Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 07:47 AM EDT

PDB ID	:	5W97
Title	:	Crystal Structure of CO-bound Cytochrome c Oxidase determined by Serial Femtosecond X-Ray Crystallography at Room Temperature
Authors	:	Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.; Zatsepin, N.A.; Grant, T.D.; Fromme, P.; Fromme, R.
Deposited on	:	2017-06-22
Resolution	:	2.30 Å(reported)

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

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

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

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

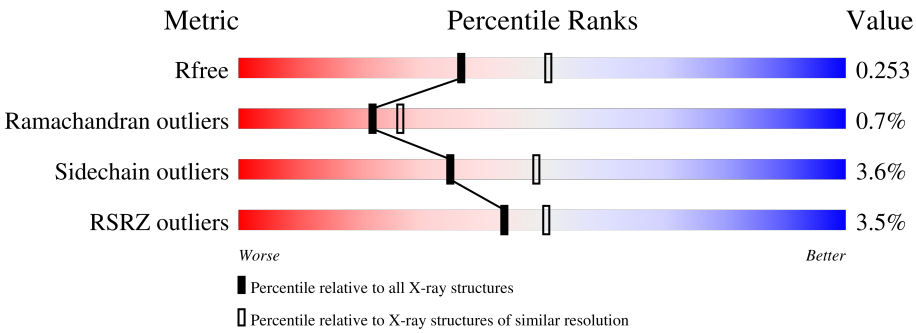
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.30 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	5042 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	98% ·
1	a	514	96% ·
2	B	227	94% 6%
2	b	227	5% 94% 6%
3	C	261	97% · ·
3	c	261	97% · ·

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Mol	Chain	Length	Quality of chain
4	D	147	%, 93%, 5%
4	d	147	8%, 93%, 5%
5	E	109	2%, 93%
5	e	109	2%, 93%
6	F	98	6%, 93%, 6%
6	f	98	7%, 98%
7	G	85	16%, 88%, 11%
7	g	85	13%, 87%, 11%
8	H	85	8%, 82%, 8%, 7%
8	h	85	7%, 91%, 7%
9	I	73	4%, 93%, 7%
9	i	73	11%, 93%, 7%
10	J	59	5%, 97%
10	j	59	8%, 81%, 15%
11	K	56	5%, 77%, 9%, 12%
11	k	56	14%, 86%, 12%
12	L	47	2%, 96%
12	l	47	2%, 85%, 11%
13	M	46	4%, 93%, 7%
13	m	46	15%, 87%, 7%, 7%

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	-	-	-
22	PSC	e	201	-	-	-	X
9	SAC	i	1	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 32025 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
			Total	C	N	O	S			
1	A	514	4027	2691	623	678	35	0	0	0
1	a	514	4027	2691	623	678	35	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

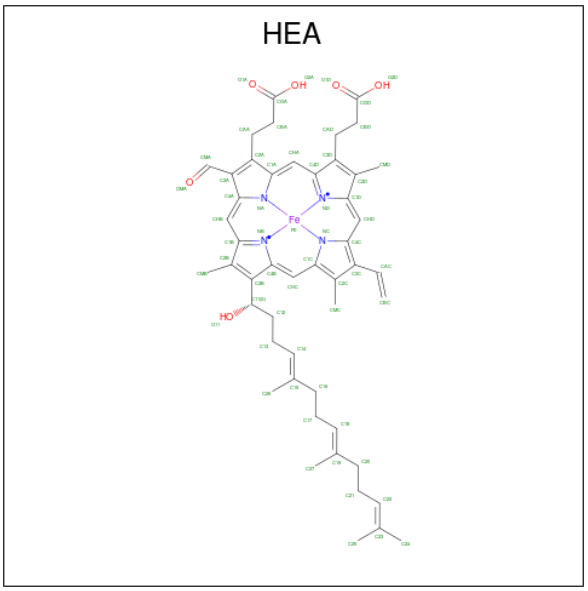
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

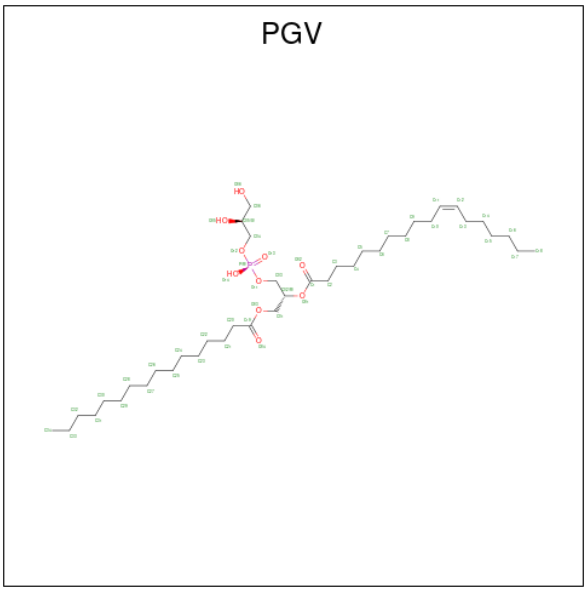
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

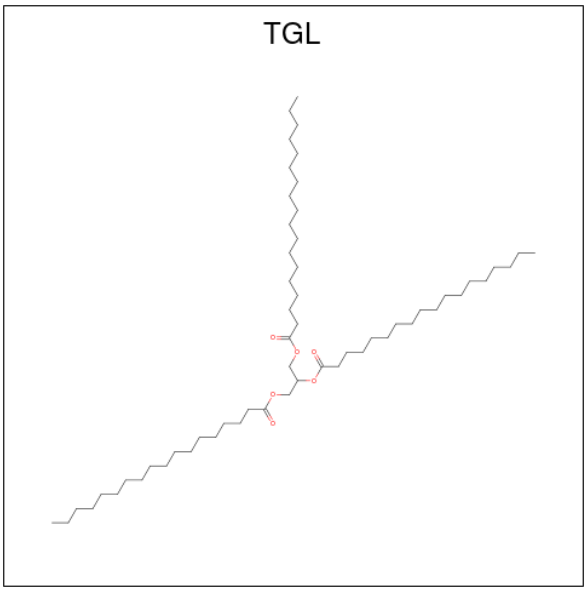
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
17	a	1	1	1	0	0

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



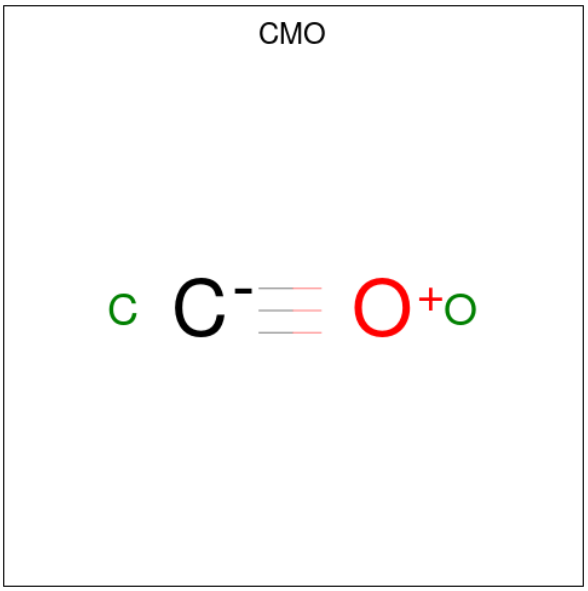
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	A	1	51	40	10	1	0	0
18	A	1	51	40	10	1	0	0
18	C	1	51	40	10	1	0	0
18	C	1	51	40	10	1	0	0
18	G	1	51	40	10	1	0	0
18	a	1	51	40	10	1	0	0
18	c	1	51	40	10	1	0	0
18	c	1	51	40	10	1	0	0

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



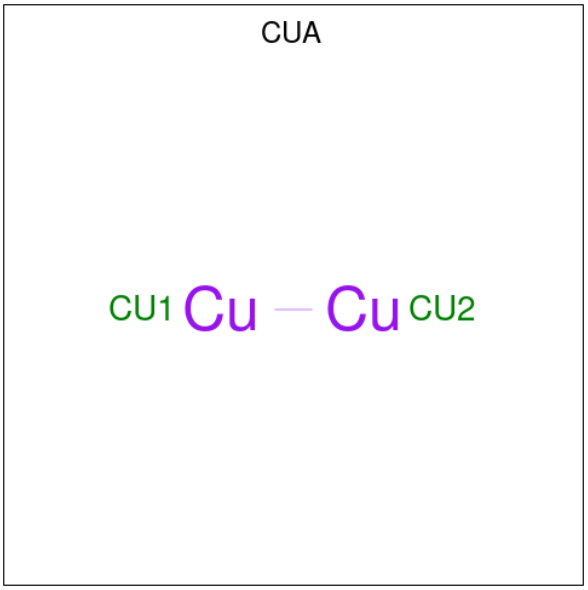
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	a	1	63	57	6	0	0
19	i	1	63	57	6	0	0
19	l	1	63	57	6	0	0

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



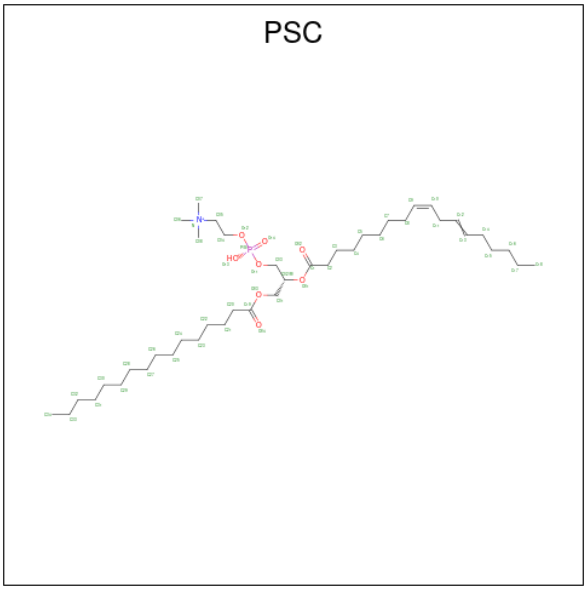
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 2 1 1	0	0
20	a	1	Total C O 2 1 1	0	0

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



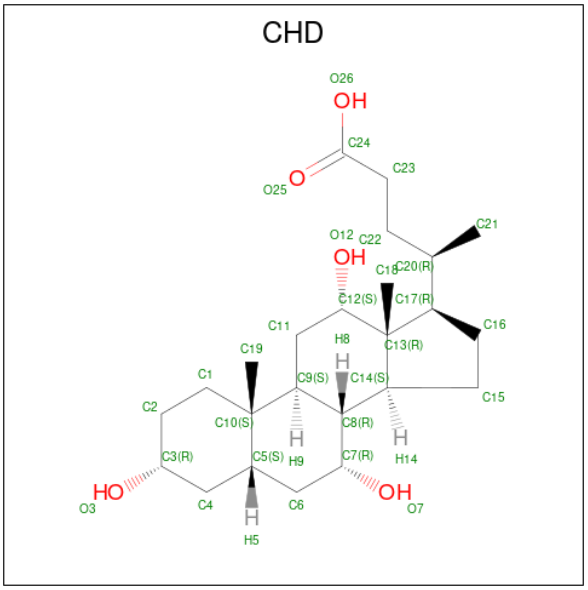
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	b	1	Total Cu 2 2	0	0

- Molecule 22 is (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: $C_{42}H_{81}NO_8P$).



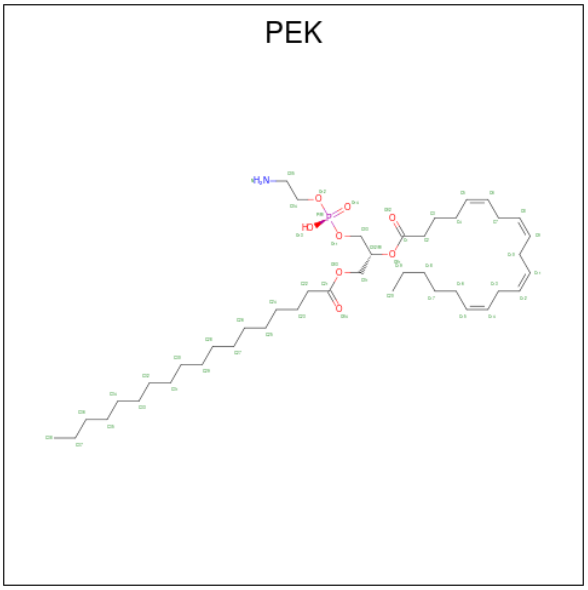
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
22	B	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
22	e	1	52	42	1	8	1	0	0

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 24 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
			Total	C	N	O	P		
24	C	1	53	43	1	8	1	0	0
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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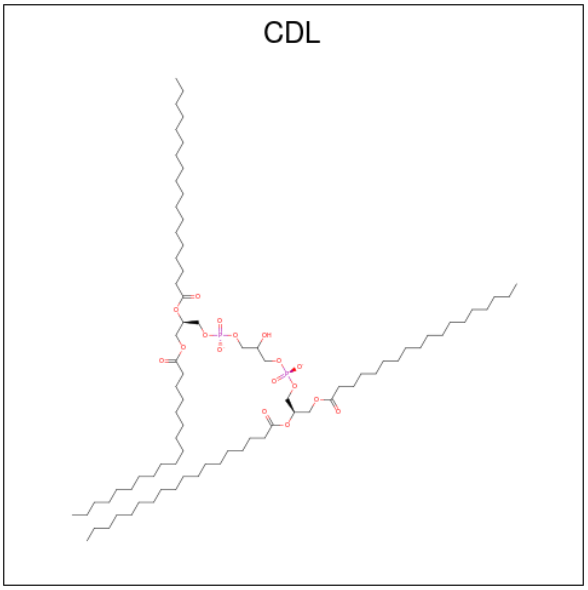
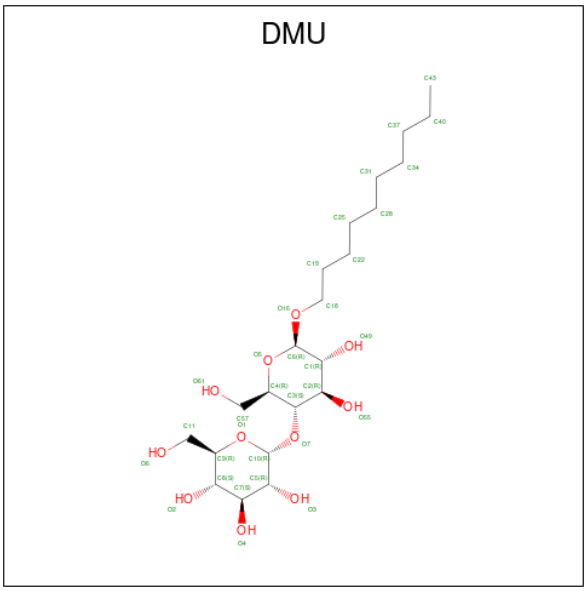
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	G	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	c	1	53	43	1	8	1	0	0
			Total	C	N	O	P		
24	g	1	53	43	1	8	1	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
28	A	197	197	197	0	0
			Total	O		
28	B	120	120	120	0	0
			Total	O		
28	C	81	81	81	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	D	85	Total O 85 85	0	0
28	E	51	Total O 51 51	0	0
28	F	66	Total O 66 66	0	0
28	G	51	Total O 51 51	0	0
28	H	33	Total O 33 33	0	0
28	I	33	Total O 33 33	0	0
28	J	26	Total O 26 26	0	0
28	K	30	Total O 30 30	0	0
28	L	35	Total O 35 35	0	0
28	M	22	Total O 22 22	0	0
28	a	140	Total O 140 140	0	0
28	b	63	Total O 63 63	0	0
28	c	59	Total O 59 59	0	0
28	d	25	Total O 25 25	0	0
28	e	36	Total O 36 36	0	0
28	f	29	Total O 29 29	0	0
28	g	29	Total O 29 29	0	0
28	h	24	Total O 24 24	0	0
28	i	14	Total O 14 14	0	0
28	j	8	Total O 8 8	0	0
28	k	8	Total O 8 8	0	0

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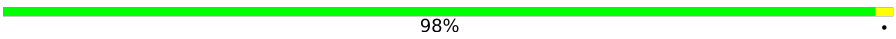
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	l	19	Total O 19 19	0	0
28	m	7	Total O 7 7	0	0

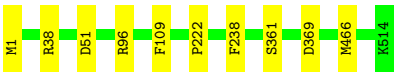
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome c oxidase subunit 1

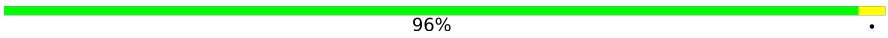
Chain A:





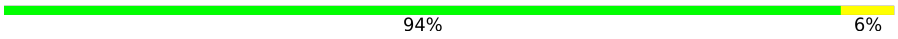
• Molecule 1: Cytochrome c oxidase subunit 1

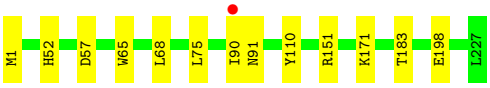
Chain a:



• Molecule 2: Cytochrome c oxidase subunit 2

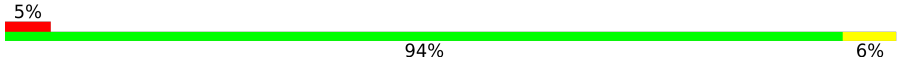
Chain B:





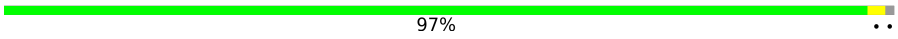
• Molecule 2: Cytochrome c oxidase subunit 2

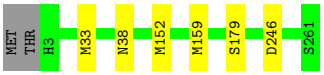
Chain b:



• Molecule 3: Cytochrome c oxidase subunit 3

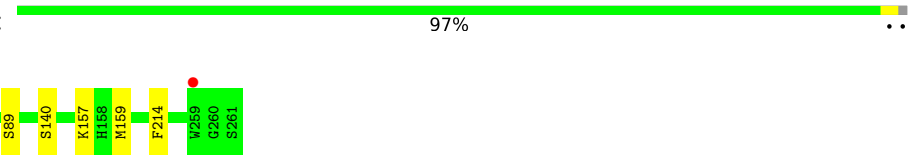
Chain C:





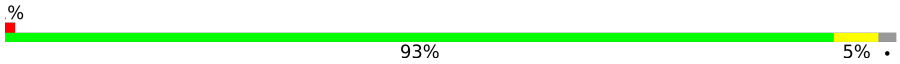
• Molecule 3: Cytochrome c oxidase subunit 3

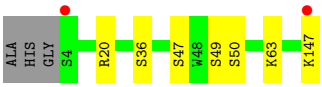
Chain c:



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

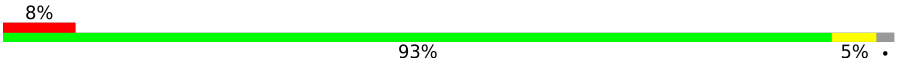
Chain D:

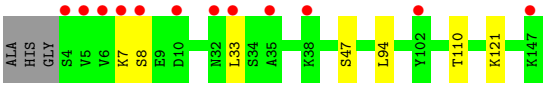




• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

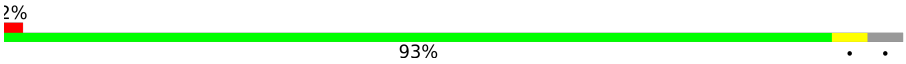
Chain d:





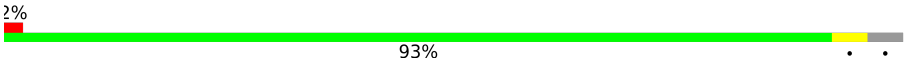
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

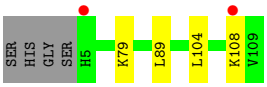
Chain E:



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

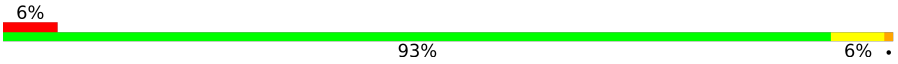
Chain e:

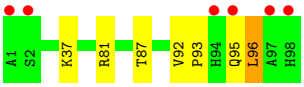




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

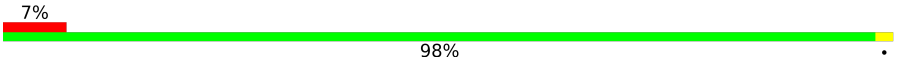
Chain F:

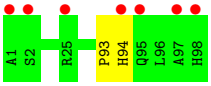




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

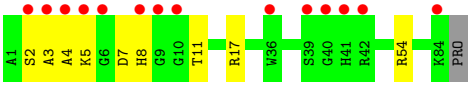
Chain f:





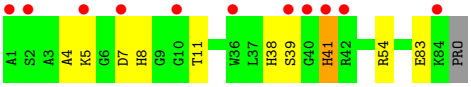
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



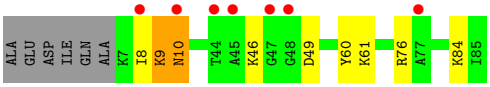
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain g:



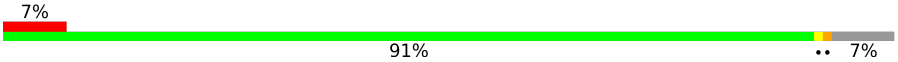
• Molecule 8: Cytochrome c oxidase subunit 6B1

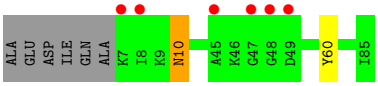
Chain H:



• Molecule 8: Cytochrome c oxidase subunit 6B1

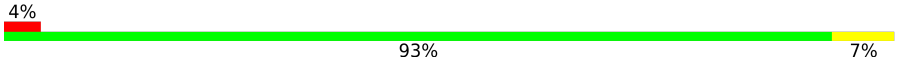
Chain h:

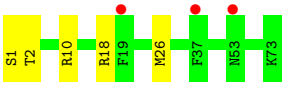




• Molecule 9: Cytochrome c oxidase subunit 6C

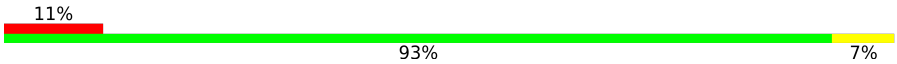
Chain I:

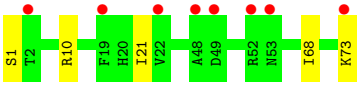




• Molecule 9: Cytochrome c oxidase subunit 6C

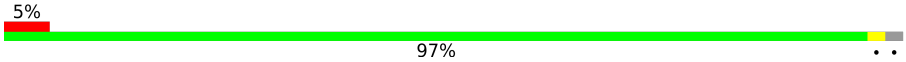
Chain i:

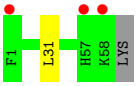




• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

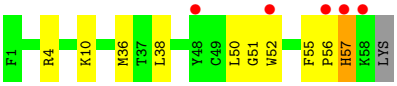
Chain J:





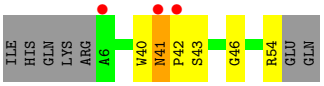
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain j:



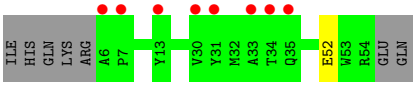
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



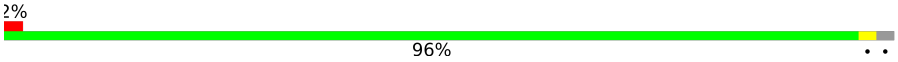
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

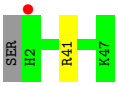
Chain k:



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

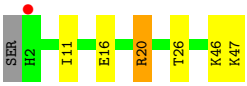
Chain L:





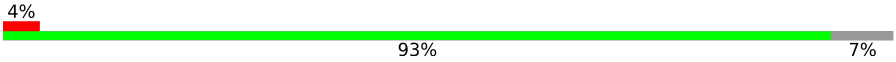
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

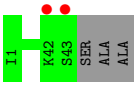
Chain l:



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

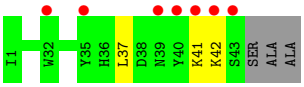
Chain M:





• 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	178.30Å 189.00Å 209.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.30 29.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.86-2.30) 100.0 (29.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.208 , 0.252 0.215 , 0.253	Depositor DCC
R_{free} test set	2994 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32025	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DMU, CMO, HEA, PGV, CDL, CU, CUA, CHD, SAC, NA, TPO, FME, MG, PEK, PSC, TGL, ZN

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	0.70	0/4156	0.78	4/5678 (0.1%)
1	a	0.65	0/4156	0.76	2/5678 (0.0%)
2	B	0.70	1/1860 (0.1%)	0.88	1/2534 (0.0%)
2	b	0.61	1/1860 (0.1%)	0.81	0/2534
3	C	0.67	0/2197	0.75	2/3005 (0.1%)
3	c	0.64	0/2197	0.72	0/3005
4	D	0.66	0/1229	0.75	1/1658 (0.1%)
4	d	0.56	0/1229	0.75	0/1658
5	E	0.59	0/871	0.72	0/1182
5	e	0.53	0/871	0.79	0/1182
6	F	0.73	0/765	0.88	1/1038 (0.1%)
6	f	0.57	0/765	0.78	0/1038
7	G	0.68	0/690	0.80	2/937 (0.2%)
7	g	0.64	0/690	0.74	0/937
8	H	0.66	0/682	0.86	0/921
8	h	0.61	0/682	0.81	0/921
9	I	0.66	0/605	0.84	1/802 (0.1%)
9	i	0.63	0/605	0.81	1/802 (0.1%)
10	J	0.62	0/471	0.77	0/636
10	j	0.72	1/471 (0.2%)	0.75	0/636
11	K	0.75	0/398	0.99	4/546 (0.7%)
11	k	0.63	0/398	0.72	0/546
12	L	0.71	0/393	0.76	1/526 (0.2%)
12	l	0.61	0/393	0.74	1/526 (0.2%)
13	M	0.59	0/345	0.68	0/470
13	m	0.56	0/345	0.66	0/470
All	All	0.65	3/29324 (0.0%)	0.78	21/39866 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	1
6	F	0	1
7	g	0	1
8	H	0	2
8	h	0	1
10	j	0	1
11	K	0	4
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	7.01	1.36	1.23
2	b	198	GLU	C-O	6.79	1.36	1.23
10	j	52	TRP	CB-CG	5.73	1.60	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	152	MET	CG-SD-CE	11.06	117.90	100.20
9	i	10	ARG	NE-CZ-NH2	-7.00	116.80	120.30
11	K	41	ASN	C-N-CA	-6.90	93.00	122.00
11	K	41	ASN	C-N-CD	6.46	141.96	128.40
11	K	43	SER	N-CA-CB	6.42	120.13	110.50
1	A	96	ARG	NE-CZ-NH2	-6.23	117.19	120.30
12	l	20	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	38	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	a	96	ARG	NE-CZ-NH1	5.84	123.22	120.30
12	L	41	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	B	151	ARG	NE-CZ-NH1	5.68	123.14	120.30
7	G	17	ARG	NE-CZ-NH2	-5.67	117.47	120.30
6	F	81	ARG	NE-CZ-NH2	-5.66	117.47	120.30
7	G	17	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	a	38	ARG	NE-CZ-NH1	5.44	123.02	120.30
4	D	20	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	96	ARG	NE-CZ-NH1	5.29	122.95	120.30
11	K	54	ARG	NE-CZ-NH2	5.22	122.91	120.30
9	I	10	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	466	MET	CG-SD-CE	5.14	108.42	100.20
3	C	246	ASP	CB-CG-OD2	-5.13	113.68	118.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	92	VAL	Peptide
8	H	10	ASN	Peptide
8	H	9	LYS	Peptide
11	K	40	TRP	Peptide
11	K	41	ASN	Peptide
11	K	42	PRO	Peptide
11	K	46	GLY	Peptide
4	d	7	LYS	Peptide
7	g	83	GLU	Peptide
8	h	10	ASN	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%)	495 (97%)	16 (3%)	1 (0%)	47	58
2	B	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	34	42
2	b	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	42
3	c	257/261 (98%)	248 (96%)	8 (3%)	1 (0%)	34	42
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	d	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	22	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	e	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	7	5
6	f	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	7	5
7	G	81/85 (95%)	71 (88%)	7 (9%)	3 (4%)	3	2
7	g	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	0
8	H	77/85 (91%)	72 (94%)	3 (4%)	2 (3%)	5	4
8	h	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	i	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11	11
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	j	56/59 (95%)	53 (95%)	0	3 (5%)	2	1
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	k	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	l	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	6	5
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	m	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	6	4
All	All	3504/3614 (97%)	3355 (96%)	123 (4%)	26 (1%)	22	26

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	96	LEU
8	H	10	ASN
7	g	4	ALA
12	l	46	LYS
2	B	90	ILE
3	C	38	ASN
7	G	4	ALA
1	a	119	GLU
4	d	8	SER
7	g	7	ASP
7	g	8	HIS
9	i	68	ILE
7	G	8	HIS

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Mol	Chain	Res	Type
3	c	38	ASN
6	f	94	HIS
7	g	39	SER
10	j	57	HIS
7	G	3	ALA
7	g	41	HIS
7	g	5	LYS
13	m	42	LYS
6	F	93	PRO
10	j	51	GLY
10	j	56	PRO
8	H	8	ILE
6	f	93	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	420 (99%)	6 (1%)	67	81
1	a	426/426 (100%)	411 (96%)	15 (4%)	36	50
2	B	210/210 (100%)	201 (96%)	9 (4%)	29	40
2	b	210/210 (100%)	198 (94%)	12 (6%)	20	28
3	C	224/226 (99%)	221 (99%)	3 (1%)	69	82
3	c	224/226 (99%)	218 (97%)	6 (3%)	44	61
4	D	128/129 (99%)	122 (95%)	6 (5%)	26	37
4	d	128/129 (99%)	123 (96%)	5 (4%)	32	46
5	E	92/95 (97%)	88 (96%)	4 (4%)	29	40
5	e	92/95 (97%)	88 (96%)	4 (4%)	29	40
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	35
6	f	81/81 (100%)	81 (100%)	0	100	100
7	G	67/68 (98%)	63 (94%)	4 (6%)	19	26
7	g	67/68 (98%)	64 (96%)	3 (4%)	27	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	71/75 (95%)	64 (90%)	7 (10%)	8	9
8	h	71/75 (95%)	69 (97%)	2 (3%)	43	60
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	31
9	i	57/57 (100%)	55 (96%)	2 (4%)	36	50
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	72
10	j	49/50 (98%)	43 (88%)	6 (12%)	5	5
11	K	39/46 (85%)	39 (100%)	0	100	100
11	k	39/46 (85%)	38 (97%)	1 (3%)	46	63
12	L	39/40 (98%)	39 (100%)	0	100	100
12	l	39/40 (98%)	34 (87%)	5 (13%)	4	4
13	M	37/38 (97%)	37 (100%)	0	100	100
13	m	37/38 (97%)	35 (95%)	2 (5%)	22	30
All	All	3040/3082 (99%)	2930 (96%)	110 (4%)	35	49

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASP
1	A	109	PHE
1	A	222	PRO
1	A	238	PHE
1	A	361	SER
1	A	369	ASP
2	B	52	HIS
2	B	57	ASP
2	B	65	TRP
2	B	68	LEU
2	B	75	LEU
2	B	91	ASN
2	B	110	TYR
2	B	171	LYS
2	B	183	THR
3	C	33	MET
3	C	159	MET
3	C	179	SER
4	D	36	SER
4	D	47	SER
4	D	49	SER

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Mol	Chain	Res	Type
4	D	50	SER
4	D	63	LYS
4	D	147	LYS
5	E	9	GLU
5	E	46	LYS
5	E	70	VAL
5	E	79	LYS
6	F	37	LYS
6	F	87	THR
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	5	LYS
7	G	7	ASP
7	G	54	ARG
8	H	9	LYS
8	H	46	LYS
8	H	49	ASP
8	H	60	TYR
8	H	61	LYS
8	H	76	ARG
8	H	84	LYS
9	I	2	THR
9	I	18	ARG
9	I	26	MET
10	J	31	LEU
1	a	38	ARG
1	a	46	THR
1	a	65	MET
1	a	90	PRO
1	a	109	PHE
1	a	238	PHE
1	a	264	LYS
1	a	265	LYS
1	a	369	ASP
1	a	382	SER
1	a	417	MET
1	a	458	SER
1	a	483	LEU
1	a	486	ASP
1	a	504	THR
2	b	60	GLU

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Mol	Chain	Res	Type
2	b	65	TRP
2	b	68	LEU
2	b	94	SER
2	b	107	SER
2	b	110	TYR
2	b	117	SER
2	b	129	LYS
2	b	156	SER
2	b	183	THR
2	b	216	LEU
2	b	217	LYS
3	c	38	ASN
3	c	89	SER
3	c	140	SER
3	c	157	LYS
3	c	159	MET
3	c	214	PHE
4	d	33	LEU
4	d	47	SER
4	d	94	LEU
4	d	110	THR
4	d	121	LYS
5	e	79	LYS
5	e	89	LEU
5	e	104	LEU
5	e	108	LYS
7	g	38	HIS
7	g	41	HIS
7	g	54	ARG
8	h	10	ASN
8	h	60	TYR
9	i	21	ILE
9	i	73	LYS
10	j	4	ARG
10	j	10	LYS
10	j	36	MET
10	j	38	LEU
10	j	50	LEU
10	j	57	HIS
11	k	52	GLU
12	l	11	ILE
12	l	16	GLU

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Mol	Chain	Res	Type
12	l	20	ARG
12	l	26	THR
12	l	47	LYS
13	m	37	LEU
13	m	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	232	GLN
1	A	422	ASN
1	A	428	GLN
2	B	91	ASN
2	B	92	ASN
2	B	195	GLN
2	B	203	ASN
3	C	36	HIS
3	C	50	ASN
3	C	76	GLN
4	D	37	GLN
5	E	59	ASN
6	F	32	ASN
6	F	47	ASN
6	F	66	ASN
6	F	88	HIS
6	F	95	GLN
7	G	38	HIS
7	G	51	HIS
7	G	76	ASN
8	H	37	HIS
10	J	9	GLN
1	a	99	ASN
1	a	232	GLN
1	a	331	ASN
1	a	503	HIS
1	a	512	ASN
2	b	6	GLN
3	c	50	ASN
3	c	161	GLN
4	d	132	GLN
6	f	95	GLN

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Mol	Chain	Res	Type
8	h	12	GLN
9	i	70	GLN
13	m	15	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SAC	i	1	9	7,8,9	1.88	1 (14%)	8,9,11	1.85	2 (25%)
2	FME	b	1	2	8,9,10	0.60	0	7,9,11	2.48	2 (28%)
1	FME	a	1	1	8,9,10	0.55	0	7,9,11	1.94	2 (28%)
1	FME	A	1	1	8,9,10	0.55	0	7,9,11	2.78	3 (42%)
7	TPO	G	11	7	8,10,11	1.52	2 (25%)	10,14,16	0.88	0
7	TPO	g	11	7	8,10,11	1.35	1 (12%)	10,14,16	0.74	0
9	SAC	I	1	9	7,8,9	1.58	1 (14%)	8,9,11	1.09	0
2	FME	B	1	2	8,9,10	1.08	0	7,9,11	3.79	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SAC	i	1	9	-	2/7/8/10	-
2	FME	b	1	2	-	1/7/9/11	-
1	FME	a	1	1	-	5/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	5/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
7	TPO	g	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	1/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	1	SAC	CA-N	4.51	1.52	1.46
9	I	1	SAC	CA-N	3.68	1.51	1.46
7	G	11	TPO	P-OG1	2.81	1.64	1.59
7	G	11	TPO	CB-CA	2.52	1.59	1.53
7	g	11	TPO	P-OG1	2.45	1.63	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-8.96	109.04	122.82
1	A	1	FME	CA-N-CN	-6.41	112.97	122.82
2	b	1	FME	CA-N-CN	-5.22	114.80	122.82
1	a	1	FME	CA-N-CN	-4.24	116.30	122.82
9	i	1	SAC	C-CA-N	3.40	115.86	109.73
2	B	1	FME	C-CA-N	3.10	115.32	109.73
2	b	1	FME	C-CA-N	2.89	114.94	109.73
2	B	1	FME	O1-CN-N	-2.74	118.04	125.27
9	i	1	SAC	OAC-C1A-C2A	-2.62	117.19	122.06
1	A	1	FME	C-CA-N	-2.55	105.13	109.73
1	A	1	FME	O-C-CA	-2.22	118.96	124.78
1	a	1	FME	O-C-CA	-2.15	119.14	124.78

There are no chirality outliers.

