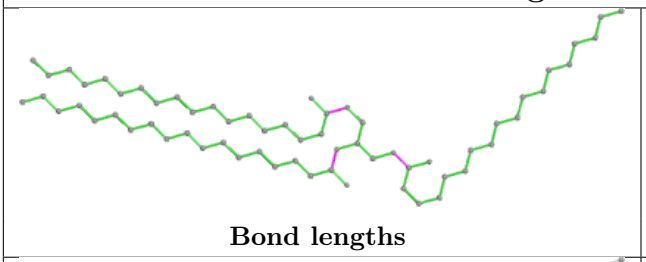


Torsions



Rings

Ligand TGL d 201



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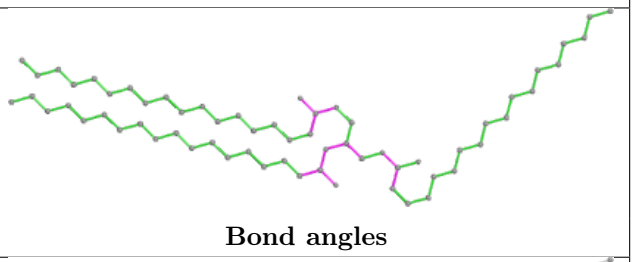
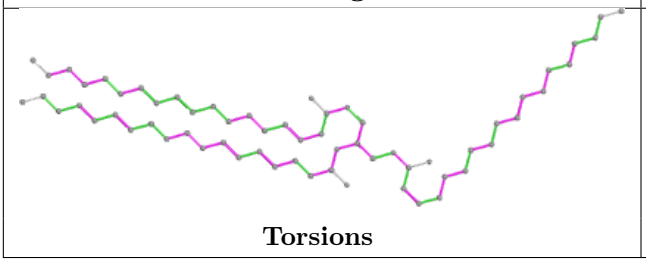


Bond angles



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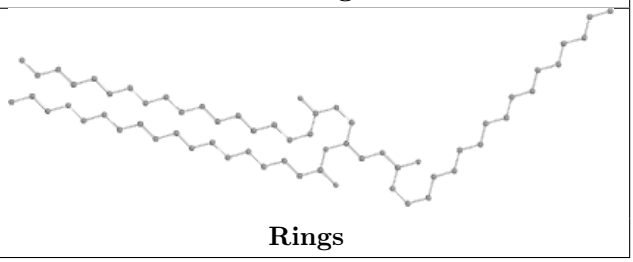
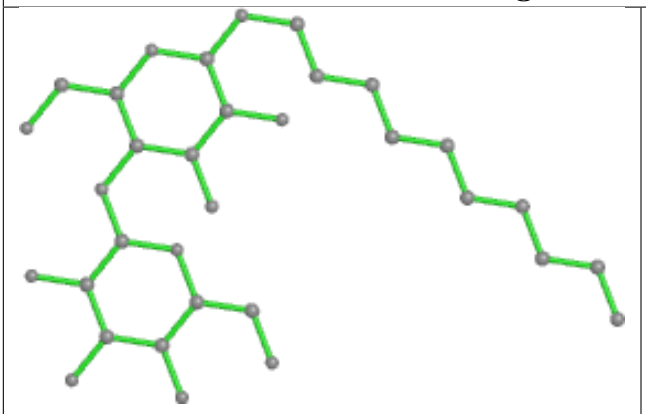


Rings

Ligand DMU m 101



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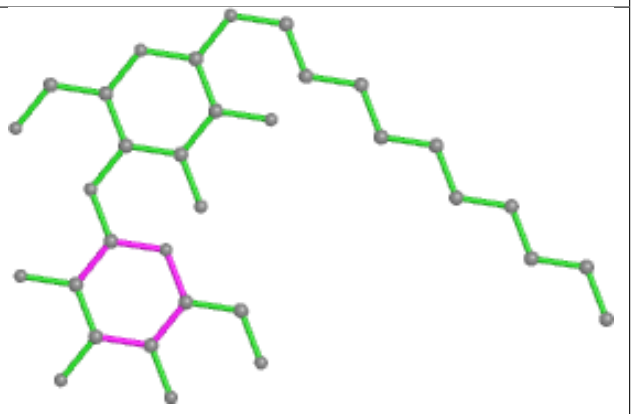
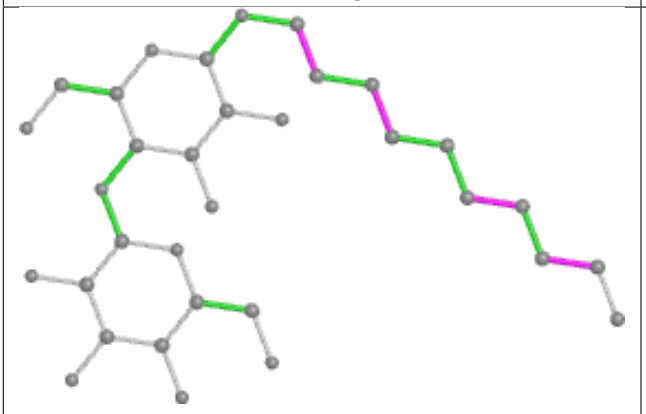
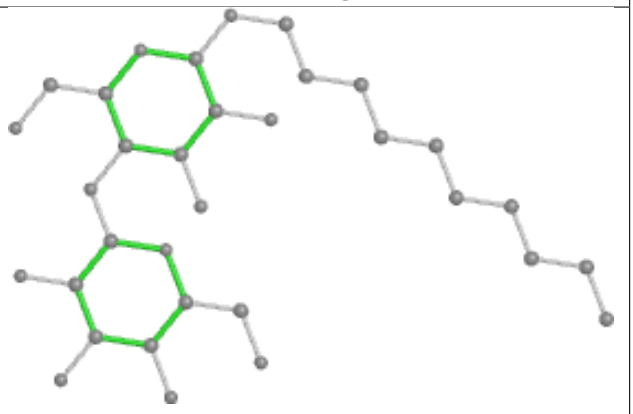


Bond angles

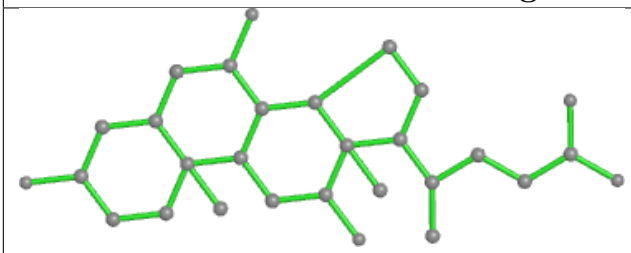


Torsions



Rings

Ligand CHD G 103



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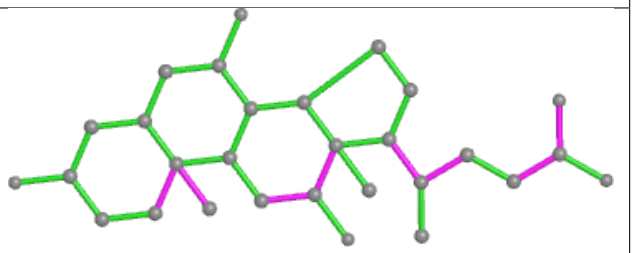
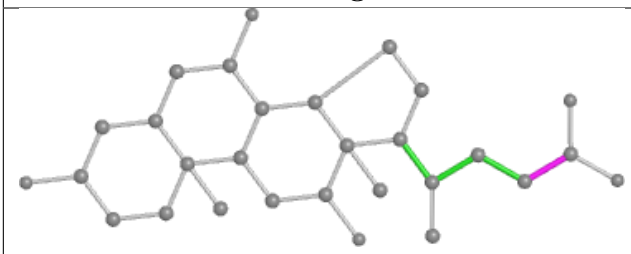
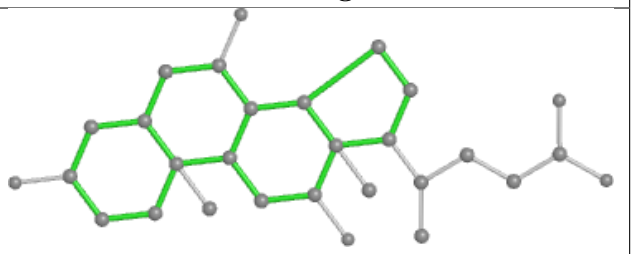


Bond angles

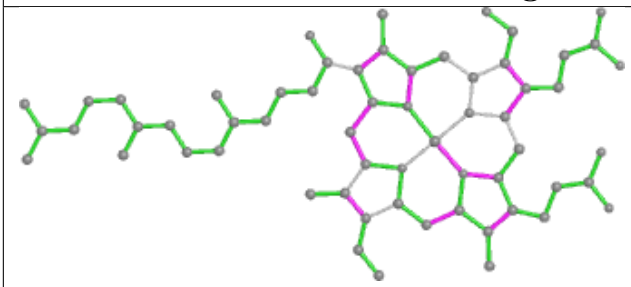


Torsions



Rings

Ligand HEA A 602



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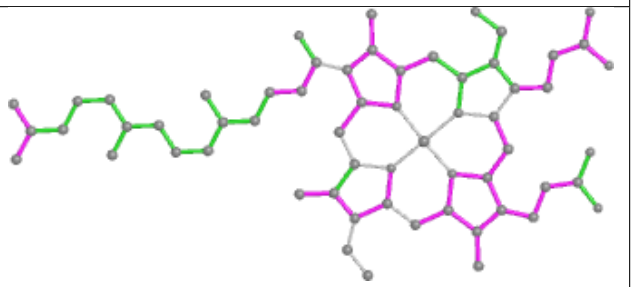
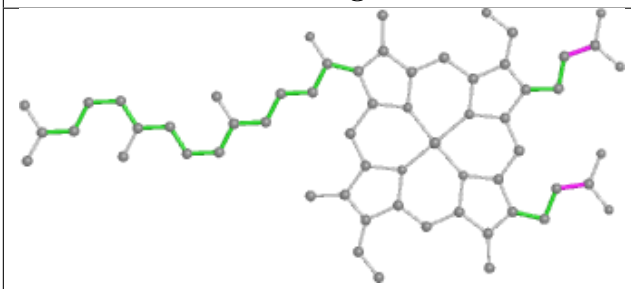
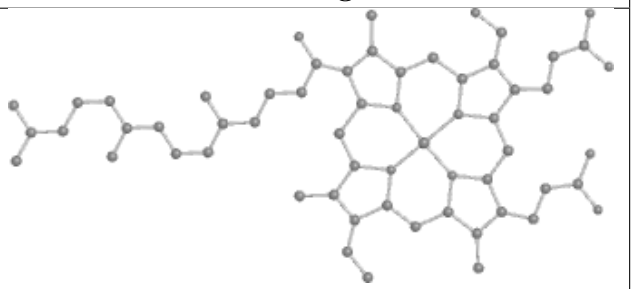


Bond angles

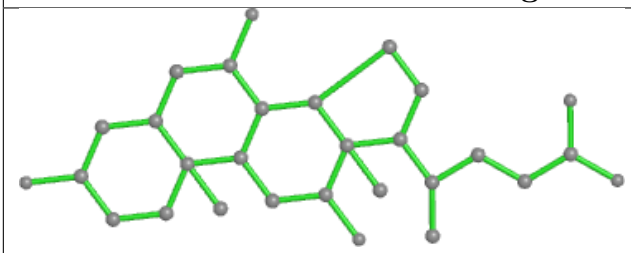


Torsions

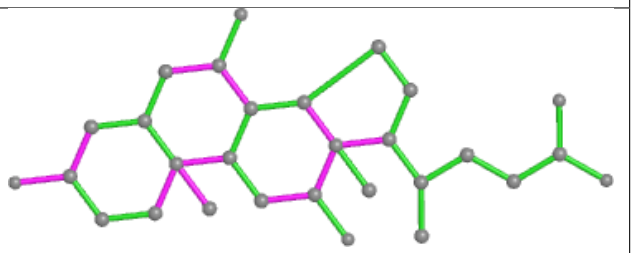


Rings

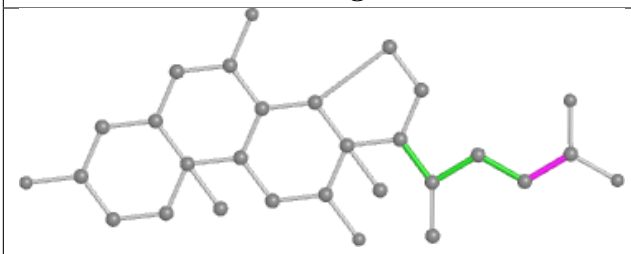
Ligand CHD B 402



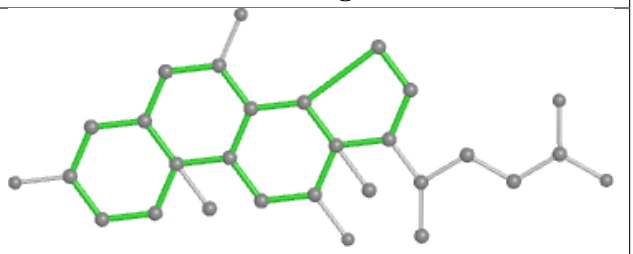
Bond lengths



Bond angles

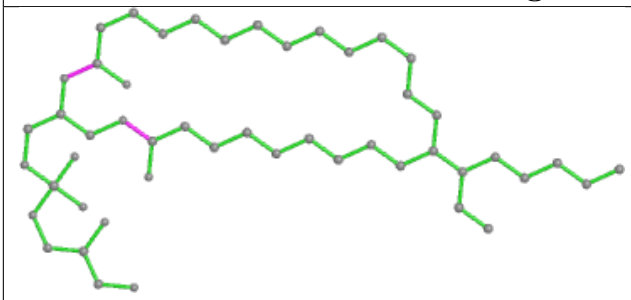


Torsions

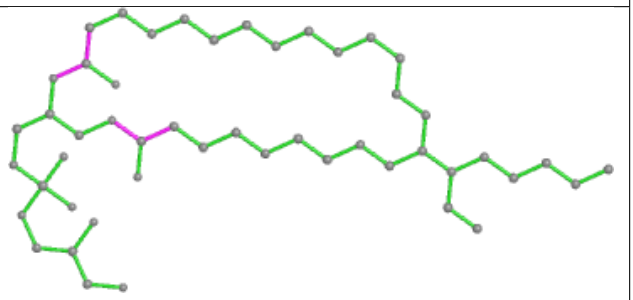


Rings

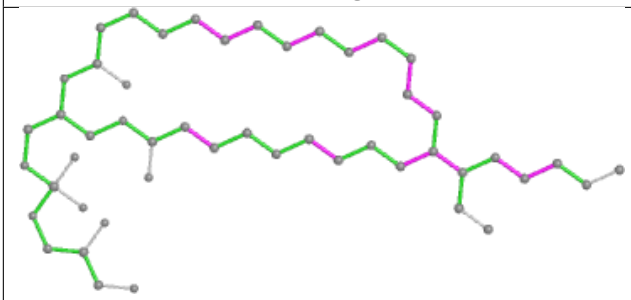
Ligand PGV a 607



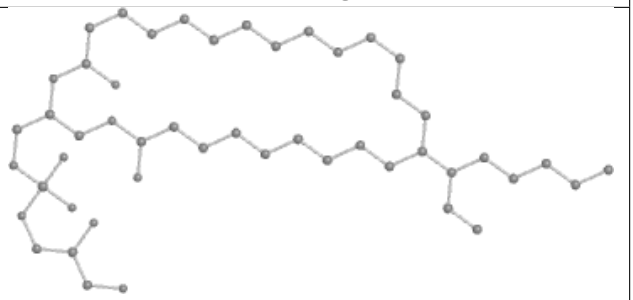
Bond lengths



Bond angles

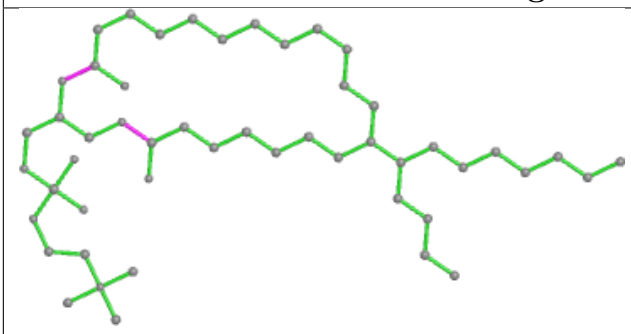


Torsions



Rings

Ligand PSC E 201



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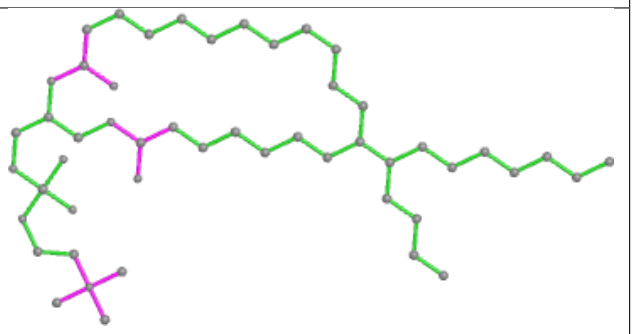
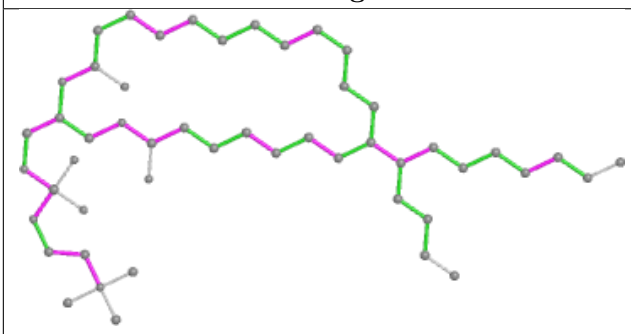
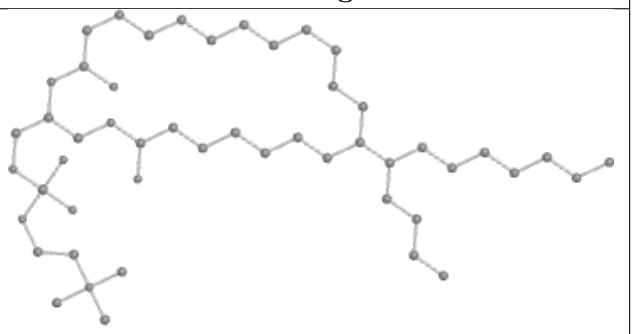