All (25) 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	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	CG2-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O3P
9	I	1	SAC	O-C-CA-CB
1	a	1	FME	O1-CN-N-CA
1	a	1	FME	C-CA-CB-CG
1	a	1	FME	CA-CB-CG-SD
2	b	1	FME	O1-CN-N-CA
7	g	11	TPO	N-CA-CB-OG1
1	A	1	FME	CA-CB-CG-SD
1	A	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
1	a	1	FME	CB-CG-SD-CE
7	g	11	TPO	CG2-CB-OG1-P
9	i	1	SAC	C-CA-CB-OG
9	i	1	SAC	N-CA-CB-OG
7	g	11	TPO	CB-OG1-P-O1P
1	a	1	FME	N-CA-CB-CG
7	g	11	TPO	CB-OG1-P-O2P
7	g	11	TPO	CB-OG1-P-O3P

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
18	PGV	C	304	-	50,50,50	1.14	2 (4%)	53,56,56	1.14	3 (5%)
25	CDL	c	305	-	99,99,99	1.09	4 (4%)	105,111,111	1.08	8 (7%)
19	TGL	L	101	-	62,62,62	1.10	3 (4%)	65,65,65	1.04	4 (6%)
25	CDL	C	305	-	99,99,99	1.02	4 (4%)	105,111,111	1.12	10 (9%)
18	PGV	A	607	-	50,50,50	0.73	2 (4%)	53,56,56	0.94	3 (5%)
14	HEA	A	602	20,1	57,67,67	1.83	15 (26%)	61,103,103	2.52	21 (34%)
21	CUA	b	302	2	0,1,1	-	-	-		
23	CHD	c	302	-	32,32,32	0.78	0	51,51,51	1.61	12 (23%)
23	CHD	C	306	-	32,32,32	0.55	0	51,51,51	1.23	5 (9%)
18	PGV	c	301	-	50,50,50	0.79	2 (4%)	53,56,56	0.85	2 (3%)
24	PEK	C	308	-	52,52,52	1.00	2 (3%)	55,57,57	1.19	4 (7%)
22	PSC	B	302	-	51,51,51	1.08	2 (3%)	57,59,59	1.91	9 (15%)
24	PEK	c	303	-	52,52,52	1.09	2 (3%)	55,57,57	1.03	3 (5%)
22	PSC	e	201	-	51,51,51	1.06	2 (3%)	57,59,59	1.83	10 (17%)
19	TGL	i	101	-	62,62,62	1.05	3 (4%)	65,65,65	1.23	5 (7%)
18	PGV	A	606	-	50,50,50	1.25	3 (6%)	53,56,56	1.28	8 (15%)
18	PGV	a	607	-	50,50,50	1.08	2 (4%)	53,56,56	0.96	3 (5%)
24	PEK	C	302	-	52,52,52	0.95	4 (7%)	55,57,57	0.97	2 (3%)
23	CHD	C	301	-	32,32,32	0.84	0	51,51,51	1.23	6 (11%)
19	TGL	A	608	-	62,62,62	1.28	3 (4%)	65,65,65	1.31	6 (9%)
19	TGL	a	606	-	62,62,62	1.16	3 (4%)	65,65,65	0.95	3 (4%)
26	DMU	M	101	-	34,34,34	0.47	0	45,45,45	1.05	4 (8%)
26	DMU	c	307	-	34,34,34	0.82	1 (2%)	45,45,45	1.13	2 (4%)
24	PEK	C	309	-	52,52,52	1.14	2 (3%)	55,57,57	0.96	4 (7%)
23	CHD	J	101	-	32,32,32	0.82	0	51,51,51	2.04	12 (23%)
19	TGL	l	101	-	62,62,62	1.16	3 (4%)	65,65,65	1.17	5 (7%)
14	HEA	a	602	20,1	57,67,67	1.85	15 (26%)	61,103,103	2.58	25 (40%)
14	HEA	a	601	1	57,67,67	2.05	15 (26%)	61,103,103	2.48	21 (34%)
20	CMO	a	608	14	0,1,1	-	-	-		
14	HEA	A	601	1	57,67,67	2.04	15 (26%)	61,103,103	2.43	25 (40%)
21	CUA	B	301	2	0,1,1	-	-	-		
18	PGV	C	303	-	50,50,50	0.87	2 (4%)	53,56,56	0.91	3 (5%)
18	PGV	c	304	-	50,50,50	0.90	2 (4%)	53,56,56	1.05	3 (5%)
23	CHD	c	306	-	32,32,32	0.59	0	51,51,51	1.49	12 (23%)
26	DMU	m	401	-	34,34,34	0.52	0	45,45,45	1.13	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CHD	B	303	-	32,32,32	1.00	1 (3%)	51,51,51	1.22	7 (13%)
24	PEK	g	102	-	52,52,52	0.89	3 (5%)	55,57,57	0.85	2 (3%)
23	CHD	j	101	-	32,32,32	0.80	0	51,51,51	2.04	12 (23%)
23	CHD	b	301	-	32,32,32	0.80	0	51,51,51	1.54	13 (25%)
25	CDL	g	103	-	99,99,99	1.07	4 (4%)	105,111,111	0.95	6 (5%)
19	TGL	D	201	-	62,62,62	1.28	3 (4%)	65,65,65	1.24	6 (9%)
24	PEK	G	102	-	52,52,52	1.11	2 (3%)	55,57,57	0.92	4 (7%)
20	CMO	A	609	14	0,1,1	-	-	-		
26	DMU	C	307	-	34,34,34	0.98	1 (2%)	45,45,45	1.46	8 (17%)
18	PGV	G	103	-	50,50,50	1.08	2 (4%)	53,56,56	0.98	4 (7%)
25	CDL	G	101	-	99,99,99	1.08	4 (4%)	105,111,111	0.95	6 (5%)

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
18	PGV	C	304	-	-	24/55/55/55	-
25	CDL	c	305	-	-	57/110/110/110	-
19	TGL	L	101	-	-	38/65/65/65	-
25	CDL	C	305	-	-	46/110/110/110	-
18	PGV	A	607	-	-	16/55/55/55	-
14	HEA	A	602	20,1	2/2/7/16	4/32/76/76	-
23	CHD	c	302	-	-	3/9/74/74	0/4/4/4
23	CHD	C	306	-	-	2/9/74/74	0/4/4/4
18	PGV	c	301	-	-	18/55/55/55	-
24	PEK	C	308	-	-	20/56/56/56	-
22	PSC	B	302	-	-	30/55/55/55	-
24	PEK	c	303	-	-	25/56/56/56	-
22	PSC	e	201	-	-	25/55/55/55	-
19	TGL	i	101	-	-	23/65/65/65	-
18	PGV	A	606	-	-	32/55/55/55	-
18	PGV	a	607	-	-	21/55/55/55	-
24	PEK	C	302	-	-	13/56/56/56	-
23	CHD	C	301	-	-	3/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	A	608	-	-	33/65/65/65	-
19	TGL	a	606	-	-	28/65/65/65	-
26	DMU	M	101	-	-	3/19/59/59	0/2/2/2
26	DMU	c	307	-	-	11/19/59/59	0/2/2/2
24	PEK	C	309	-	-	25/56/56/56	-
23	CHD	J	101	-	-	6/9/74/74	1/4/4/4
19	TGL	l	101	-	-	34/65/65/65	-
14	HEA	a	602	20,1	2/2/7/16	5/32/76/76	-
14	HEA	a	601	1	2/2/7/16	2/32/76/76	-
14	HEA	A	601	1	2/2/7/16	3/32/76/76	-
18	PGV	C	303	-	-	12/55/55/55	-
18	PGV	c	304	-	-	15/55/55/55	-
23	CHD	c	306	-	-	3/9/74/74	0/4/4/4
26	DMU	m	401	-	-	6/19/59/59	0/2/2/2
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
24	PEK	g	102	-	-	17/56/56/56	-
23	CHD	j	101	-	-	7/9/74/74	0/4/4/4
23	CHD	b	301	-	-	3/9/74/74	0/4/4/4
25	CDL	g	103	-	-	58/110/110/110	-
19	TGL	D	201	-	-	30/65/65/65	-
24	PEK	G	102	-	-	24/56/56/56	-
26	DMU	C	307	-	-	8/19/59/59	0/2/2/2
18	PGV	G	103	-	-	26/55/55/55	-
25	CDL	G	101	-	-	58/110/110/110	-

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	608	TGL	OG1-CA1	6.07	1.51	1.33
14	a	601	HEA	C3B-C2B	5.81	1.47	1.34
14	A	601	HEA	C3D-C2D	5.67	1.48	1.36
19	D	201	TGL	OG2-CB1	5.55	1.50	1.34
14	a	601	HEA	C3C-C2C	5.35	1.47	1.40
18	A	606	PGV	O03-C19	5.34	1.48	1.33
19	A	608	TGL	OG2-CB1	5.26	1.49	1.34
19	D	201	TGL	OG3-CC1	5.23	1.48	1.33
14	A	601	HEA	C3B-C2B	5.20	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	309	PEK	O01-C1	5.12	1.48	1.34
24	G	102	PEK	O03-C21	5.08	1.48	1.33
19	l	101	TGL	OG3-CC1	5.04	1.48	1.33
24	C	309	PEK	O03-C21	5.04	1.48	1.33
19	L	101	TGL	OG2-CB1	5.01	1.48	1.34
19	a	606	TGL	OG2-CB1	4.98	1.48	1.34
24	c	303	PEK	O01-C1	4.95	1.48	1.34
25	g	103	CDL	OB6-CB5	4.91	1.48	1.34
18	C	304	PGV	O03-C19	4.90	1.47	1.33
14	A	601	HEA	C3C-C2C	4.89	1.47	1.40
18	a	607	PGV	O03-C19	4.81	1.47	1.33
25	c	305	CDL	OB8-CB7	4.80	1.47	1.33
24	c	303	PEK	O03-C21	4.79	1.47	1.33
18	A	606	PGV	O01-C1	4.78	1.47	1.34
25	G	101	CDL	OB8-CB7	4.78	1.47	1.33
24	G	102	PEK	O01-C1	4.75	1.47	1.34
18	C	304	PGV	O01-C1	4.75	1.47	1.34
19	i	101	TGL	OG2-CB1	4.74	1.47	1.34
22	e	201	PSC	O03-C19	4.74	1.47	1.33
25	c	305	CDL	OB6-CB5	4.73	1.47	1.34
25	C	305	CDL	OA6-CA5	4.73	1.47	1.34
19	l	101	TGL	OG2-CB1	4.72	1.47	1.34
22	e	201	PSC	O01-C1	4.70	1.47	1.34
25	c	305	CDL	OA8-CA7	4.69	1.47	1.33
18	G	103	PGV	O01-C1	4.69	1.47	1.34
22	B	302	PSC	O01-C1	4.69	1.47	1.34
19	a	606	TGL	OG3-CC1	4.68	1.47	1.33
19	L	101	TGL	OG3-CC1	4.66	1.47	1.33
19	i	101	TGL	OG1-CA1	4.66	1.46	1.33
24	C	308	PEK	O01-C1	4.64	1.47	1.34
25	G	101	CDL	OB6-CB5	4.63	1.47	1.34
25	g	103	CDL	OA6-CA5	4.61	1.47	1.34
19	D	201	TGL	OG1-CA1	4.58	1.46	1.33
25	c	305	CDL	OA6-CA5	4.58	1.47	1.34
22	B	302	PSC	O03-C19	4.57	1.46	1.33
19	a	606	TGL	OG1-CA1	4.56	1.46	1.33
14	A	602	HEA	C3B-C2B	4.54	1.45	1.34
18	G	103	PGV	O03-C19	4.54	1.46	1.33
25	C	305	CDL	OB8-CB7	4.53	1.46	1.33
14	a	602	HEA	C4B-NB	-4.53	1.32	1.40
14	A	602	HEA	C3D-C2D	4.52	1.46	1.36
25	g	103	CDL	OB8-CB7	4.49	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	103	CDL	OA8-CA7	4.48	1.46	1.33
25	G	101	CDL	OA6-CA5	4.47	1.46	1.34
24	C	308	PEK	O03-C21	4.44	1.46	1.33
19	l	101	TGL	OG1-CA1	4.42	1.46	1.33
25	G	101	CDL	OA8-CA7	4.38	1.46	1.33
14	a	601	HEA	C3A-C2A	4.38	1.46	1.40
14	a	601	HEA	C3D-C2D	4.34	1.45	1.36
14	a	601	HEA	CHD-C1D	4.32	1.46	1.35
14	a	602	HEA	C1D-ND	-4.31	1.32	1.40
14	A	601	HEA	C4B-NB	-4.31	1.32	1.40
25	C	305	CDL	OA8-CA7	4.29	1.45	1.33
14	A	601	HEA	CHD-C1D	4.29	1.46	1.35
14	a	602	HEA	C3D-C2D	4.22	1.45	1.36
18	C	303	PGV	O01-C1	4.16	1.46	1.34
19	A	608	TGL	OG3-CC1	4.12	1.45	1.33
18	a	607	PGV	O01-C1	4.09	1.45	1.34
24	C	302	PEK	O03-C21	4.07	1.45	1.33
14	a	602	HEA	C3B-C2B	4.06	1.43	1.34
14	a	601	HEA	C4B-NB	-4.03	1.33	1.40
14	A	602	HEA	CHC-C4B	3.99	1.45	1.35
14	A	602	HEA	CHD-C1D	3.91	1.45	1.35
14	A	601	HEA	C1D-ND	-3.88	1.33	1.40
25	C	305	CDL	OB6-CB5	3.87	1.45	1.34
14	a	601	HEA	C1D-ND	-3.85	1.33	1.40
18	c	304	PGV	O01-C1	3.83	1.45	1.34
19	L	101	TGL	OG1-CA1	3.80	1.44	1.33
14	A	601	HEA	C3A-C2A	3.76	1.45	1.40
18	c	304	PGV	O03-C19	3.72	1.44	1.33
14	a	602	HEA	C3A-C2A	3.69	1.45	1.40
14	A	602	HEA	C1D-ND	-3.63	1.34	1.40
14	a	601	HEA	CHC-C4B	3.60	1.44	1.35
24	g	102	PEK	O03-C21	3.59	1.43	1.33
14	A	601	HEA	CHC-C4B	3.59	1.44	1.35
24	g	102	PEK	O01-C1	3.58	1.44	1.34
14	a	602	HEA	C4D-ND	-3.57	1.31	1.38
14	a	602	HEA	C3C-C2C	3.52	1.45	1.40
24	C	302	PEK	O01-C1	3.49	1.44	1.34
26	C	307	DMU	O16-C6	3.44	1.46	1.40
18	c	301	PGV	O01-C1	3.41	1.43	1.34
14	a	602	HEA	CHD-C1D	3.40	1.43	1.35
14	a	602	HEA	CHC-C4B	3.32	1.43	1.35
18	C	303	PGV	O03-C19	3.31	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	i	101	TGL	OG3-CC1	3.29	1.43	1.33
18	c	301	PGV	O03-C19	3.27	1.42	1.33
14	A	602	HEA	C1B-NB	-3.25	1.32	1.38
14	A	602	HEA	C4B-NB	-3.22	1.34	1.40
18	A	607	PGV	O03-C19	3.14	1.42	1.33
14	a	601	HEA	FE-NB	3.02	2.11	1.96
26	c	307	DMU	O16-C6	2.90	1.45	1.40
24	C	302	PEK	O01-C02	-2.89	1.39	1.46
18	A	607	PGV	O01-C1	2.87	1.42	1.34
14	A	602	HEA	C3C-C2C	2.86	1.44	1.40
14	A	602	HEA	C4D-ND	-2.84	1.33	1.38
14	A	601	HEA	C1B-C2B	2.71	1.49	1.44
14	A	602	HEA	C3A-C2A	2.70	1.44	1.40
14	a	601	HEA	FE-ND	2.68	2.10	1.96
14	A	601	HEA	FE-NB	2.54	2.09	1.96
14	a	601	HEA	C4D-ND	-2.54	1.33	1.38
14	A	602	HEA	C1D-C2D	2.50	1.49	1.44
23	B	303	CHD	C13-C14	-2.46	1.51	1.55
14	A	601	HEA	C4D-ND	-2.45	1.33	1.38
14	a	601	HEA	C4B-C3B	2.42	1.48	1.44
14	a	601	HEA	C2A-C1A	2.41	1.48	1.42
14	a	602	HEA	FE-NB	2.40	2.08	1.96
24	g	102	PEK	O03-C01	-2.39	1.39	1.45
14	a	601	HEA	C1C-CHC	2.33	1.47	1.41
14	A	601	HEA	C4B-C3B	2.31	1.48	1.44
14	a	602	HEA	FE-ND	2.31	2.08	1.96
14	a	602	HEA	C1B-NB	-2.29	1.34	1.38
14	A	601	HEA	O1A-CGA	2.27	1.29	1.22
14	A	601	HEA	FE-ND	2.22	2.07	1.96
14	A	602	HEA	C4D-C3D	2.15	1.48	1.45
14	A	601	HEA	C1B-NB	-2.12	1.34	1.38
14	A	602	HEA	C1C-CHC	2.12	1.46	1.41
14	a	602	HEA	C4B-C3B	2.09	1.48	1.44
14	A	602	HEA	FE-NB	2.09	2.07	1.96
14	a	601	HEA	CAA-C2A	-2.07	1.48	1.52
14	a	602	HEA	C1C-NC	-2.07	1.31	1.36
14	A	602	HEA	C2A-C1A	2.06	1.47	1.42
14	a	602	HEA	C2A-C1A	2.02	1.47	1.42
18	A	606	PGV	C01-C02	2.02	1.56	1.50
24	C	302	PEK	O03-C01	-2.00	1.40	1.45

All (314) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	302	PSC	C08-N-C07	-7.43	89.88	108.97
14	a	602	HEA	C3D-C4D-ND	7.21	117.33	110.36
14	a	601	HEA	C3D-C4D-ND	6.91	117.05	110.36
22	B	302	PSC	C08-N-C06	-6.65	91.89	108.97
14	a	602	HEA	C2D-C1D-ND	6.46	117.50	109.84
19	i	101	TGL	OG2-CB1-CB2	6.30	125.07	111.50
14	a	601	HEA	C13-C12-C11	-6.26	104.94	114.35
22	e	201	PSC	C08-N-C07	-6.23	92.96	108.97
22	e	201	PSC	C08-N-C06	-6.11	93.25	108.97
14	a	602	HEA	C1D-C2D-C3D	-5.99	100.66	106.96
14	a	601	HEA	C2B-C1B-NB	5.96	117.02	109.88
14	A	602	HEA	C3D-C4D-ND	5.96	116.13	110.36
19	D	201	TGL	OG2-CB1-CB2	5.93	124.28	111.50
14	a	602	HEA	C2B-C1B-NB	5.90	116.94	109.88
14	A	601	HEA	C2B-C1B-NB	5.87	116.91	109.88
23	J	101	CHD	C6-C5-C10	5.82	118.84	112.66
14	A	602	HEA	C2B-C1B-NB	5.82	116.85	109.88
22	B	302	PSC	C07-N-C06	5.76	123.79	108.97
19	A	608	TGL	OG2-CB1-CB2	5.67	123.73	111.50
19	l	101	TGL	OG2-CB1-CB2	5.64	123.66	111.50
23	j	101	CHD	C6-C5-C10	5.61	118.61	112.66
14	A	601	HEA	C3D-C4D-ND	5.59	115.77	110.36
24	C	308	PEK	O01-C1-C2	5.56	123.48	111.50
14	A	602	HEA	C3B-C4B-NB	5.53	116.39	109.84
14	A	602	HEA	CAD-CBD-CGD	-5.44	101.89	113.60
25	C	305	CDL	OA6-CA5-C11	5.38	123.09	111.50
14	A	601	HEA	C3B-C4B-NB	5.35	116.17	109.84
14	A	601	HEA	C13-C12-C11	-5.33	106.35	114.35
23	j	101	CHD	C9-C10-C5	5.27	115.98	108.58
14	A	601	HEA	C1D-C2D-C3D	-5.23	101.45	106.96
14	a	601	HEA	C3B-C4B-NB	5.18	115.98	109.84
23	J	101	CHD	C6-C7-C8	5.17	116.99	111.48
14	a	602	HEA	CAD-CBD-CGD	-5.15	102.53	113.60
14	A	601	HEA	C1B-C2B-C3B	-5.14	100.66	106.80
14	a	601	HEA	C2D-C1D-ND	5.05	115.82	109.84
23	J	101	CHD	C22-C20-C17	5.04	120.70	110.28
22	e	201	PSC	O01-C1-C2	5.03	122.35	111.50
25	c	305	CDL	OB6-CB5-C51	4.94	122.15	111.50
14	A	602	HEA	C2D-C1D-ND	4.90	115.65	109.84
25	g	103	CDL	OB6-CB5-C51	4.85	121.95	111.50
14	a	601	HEA	C1B-C2B-C3B	-4.83	101.02	106.80
23	j	101	CHD	C13-C17-C20	4.73	125.14	119.50
25	c	305	CDL	OA6-CA5-C11	4.65	121.52	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	602	HEA	C3B-C4B-NB	4.63	115.32	109.84
14	A	602	HEA	C1D-C2D-C3D	-4.61	102.11	106.96
14	A	601	HEA	C2D-C1D-ND	4.53	115.21	109.84
25	G	101	CDL	OA6-CA5-C11	4.48	121.16	111.50
18	C	304	PGV	O01-C1-C2	4.47	121.14	111.50
18	C	304	PGV	O03-C19-C20	4.42	125.78	111.91
23	j	101	CHD	C5-C6-C7	4.42	119.34	114.46
23	j	101	CHD	C22-C20-C17	4.41	119.39	110.28
23	J	101	CHD	C5-C6-C7	4.38	119.29	114.46
18	a	607	PGV	O01-C1-C2	4.36	120.90	111.50
25	C	305	CDL	OB6-CB5-C51	4.33	120.83	111.50
14	A	602	HEA	CMD-C2D-C1D	4.26	131.53	125.04
25	g	103	CDL	OA6-CA5-C11	4.25	120.66	111.50
24	c	303	PEK	O03-C21-C22	4.23	125.17	111.91
26	m	401	DMU	C7-C8-C9	4.16	117.65	110.24
22	B	302	PSC	O01-C1-C2	4.14	120.43	111.50
14	A	602	HEA	C3C-C4C-NC	4.09	114.50	109.21
14	a	602	HEA	C3C-C4C-NC	4.07	114.47	109.21
18	A	606	PGV	O03-C19-C20	4.06	124.64	111.91
14	A	602	HEA	C13-C12-C11	-4.01	108.32	114.35
18	A	606	PGV	C02-O01-C1	3.96	127.54	117.79
25	G	101	CDL	OB6-CB5-C51	3.94	119.98	111.50
23	c	302	CHD	C22-C20-C17	3.93	118.40	110.28
18	G	103	PGV	O03-C19-C20	3.89	124.10	111.91
14	A	602	HEA	CHA-C4D-C3D	-3.88	119.14	124.84
22	e	201	PSC	C07-N-C06	3.85	118.87	108.97
19	L	101	TGL	OG2-CB1-CB2	3.84	119.78	111.50
23	b	301	CHD	C13-C17-C20	-3.83	114.92	119.50
23	C	306	CHD	C6-C5-C4	-3.82	106.79	111.19
14	a	602	HEA	C1B-C2B-C3B	-3.82	102.23	106.80
14	a	601	HEA	C1D-C2D-C3D	-3.81	102.95	106.96
19	a	606	TGL	OG2-CB1-CB2	3.81	119.70	111.50
25	c	305	CDL	OB8-CB7-C71	3.80	123.83	111.91
24	C	309	PEK	O01-C1-C2	3.77	119.63	111.50
14	A	602	HEA	C1B-C2B-C3B	-3.77	102.30	106.80
18	C	303	PGV	O03-C19-O04	-3.74	114.14	123.59
26	C	307	DMU	C10-C5-C7	3.73	117.76	110.00
23	J	101	CHD	C13-C17-C20	3.70	123.92	119.50
14	a	601	HEA	C4D-C3D-C2D	-3.67	101.55	106.90
14	a	602	HEA	CHB-C1B-C2B	-3.65	119.27	124.98
24	C	302	PEK	O01-C1-C2	3.65	119.36	111.50
19	a	606	TGL	OG3-CC1-CC2	3.63	123.31	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	c	304	PGV	O01-C1-C2	3.63	119.33	111.50
24	c	303	PEK	O01-C1-C2	3.62	119.31	111.50
19	D	201	TGL	OG1-CA1-CA2	3.60	123.20	111.91
22	e	201	PSC	O03-C19-C20	3.60	123.19	111.91
19	A	608	TGL	OG3-CC1-CC2	3.59	123.19	111.91
14	a	601	HEA	C3C-C4C-NC	3.59	113.85	109.21
22	e	201	PSC	C08-N-C05	-3.56	95.34	109.92
23	C	306	CHD	C4-C5-C10	3.53	116.41	112.66
19	A	608	TGL	OG1-CA1-CA2	3.47	122.80	111.91
14	A	602	HEA	CAD-C3D-C4D	3.44	130.67	124.66
19	D	201	TGL	OG3-CC1-CC2	3.43	122.67	111.91
14	a	601	HEA	CBA-CAA-C2A	-3.42	106.84	112.60
14	A	602	HEA	CMC-C2C-C3C	3.41	131.06	124.68
14	a	601	HEA	CHA-C4D-C3D	-3.40	119.83	124.84
14	A	601	HEA	C3C-C4C-NC	3.40	113.61	109.21
24	c	303	PEK	O03-C21-O04	-3.40	115.02	123.59
18	A	606	PGV	O01-C1-C2	3.37	118.77	111.50
23	J	101	CHD	C6-C5-C4	-3.36	107.32	111.19
26	c	307	DMU	C6-C1-C2	3.33	116.92	110.00
14	A	601	HEA	CMC-C2C-C3C	3.30	130.86	124.68
24	G	102	PEK	O01-C1-C2	3.30	118.60	111.50
25	C	305	CDL	OB8-CB7-C71	3.29	122.23	111.91
14	a	602	HEA	CMD-C2D-C1D	3.27	130.02	125.04
26	C	307	DMU	C8-C7-C5	3.27	116.53	110.82
14	a	602	HEA	CHA-C4D-C3D	-3.25	120.06	124.84
14	a	601	HEA	CHB-C1B-C2B	-3.23	119.93	124.98
22	e	201	PSC	C07-N-C05	3.22	123.09	109.92
14	A	601	HEA	CHA-C4D-C3D	-3.22	120.11	124.84
23	c	302	CHD	O26-C24-C23	3.19	124.27	114.03
25	c	305	CDL	OA8-CA7-C31	3.18	121.89	111.91
14	a	601	HEA	CMC-C2C-C3C	3.18	130.63	124.68
24	C	308	PEK	O03-C21-C22	3.18	121.89	111.91
23	b	301	CHD	C6-C5-C4	-3.17	107.55	111.19
23	c	302	CHD	C13-C17-C20	-3.13	115.76	119.50
14	a	602	HEA	C1D-ND-C4D	-3.10	101.87	105.07
24	C	308	PEK	O03-C21-O04	-3.10	115.77	123.59
18	G	103	PGV	O01-C1-C2	3.06	118.11	111.50
14	A	602	HEA	CHB-C1B-C2B	-3.06	120.19	124.98
14	A	601	HEA	CMB-C2B-C1B	3.05	129.69	125.04
14	A	602	HEA	C4D-C3D-C2D	-3.04	102.47	106.90
14	A	602	HEA	C4B-C3B-C2B	-3.02	102.24	107.41
19	A	608	TGL	OG3-CG3-CG2	3.02	117.24	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	M	101	DMU	O49-C1-C6	-2.95	102.88	110.05
18	A	607	PGV	O01-C1-C2	2.94	117.85	111.50
26	C	307	DMU	C18-O16-C6	2.94	118.72	113.84
23	j	101	CHD	C1-C2-C3	2.94	114.24	110.47
23	c	302	CHD	O25-C24-C23	-2.94	113.64	123.08
19	D	201	TGL	OG2-CB1-OB1	-2.94	116.60	123.70
14	a	602	HEA	C4D-C3D-C2D	-2.93	102.62	106.90
24	G	102	PEK	O03-C21-C22	2.93	121.11	111.91
23	c	306	CHD	C4-C3-C2	-2.93	107.05	110.55
19	l	101	TGL	OG3-CC1-CC2	2.93	121.09	111.91
23	j	101	CHD	C10-C9-C8	2.93	114.96	111.82
23	C	306	CHD	C4-C3-C2	-2.91	107.08	110.55
19	i	101	TGL	OG2-CB1-OB1	-2.91	116.67	123.70
14	A	601	HEA	CHB-C1B-C2B	-2.90	120.44	124.98
23	c	302	CHD	C1-C2-C3	-2.89	106.76	110.47
18	A	606	PGV	O03-C01-C02	2.89	116.84	108.43
14	a	602	HEA	CMC-C2C-C3C	2.88	130.07	124.68
18	C	304	PGV	O03-C19-O04	-2.88	116.32	123.59
26	C	307	DMU	C2-C3-C4	-2.88	104.32	110.93
25	C	305	CDL	OA6-CA5-OA7	-2.88	116.74	123.70
22	B	302	PSC	C08-N-C05	-2.87	98.19	109.92
19	i	101	TGL	OG3-CC1-CC2	2.86	120.88	111.91
23	j	101	CHD	C6-C5-C4	-2.86	107.90	111.19
25	C	305	CDL	OA8-CA7-C31	2.85	120.85	111.91
25	c	305	CDL	OB6-CB5-OB7	-2.85	116.82	123.70
26	M	101	DMU	C18-O16-C6	-2.84	109.13	113.84
23	J	101	CHD	C11-C9-C8	2.83	115.01	110.88
14	A	602	HEA	C4B-NB-C1B	-2.82	102.16	105.07
22	B	302	PSC	C06-N-C05	2.82	121.45	109.92
26	C	307	DMU	O7-C3-C2	2.81	114.76	107.28
19	L	101	TGL	OG3-CC1-CC2	2.79	120.65	111.91
23	c	306	CHD	C11-C9-C8	-2.78	106.81	110.88
22	e	201	PSC	C01-O03-C19	2.78	127.42	117.12
23	J	101	CHD	C16-C17-C20	2.78	116.45	112.15
18	G	103	PGV	O03-C19-O04	-2.77	116.60	123.59
23	b	301	CHD	C22-C20-C17	2.76	115.99	110.28
26	C	307	DMU	C6-C1-C2	2.76	115.73	110.00
19	D	201	TGL	OG1-CA1-OA1	-2.75	116.64	123.59
19	i	101	TGL	OG1-CA1-CA2	2.74	120.50	111.91
19	l	101	TGL	OG1-CA1-CA2	2.73	120.47	111.91
23	j	101	CHD	C19-C10-C1	-2.72	103.88	108.26
23	j	101	CHD	C13-C14-C8	2.71	118.20	114.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	309	PEK	C01-O03-C21	2.70	127.11	117.12
25	C	305	CDL	CB4-OB6-CB5	-2.70	111.15	117.79
23	B	303	CHD	C5-C6-C7	2.69	117.43	114.46
19	l	101	TGL	OG2-CB1-OB1	-2.69	117.20	123.70
25	G	101	CDL	OA6-CA5-OA7	-2.68	117.23	123.70
14	A	601	HEA	O2D-CGD-CBD	2.67	122.61	114.03
23	J	101	CHD	O26-C24-C23	2.66	122.58	114.03
26	m	401	DMU	O1-C9-C8	2.65	114.51	109.69
23	c	306	CHD	C10-C9-C8	2.64	114.66	111.82
24	C	302	PEK	O01-C1-O02	-2.64	117.31	123.70
23	c	306	CHD	C23-C22-C20	-2.64	109.69	114.52
14	a	602	HEA	C4B-C3B-C2B	-2.64	102.90	107.41
25	g	103	CDL	OA8-CA7-C31	2.64	120.20	111.91
14	A	601	HEA	C13-C14-C15	-2.64	121.31	127.66
23	B	303	CHD	C19-C10-C1	-2.63	104.02	108.26
25	G	101	CDL	OA8-CA7-C31	2.62	120.12	111.91
14	a	602	HEA	C4D-CHA-C1A	2.61	126.01	122.56
18	C	303	PGV	O01-C1-C2	2.60	117.11	111.50
18	A	606	PGV	O03-C19-O04	-2.60	117.03	123.59
14	a	601	HEA	CAD-C3D-C4D	2.58	129.16	124.66
14	A	601	HEA	C4D-C3D-C2D	-2.58	103.14	106.90
14	a	602	HEA	O1D-CGD-CBD	-2.57	114.84	123.08
19	L	101	TGL	OG3-CC1-OC1	-2.56	117.12	123.59
23	b	301	CHD	C1-C10-C9	2.56	115.38	111.35
22	B	302	PSC	O03-C19-C20	2.56	119.93	111.91
23	J	101	CHD	C19-C10-C1	-2.56	104.14	108.26
23	c	306	CHD	C1-C10-C9	2.56	115.37	111.35
14	a	602	HEA	C4B-NB-C1B	-2.55	102.44	105.07
23	b	301	CHD	C4-C5-C10	2.54	115.36	112.66
23	c	302	CHD	C6-C7-C8	2.54	114.19	111.48
25	G	101	CDL	OB8-CB7-C71	2.54	119.87	111.91
18	c	304	PGV	O01-C1-O02	-2.53	117.59	123.70
18	a	607	PGV	O03-C19-C20	2.52	119.83	111.91
14	A	601	HEA	O1D-CGD-CBD	-2.51	115.00	123.08
14	A	601	HEA	C4A-CHB-C1B	2.51	125.87	122.56
19	A	608	TGL	CG1-OG1-CA1	2.51	126.42	117.12
14	A	602	HEA	CHD-C1D-C2D	-2.51	119.78	126.72
14	a	602	HEA	C26-C15-C16	2.50	119.48	115.27
26	M	101	DMU	O1-C10-C5	-2.49	105.07	110.35
25	C	305	CDL	O1-C1-CB2	2.49	118.30	109.56
14	a	602	HEA	CHD-C1D-C2D	-2.49	119.82	126.72
22	B	302	PSC	C04-C05-N	2.49	124.10	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	305	CDL	OB6-CB5-OB7	-2.49	117.68	123.70
23	b	301	CHD	C5-C4-C3	2.49	116.42	112.76
19	i	101	TGL	OG3-CG3-CG2	2.48	115.66	108.43
14	A	601	HEA	CHD-C1D-C2D	-2.48	119.86	126.72
26	c	307	DMU	C1-C2-C3	2.47	115.31	109.68
24	C	308	PEK	O01-C1-O02	-2.45	117.78	123.70
23	c	306	CHD	C6-C5-C4	-2.44	108.38	111.19
14	a	601	HEA	C4B-C3B-C2B	-2.43	103.25	107.41
22	e	201	PSC	O01-C1-O02	-2.43	117.82	123.70
22	e	201	PSC	O03-C19-O04	-2.42	117.47	123.59
19	a	606	TGL	OG3-CC1-OC1	-2.42	117.48	123.59
19	A	608	TGL	CC3-CC2-CC1	-2.42	104.81	113.62
25	G	101	CDL	OB6-CB5-OB7	-2.42	117.85	123.70
18	c	304	PGV	O03-C19-O04	-2.42	117.48	123.59
18	a	607	PGV	O01-C1-O02	-2.41	117.87	123.70
14	a	601	HEA	CAD-CBD-CGD	-2.40	108.43	113.60
23	j	101	CHD	C6-C7-C8	2.40	114.05	111.48
14	a	601	HEA	C1D-ND-C4D	-2.40	102.59	105.07
14	A	602	HEA	O1A-CGA-CBA	-2.40	115.38	123.08
24	C	309	PEK	O03-C01-C02	2.39	115.40	108.43
14	a	601	HEA	CHD-C1D-C2D	-2.39	120.12	126.72
25	g	103	CDL	OB8-CB7-OB9	-2.39	117.57	123.59
23	c	306	CHD	C9-C10-C5	2.38	111.93	108.58
23	B	303	CHD	O26-C24-C23	2.38	121.67	114.03
18	c	301	PGV	O01-C1-C2	2.37	116.60	111.50
25	C	305	CDL	OB8-CB7-OB9	-2.37	117.62	123.59
25	c	305	CDL	OA8-CA7-OA9	-2.36	117.64	123.59
23	b	301	CHD	C18-C13-C12	-2.36	106.67	109.07
23	c	306	CHD	C1-C2-C3	2.34	113.47	110.47
24	G	102	PEK	C01-O03-C21	2.34	125.80	117.12
19	l	101	TGL	CG3-OG3-CC1	2.33	125.75	117.12
26	C	307	DMU	O5-C4-C57	2.33	112.23	106.44
19	L	101	TGL	OG3-CG3-CG2	2.32	115.19	108.43
23	j	101	CHD	C14-C13-C12	-2.31	105.25	107.40
14	a	601	HEA	C4B-NB-C1B	-2.31	102.68	105.07
14	A	601	HEA	C4B-C3B-C2B	-2.31	103.47	107.41
23	b	301	CHD	C11-C12-C13	2.30	113.60	111.24
23	c	306	CHD	C2-C1-C10	2.30	116.72	112.78
23	c	302	CHD	C19-C10-C1	-2.29	104.56	108.26
23	B	303	CHD	C22-C20-C17	2.29	115.02	110.28
23	C	301	CHD	C19-C10-C1	-2.28	104.59	108.26
23	J	101	CHD	C21-C20-C17	-2.28	109.43	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	309	PEK	O03-C21-C22	2.28	119.05	111.91
24	g	102	PEK	O01-C1-C2	2.28	116.40	111.50
23	c	306	CHD	O25-C24-C23	-2.27	115.80	123.08
14	A	602	HEA	O2A-CGA-CBA	2.26	121.30	114.03
18	A	607	PGV	O03-C19-C20	2.26	119.00	111.91
24	g	102	PEK	O03-C21-O04	-2.26	117.89	123.59
14	a	601	HEA	O2D-CGD-CBD	2.25	121.27	114.03
14	A	601	HEA	C4B-NB-C1B	-2.25	102.75	105.07
23	C	306	CHD	C9-C10-C5	2.25	111.73	108.58
25	c	305	CDL	OB8-CB7-OB9	-2.24	117.94	123.59
18	A	607	PGV	O01-C1-O02	-2.24	118.30	123.70
18	A	606	PGV	O01-C02-C03	2.23	116.47	108.40
23	c	302	CHD	C18-C13-C12	2.23	111.33	109.07
23	c	302	CHD	C11-C9-C8	2.22	114.12	110.88
23	c	302	CHD	C5-C4-C3	-2.22	109.50	112.76
18	C	303	PGV	O03-C19-C20	2.22	118.86	111.91
24	G	102	PEK	O03-C01-C02	2.22	114.89	108.43
19	D	201	TGL	CG3-OG3-CC1	2.21	125.29	117.12
14	A	601	HEA	O1A-CGA-CBA	-2.20	116.01	123.08
23	b	301	CHD	C19-C10-C1	-2.20	104.72	108.26
14	A	602	HEA	C26-C15-C16	2.20	118.97	115.27
23	B	303	CHD	C6-C5-C4	-2.19	108.67	111.19
26	C	307	DMU	C10-O1-C9	2.19	117.98	113.69
26	M	101	DMU	O1-C9-C11	2.19	111.87	106.44
18	G	103	PGV	O03-C01-C02	2.17	114.76	108.43
14	a	602	HEA	CBA-CAA-C2A	-2.17	108.94	112.60
14	a	602	HEA	OMA-CMA-C3A	-2.17	120.18	124.91
23	B	303	CHD	C11-C12-C13	2.16	113.46	111.24
14	A	601	HEA	CAD-C3D-C4D	2.14	128.40	124.66
23	c	302	CHD	C14-C13-C12	-2.14	105.41	107.40
25	g	103	CDL	OA8-CA7-OA9	-2.14	118.20	123.59
14	a	601	HEA	CHC-C4B-NB	-2.13	121.75	124.38
14	A	601	HEA	CMD-C2D-C1D	2.13	128.28	125.04
22	B	302	PSC	O03-C01-C02	2.12	114.61	108.43
23	J	101	CHD	C18-C13-C17	2.12	114.53	111.21
25	C	305	CDL	OA8-CA7-OA9	-2.11	118.26	123.59
23	b	301	CHD	C18-C13-C14	2.11	114.51	111.21
23	C	301	CHD	O7-C7-C8	2.10	114.12	109.43
14	a	602	HEA	C27-C19-C20	2.10	118.80	115.27
23	B	303	CHD	C1-C10-C9	2.09	114.64	111.35
18	A	606	PGV	C21-C20-C19	2.09	121.22	113.62
25	g	103	CDL	OA6-CA5-OA7	-2.09	118.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	301	CHD	C1-C10-C5	-2.08	104.68	107.77
23	b	301	CHD	O26-C24-C23	2.08	120.72	114.03
14	a	602	HEA	O2D-CGD-O1D	2.07	128.46	123.30
23	C	301	CHD	C23-C22-C20	-2.07	110.73	114.52
25	c	305	CDL	OA6-CA5-OA7	-2.07	118.71	123.70
23	C	306	CHD	C19-C10-C1	-2.06	104.94	108.26
14	A	601	HEA	CAD-CBD-CGD	-2.05	109.18	113.60
23	C	301	CHD	C1-C2-C3	-2.05	107.84	110.47
23	c	306	CHD	C19-C10-C9	-2.03	108.38	111.18
18	c	301	PGV	C02-O01-C1	-2.03	112.80	117.79
26	m	401	DMU	O1-C10-C5	-2.03	106.06	110.35
18	A	606	PGV	C01-O03-C19	2.03	124.62	117.12
14	A	601	HEA	CHC-C4B-C3B	-2.02	120.59	125.80
23	b	301	CHD	C9-C8-C7	-2.02	109.46	111.88
23	c	306	CHD	C4-C5-C10	2.01	114.79	112.66
23	c	302	CHD	C11-C12-C13	2.01	113.31	111.24
23	C	301	CHD	C21-C20-C22	-2.01	107.22	110.36
14	a	602	HEA	CMB-C2B-C1B	2.00	128.09	125.04
23	C	301	CHD	C6-C7-C8	2.00	113.62	111.48

All (8) chirality outliers are listed below:

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

All (819) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C03-O11-P-O13
18	A	606	PGV	C03-O11-P-O14
18	A	606	PGV	O12-C04-C05-O05
18	C	304	PGV	C03-O11-P-O12
18	C	304	PGV	C03-O11-P-O13
18	C	304	PGV	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
18	C	304	PGV	C04-O12-P-O11
18	C	304	PGV	C04-O12-P-O13
18	C	304	PGV	C04-O12-P-O14
18	G	103	PGV	C03-O11-P-O13
18	G	103	PGV	C04-C05-C06-O06
18	a	607	PGV	C03-O11-P-O14
18	a	607	PGV	C04-O12-P-O11
18	a	607	PGV	C2-C1-O01-C02
19	A	608	TGL	CB2-CB1-OG2-CG2
19	A	608	TGL	OB1-CB1-OG2-CG2
19	L	101	TGL	CB2-CB1-OG2-CG2
19	a	606	TGL	CB2-CB1-OG2-CG2
22	B	302	PSC	C04-O12-P-O13
22	B	302	PSC	O12-C04-C05-N
22	B	302	PSC	C05-C04-O12-P
22	e	201	PSC	C03-O11-P-O13
22	e	201	PSC	C04-O12-P-O11
22	e	201	PSC	C04-O12-P-O14
22	e	201	PSC	O02-C1-O01-C02
22	e	201	PSC	O04-C19-O03-C01
22	e	201	PSC	C20-C19-O03-C01
24	C	308	PEK	C04-O12-P-O11
24	C	308	PEK	C04-O12-P-O14
24	C	308	PEK	O02-C1-O01-C02
24	C	308	PEK	C2-C1-O01-C02
24	C	309	PEK	C04-O12-P-O13
24	C	309	PEK	O12-C04-C05-N
24	G	102	PEK	C03-O11-P-O12
24	G	102	PEK	C03-O11-P-O14
24	c	303	PEK	C2-C1-O01-C02
24	g	102	PEK	C9-C10-C11-C12
25	C	305	CDL	C1-CA2-OA2-PA1
25	C	305	CDL	OA7-CA5-OA6-CA4
25	C	305	CDL	C11-CA5-OA6-CA4
25	C	305	CDL	CB3-OB5-PB2-OB3
25	G	101	CDL	CA2-C1-CB2-OB2
25	G	101	CDL	CA2-OA2-PA1-OA4
25	G	101	CDL	CA3-OA5-PA1-OA2
25	G	101	CDL	CA3-OA5-PA1-OA3
25	G	101	CDL	OA7-CA5-OA6-CA4
25	G	101	CDL	CB3-OB5-PB2-OB2
25	G	101	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
25	G	101	CDL	CB3-OB5-PB2-OB4
25	c	305	CDL	C1-CA2-OA2-PA1
25	c	305	CDL	CA2-OA2-PA1-OA3
25	c	305	CDL	CA2-OA2-PA1-OA4
25	c	305	CDL	CA2-OA2-PA1-OA5
25	c	305	CDL	C11-CA5-OA6-CA4
25	c	305	CDL	CB3-OB5-PB2-OB2
25	c	305	CDL	CB3-OB5-PB2-OB3
25	c	305	CDL	CB3-OB5-PB2-OB4
25	g	103	CDL	CA2-OA2-PA1-OA3
25	g	103	CDL	CA3-OA5-PA1-OA3
25	g	103	CDL	OA7-CA5-OA6-CA4
25	g	103	CDL	OB6-CB4-CB6-OB8
26	c	307	DMU	O5-C6-O16-C18
19	a	606	TGL	CC2-CC1-OG3-CG3
18	G	103	PGV	O04-C19-O03-C01
19	a	606	TGL	OC1-CC1-OG3-CG3
25	G	101	CDL	OB9-CB7-OB8-CB6
18	a	607	PGV	O02-C1-O01-C02
19	L	101	TGL	OB1-CB1-OG2-CG2
19	a	606	TGL	OB1-CB1-OG2-CG2
24	c	303	PEK	O02-C1-O01-C02
25	c	305	CDL	OA7-CA5-OA6-CA4
24	C	308	PEK	O04-C21-O03-C01
18	G	103	PGV	C20-C19-O03-C01
25	G	101	CDL	C31-CA7-OA8-CA6
22	e	201	PSC	C2-C1-O01-C02
25	G	101	CDL	C11-CA5-OA6-CA4
25	g	103	CDL	C11-CA5-OA6-CA4
19	D	201	TGL	OC1-CC1-OG3-CG3
19	L	101	TGL	CA2-CA1-OG1-CG1
24	C	308	PEK	C22-C21-O03-C01
24	g	102	PEK	C22-C21-O03-C01
25	G	101	CDL	C71-CB7-OB8-CB6
18	C	304	PGV	O02-C1-O01-C02
19	l	101	TGL	OA1-CA1-OG1-CG1
25	G	101	CDL	OA9-CA7-OA8-CA6
23	J	101	CHD	C13-C17-C20-C22
23	j	101	CHD	C13-C17-C20-C22
25	C	305	CDL	O1-C1-CB2-OB2
25	G	101	CDL	O1-C1-CB2-OB2
19	A	608	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CC2-CC1-OG3-CG3
25	g	103	CDL	C31-CA7-OA8-CA6
18	C	304	PGV	C2-C1-O01-C02
19	i	101	TGL	CB2-CB1-OG2-CG2
24	g	102	PEK	O04-C21-O03-C01
19	l	101	TGL	CA2-CA1-OG1-CG1
25	C	305	CDL	C31-CA7-OA8-CA6
26	c	307	DMU	O5-C4-C57-O61
19	L	101	TGL	OA1-CA1-OG1-CG1
25	g	103	CDL	OA9-CA7-OA8-CA6
25	C	305	CDL	OA9-CA7-OA8-CA6
25	G	101	CDL	C51-CB5-OB6-CB4
26	m	401	DMU	C3-C4-C57-O61
18	A	606	PGV	O12-C04-C05-C06
25	C	305	CDL	CA2-C1-CB2-OB2
19	i	101	TGL	OB1-CB1-OG2-CG2
19	A	608	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	CA2-CA1-OG1-CG1
25	c	305	CDL	C31-CA7-OA8-CA6
26	c	307	DMU	C3-C4-C57-O61
23	J	101	CHD	C13-C17-C20-C21
18	C	304	PGV	O12-C04-C05-O05
25	g	103	CDL	O1-C1-CA2-OA2
26	c	307	DMU	C1-C6-O16-C18
25	c	305	CDL	OA9-CA7-OA8-CA6
23	C	306	CHD	C17-C20-C22-C23
23	j	101	CHD	C17-C20-C22-C23
26	m	401	DMU	O6-C11-C9-C8
24	C	302	PEK	C1-C2-C3-C4
24	C	308	PEK	C21-C22-C23-C24
23	j	101	CHD	C13-C17-C20-C21
18	a	607	PGV	C1-C2-C3-C4
19	L	101	TGL	CA1-CA2-CA3-CA4
25	c	305	CDL	CB7-C71-C72-C73
23	J	101	CHD	C17-C20-C22-C23
18	a	607	PGV	C20-C19-O03-C01
25	C	305	CDL	C71-CB7-OB8-CB6
25	G	101	CDL	OB7-CB5-OB6-CB4
23	J	101	CHD	C21-C20-C22-C23
18	G	103	PGV	C1-C2-C3-C4
18	c	301	PGV	C19-C20-C21-C22
19	D	201	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
19	i	101	TGL	CC1-CC2-CC3-CC4
25	C	305	CDL	CB7-C71-C72-C73
26	C	307	DMU	O1-C10-O7-C3
19	D	201	TGL	OA1-CA1-OG1-CG1
23	b	301	CHD	C17-C20-C22-C23
23	C	306	CHD	C21-C20-C22-C23
23	j	101	CHD	C21-C20-C22-C23
26	m	401	DMU	O5-C4-C57-O61
18	G	103	PGV	C2-C1-O01-C02
25	C	305	CDL	C51-CB5-OB6-CB4
18	A	606	PGV	C04-O12-P-O11
18	G	103	PGV	C03-O11-P-O12
18	a	607	PGV	C03-O11-P-O12
22	B	302	PSC	C04-O12-P-O11
24	C	309	PEK	C04-O12-P-O11
25	G	101	CDL	CA2-OA2-PA1-OA5
25	c	305	CDL	CA3-OA5-PA1-OA2
25	g	103	CDL	CB2-OB2-PB2-OB5
18	c	301	PGV	C1-C2-C3-C4
19	L	101	TGL	CC2-CC1-OG3-CG3
25	g	103	CDL	C71-CB7-OB8-CB6
25	g	103	CDL	CB2-C1-CA2-OA2
18	G	103	PGV	O02-C1-O01-C02
19	D	201	TGL	OB1-CB1-OG2-CG2
25	C	305	CDL	OB7-CB5-OB6-CB4
22	B	302	PSC	C20-C19-O03-C01
23	j	101	CHD	C16-C17-C20-C21
25	G	101	CDL	CB5-C51-C52-C53
18	c	301	PGV	C7-C8-C9-C10
25	c	305	CDL	C59-C60-C61-C62
19	D	201	TGL	CB2-CB1-OG2-CG2
19	A	608	TGL	C18-C19-C33-C34
19	L	101	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	C11-C10-CB9-CB8
19	i	101	TGL	C11-C12-C13-C14
19	l	101	TGL	CC9-C15-C16-C17
24	C	309	PEK	C27-C28-C29-C30
24	c	303	PEK	C16-C17-C18-C19
25	G	101	CDL	C80-C81-C82-C83
25	c	305	CDL	C16-C17-C18-C19
25	g	103	CDL	C52-C53-C54-C55
19	l	101	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
24	G	102	PEK	C29-C30-C31-C32
25	C	305	CDL	C16-C17-C18-C19
25	G	101	CDL	C38-C39-C40-C41
25	c	305	CDL	C43-C44-C45-C46
26	c	307	DMU	C25-C28-C31-C34
18	A	606	PGV	C03-C02-O01-C1
25	c	305	CDL	OB7-CB5-OB6-CB4
18	A	607	PGV	C22-C23-C24-C25
19	A	608	TGL	C15-C16-C17-C18
19	l	101	TGL	C20-C21-C22-C23
18	A	606	PGV	C5-C6-C7-C8
19	D	201	TGL	C18-C19-C33-C34
19	a	606	TGL	C21-C20-CA9-CA8
19	l	101	TGL	CA3-CA4-CA5-CA6
19	l	101	TGL	CA5-CA6-CA7-CA8
18	a	607	PGV	O12-C04-C05-O05
18	G	103	PGV	C7-C8-C9-C10
22	e	201	PSC	C29-C30-C31-C32
25	C	305	CDL	C12-C13-C14-C15
25	C	305	CDL	C32-C33-C34-C35
25	G	101	CDL	C32-C33-C34-C35
25	C	305	CDL	C33-C34-C35-C36
25	g	103	CDL	C19-C20-C21-C22
18	a	607	PGV	O04-C19-O03-C01
19	L	101	TGL	OC1-CC1-OG3-CG3
18	C	304	PGV	C5-C6-C7-C8
19	L	101	TGL	C22-C23-C24-C25
25	C	305	CDL	C22-C23-C24-C25
25	G	101	CDL	C34-C35-C36-C37
25	g	103	CDL	C59-C60-C61-C62
26	c	307	DMU	C28-C31-C34-C37
26	C	307	DMU	C3-C4-C57-O61
18	C	303	PGV	C19-C20-C21-C22
19	L	101	TGL	CC9-C15-C16-C17
19	a	606	TGL	C15-C16-C17-C18
19	l	101	TGL	CC7-CC8-CC9-C15
24	c	303	PEK	C25-C26-C27-C28
25	C	305	CDL	C51-C52-C53-C54
25	G	101	CDL	C56-C57-C58-C59
26	c	307	DMU	C22-C25-C28-C31
26	m	401	DMU	C25-C28-C31-C34
25	C	305	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
18	c	301	PGV	C26-C27-C28-C29
24	C	302	PEK	C16-C17-C18-C19
18	A	606	PGV	C04-C05-C06-O06
25	c	305	CDL	C51-CB5-OB6-CB4
18	G	103	PGV	C5-C6-C7-C8
19	A	608	TGL	CA4-CA5-CA6-CA7
19	D	201	TGL	CA9-C20-C21-C22
25	G	101	CDL	C37-C38-C39-C40
25	G	101	CDL	C79-C80-C81-C82
25	c	305	CDL	C52-C53-C54-C55
25	g	103	CDL	C56-C57-C58-C59
19	L	101	TGL	CC1-CC2-CC3-CC4
19	A	608	TGL	CC9-C15-C16-C17
19	D	201	TGL	C17-C18-C19-C33
19	l	101	TGL	CB4-CB5-CB6-CB7
24	C	308	PEK	C33-C34-C35-C36
24	C	309	PEK	C28-C29-C30-C31
24	g	102	PEK	C30-C31-C32-C33
25	C	305	CDL	C81-C82-C83-C84
25	c	305	CDL	C75-C76-C77-C78
25	c	305	CDL	C77-C78-C79-C80
25	g	103	CDL	C13-C14-C15-C16
25	g	103	CDL	C14-C15-C16-C17
25	g	103	CDL	C80-C81-C82-C83
18	G	103	PGV	C21-C22-C23-C24
18	c	304	PGV	C23-C24-C25-C26
19	D	201	TGL	CC6-CC7-CC8-CC9
19	a	606	TGL	C10-C11-C12-C13
19	a	606	TGL	CC7-CC8-CC9-C15
19	i	101	TGL	CB5-CB6-CB7-CB8
19	i	101	TGL	CC3-CC4-CC5-CC6
19	l	101	TGL	C19-C33-C34-C35
25	c	305	CDL	C36-C37-C38-C39
19	D	201	TGL	CB6-CB7-CB8-CB9
19	a	606	TGL	CB5-CB6-CB7-CB8
22	B	302	PSC	C24-C25-C26-C27
25	c	305	CDL	C39-C40-C41-C42
25	g	103	CDL	C31-C32-C33-C34
25	c	305	CDL	CA5-C11-C12-C13
25	g	103	CDL	CA5-C11-C12-C13
18	G	103	PGV	C4-C5-C6-C7
19	A	608	TGL	C11-C10-CB9-CB8

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	CB6-CB7-CB8-CB9
19	i	101	TGL	C13-C14-C29-C30
23	J	101	CHD	C16-C17-C20-C21
18	C	303	PGV	C21-C22-C23-C24
25	c	305	CDL	C41-C42-C43-C44
25	c	305	CDL	C56-C57-C58-C59
25	g	103	CDL	C53-C54-C55-C56
25	g	103	CDL	OB9-CB7-OB8-CB6
18	C	304	PGV	C22-C23-C24-C25
18	a	607	PGV	C6-C7-C8-C9
19	D	201	TGL	CA7-CA8-CA9-C20
25	c	305	CDL	C63-C64-C65-C66
19	A	608	TGL	C20-C21-C22-C23
24	C	308	PEK	C24-C25-C26-C27
24	c	303	PEK	C28-C29-C30-C31
25	G	101	CDL	C14-C15-C16-C17
19	l	101	TGL	CB2-CB1-OG2-CG2
19	i	101	TGL	CA4-CA5-CA6-CA7
18	G	103	PGV	O05-C05-C06-O06
18	c	301	PGV	C2-C3-C4-C5
19	L	101	TGL	C15-C16-C17-C18
19	L	101	TGL	C17-C18-C19-C33
24	c	303	PEK	C2-C3-C4-C5
25	C	305	CDL	CA7-C31-C32-C33
18	A	607	PGV	C27-C28-C29-C30
18	G	103	PGV	C24-C25-C26-C27
18	A	606	PGV	C20-C21-C22-C23
25	G	101	CDL	C19-C20-C21-C22
22	B	302	PSC	O04-C19-O03-C01
25	G	101	CDL	C23-C24-C25-C26
25	g	103	CDL	C62-C63-C64-C65
19	D	201	TGL	CA2-CA3-CA4-CA5
19	i	101	TGL	C20-C21-C22-C23
25	C	305	CDL	C41-C42-C43-C44
25	G	101	CDL	C11-C12-C13-C14
25	g	103	CDL	C54-C55-C56-C57
23	J	101	CHD	C16-C17-C20-C22
18	c	304	PGV	C7-C8-C9-C10
19	L	101	TGL	C23-C24-C25-C26
19	a	606	TGL	C19-C33-C34-C35
25	C	305	CDL	C43-C44-C45-C46
22	e	201	PSC	C04-C05-N-C07

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Mol	Chain	Res	Type	Atoms
25	g	103	CDL	CA7-C31-C32-C33
18	A	607	PGV	C5-C6-C7-C8
18	G	103	PGV	C27-C28-C29-C30
19	D	201	TGL	CB7-CB8-CB9-C10
19	D	201	TGL	C10-C11-C12-C13
25	C	305	CDL	C58-C59-C60-C61
25	G	101	CDL	C72-C73-C74-C75
19	i	101	TGL	CC2-CC1-OG3-CG3
25	g	103	CDL	C51-CB5-OB6-CB4
18	a	607	PGV	C3-C4-C5-C6
19	L	101	TGL	C14-C29-C30-C31
19	l	101	TGL	CC6-CC7-CC8-CC9
24	C	309	PEK	C26-C27-C28-C29
22	B	302	PSC	C2-C3-C4-C5
24	c	303	PEK	C34-C35-C36-C37
18	C	303	PGV	C11-C10-C9-C8
18	G	103	PGV	C12-C13-C14-C15
18	c	304	PGV	C12-C13-C14-C15
22	e	201	PSC	C6-C7-C8-C9
19	l	101	TGL	OB1-CB1-OG2-CG2
22	B	302	PSC	C1-C2-C3-C4
25	g	103	CDL	CB7-C71-C72-C73
19	L	101	TGL	CC3-CC4-CC5-CC6
19	i	101	TGL	C15-C16-C17-C18
22	e	201	PSC	C27-C28-C29-C30
19	L	101	TGL	CB2-CB3-CB4-CB5
24	C	308	PEK	C22-C23-C24-C25
18	A	607	PGV	C19-C20-C21-C22
19	A	608	TGL	CC4-CC5-CC6-CC7
19	i	101	TGL	CC7-CC8-CC9-C15
19	i	101	TGL	C16-C17-C18-C19
25	c	305	CDL	C62-C63-C64-C65
25	g	103	CDL	C37-C38-C39-C40
23	j	101	CHD	C16-C17-C20-C22
19	A	608	TGL	CC3-CC4-CC5-CC6
19	A	608	TGL	C22-C23-C24-C25
19	L	101	TGL	C11-C12-C13-C14
19	L	101	TGL	C21-C22-C23-C24
19	i	101	TGL	CB2-CB3-CB4-CB5
22	e	201	PSC	C28-C29-C30-C31
25	C	305	CDL	C36-C37-C38-C39
18	A	606	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
22	B	302	PSC	C2-C1-O01-C02
24	G	102	PEK	C2-C1-O01-C02
18	C	304	PGV	O01-C02-C03-O11
19	L	101	TGL	C16-C15-CC9-CC8
25	g	103	CDL	C34-C35-C36-C37
19	a	606	TGL	CA6-CA7-CA8-CA9
22	B	302	PSC	C20-C21-C22-C23
18	A	606	PGV	O02-C1-O01-C02
22	B	302	PSC	O02-C1-O01-C02
24	G	102	PEK	O02-C1-O01-C02
19	l	101	TGL	CB5-CB6-CB7-CB8
24	G	102	PEK	C25-C26-C27-C28
18	A	606	PGV	O03-C01-C02-O01
25	g	103	CDL	C74-C75-C76-C77
19	D	201	TGL	CC5-CC6-CC7-CC8
24	g	102	PEK	C28-C29-C30-C31
26	c	307	DMU	C31-C34-C37-C40
18	A	606	PGV	C11-C10-C9-C8
22	B	302	PSC	C13-C14-C15-C16
19	L	101	TGL	CA6-CA7-CA8-CA9
23	c	306	CHD	C20-C22-C23-C24
24	C	308	PEK	C23-C24-C25-C26
24	C	309	PEK	C24-C25-C26-C27
25	G	101	CDL	C39-C40-C41-C42
25	G	101	CDL	C76-C77-C78-C79
25	c	305	CDL	C55-C56-C57-C58
25	g	103	CDL	C63-C64-C65-C66
25	g	103	CDL	OB7-CB5-OB6-CB4
18	A	607	PGV	C7-C8-C9-C10
25	G	101	CDL	C82-C83-C84-C85
22	e	201	PSC	C03-O11-P-O12
25	C	305	CDL	CB3-OB5-PB2-OB2
25	g	103	CDL	CA3-OA5-PA1-OA2
24	g	102	PEK	C27-C28-C29-C30
24	C	309	PEK	C01-C02-C03-O11
25	g	103	CDL	OB5-CB3-CB4-CB6
18	A	606	PGV	C27-C28-C29-C30
18	C	304	PGV	C20-C21-C22-C23
19	L	101	TGL	C12-C13-C14-C29
24	g	102	PEK	C24-C25-C26-C27
25	c	305	CDL	C15-C16-C17-C18
18	c	301	PGV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	C	308	PEK	C15-C16-C17-C18
18	C	304	PGV	O12-C04-C05-C06
18	C	303	PGV	C24-C25-C26-C27
18	c	304	PGV	C25-C26-C27-C28
19	A	608	TGL	CB6-CB7-CB8-CB9
19	D	201	TGL	C14-C29-C30-C31
24	C	302	PEK	C25-C26-C27-C28
24	G	102	PEK	C26-C27-C28-C29
25	C	305	CDL	C77-C78-C79-C80
25	c	305	CDL	C38-C39-C40-C41
19	i	101	TGL	CA6-CA7-CA8-CA9
19	l	101	TGL	CB9-C10-C11-C12
19	i	101	TGL	OC1-CC1-OG3-CG3
18	a	607	PGV	C13-C14-C15-C16
19	L	101	TGL	CB5-CB6-CB7-CB8
22	B	302	PSC	C23-C24-C25-C26
25	c	305	CDL	C33-C34-C35-C36
18	A	606	PGV	O03-C01-C02-C03
19	D	201	TGL	OG1-CG1-CG2-CG3
24	C	309	PEK	C30-C31-C32-C33
25	C	305	CDL	CB3-CB4-CB6-OB8
25	G	101	CDL	CB3-CB4-CB6-OB8
24	C	309	PEK	C31-C32-C33-C34
18	C	304	PGV	C13-C14-C15-C16
18	C	303	PGV	C22-C23-C24-C25
18	c	304	PGV	C15-C16-C17-C18
22	e	201	PSC	C25-C26-C27-C28
24	G	102	PEK	C22-C23-C24-C25
25	G	101	CDL	C12-C13-C14-C15
25	G	101	CDL	C44-C45-C46-C47
18	a	607	PGV	C24-C25-C26-C27
22	B	302	PSC	C15-C16-C17-C18
18	G	103	PGV	C20-C21-C22-C23
19	L	101	TGL	CC7-CC8-CC9-C15
19	a	606	TGL	C33-C34-C35-C36
19	a	606	TGL	C20-C21-C22-C23
25	c	305	CDL	C19-C20-C21-C22
25	c	305	CDL	C20-C21-C22-C23
18	C	304	PGV	C11-C10-C9-C8
24	G	102	PEK	C32-C33-C34-C35
19	A	608	TGL	C16-C17-C18-C19
19	A	608	TGL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
22	e	201	PSC	C15-C16-C17-C18
26	C	307	DMU	O6-C11-C9-O1
26	c	307	DMU	O6-C11-C9-O1
19	a	606	TGL	CA9-C20-C21-C22
25	G	101	CDL	C81-C82-C83-C84
19	i	101	TGL	C29-C30-C31-C32
25	G	101	CDL	C75-C76-C77-C78
18	G	103	PGV	C15-C16-C17-C18
19	D	201	TGL	C16-C15-CC9-CC8
18	c	301	PGV	C6-C7-C8-C9
18	c	301	PGV	C22-C23-C24-C25
24	c	303	PEK	C29-C30-C31-C32
22	B	302	PSC	O01-C02-C03-O11
19	L	101	TGL	C33-C34-C35-C36
19	D	201	TGL	C21-C20-CA9-CA8
19	i	101	TGL	C21-C20-CA9-CA8
22	B	302	PSC	C5-C6-C7-C8
18	G	103	PGV	C11-C10-C9-C8
25	G	101	CDL	C64-C65-C66-C67
26	c	307	DMU	C18-C19-C22-C25
18	A	606	PGV	C29-C30-C31-C32
19	L	101	TGL	CA5-CA6-CA7-CA8
19	L	101	TGL	C21-C20-CA9-CA8
19	D	201	TGL	C25-C26-C27-C28
24	C	302	PEK	C31-C32-C33-C34
25	C	305	CDL	C84-C85-C86-C87
25	g	103	CDL	C76-C77-C78-C79
19	L	101	TGL	CA4-CA5-CA6-CA7
18	A	606	PGV	C01-C02-C03-O11
18	C	304	PGV	C01-C02-C03-O11
25	G	101	CDL	OA5-CA3-CA4-CA6
25	c	305	CDL	OA5-CA3-CA4-CA6
25	g	103	CDL	OA5-CA3-CA4-CA6
24	C	309	PEK	C25-C26-C27-C28
26	C	307	DMU	O5-C4-C57-O61
18	c	304	PGV	C1-C2-C3-C4
19	D	201	TGL	C11-C10-CB9-CB8
19	i	101	TGL	C25-C26-C27-C28
25	G	101	CDL	C24-C25-C26-C27
18	C	304	PGV	C24-C25-C26-C27
18	C	304	PGV	C20-C19-O03-C01
24	C	308	PEK	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	C	305	CDL	C31-C32-C33-C34
25	g	103	CDL	C11-C12-C13-C14
24	G	102	PEK	C34-C35-C36-C37
19	A	608	TGL	OG1-CG1-CG2-CG3
26	m	401	DMU	O6-C11-C9-O1
18	A	606	PGV	C23-C24-C25-C26
24	C	309	PEK	C17-C18-C19-C20
25	G	101	CDL	C51-C52-C53-C54
24	C	308	PEK	C35-C36-C37-C38
22	B	302	PSC	C04-C05-N-C07
26	M	101	DMU	O6-C11-C9-C8
24	C	302	PEK	C5-C6-C7-C8
24	C	302	PEK	C9-C10-C11-C12
24	C	308	PEK	C9-C10-C11-C12
24	C	309	PEK	C5-C6-C7-C8
24	C	309	PEK	C6-C7-C8-C9
24	C	309	PEK	C11-C12-C13-C14
24	C	309	PEK	C12-C13-C14-C15
24	G	102	PEK	C11-C10-C9-C8
24	c	303	PEK	C5-C6-C7-C8
24	c	303	PEK	C6-C7-C8-C9
24	c	303	PEK	C11-C12-C13-C14
24	g	102	PEK	C12-C13-C14-C15
19	l	101	TGL	CB1-CB2-CB3-CB4
24	c	303	PEK	C23-C24-C25-C26
18	c	304	PGV	O05-C05-C06-O06
18	c	301	PGV	C4-C5-C6-C7
19	D	201	TGL	C23-C24-C25-C26
25	g	103	CDL	C58-C59-C60-C61
18	a	607	PGV	C11-C10-C9-C8
24	C	302	PEK	C15-C16-C17-C18
24	c	303	PEK	O03-C01-C02-O01
25	G	101	CDL	OB6-CB4-CB6-OB8
18	c	304	PGV	C20-C19-O03-C01
25	C	305	CDL	C18-C19-C20-C21
19	L	101	TGL	C24-C25-C26-C27
25	g	103	CDL	C17-C18-C19-C20
18	A	606	PGV	C02-C03-O11-P
18	C	303	PGV	C02-C03-O11-P
18	C	304	PGV	C02-C03-O11-P
18	G	103	PGV	C02-C03-O11-P
19	A	608	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
25	G	101	CDL	C54-C55-C56-C57
24	g	102	PEK	C16-C17-C18-C19
25	g	103	CDL	C21-C22-C23-C24
19	i	101	TGL	C17-C18-C19-C33
25	c	305	CDL	C79-C80-C81-C82
18	a	607	PGV	C20-C21-C22-C23
24	c	303	PEK	C30-C31-C32-C33
25	C	305	CDL	C42-C43-C44-C45
26	m	401	DMU	C31-C34-C37-C40
24	C	309	PEK	C29-C30-C31-C32
18	C	303	PGV	C26-C27-C28-C29
24	G	102	PEK	C16-C17-C18-C19
18	A	606	PGV	C6-C7-C8-C9
25	g	103	CDL	C41-C42-C43-C44
19	a	606	TGL	CG1-CG2-OG2-CB1
18	C	304	PGV	C4-C5-C6-C7
24	c	303	PEK	C24-C25-C26-C27
25	G	101	CDL	C61-C62-C63-C64
24	G	102	PEK	O03-C01-C02-C03
25	c	305	CDL	CB3-CB4-CB6-OB8
25	g	103	CDL	C1-CA2-OA2-PA1
25	g	103	CDL	CB3-CB4-CB6-OB8
25	c	305	CDL	OA5-CA3-CA4-OA6
25	g	103	CDL	OA5-CA3-CA4-OA6
19	l	101	TGL	CC5-CC6-CC7-CC8
18	C	304	PGV	O04-C19-O03-C01
19	i	101	TGL	CB6-CB7-CB8-CB9
19	L	101	TGL	OG2-CG2-CG3-OG3
19	a	606	TGL	OG2-CG2-CG3-OG3
22	B	302	PSC	O03-C01-C02-O01
24	G	102	PEK	O03-C01-C02-O01
25	C	305	CDL	OB6-CB4-CB6-OB8
18	c	304	PGV	O04-C19-O03-C01
24	c	303	PEK	C22-C23-C24-C25
24	g	102	PEK	C34-C35-C36-C37
25	g	103	CDL	C15-C16-C17-C18
18	C	304	PGV	C30-C31-C32-C33
24	C	309	PEK	O04-C21-O03-C01
18	A	607	PGV	C25-C26-C27-C28
19	l	101	TGL	C25-C26-C27-C28
18	c	301	PGV	C29-C30-C31-C32
25	C	305	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
24	g	102	PEK	C33-C34-C35-C36
25	C	305	CDL	CA2-OA2-PA1-OA5
25	g	103	CDL	CA2-OA2-PA1-OA5
25	c	305	CDL	C23-C24-C25-C26
18	c	304	PGV	C02-C03-O11-P
22	B	302	PSC	C27-C28-C29-C30
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
18	G	103	PGV	C03-O11-P-O14
18	a	607	PGV	C04-O12-P-O14
22	e	201	PSC	C03-O11-P-O14
24	C	309	PEK	C04-O12-P-O14
24	c	303	PEK	C04-O12-P-O14
25	C	305	CDL	CB3-OB5-PB2-OB4
25	G	101	CDL	CA2-OA2-PA1-OA3
25	c	305	CDL	CA3-OA5-PA1-OA3
25	c	305	CDL	CA3-OA5-PA1-OA4
25	g	103	CDL	CB2-OB2-PB2-OB3
19	l	101	TGL	CC2-CC1-OG3-CG3
19	l	101	TGL	C22-C23-C24-C25
24	C	302	PEK	C35-C36-C37-C38
19	l	101	TGL	OG2-CB1-CB2-CB3
22	e	201	PSC	C22-C23-C24-C25
24	g	102	PEK	C1-C2-C3-C4
18	C	304	PGV	C3-C4-C5-C6
25	C	305	CDL	C54-C55-C56-C57
19	A	608	TGL	CA3-CA4-CA5-CA6
25	g	103	CDL	CB5-C51-C52-C53
18	A	606	PGV	O01-C02-C03-O11
25	G	101	CDL	OA5-CA3-CA4-OA6
18	A	607	PGV	C4-C5-C6-C7
19	L	101	TGL	CG1-CG2-CG3-OG3
19	a	606	TGL	CG1-CG2-CG3-OG3
22	B	302	PSC	O03-C01-C02-C03
22	e	201	PSC	O12-C04-C05-N
19	l	101	TGL	OG2-CG2-CG3-OG3
25	c	305	CDL	OB6-CB4-CB6-OB8
25	C	305	CDL	C37-C38-C39-C40
18	c	301	PGV	C11-C10-C9-C8
25	G	101	CDL	C21-C22-C23-C24
22	e	201	PSC	C3-C4-C5-C6
18	A	606	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
24	C	309	PEK	C22-C21-O03-C01
18	A	607	PGV	C21-C22-C23-C24
19	D	201	TGL	C21-C22-C23-C24
24	C	302	PEK	C23-C24-C25-C26
22	e	201	PSC	C26-C27-C28-C29
18	c	301	PGV	C30-C31-C32-C33
26	c	307	DMU	C19-C22-C25-C28
19	l	101	TGL	OC1-CC1-OG3-CG3
19	L	101	TGL	CC6-CC7-CC8-CC9
19	a	606	TGL	CC4-CC5-CC6-CC7
24	c	303	PEK	C33-C34-C35-C36
18	A	606	PGV	C11-C12-C13-C14
25	c	305	CDL	C72-C73-C74-C75
25	g	103	CDL	C81-C82-C83-C84
22	B	302	PSC	C01-C02-C03-O11
25	G	101	CDL	C36-C37-C38-C39
24	c	303	PEK	C22-C21-O03-C01
18	C	303	PGV	C1-C2-C3-C4
19	A	608	TGL	C14-C29-C30-C31
19	l	101	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	C25-C26-C27-C28
18	c	304	PGV	C05-C04-O12-P
25	g	103	CDL	C83-C84-C85-C86
24	C	309	PEK	O01-C02-C03-O11
25	g	103	CDL	OB5-CB3-CB4-OB6
18	G	103	PGV	C26-C27-C28-C29
25	C	305	CDL	C24-C25-C26-C27
18	A	606	PGV	C9-C10-C11-C12
18	c	301	PGV	C21-C22-C23-C24
19	A	608	TGL	OG1-CG1-CG2-OG2
22	B	302	PSC	C03-O11-P-O12
24	G	102	PEK	C04-O12-P-O11
25	G	101	CDL	CB2-OB2-PB2-OB5
25	g	103	CDL	CB3-OB5-PB2-OB2
18	c	304	PGV	C27-C28-C29-C30
25	c	305	CDL	CA3-CA4-CA6-OA8
19	A	608	TGL	C21-C20-CA9-CA8
25	C	305	CDL	C76-C77-C78-C79
19	i	101	TGL	CA5-CA6-CA7-CA8
22	B	302	PSC	C31-C32-C33-C34
19	l	101	TGL	CA1-CA2-CA3-CA4
18	C	303	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
18	C	303	PGV	C27-C28-C29-C30
19	i	101	TGL	CB4-CB5-CB6-CB7
24	C	309	PEK	C3-C4-C5-C6
19	A	608	TGL	CA6-CA7-CA8-CA9
25	c	305	CDL	C17-C18-C19-C20
18	a	607	PGV	O12-C04-C05-C06
24	C	308	PEK	C2-C3-C4-C5
24	C	308	PEK	C28-C29-C30-C31
25	c	305	CDL	C84-C85-C86-C87
19	l	101	TGL	C11-C12-C13-C14
18	A	607	PGV	C24-C25-C26-C27
22	e	201	PSC	C01-C02-C03-O11
14	A	601	HEA	CAD-CBD-CGD-O1D
24	c	303	PEK	O01-C02-C03-O11
25	G	101	CDL	C55-C56-C57-C58
14	A	602	HEA	CAD-CBD-CGD-O2D
23	b	301	CHD	C22-C23-C24-O26
18	A	606	PGV	O04-C19-O03-C01
19	a	606	TGL	CA1-CA2-CA3-CA4
18	A	606	PGV	C30-C31-C32-C33
25	c	305	CDL	C51-C52-C53-C54
23	b	301	CHD	C22-C23-C24-O25
24	g	102	PEK	O03-C01-C02-O01
19	a	606	TGL	C11-C12-C13-C14
25	G	101	CDL	C43-C44-C45-C46
23	B	303	CHD	C22-C23-C24-O25
18	c	304	PGV	C9-C10-C11-C12
24	G	102	PEK	C23-C24-C25-C26
25	c	305	CDL	C31-C32-C33-C34
18	c	301	PGV	C24-C25-C26-C27
14	a	601	HEA	CAD-CBD-CGD-O1D
25	g	103	CDL	C18-C19-C20-C21
22	B	302	PSC	C28-C29-C30-C31
25	g	103	CDL	C72-C73-C74-C75
22	e	201	PSC	C2-C3-C4-C5
24	C	309	PEK	C33-C34-C35-C36
18	A	607	PGV	C31-C32-C33-C34
18	c	301	PGV	C9-C10-C11-C12
24	C	302	PEK	C11-C12-C13-C14
24	C	308	PEK	C5-C6-C7-C8
24	C	308	PEK	C11-C12-C13-C14
24	G	102	PEK	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	G	102	PEK	C12-C13-C14-C15
24	c	303	PEK	C11-C10-C9-C8
24	g	102	PEK	C5-C6-C7-C8
25	g	103	CDL	C82-C83-C84-C85
26	M	101	DMU	O6-C11-C9-O1
25	C	305	CDL	CA4-CA3-OA5-PA1
24	c	303	PEK	O04-C21-O03-C01
26	M	101	DMU	C19-C22-C25-C28
25	G	101	CDL	C63-C64-C65-C66
26	C	307	DMU	O16-C18-C19-C22
19	A	608	TGL	CA5-CA6-CA7-CA8
25	G	101	CDL	C18-C19-C20-C21
25	G	101	CDL	C57-C58-C59-C60
19	a	606	TGL	CB1-CB2-CB3-CB4
25	C	305	CDL	C14-C15-C16-C17
23	c	302	CHD	C17-C20-C22-C23
24	G	102	PEK	C28-C29-C30-C31
14	A	601	HEA	C19-C20-C21-C22
25	C	305	CDL	C52-C51-CB5-OB6
18	G	103	PGV	C28-C29-C30-C31
18	G	103	PGV	C3-C4-C5-C6
19	A	608	TGL	CA2-CA3-CA4-CA5
18	c	304	PGV	C04-C05-C06-O06
25	c	305	CDL	C58-C59-C60-C61
24	G	102	PEK	C27-C28-C29-C30
24	C	302	PEK	C32-C33-C34-C35
22	B	302	PSC	C12-C13-C14-C15
25	G	101	CDL	C59-C60-C61-C62
24	C	309	PEK	C35-C36-C37-C38
24	c	303	PEK	C01-C02-C03-O11
23	B	303	CHD	C22-C23-C24-O26
19	D	201	TGL	OG2-CG2-CG3-OG3
19	l	101	TGL	OG1-CG1-CG2-OG2
25	C	305	CDL	C64-C65-C66-C67
14	a	602	HEA	CAD-CBD-CGD-O1D
18	a	607	PGV	O01-C1-C2-C3
19	a	606	TGL	OG2-CB1-CB2-CB3
25	c	305	CDL	C14-C15-C16-C17
26	C	307	DMU	C5-C10-O7-C3
14	a	602	HEA	CAD-CBD-CGD-O2D
18	C	303	PGV	C20-C19-O03-C01
18	a	607	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	a	606	TGL	CA5-CA6-CA7-CA8
18	a	607	PGV	C15-C16-C17-C18
14	A	601	HEA	CAD-CBD-CGD-O2D
14	a	601	HEA	CAD-CBD-CGD-O2D
19	A	608	TGL	OG3-CC1-CC2-CC3
24	G	102	PEK	C14-C15-C16-C17
24	g	102	PEK	C14-C15-C16-C17
18	A	607	PGV	C13-C14-C15-C16
24	g	102	PEK	O01-C1-C2-C3
23	C	301	CHD	C21-C20-C22-C23
14	a	602	HEA	C26-C15-C16-C17
24	C	302	PEK	C2-C3-C4-C5
24	c	303	PEK	C15-C16-C17-C18
19	D	201	TGL	CB2-CB3-CB4-CB5
19	l	101	TGL	CG1-CG2-CG3-OG3
24	c	303	PEK	O03-C01-C02-C03
25	g	103	CDL	C32-C33-C34-C35
19	a	606	TGL	OG3-CC1-CC2-CC3
19	a	606	TGL	C29-C30-C31-C32
23	C	301	CHD	C16-C17-C20-C22
14	A	602	HEA	CAD-CBD-CGD-O1D
26	C	307	DMU	C19-C22-C25-C28
25	c	305	CDL	C32-C31-CA7-OA8
23	C	301	CHD	C17-C20-C22-C23
14	A	602	HEA	CAA-CBA-CGA-O1A
14	a	602	HEA	CAA-CBA-CGA-O1A
18	c	304	PGV	C11-C12-C13-C14
19	L	101	TGL	OG2-CB1-CB2-CB3
18	A	607	PGV	C6-C7-C8-C9
19	A	608	TGL	CC5-CC6-CC7-CC8
19	A	608	TGL	OG2-CG2-CG3-OG3
18	C	303	PGV	O04-C19-O03-C01
18	A	607	PGV	C9-C10-C11-C12
24	C	309	PEK	C14-C15-C16-C17
18	A	607	PGV	C14-C15-C16-C17
18	A	606	PGV	O01-C1-C2-C3
25	g	103	CDL	C52-C51-CB5-OB6
18	A	606	PGV	O05-C05-C06-O06
19	a	606	TGL	C23-C24-C25-C26
18	A	607	PGV	O03-C19-C20-C21
19	L	101	TGL	CC2-CC3-CC4-CC5
19	l	101	TGL	CA7-CA8-CA9-C20

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Mol	Chain	Res	Type	Atoms
22	B	302	PSC	C7-C8-C9-C10
26	C	307	DMU	O5-C6-O16-C18
14	a	602	HEA	CAA-CBA-CGA-O2A
22	e	201	PSC	C5-C6-C7-C8
18	c	301	PGV	C2-C1-O01-C02
25	c	305	CDL	C32-C31-CA7-OA9
18	c	301	PGV	O03-C19-C20-C21
18	a	607	PGV	C21-C22-C23-C24
19	A	608	TGL	C11-C12-C13-C14
22	B	302	PSC	C26-C27-C28-C29
19	D	201	TGL	C11-C12-C13-C14
24	g	102	PEK	O02-C1-C2-C3
18	G	103	PGV	C2-C3-C4-C5
19	A	608	TGL	CG1-CG2-CG3-OG3
19	D	201	TGL	CG1-CG2-CG3-OG3
19	l	101	TGL	OG1-CG1-CG2-CG3
24	G	102	PEK	C30-C31-C32-C33
19	A	608	TGL	CB4-CB5-CB6-CB7
25	c	305	CDL	C82-C83-C84-C85
18	A	607	PGV	O04-C19-C20-C21
24	G	102	PEK	C04-O12-P-O14
25	C	305	CDL	CA2-OA2-PA1-OA4
25	c	305	CDL	CB2-OB2-PB2-OB3
25	c	305	CDL	CB2-OB2-PB2-OB4
19	L	101	TGL	OB1-CB1-CB2-CB3
14	A	602	HEA	CAA-CBA-CGA-O2A
19	l	101	TGL	C21-C20-CA9-CA8
18	c	301	PGV	O04-C19-C20-C21
23	c	302	CHD	C22-C23-C24-O26
19	A	608	TGL	CB2-CB3-CB4-CB5
19	a	606	TGL	OC1-CC1-CC2-CC3
25	G	101	CDL	C53-C54-C55-C56
23	j	101	CHD	C22-C23-C24-O26
19	l	101	TGL	C11-C10-CB9-CB8
19	D	201	TGL	C15-C16-C17-C18
24	C	302	PEK	C3-C4-C5-C6
24	C	308	PEK	C25-C26-C27-C28
25	C	305	CDL	C72-C73-C74-C75
19	a	606	TGL	C14-C29-C30-C31
19	A	608	TGL	OC1-CC1-CC2-CC3
22	e	201	PSC	O01-C1-C2-C3
25	G	101	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
25	c	305	CDL	C81-C82-C83-C84
23	c	306	CHD	C22-C23-C24-O25
19	l	101	TGL	OG1-CA1-CA2-CA3
22	B	302	PSC	O03-C19-C20-C21
22	B	302	PSC	C30-C31-C32-C33
18	G	103	PGV	C6-C7-C8-C9
22	e	201	PSC	O02-C1-C2-C3
23	c	302	CHD	C22-C23-C24-O25
19	l	101	TGL	C15-C16-C17-C18
25	g	103	CDL	C52-C51-CB5-OB7
18	A	606	PGV	C22-C23-C24-C25
25	c	305	CDL	C83-C84-C85-C86
24	G	102	PEK	O01-C1-C2-C3
23	c	306	CHD	C22-C23-C24-O26

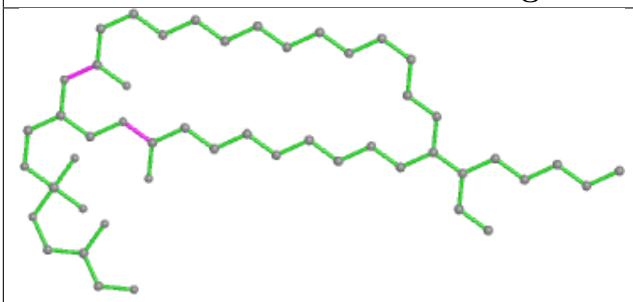
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	J	101	CHD	C1-C10-C2-C3-C4-C5

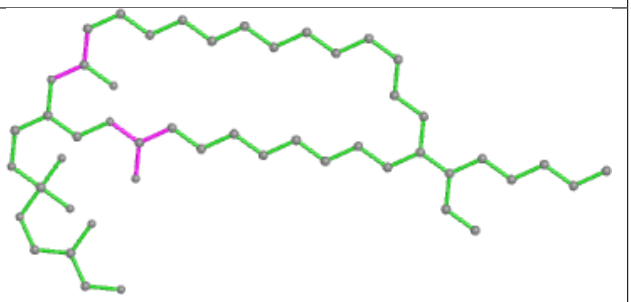
No monomer is involved in short contacts.

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.

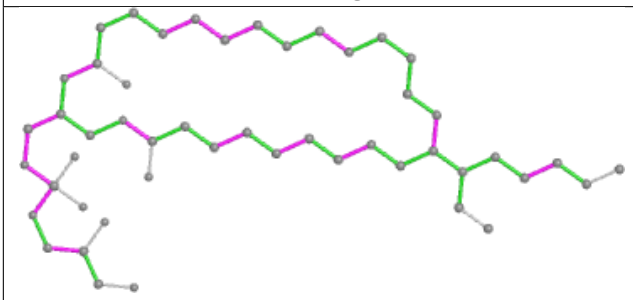
Ligand PGV C 304



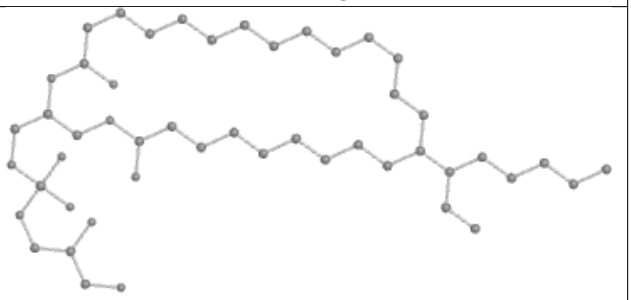
Bond lengths



Bond angles

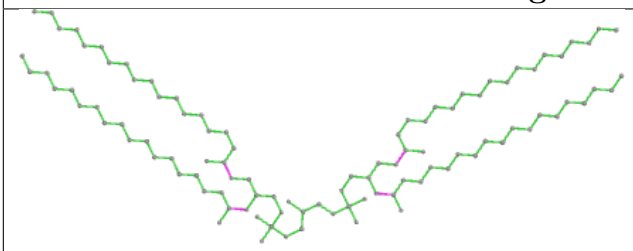


Torsions

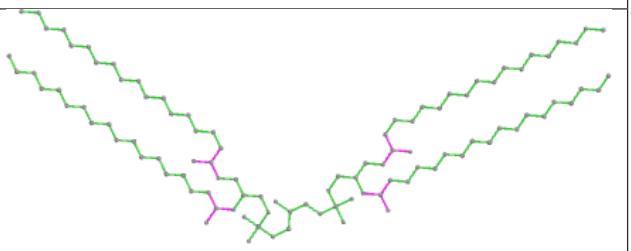


Rings

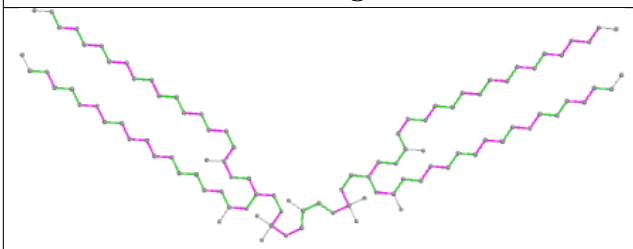
Ligand CDL c 305



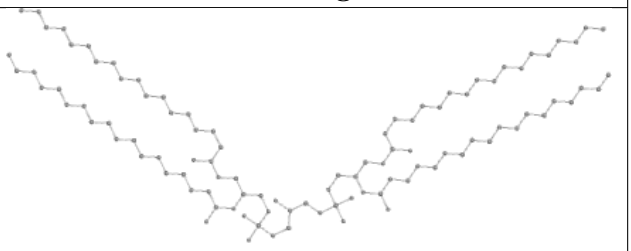
Bond lengths



Bond angles

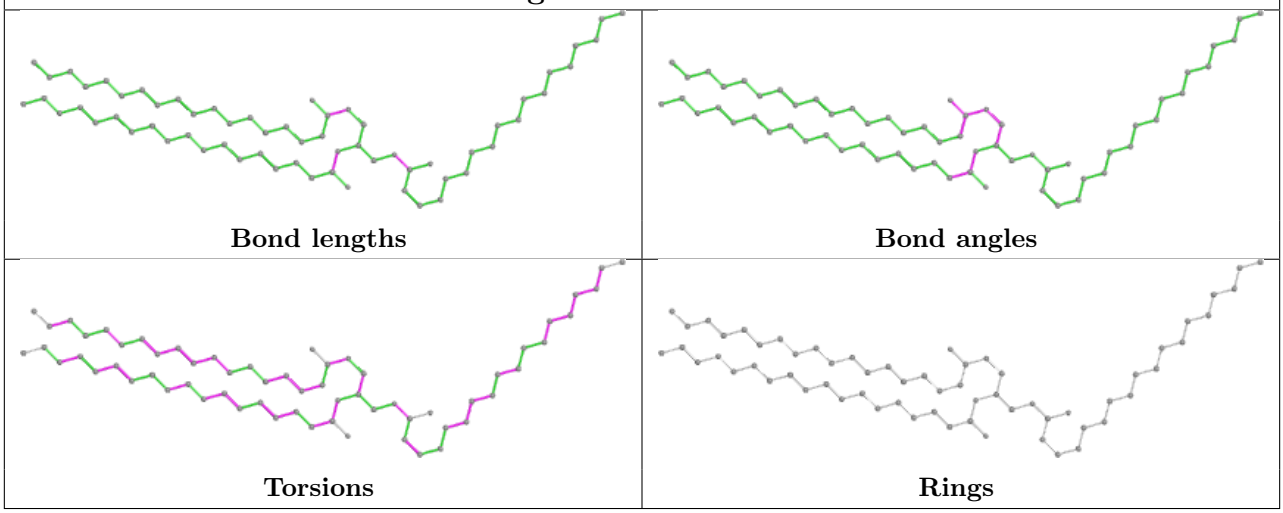


Torsions

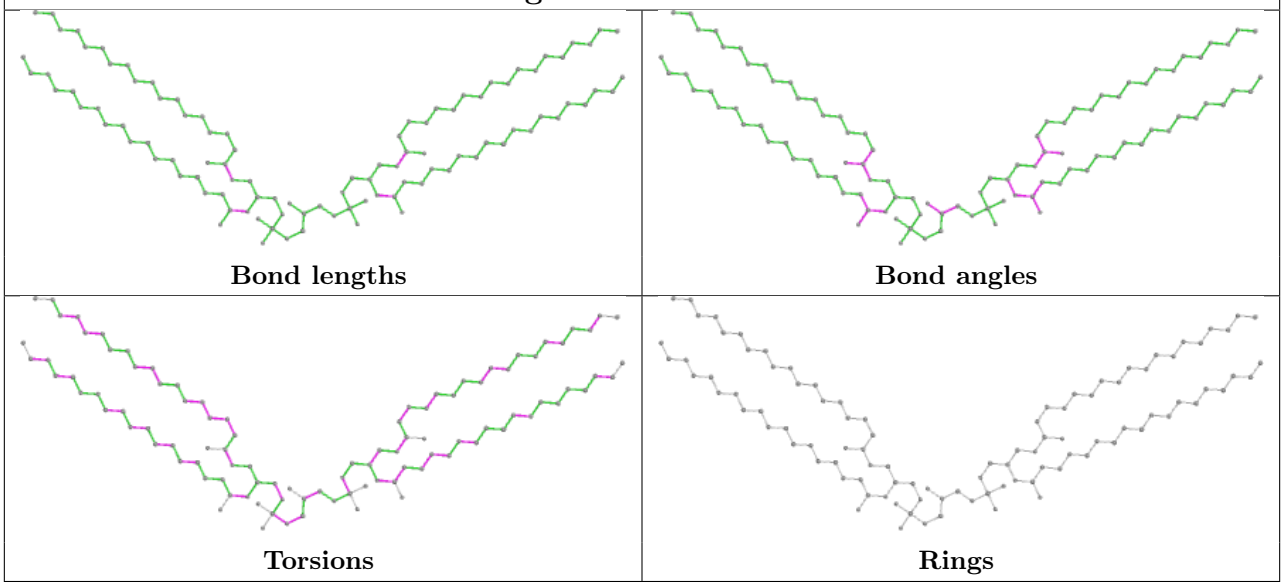


Rings

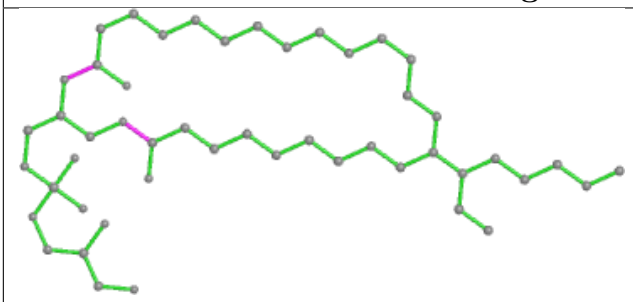
Ligand TGL L 101



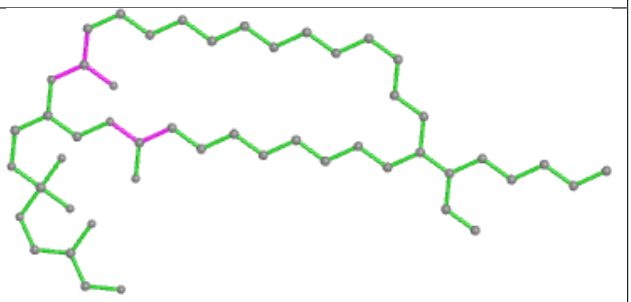
Ligand CDL C 305



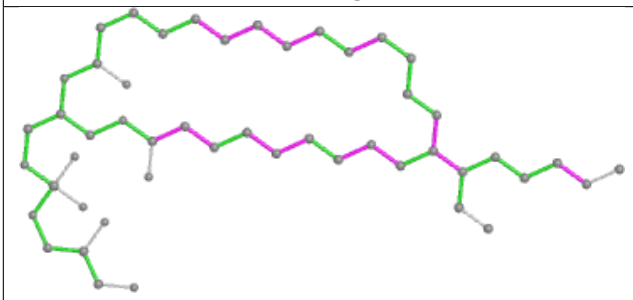
Ligand PGV A 607



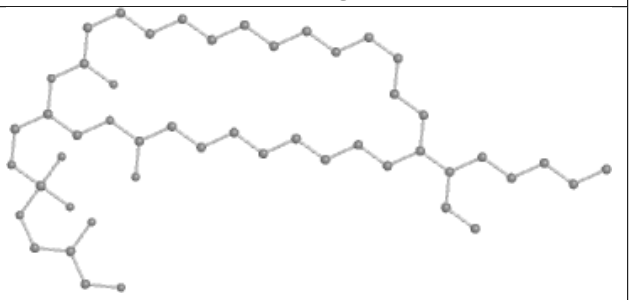
Bond lengths



Bond angles

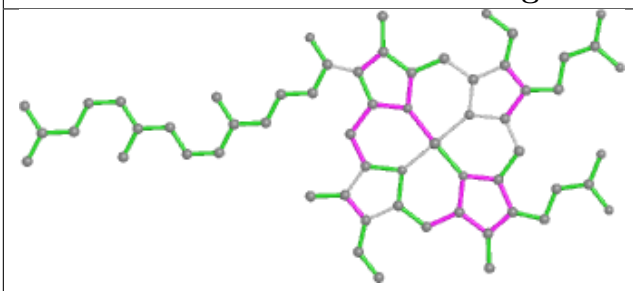


Torsions

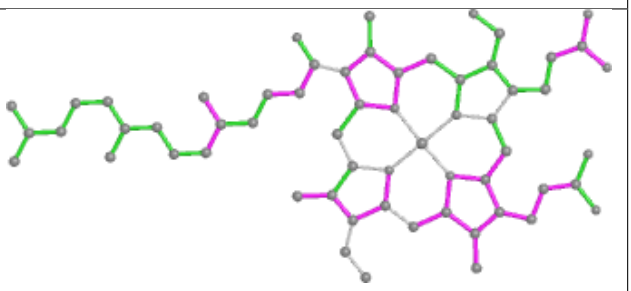


Rings

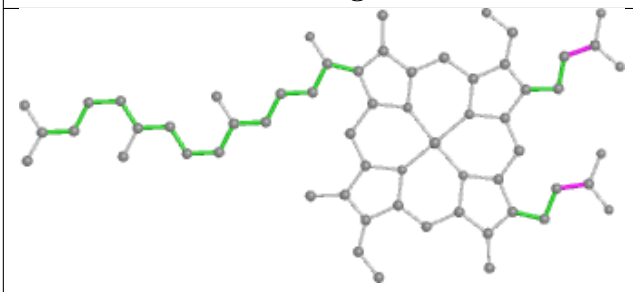
Ligand HEA A 602



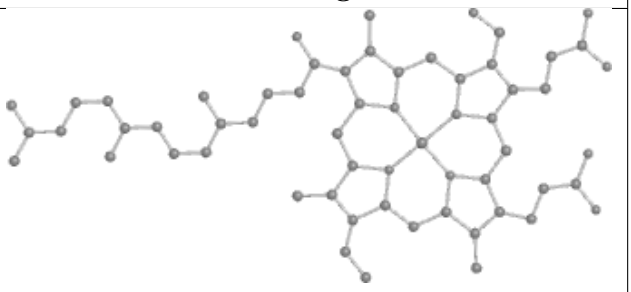
Bond lengths



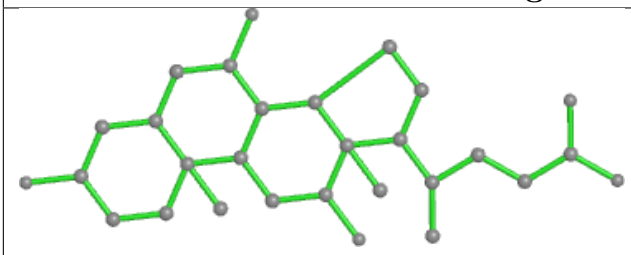
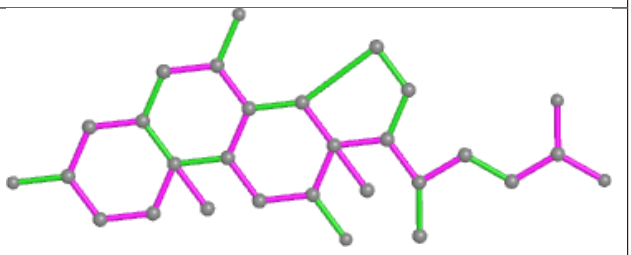
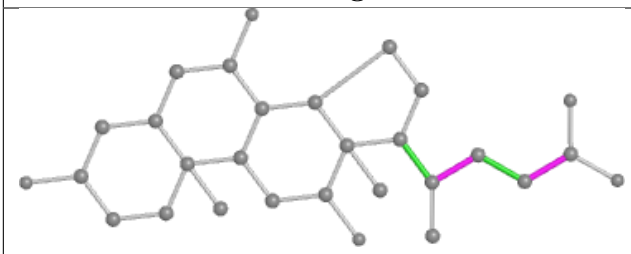
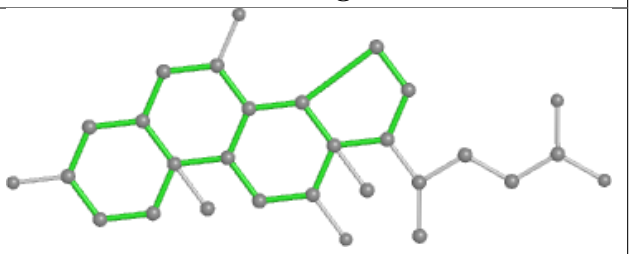
Bond angles



Torsions



Rings

Ligand CHD c 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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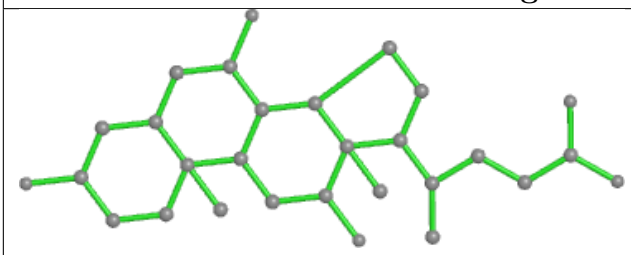
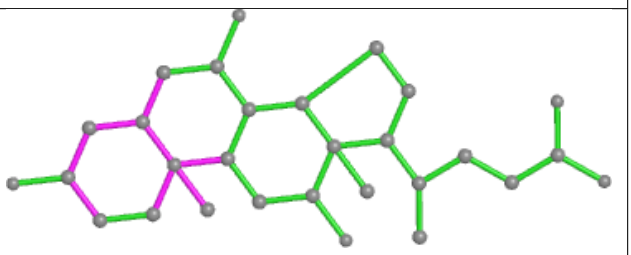
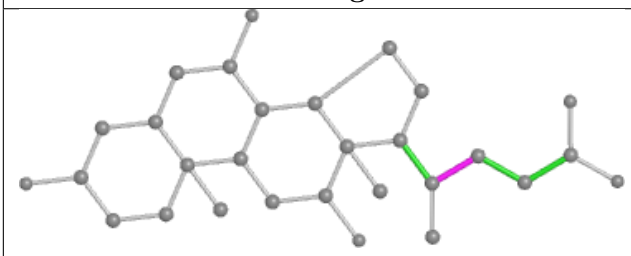
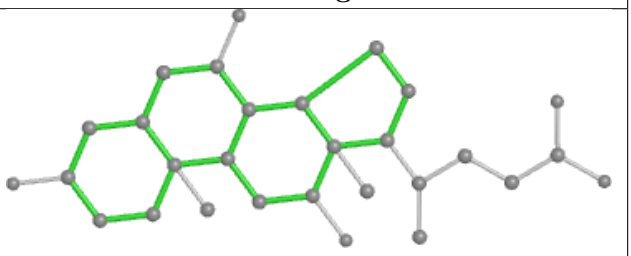
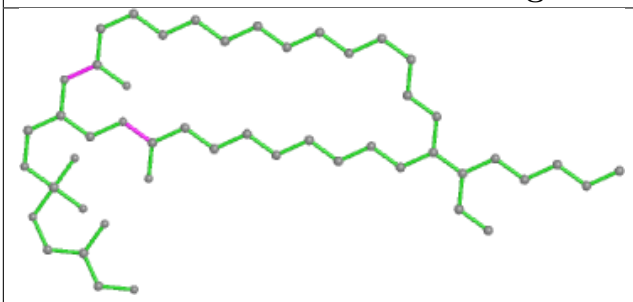
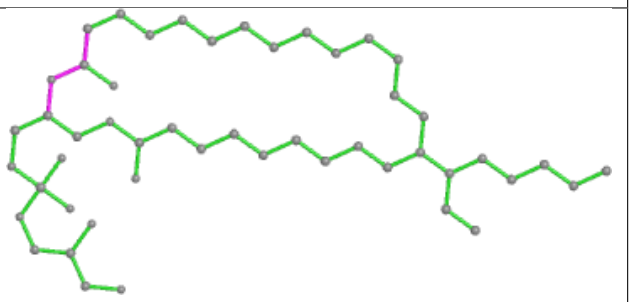
 Bond lengths	 Bond angles
 Torsions	 Rings

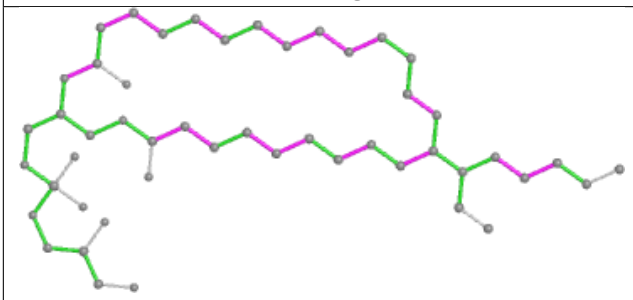
Ligand PGV c 301



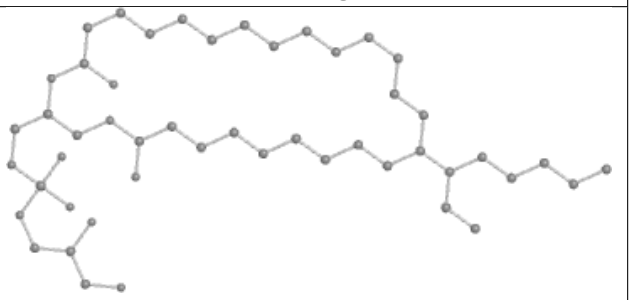
Bond lengths



Bond angles

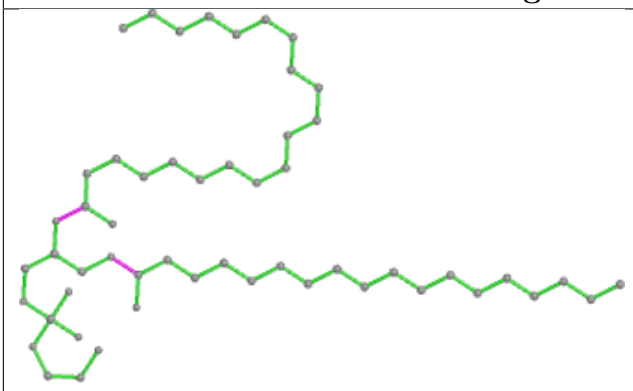


Torsions



Rings

Ligand PEK C 308



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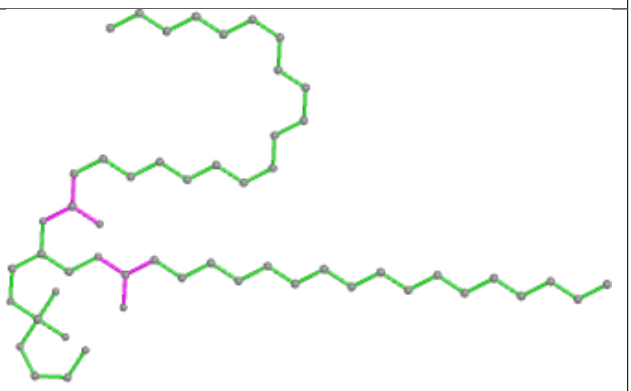
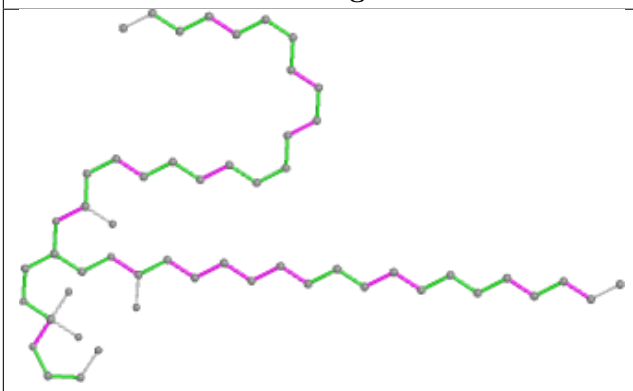
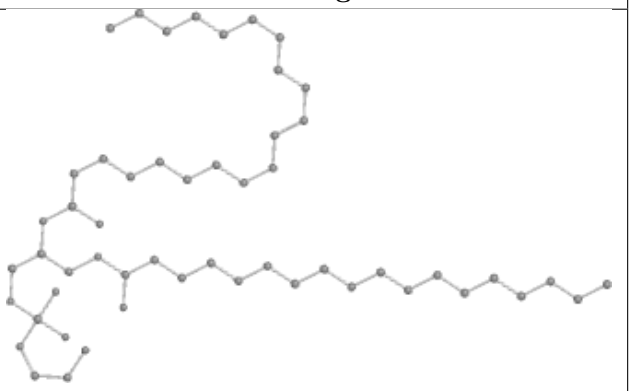


Bond angles

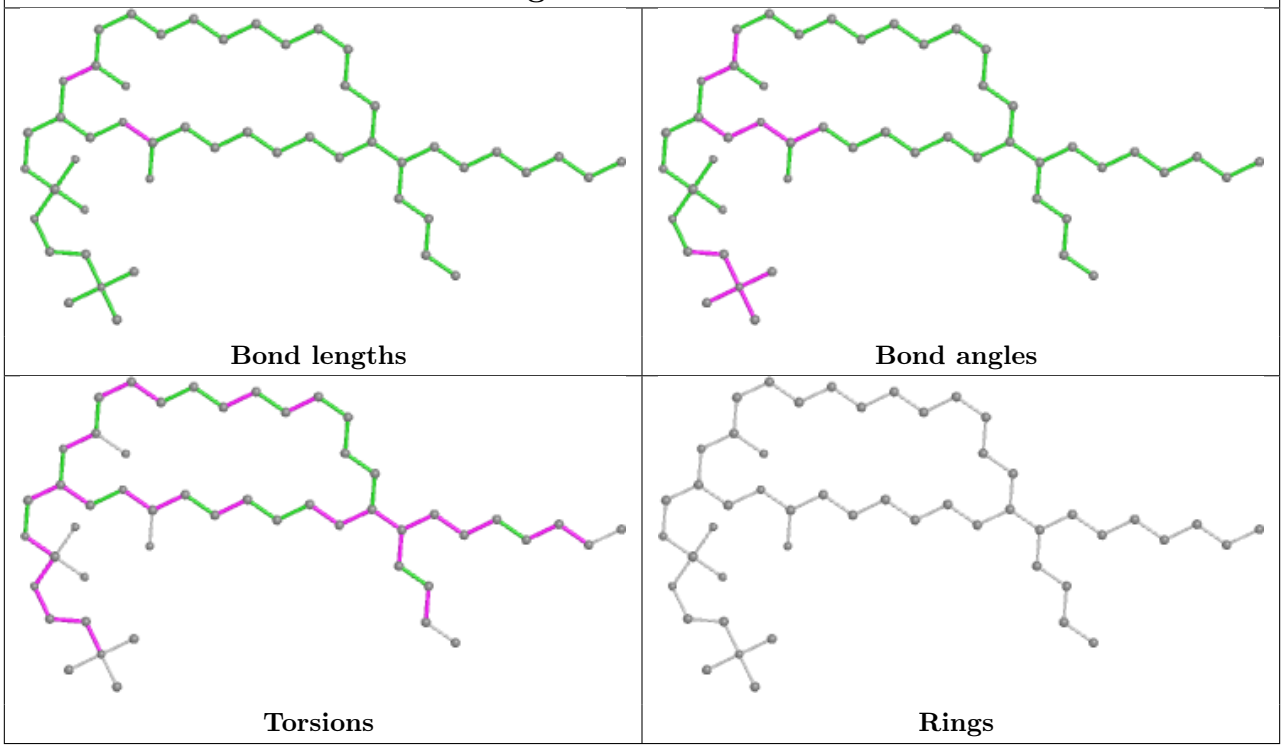


Torsions



Rings

Ligand PSC B 302



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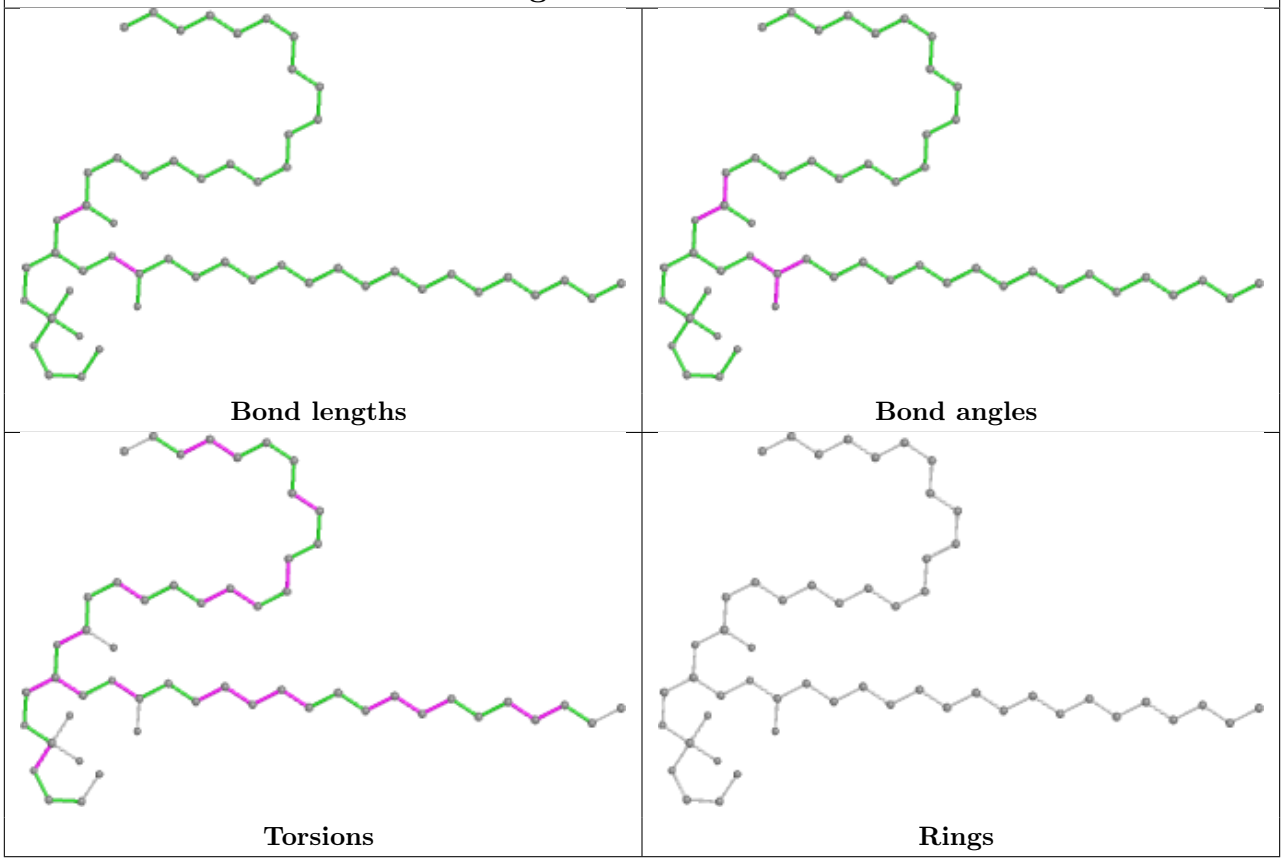
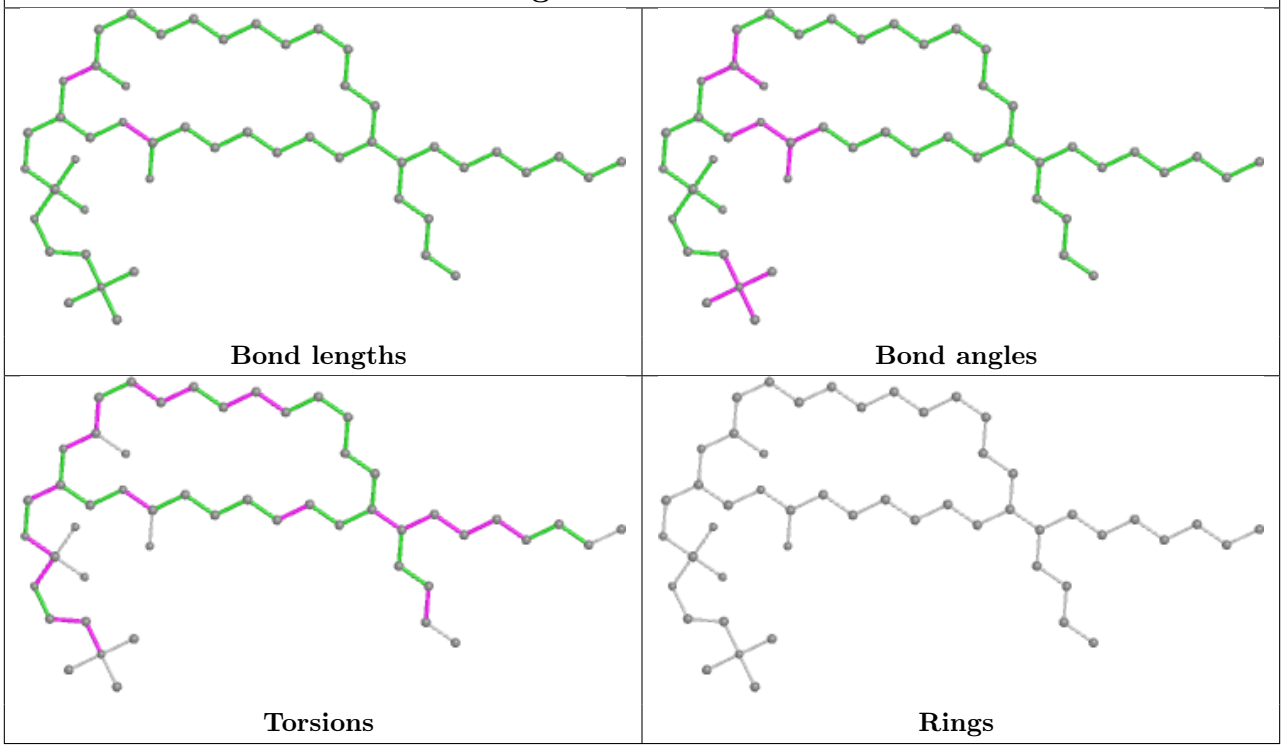
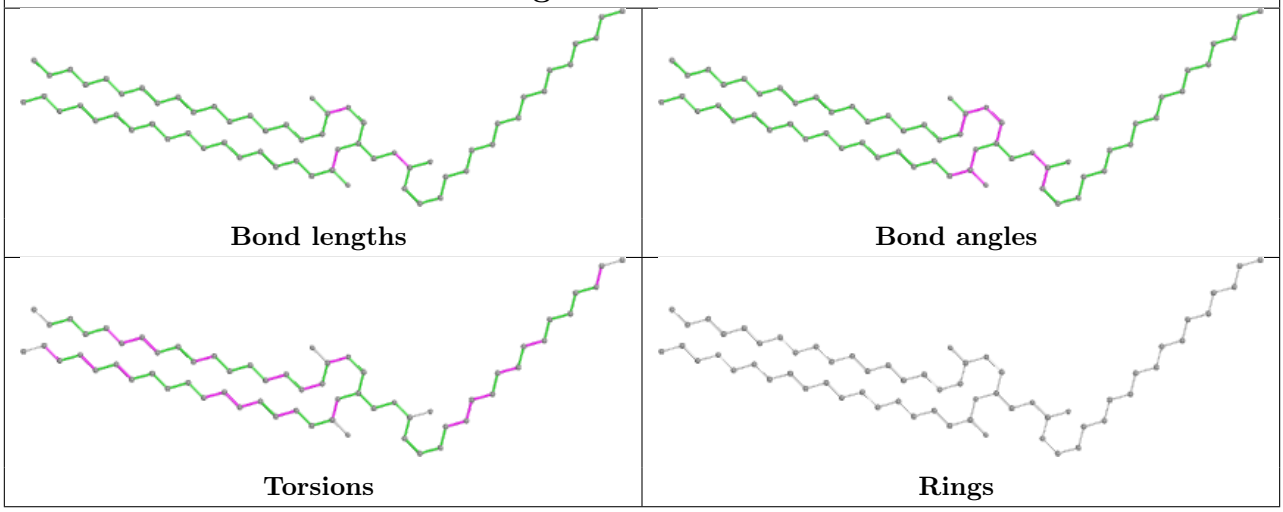
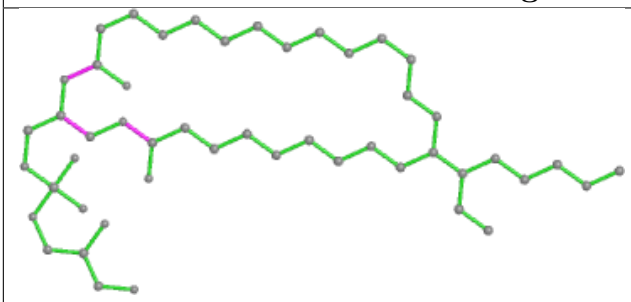
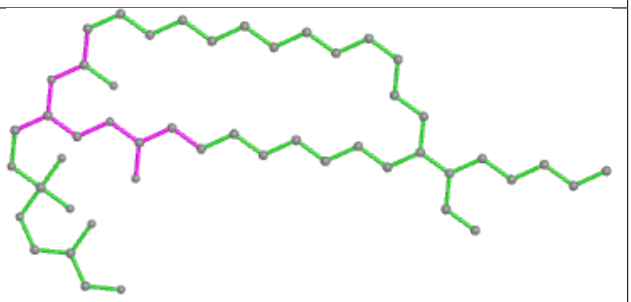
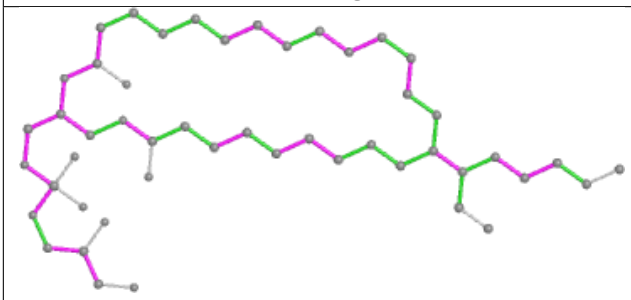
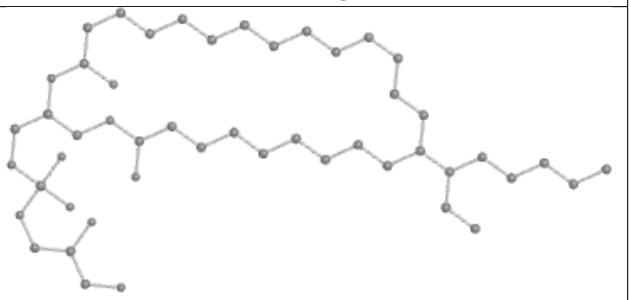


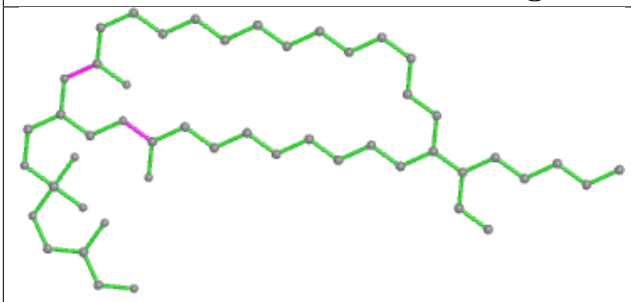
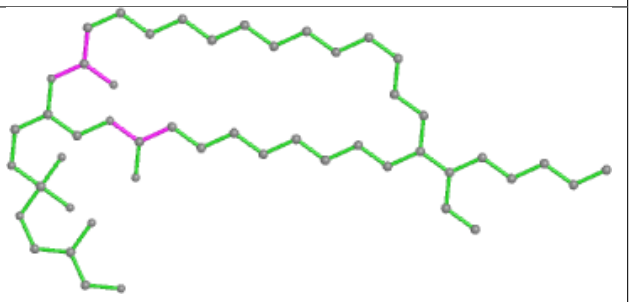
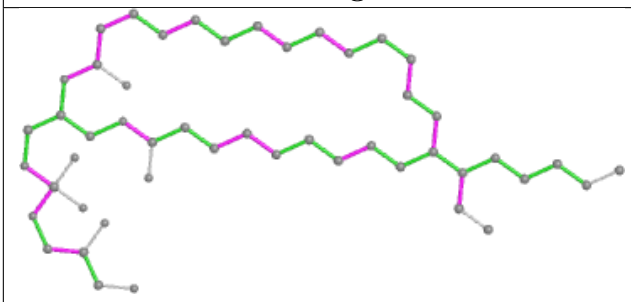
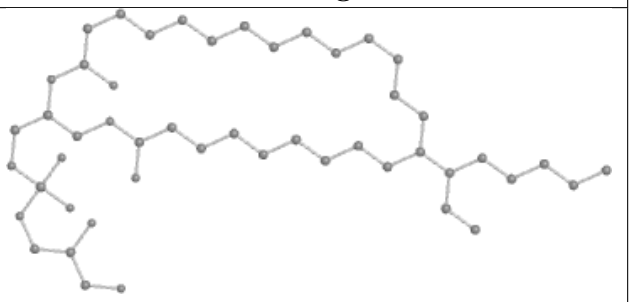
Ligand PSC e 201