Bond angles

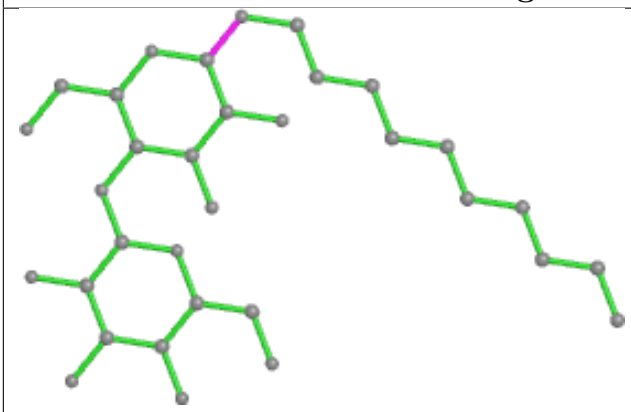


Torsions

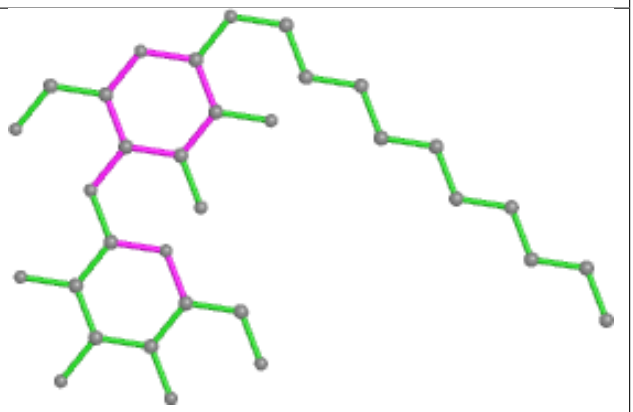


Rings

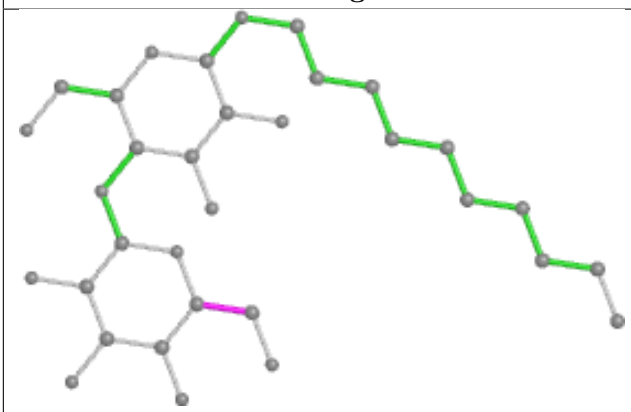
Ligand DMU C 308



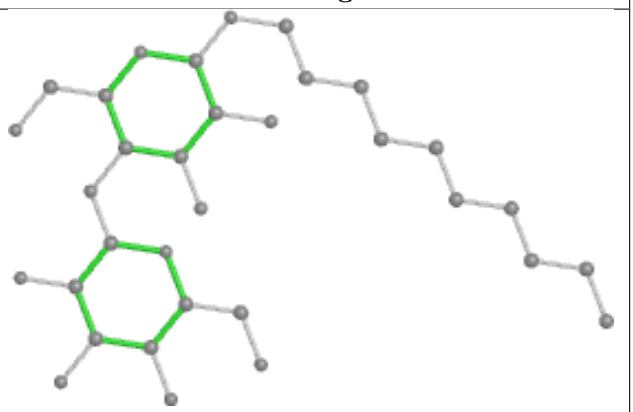
Bond lengths



Bond angles

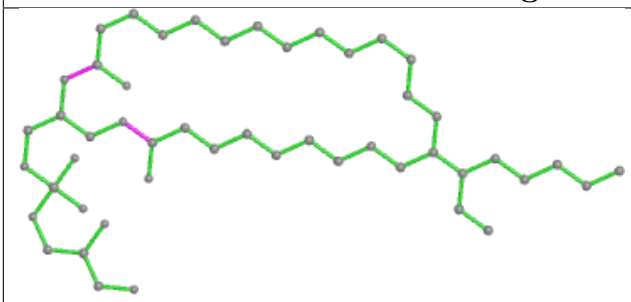


Torsions

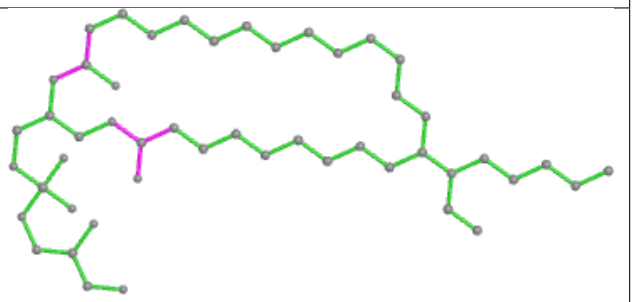


Rings

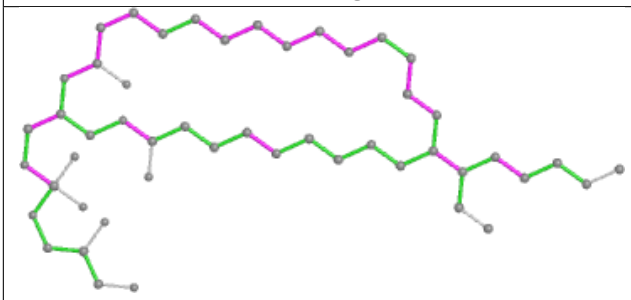
Ligand PGV A 606



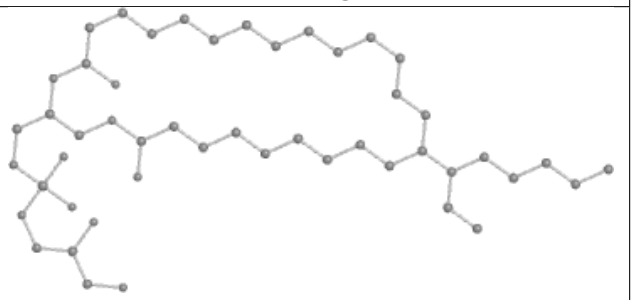
Bond lengths



Bond angles

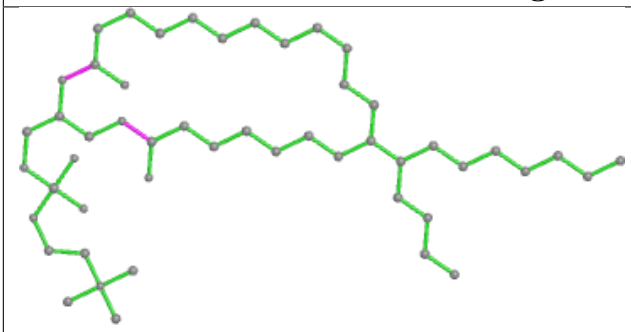


Torsions

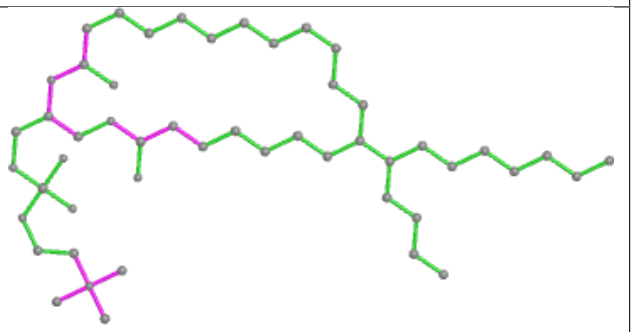


Rings

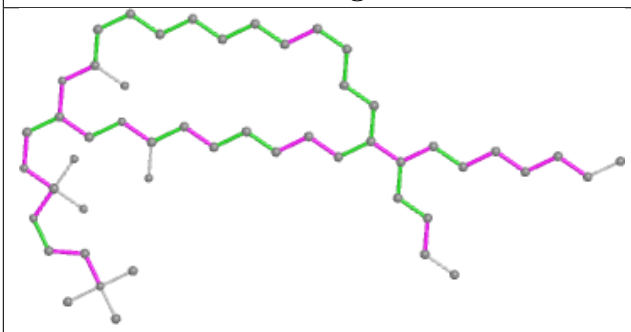
Ligand PSC b 303



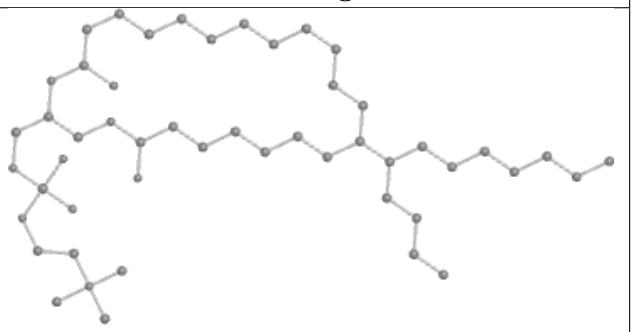
Bond lengths



Bond angles

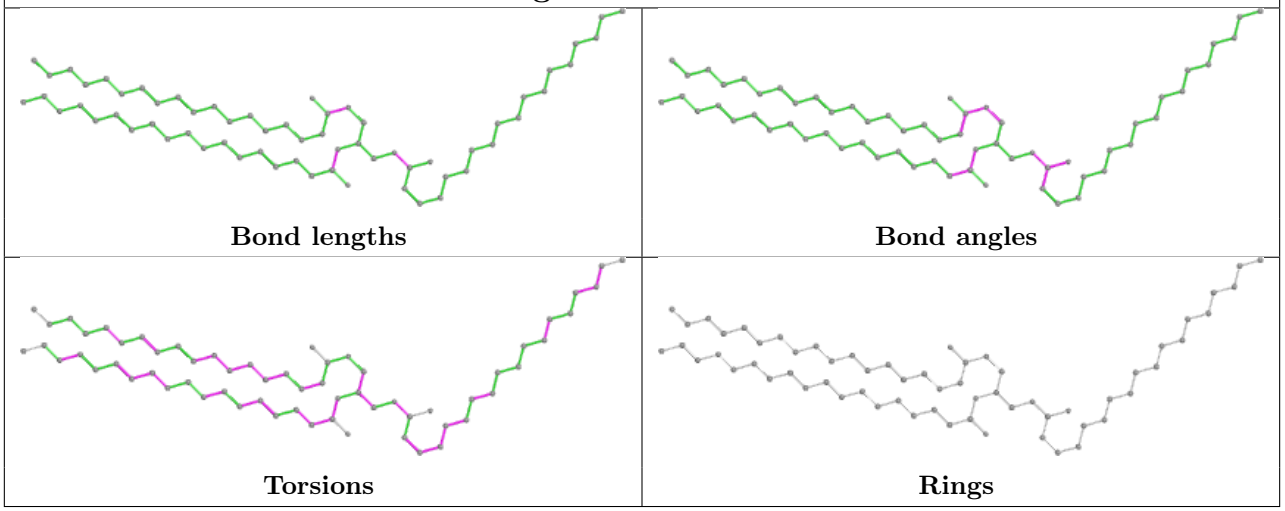


Torsions

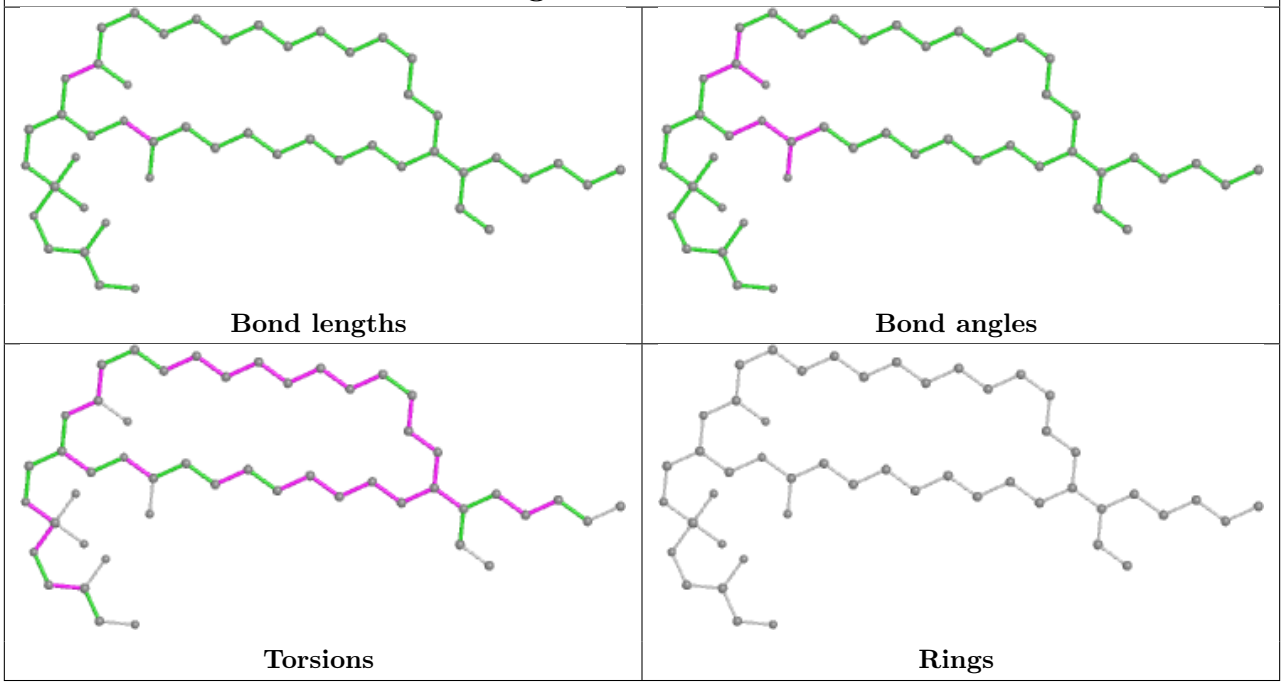


Rings

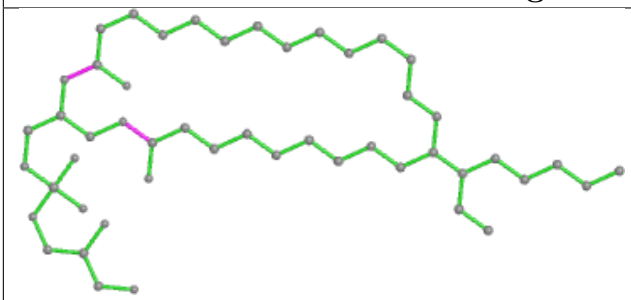
Ligand TGL l 101



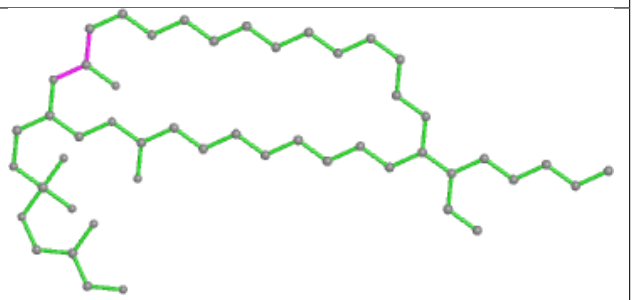
Ligand PGV c 302



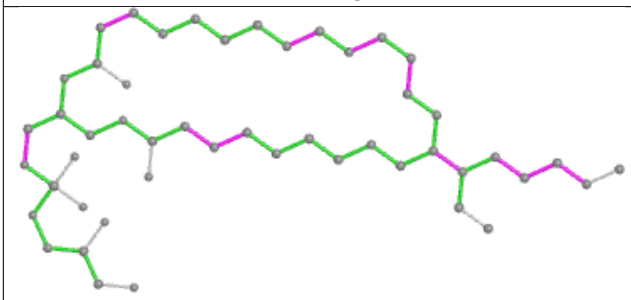
Ligand PGV c 306



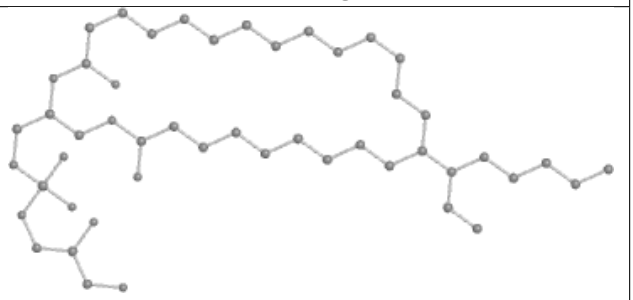
Bond lengths



Bond angles

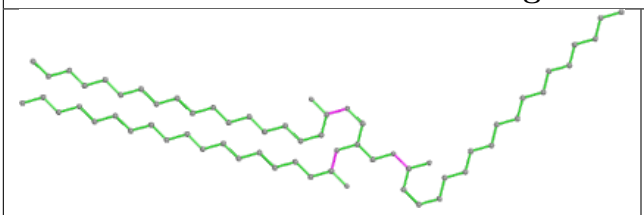


Torsions

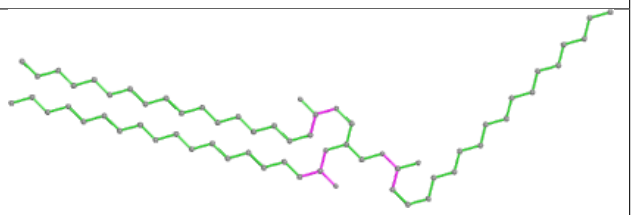


Rings

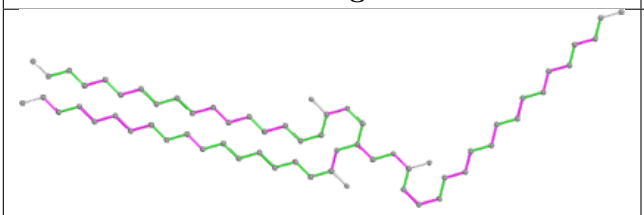
Ligand TGL D 201



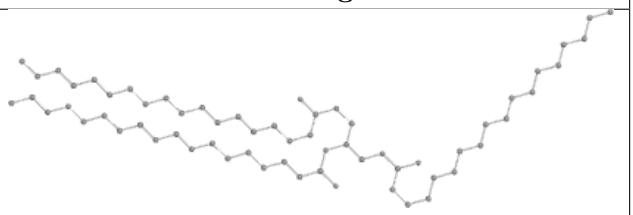
Bond lengths



Bond angles

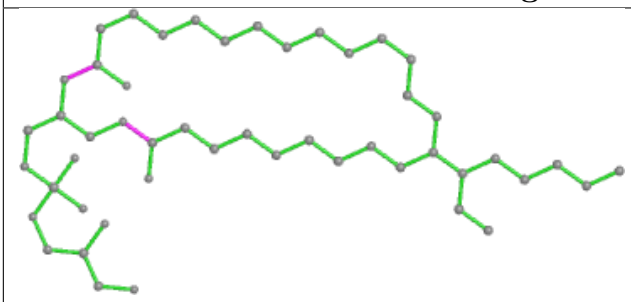


Torsions

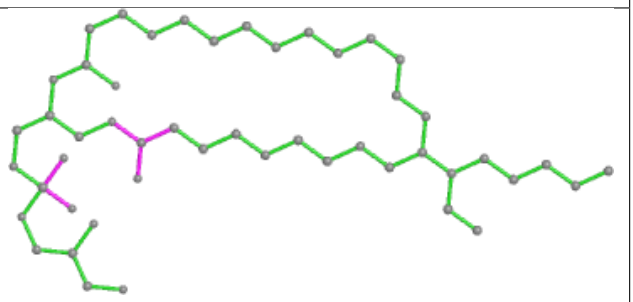


Rings

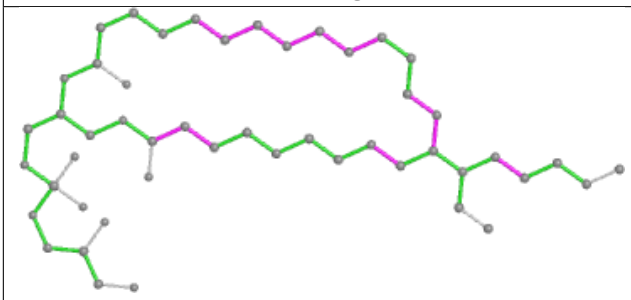
Ligand PGV A 607



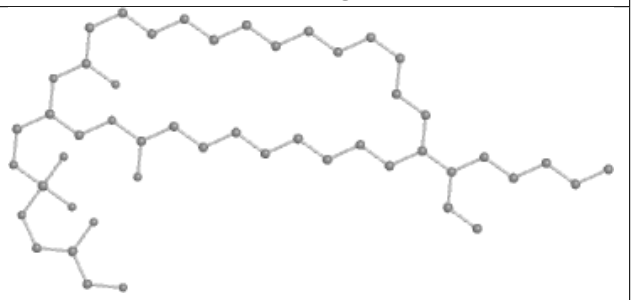
Bond lengths



Bond angles

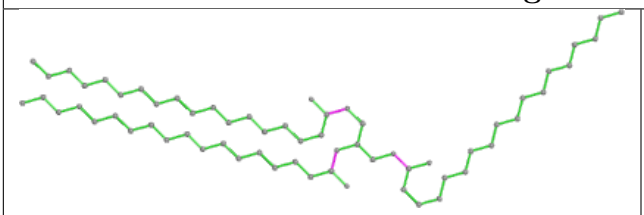


Torsions

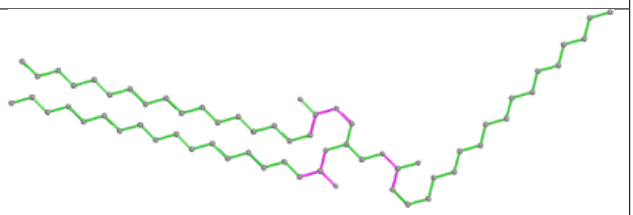


Rings

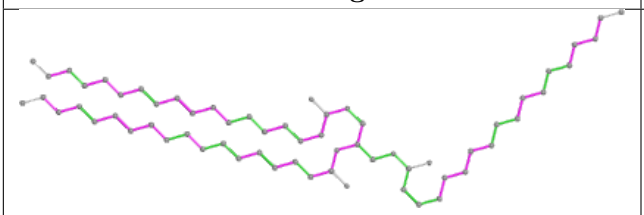
Ligand TGL A 609



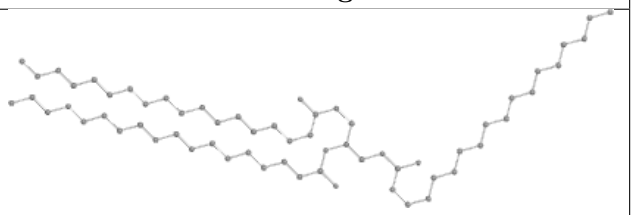
Bond lengths



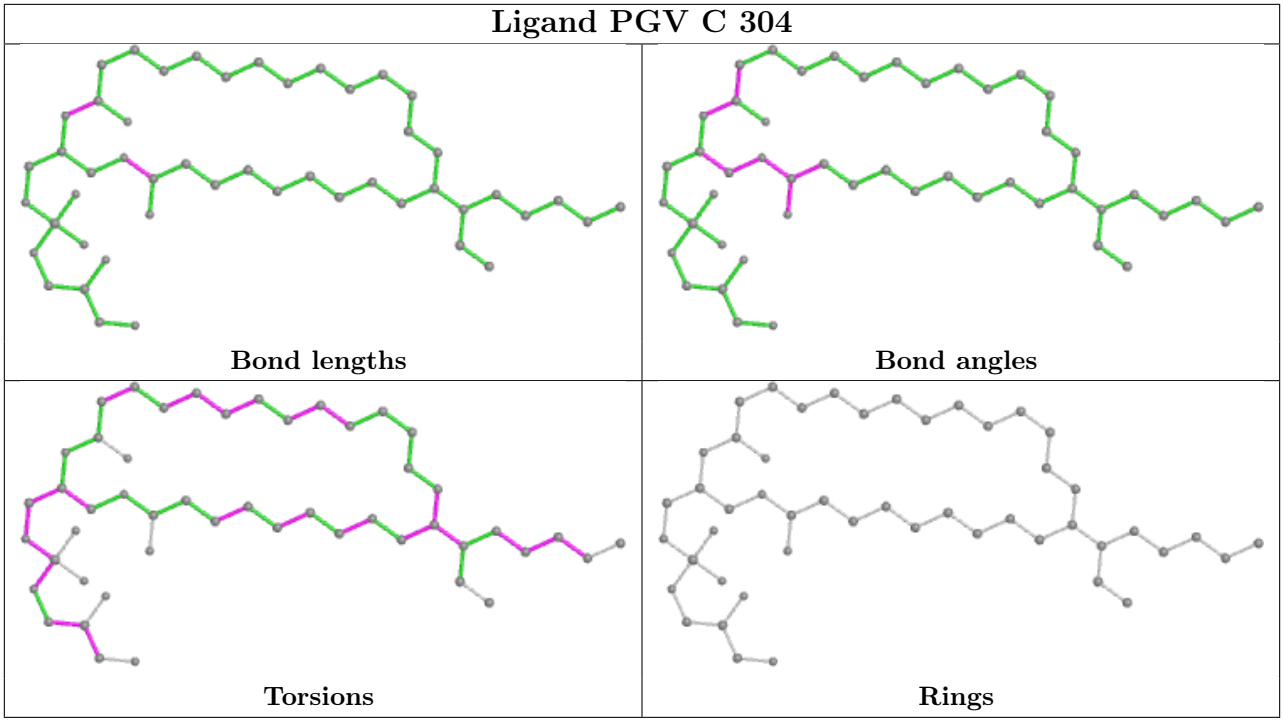
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