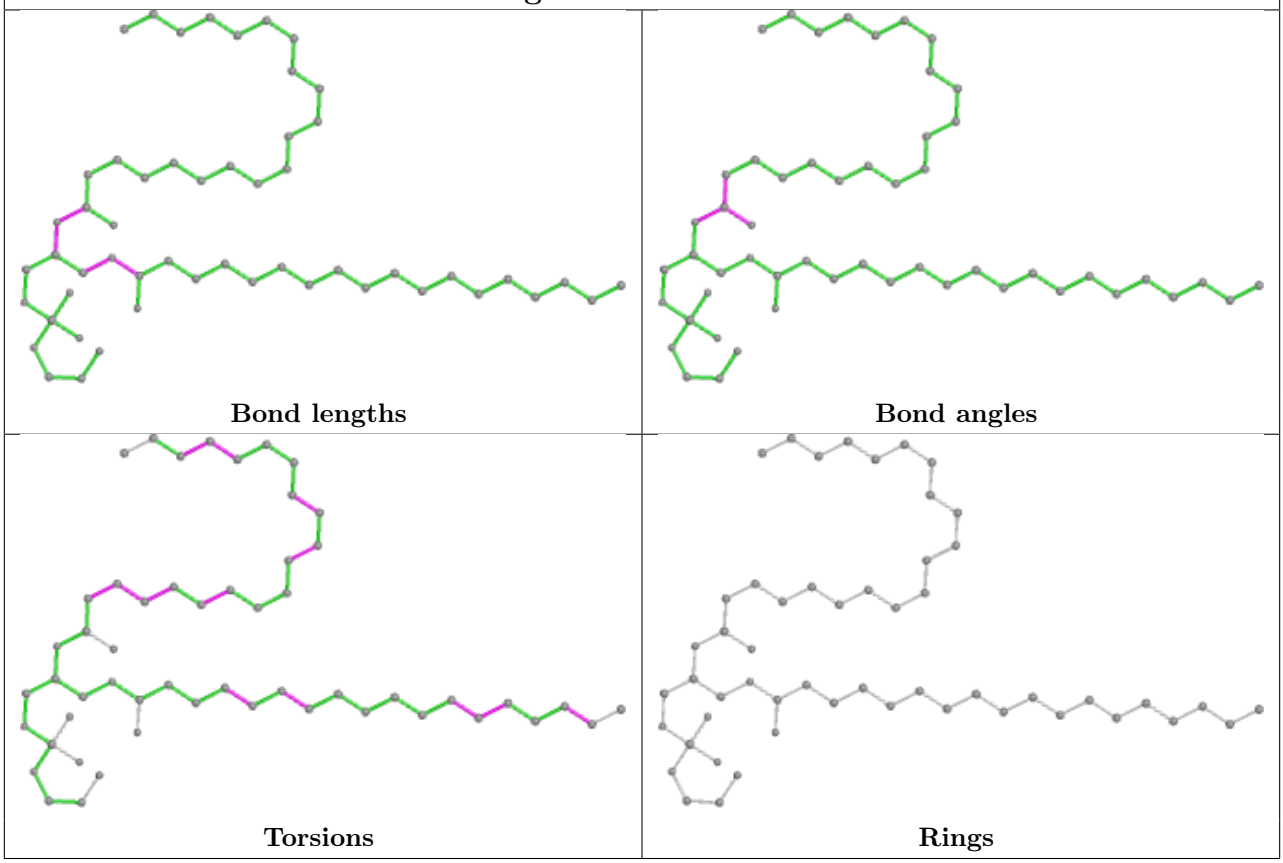
Ligand TGL i 101



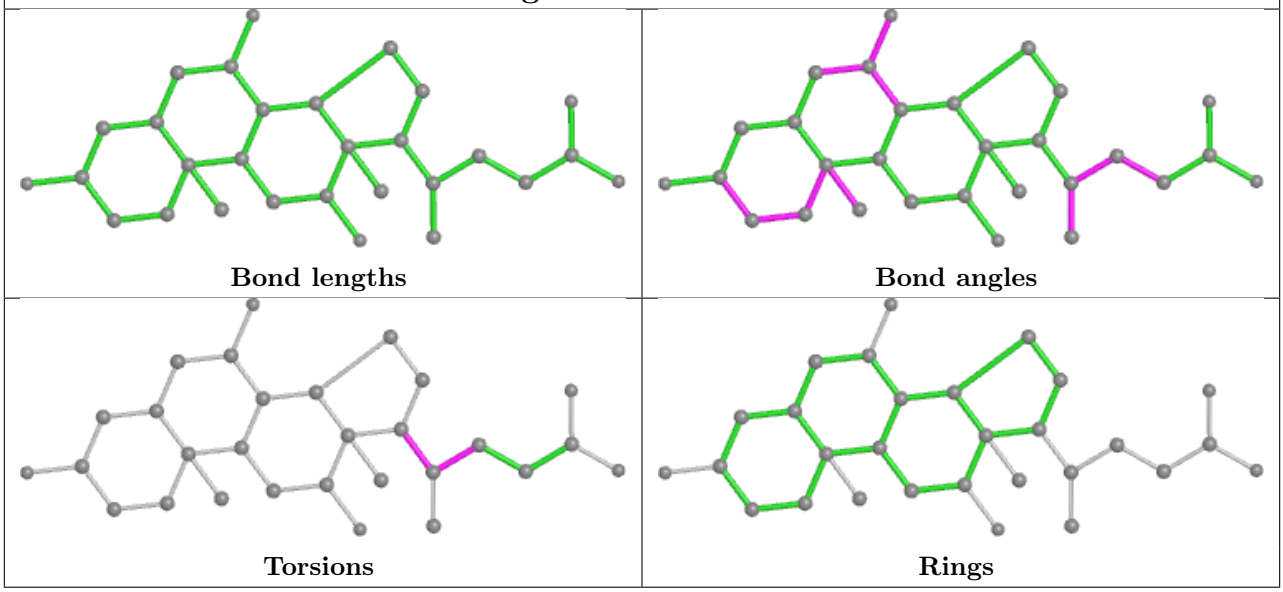
Ligand PGV A 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV a 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

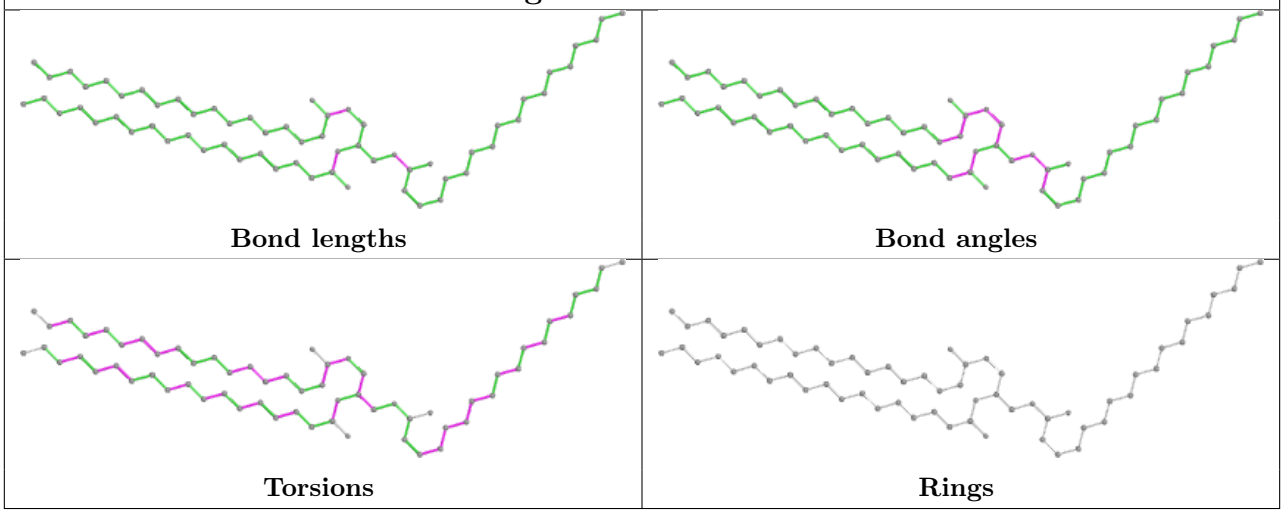
Ligand PEK C 302



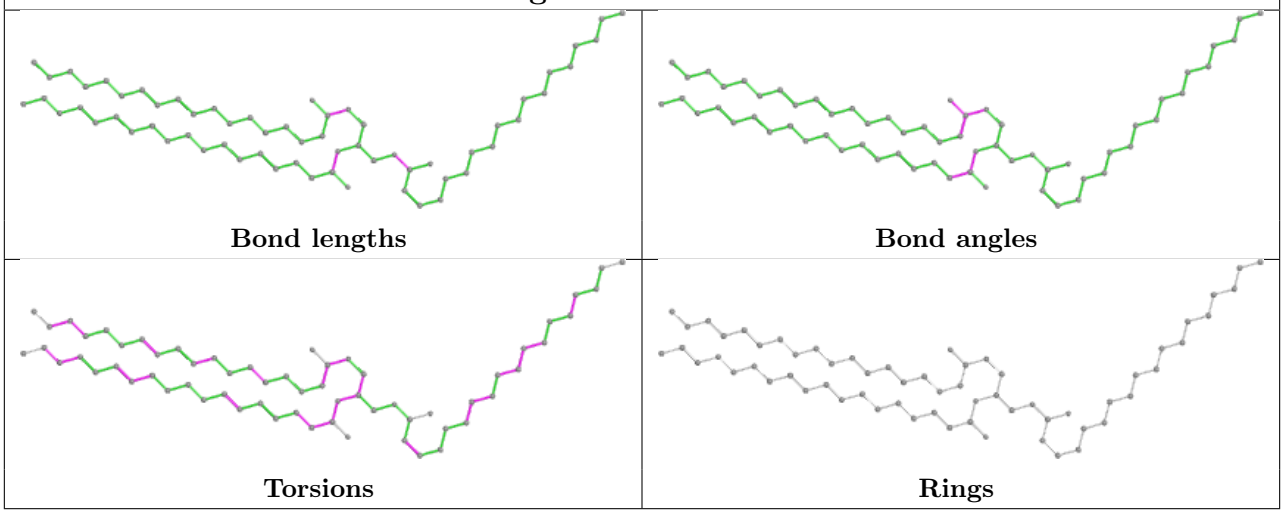
Ligand CHD C 301

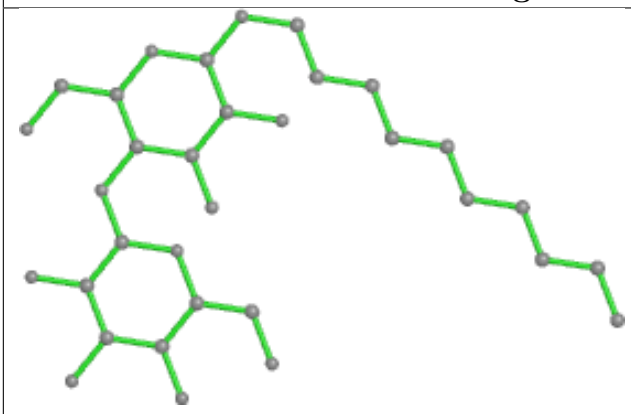
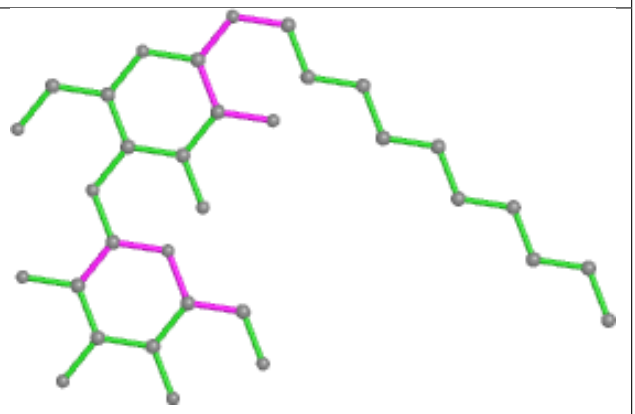
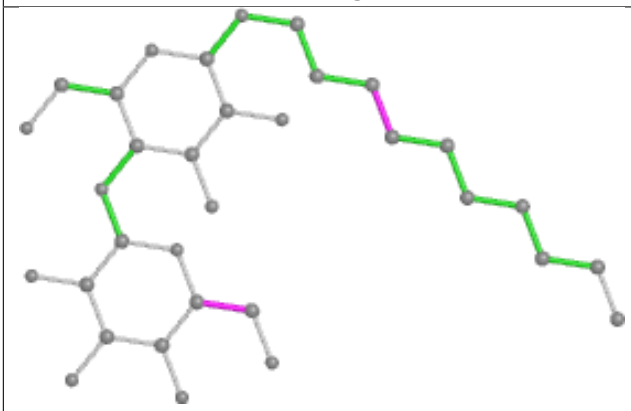
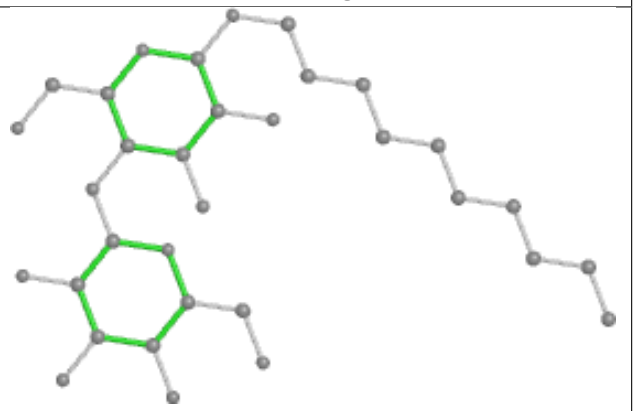


Ligand TGL A 608

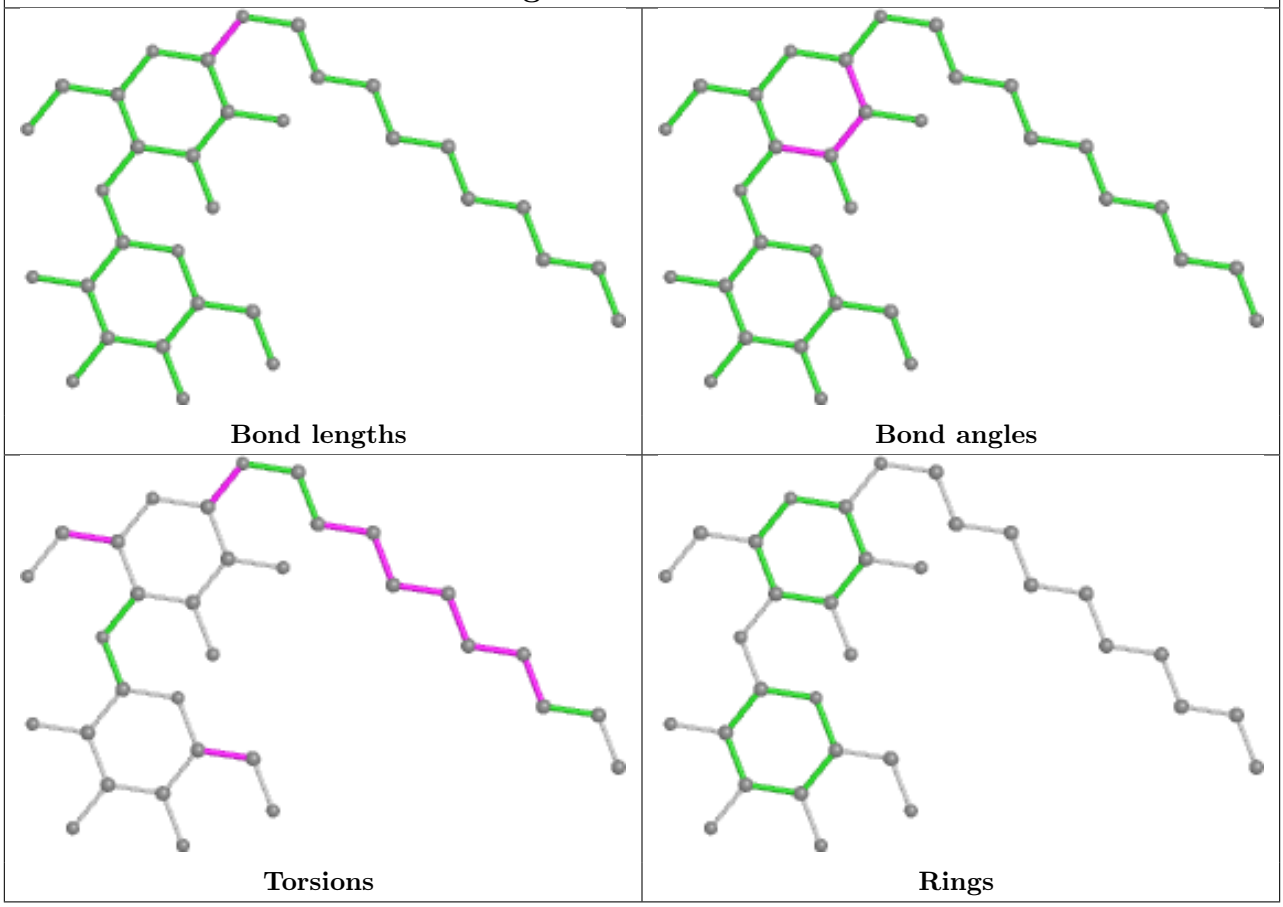


Ligand TGL a 606

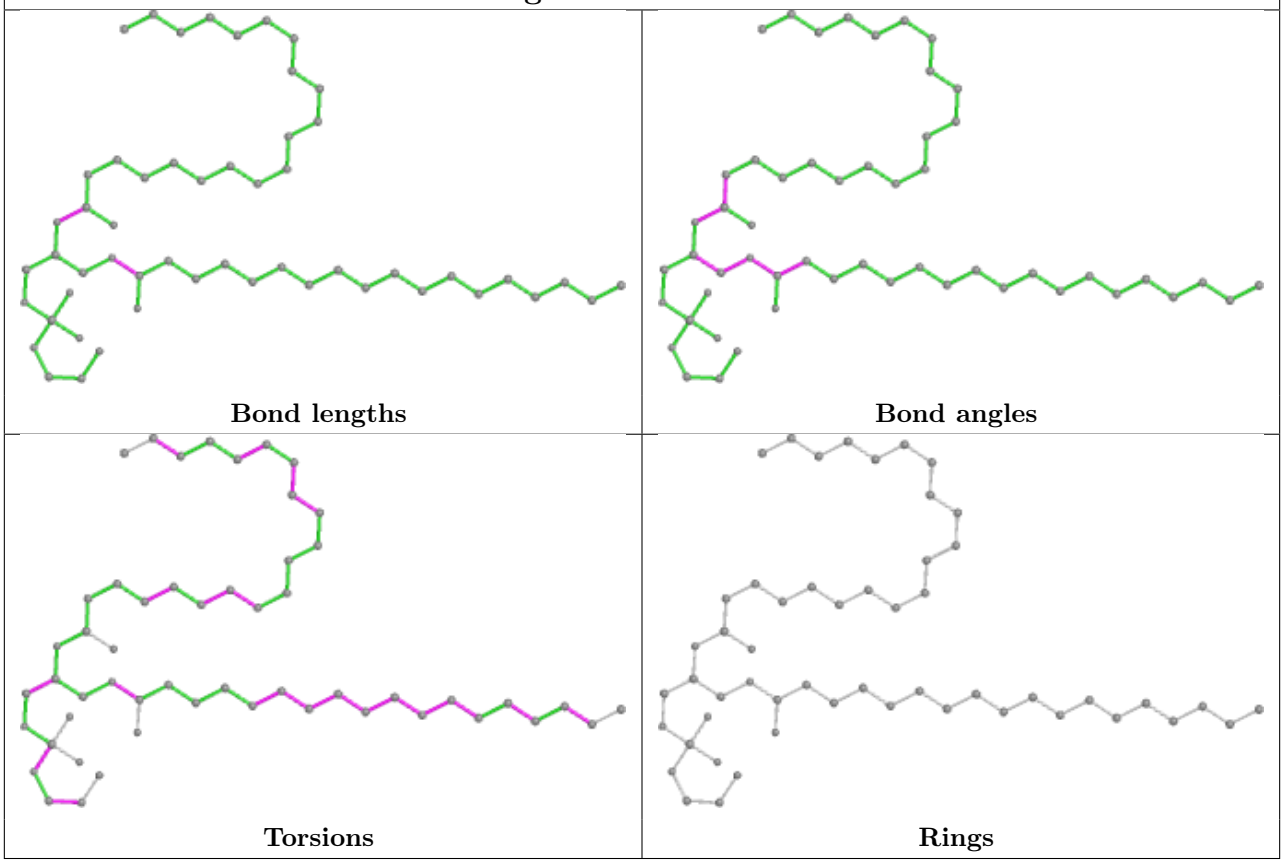


Ligand DMU M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

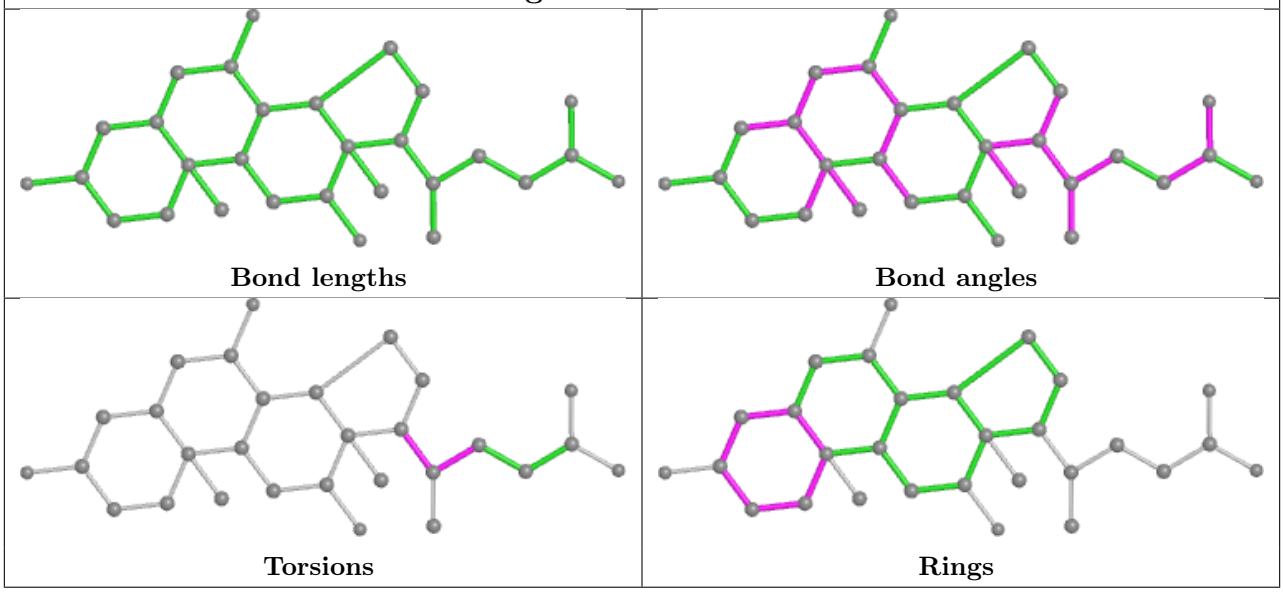
Ligand DMU c 307



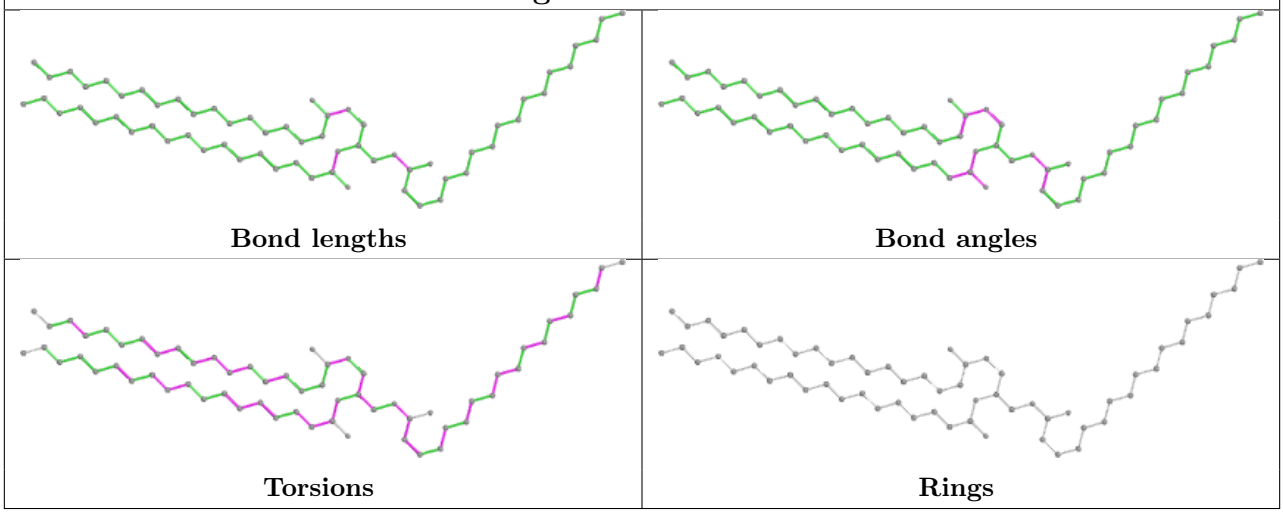
Ligand PEK C 309



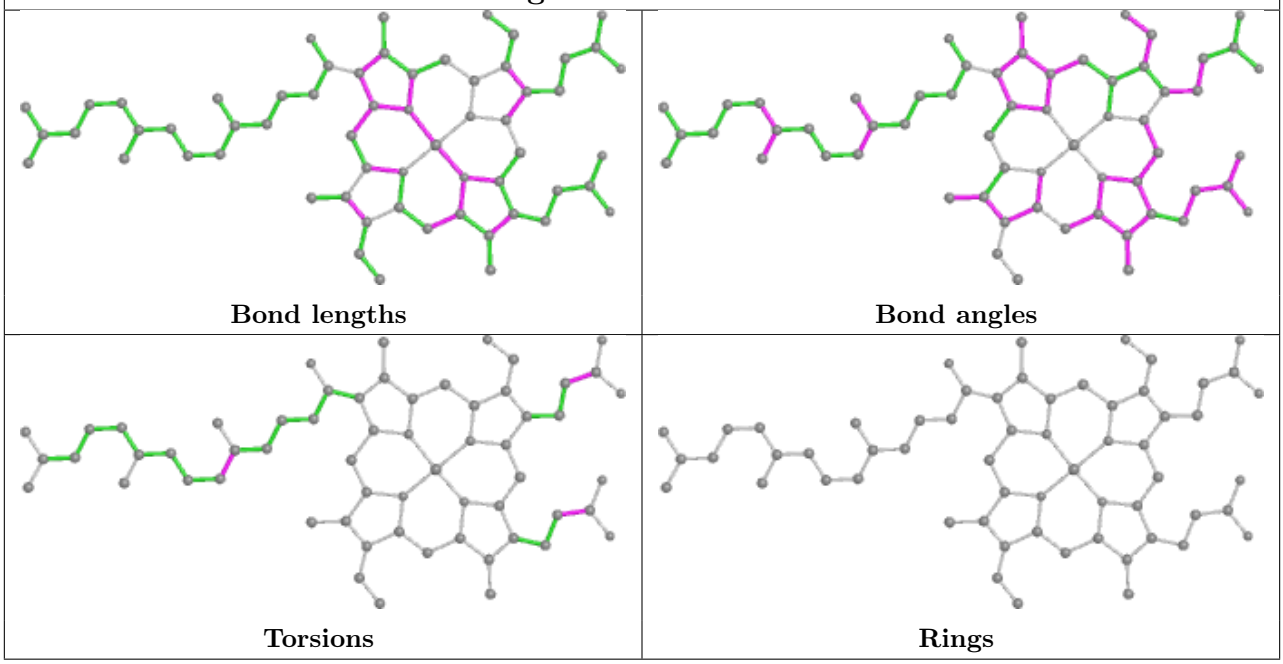
Ligand CHD J 101



Ligand TGL l 101



Ligand HEA a 602



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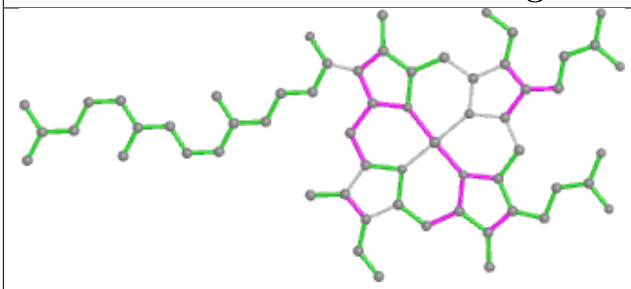
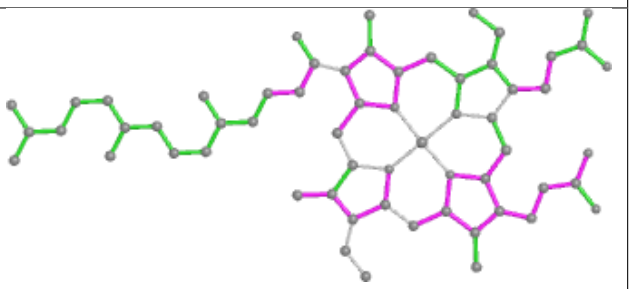
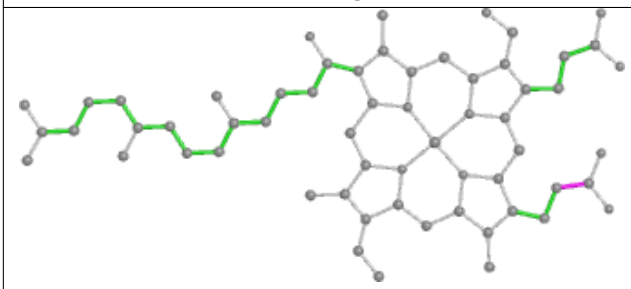
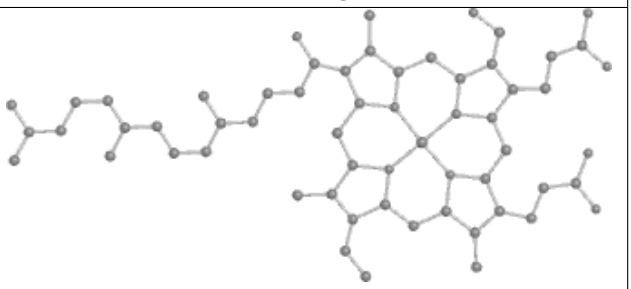
 Bond lengths	 Bond angles
 Torsions	 Rings

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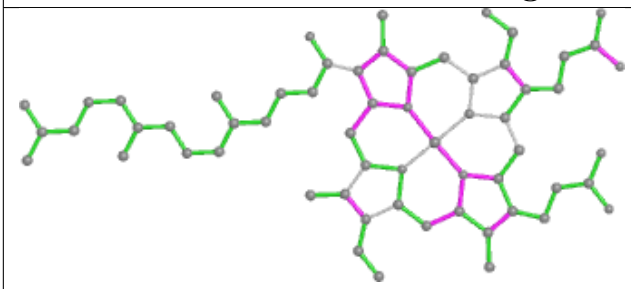
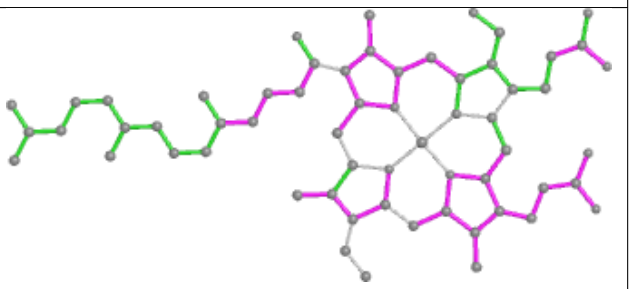
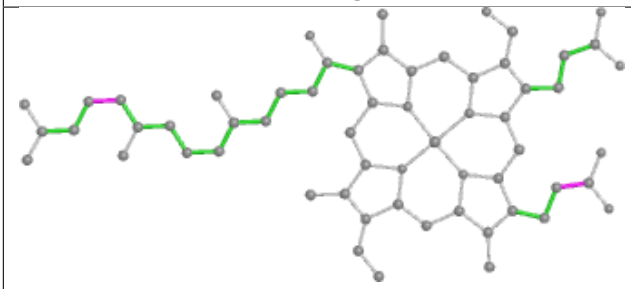
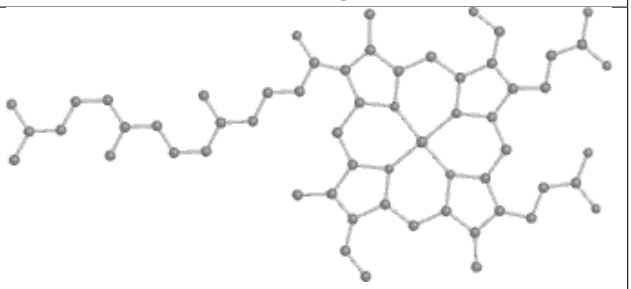
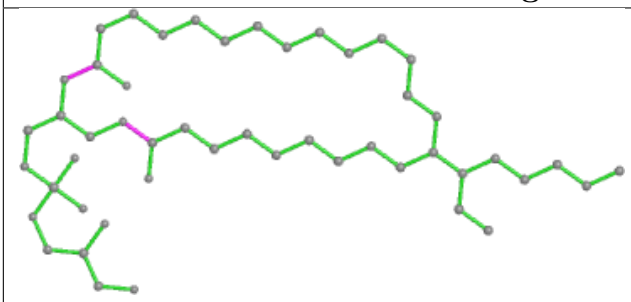
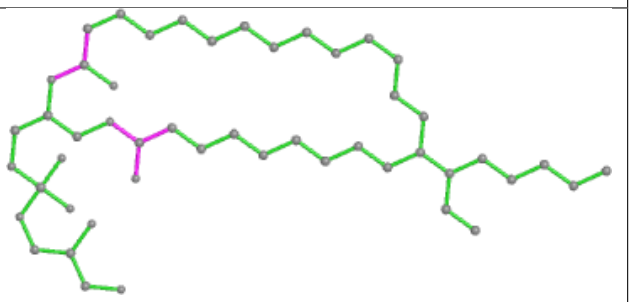
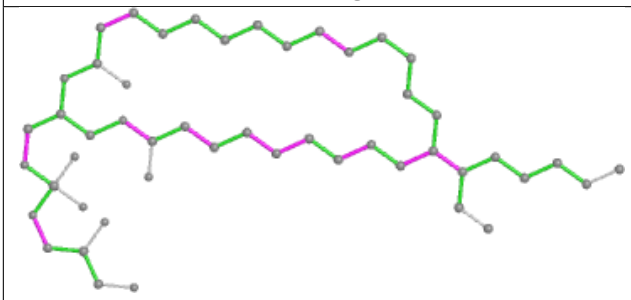
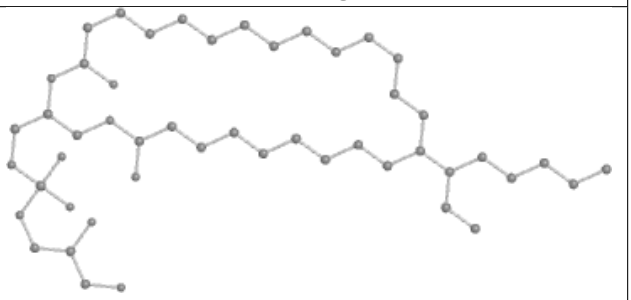
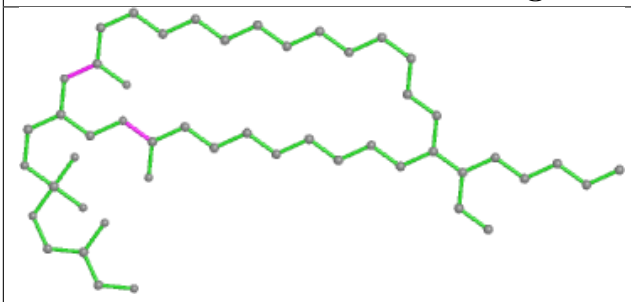
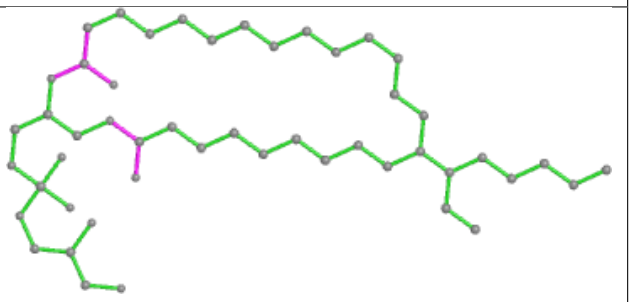
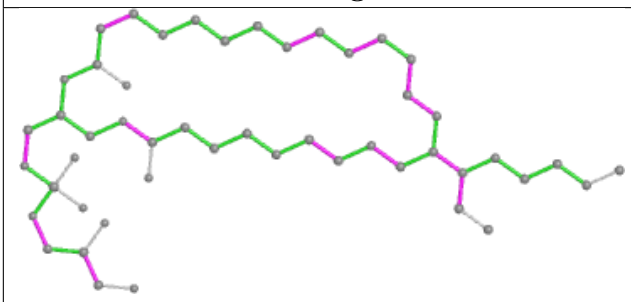
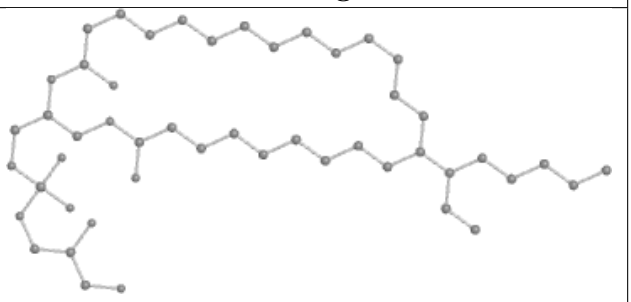
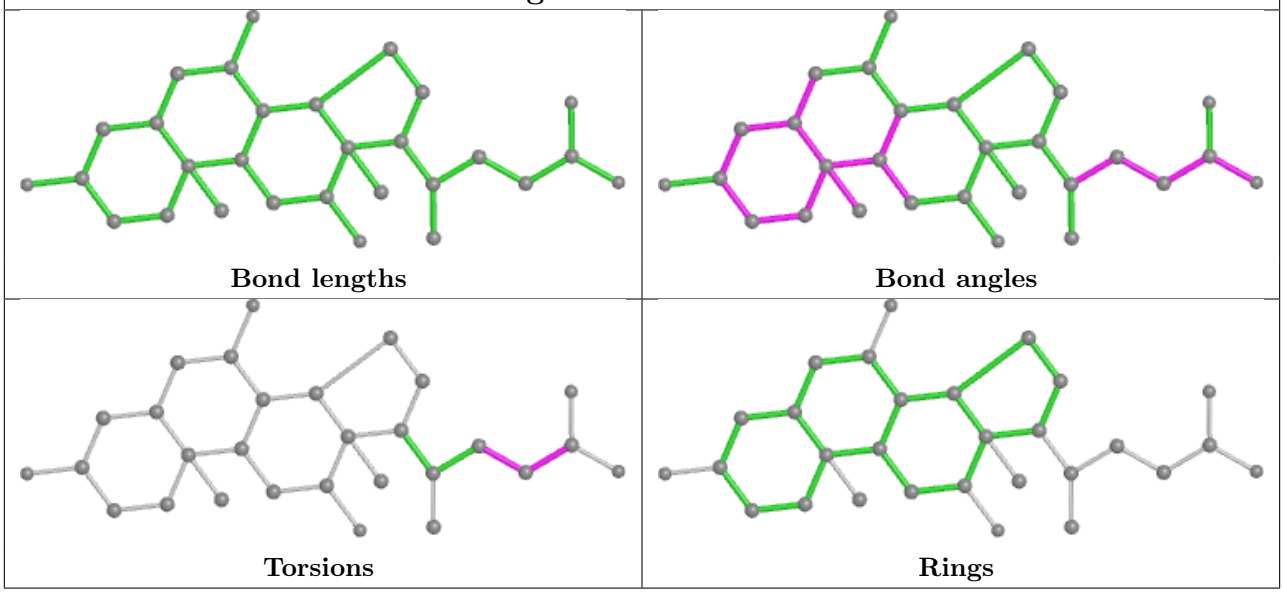
 Bond lengths	 Bond angles
 Torsions	 Rings

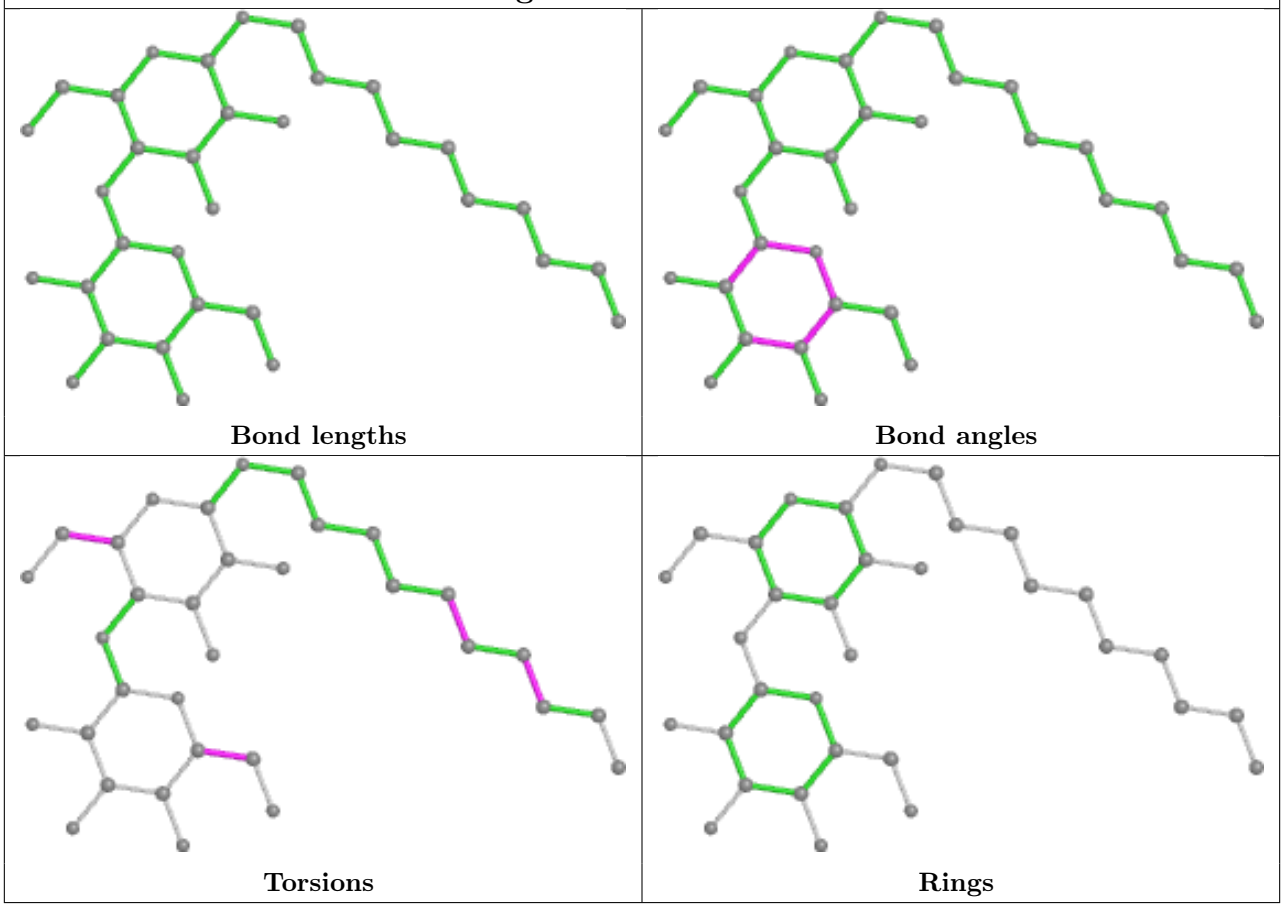
Ligand PGV C 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV c 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