All (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
4	d	7	LYS	13.9
10	j	57	HIS	12.7
13	m	43	SER	11.6
4	d	6	VAL	11.3
6	F	97	ALA	11.3
6	f	98	HIS	10.5
6	F	98	HIS	10.4
7	G	2	SER	10.3
5	e	109	VAL	10.0
6	F	2	SER	9.9
8	h	8	ILE	9.9
6	F	1	ALA	9.8
7	G	3	ALA	9.1
6	F	94	HIS	8.5
6	f	1	ALA	8.1
10	J	57	HIS	7.6
5	E	5	HIS	7.5
8	H	45	ALA	7.4
10	J	58	LYS	7.2
7	g	1	ALA	7.2
7	g	3	ALA	7.1
13	m	42	LYS	7.1
4	d	33	LEU	7.0
6	f	94	HIS	7.0
11	k	7	PRO	6.9
7	G	10	GLY	6.7
12	l	47	LYS	6.6
7	G	36	TRP	6.4
13	M	43	SER	6.4

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Mol	Chain	Res	Type	RSRZ
7	g	41	HIS	6.3
7	g	10	GLY	6.3
9	I	37	PHE	6.2
8	h	45	ALA	6.2
4	d	147	LYS	6.1
9	i	37	PHE	6.0
7	g	36	TRP	5.9
5	e	5	HIS	5.8
2	b	227	LEU	5.8
6	F	95	GLN	5.8
7	G	1	ALA	5.7
6	f	95	GLN	5.6
7	G	40	GLY	5.6
8	H	8	ILE	5.6
2	b	113	TYR	5.6
7	G	5	LYS	5.5
8	H	47	GLY	5.4
7	G	9	GLY	5.4
4	d	8	SER	5.3
8	h	44	THR	5.3
10	j	52	TRP	5.2
11	k	13	TYR	5.2
7	g	5	LYS	5.2
7	g	40	GLY	5.2
8	h	10	ASN	5.1
10	J	1	PHE	5.1
2	b	90	ILE	5.0
10	j	48	TYR	5.0
6	f	2	SER	4.9
7	g	84	LYS	4.9
7	G	41	HIS	4.9
4	D	147	LYS	4.8
10	J	56	PRO	4.7
13	m	41	LYS	4.7
11	k	23	THR	4.6
9	i	2	THR	4.5
8	h	7	LYS	4.5
4	d	51	LEU	4.4
7	G	39	SER	4.4
4	d	48	TRP	4.4
5	E	109	VAL	4.4
11	k	6	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
7	G	43	GLU	4.4
8	H	50	VAL	4.4
7	g	8	HIS	4.3
7	g	2	SER	4.3
7	G	42	ARG	4.2
7	G	84	LYS	4.2
3	c	3	HIS	4.1
8	h	48	GLY	4.1
11	K	7	PRO	4.1
7	G	37	LEU	4.0
10	J	52	TRP	4.0
7	g	4	ALA	4.0
4	d	39	ALA	4.0
3	C	3	HIS	4.0
9	i	26	MET	3.9
8	h	9	LYS	3.9
10	j	1	PHE	3.9
7	g	42	ARG	3.9
7	G	6	GLY	3.9
5	e	108	LYS	3.8
10	j	30	ILE	3.8
9	i	25	PHE	3.8
11	K	42	PRO	3.8
4	d	46	ALA	3.8
5	e	96	LEU	3.8
11	k	12	LYS	3.7
4	d	58	GLU	3.7
2	B	90	ILE	3.7
11	k	19	ALA	3.5
13	M	42	LYS	3.5
8	H	48	GLY	3.5
1	a	381	LEU	3.5
9	I	34	PHE	3.5
7	g	39	SER	3.5
8	H	44	THR	3.4
9	i	34	PHE	3.4
4	d	128	VAL	3.4
11	k	18	LEU	3.4
11	K	6	ALA	3.4
2	b	218	TYR	3.4
8	H	10	ASN	3.4
10	j	56	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
10	j	27	THR	3.4
2	b	170	LEU	3.4
2	b	224	ALA	3.3
10	J	55	PHE	3.3
9	I	30	GLY	3.3
8	H	85	ILE	3.3
6	F	22	LEU	3.3
2	b	221	LYS	3.2
11	k	26	VAL	3.2
5	e	92	THR	3.2
13	m	40	TYR	3.2
11	k	47	ARG	3.2
3	c	37	PHE	3.2
9	I	25	PHE	3.2
8	H	42	ALA	3.2
9	I	29	LEU	3.2
9	I	33	THR	3.2
13	M	39	ASN	3.2
8	h	42	ALA	3.1
11	k	16	ALA	3.1
7	G	45	PRO	3.1
12	L	47	LYS	3.1
1	A	381	LEU	3.1
9	i	33	THR	3.1
12	L	2	HIS	3.0
6	f	27	GLY	3.0
13	m	39	ASN	3.0
11	k	9	PHE	3.0
7	g	82	TYR	3.0
9	I	26	MET	3.0
1	A	70	VAL	3.0
1	a	366	VAL	3.0
4	d	34	SER	3.0
4	d	49	SER	3.0
4	d	10	ASP	3.0
10	j	55	PHE	3.0
8	H	46	LYS	3.0
10	j	26	ALA	3.0
8	h	49	ASP	3.0
13	M	40	TYR	2.9
7	G	7	ASP	2.9
13	m	35	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
6	f	22	LEU	2.9
2	B	170	LEU	2.9
7	g	43	GLU	2.9
4	d	102	TYR	2.9
9	I	53	ASN	2.9
8	h	52	VAL	2.8
10	j	24	GLY	2.8
11	k	17	VAL	2.8
11	k	20	SER	2.8
13	m	13	LYS	2.8
4	d	40	LEU	2.8
7	g	45	PRO	2.8
4	d	101	HIS	2.8
11	k	8	ASP	2.7
4	d	142	LYS	2.7
11	k	34	THR	2.7
9	i	31	PHE	2.7
7	g	7	ASP	2.7
9	i	30	GLY	2.7
1	a	73	ILE	2.6
8	H	43	MET	2.6
4	d	35	ALA	2.6
4	d	53	ILE	2.6
8	h	55	TRP	2.6
4	d	9	GLU	2.6
6	f	44	GLU	2.6
8	h	47	GLY	2.6
9	i	29	LEU	2.6
10	j	4	ARG	2.6
7	G	4	ALA	2.6
7	g	6	GLY	2.6
1	A	73	ILE	2.6
3	c	38	ASN	2.6
8	H	7	LYS	2.5
5	e	7	THR	2.5
7	g	38	HIS	2.5
2	b	217	LYS	2.5
12	l	38	PHE	2.5
6	f	93	PRO	2.5
1	a	70	VAL	2.5
11	k	46	GLY	2.5
7	G	8	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
4	d	43	LYS	2.5
1	A	513	LEU	2.4
9	i	57	MET	2.4
6	f	43	LYS	2.4
7	g	37	LEU	2.4
1	A	66	ILE	2.4
1	a	433	LEU	2.4
5	e	94	ASN	2.4
1	a	203	ALA	2.4
2	b	59	GLN	2.4
2	b	65	TRP	2.4
4	D	78	TRP	2.4
10	j	58	LYS	2.4
2	b	165	VAL	2.4
12	l	20	ARG	2.3
11	k	31	TYR	2.3
10	j	2	GLU	2.3
4	d	141	ASP	2.3
4	d	38	LYS	2.3
9	i	53	ASN	2.3
12	l	45	LEU	2.3
2	B	168	LEU	2.3
8	h	84	LYS	2.3
2	B	113	TYR	2.2
11	k	35	GLN	2.2
7	G	38	HIS	2.2
1	A	382	SER	2.2
1	A	380	VAL	2.2
5	E	9	GLU	2.2
7	G	35	SER	2.2
2	B	91	ASN	2.2
10	j	50	LEU	2.2
4	d	31	LYS	2.2
8	h	43	MET	2.1
4	d	42	GLU	2.1
11	k	22	ALA	2.1
11	k	24	PHE	2.1
1	a	380	VAL	2.1
5	e	10	GLU	2.1
4	d	54	ASP	2.1
1	a	136	LEU	2.1
1	a	462	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
7	g	49	PRO	2.1
1	a	66	ILE	2.1
1	a	206	ILE	2.1
11	k	52	GLU	2.1
9	i	32	ALA	2.1
7	g	9	GLY	2.1
4	d	47	SER	2.1
11	k	11	ASP	2.1
6	F	3	GLY	2.1
5	e	23	ASP	2.0
8	h	11	TYR	2.0
1	A	374	VAL	2.0
6	f	25	ARG	2.0
1	a	365	ILE	2.0
3	c	33	MET	2.0
11	k	14	GLY	2.0
13	m	32	TRP	2.0
8	H	49	ASP	2.0
9	i	52	ARG	2.0
10	j	33	ARG	2.0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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

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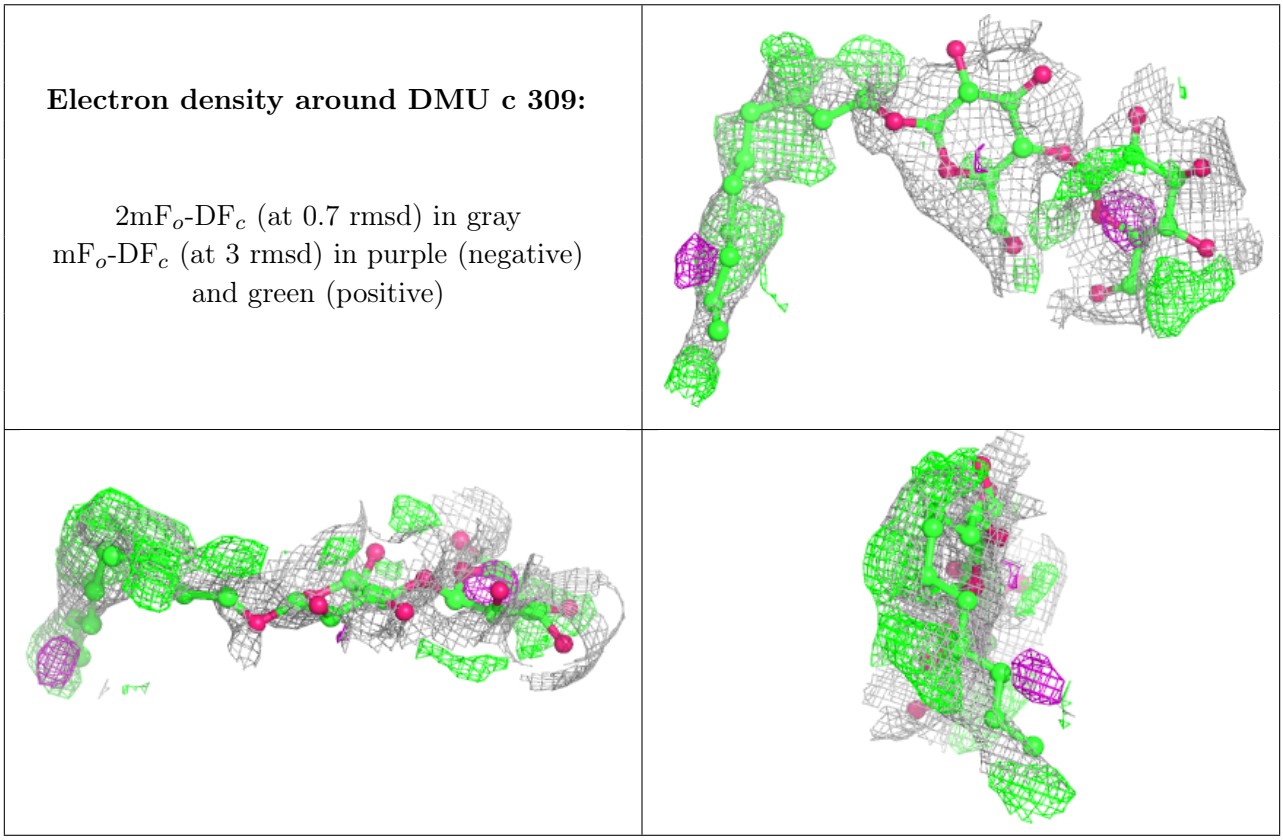
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	PEK	C	302	53/53	0.95	0.22	31,53,83,89	0
14	HEA	a	601	60/60	0.96	0.18	32,37,55,62	0
14	HEA	a	602	60/60	0.96	0.16	29,32,40,43	0
22	CHD	c	303	29/29	0.96	0.08	34,36,40,41	0
18	PGV	a	607	51/51	0.96	0.20	32,48,74,83	0
18	PGV	A	607	51/51	0.96	0.18	25,42,65,69	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.

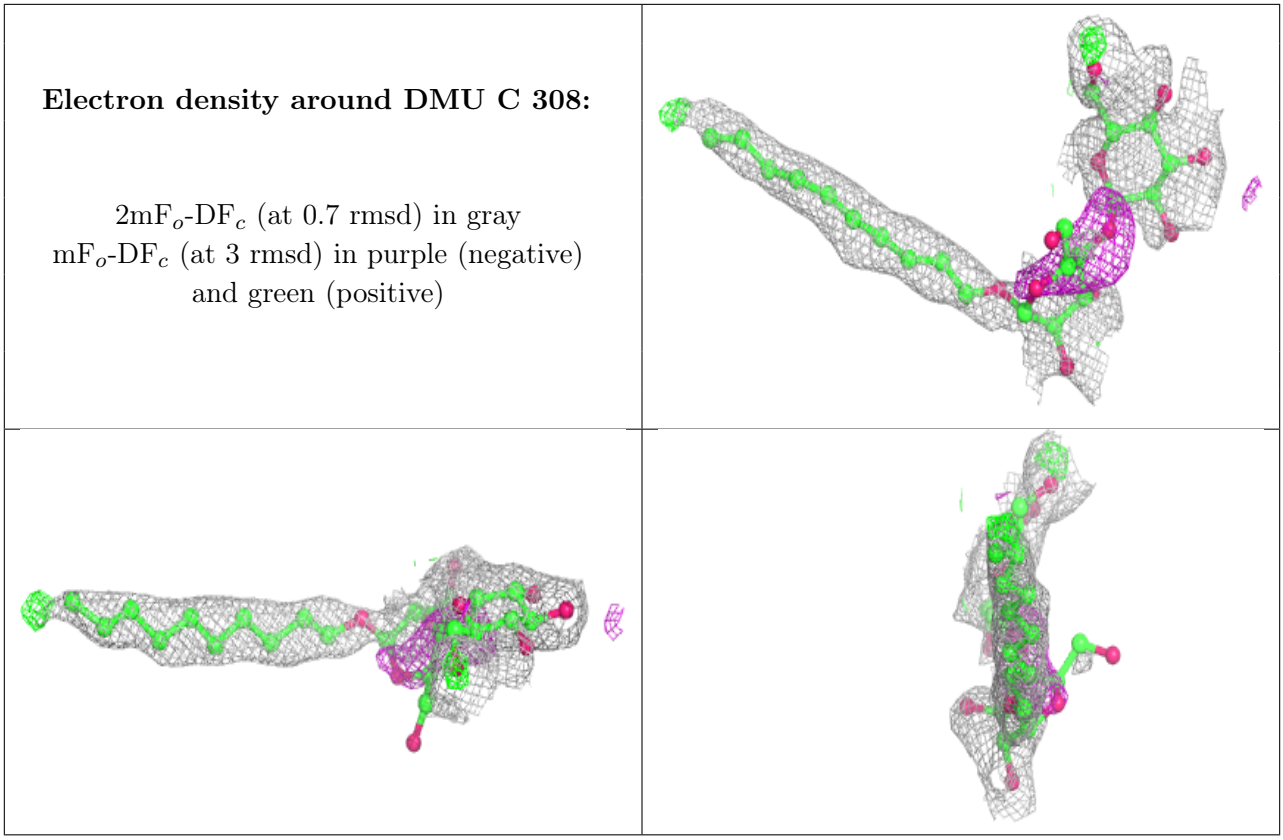
Electron density around DMU c 309:

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



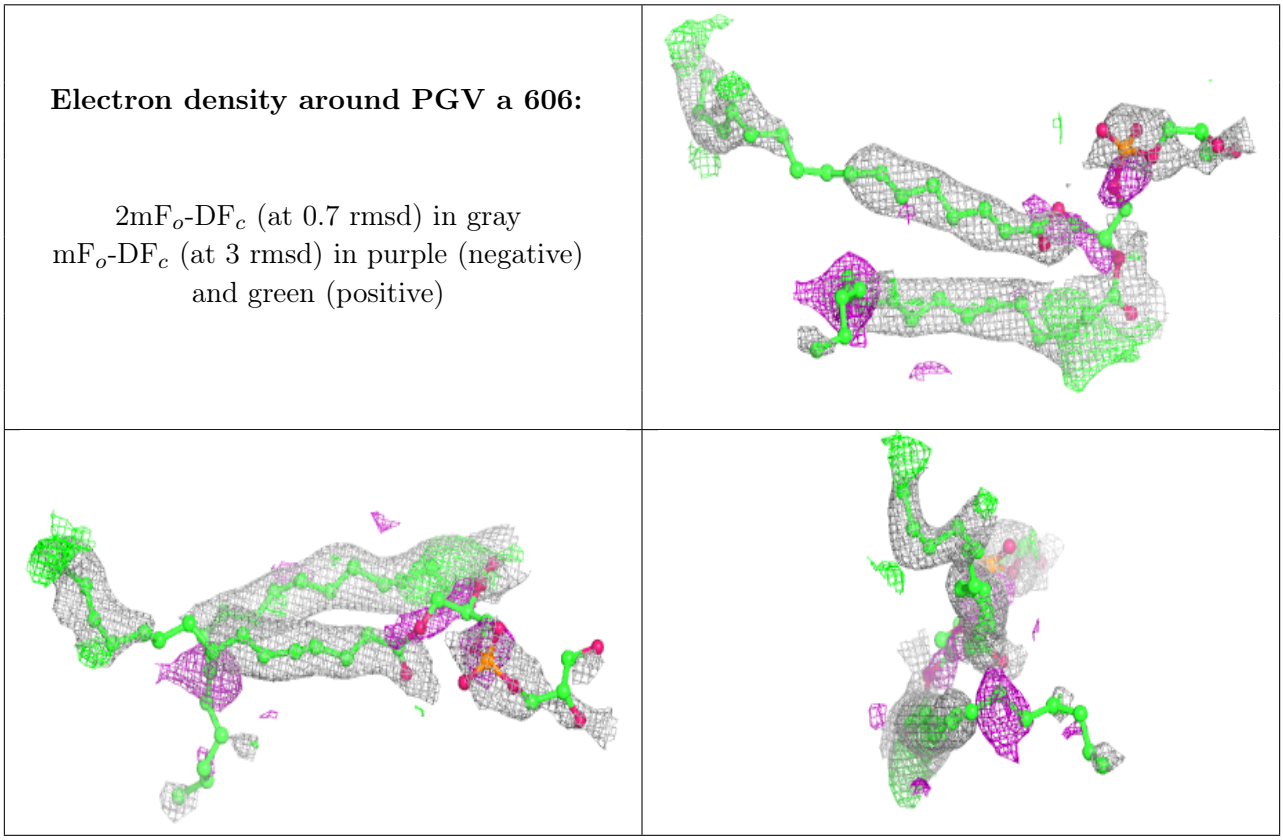
Electron density around DMU C 308:

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



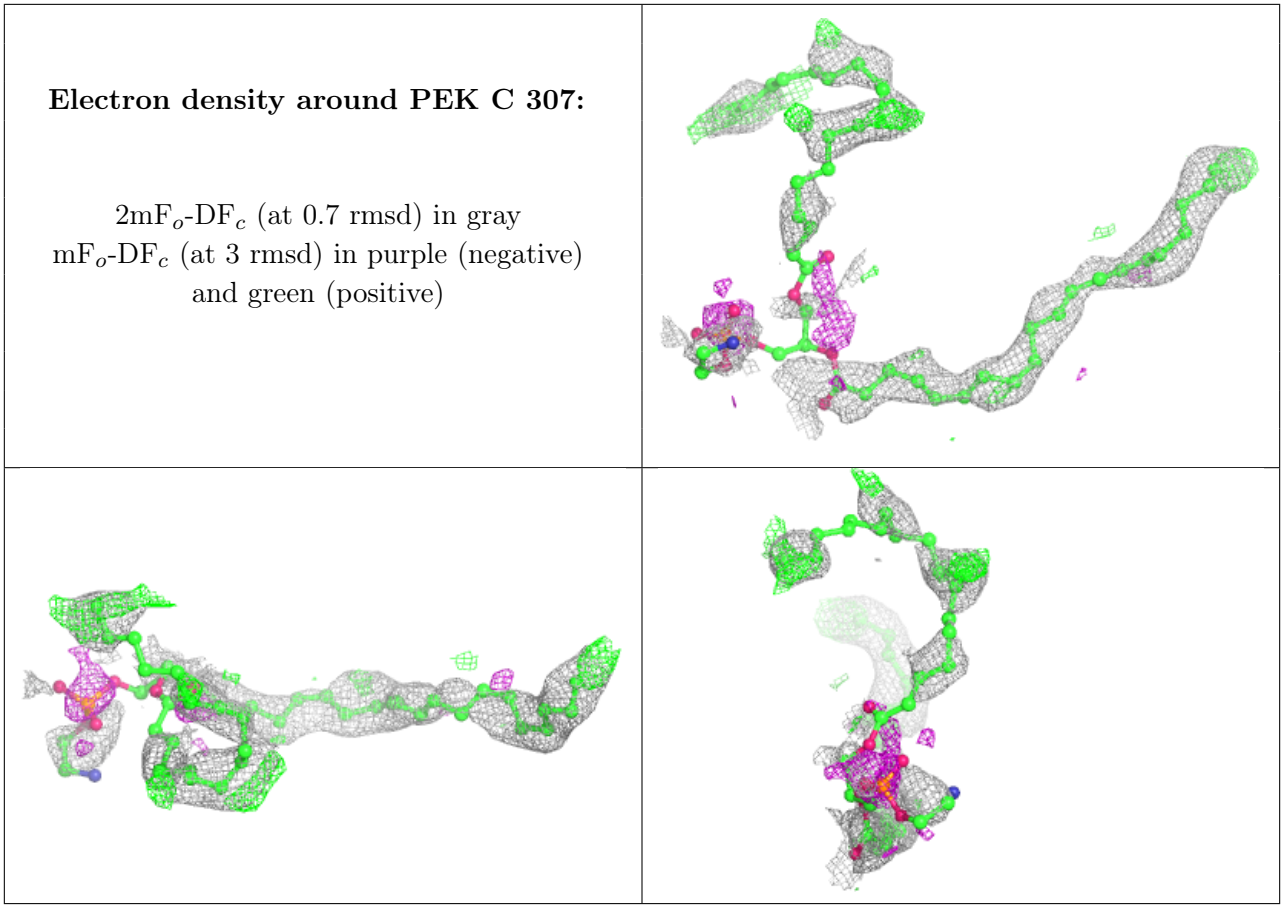
Electron density around PGV a 606:

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



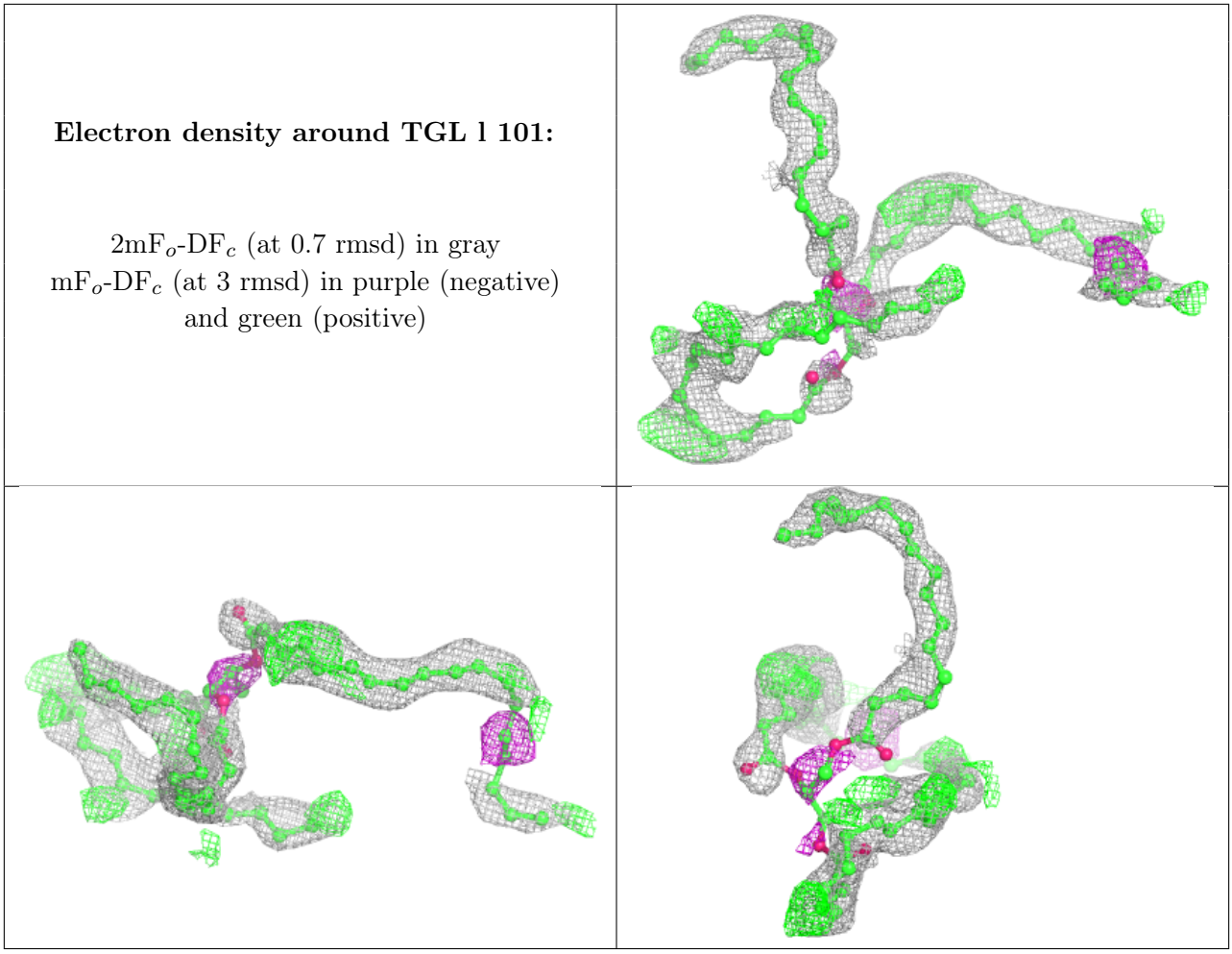
Electron density around PEK C 307:

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



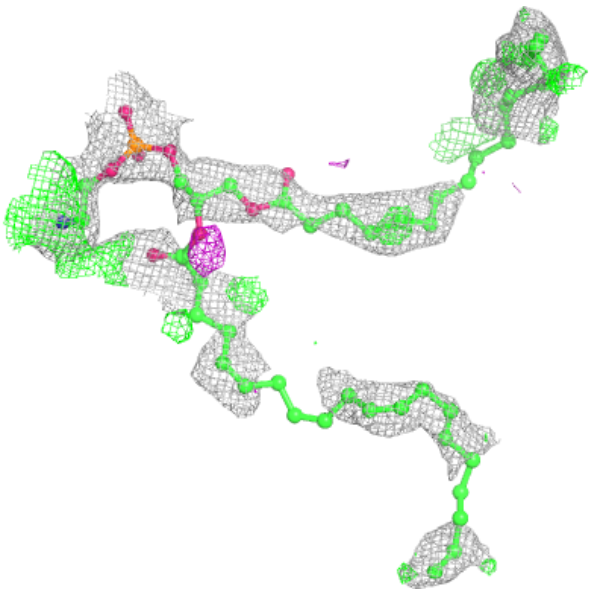
Electron density around TGL l 101:

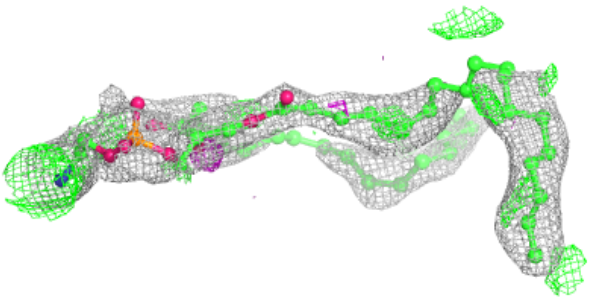
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

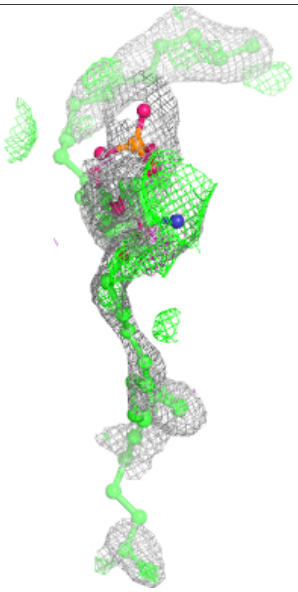


Electron density around PEK c 305:

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

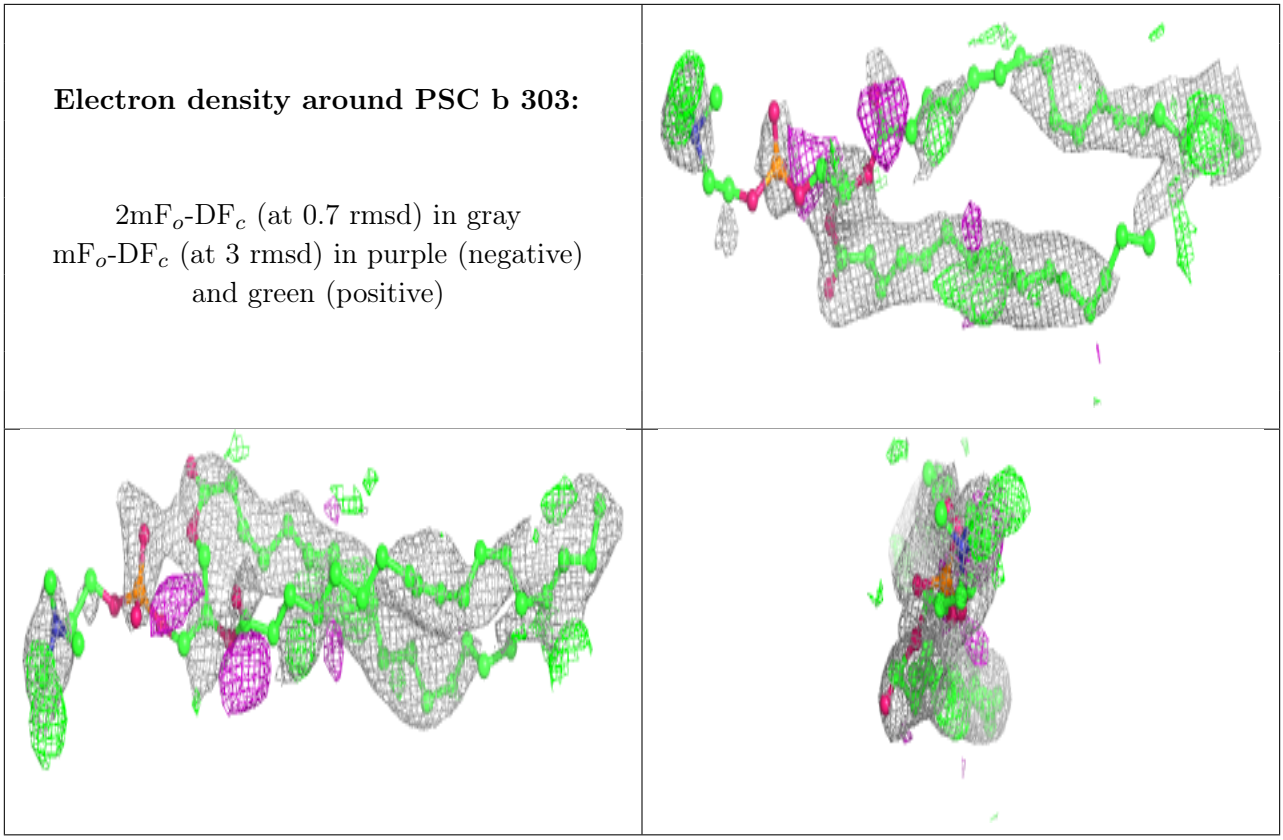






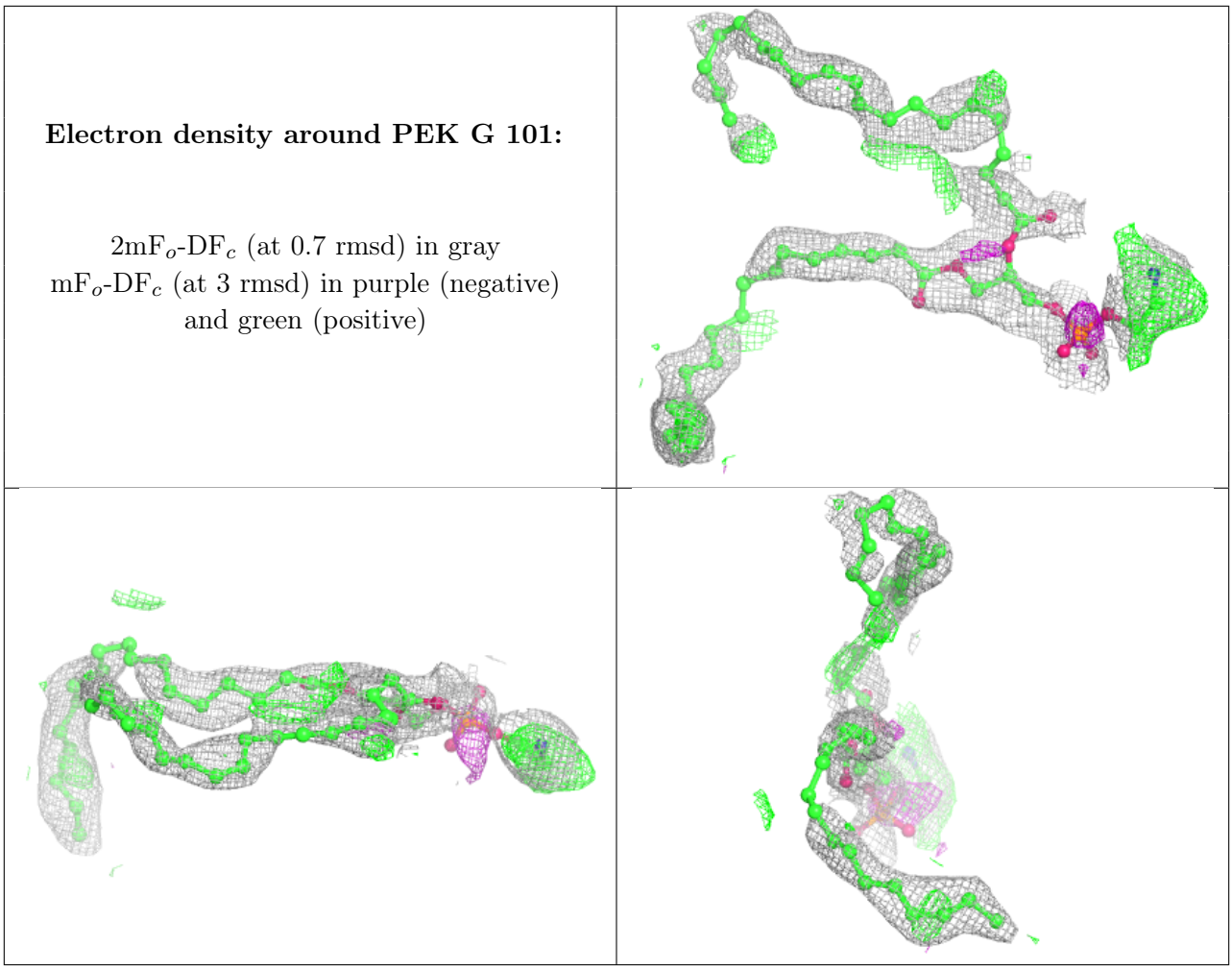
Electron density around PSC b 303:

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



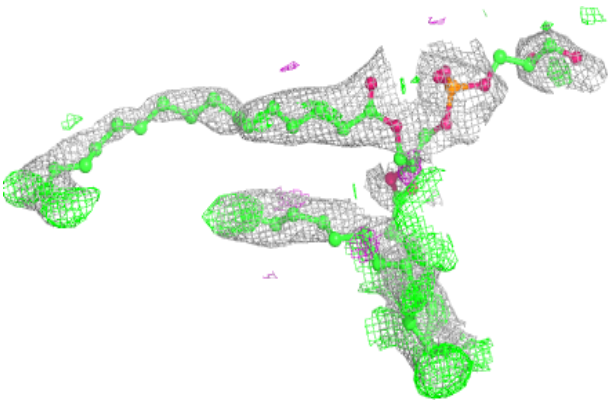
Electron density around PEK G 101:

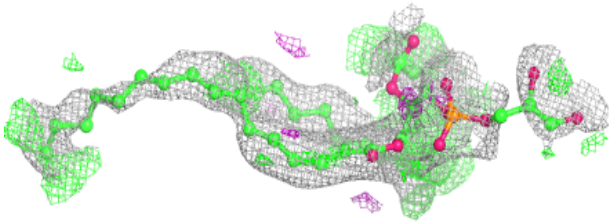
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

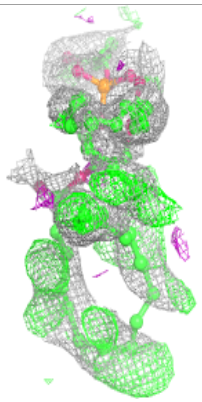


Electron density around PGV c 302:

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

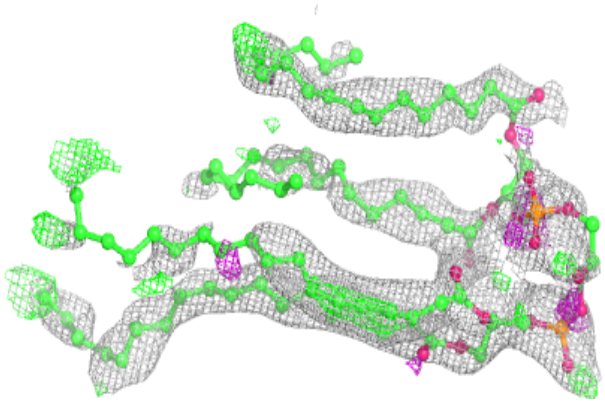


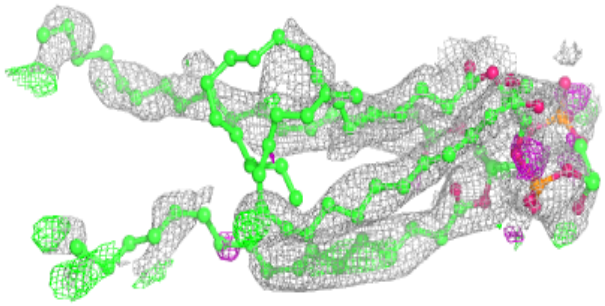


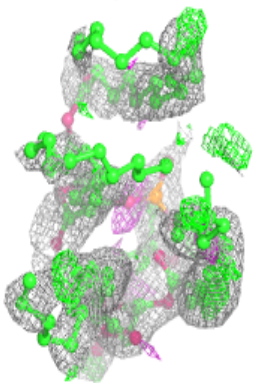


Electron density around CDL c 307:

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

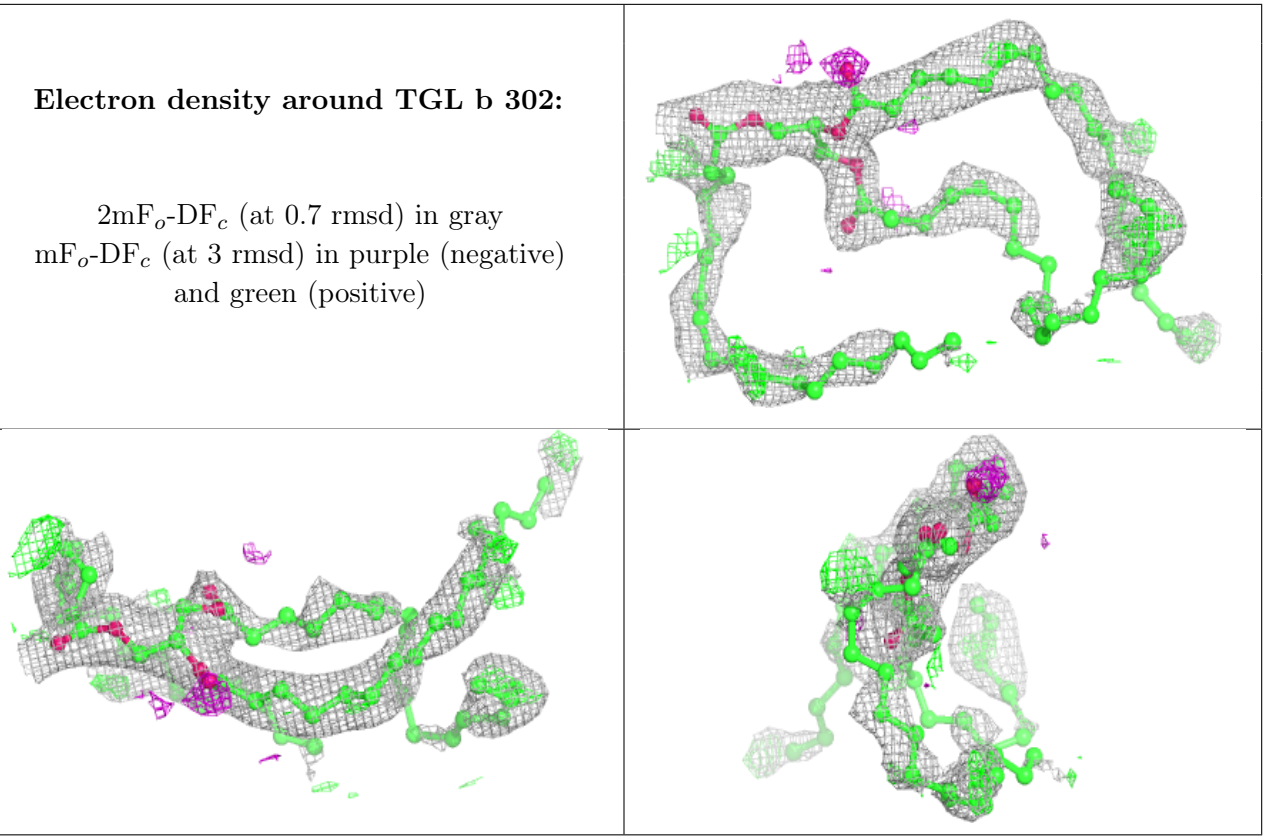






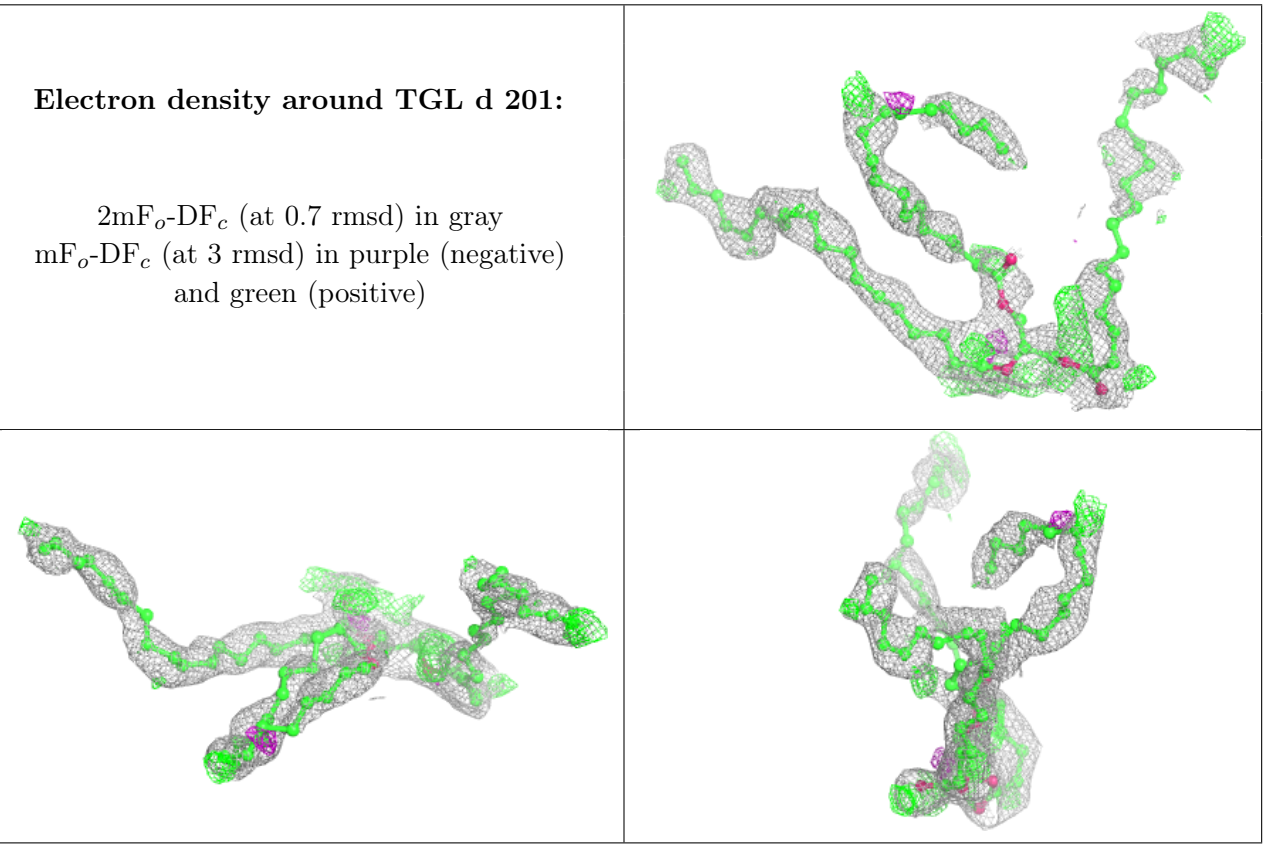
Electron density around TGL b 302:

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



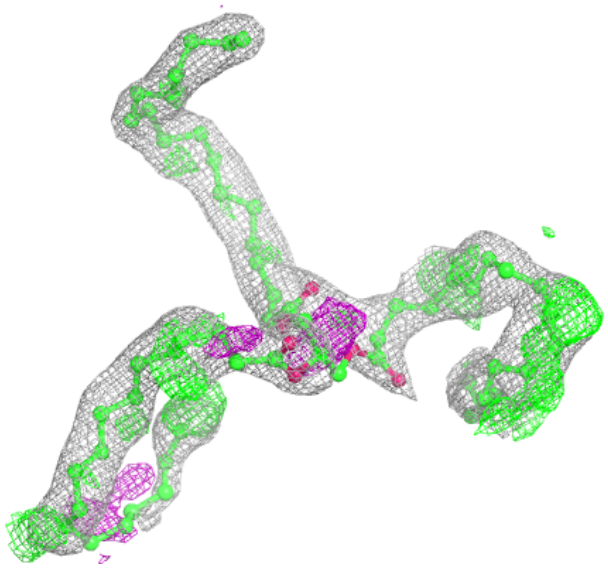
Electron density around TGL d 201:

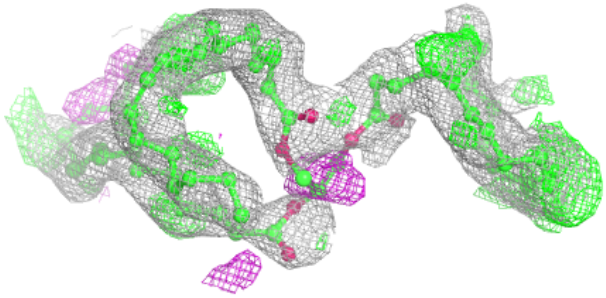
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

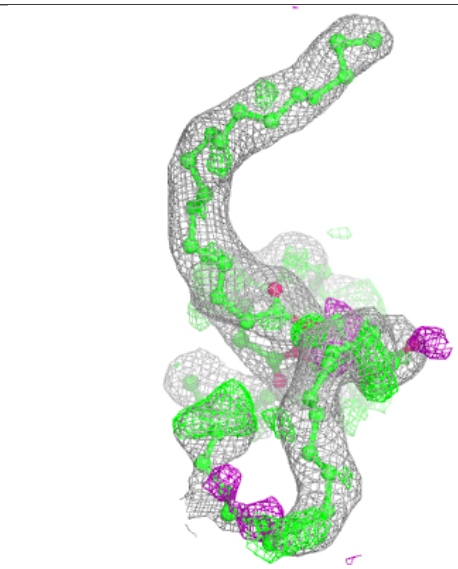


Electron density around TGL A 609:

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

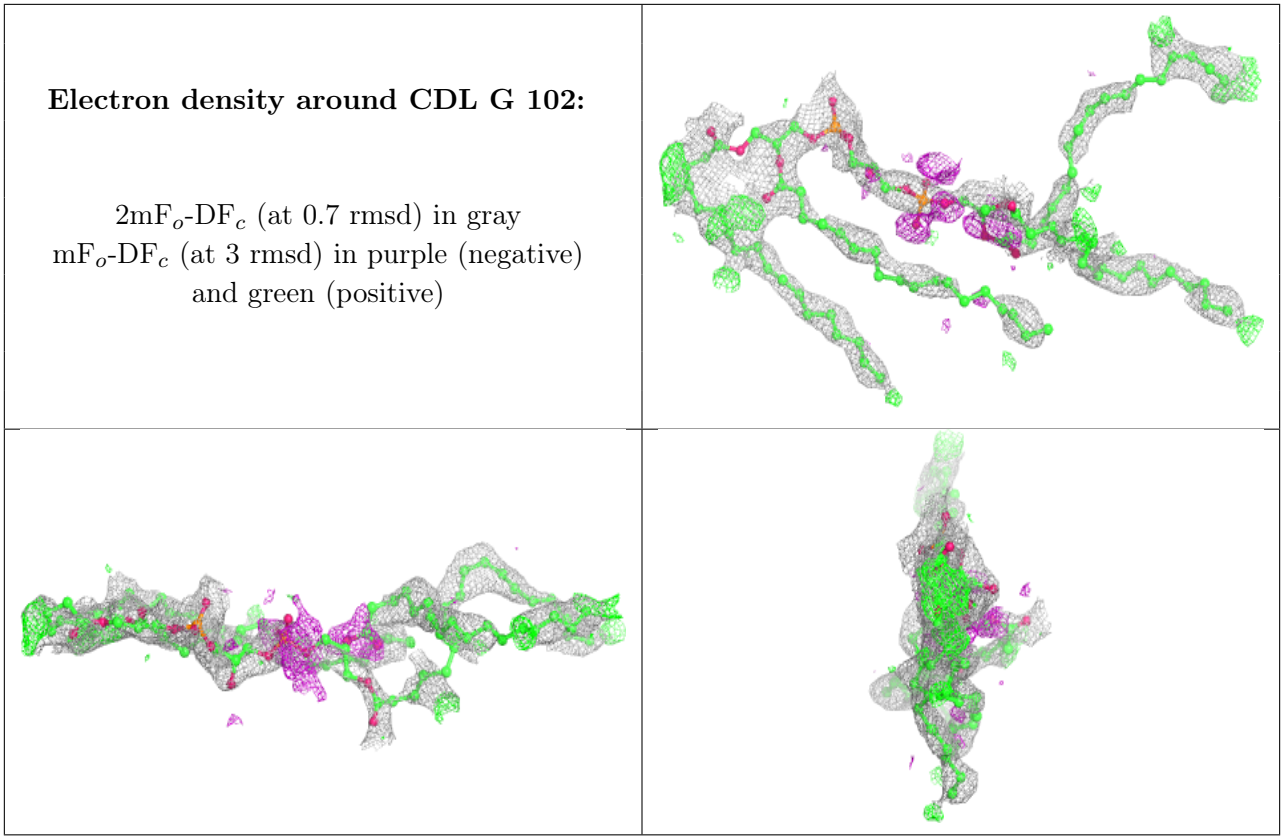






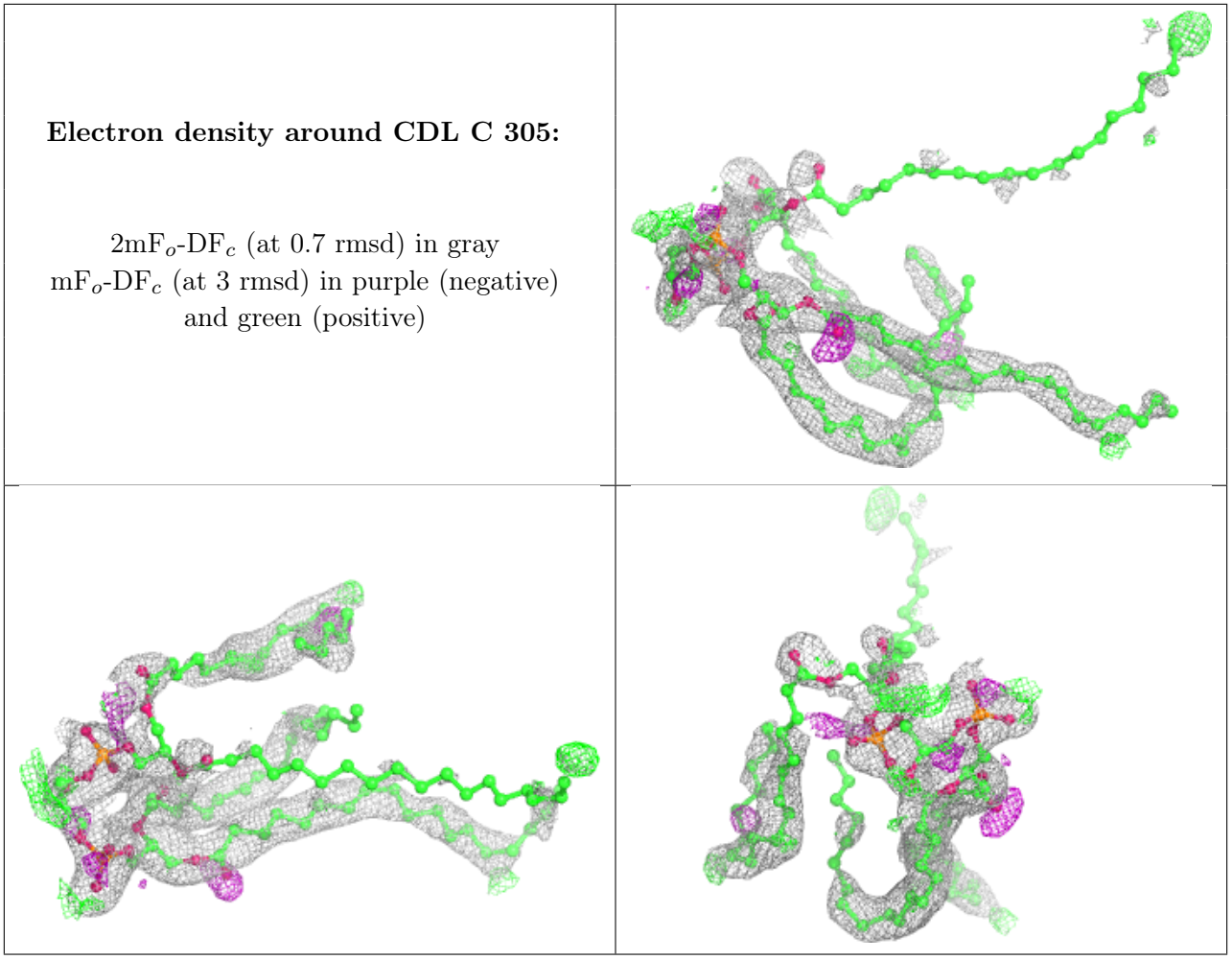
Electron density around CDL G 102:

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



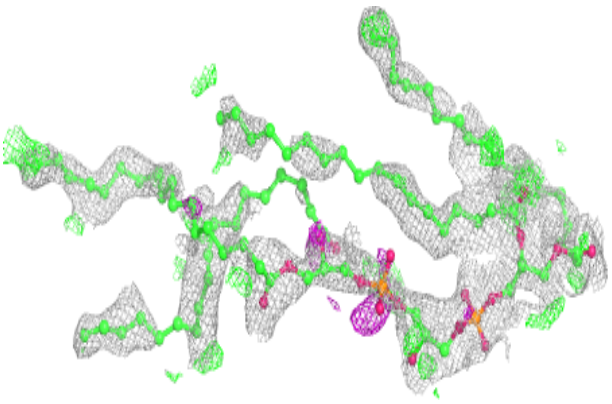
Electron density around CDL C 305:

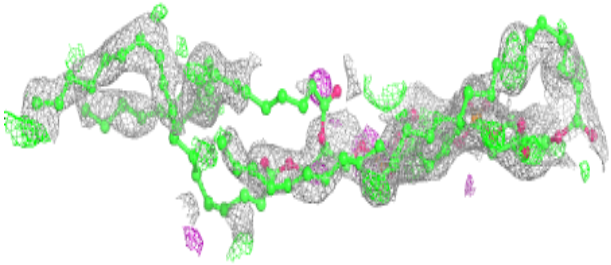
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

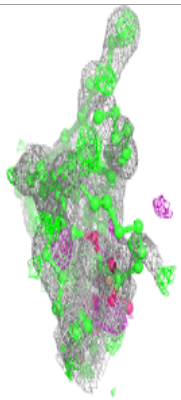


Electron density around CDL g 101:

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

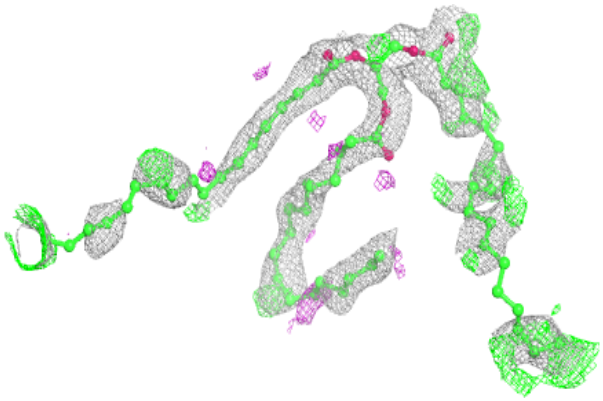


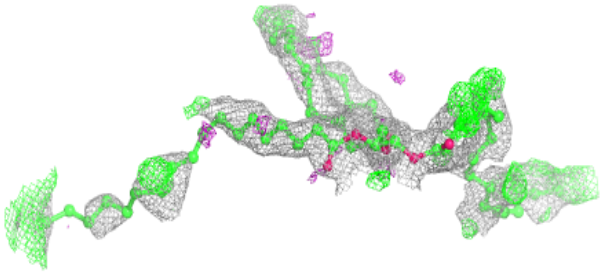


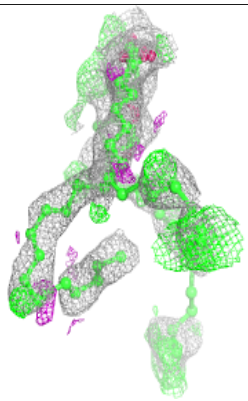


Electron density around TGL D 201:

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

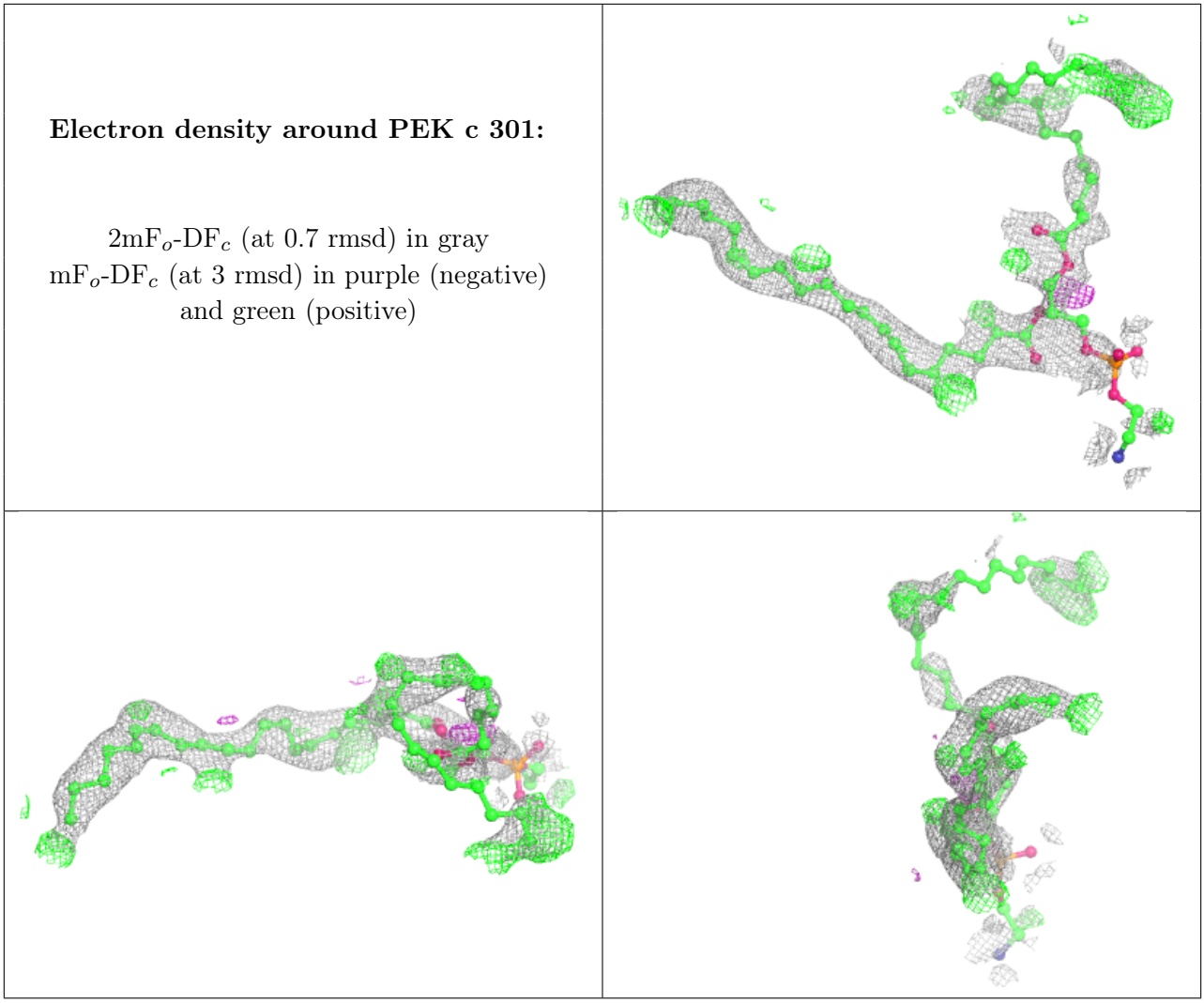






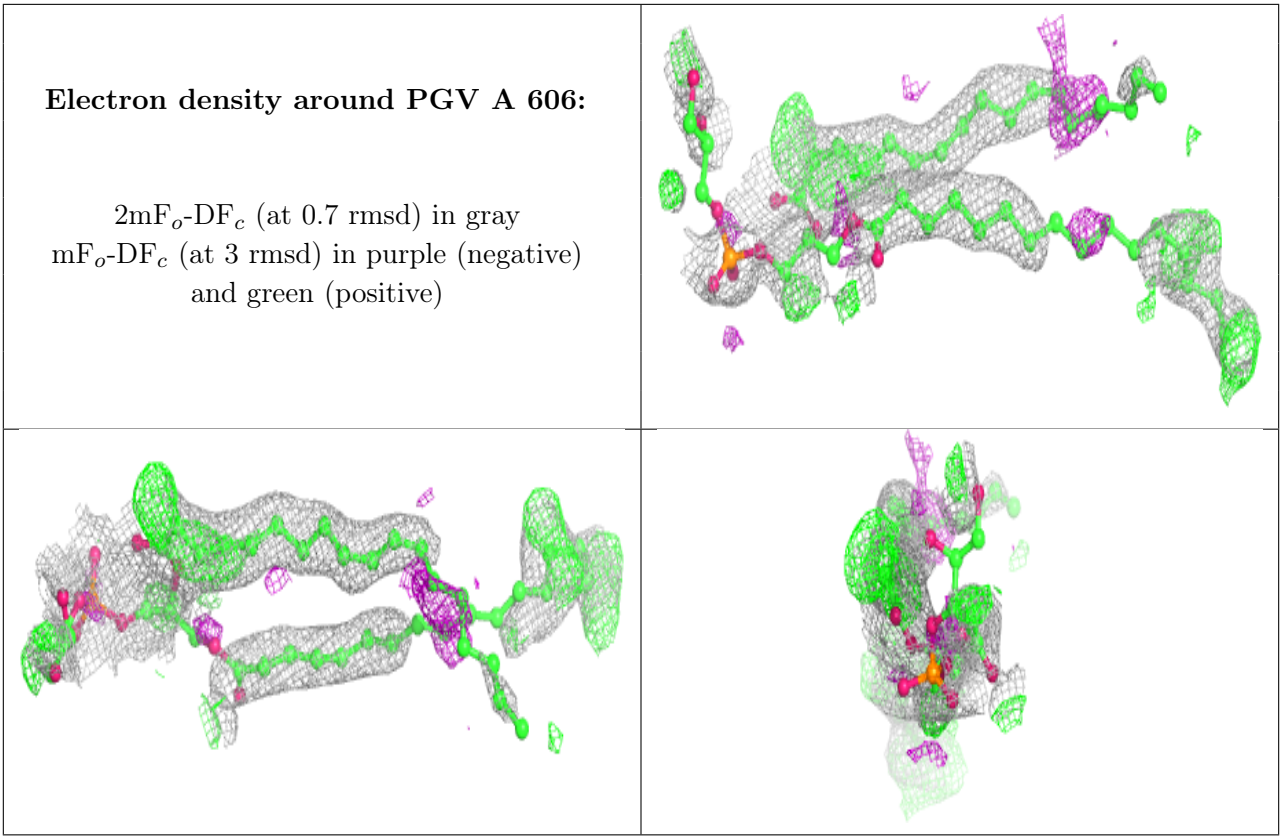
Electron density around PEK c 301:

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



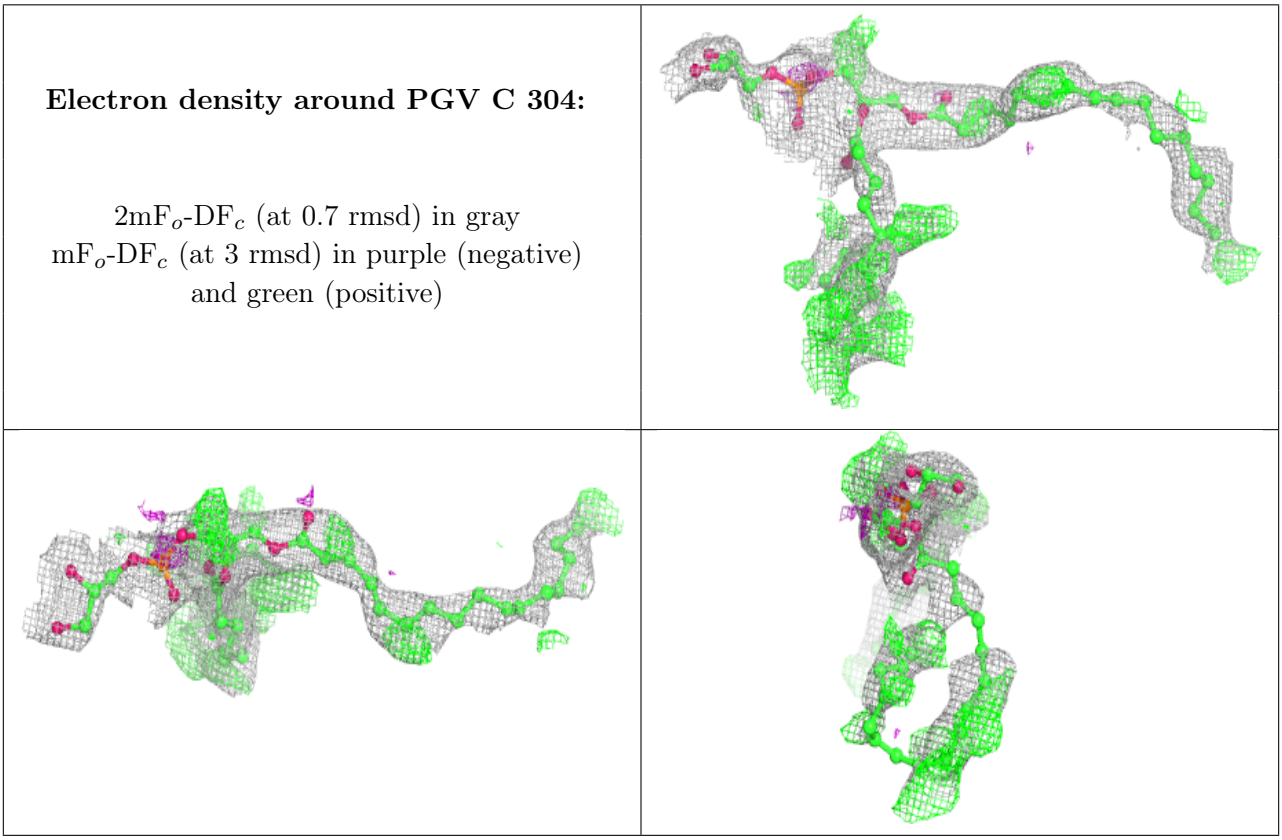
Electron density around PGV A 606:

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



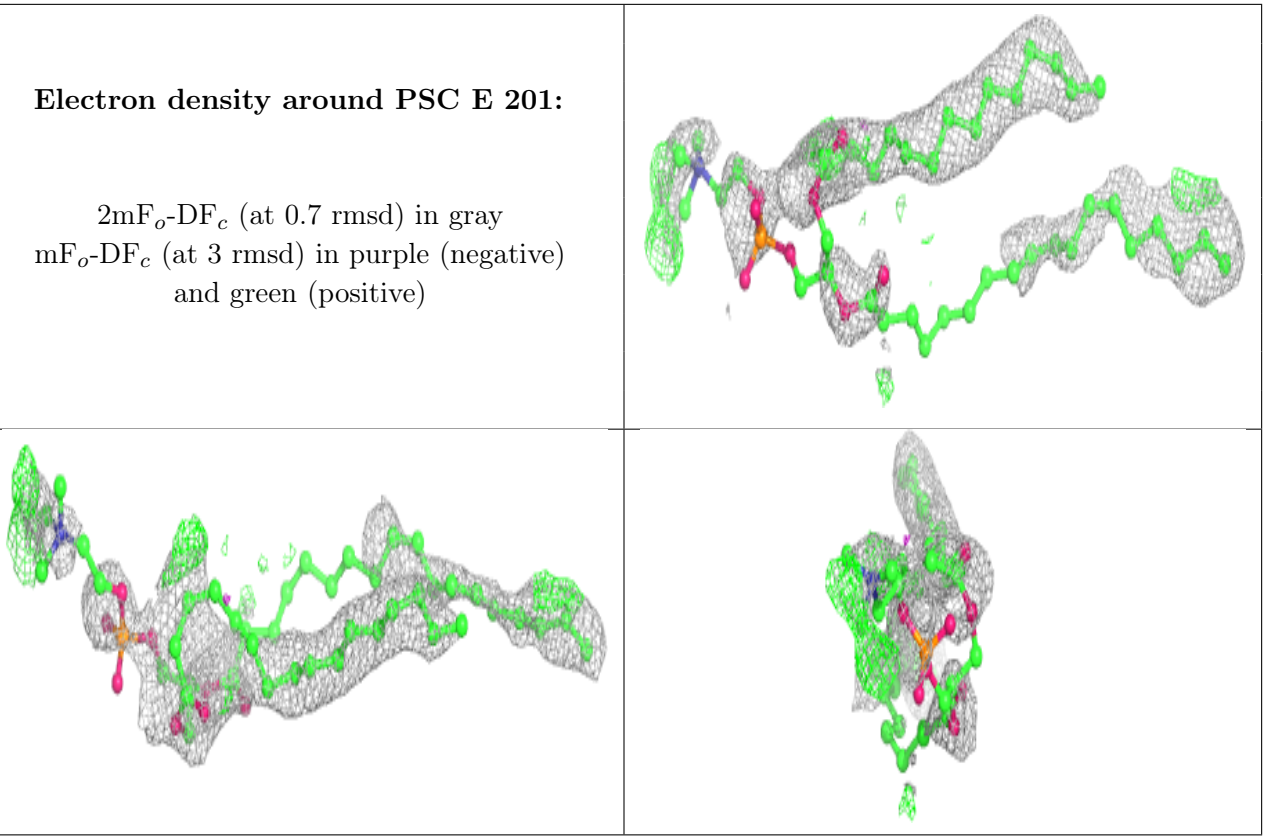
Electron density around PGV C 304:

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



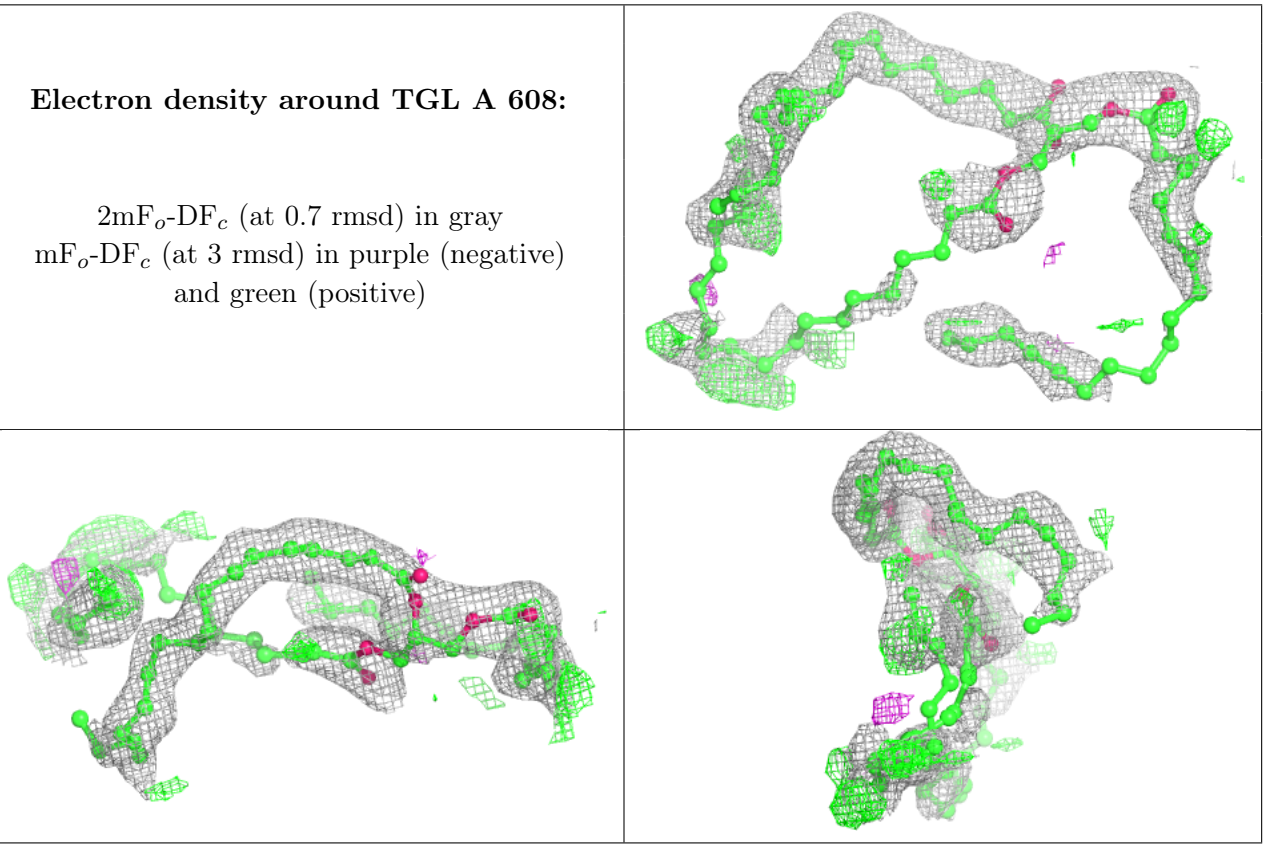
Electron density around PSC E 201:

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



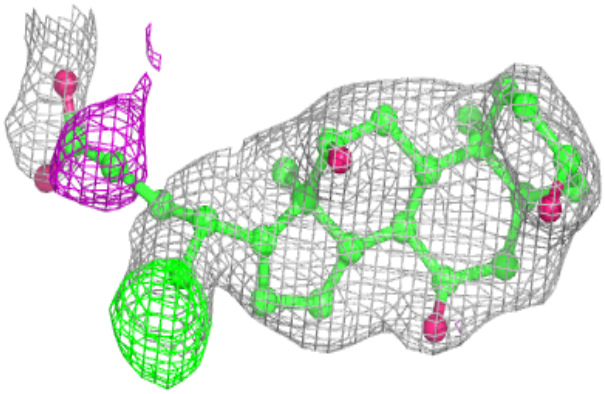
Electron density around TGL A 608:

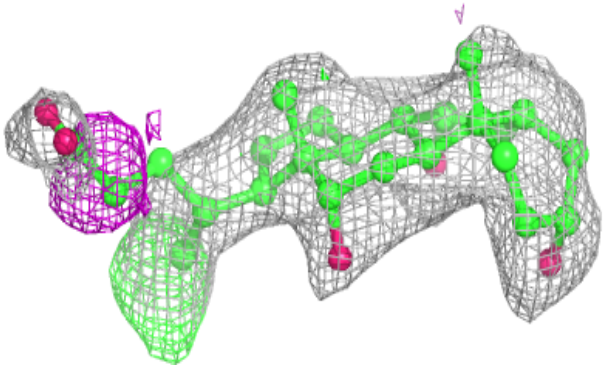
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

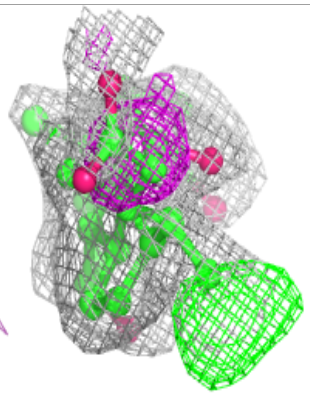


Electron density around CHD J 101:

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

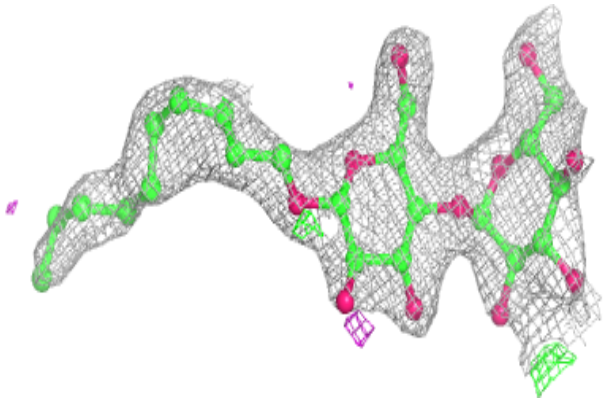


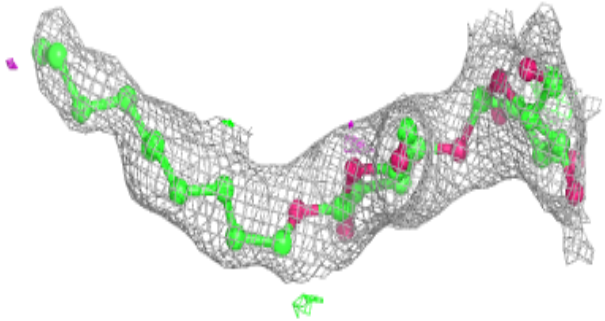


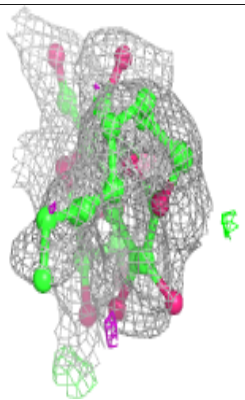


Electron density around DMU m 101:

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

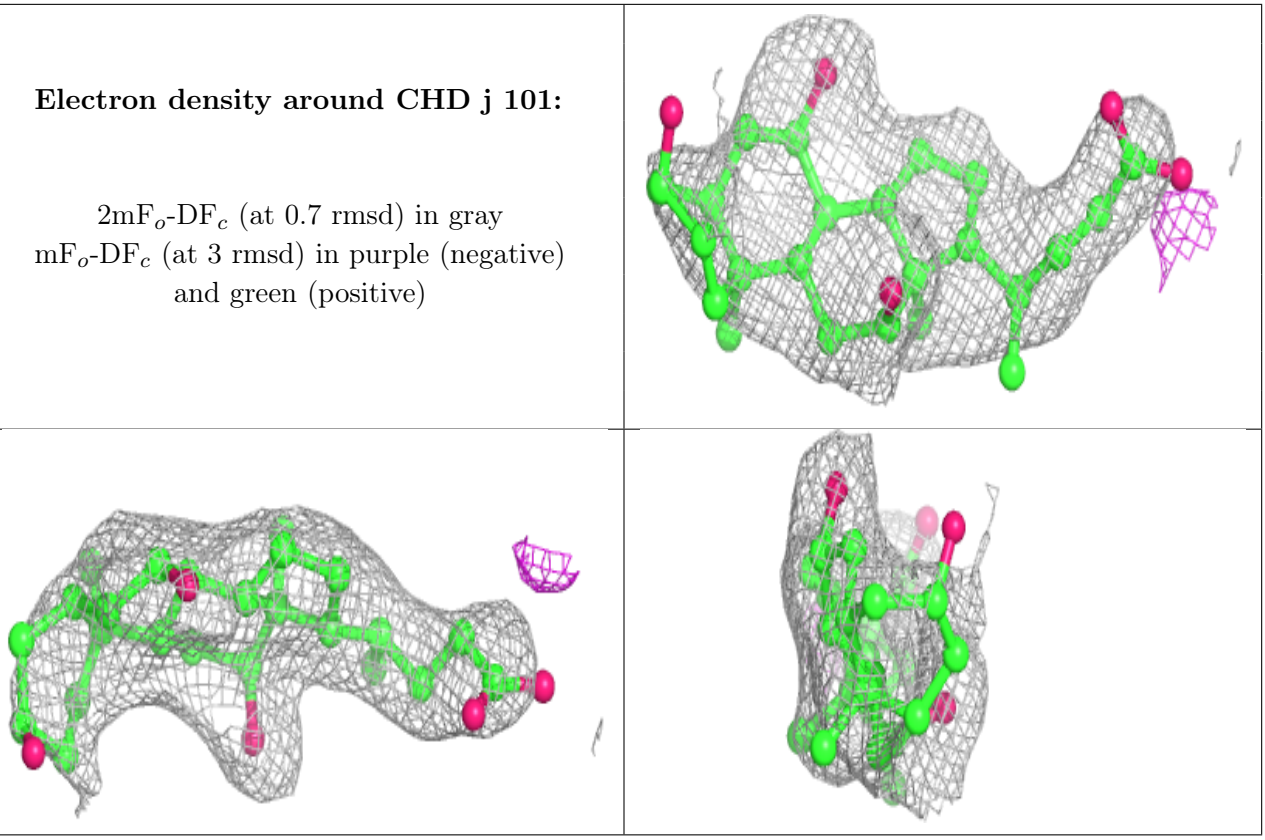






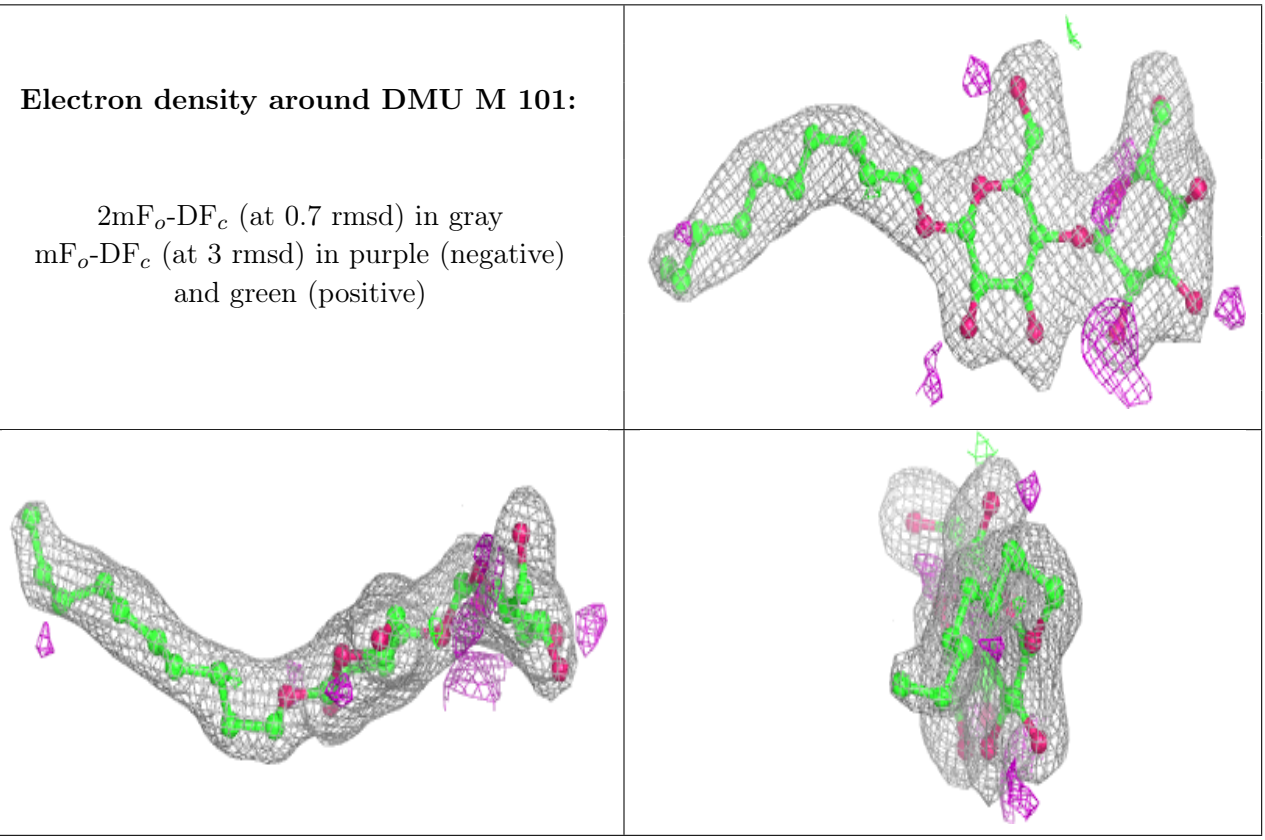
Electron density around CHD j 101:

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



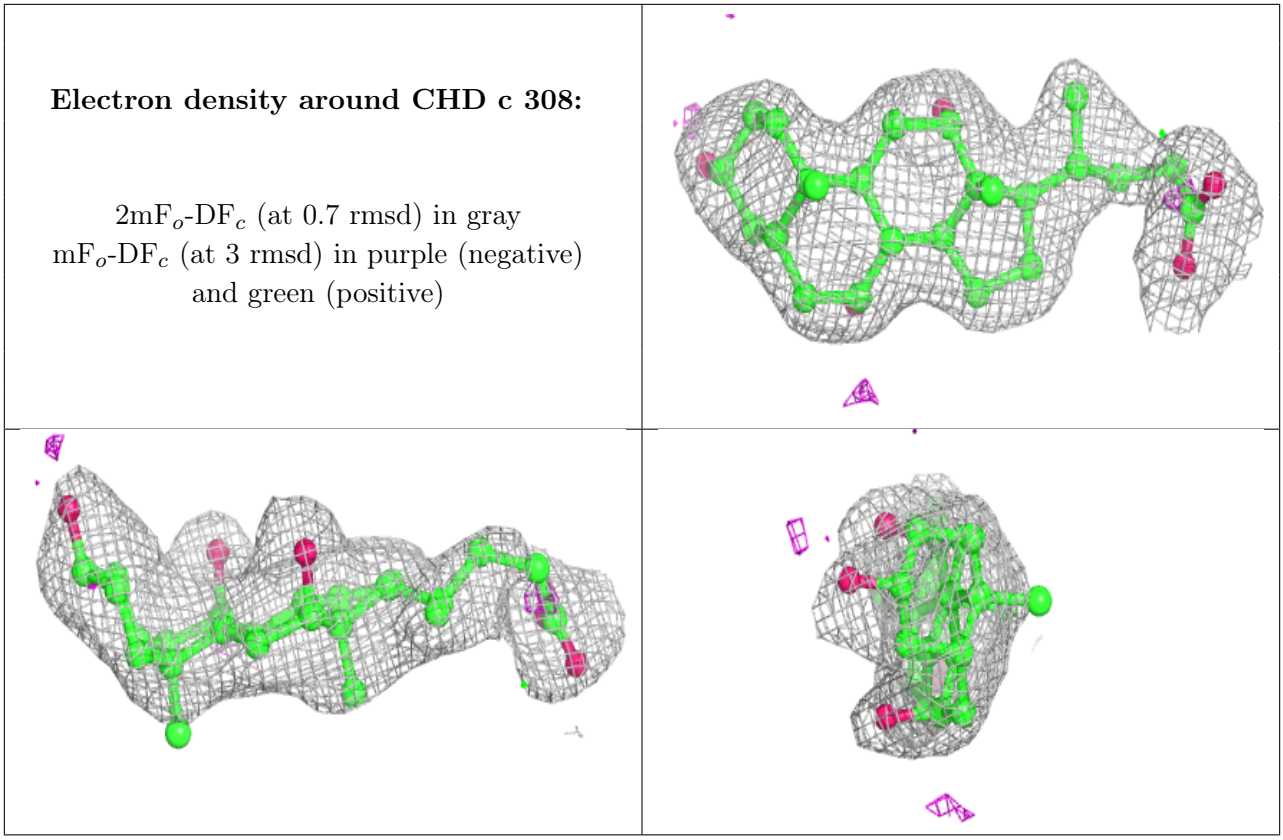
Electron density around DMU M 101:

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



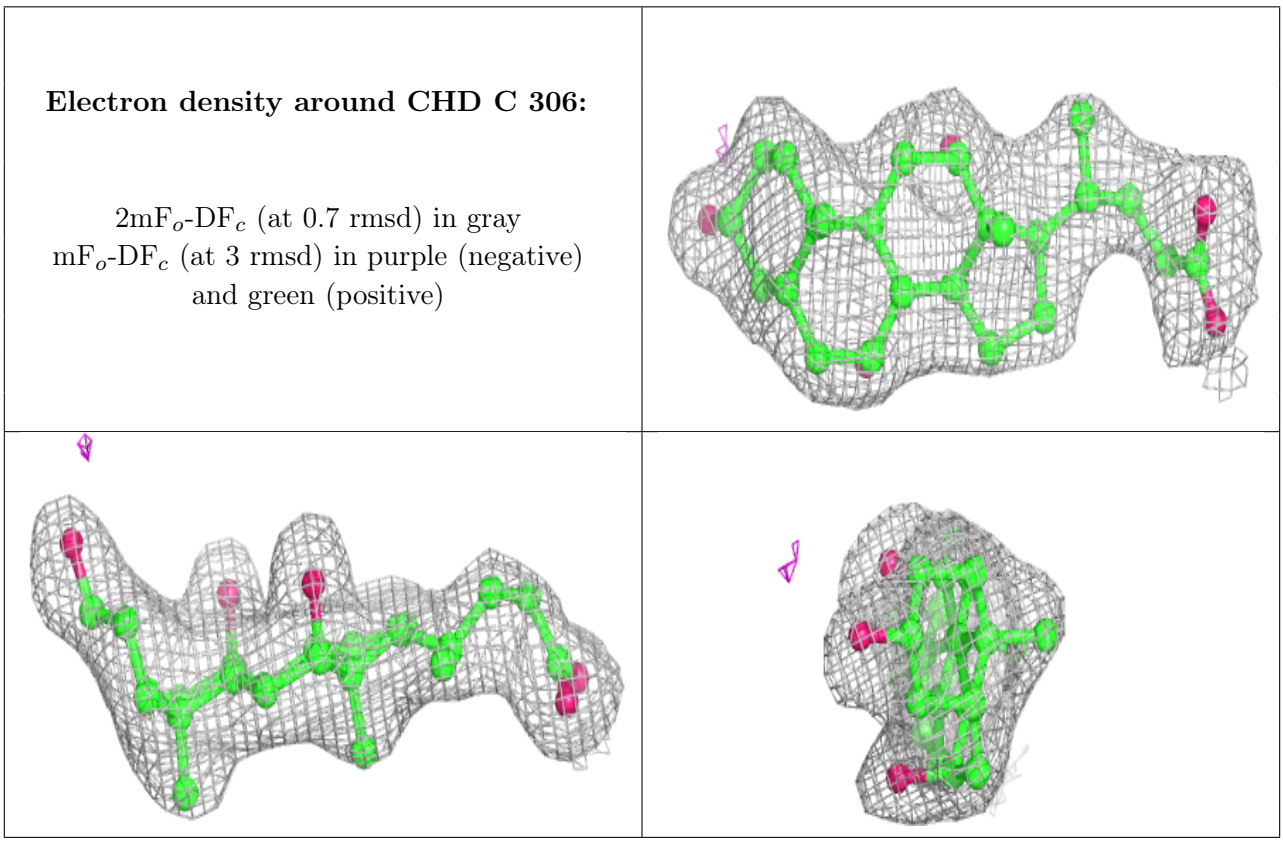
Electron density around CHD c 308:

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



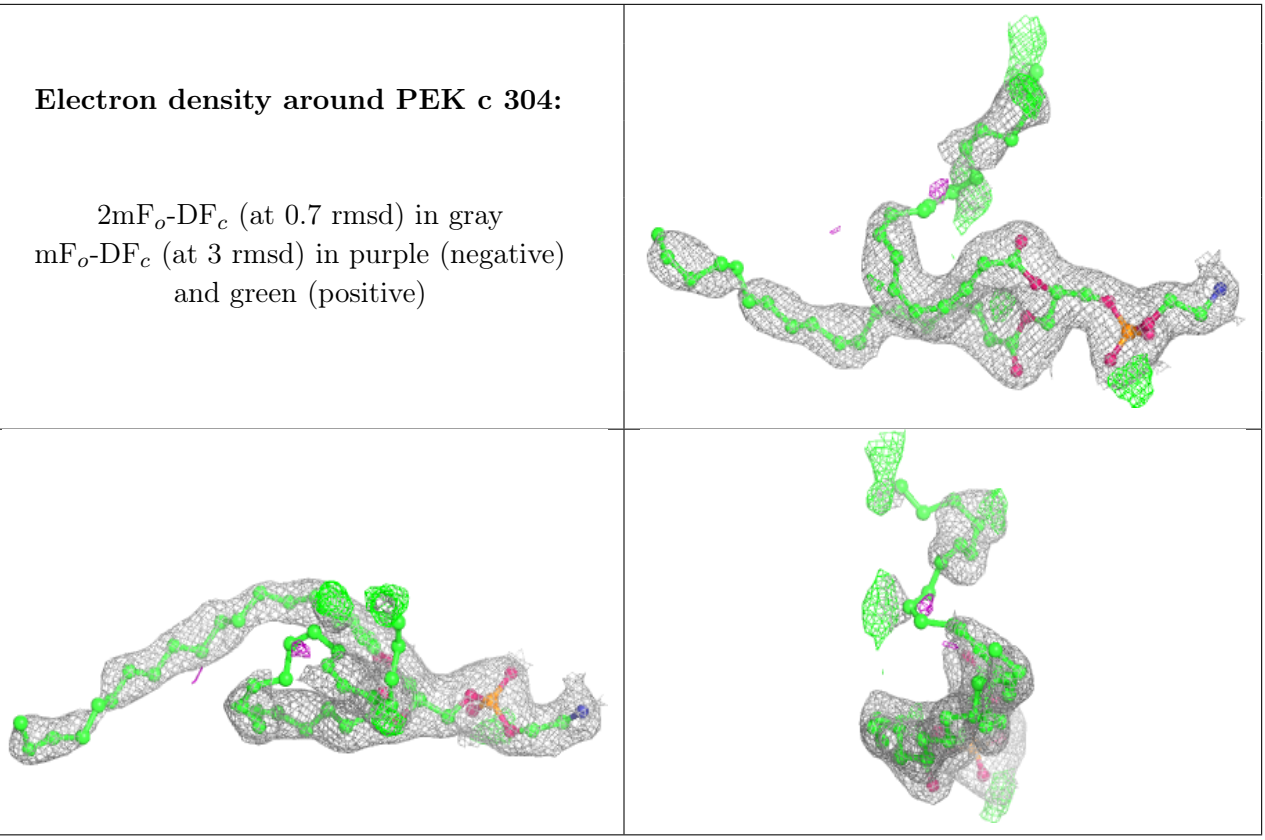
Electron density around CHD C 306:

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



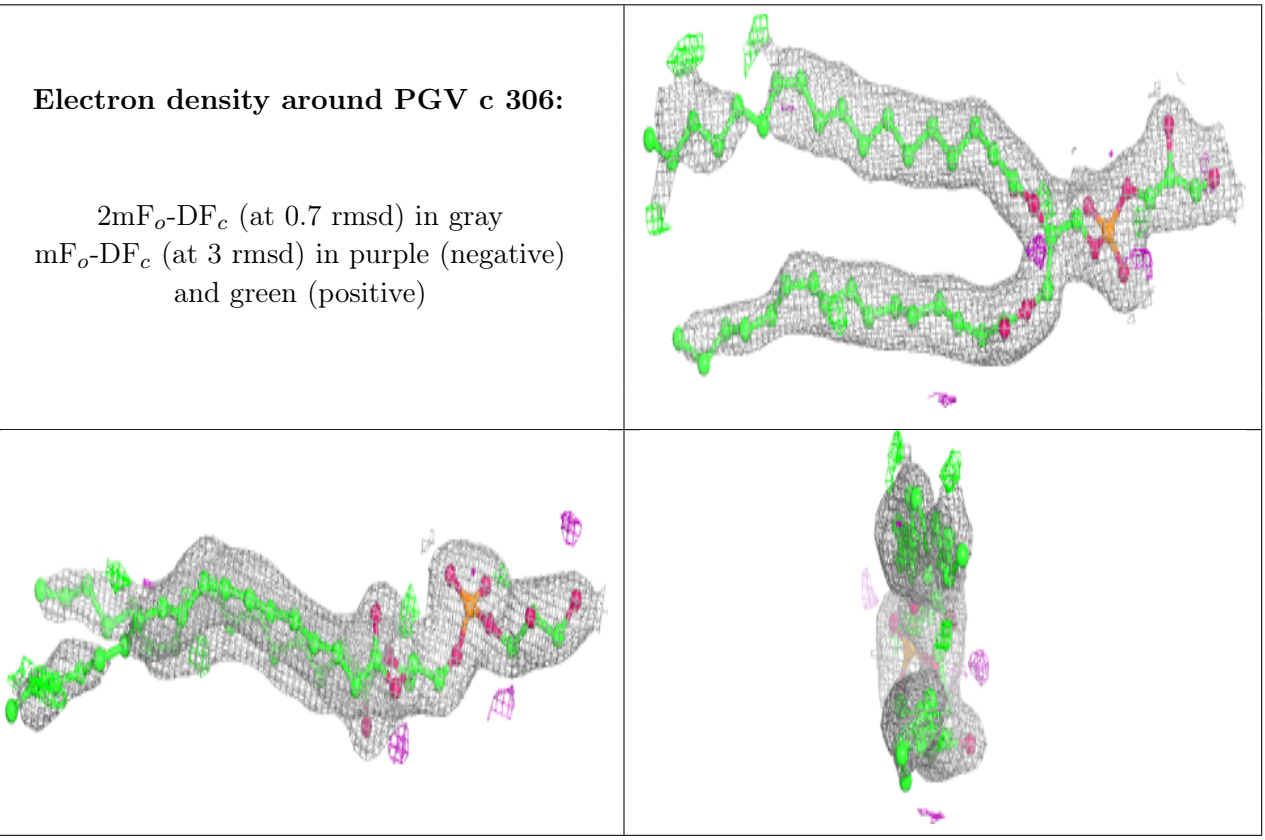
Electron density around PEK c 304:

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



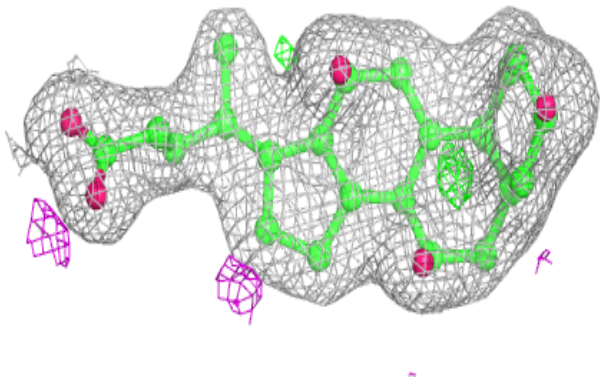
Electron density around PGV c 306:

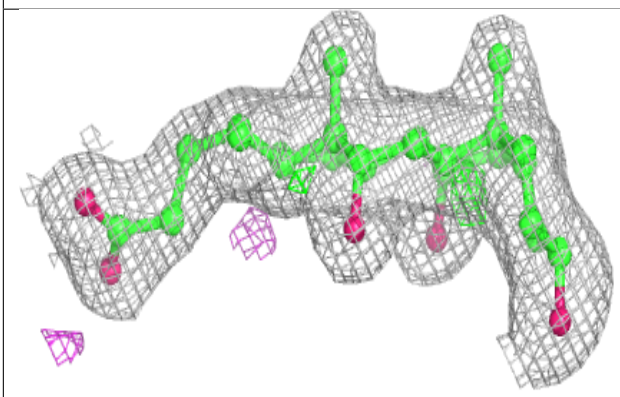
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

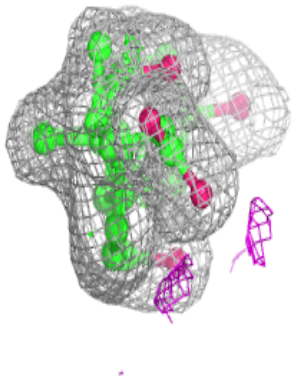


Electron density around CHD G 103:

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

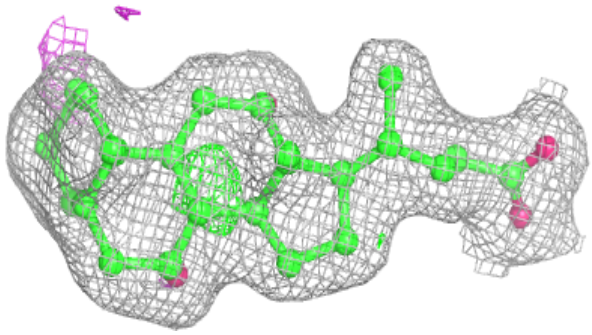


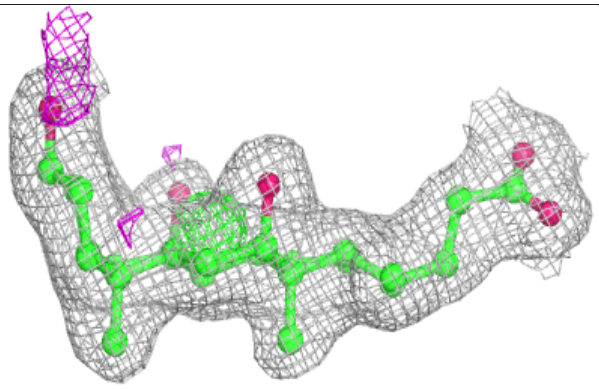


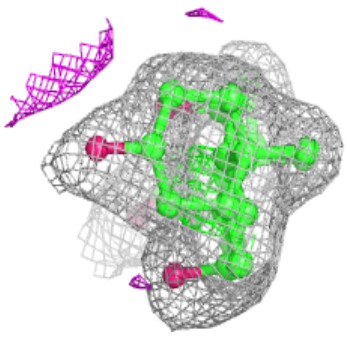


Electron density around CHD B 402:

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

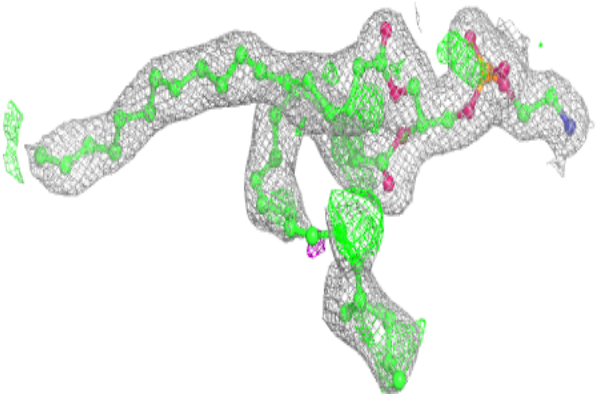


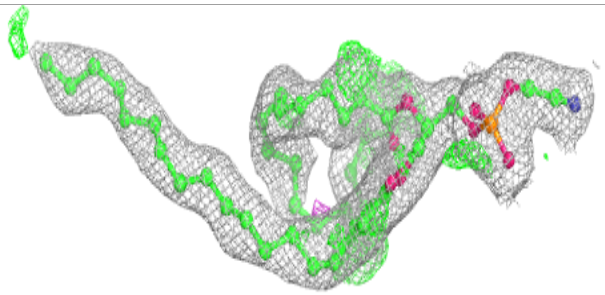


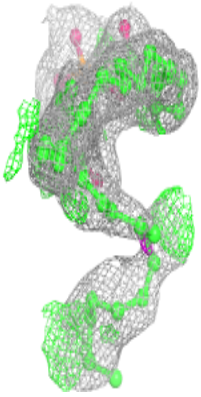


Electron density around PEK C 302:

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

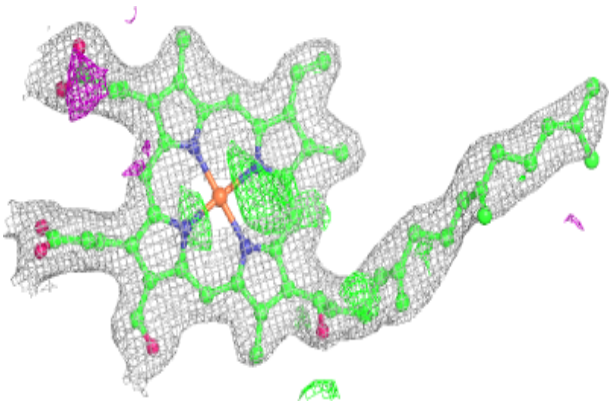


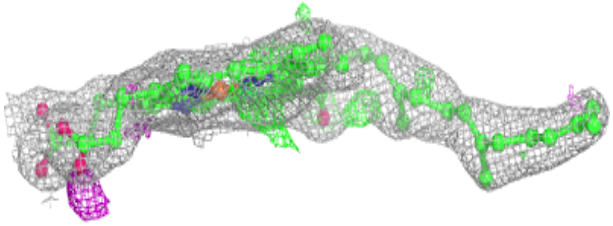


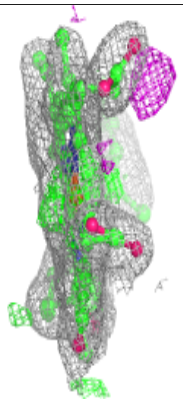


Electron density around HEA a 601:

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

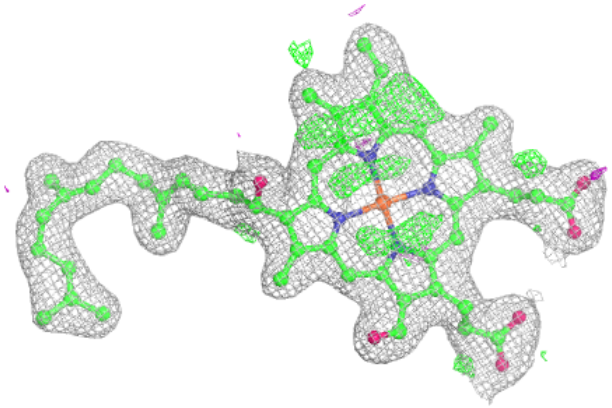


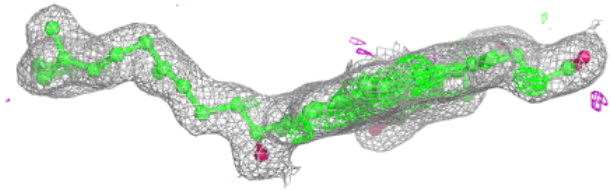


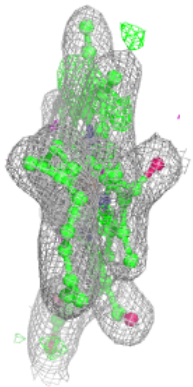


Electron density around HEA a 602:

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

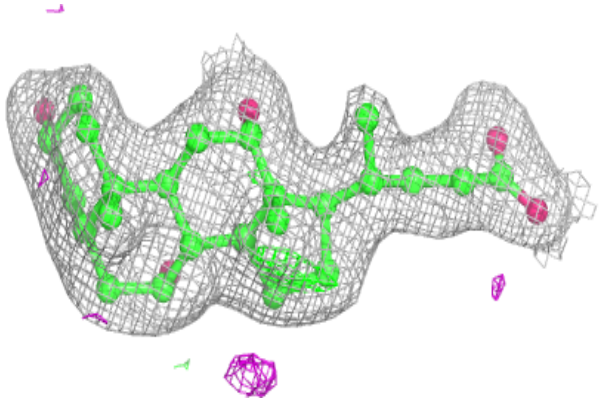


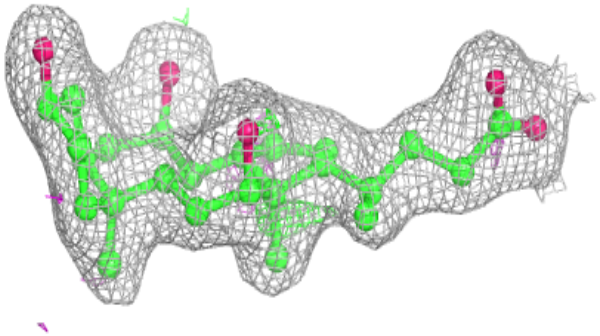


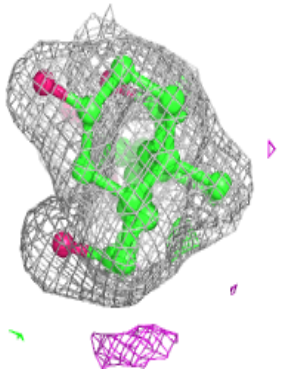


Electron density around CHD c 303:

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

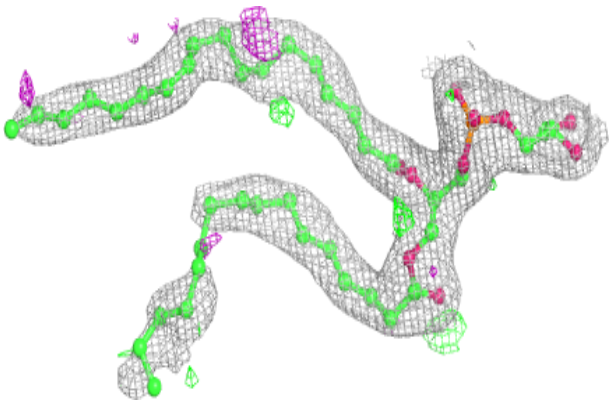


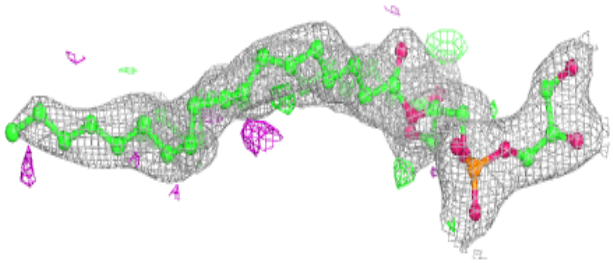


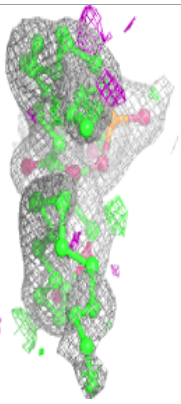


Electron density around PGV a 607:

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

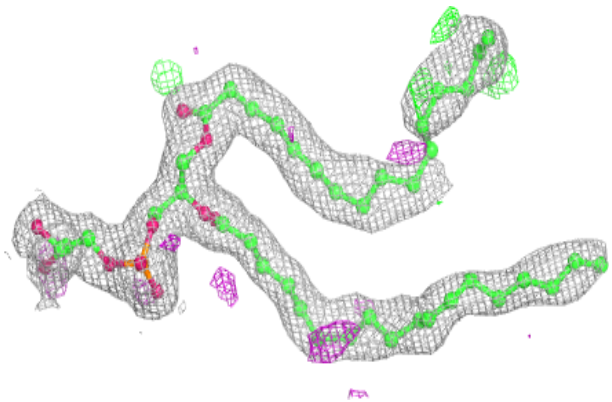


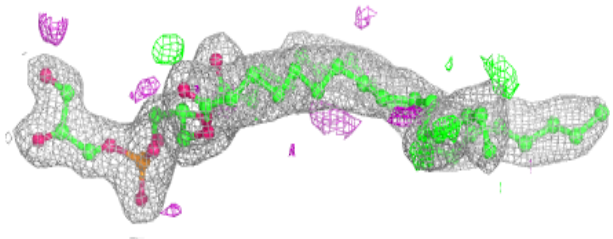


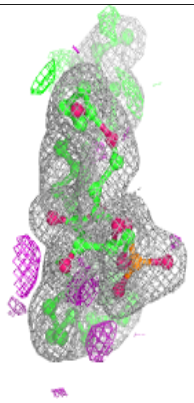


Electron density around PGV A 607:

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

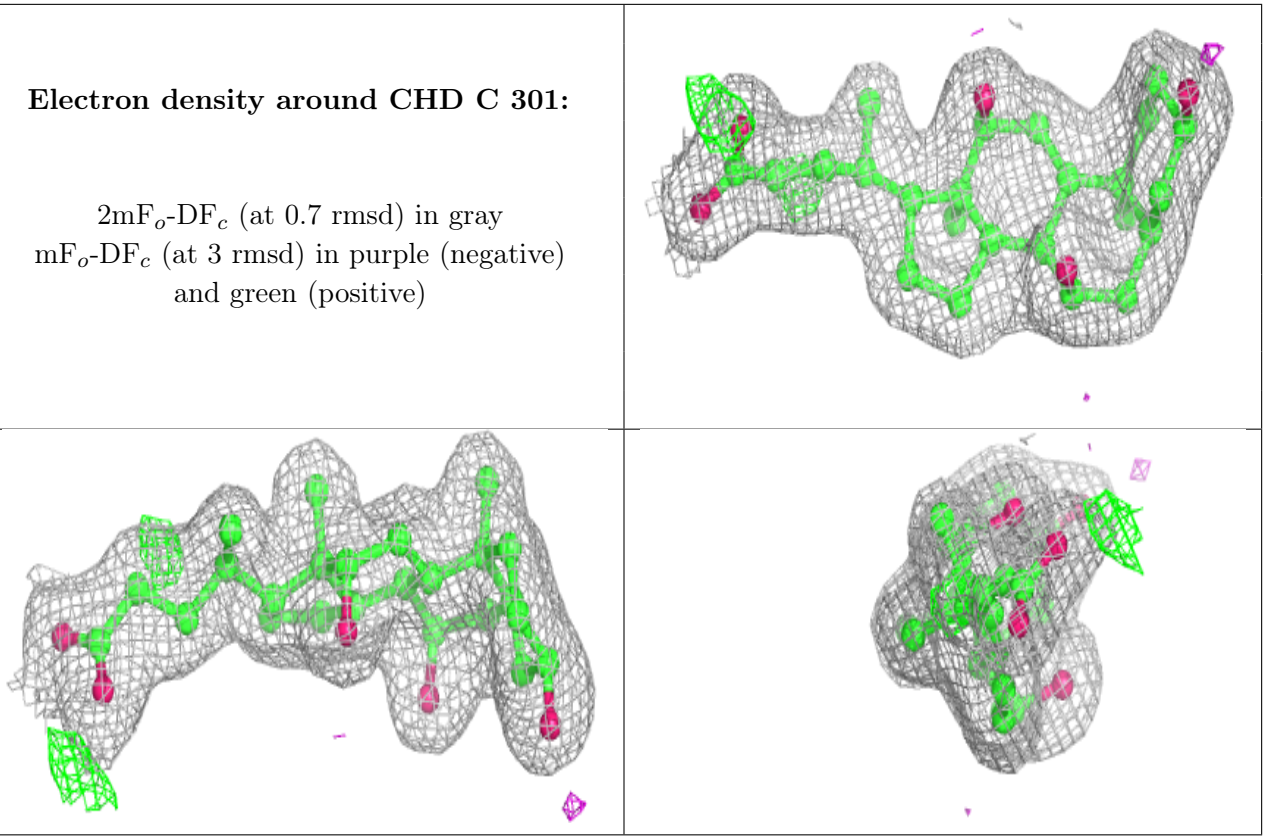






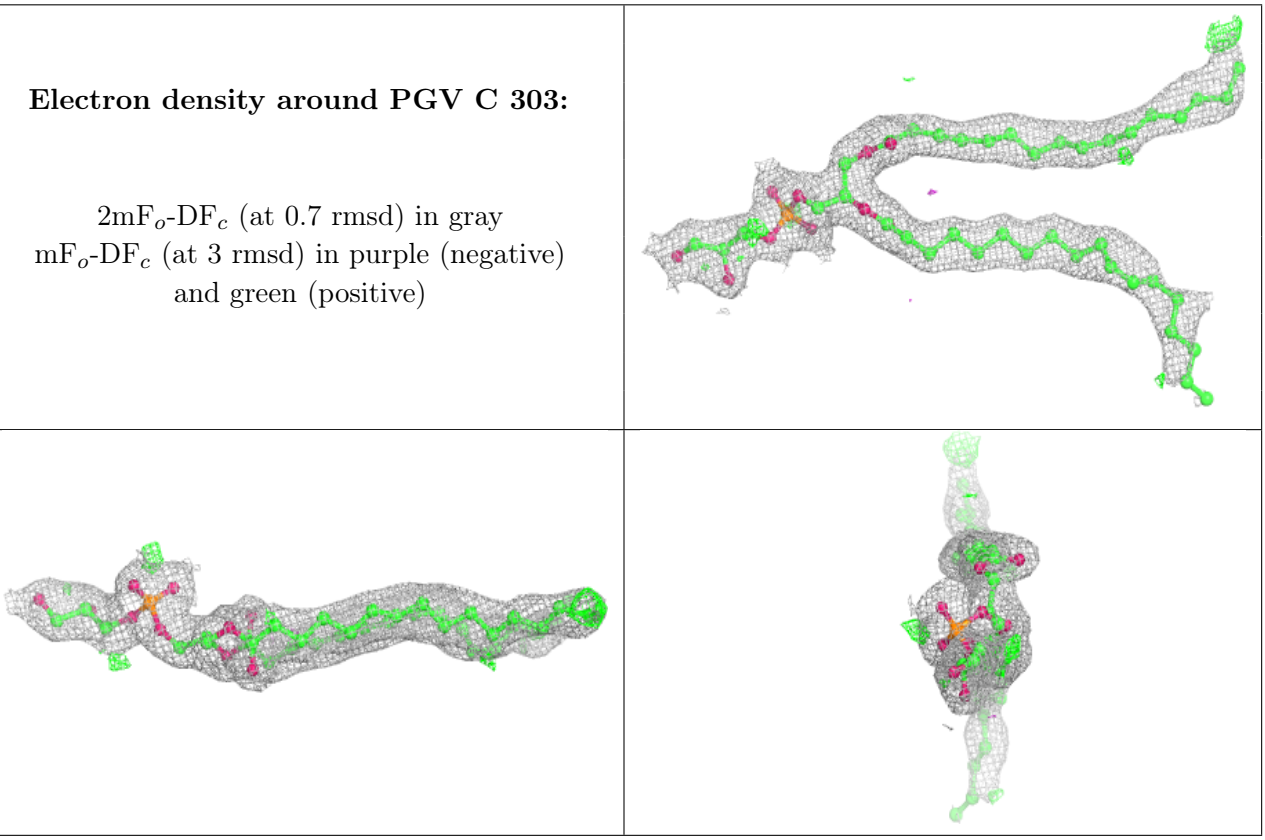
Electron density around CHD C 301:

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



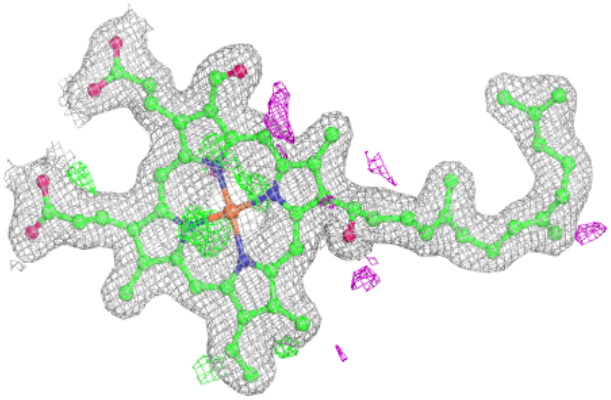
Electron density around PGV C 303:

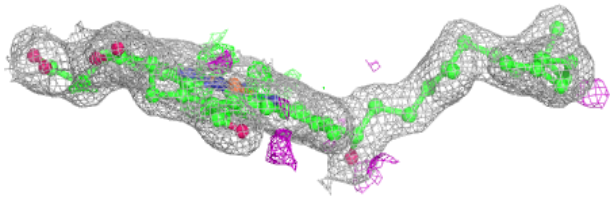
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

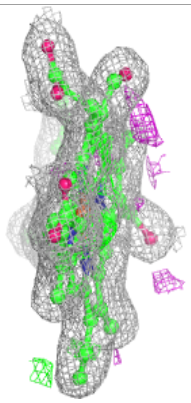


Electron density around HEA A 602:

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

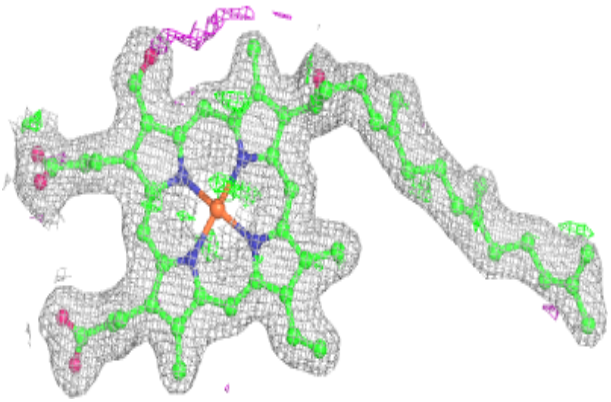


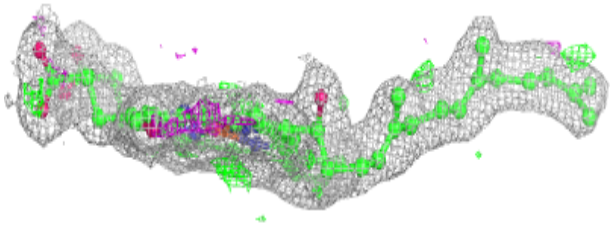


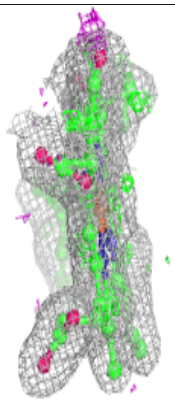


Electron density around HEA A 601:

$2mF_o$-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.