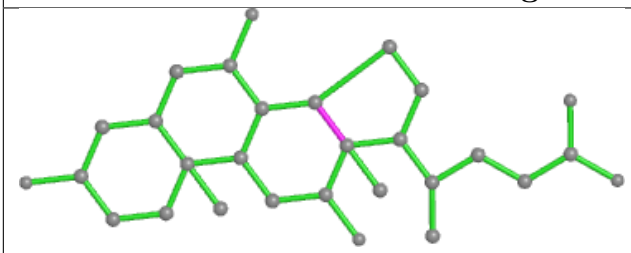
Ligand CHD c 306



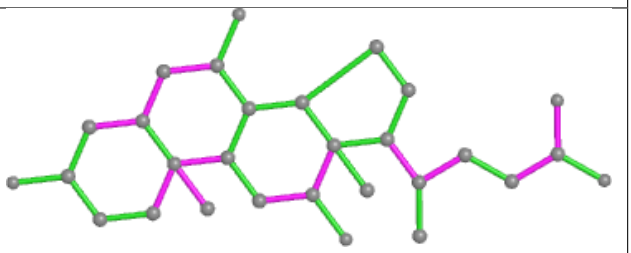
Ligand DMU m 401



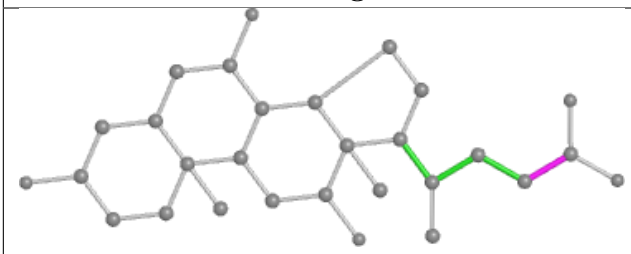
Ligand CHD B 303



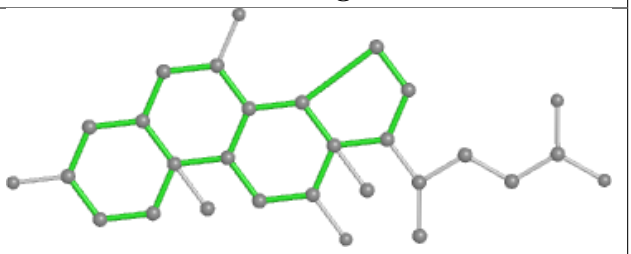
Bond lengths



Bond angles

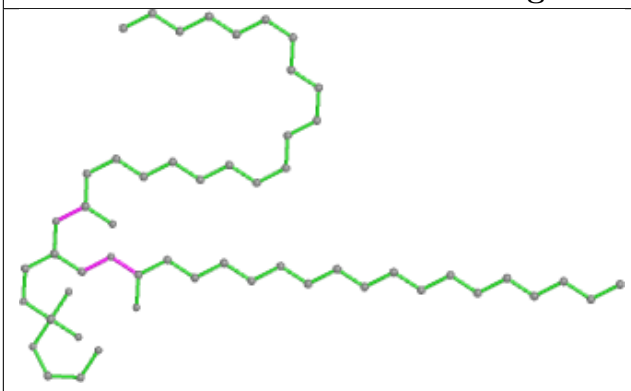


Torsions



Rings

Ligand PEK g 102



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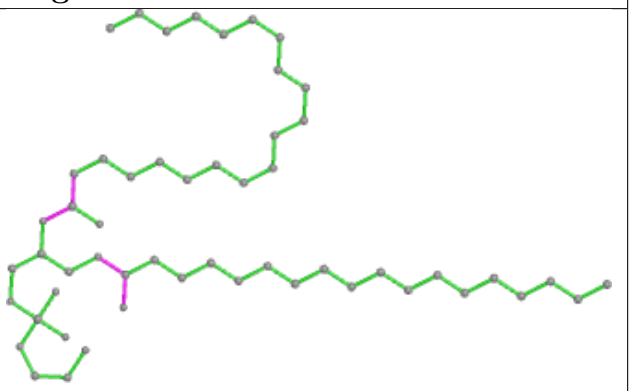
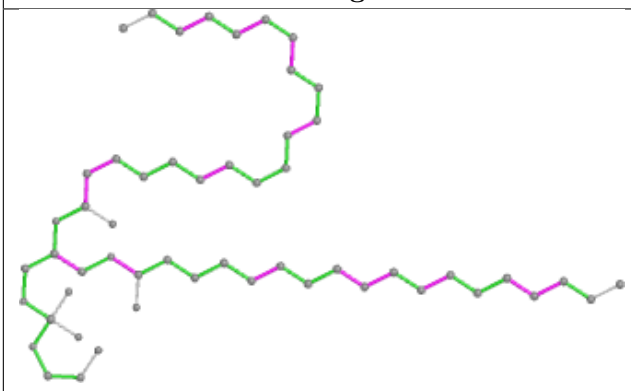


Bond angles



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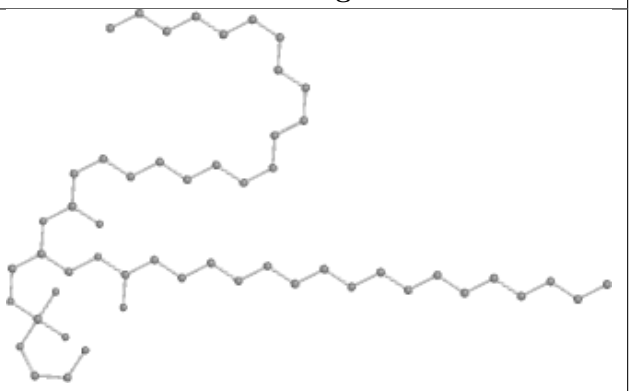
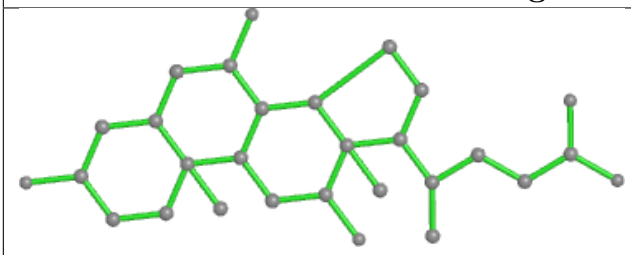
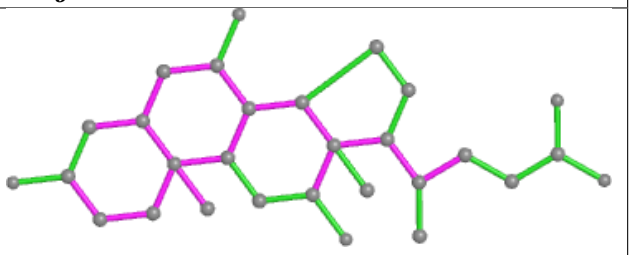
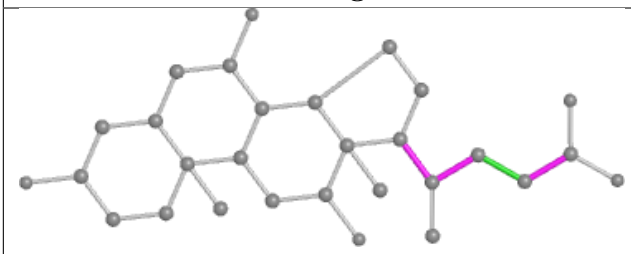
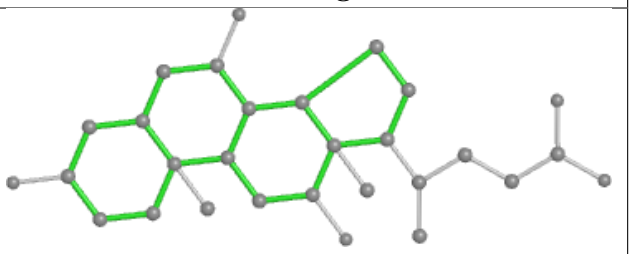
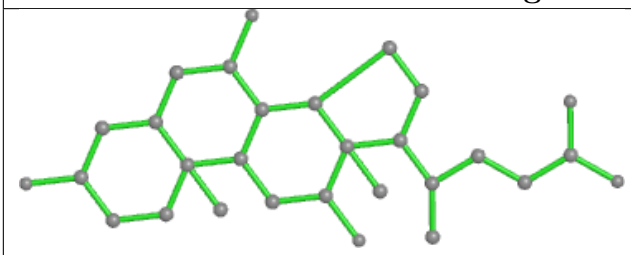
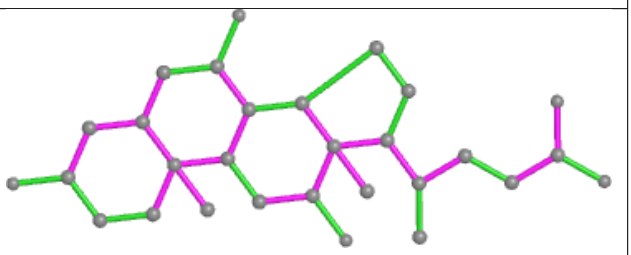
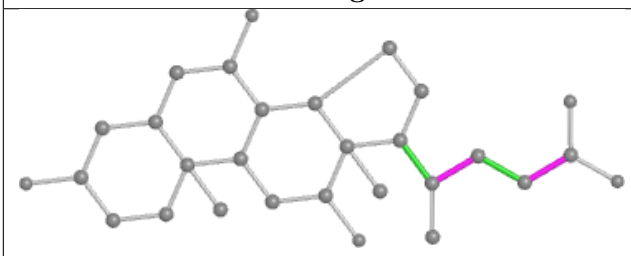
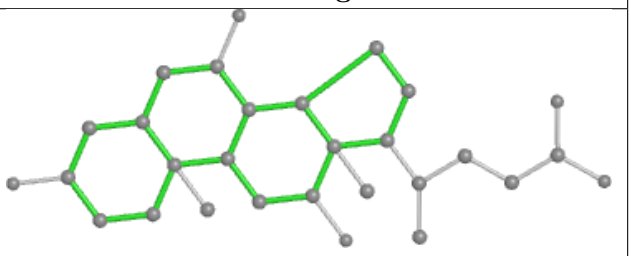
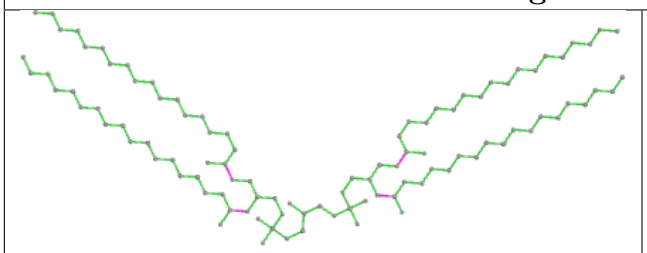


Rings

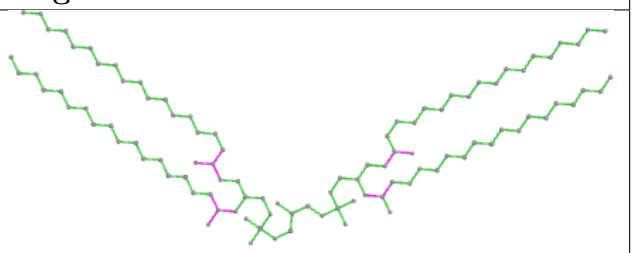
Ligand CHD j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD b 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

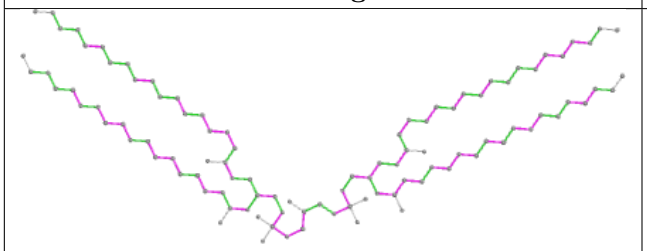
Ligand CDL g 103



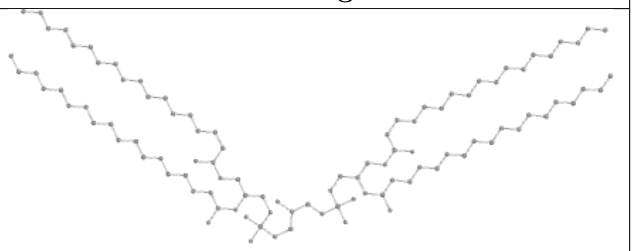
Bond lengths



Bond angles

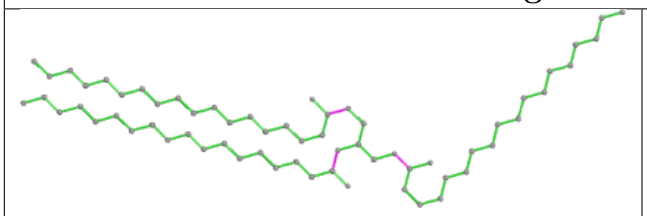


Torsions

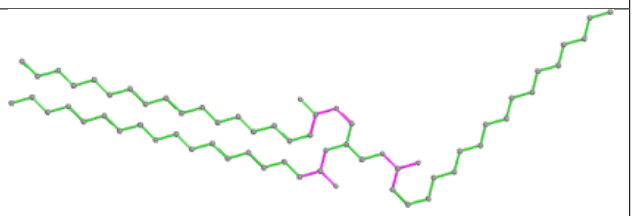


Rings

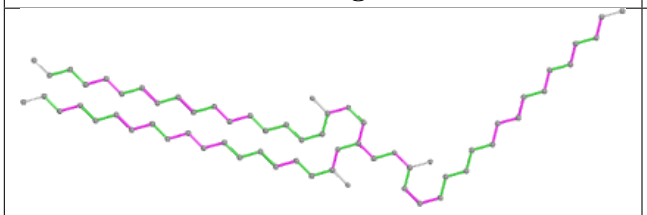
Ligand TGL D 201



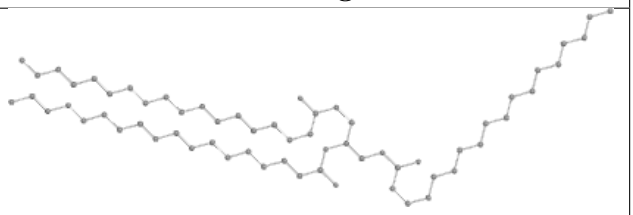
Bond lengths



Bond angles

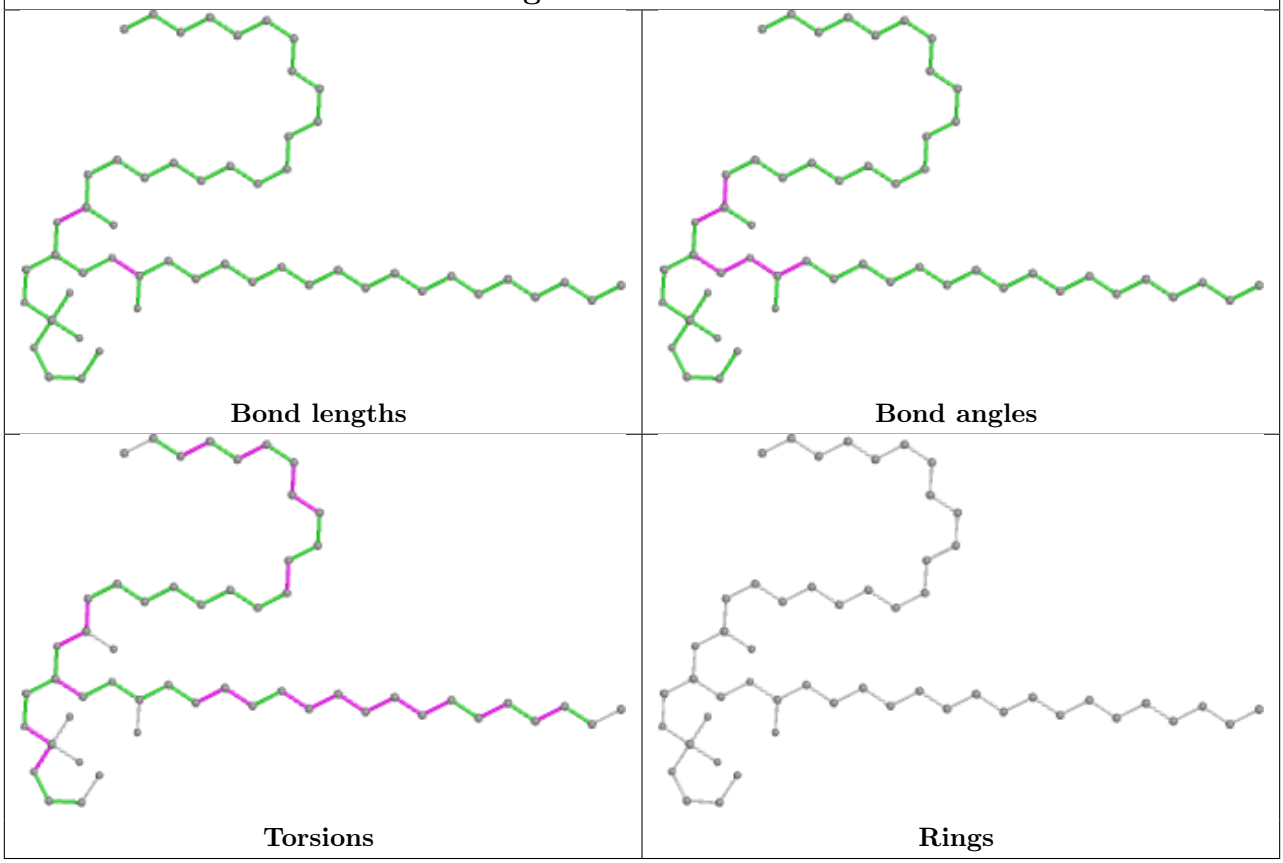


Torsions

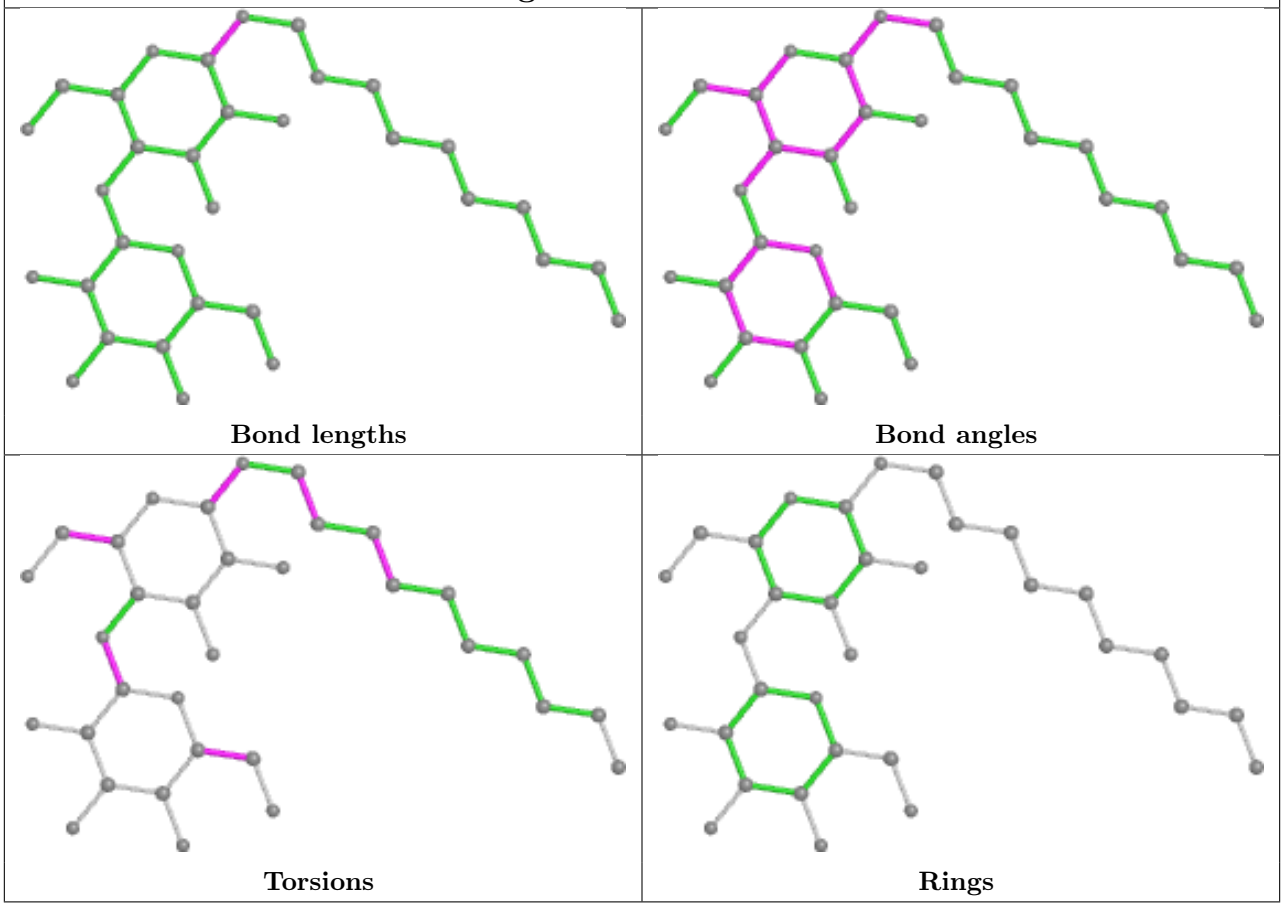


Rings

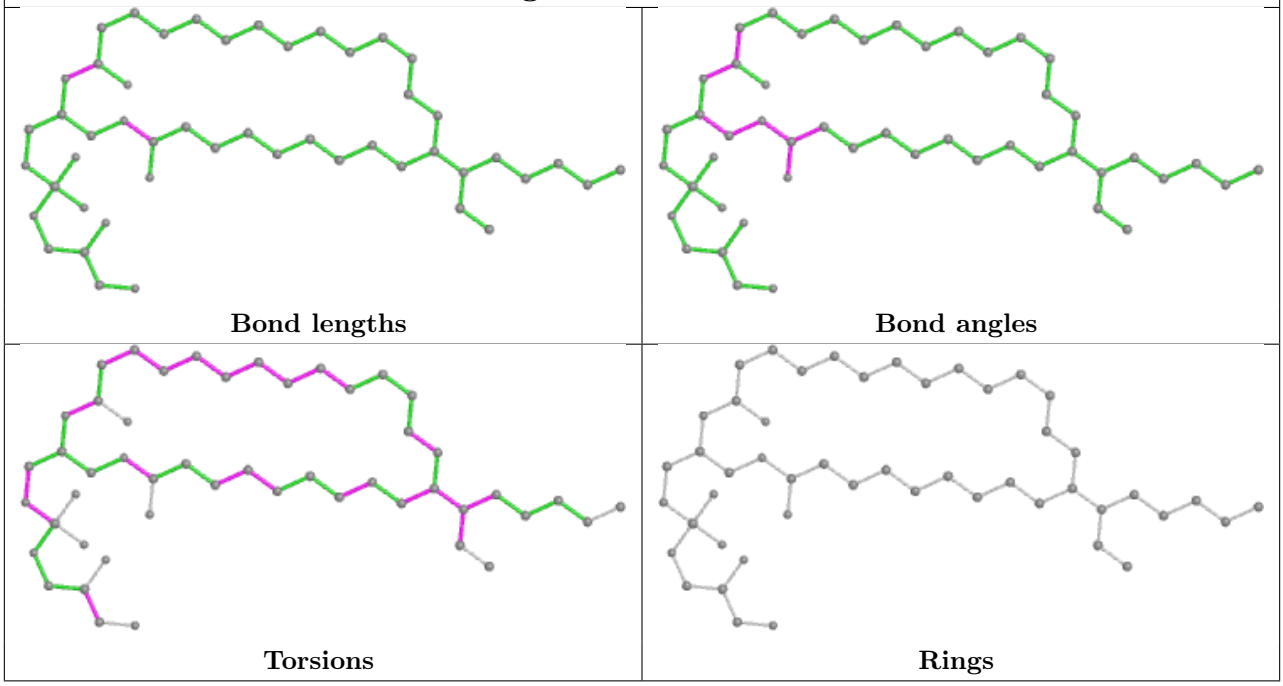
Ligand PEK G 102

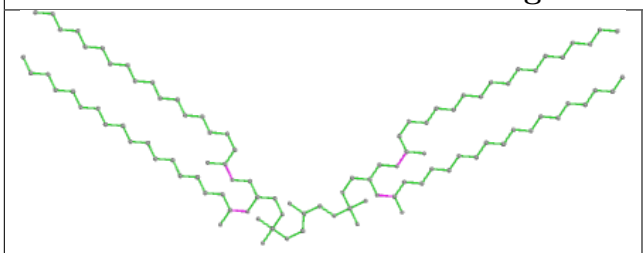
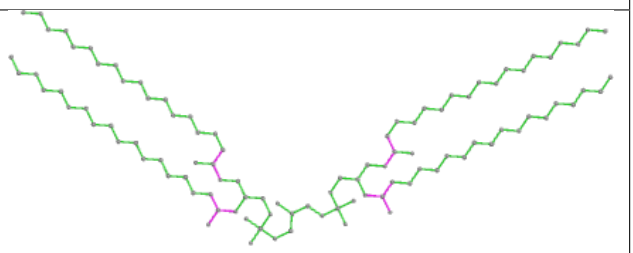
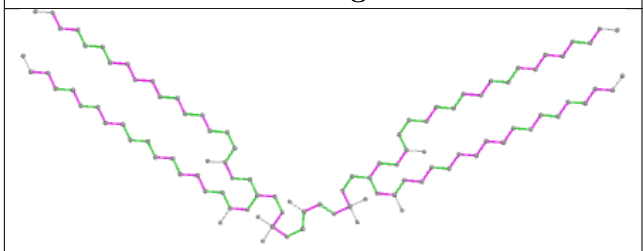
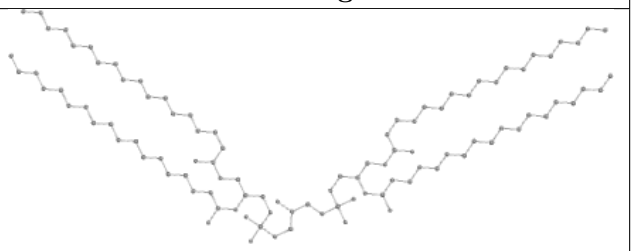


Ligand DMU C 307



Ligand PGV G 103



Ligand CDL G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	-0.64	0	100	100	22, 28, 39, 85	0
1	a	513/514 (99%)	-0.50	0	100	100	27, 41, 58, 93	0
2	B	226/227 (99%)	-0.53	1 (0%)	92	95	23, 35, 62, 123	0
2	b	226/227 (99%)	-0.08	11 (4%)	29	36	36, 52, 90, 134	0
3	C	259/261 (99%)	-0.62	0	100	100	25, 33, 52, 87	0
3	c	259/261 (99%)	-0.50	1 (0%)	92	95	31, 41, 64, 92	0
4	D	144/147 (97%)	-0.52	2 (1%)	75	80	29, 39, 65, 108	0
4	d	144/147 (97%)	0.35	12 (8%)	11	15	49, 67, 109, 200	0
5	E	105/109 (96%)	-0.40	2 (1%)	66	73	29, 40, 77, 124	0
5	e	105/109 (96%)	-0.12	2 (1%)	66	73	37, 56, 79, 118	0
6	F	98/98 (100%)	-0.10	6 (6%)	21	27	28, 43, 118, 148	0
6	f	98/98 (100%)	0.23	7 (7%)	16	21	37, 53, 130, 160	0
7	G	83/85 (97%)	0.17	14 (16%)	1	2	31, 43, 128, 140	0
7	g	83/85 (97%)	0.31	11 (13%)	3	4	33, 55, 133, 156	0
8	H	79/85 (92%)	-0.15	7 (8%)	9	13	30, 46, 113, 133	0
8	h	79/85 (92%)	0.19	6 (7%)	13	18	40, 62, 133, 154	0
9	I	72/73 (98%)	-0.20	3 (4%)	36	43	33, 47, 73, 76	0
9	i	72/73 (98%)	0.30	8 (11%)	5	7	38, 65, 90, 129	0
10	J	58/59 (98%)	-0.16	3 (5%)	27	34	36, 48, 82, 130	0
10	j	58/59 (98%)	0.09	5 (8%)	10	14	49, 62, 106, 176	0
11	K	49/56 (87%)	-0.03	3 (6%)	21	27	30, 46, 76, 107	0
11	k	49/56 (87%)	0.58	8 (16%)	1	2	53, 68, 91, 111	0
12	L	46/47 (97%)	-0.69	1 (2%)	62	69	28, 36, 58, 118	0
12	l	46/47 (97%)	-0.31	1 (2%)	62	69	42, 59, 89, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.36	2 (4%) 31 38	33, 38, 69, 116	0
13	m	43/46 (93%)	0.50	7 (16%) 1 2	51, 60, 97, 163	0
All	All	3550/3614 (98%)	-0.29	123 (3%) 44 51	22, 42, 87, 200	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	f	1	ALA	18.4
4	d	6	VAL	14.3
4	d	5	VAL	9.7
13	m	43	SER	9.7
10	j	57	HIS	9.3
6	f	2	SER	9.2
7	g	41	HIS	9.1
13	m	42	LYS	8.3
6	f	98	HIS	8.2
6	F	1	ALA	7.8
4	d	4	SER	7.8
8	h	48	GLY	7.7
6	F	94	HIS	7.2
6	f	97	ALA	6.9
6	f	94	HIS	6.6
7	G	3	ALA	6.5
7	g	39	SER	6.4
6	F	2	SER	6.2
7	G	41	HIS	6.0
12	l	2	HIS	5.8
6	F	98	HIS	5.7
7	G	40	GLY	5.6
7	g	36	TRP	5.6
7	g	40	GLY	5.5
4	d	7	LYS	5.4
10	J	58	LYS	5.2
2	b	90	ILE	5.0
9	i	2	THR	4.9
2	B	90	ILE	4.9
8	h	7	LYS	4.8
8	h	8	ILE	4.8
5	e	5	HIS	4.5
7	G	39	SER	4.3
7	G	10	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
6	F	95	GLN	4.1
9	i	53	ASN	4.0
10	j	52	TRP	4.0
6	F	97	ALA	3.9
11	K	42	PRO	3.8
4	D	4	SER	3.8
10	J	57	HIS	3.7
11	K	6	ALA	3.6
2	b	170	LEU	3.6
7	G	5	LYS	3.5
12	L	2	HIS	3.5
11	k	7	PRO	3.5
8	H	8	ILE	3.5
2	b	165	VAL	3.5
8	H	45	ALA	3.5
7	g	7	ASP	3.4
7	G	36	TRP	3.4
8	H	48	GLY	3.4
13	M	43	SER	3.4
2	b	59	GLN	3.3
7	g	5	LYS	3.2
7	g	42	ARG	3.2
7	G	42	ARG	3.2
9	i	52	ARG	3.2
7	G	2	SER	3.1
9	I	37	PHE	3.1
7	G	4	ALA	3.1
8	h	49	ASP	3.1
4	d	32	ASN	3.0
10	j	56	PRO	3.0
8	H	47	GLY	3.0
7	G	9	GLY	3.0
4	d	147	LYS	2.9
13	m	32	TRP	2.9
11	K	41	ASN	2.8
13	m	35	TYR	2.8
9	i	73	LYS	2.8
8	H	44	THR	2.8
4	d	8	SER	2.7
4	d	38	LYS	2.7
9	I	19	PHE	2.7
11	k	31	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
11	k	30	VAL	2.7
11	k	13	TYR	2.6
7	g	84	LYS	2.6
10	j	48	TYR	2.6
3	c	259	TRP	2.6
7	g	10	GLY	2.6
4	d	102	TYR	2.6
10	j	58	LYS	2.6
11	k	6	ALA	2.6
7	G	8	HIS	2.5
6	f	95	GLN	2.5
13	M	42	LYS	2.5
5	E	5	HIS	2.5
9	i	22	VAL	2.5
13	m	41	LYS	2.4
11	k	35	GLN	2.4
2	b	227	LEU	2.4
9	i	19	PHE	2.4
2	b	2	ALA	2.4
2	b	131	GLY	2.4
7	G	6	GLY	2.4
7	g	1	ALA	2.3
9	I	53	ASN	2.3
2	b	130	PRO	2.3
13	m	40	TYR	2.3
8	H	10	ASN	2.3
2	b	92	ASN	2.2
2	b	113	TYR	2.2
7	G	84	LYS	2.2
11	k	33	ALA	2.2
8	H	77	ALA	2.2
8	h	45	ALA	2.2
9	i	48	ALA	2.2
11	k	34	THR	2.2
7	g	2	SER	2.2
2	b	166	PRO	2.1
13	m	39	ASN	2.1
4	d	35	ALA	2.1
9	i	49	ASP	2.1
10	J	1	PHE	2.1
6	f	25	ARG	2.1
4	d	10	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	33	LEU	2.1
8	h	47	GLY	2.0
5	e	108	LYS	2.0
5	E	109	VAL	2.0
4	D	147	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.66	0.30	92,134,145,151	0
9	SAC	i	1	9/10	0.66	0.60	117,152,162,171	0
7	TPO	g	11	11/12	0.77	0.26	93,121,137,145	0
9	SAC	I	1	9/10	0.82	0.32	86,107,126,130	0
1	FME	a	1	10/11	0.89	0.32	80,89,130,142	0
1	FME	A	1	10/11	0.95	0.23	53,62,98,100	0
2	FME	b	1	10/11	0.95	0.23	48,55,57,58	0
2	FME	B	1	10/11	0.97	0.22	29,35,42,44	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	PSC	e	201	52/52	0.48	0.42	56,121,231,239	0
24	PEK	G	102	53/53	0.54	0.35	64,117,204,226	0
26	DMU	C	307	33/33	0.54	0.32	66,126,146,150	0
24	PEK	C	309	53/53	0.55	0.36	66,98,168,173	0
19	TGL	l	101	63/63	0.59	0.27	55,100,146,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	PSC	B	302	52/52	0.59	0.35	57,118,223,244	0
24	PEK	C	308	53/53	0.62	0.29	67,103,158,173	0
26	DMU	c	307	33/33	0.62	0.38	90,138,163,171	0
24	PEK	c	303	53/53	0.63	0.26	59,104,133,143	0
25	CDL	c	305	100/100	0.65	0.29	49,107,143,157	0
19	TGL	a	606	63/63	0.65	0.23	74,95,131,133	0
25	CDL	C	305	100/100	0.65	0.29	46,102,140,147	0
25	CDL	g	103	100/100	0.67	0.30	63,112,158,182	0
25	CDL	G	101	100/100	0.70	0.28	71,112,154,164	0
17	NA	a	605	1/1	0.71	0.12	50,50,50,50	0
19	TGL	L	101	63/63	0.71	0.27	43,88,128,130	0
19	TGL	D	201	63/63	0.72	0.21	66,92,121,126	0
18	PGV	A	606	51/51	0.73	0.26	53,89,136,151	0
18	PGV	a	607	51/51	0.74	0.29	58,96,149,171	0
26	DMU	m	401	33/33	0.75	0.31	67,94,108,112	0
18	PGV	G	103	51/51	0.78	0.21	54,108,130,139	0
23	CHD	j	101	29/29	0.82	0.24	104,119,130,134	0
18	PGV	C	304	51/51	0.83	0.20	61,95,132,142	0
26	DMU	M	101	33/33	0.83	0.19	42,54,66,67	0
19	TGL	A	608	63/63	0.85	0.21	37,87,127,146	0
19	TGL	i	101	63/63	0.85	0.21	46,99,142,151	0
23	CHD	J	101	29/29	0.88	0.23	76,89,111,117	0
23	CHD	C	306	29/29	0.89	0.21	72,84,88,90	0
23	CHD	c	306	29/29	0.92	0.19	78,83,100,101	0
24	PEK	g	102	53/53	0.94	0.20	41,65,100,105	0
18	PGV	C	303	51/51	0.95	0.23	27,39,95,97	0
23	CHD	b	301	29/29	0.96	0.10	32,39,46,51	0
23	CHD	c	302	29/29	0.96	0.08	34,38,40,44	0
16	MG	a	604	1/1	0.96	0.15	42,42,42,42	0
18	PGV	c	304	51/51	0.96	0.24	31,44,93,100	0
24	PEK	C	302	53/53	0.96	0.21	28,56,114,116	0
14	HEA	a	601	60/60	0.96	0.13	34,41,52,53	0
18	PGV	c	301	51/51	0.97	0.21	29,56,75,82	0
20	CMO	a	608	2/2	0.97	0.11	33,33,33,36	0
23	CHD	B	303	29/29	0.97	0.10	32,36,45,49	0
23	CHD	C	301	29/29	0.97	0.07	29,32,37,41	0
21	CUA	B	301	2/2	0.97	0.04	29,29,29,31	0
21	CUA	b	302	2/2	0.97	0.03	46,46,46,47	0
14	HEA	A	601	60/60	0.98	0.10	20,25,42,54	0
14	HEA	a	602	60/60	0.98	0.13	27,31,41,45	0
18	PGV	A	607	51/51	0.98	0.21	24,46,64,72	0
16	MG	A	604	1/1	0.98	0.07	26,26,26,26	0

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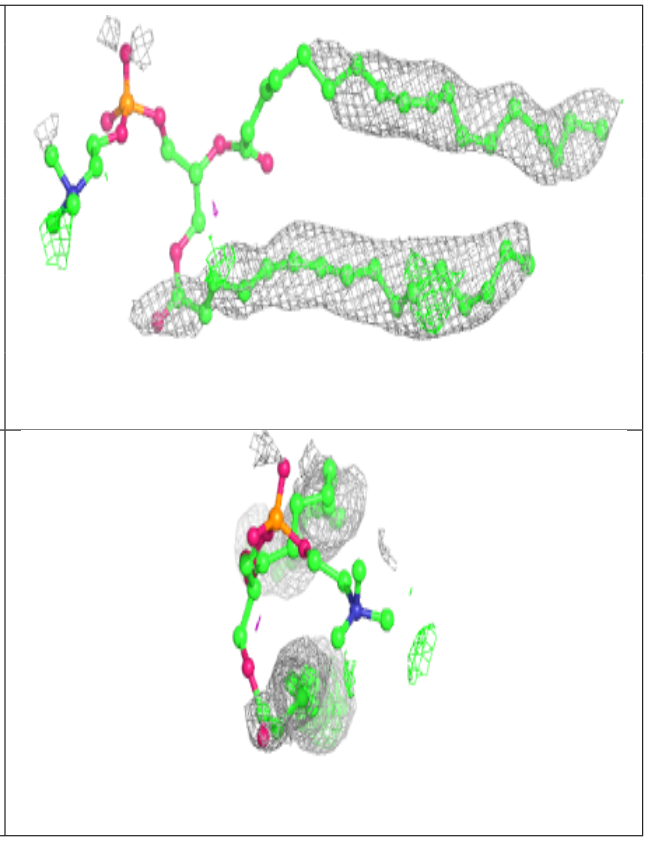
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	HEA	A	602	60/60	0.98	0.12	20,23,36,43	0
17	NA	A	605	1/1	0.98	0.04	31,31,31,31	0
20	CMO	A	609	2/2	0.99	0.09	23,23,23,24	0
15	CU	a	603	1/1	0.99	0.06	39,39,39,39	0
27	ZN	F	101	1/1	0.99	0.02	45,45,45,45	0
15	CU	A	603	1/1	1.00	0.05	28,28,28,28	0
27	ZN	f	101	1/1	1.00	0.03	52,52,52,52	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.

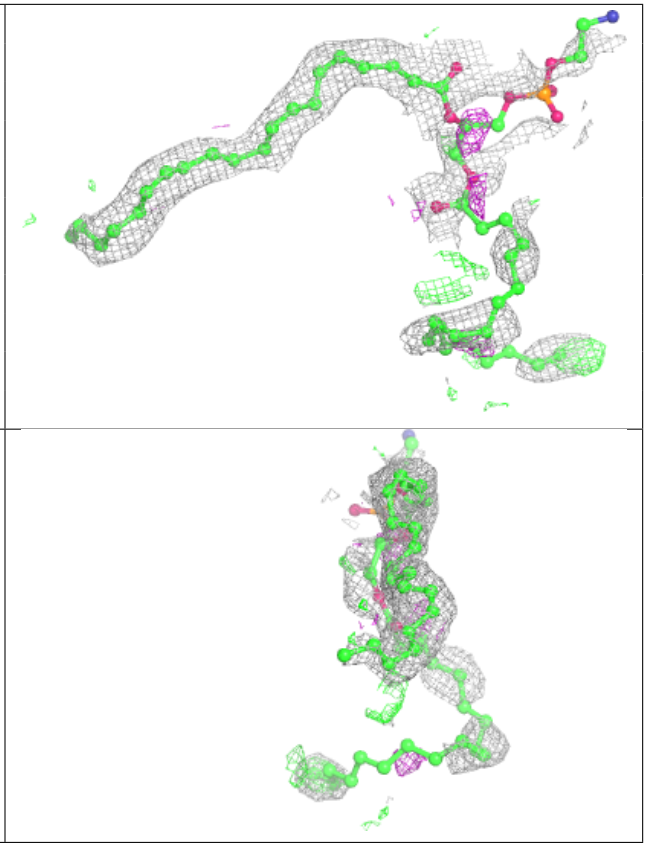
Electron density around PSC e 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



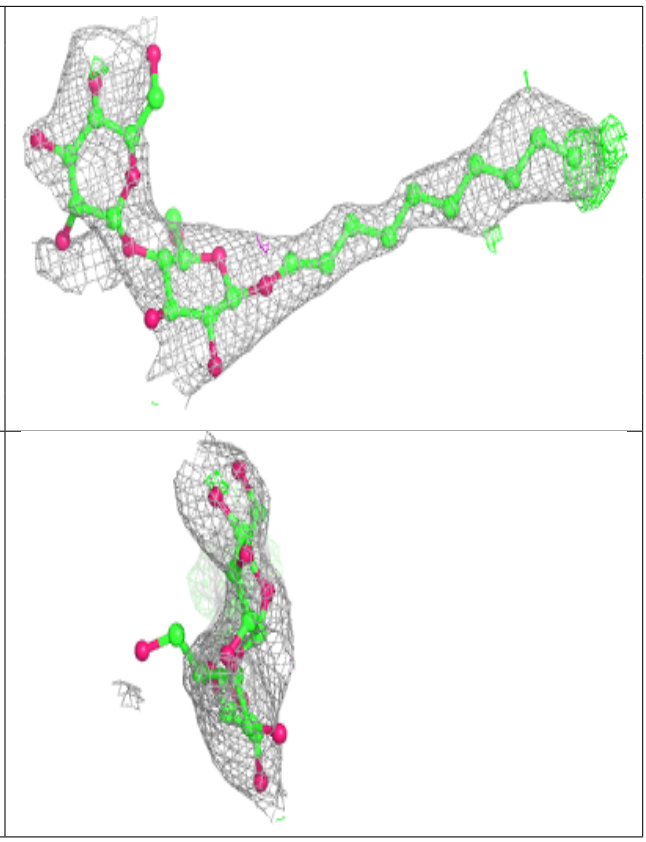
Electron density around PEK G 102:

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



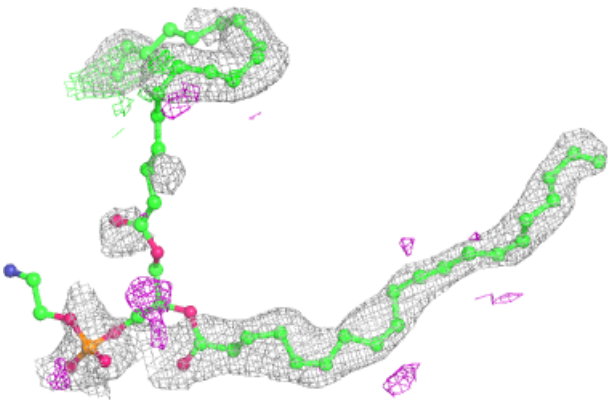
Electron density around DMU C 307:

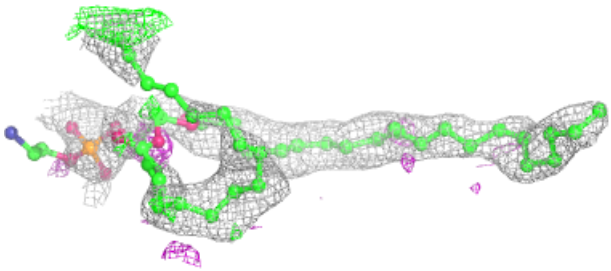
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

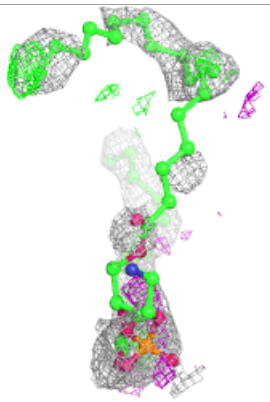


Electron density around PEK C 309:

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

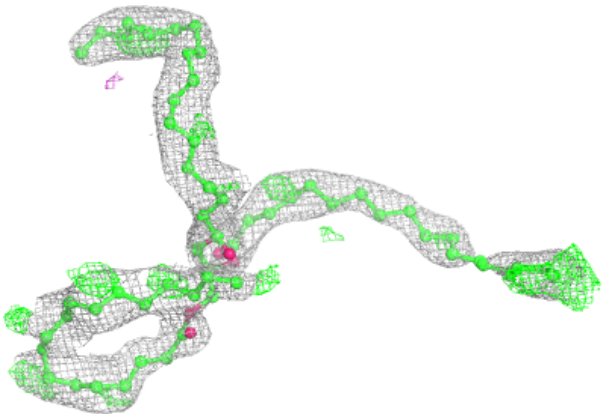


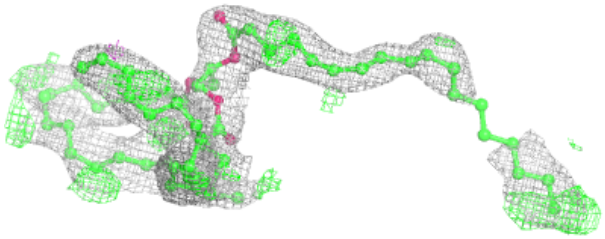


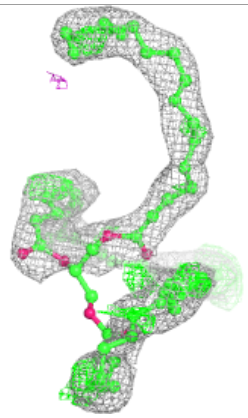


Electron density around TGL l 101:

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

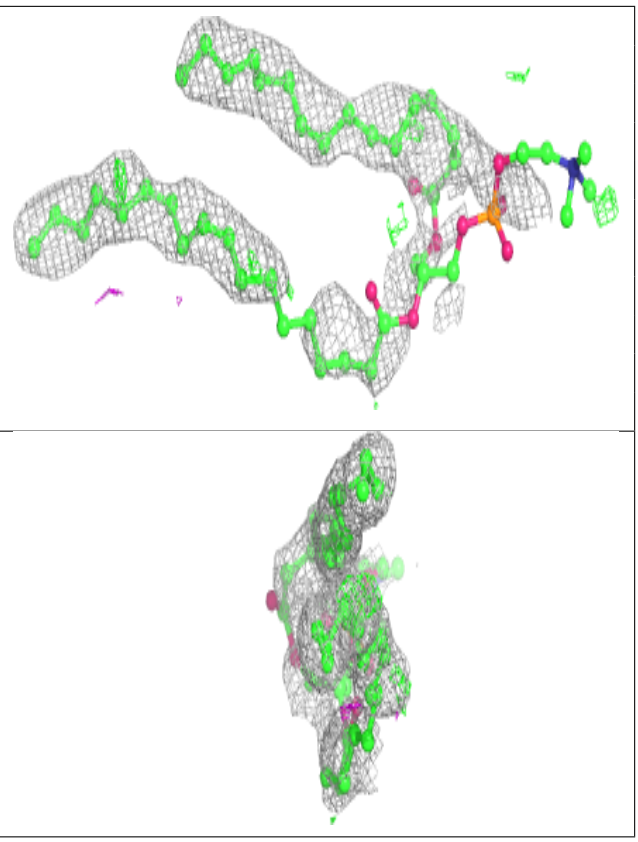






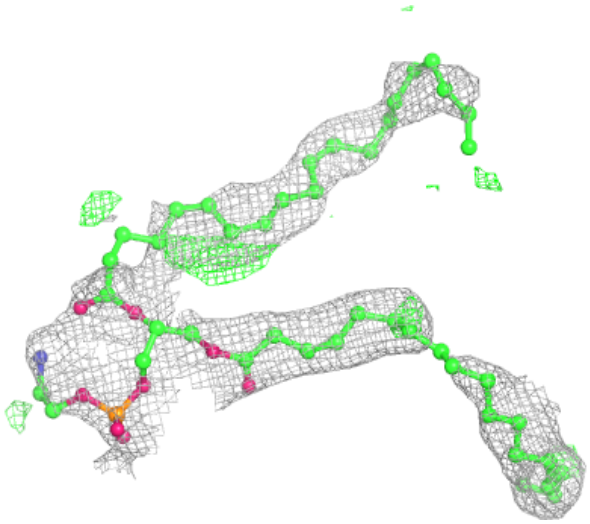
Electron density around PSC B 302:

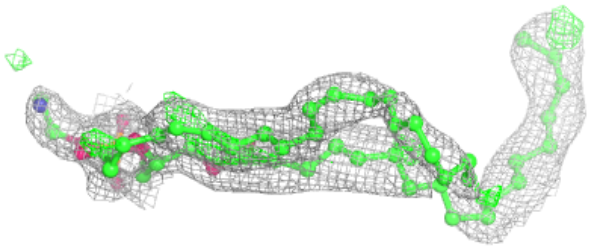
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

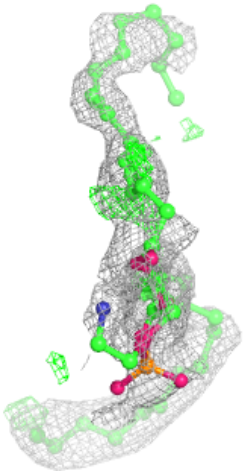


Electron density around PEK C 308:

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

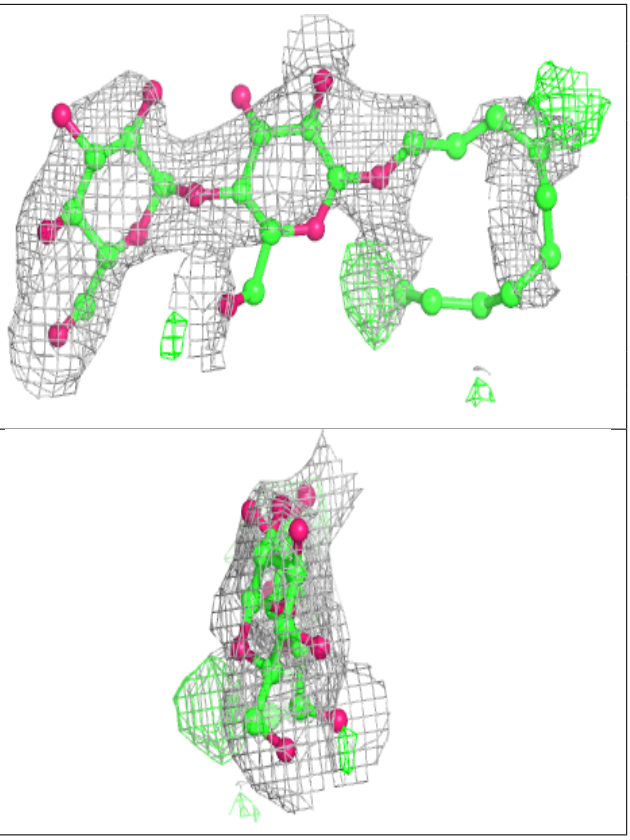


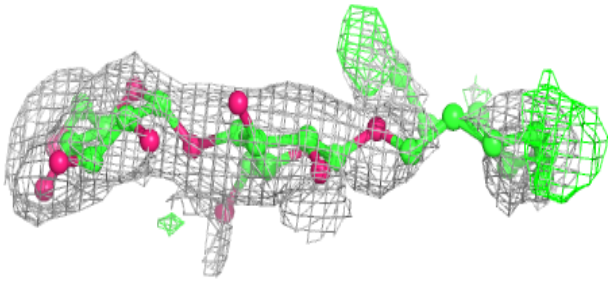




Electron density around DMU c 307:

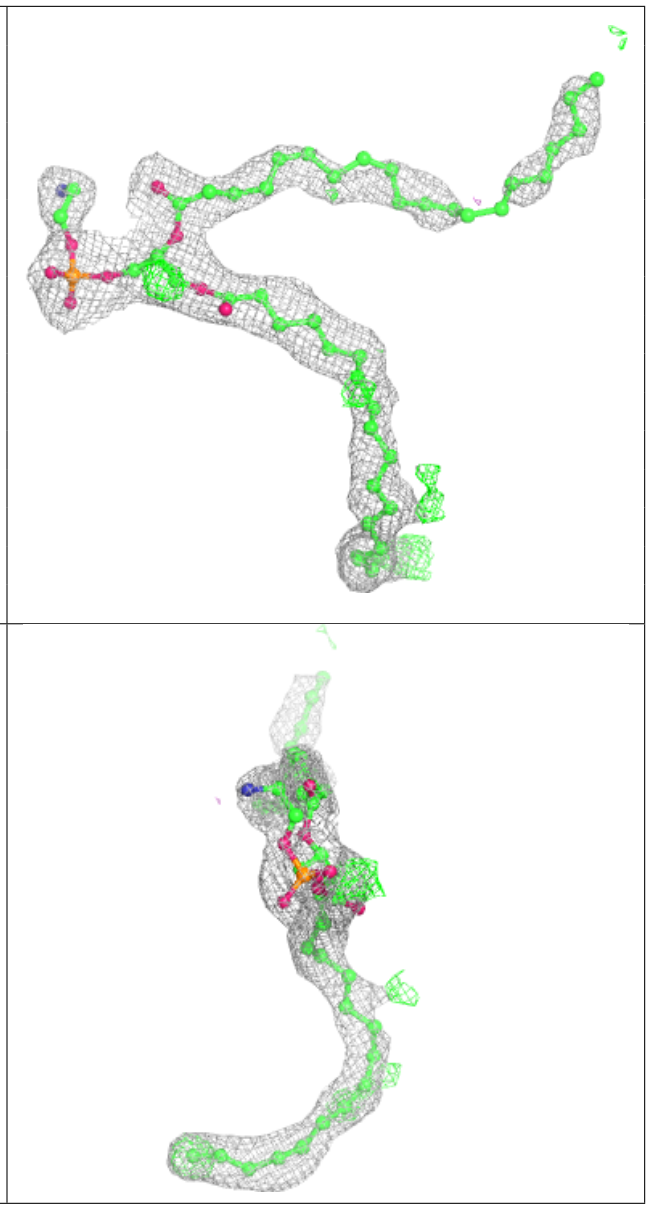
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





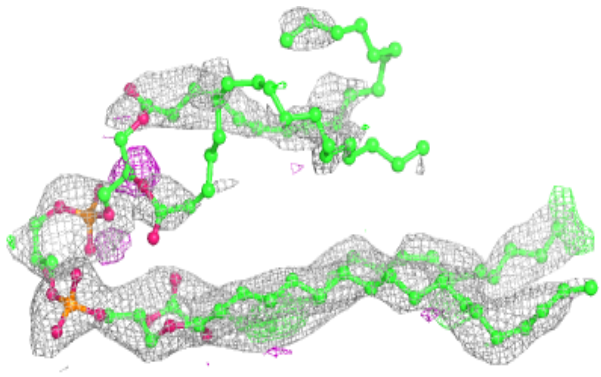
Electron density around PEK c 303:

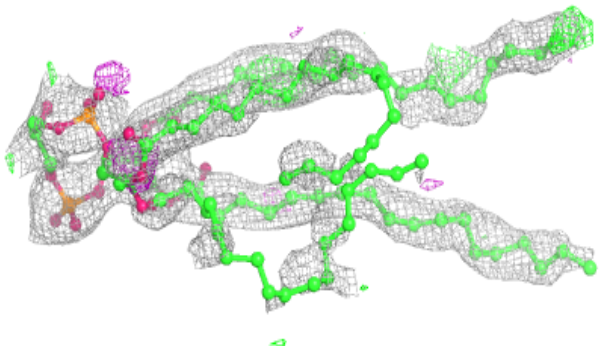
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

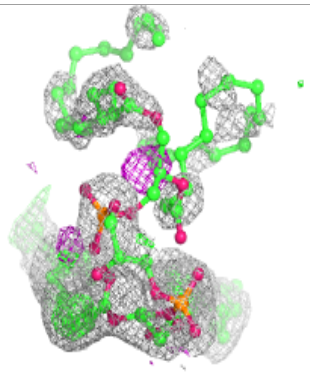


Electron density around CDL c 305:

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

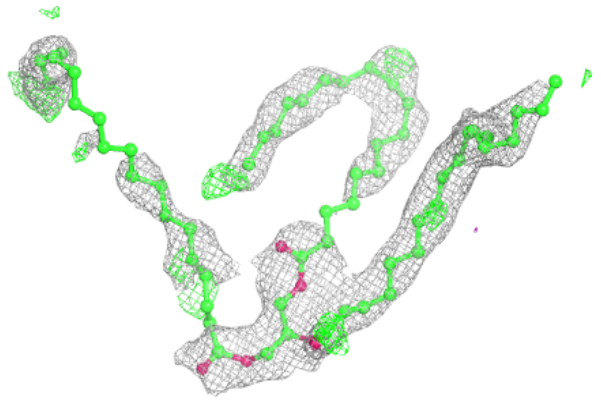


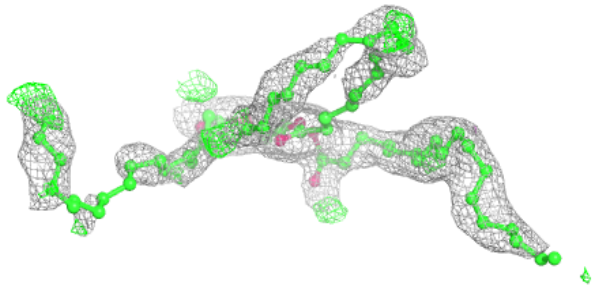


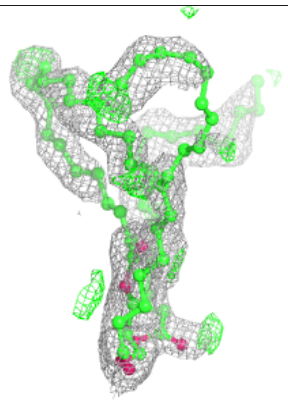


Electron density around TGL a 606:

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

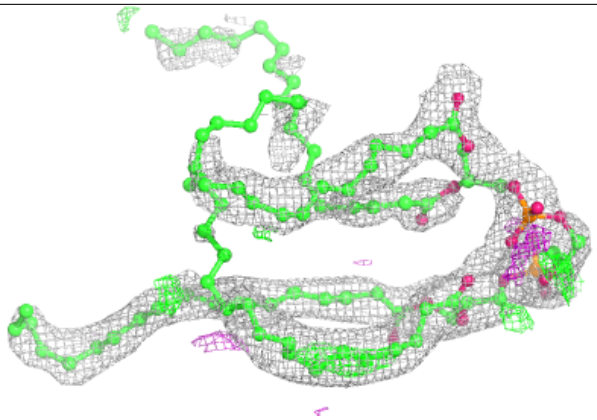


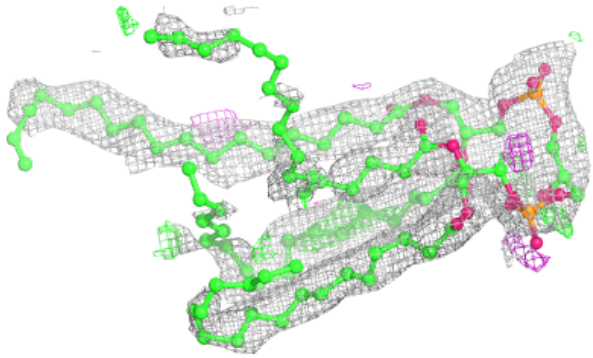


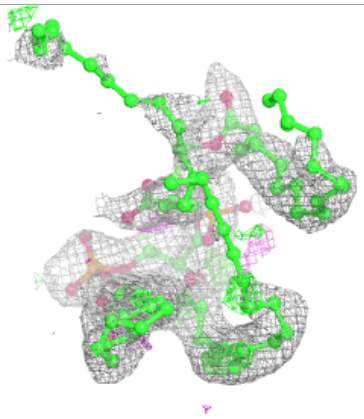


Electron density around CDL C 305:

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

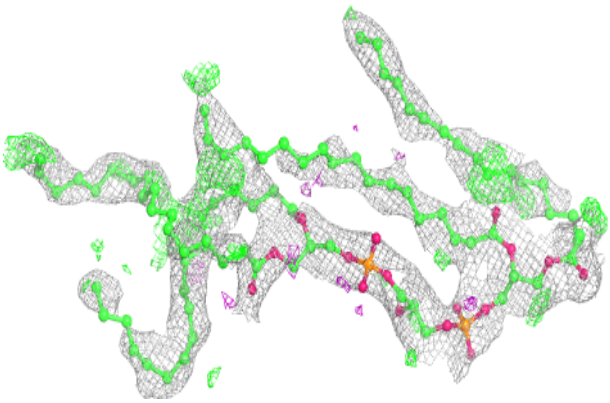


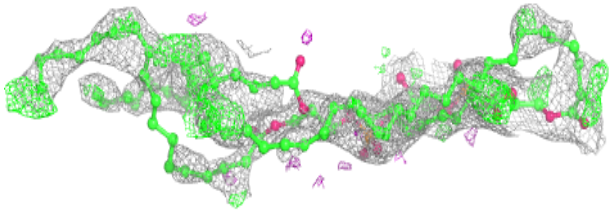


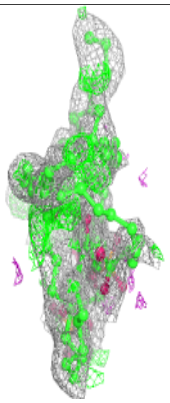


Electron density around CDL g 103:

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

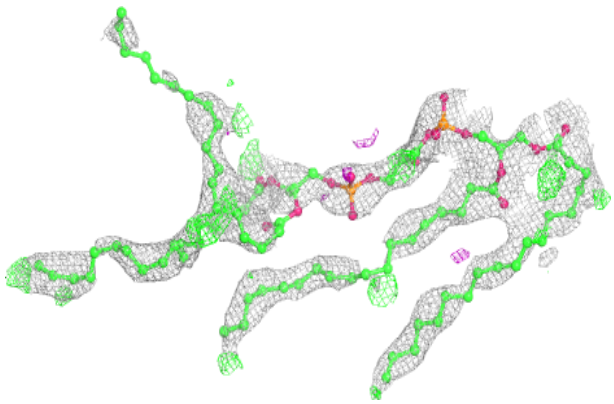


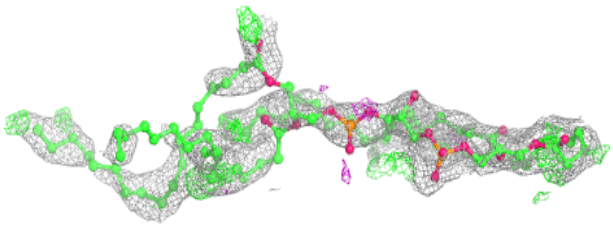


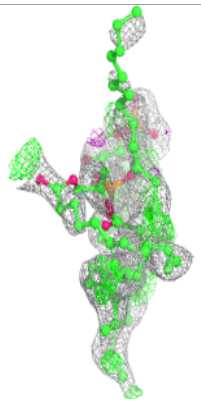


Electron density around CDL G 101:

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

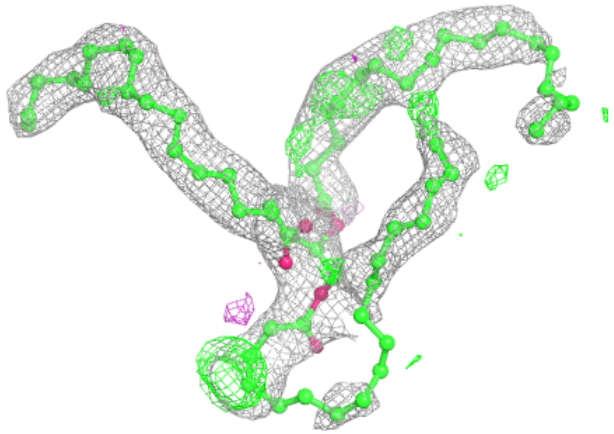


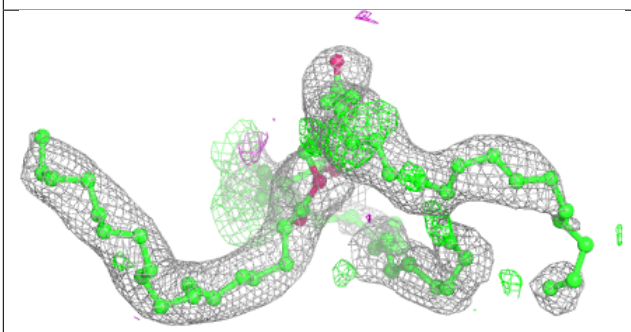


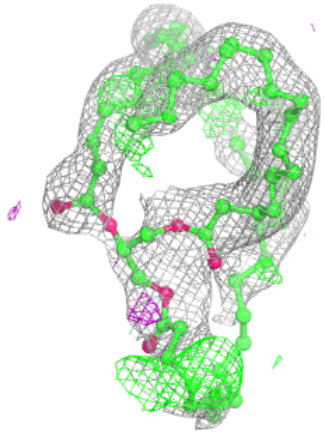


Electron density around TGL L 101:

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

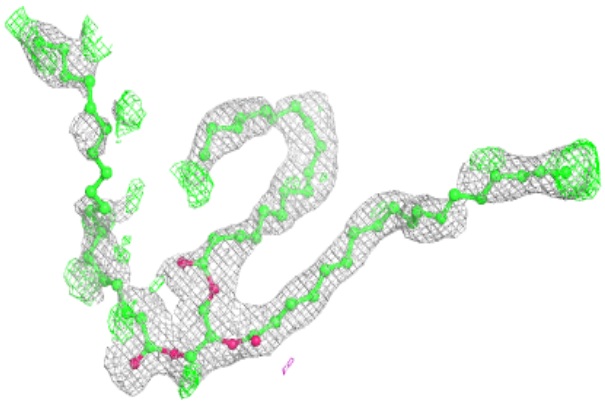


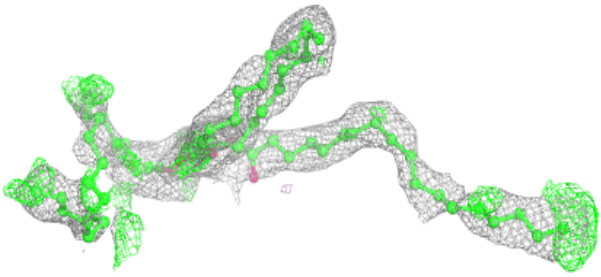


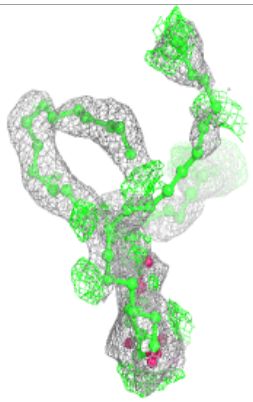


Electron density around TGL D 201:

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

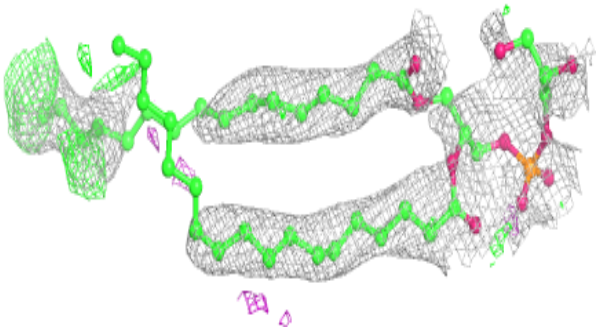


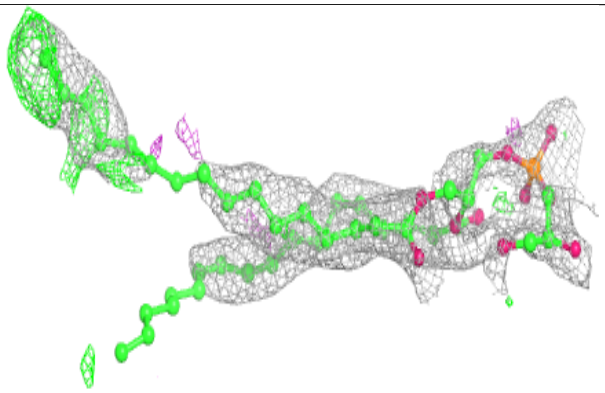


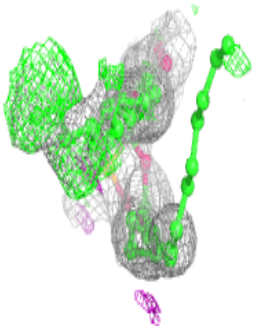


Electron density around PGV A 606:

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

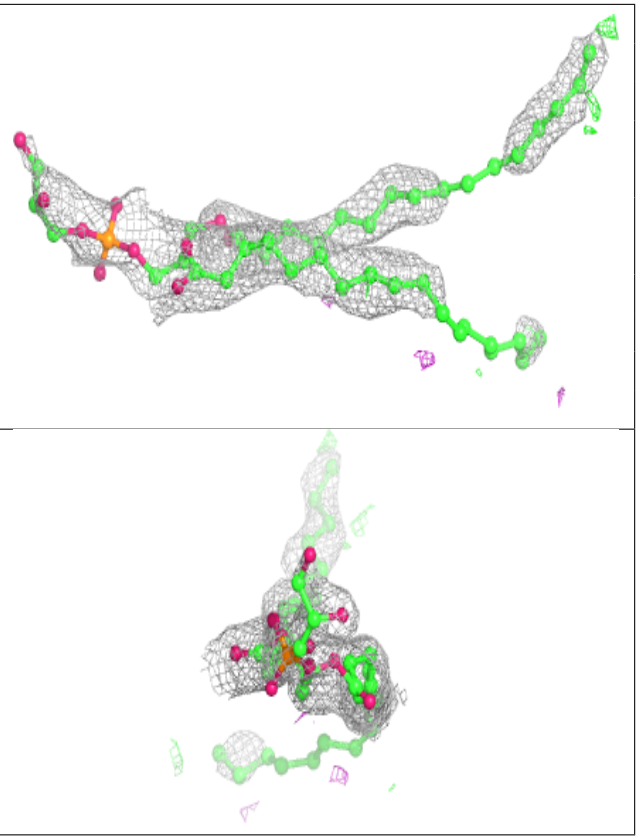






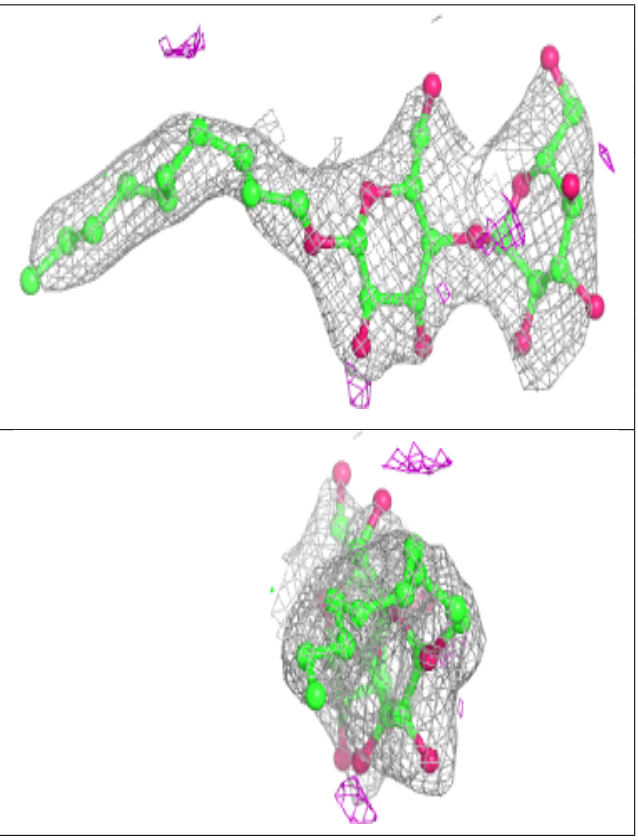
Electron density around PGV a 607:

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



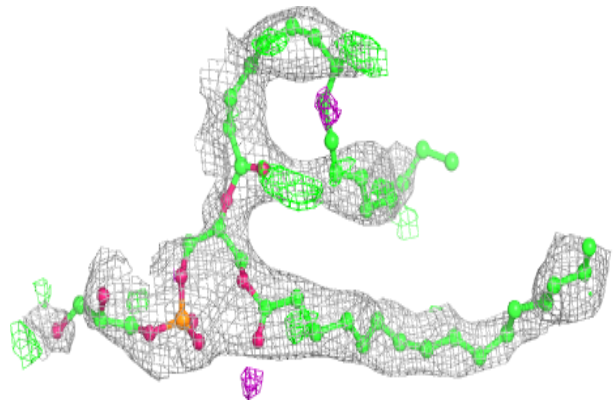
Electron density around DMU m 401:

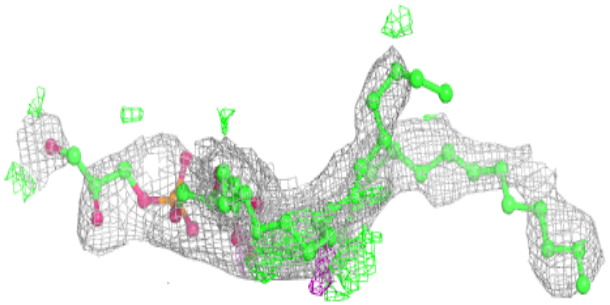
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

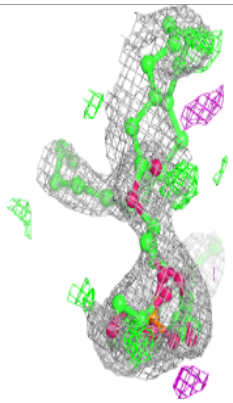


Electron density around PGV G 103:

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

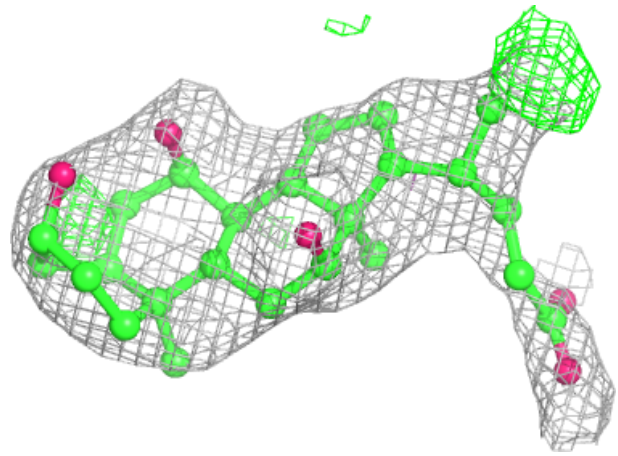


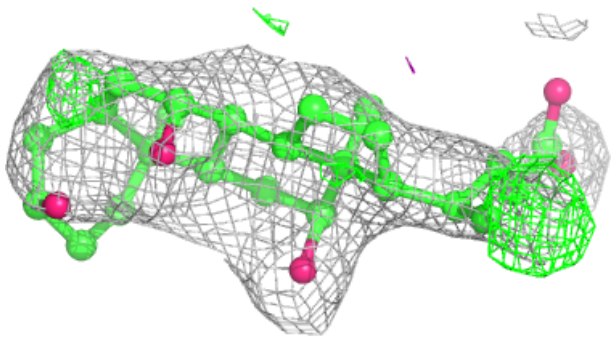


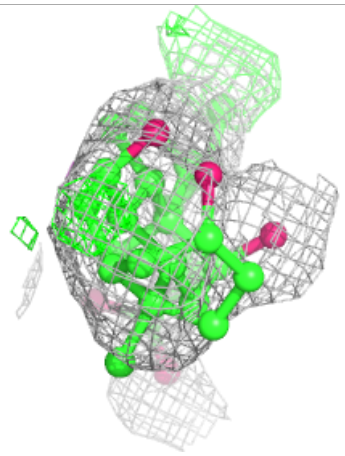


Electron density around CHD j 101:

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

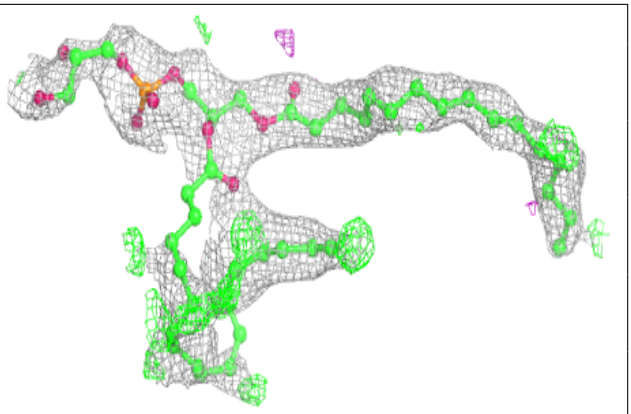


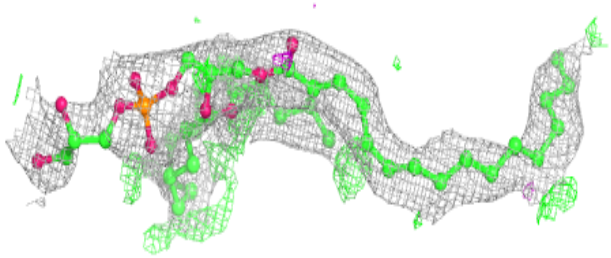


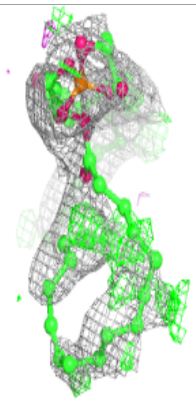


Electron density around PGV C 304:

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

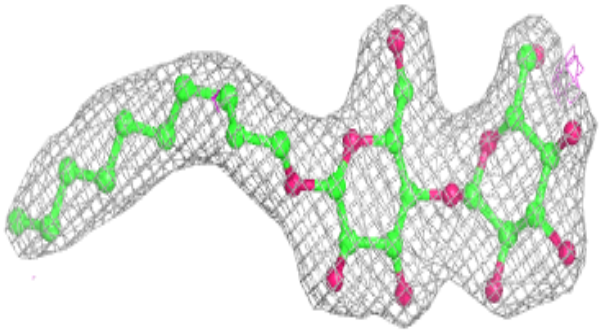


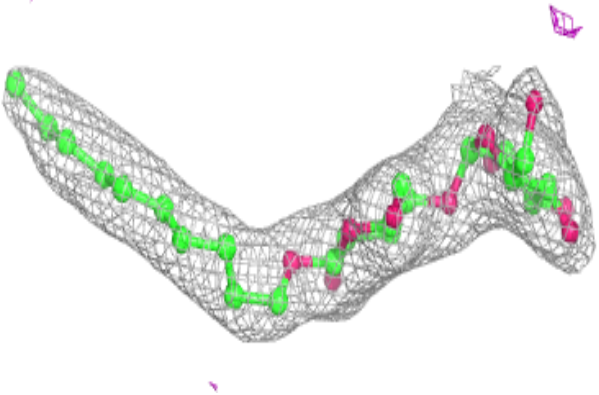


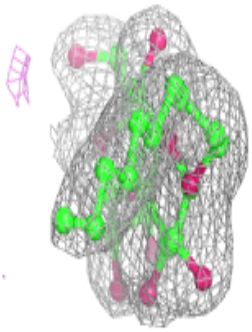


Electron density around DMU M 101:

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

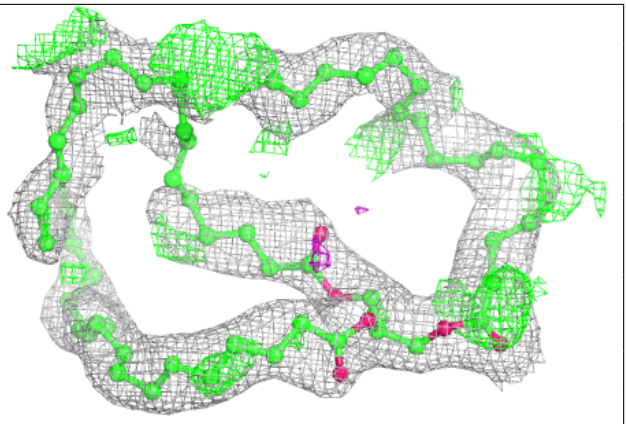


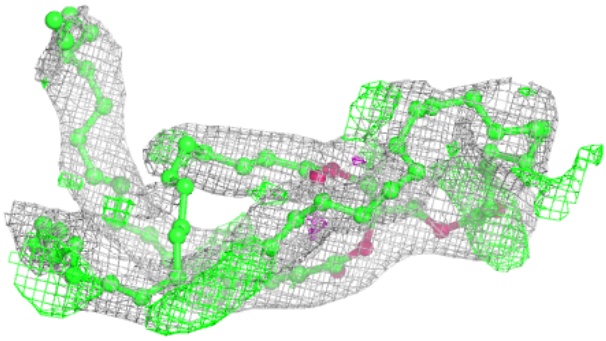


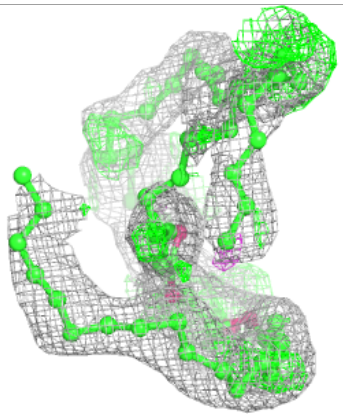


Electron density around TGL A 608:

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

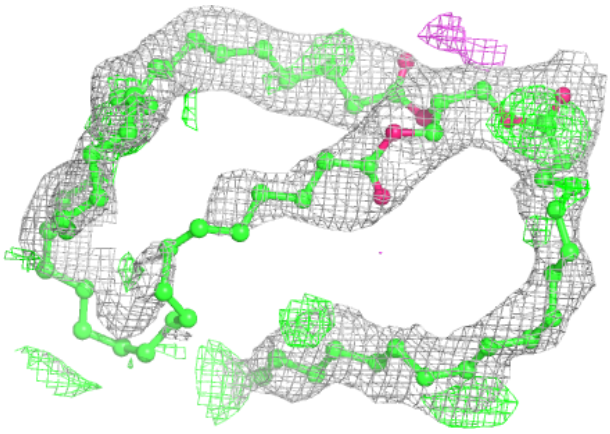


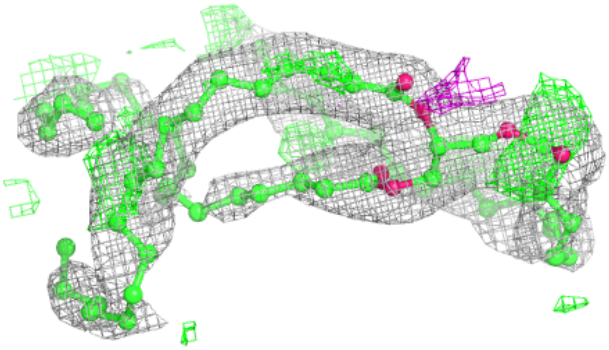


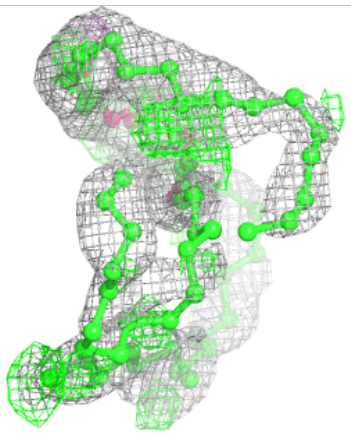


Electron density around TGL i 101:

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

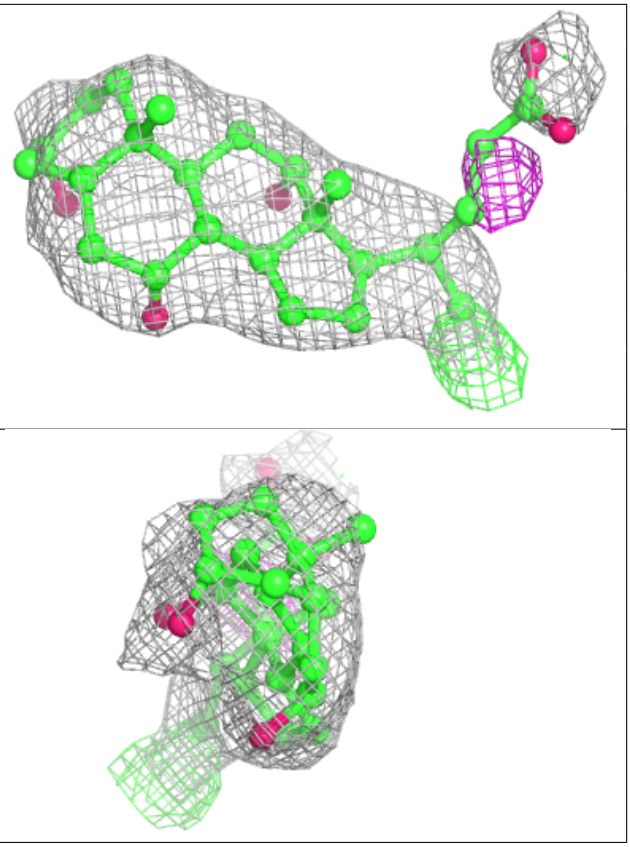






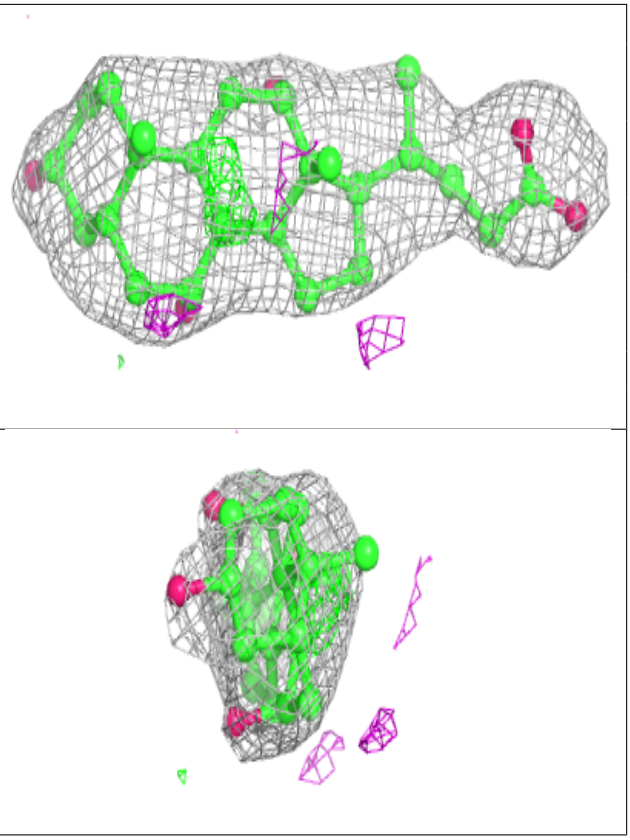
Electron density around CHD J 101:

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



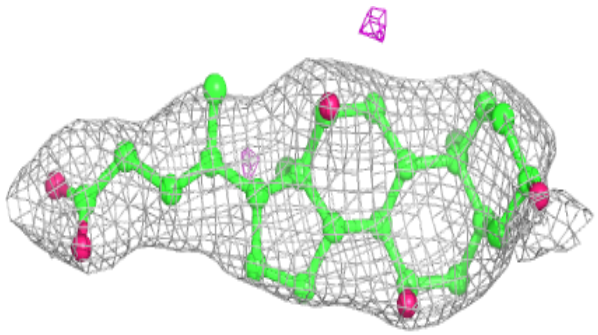
Electron density around CHD C 306:

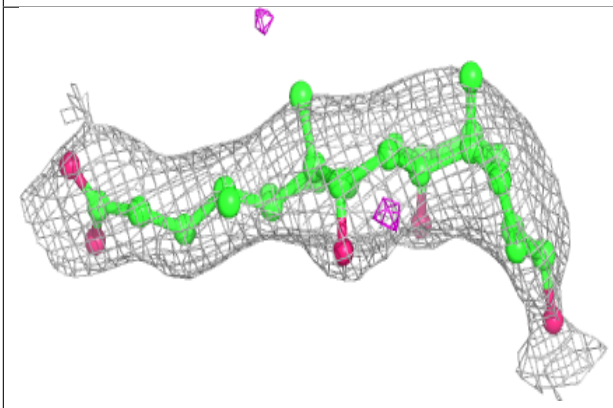
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

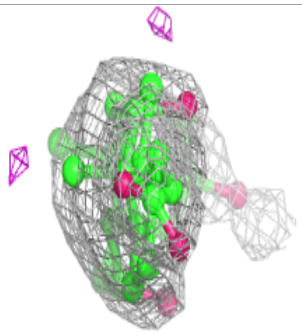


Electron density around CHD c 306:

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

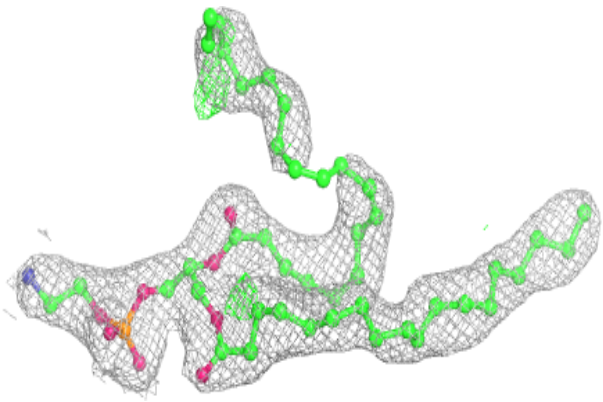


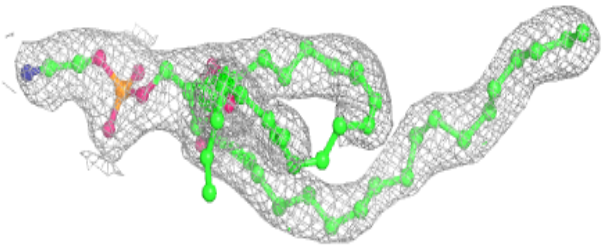


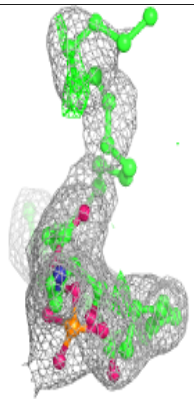


Electron density around PEK g 102:

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

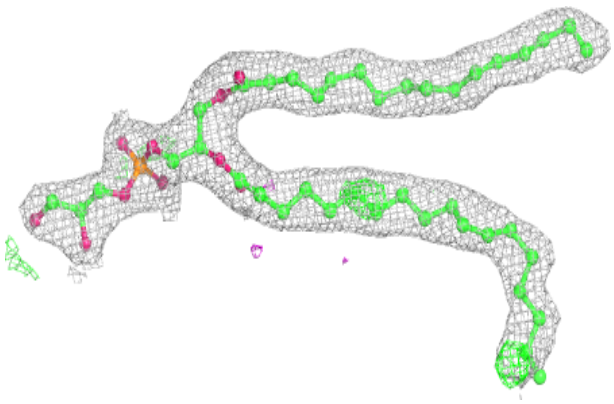


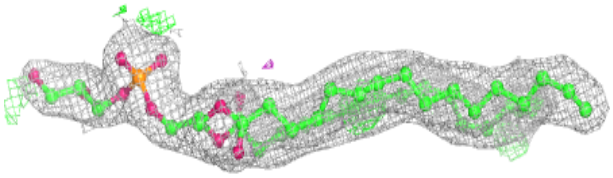


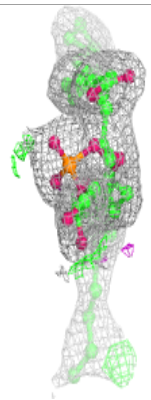


Electron density around PGV C 303:

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

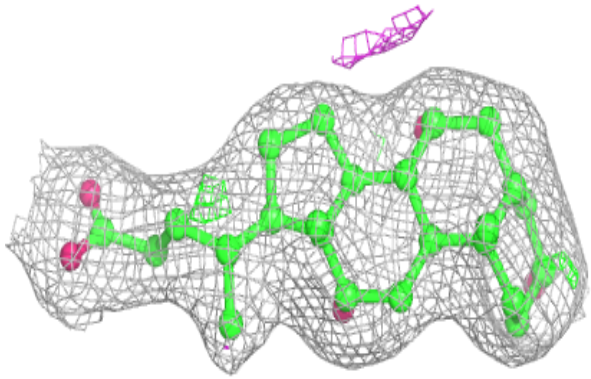


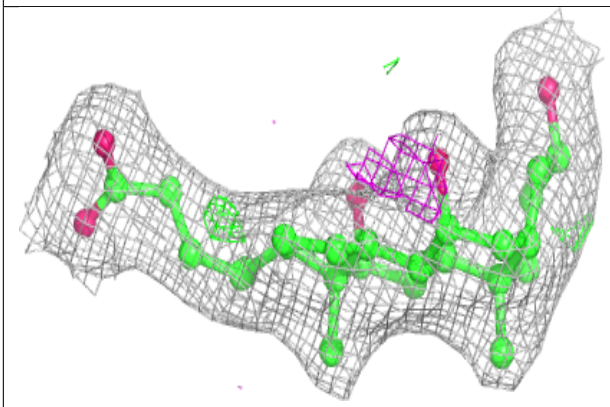


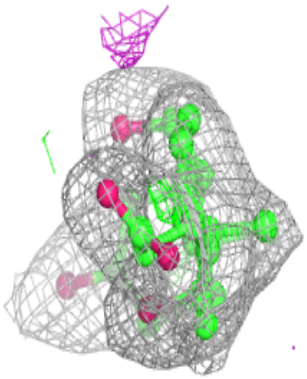


Electron density around CHD b 301:

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

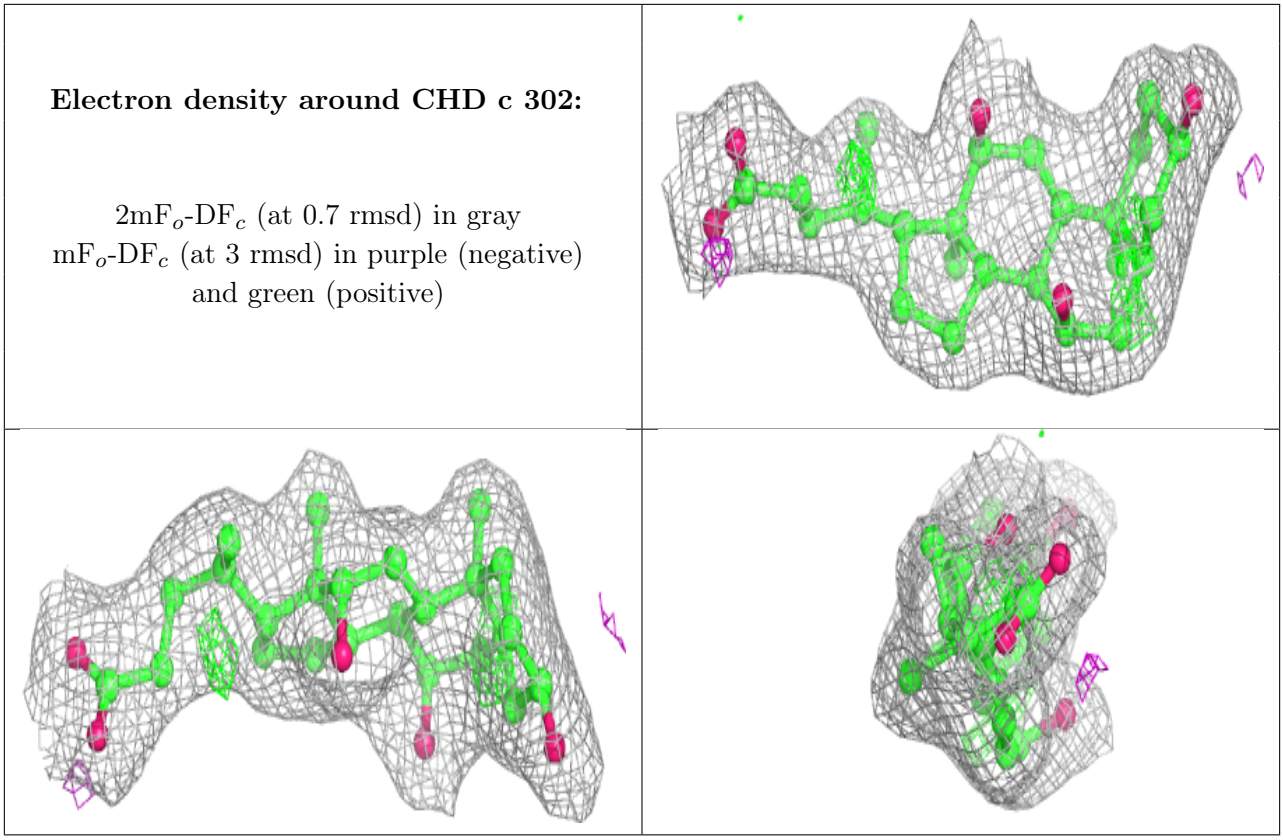






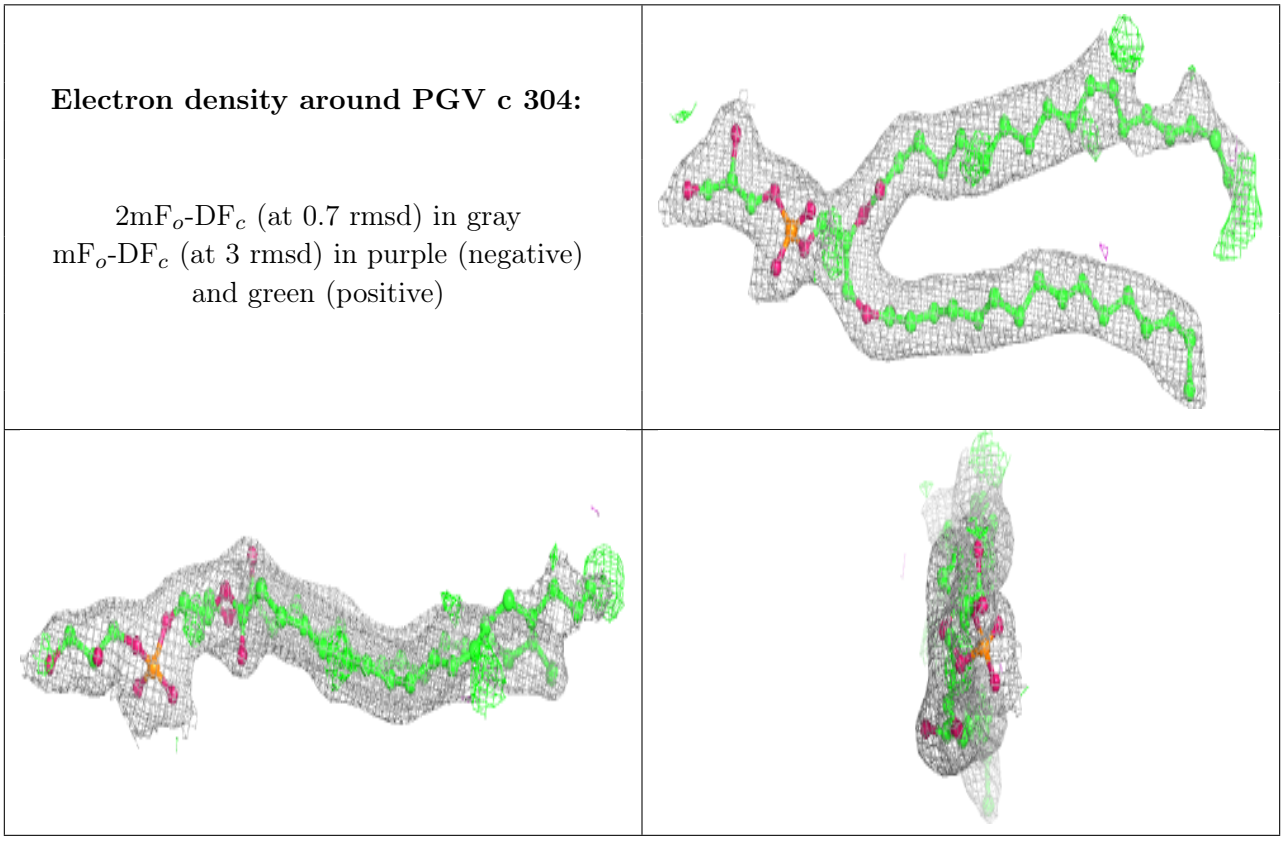
Electron density around CHD c 302:

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



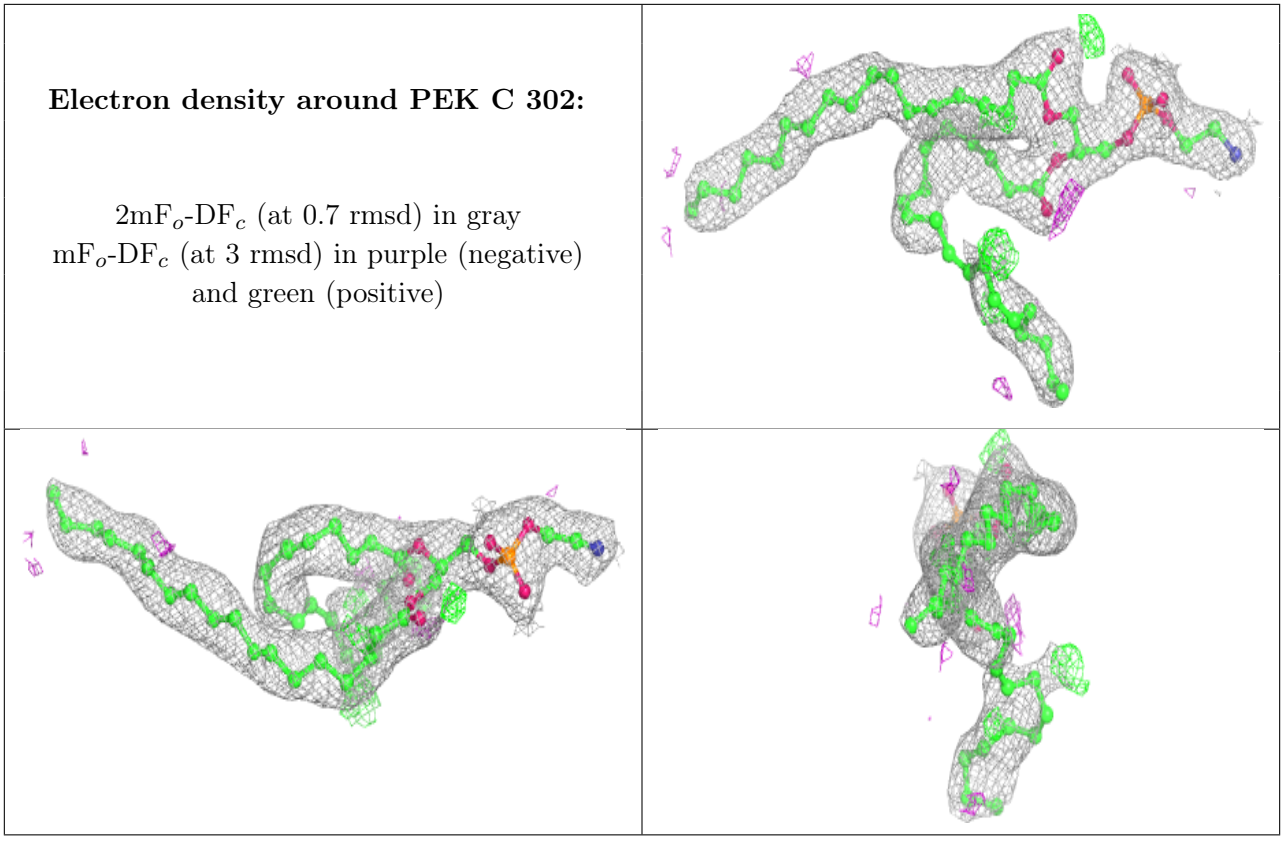
Electron density around PGV c 304:

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



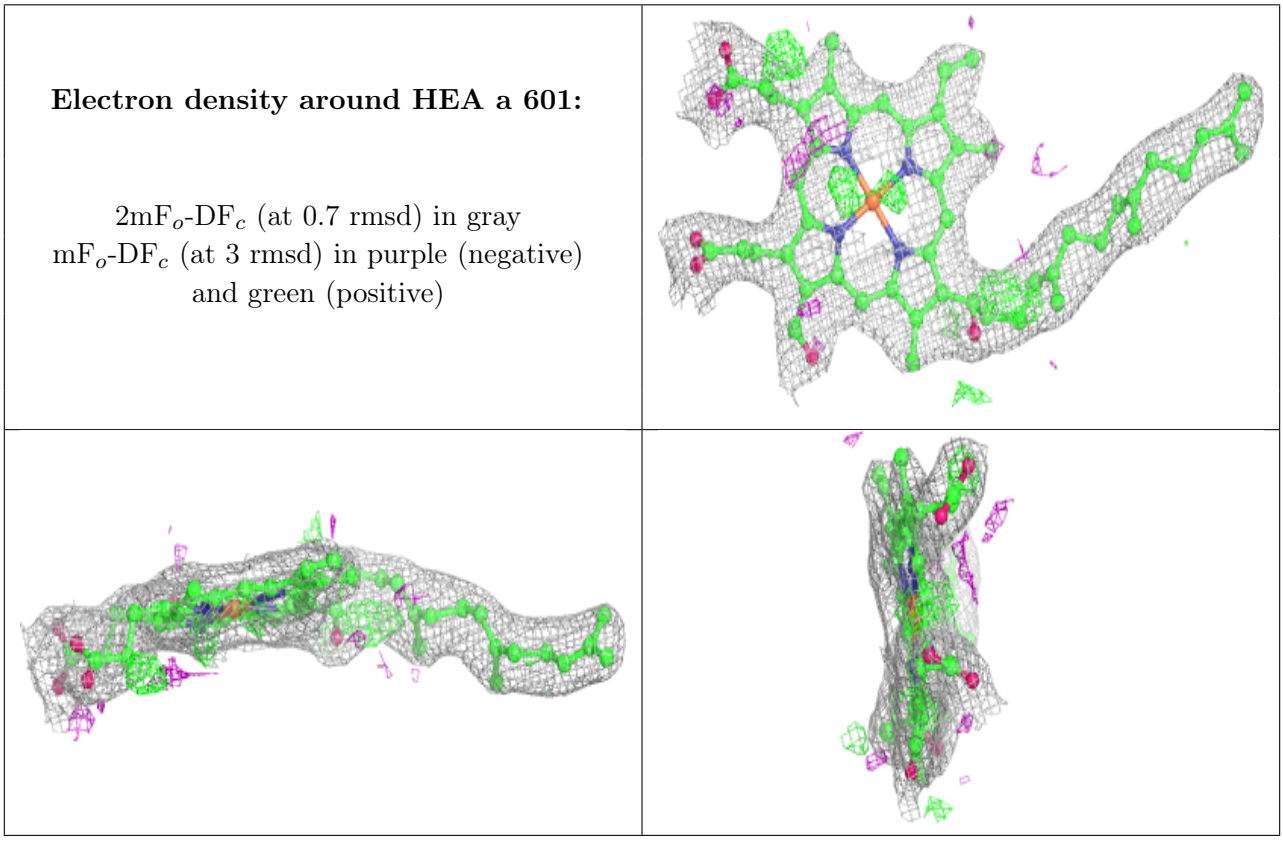
Electron density around PEK C 302:

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



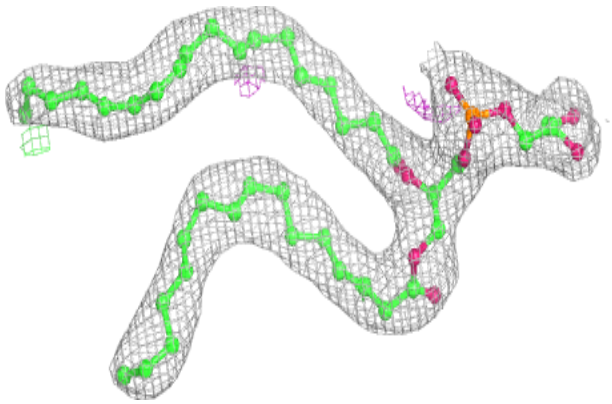
Electron density around HEA a 601:

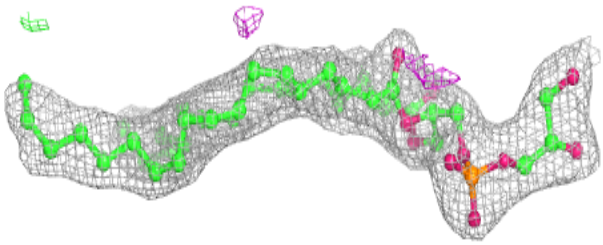
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

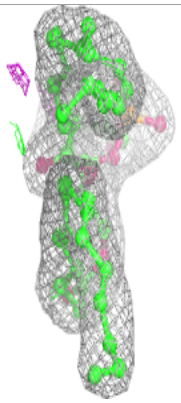


Electron density around PGV c 301:

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

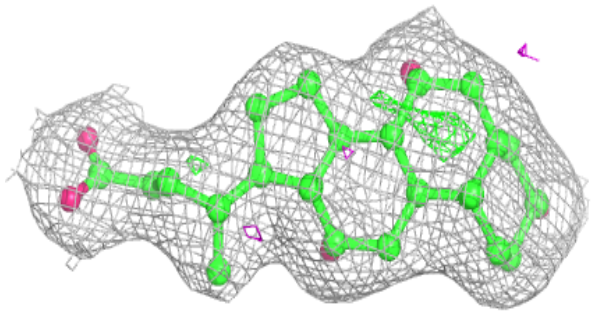


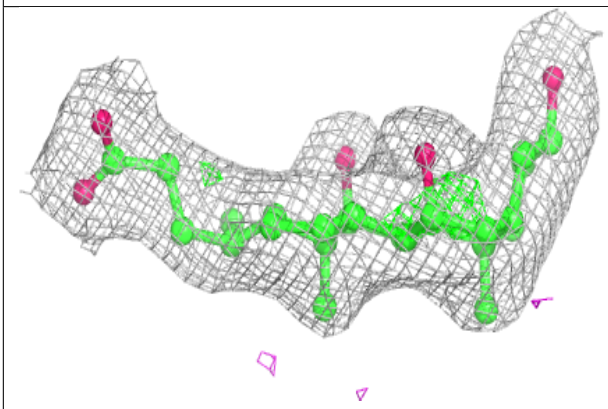


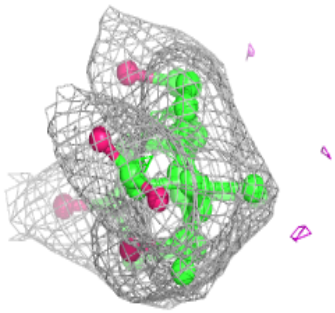


Electron density around CHD B 303:

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

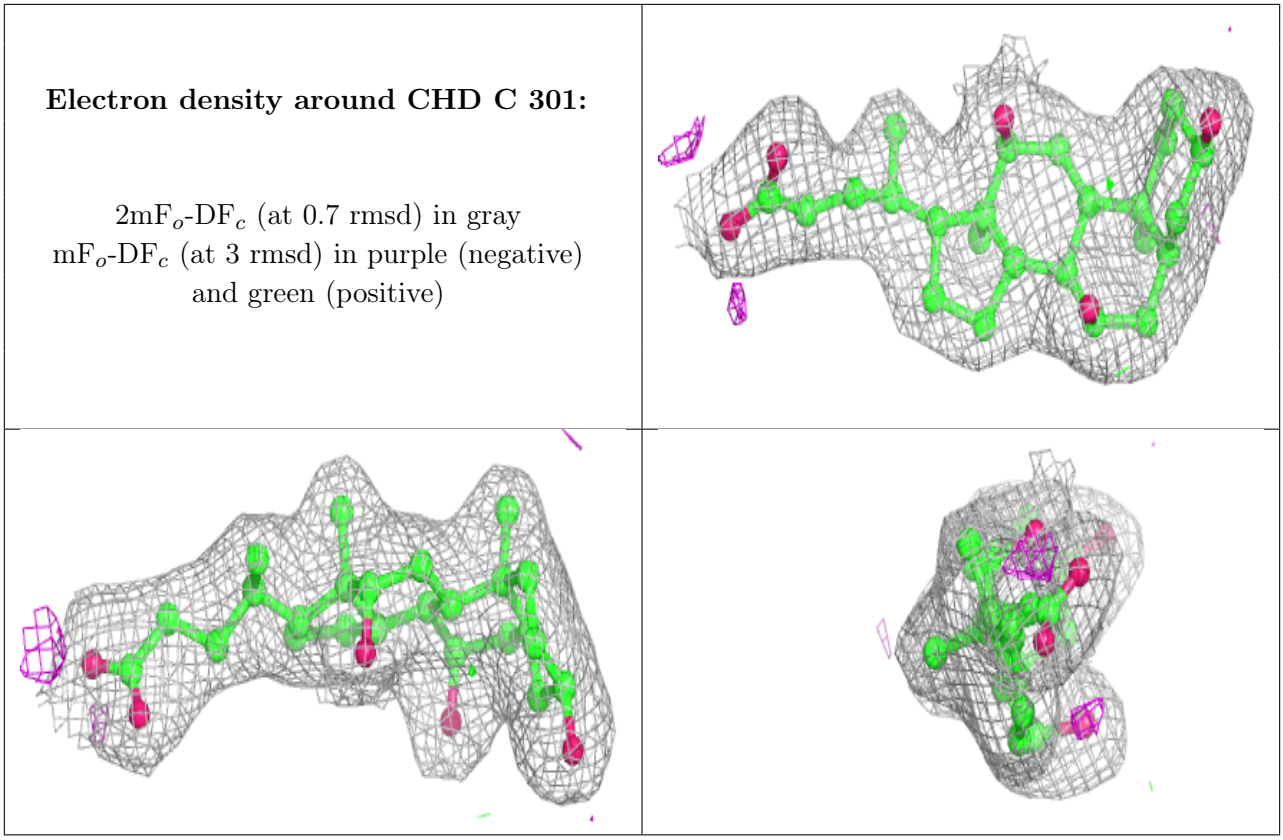






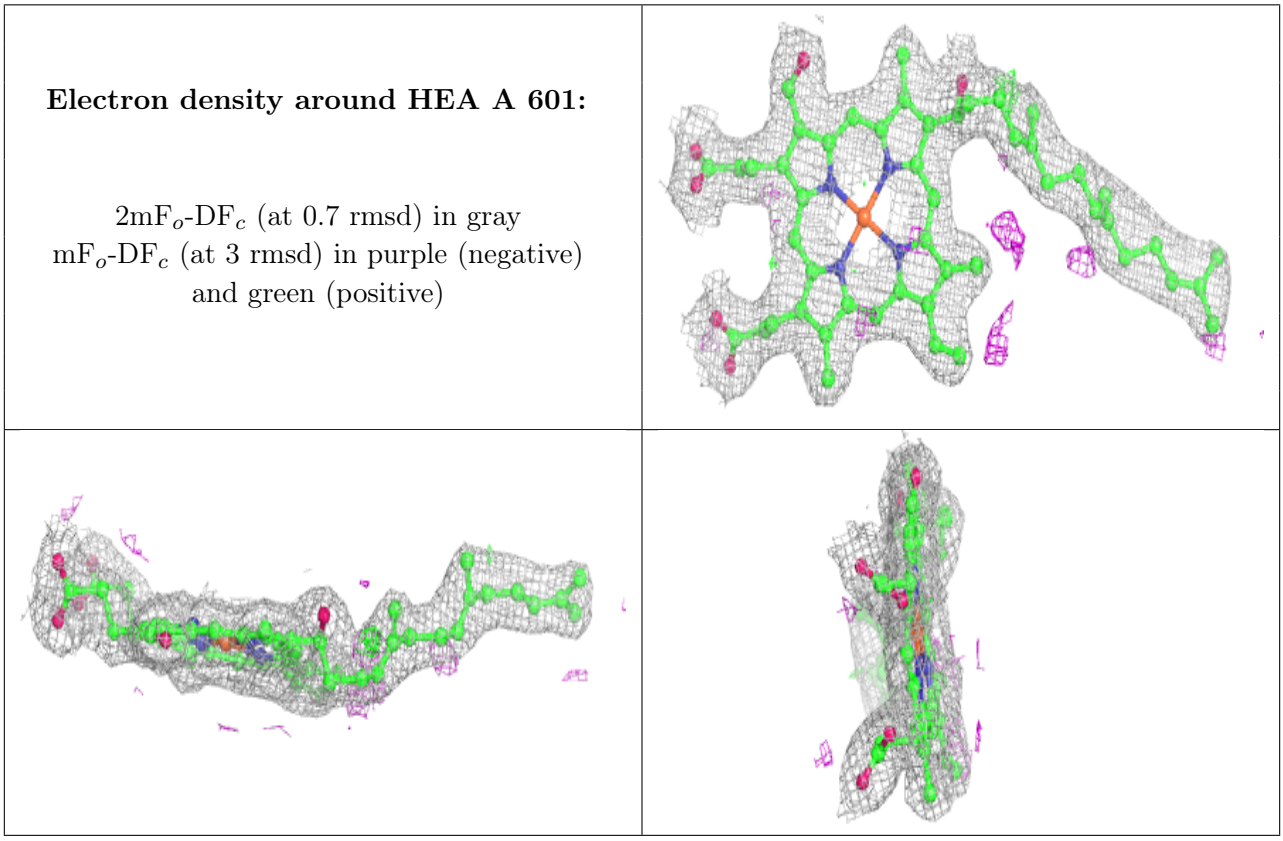
Electron density around CHD C 301:

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



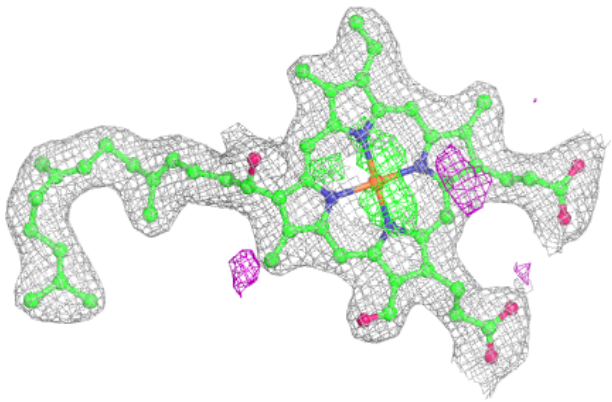
Electron density around HEA A 601:

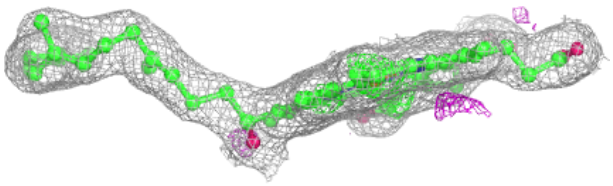
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

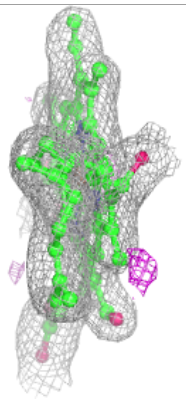


Electron density around HEA a 602:

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

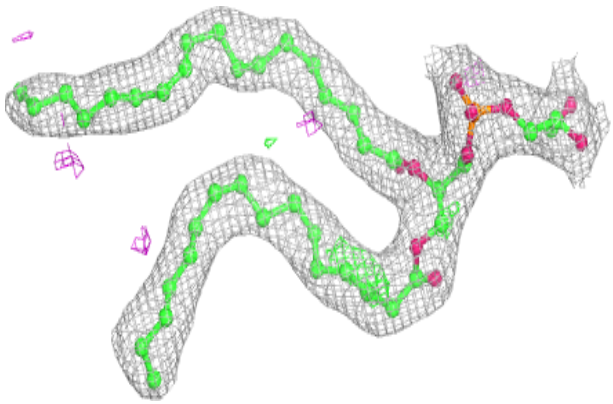


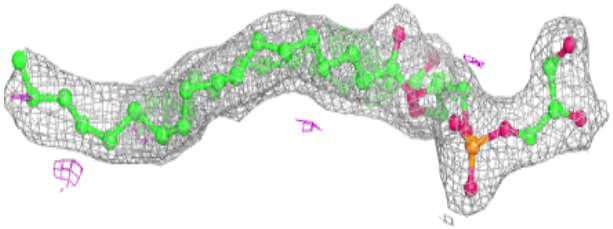


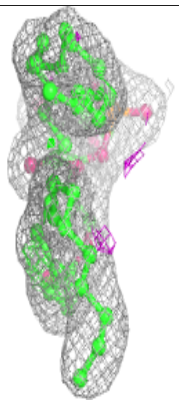


Electron density around PGV A 607:

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

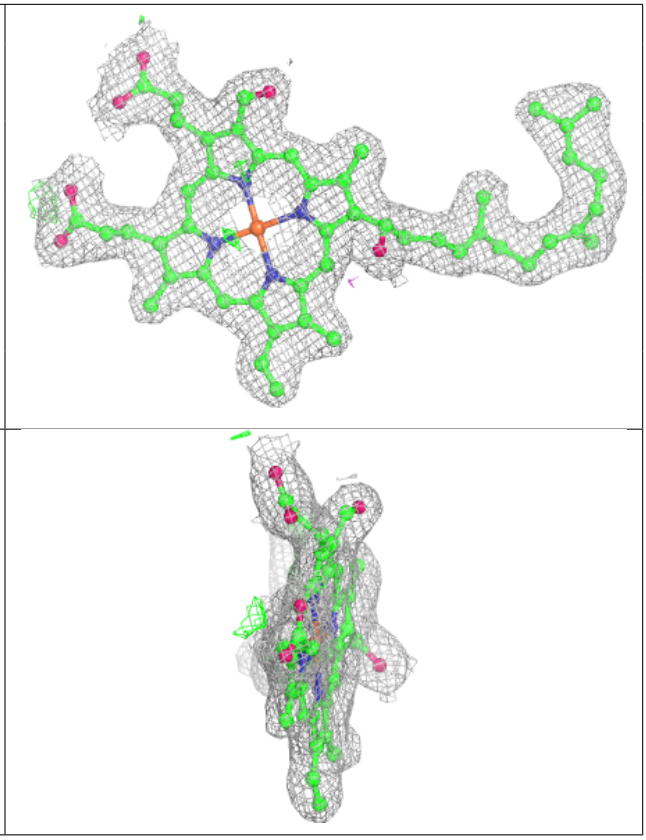






Electron density around HEA A 602:

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



6.5 Other polymers (i)

There are no such residues in this entry.